Full wwPDB X-ray Structure Validation Report (i)

Feb 11, 2024 – 01:51 AM EST

PDB ID	:	3BFJ
Title	:	Crystal structure analysis of 1,3-propanediol oxidoreductase
Authors	:	Marcal, D.; Enguita, F.J.; Carrondo, M.A.; Structural Proteomics in Europe (SPINE)
Deposited on	:	2007-11-21
Resolution	:	2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

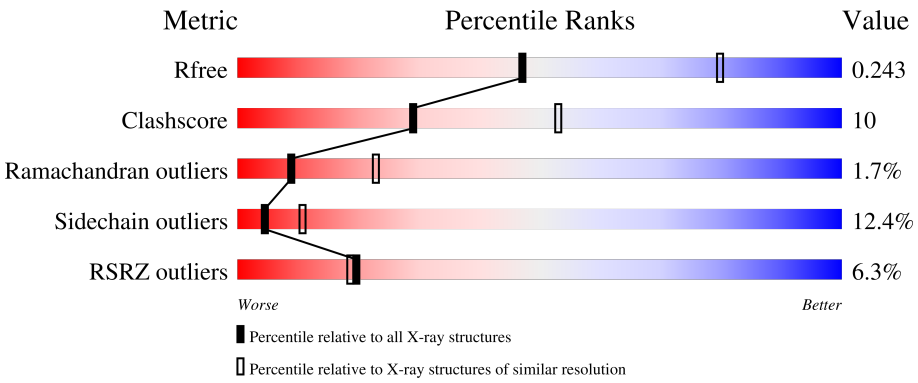
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	387	4% 74% 21% • •
1	B	387	5% 73% 21% • ••
1	C	387	8% 76% 19% • •
1	D	387	6% 75% 19% 5% •
1	E	387	3% 75% 19% 5% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	387	10% 75% 19% 5%
1	G	387	7% 74% 19% 5%
1	H	387	4% 71% 21% 5%
1	I	387	5% 73% 20% 5%
1	J	387	5% 78% 17%
1	K	387	4% 72% 20% 6%
1	L	387	6% 73% 20% 5%
1	M	387	5% 76% 18% 5%
1	N	387	4% 75% 19% 5%
1	O	387	4% 78% 16% 5%
1	P	387	2% 70% 22% 6%
1	Q	387	6% 73% 20% 5%
1	R	387	5% 77% 17% 5%
1	S	387	12% 71% 22% 5%
1	T	387	17% 76% 20%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 58348 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 1,3-propanediol oxidoreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	382	2871	1810	505	540	16	0	0	0
1	B	382	2871	1810	505	540	16	0	0	0
1	C	382	2871	1810	505	540	16	0	0	0
1	D	382	2871	1810	505	540	16	0	0	0
1	E	382	2871	1810	505	540	16	0	0	0
1	F	382	2871	1810	505	540	16	0	0	0
1	G	382	2871	1810	505	540	16	0	0	0
1	H	382	2871	1810	505	540	16	0	0	0
1	I	382	2871	1810	505	540	16	0	0	0
1	J	382	2871	1810	505	540	16	0	0	0
1	K	382	2871	1810	505	540	16	0	0	0
1	L	382	2871	1810	505	540	16	0	0	0
1	M	382	2871	1810	505	540	16	0	0	0
1	N	382	2871	1810	505	540	16	0	0	0
1	O	382	2871	1810	505	540	16	0	0	0
1	P	382	2871	1810	505	540	16	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	Q	382	2871	1810	505	540	16	0	0	0
			Total	C	N	O	S			
1	R	382	2871	1810	505	540	16	0	0	0
			Total	C	N	O	S			
1	S	382	2871	1810	505	540	16	0	0	0
			Total	C	N	O	S			
1	T	382	2871	1810	505	540	16	0	0	0

- Molecule 2 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
2	A	1	1	1	0	0
			Total	Fe		
2	B	1	1	1	0	0
			Total	Fe		
2	C	1	1	1	0	0
			Total	Fe		
2	D	1	1	1	0	0
			Total	Fe		
2	E	1	1	1	0	0
			Total	Fe		
2	F	1	1	1	0	0
			Total	Fe		
2	G	1	1	1	0	0
			Total	Fe		
2	H	1	1	1	0	0
			Total	Fe		
2	I	1	1	1	0	0
			Total	Fe		
2	J	1	1	1	0	0
			Total	Fe		
2	K	1	1	1	0	0
			Total	Fe		
2	L	1	1	1	0	0
			Total	Fe		
2	M	1	1	1	0	0
			Total	Fe		
2	N	1	1	1	0	0
			Total	Fe		
2	O	1	1	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
2	P	1	1	1	0	0
2	Q	1	1	1	0	0
2	R	1	1	1	0	0
2	S	1	1	1	0	0
2	T	1	1	1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	36	36	36	0	0
3	B	45	45	45	0	0
3	C	27	27	27	0	0
3	D	49	49	49	0	0
3	E	76	76	76	0	0
3	F	19	19	19	0	0
3	G	41	41	41	0	0
3	H	61	61	61	0	0
3	I	51	51	51	0	0
3	J	31	31	31	0	0
3	K	89	89	89	0	0
3	L	42	42	42	0	0
3	M	58	58	58	0	0
3	N	33	33	33	0	0

Continued on next page...

Continued from previous page...

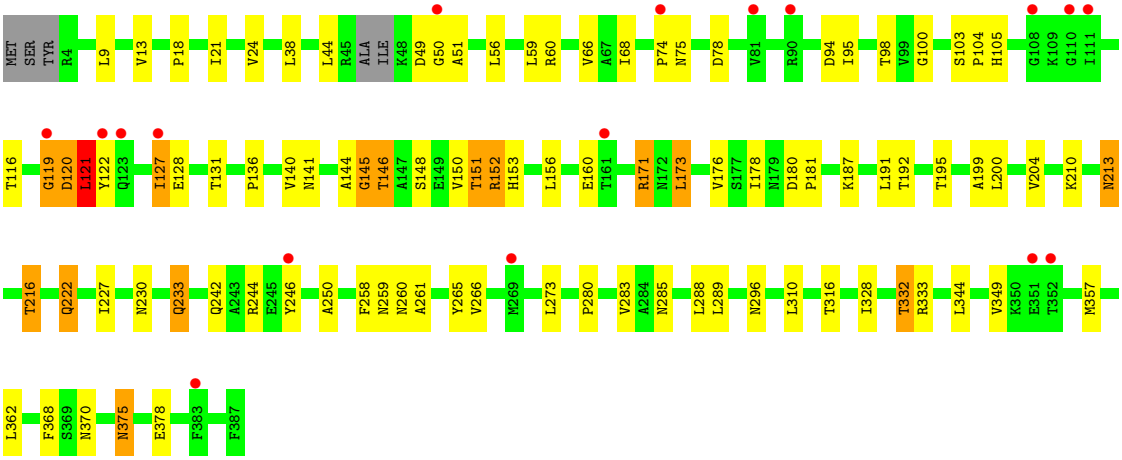
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	O	50	50	50	0	0
			Total	O		
3	P	64	64	64	0	0
			Total	O		
3	Q	43	43	43	0	0
			Total	O		
3	R	39	39	39	0	0
			Total	O		
3	S	19	19	19	0	0
			Total	O		
3	T	35	35	35	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

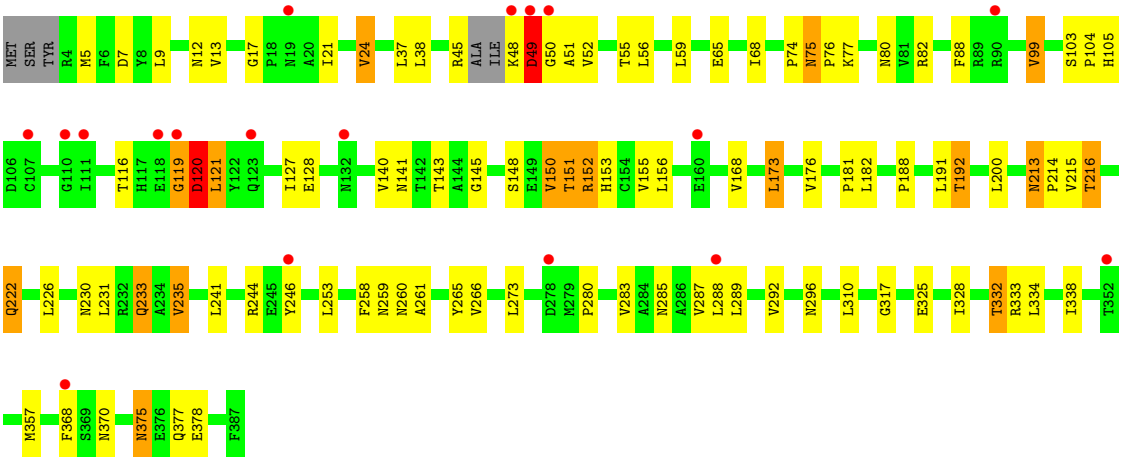
• Molecule 1: 1,3-propanediol oxidoreductase

Chain A:



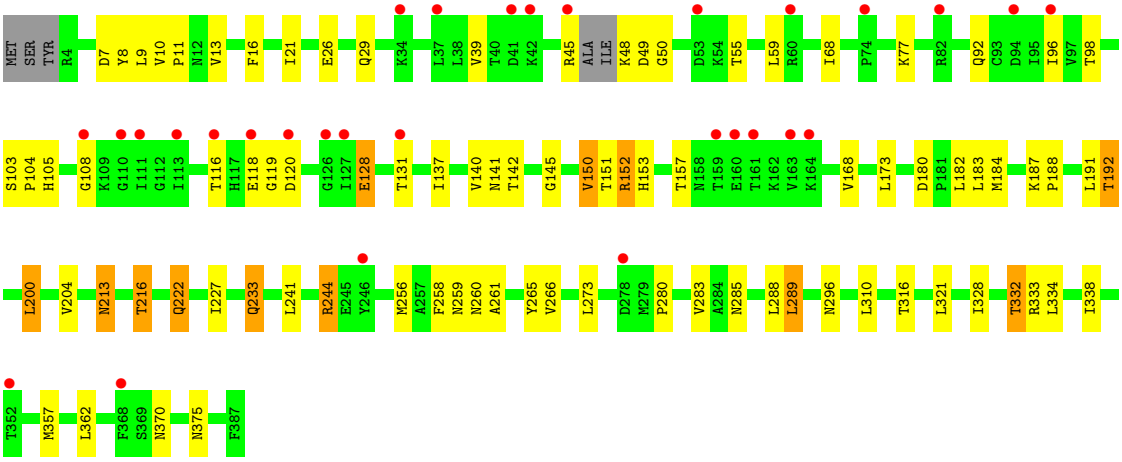
• Molecule 1: 1,3-propanediol oxidoreductase

Chain B:



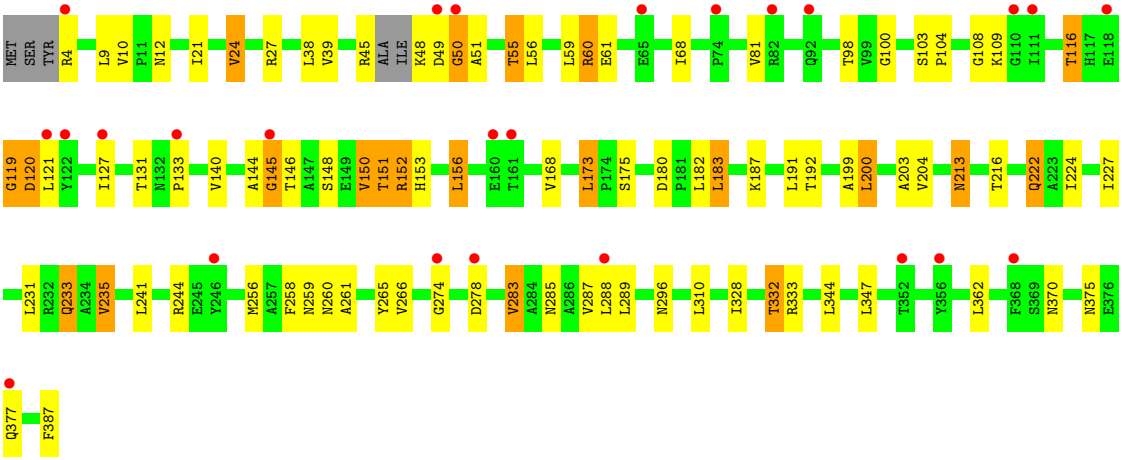
• Molecule 1: 1,3-propanediol oxidoreductase

Chain C:



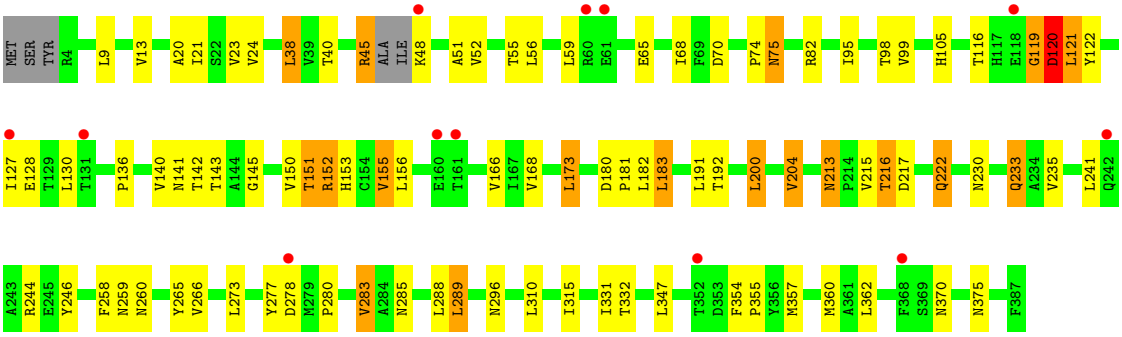
• Molecule 1: 1,3-propanediol oxidoreductase

Chain D:



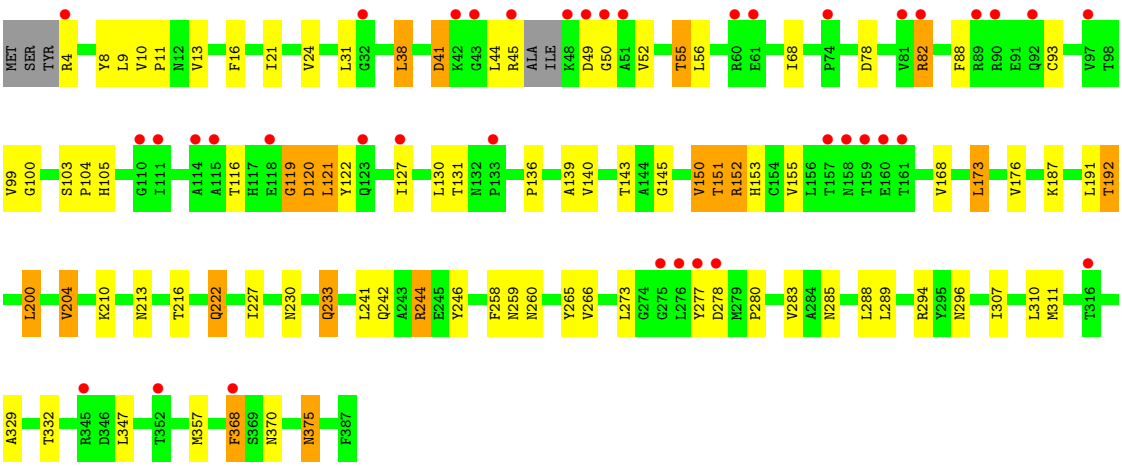
• Molecule 1: 1,3-propanediol oxidoreductase

Chain E:



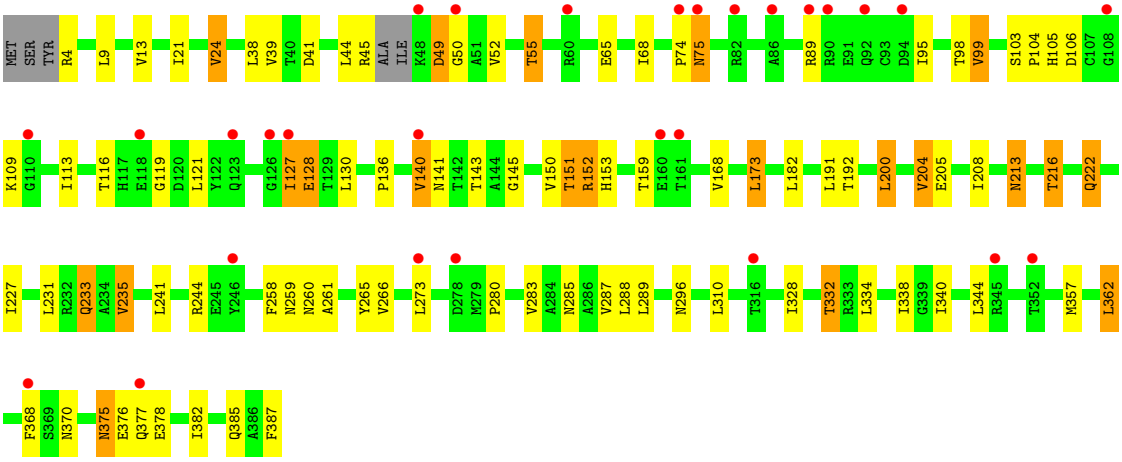
• Molecule 1: 1,3-propanediol oxidoreductase

Chain F:



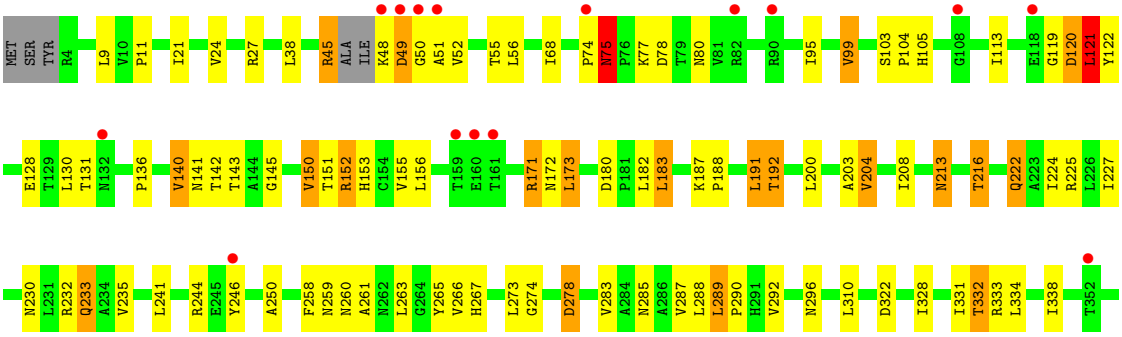
- Molecule 1: 1,3-propanediol oxidoreductase

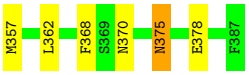
Chain G:



- Molecule 1: 1,3-propanediol oxidoreductase

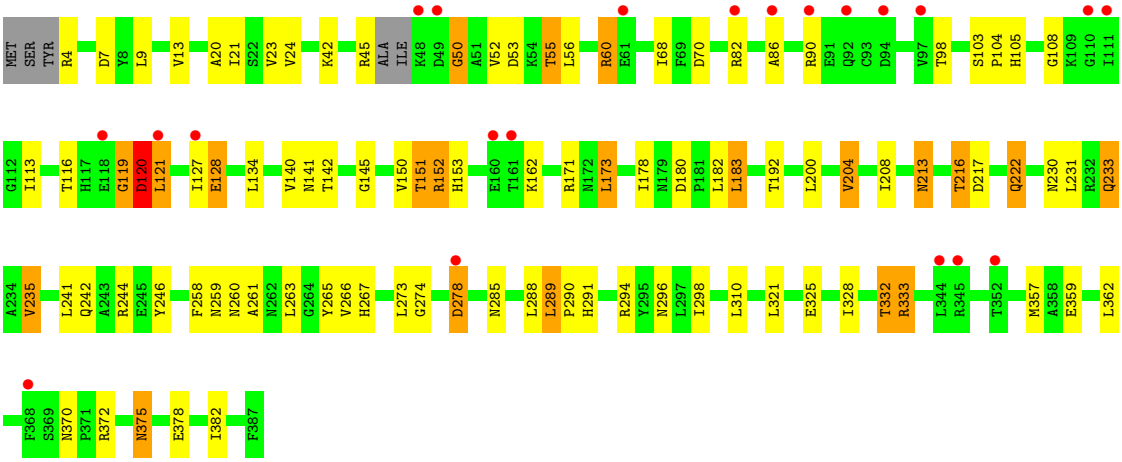
Chain H:





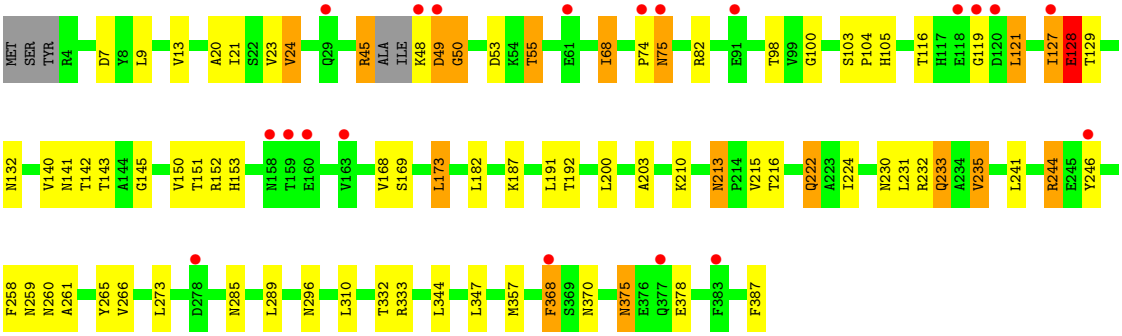
• Molecule 1: 1,3-propanediol oxidoreductase

Chain I:



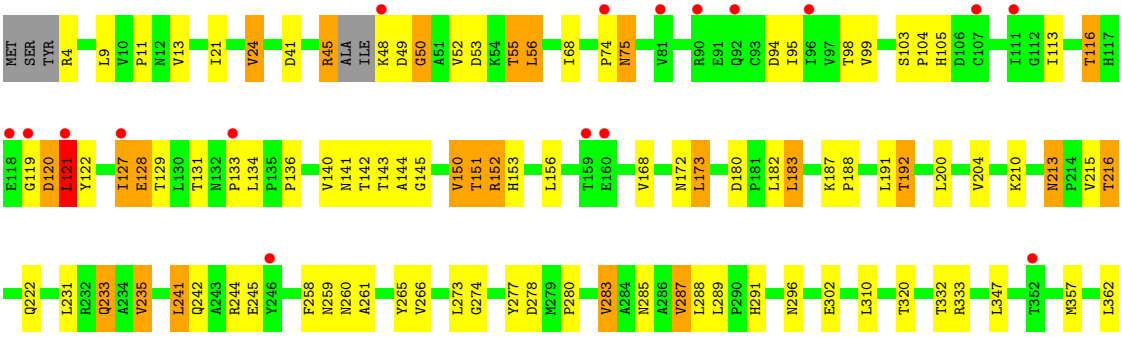
• Molecule 1: 1,3-propanediol oxidoreductase

Chain J:



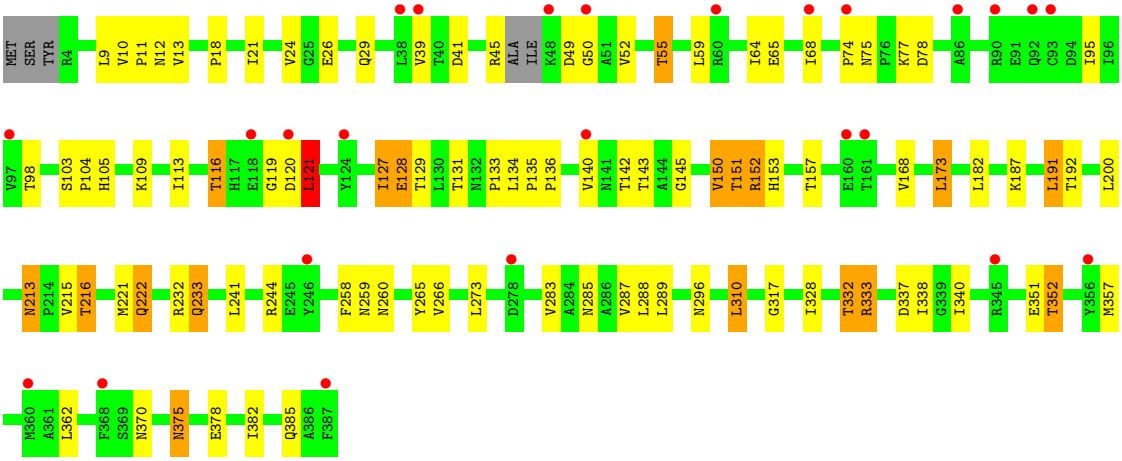
• Molecule 1: 1,3-propanediol oxidoreductase

Chain K:



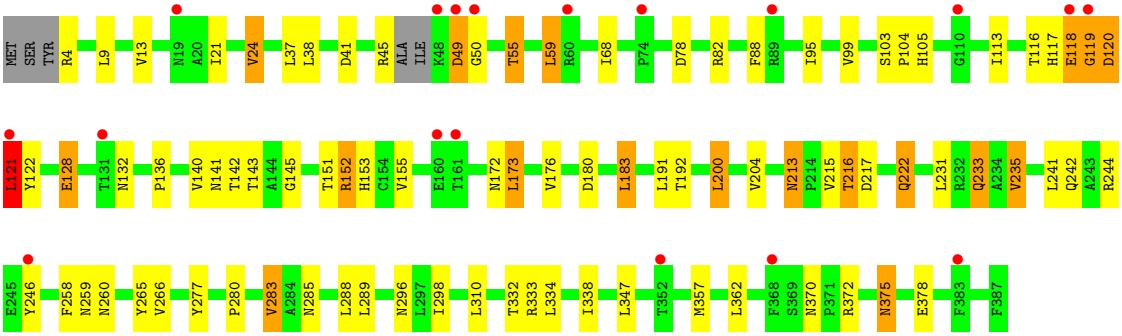
• Molecule 1: 1,3-propanediol oxidoreductase

Chain L:



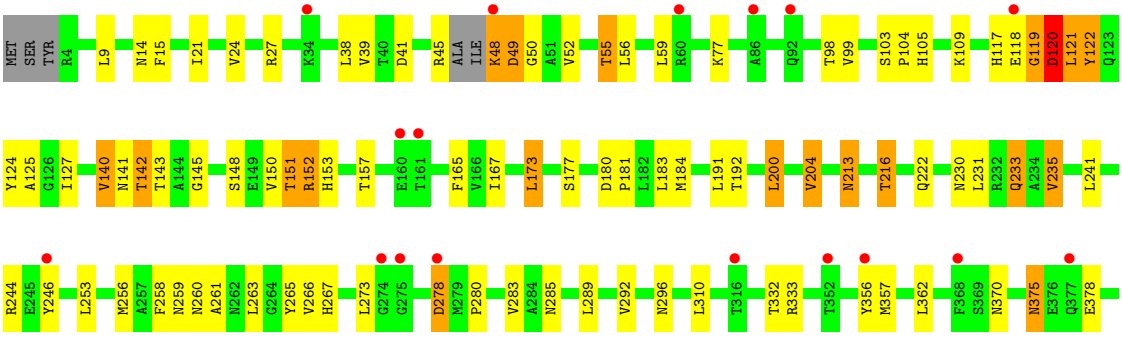
• Molecule 1: 1,3-propanediol oxidoreductase

Chain M:



• Molecule 1: 1,3-propanediol oxidoreductase

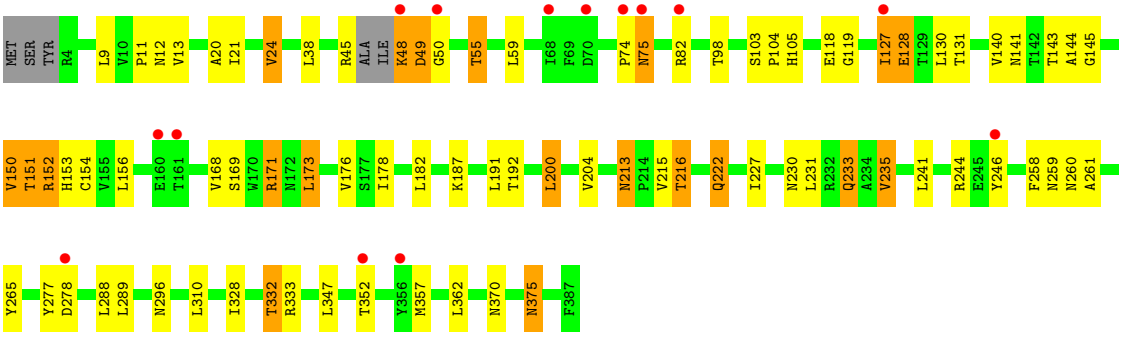
Chain N:



F387

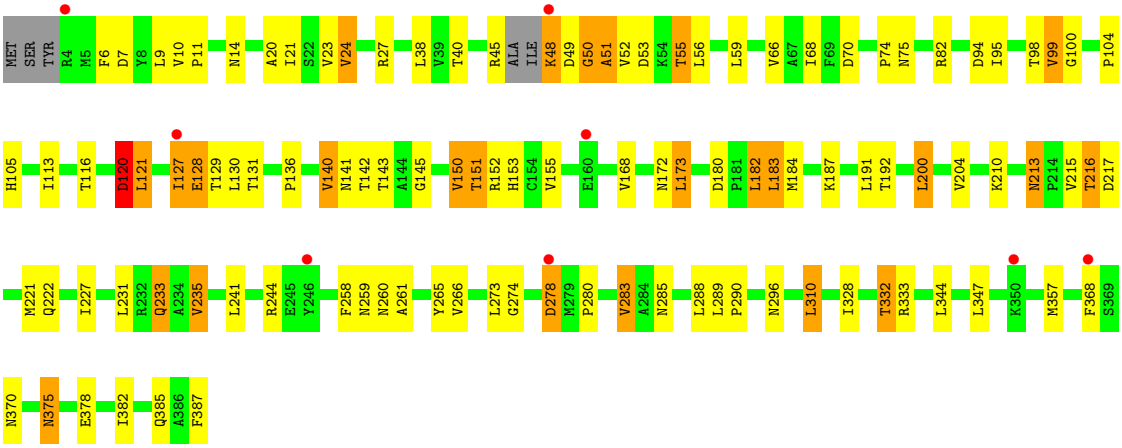
- Molecule 1: 1,3-propanediol oxidoreductase

Chain O:



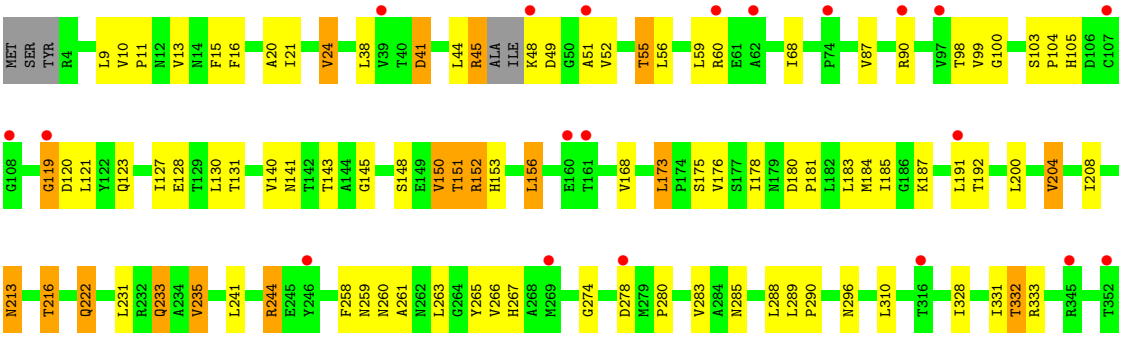
- Molecule 1: 1,3-propanediol oxidoreductase

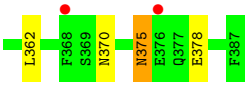
Chain P:



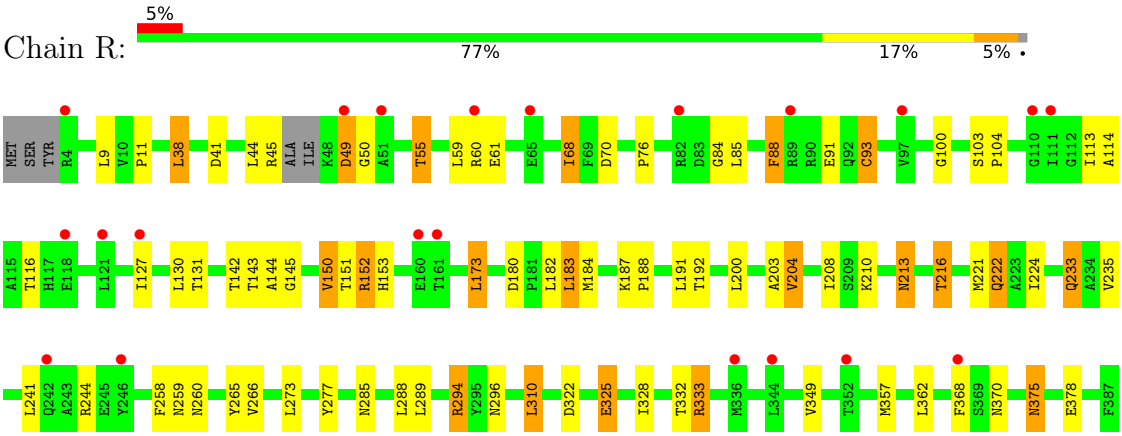
- Molecule 1: 1,3-propanediol oxidoreductase

Chain Q:

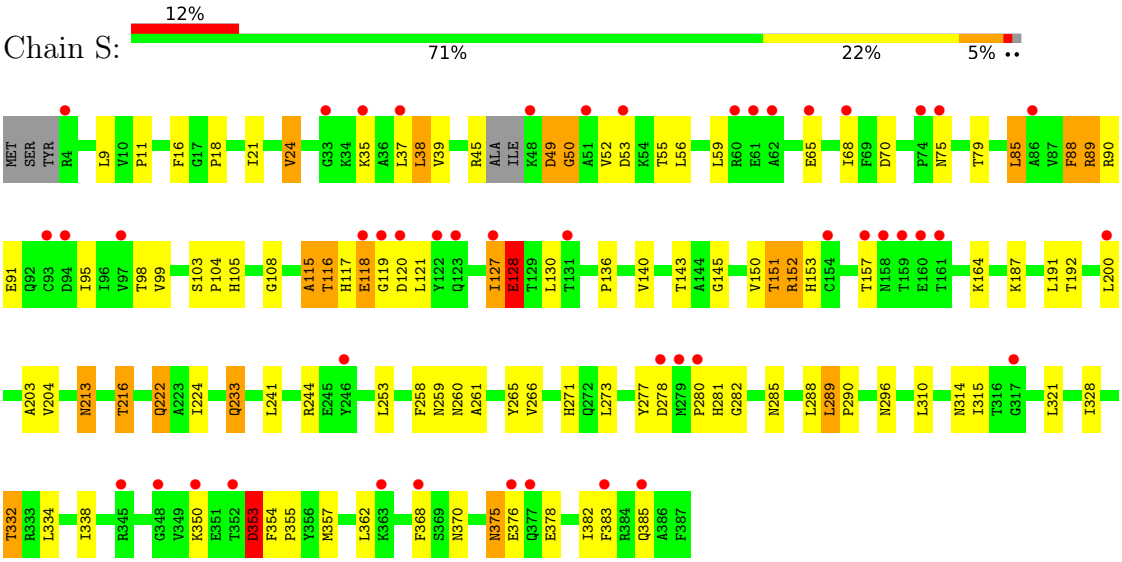




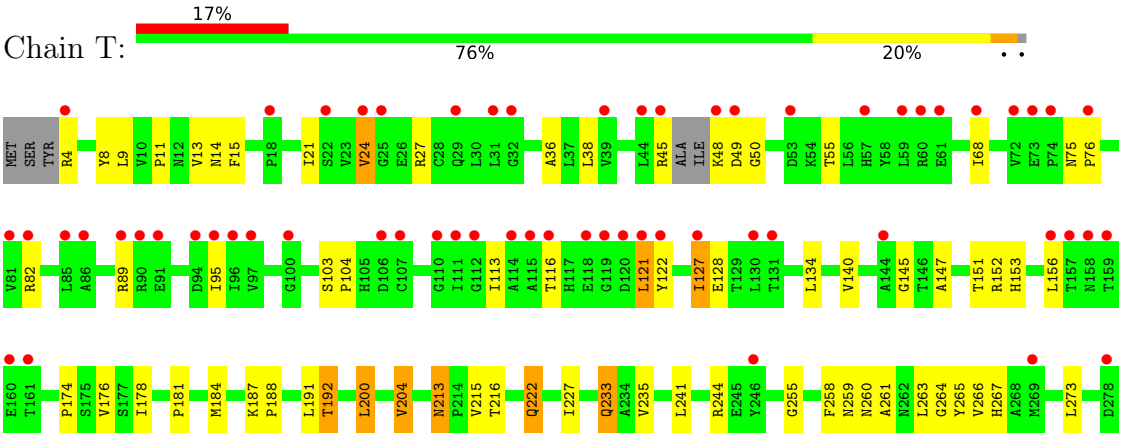
• Molecule 1: 1,3-propanediol oxidoreductase

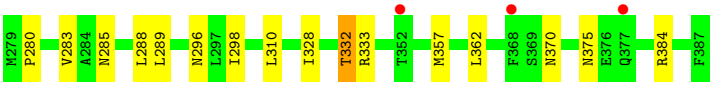


• Molecule 1: 1,3-propanediol oxidoreductase



• Molecule 1: 1,3-propanediol oxidoreductase




M279
P280
V283
A284
N285
L288
L289
N296
L297
I298
L310
I328
T332
R333
T352
M357
L362
F368
S369
N370
N375
E376
Q377
R384
F387

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	91.94Å 226.61Å 232.63Å 90.00° 92.91° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70 20.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.7 (20.00-2.70) 97.7 (20.00-2.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.92 (at 2.71Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.203 , 0.251 0.198 , 0.243	Depositor DCC
R_{free} test set	12840 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	48.0	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 57.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.004 for -h,l,k 0.009 for -h,-l,-k 0.021 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	58348	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FE2

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.38	0/2922	0.56	0/3969
1	B	0.38	0/2922	0.56	0/3969
1	C	0.36	0/2922	0.53	0/3969
1	D	0.37	0/2922	0.58	0/3969
1	E	0.43	0/2922	0.62	2/3969 (0.1%)
1	F	0.36	0/2922	0.54	0/3969
1	G	0.43	2/2922 (0.1%)	0.60	2/3969 (0.1%)
1	H	0.41	0/2922	0.61	0/3969
1	I	0.84	8/2922 (0.3%)	0.69	3/3969 (0.1%)
1	J	0.37	0/2922	0.54	0/3969
1	K	0.42	0/2922	0.59	0/3969
1	L	0.50	2/2922 (0.1%)	0.56	0/3969
1	M	0.39	0/2922	0.58	0/3969
1	N	0.47	4/2922 (0.1%)	0.57	0/3969
1	O	0.38	0/2922	0.57	0/3969
1	P	0.39	0/2922	0.58	0/3969
1	Q	0.38	0/2922	0.57	1/3969 (0.0%)
1	R	0.71	8/2922 (0.3%)	0.65	4/3969 (0.1%)
1	S	1.23	25/2922 (0.9%)	1.16	13/3969 (0.3%)
1	T	0.54	7/2922 (0.2%)	0.74	5/3969 (0.1%)
All	All	0.53	56/58440 (0.1%)	0.63	30/79380 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	S	0	3

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S	89	ARG	NE-CZ	31.52	1.74	1.33
1	I	60	ARG	CZ-NH1	27.64	1.69	1.33
1	I	90	ARG	NE-CZ	18.03	1.56	1.33
1	S	89	ARG	CZ-NH2	17.00	1.55	1.33
1	S	376	GLU	CD-OE1	16.53	1.43	1.25
1	R	93	CYS	CB-SG	16.24	2.09	1.82
1	S	383	PHE	CE1-CZ	14.68	1.65	1.37
1	L	351	GLU	CD-OE2	14.58	1.41	1.25
1	S	271	HIS	CG-CD2	13.48	1.58	1.35
1	T	27	ARG	CZ-NH1	13.01	1.50	1.33
1	S	353	ASP	CG-OD1	11.87	1.52	1.25
1	R	60	ARG	CZ-NH1	11.68	1.48	1.33
1	I	90	ARG	CZ-NH2	11.44	1.48	1.33
1	S	353	ASP	C-N	11.21	1.59	1.34
1	S	383	PHE	CG-CD1	11.03	1.55	1.38
1	S	115	ALA	C-O	10.43	1.43	1.23
1	R	84	GLY	C-O	9.85	1.39	1.23
1	S	88	PHE	CG-CD1	9.55	1.53	1.38
1	I	86	ALA	C-N	9.53	1.55	1.34
1	G	89	ARG	CZ-NH1	9.51	1.45	1.33
1	L	351	GLU	CD-OE1	9.40	1.35	1.25
1	S	89	ARG	CD-NE	9.35	1.62	1.46
1	T	89	ARG	CZ-NH1	9.18	1.45	1.33
1	S	353	ASP	CG-OD2	9.13	1.46	1.25
1	S	89	ARG	CZ-NH1	-9.04	1.21	1.33
1	S	91	GLU	CD-OE2	8.78	1.35	1.25
1	R	70	ASP	C-O	8.50	1.39	1.23
1	S	91	GLU	CD-OE1	8.44	1.34	1.25
1	N	356	TYR	CE1-CZ	8.38	1.49	1.38
1	T	27	ARG	CZ-NH2	8.16	1.43	1.33
1	N	356	TYR	CE2-CZ	8.14	1.49	1.38
1	S	376	GLU	C-O	7.79	1.38	1.23
1	N	356	TYR	CG-CD2	7.70	1.49	1.39
1	S	88	PHE	CE2-CZ	7.54	1.51	1.37
1	R	70	ASP	C-N	7.45	1.46	1.33
1	T	27	ARG	NE-CZ	7.44	1.42	1.33
1	S	88	PHE	CE1-CZ	7.39	1.51	1.37
1	N	356	TYR	CG-CD1	7.33	1.48	1.39
1	S	383	PHE	CG-CD2	7.11	1.49	1.38
1	S	271	HIS	CE1-NE2	6.85	1.48	1.32
1	S	89	ARG	CG-CD	6.78	1.68	1.51
1	I	90	ARG	CD-NE	6.66	1.57	1.46
1	S	376	GLU	CD-OE2	6.54	1.32	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S	353	ASP	CA-CB	6.38	1.68	1.53
1	I	60	ARG	CD-NE	6.26	1.57	1.46
1	S	85	LEU	CG-CD1	6.22	1.74	1.51
1	I	68	ILE	CB-CG1	6.05	1.71	1.54
1	T	89	ARG	CZ-NH2	6.04	1.40	1.33
1	R	61	GLU	CD-OE2	5.64	1.31	1.25
1	R	88	PHE	CE2-CZ	5.51	1.47	1.37
1	G	89	ARG	CZ-NH2	5.47	1.40	1.33
1	R	91	GLU	CD-OE2	5.44	1.31	1.25
1	T	27	ARG	CD-NE	5.43	1.55	1.46
1	T	89	ARG	NE-CZ	5.23	1.39	1.33
1	S	271	HIS	CG-ND1	5.09	1.50	1.38
1	I	60	ARG	CG-CD	5.02	1.64	1.51

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	S	89	ARG	NE-CZ-NH2	-48.18	96.21	120.30
1	S	89	ARG	NH1-CZ-NH2	23.44	145.18	119.40
1	T	27	ARG	NE-CZ-NH2	-23.04	108.78	120.30
1	I	90	ARG	NE-CZ-NH2	-20.39	110.11	120.30
1	S	89	ARG	CD-NE-CZ	-16.11	101.05	123.60
1	T	89	ARG	NE-CZ-NH2	-16.11	112.25	120.30
1	G	89	ARG	NE-CZ-NH2	-13.88	113.36	120.30
1	T	27	ARG	NE-CZ-NH1	12.94	126.77	120.30
1	R	60	ARG	NE-CZ-NH2	-12.52	114.04	120.30
1	S	90	ARG	NE-CZ-NH2	-11.87	114.37	120.30
1	R	60	ARG	NE-CZ-NH1	9.16	124.88	120.30
1	S	383	PHE	CB-CG-CD1	-8.28	115.00	120.80
1	S	89	ARG	CG-CD-NE	-8.16	94.67	111.80
1	S	353	ASP	CB-CG-OD2	-7.80	111.28	118.30
1	S	353	ASP	O-C-N	7.35	134.46	122.70
1	T	27	ARG	CD-NE-CZ	-7.27	113.42	123.60
1	S	353	ASP	CA-C-N	-7.04	101.70	117.20
1	T	89	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	I	90	ARG	NE-CZ-NH1	6.63	123.61	120.30
1	S	271	HIS	CG-ND1-CE1	-6.57	97.16	105.70
1	R	88	PHE	CB-CG-CD2	-6.38	116.33	120.80
1	S	90	ARG	NH1-CZ-NH2	5.79	125.77	119.40
1	S	383	PHE	CD1-CG-CD2	5.63	125.62	118.30
1	I	90	ARG	NH1-CZ-NH2	5.56	125.51	119.40
1	G	89	ARG	NE-CZ-NH1	5.47	123.04	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	156	LEU	CA-CB-CG	5.26	127.41	115.30
1	E	38	LEU	CA-CB-CG	5.17	127.20	115.30
1	S	383	PHE	CG-CD1-CE1	-5.15	115.13	120.80
1	Q	156	LEU	CA-CB-CG	5.11	127.06	115.30
1	R	93	CYS	CA-CB-SG	-5.02	104.96	114.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	S	116	THR	Mainchain
1	S	353	ASP	Sidechain,Mainchain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2871	0	2872	58	0
1	B	2871	0	2872	60	0
1	C	2871	0	2872	51	0
1	D	2871	0	2872	54	0
1	E	2871	0	2872	50	0
1	F	2871	0	2872	51	0
1	G	2871	0	2872	57	0
1	H	2871	0	2872	79	0
1	I	2871	0	2872	63	0
1	J	2871	0	2872	48	0
1	K	2871	0	2872	66	0
1	L	2871	0	2872	56	0
1	M	2871	0	2872	53	0
1	N	2871	0	2872	55	0
1	O	2871	0	2872	53	0
1	P	2871	0	2872	67	0
1	Q	2871	0	2872	50	0
1	R	2871	0	2872	49	0
1	S	2871	0	2872	68	0
1	T	2871	0	2872	50	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
2	N	1	0	0	0	0
2	O	1	0	0	0	0
2	P	1	0	0	0	0
2	Q	1	0	0	0	0
2	R	1	0	0	0	0
2	S	1	0	0	0	0
2	T	1	0	0	0	0
3	A	36	0	0	3	0
3	B	45	0	0	4	0
3	C	27	0	0	3	0
3	D	49	0	0	6	0
3	E	76	0	0	3	0
3	F	19	0	0	2	0
3	G	41	0	0	1	0
3	H	61	0	0	7	0
3	I	51	0	0	5	0
3	J	31	0	0	1	0
3	K	89	0	0	6	0
3	L	42	0	0	0	0
3	M	58	0	0	1	0
3	N	33	0	0	2	0
3	O	50	0	0	3	0
3	P	64	0	0	5	0
3	Q	43	0	0	1	0
3	R	39	0	0	0	0
3	S	19	0	0	6	0
3	T	35	0	0	1	0
All	All	58348	0	57440	1102	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 10.

All (1102) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:85:LEU:CG	1:S:85:LEU:CD1	1.74	1.63
1:I:60:ARG:CZ	1:I:60:ARG:NH1	1.69	1.52
1:S:89:ARG:NE	1:S:89:ARG:CZ	1.74	1.49
1:R:93:CYS:CB	1:R:93:CYS:SG	2.09	1.39
1:H:171:ARG:HG2	1:H:171:ARG:HH11	1.16	1.05
1:A:171:ARG:HG2	1:A:171:ARG:HH11	1.28	0.97
1:C:233:GLN:H	1:C:233:GLN:HE21	1.11	0.96
1:T:216:THR:HG21	1:T:261:ALA:HB2	1.47	0.96
1:H:233:GLN:H	1:H:233:GLN:HE21	0.97	0.95
1:D:216:THR:HG22	3:D:1429:HOH:O	1.66	0.95
1:N:233:GLN:H	1:N:233:GLN:HE21	1.15	0.94
1:J:233:GLN:H	1:J:233:GLN:HE21	1.11	0.94
1:G:233:GLN:H	1:G:233:GLN:HE21	1.04	0.94
1:E:9:LEU:H	1:E:260:ASN:HD21	1.16	0.93
1:E:21:ILE:O	1:E:24:VAL:HG23	1.69	0.93
1:M:233:GLN:H	1:M:233:GLN:HE21	1.17	0.93
1:O:233:GLN:H	1:O:233:GLN:HE21	1.12	0.91
1:O:9:LEU:H	1:O:260:ASN:HD21	1.17	0.91
1:A:233:GLN:H	1:A:233:GLN:HE21	1.18	0.91
1:D:233:GLN:H	1:D:233:GLN:HE21	1.16	0.91
1:L:233:GLN:H	1:L:233:GLN:HE21	1.11	0.91
1:K:233:GLN:HE21	1:K:233:GLN:H	0.97	0.90
1:E:233:GLN:H	1:E:233:GLN:HE21	1.16	0.89
1:Q:233:GLN:H	1:Q:233:GLN:HE21	1.15	0.89
1:K:9:LEU:H	1:K:260:ASN:HD21	1.18	0.89
1:E:9:LEU:H	1:E:260:ASN:ND2	1.71	0.88
1:P:9:LEU:H	1:P:260:ASN:HD21	1.23	0.87
1:E:82:ARG:HB3	3:E:1462:HOH:O	1.74	0.85
1:K:233:GLN:HE21	1:K:233:GLN:N	1.76	0.84
1:I:119:GLY:O	1:I:120:ASP:HB2	1.78	0.84
1:B:9:LEU:H	1:B:260:ASN:HD21	1.23	0.83
1:J:216:THR:HG21	1:J:261:ALA:HB2	1.61	0.83
1:M:152:ARG:H	1:M:259:ASN:HD21	1.26	0.83
1:T:233:GLN:H	1:T:233:GLN:HE21	1.26	0.83
1:P:233:GLN:HE21	1:P:233:GLN:H	1.26	0.83
1:B:233:GLN:H	1:B:233:GLN:HE21	1.25	0.83
1:G:216:THR:HG21	1:G:261:ALA:HB2	1.60	0.83
1:J:21:ILE:O	1:J:24:VAL:HG22	1.80	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:151:THR:HG22	1:M:153:HIS:H	1.42	0.82
1:O:152:ARG:H	1:O:259:ASN:HD21	1.27	0.82
1:B:9:LEU:H	1:B:260:ASN:ND2	1.78	0.81
1:O:9:LEU:H	1:O:260:ASN:ND2	1.77	0.81
1:F:9:LEU:H	1:F:260:ASN:ND2	1.78	0.81
1:R:296:ASN:HD21	1:R:370:ASN:HD21	1.25	0.81
1:C:233:GLN:HE21	1:C:233:GLN:N	1.79	0.80
1:H:233:GLN:H	1:H:233:GLN:NE2	1.76	0.80
1:C:9:LEU:H	1:C:260:ASN:ND2	1.79	0.80
1:E:151:THR:HG23	1:E:153:HIS:H	1.46	0.80
1:S:89:ARG:CZ	1:S:89:ARG:CD	2.59	0.80
1:H:233:GLN:HE21	1:H:233:GLN:N	1.78	0.79
1:K:9:LEU:H	1:K:260:ASN:ND2	1.80	0.79
1:A:328:ILE:O	1:A:332:THR:HG22	1.81	0.78
1:S:233:GLN:H	1:S:233:GLN:HE21	1.29	0.78
1:H:9:LEU:H	1:H:260:ASN:HD21	1.30	0.78
1:Q:60:ARG:HG3	1:Q:60:ARG:HH11	1.48	0.78
1:C:216:THR:HG21	1:C:261:ALA:HB2	1.65	0.78
1:N:151:THR:HG23	1:N:153:HIS:H	1.47	0.78
1:R:233:GLN:H	1:R:233:GLN:HE21	1.31	0.77
1:H:9:LEU:H	1:H:260:ASN:ND2	1.82	0.77
1:A:9:LEU:H	1:A:260:ASN:HD21	1.30	0.77
1:K:296:ASN:HD21	1:K:370:ASN:HD21	1.33	0.77
1:F:233:GLN:H	1:F:233:GLN:HE21	1.33	0.77
1:I:171:ARG:HG2	1:I:171:ARG:HH11	1.50	0.77
1:O:328:ILE:O	1:O:332:THR:HG22	1.86	0.76
1:S:117:HIS:HB3	3:S:1390:HOH:O	1.84	0.76
1:D:119:GLY:O	1:D:120:ASP:HB2	1.86	0.76
1:M:9:LEU:HB3	1:M:173:LEU:HD21	1.68	0.76
1:S:204:VAL:HG21	1:S:289:LEU:HD21	1.67	0.76
1:D:216:THR:HG21	1:D:261:ALA:HB2	1.68	0.76
1:H:171:ARG:HH11	1:H:171:ARG:CG	1.97	0.76
1:I:233:GLN:H	1:I:233:GLN:HE21	1.33	0.76
1:C:9:LEU:H	1:C:260:ASN:HD21	1.29	0.75
1:R:152:ARG:H	1:R:259:ASN:HD21	1.34	0.75
1:D:222:GLN:HE21	1:D:222:GLN:HA	1.51	0.75
1:B:119:GLY:O	1:B:120:ASP:HB2	1.84	0.75
1:D:9:LEU:H	1:D:260:ASN:HD21	1.31	0.75
1:F:280:PRO:HB2	1:F:283:VAL:HG12	1.67	0.75
1:H:296:ASN:HD21	1:H:370:ASN:HD21	1.35	0.75
1:Q:9:LEU:H	1:Q:260:ASN:HD21	1.35	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:171:ARG:HH11	1:O:171:ARG:HG2	1.52	0.75
1:D:9:LEU:H	1:D:260:ASN:ND2	1.83	0.74
1:M:9:LEU:H	1:M:260:ASN:HD21	1.35	0.74
1:K:21:ILE:O	1:K:24:VAL:HG22	1.88	0.74
1:N:9:LEU:H	1:N:260:ASN:HD21	1.35	0.74
1:A:171:ARG:HH11	1:A:171:ARG:CG	2.00	0.74
1:T:151:THR:HG22	1:T:153:HIS:H	1.51	0.73
1:E:152:ARG:H	1:E:259:ASN:HD21	1.35	0.73
1:S:103:SER:HB2	1:S:104:PRO:HD3	1.70	0.73
1:G:9:LEU:H	1:G:260:ASN:HD21	1.33	0.73
1:G:233:GLN:H	1:G:233:GLN:NE2	1.85	0.73
1:N:105:HIS:HE1	1:N:141:ASN:HD22	1.36	0.73
1:C:151:THR:HG22	1:C:153:HIS:H	1.53	0.73
1:F:296:ASN:HD21	1:F:370:ASN:HD21	1.33	0.73
1:F:9:LEU:H	1:F:260:ASN:HD21	1.37	0.73
1:H:216:THR:HG21	1:H:261:ALA:HB2	1.71	0.73
1:I:291:HIS:HD2	3:I:1415:HOH:O	1.72	0.72
1:I:296:ASN:HD21	1:I:370:ASN:HD21	1.38	0.72
1:J:152:ARG:H	1:J:259:ASN:HD21	1.36	0.72
1:S:9:LEU:H	1:S:260:ASN:ND2	1.86	0.72
1:T:328:ILE:O	1:T:332:THR:HG22	1.90	0.72
1:O:171:ARG:HH11	1:O:171:ARG:CG	2.02	0.72
1:C:216:THR:HG22	3:C:1400:HOH:O	1.88	0.72
1:M:9:LEU:H	1:M:260:ASN:ND2	1.86	0.72
1:F:121:LEU:HG	1:F:122:TYR:H	1.54	0.72
1:K:21:ILE:HD11	1:K:55:THR:HB	1.72	0.72
1:A:151:THR:HG23	1:A:153:HIS:H	1.53	0.72
1:B:9:LEU:HB3	1:B:173:LEU:HD21	1.71	0.71
1:R:222:GLN:HA	1:R:222:GLN:HE21	1.55	0.71
1:S:85:LEU:CD1	1:S:85:LEU:CB	2.68	0.71
1:P:9:LEU:H	1:P:260:ASN:ND2	1.87	0.71
1:G:368:PHE:HB2	3:G:1428:HOH:O	1.91	0.71
1:B:368:PHE:HB2	3:B:1400:HOH:O	1.90	0.71
1:D:60:ARG:HG3	1:D:60:ARG:HH11	1.55	0.71
1:F:151:THR:HG23	1:F:153:HIS:H	1.55	0.71
1:J:9:LEU:H	1:J:260:ASN:ND2	1.89	0.71
1:D:266:VAL:HG12	1:D:285:ASN:HD22	1.55	0.70
1:L:151:THR:HG23	1:L:153:HIS:H	1.55	0.70
1:O:21:ILE:O	1:O:24:VAL:HG22	1.91	0.70
1:T:152:ARG:H	1:T:259:ASN:HD21	1.37	0.70
1:A:9:LEU:H	1:A:260:ASN:ND2	1.90	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:9:LEU:H	1:G:260:ASN:ND2	1.88	0.70
1:J:45:ARG:HH21	1:J:68:ILE:HD11	1.57	0.70
1:J:98:THR:OG1	1:J:105:HIS:HD2	1.74	0.69
1:I:273:LEU:HD23	1:I:357:MET:HE1	1.74	0.69
1:J:9:LEU:H	1:J:260:ASN:HD21	1.38	0.69
1:G:233:GLN:HE21	1:G:233:GLN:N	1.84	0.69
1:K:291:HIS:HD2	3:K:1447:HOH:O	1.75	0.69
1:E:152:ARG:H	1:E:259:ASN:ND2	1.90	0.69
1:H:171:ARG:HG2	1:H:171:ARG:NH1	1.97	0.69
1:N:9:LEU:H	1:N:260:ASN:ND2	1.90	0.69
1:Q:328:ILE:O	1:Q:332:THR:HG22	1.93	0.69
1:K:152:ARG:H	1:K:259:ASN:HD21	1.39	0.69
1:J:265:TYR:H	1:J:370:ASN:ND2	1.91	0.68
1:L:266:VAL:HG12	1:L:285:ASN:HD22	1.57	0.68
1:A:213:ASN:ND2	1:A:216:THR:H	1.91	0.68
1:J:233:GLN:HE21	1:J:233:GLN:N	1.90	0.68
1:H:9:LEU:HB3	1:H:173:LEU:HD21	1.73	0.68
1:P:121:LEU:HA	3:P:1449:HOH:O	1.93	0.68
1:Q:266:VAL:HG12	1:Q:285:ASN:HD22	1.57	0.68
1:S:213:ASN:ND2	1:S:216:THR:H	1.91	0.68
1:N:230:ASN:OD1	1:N:246:TYR:HD2	1.75	0.68
1:G:121:LEU:HD23	1:G:121:LEU:H	1.58	0.68
1:M:128:GLU:HG3	3:M:1400:HOH:O	1.93	0.68
1:E:233:GLN:H	1:E:233:GLN:NE2	1.90	0.68
1:H:266:VAL:HG12	1:H:285:ASN:HD22	1.58	0.68
1:L:233:GLN:HE21	1:L:233:GLN:N	1.90	0.68
1:A:21:ILE:O	1:A:24:VAL:HG23	1.94	0.67
1:D:265:TYR:H	1:D:370:ASN:ND2	1.92	0.67
1:F:152:ARG:H	1:F:259:ASN:HD21	1.42	0.67
1:L:152:ARG:H	1:L:259:ASN:HD21	1.39	0.67
1:R:9:LEU:H	1:R:260:ASN:ND2	1.92	0.67
1:G:328:ILE:O	1:G:332:THR:HG22	1.95	0.67
1:A:105:HIS:HE1	1:A:141:ASN:HD22	1.42	0.67
1:G:213:ASN:ND2	1:G:216:THR:H	1.93	0.67
1:L:103:SER:HB2	1:L:104:PRO:HD3	1.77	0.67
1:Q:152:ARG:H	1:Q:259:ASN:HD21	1.42	0.67
1:F:9:LEU:HB3	1:F:173:LEU:HD21	1.74	0.67
1:K:9:LEU:HB3	1:K:173:LEU:HD21	1.76	0.67
1:N:233:GLN:H	1:N:233:GLN:NE2	1.91	0.67
1:P:21:ILE:O	1:P:24:VAL:HG22	1.94	0.67
1:H:152:ARG:H	1:H:259:ASN:HD21	1.43	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:THR:HG23	1:B:153:HIS:H	1.59	0.66
1:I:105:HIS:HE1	1:I:141:ASN:HD22	1.43	0.66
1:M:103:SER:HB2	1:M:104:PRO:HD3	1.78	0.66
1:N:296:ASN:HD21	1:N:370:ASN:HD21	1.43	0.66
1:B:283:VAL:O	1:B:287:VAL:HG12	1.95	0.66
1:M:296:ASN:HD21	1:M:370:ASN:HD21	1.43	0.66
1:B:296:ASN:HD21	1:B:370:ASN:HD21	1.43	0.66
1:K:233:GLN:H	1:K:233:GLN:NE2	1.82	0.66
1:R:9:LEU:H	1:R:260:ASN:HD21	1.44	0.66
1:Q:222:GLN:HA	1:Q:222:GLN:HE21	1.60	0.66
1:L:13:VAL:HG22	1:M:9:LEU:HD22	1.77	0.65
1:H:151:THR:HG22	1:H:153:HIS:H	1.62	0.65
1:K:152:ARG:H	1:K:259:ASN:ND2	1.94	0.65
1:P:27:ARG:HD3	3:P:1406:HOH:O	1.95	0.65
1:R:151:THR:HG22	1:R:153:HIS:H	1.62	0.65
1:O:233:GLN:H	1:O:233:GLN:NE2	1.91	0.65
1:G:152:ARG:H	1:G:259:ASN:HD21	1.44	0.65
1:P:296:ASN:HD21	1:P:370:ASN:HD21	1.43	0.65
1:T:233:GLN:H	1:T:233:GLN:NE2	1.95	0.65
1:G:52:VAL:HG12	1:G:99:VAL:HG21	1.79	0.65
1:O:216:THR:CG2	3:O:1436:HOH:O	2.45	0.65
1:H:121:LEU:HG	1:H:122:TYR:H	1.62	0.64
1:C:21:ILE:HD11	1:C:55:THR:HB	1.77	0.64
1:L:9:LEU:H	1:L:260:ASN:HD21	1.46	0.64
1:P:265:TYR:H	1:P:370:ASN:ND2	1.96	0.64
1:H:45:ARG:O	1:H:48:LYS:N	2.31	0.64
1:L:152:ARG:H	1:L:259:ASN:ND2	1.95	0.64
1:P:7:ASP:HB3	1:Q:15:PHE:CE2	2.32	0.64
1:I:180:ASP:HB3	1:I:183:LEU:HD22	1.79	0.64
1:S:89:ARG:NE	1:S:89:ARG:NH2	2.45	0.64
1:I:21:ILE:O	1:I:24:VAL:HG23	1.98	0.64
1:O:216:THR:HG21	1:O:261:ALA:HB2	1.79	0.63
1:A:78:ASP:HB2	1:A:121:LEU:HD13	1.80	0.63
1:O:151:THR:HG23	1:O:153:HIS:H	1.63	0.63
1:P:51:ALA:HB3	3:P:1394:HOH:O	1.98	0.63
1:R:266:VAL:HG12	1:R:285:ASN:HD22	1.63	0.63
1:D:60:ARG:HH11	1:D:60:ARG:CG	2.11	0.63
1:I:4:ARG:N	3:I:1393:HOH:O	2.30	0.63
1:L:9:LEU:H	1:L:260:ASN:ND2	1.96	0.63
1:K:273:LEU:HD23	1:K:357:MET:HE1	1.80	0.63
1:N:231:LEU:O	1:N:235:VAL:HG13	1.98	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:213:ASN:ND2	1:O:216:THR:H	1.96	0.63
1:N:103:SER:HB2	1:N:104:PRO:HD3	1.79	0.63
1:T:82:ARG:HH22	1:T:121:LEU:HD22	1.63	0.63
1:C:216:THR:CG2	3:C:1400:HOH:O	2.45	0.63
1:P:290:PRO:HB3	1:P:332:THR:HG22	1.79	0.63
1:C:152:ARG:H	1:C:259:ASN:HD21	1.47	0.62
1:J:265:TYR:H	1:J:370:ASN:HD22	1.46	0.62
1:Q:9:LEU:H	1:Q:260:ASN:ND2	1.96	0.62
1:Q:213:ASN:ND2	1:Q:216:THR:H	1.97	0.62
1:D:27:ARG:HD3	3:D:1393:HOH:O	1.99	0.62
1:P:274:GLY:O	1:P:278:ASP:HA	1.99	0.62
1:R:103:SER:HB2	1:R:104:PRO:HD3	1.82	0.62
1:A:233:GLN:HE21	1:A:233:GLN:N	1.95	0.62
1:E:180:ASP:HB3	1:E:183:LEU:HD22	1.80	0.62
1:K:105:HIS:HE1	1:K:141:ASN:HD22	1.47	0.62
1:M:233:GLN:H	1:M:233:GLN:NE2	1.93	0.62
1:N:213:ASN:ND2	1:N:216:THR:H	1.97	0.62
1:O:153:HIS:HD2	1:O:168:VAL:HG22	1.64	0.62
1:D:152:ARG:H	1:D:259:ASN:HD21	1.47	0.62
1:E:98:THR:OG1	1:E:105:HIS:HD2	1.82	0.62
1:D:180:ASP:HB3	1:D:183:LEU:HD22	1.80	0.62
1:P:233:GLN:HE21	1:P:233:GLN:N	1.98	0.62
1:S:21:ILE:O	1:S:24:VAL:HG22	2.00	0.62
1:A:119:GLY:O	1:A:120:ASP:HB2	1.98	0.62
1:G:55:THR:HG21	1:G:99:VAL:HG11	1.82	0.62
1:D:21:ILE:O	1:D:24:VAL:HG22	2.00	0.62
1:G:283:VAL:O	1:G:287:VAL:HG12	1.99	0.62
1:E:121:LEU:HB2	3:E:1404:HOH:O	1.98	0.62
1:O:265:TYR:H	1:O:370:ASN:ND2	1.98	0.62
1:M:119:GLY:O	1:M:120:ASP:HB2	2.00	0.61
1:T:213:ASN:ND2	1:T:216:THR:H	1.98	0.61
1:C:328:ILE:O	1:C:332:THR:HG22	2.00	0.61
1:J:216:THR:HG21	1:J:261:ALA:CB	2.30	0.61
1:M:82:ARG:NH1	1:M:121:LEU:HD21	2.14	0.61
1:E:45:ARG:C	1:E:48:LYS:HE3	2.20	0.61
1:G:152:ARG:H	1:G:259:ASN:ND2	1.99	0.61
1:P:265:TYR:H	1:P:370:ASN:HD22	1.49	0.61
1:S:85:LEU:CD1	1:S:85:LEU:CD2	2.75	0.61
1:D:231:LEU:O	1:D:235:VAL:HG13	2.00	0.61
1:J:213:ASN:ND2	1:J:216:THR:H	1.99	0.61
1:R:11:PRO:HD2	1:R:150:VAL:HG22	1.83	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:230:ASN:OD1	1:J:246:TYR:HD2	1.83	0.61
1:Q:265:TYR:H	1:Q:370:ASN:ND2	1.97	0.61
1:J:231:LEU:O	1:J:235:VAL:HG13	2.00	0.61
1:O:152:ARG:H	1:O:259:ASN:ND2	1.97	0.61
1:C:204:VAL:HG21	1:C:289:LEU:HD21	1.83	0.61
1:T:266:VAL:HG12	1:T:285:ASN:HD22	1.64	0.61
1:K:103:SER:HB2	1:K:104:PRO:HD3	1.81	0.61
1:Q:187:LYS:HD2	1:Q:191:LEU:HD12	1.82	0.61
1:I:375:ASN:C	1:I:375:ASN:HD22	2.04	0.61
1:Q:233:GLN:HE21	1:Q:233:GLN:N	1.94	0.61
1:E:222:GLN:HE21	1:E:222:GLN:HA	1.66	0.60
1:G:103:SER:HB2	1:G:104:PRO:HD3	1.83	0.60
1:G:105:HIS:HE1	1:G:141:ASN:HD22	1.50	0.60
1:I:266:VAL:HG12	1:I:285:ASN:HD22	1.65	0.60
1:P:82:ARG:HD2	3:P:1399:HOH:O	2.00	0.60
1:D:265:TYR:H	1:D:370:ASN:HD22	1.49	0.60
1:J:222:GLN:HA	1:J:222:GLN:HE21	1.65	0.60
1:M:200:LEU:O	1:M:204:VAL:HG13	2.01	0.60
1:R:265:TYR:H	1:R:370:ASN:ND2	1.99	0.60
1:L:9:LEU:HD22	1:M:13:VAL:HG22	1.81	0.60
1:A:242:GLN:HE21	1:A:246:TYR:HE2	1.50	0.60
1:R:55:THR:O	1:R:59:LEU:HB2	2.02	0.60
1:S:354:PHE:N	1:S:355:PRO:CD	2.64	0.60
1:N:280:PRO:HB2	1:N:283:VAL:HG22	1.84	0.60
1:D:152:ARG:H	1:D:259:ASN:ND2	2.00	0.60
1:I:9:LEU:H	1:I:260:ASN:ND2	2.00	0.60
1:R:213:ASN:ND2	1:R:216:THR:H	1.99	0.60
1:F:329:ALA:HA	1:F:332:THR:HG22	1.84	0.60
1:K:45:ARG:O	1:K:48:LYS:N	2.35	0.60
1:K:151:THR:HG23	1:K:153:HIS:H	1.66	0.60
1:D:216:THR:HG21	1:D:261:ALA:CB	2.32	0.59
1:E:121:LEU:HD23	1:E:122:TYR:H	1.67	0.59
1:I:24:VAL:HG22	1:I:178:ILE:HD13	1.82	0.59
1:B:103:SER:HB2	1:B:104:PRO:HD3	1.83	0.59
1:P:273:LEU:HD23	1:P:357:MET:HE1	1.85	0.59
1:J:266:VAL:HG12	1:J:285:ASN:HD22	1.67	0.59
1:L:382:ILE:HA	1:L:385:GLN:HE21	1.66	0.59
1:P:213:ASN:ND2	1:P:216:THR:H	2.00	0.59
1:D:146:THR:HG22	1:D:148:SER:H	1.67	0.59
1:G:362:LEU:HD12	1:G:376:GLU:HG3	1.83	0.59
1:O:49:ASP:N	1:O:49:ASP:OD1	2.36	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:277:TYR:CE2	1:K:357:MET:HE3	2.36	0.59
1:L:9:LEU:HB3	1:L:173:LEU:HD21	1.83	0.59
1:L:26:GLU:HA	1:L:29:GLN:HE21	1.66	0.59
1:M:152:ARG:H	1:M:259:ASN:ND2	1.97	0.59
1:H:9:LEU:HD22	1:K:13:VAL:HG22	1.85	0.59
1:R:151:THR:CG2	1:R:153:HIS:H	2.16	0.59
1:A:171:ARG:HG2	1:A:171:ARG:NH1	2.09	0.58
1:L:187:LYS:HD2	1:L:191:LEU:HD13	1.84	0.58
1:O:296:ASN:HD21	1:O:370:ASN:HD21	1.51	0.58
1:Q:21:ILE:O	1:Q:24:VAL:HG22	2.03	0.58
1:B:273:LEU:HD23	1:B:357:MET:HE1	1.85	0.58
1:H:213:ASN:ND2	1:H:216:THR:H	2.00	0.58
1:P:152:ARG:H	1:P:259:ASN:HD21	1.50	0.58
1:F:273:LEU:HD23	1:F:357:MET:HE1	1.85	0.58
1:H:216:THR:CG2	3:H:1429:HOH:O	2.51	0.58
1:Q:105:HIS:HE1	1:Q:141:ASN:HD22	1.50	0.58
1:F:100:GLY:HA3	1:F:104:PRO:HG2	1.84	0.58
1:B:328:ILE:O	1:B:332:THR:HG22	2.03	0.58
1:Q:151:THR:HG23	1:Q:153:HIS:H	1.68	0.58
1:F:200:LEU:HG	1:F:227:ILE:HG21	1.85	0.58
1:R:294:ARG:NH1	1:R:328:ILE:HG21	2.18	0.58
1:S:273:LEU:HD23	1:S:357:MET:HE1	1.85	0.58
1:D:9:LEU:HB3	1:D:173:LEU:HD21	1.85	0.58
1:I:9:LEU:HB3	1:I:173:LEU:HD21	1.84	0.58
1:I:213:ASN:ND2	1:I:216:THR:H	2.02	0.58
1:I:230:ASN:OD1	1:I:246:TYR:HD2	1.87	0.58
1:K:273:LEU:HA	1:K:357:MET:HE1	1.85	0.58
1:O:233:GLN:HE21	1:O:233:GLN:N	1.94	0.58
1:L:142:THR:HG22	1:L:142:THR:O	2.04	0.58
1:R:296:ASN:HD21	1:R:370:ASN:ND2	1.99	0.58
1:C:296:ASN:HD21	1:C:370:ASN:HD21	1.52	0.58
1:K:216:THR:HG21	1:K:261:ALA:HB2	1.85	0.58
1:B:213:ASN:ND2	1:B:216:THR:H	2.03	0.57
1:L:74:PRO:O	1:L:75:ASN:HB2	2.03	0.57
1:Q:153:HIS:HD2	1:Q:168:VAL:HG22	1.68	0.57
1:N:48:LYS:HD2	1:N:49:ASP:OD1	2.04	0.57
1:I:233:GLN:HE21	1:I:233:GLN:N	2.02	0.57
1:B:82:ARG:HB3	3:B:1397:HOH:O	2.04	0.57
1:H:105:HIS:HE1	1:H:141:ASN:HD22	1.51	0.57
1:N:9:LEU:HB3	1:N:173:LEU:HD21	1.86	0.57
1:O:216:THR:HG23	3:O:1436:HOH:O	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:296:ASN:HD21	1:Q:370:ASN:HD21	1.52	0.57
1:E:105:HIS:HE1	1:E:141:ASN:HD22	1.52	0.57
1:G:151:THR:HG23	1:G:153:HIS:H	1.69	0.57
1:B:74:PRO:O	1:B:75:ASN:HB2	2.04	0.57
1:H:21:ILE:O	1:H:24:VAL:HG22	2.04	0.57
1:K:375:ASN:C	1:K:375:ASN:HD22	2.08	0.57
1:T:9:LEU:H	1:T:260:ASN:ND2	2.03	0.57
1:T:296:ASN:HD21	1:T:370:ASN:HD21	1.53	0.57
1:G:45:ARG:HA	1:G:52:VAL:HG21	1.86	0.57
1:P:21:ILE:HD11	1:P:55:THR:HB	1.85	0.57
1:S:89:ARG:CD	1:S:89:ARG:NH1	2.67	0.57
1:M:265:TYR:H	1:M:370:ASN:ND2	2.03	0.57
1:B:266:VAL:HG12	1:B:285:ASN:HD22	1.70	0.57
1:H:51:ALA:HB3	3:H:1441:HOH:O	2.03	0.57
1:H:273:LEU:HD23	1:H:357:MET:HE1	1.86	0.57
1:P:180:ASP:HB3	1:P:183:LEU:HD22	1.87	0.56
1:F:4:ARG:N	3:F:1394:HOH:O	2.38	0.56
1:L:222:GLN:HE21	1:L:222:GLN:HA	1.70	0.56
1:P:153:HIS:HD2	1:P:168:VAL:HG22	1.70	0.56
1:R:9:LEU:HB3	1:R:173:LEU:HD21	1.87	0.56
1:A:265:TYR:H	1:A:370:ASN:HD22	1.52	0.56
1:D:213:ASN:ND2	1:D:216:THR:H	2.03	0.56
1:E:266:VAL:HG12	1:E:285:ASN:HD22	1.69	0.56
1:J:152:ARG:H	1:J:259:ASN:ND2	2.02	0.56
1:K:277:TYR:HE2	1:K:357:MET:HE3	1.70	0.56
1:M:233:GLN:HE21	1:M:233:GLN:N	1.95	0.56
1:N:27:ARG:HD3	3:N:1391:HOH:O	2.03	0.56
1:A:296:ASN:HD21	1:A:370:ASN:HD21	1.53	0.56
1:B:152:ARG:H	1:B:259:ASN:HD21	1.54	0.56
1:D:55:THR:O	1:D:59:LEU:HB2	2.05	0.56
1:S:89:ARG:CD	1:S:89:ARG:HH11	2.18	0.56
1:D:328:ILE:O	1:D:332:THR:HG22	2.06	0.56
1:I:9:LEU:H	1:I:260:ASN:HD21	1.52	0.56
1:O:230:ASN:OD1	1:O:246:TYR:HD2	1.88	0.56
1:D:144:ALA:H	1:D:187:LYS:NZ	2.03	0.56
1:H:152:ARG:H	1:H:259:ASN:ND2	2.03	0.56
1:J:210:LYS:HE2	1:J:368:PHE:O	2.05	0.56
1:I:152:ARG:NH1	1:I:259:ASN:O	2.38	0.56
1:C:222:GLN:HE21	1:C:222:GLN:HA	1.70	0.56
1:O:222:GLN:HE21	1:O:222:GLN:HA	1.71	0.56
1:S:233:GLN:HE21	1:S:233:GLN:N	2.03	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:213:ASN:HD22	1:L:215:VAL:H	1.51	0.55
1:R:152:ARG:H	1:R:259:ASN:ND2	2.01	0.55
1:E:280:PRO:HB2	1:E:283:VAL:HG13	1.87	0.55
1:F:152:ARG:HG3	1:F:168:VAL:HG13	1.88	0.55
1:H:142:THR:O	1:H:142:THR:HG22	2.06	0.55
1:J:187:LYS:HB2	1:J:244:ARG:HH22	1.71	0.55
1:C:55:THR:O	1:C:59:LEU:HB2	2.06	0.55
1:M:277:TYR:CE2	1:M:357:MET:HE3	2.42	0.55
1:T:265:TYR:H	1:T:370:ASN:ND2	2.04	0.55
1:B:233:GLN:HE21	1:B:233:GLN:N	2.00	0.55
1:C:273:LEU:HD23	1:C:357:MET:HE1	1.88	0.55
1:H:266:VAL:HG22	1:H:292:VAL:HB	1.89	0.55
1:J:105:HIS:HE1	1:J:141:ASN:HD22	1.55	0.55
1:T:103:SER:HB2	1:T:104:PRO:HD3	1.89	0.55
1:N:265:TYR:H	1:N:370:ASN:ND2	2.05	0.55
1:P:105:HIS:HE1	1:P:141:ASN:HD22	1.55	0.55
1:J:98:THR:OG1	1:J:105:HIS:CD2	2.58	0.55
1:M:142:THR:O	1:M:142:THR:HG22	2.06	0.55
1:D:233:GLN:H	1:D:233:GLN:NE2	1.96	0.55
1:Q:216:THR:HG21	1:Q:261:ALA:HB2	1.89	0.55
1:Q:280:PRO:HB2	1:Q:283:VAL:HG12	1.89	0.55
1:A:216:THR:HG21	1:A:261:ALA:HB2	1.89	0.54
1:D:4:ARG:N	3:D:1435:HOH:O	2.40	0.54
1:F:200:LEU:O	1:F:204:VAL:HG13	2.07	0.54
1:O:13:VAL:HB	1:O:176:VAL:HG22	1.87	0.54
1:P:151:THR:CG2	1:P:153:HIS:H	2.20	0.54
1:E:296:ASN:HD21	1:E:370:ASN:HD21	1.53	0.54
1:K:265:TYR:H	1:K:370:ASN:ND2	2.05	0.54
1:S:382:ILE:HA	1:S:385:GLN:HE21	1.72	0.54
1:G:21:ILE:O	1:G:24:VAL:HG22	2.07	0.54
1:G:49:ASP:N	1:G:49:ASP:OD1	2.41	0.54
1:G:273:LEU:HD23	1:G:357:MET:HE1	1.88	0.54
1:N:152:ARG:H	1:N:259:ASN:HD21	1.54	0.54
1:P:9:LEU:HB3	1:P:173:LEU:HD21	1.90	0.54
1:A:145:GLY:HA3	1:A:195:THR:O	2.07	0.54
1:I:151:THR:CG2	1:I:153:HIS:H	2.20	0.54
1:J:273:LEU:HD23	1:J:357:MET:HE1	1.89	0.54
1:R:93:CYS:SG	1:R:93:CYS:CA	2.93	0.54
1:B:55:THR:HG21	1:B:99:VAL:HG11	1.90	0.54
1:C:45:ARG:C	1:C:48:LYS:N	2.61	0.54
1:K:188:PRO:O	1:K:192:THR:HG22	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:233:GLN:H	1:Q:233:GLN:NE2	1.96	0.54
1:G:265:TYR:H	1:G:370:ASN:ND2	2.06	0.54
1:P:280:PRO:HB2	1:P:283:VAL:CG1	2.38	0.54
1:G:216:THR:HG21	1:G:261:ALA:CB	2.35	0.54
1:G:280:PRO:HB2	1:G:283:VAL:HG22	1.89	0.54
1:I:152:ARG:H	1:I:259:ASN:HD21	1.55	0.54
1:R:88:PHE:CD1	1:R:93:CYS:HB2	2.43	0.54
1:D:100:GLY:HA3	1:D:104:PRO:HG2	1.90	0.54
1:E:21:ILE:O	1:E:24:VAL:CG2	2.52	0.54
1:I:50:GLY:HA2	1:I:53:ASP:HB2	1.90	0.54
1:S:187:LYS:HE3	1:S:192:THR:HG22	1.89	0.54
1:B:7:ASP:OD2	1:B:152:ARG:NH2	2.36	0.54
1:E:265:TYR:H	1:E:370:ASN:ND2	2.06	0.54
1:K:50:GLY:HA3	3:K:1477:HOH:O	2.07	0.54
1:M:113:ILE:HD11	1:M:172:ASN:HD21	1.72	0.54
1:H:121:LEU:HD22	3:H:1410:HOH:O	2.08	0.53
1:J:20:ALA:O	1:J:23:VAL:HG22	2.07	0.53
1:K:210:LYS:HE2	1:K:368:PHE:O	2.09	0.53
1:S:265:TYR:H	1:S:370:ASN:ND2	2.06	0.53
1:N:125:ALA:HA	1:N:167:ILE:HG12	1.90	0.53
1:O:105:HIS:HE1	1:O:141:ASN:HD22	1.56	0.53
1:S:55:THR:O	1:S:59:LEU:HB2	2.08	0.53
1:G:52:VAL:HG12	1:G:99:VAL:CG2	2.38	0.53
1:P:9:LEU:HD22	1:Q:13:VAL:HG22	1.91	0.53
1:H:274:GLY:O	1:H:278:ASP:HA	2.08	0.53
1:C:180:ASP:HB3	1:C:183:LEU:HD22	1.90	0.53
1:D:151:THR:HG23	1:D:153:HIS:H	1.73	0.53
1:O:277:TYR:CE2	1:O:357:MET:HE1	2.44	0.53
1:Q:24:VAL:HG13	1:Q:178:ILE:HD12	1.91	0.53
1:B:48:LYS:HB3	1:B:49:ASP:OD2	2.08	0.53
1:E:13:VAL:HG22	1:I:9:LEU:HD22	1.90	0.53
1:F:222:GLN:HE21	1:F:222:GLN:HA	1.73	0.53
1:H:216:THR:HG22	3:H:1429:HOH:O	2.07	0.53
1:J:128:GLU:OE2	1:J:169:SER:HA	2.08	0.53
1:L:109:LYS:NZ	1:L:151:THR:HG22	2.23	0.53
1:N:45:ARG:O	1:N:48:LYS:HE2	2.09	0.53
1:K:266:VAL:HG12	1:K:285:ASN:HD22	1.74	0.53
1:T:151:THR:HG22	1:T:153:HIS:N	2.22	0.53
1:B:173:LEU:HD23	1:O:12:ASN:OD1	2.09	0.53
1:H:121:LEU:CG	1:H:122:TYR:H	2.20	0.53
1:N:121:LEU:HG	1:N:122:TYR:H	1.72	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:LEU:HD23	1:D:12:ASN:OD1	2.09	0.53
1:E:119:GLY:O	1:E:120:ASP:HB2	2.09	0.53
1:M:119:GLY:O	1:M:120:ASP:CB	2.57	0.53
1:N:375:ASN:ND2	1:N:378:GLU:H	2.07	0.53
1:L:296:ASN:HD21	1:L:370:ASN:HD21	1.57	0.52
1:B:21:ILE:O	1:B:24:VAL:HG22	2.10	0.52
1:G:153:HIS:HD2	1:G:168:VAL:HG22	1.74	0.52
1:J:375:ASN:ND2	1:J:378:GLU:H	2.07	0.52
1:A:105:HIS:CE1	1:A:141:ASN:HD22	2.25	0.52
1:E:9:LEU:HB3	1:E:173:LEU:HD21	1.90	0.52
1:H:265:TYR:H	1:H:370:ASN:ND2	2.08	0.52
1:R:333:ARG:NH1	1:S:321:LEU:HB3	2.24	0.52
1:T:13:VAL:O	1:T:176:VAL:HA	2.09	0.52
1:A:98:THR:OG1	1:A:105:HIS:HD2	1.93	0.52
1:B:213:ASN:HD22	1:B:215:VAL:H	1.56	0.52
1:P:328:ILE:O	1:P:332:THR:HG23	2.09	0.52
1:C:16:PHE:HE1	1:F:8:TYR:HB2	1.74	0.52
1:G:296:ASN:HD21	1:G:370:ASN:HD21	1.57	0.52
1:O:128:GLU:OE2	1:O:169:SER:HA	2.09	0.52
1:C:45:ARG:O	1:C:48:LYS:N	2.42	0.52
1:C:105:HIS:HE1	1:C:141:ASN:HD22	1.57	0.52
1:E:74:PRO:O	1:E:75:ASN:HB2	2.10	0.52
1:G:231:LEU:O	1:G:235:VAL:HG13	2.09	0.52
1:K:231:LEU:O	1:K:235:VAL:HG13	2.09	0.52
1:M:49:ASP:OD1	1:M:49:ASP:N	2.42	0.52
1:A:265:TYR:H	1:A:370:ASN:ND2	2.08	0.52
1:H:222:GLN:HE21	1:H:222:GLN:HA	1.73	0.52
1:M:213:ASN:ND2	1:M:216:THR:H	2.08	0.52
1:S:49:ASP:OD1	1:S:49:ASP:N	2.42	0.52
1:A:171:ARG:CG	1:A:171:ARG:NH1	2.66	0.52
1:F:273:LEU:HA	1:F:357:MET:HE1	1.92	0.52
1:P:151:THR:HG23	1:P:153:HIS:H	1.74	0.52
1:S:334:LEU:O	1:S:338:ILE:HG12	2.10	0.52
1:F:41:ASP:HB2	1:F:44:LEU:HD12	1.91	0.52
1:M:78:ASP:CB	1:M:121:LEU:HD13	2.40	0.52
1:N:181:PRO:HA	1:N:184:MET:HG3	1.92	0.52
1:G:265:TYR:H	1:G:370:ASN:HD22	1.57	0.52
1:O:200:LEU:HG	1:O:227:ILE:HG21	1.92	0.52
1:F:13:VAL:O	1:F:176:VAL:HA	2.11	0.51
1:T:280:PRO:HB2	1:T:283:VAL:HG22	1.91	0.51
1:M:82:ARG:HH11	1:M:121:LEU:HD21	1.74	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:266:VAL:HG12	1:N:285:ASN:HD22	1.74	0.51
1:A:266:VAL:HG12	1:A:285:ASN:HD22	1.75	0.51
1:I:328:ILE:O	1:I:332:THR:HG22	2.09	0.51
1:O:48:LYS:N	3:O:1407:HOH:O	2.43	0.51
1:Q:274:GLY:HA2	1:Q:278:ASP:HA	1.92	0.51
1:S:65:GLU:HB2	3:S:1394:HOH:O	2.09	0.51
1:A:24:VAL:HG22	1:A:178:ILE:CD1	2.41	0.51
1:B:152:ARG:HG3	1:B:168:VAL:HG13	1.92	0.51
1:I:222:GLN:HA	1:I:222:GLN:HE21	1.75	0.51
1:I:265:TYR:H	1:I:370:ASN:ND2	2.08	0.51
1:J:296:ASN:HD21	1:J:370:ASN:HD21	1.58	0.51
1:N:119:GLY:O	1:N:120:ASP:HB2	2.10	0.51
1:Q:151:THR:CG2	1:Q:153:HIS:H	2.23	0.51
1:D:50:GLY:HA3	3:D:1391:HOH:O	2.11	0.51
1:G:344:LEU:HB2	1:G:387:PHE:HA	1.91	0.51
1:S:16:PHE:HE1	1:T:8:TYR:HB2	1.76	0.51
1:T:263:LEU:HD13	1:T:267:HIS:CG	2.45	0.51
1:A:44:LEU:HD11	1:A:100:GLY:HA2	1.93	0.51
1:B:152:ARG:H	1:B:259:ASN:ND2	2.09	0.51
1:S:21:ILE:HD11	1:S:55:THR:HG22	1.92	0.51
1:K:4:ARG:NH2	3:K:1453:HOH:O	2.44	0.51
1:Q:60:ARG:HG3	1:Q:60:ARG:NH1	2.21	0.51
1:D:81:VAL:HG21	1:D:156:LEU:HD21	1.92	0.51
1:K:283:VAL:O	1:K:287:VAL:HG12	2.11	0.51
1:S:16:PHE:CE1	1:T:8:TYR:HB2	2.45	0.51
1:F:266:VAL:HG12	1:F:285:ASN:HD22	1.76	0.51
1:H:328:ILE:O	1:H:332:THR:HG22	2.11	0.51
1:K:280:PRO:HB2	1:K:283:VAL:HG13	1.93	0.51
1:N:375:ASN:C	1:N:375:ASN:HD22	2.13	0.51
1:T:9:LEU:H	1:T:260:ASN:HD21	1.59	0.51
1:L:213:ASN:ND2	1:L:216:THR:H	2.09	0.50
1:H:375:ASN:C	1:H:375:ASN:HD22	2.15	0.50
1:A:13:VAL:HB	1:A:176:VAL:HG22	1.92	0.50
1:B:230:ASN:OD1	1:B:246:TYR:HD2	1.93	0.50
1:F:187:LYS:HB3	1:F:192:THR:HG22	1.93	0.50
1:H:216:THR:CG2	1:H:261:ALA:HB2	2.41	0.50
1:J:74:PRO:O	1:J:75:ASN:HB2	2.11	0.50
1:L:78:ASP:HB2	1:L:121:LEU:HD13	1.94	0.50
1:O:153:HIS:CD2	1:O:168:VAL:HG22	2.45	0.50
1:E:230:ASN:OD1	1:E:246:TYR:HD2	1.95	0.50
1:F:152:ARG:H	1:F:259:ASN:ND2	2.06	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:216:THR:HG23	3:K:1395:HOH:O	2.11	0.50
1:I:42:LYS:HG2	1:I:70:ASP:O	2.12	0.50
1:K:98:THR:OG1	1:K:105:HIS:HD2	1.94	0.50
1:P:48:LYS:C	1:P:49:ASP:OD1	2.50	0.50
1:S:296:ASN:HD21	1:S:370:ASN:HD21	1.58	0.50
1:H:187:LYS:HD2	1:H:191:LEU:HD13	1.94	0.50
1:P:216:THR:HG21	1:P:261:ALA:HB2	1.92	0.50
1:R:375:ASN:ND2	1:R:378:GLU:H	2.09	0.50
1:I:378:GLU:O	1:I:382:ILE:HG13	2.12	0.50
1:J:103:SER:HB2	1:J:104:PRO:HD3	1.93	0.50
1:S:290:PRO:HB3	1:S:332:THR:HG22	1.93	0.50
1:A:222:GLN:HA	1:A:222:GLN:HE21	1.75	0.50
1:B:216:THR:HG21	1:B:261:ALA:HB2	1.93	0.50
1:M:116:THR:HG22	1:M:132:ASN:HB2	1.94	0.50
1:O:277:TYR:HE2	1:O:357:MET:HE1	1.77	0.50
1:Q:21:ILE:HD11	1:Q:55:THR:HB	1.93	0.50
1:S:11:PRO:HD2	1:S:150:VAL:HG23	1.94	0.50
1:T:21:ILE:HD11	1:T:55:THR:HB	1.93	0.50
1:B:317:GLY:HA3	3:B:1401:HOH:O	2.11	0.50
1:H:142:THR:O	1:H:142:THR:CG2	2.60	0.50
1:H:151:THR:CG2	1:H:153:HIS:H	2.25	0.50
1:H:152:ARG:HH12	1:H:260:ASN:HD22	1.60	0.50
1:H:290:PRO:HG3	1:H:331:ILE:HG22	1.93	0.50
1:J:45:ARG:O	1:J:48:LYS:HB2	2.11	0.50
1:L:317:GLY:O	1:S:314:ASN:ND2	2.43	0.50
1:N:49:ASP:HB3	3:N:1415:HOH:O	2.12	0.50
1:D:152:ARG:HG3	1:D:168:VAL:HG13	1.93	0.49
1:J:50:GLY:HA2	1:J:53:ASP:HB2	1.94	0.49
1:K:119:GLY:O	1:K:120:ASP:HB2	2.12	0.49
1:C:265:TYR:H	1:C:370:ASN:ND2	2.10	0.49
1:H:180:ASP:HB3	1:H:183:LEU:HD22	1.93	0.49
1:M:266:VAL:HG12	1:M:285:ASN:HD22	1.77	0.49
1:M:375:ASN:C	1:M:375:ASN:HD22	2.15	0.49
1:N:52:VAL:O	1:N:56:LEU:HB2	2.12	0.49
1:A:273:LEU:HD23	1:A:357:MET:HE1	1.93	0.49
1:E:82:ARG:HH22	1:E:121:LEU:CD2	2.24	0.49
1:H:230:ASN:OD1	1:H:246:TYR:HD2	1.94	0.49
1:L:273:LEU:HD23	1:L:357:MET:HE1	1.94	0.49
1:M:21:ILE:HD11	1:M:55:THR:HB	1.94	0.49
1:P:152:ARG:H	1:P:259:ASN:ND2	2.09	0.49
1:I:82:ARG:NH1	1:I:121:LEU:HD21	2.27	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:188:PRO:O	1:H:192:THR:HG23	2.11	0.49
1:I:231:LEU:O	1:I:235:VAL:HG13	2.13	0.49
1:R:273:LEU:HD23	1:R:357:MET:HE1	1.95	0.49
1:B:253:LEU:HD11	1:O:215:VAL:HA	1.94	0.49
1:C:266:VAL:HG12	1:C:285:ASN:HD22	1.77	0.49
1:F:307:ILE:O	1:F:311:MET:HG3	2.12	0.49
1:G:109:LYS:NZ	1:G:151:THR:HG22	2.28	0.49
1:I:45:ARG:HA	1:I:52:VAL:HG21	1.95	0.49
1:L:45:ARG:HA	1:L:52:VAL:HG21	1.93	0.49
1:P:40:THR:O	1:P:70:ASP:HA	2.12	0.49
1:A:151:THR:HG21	3:A:1404:HOH:O	2.13	0.49
1:C:103:SER:HB2	1:C:104:PRO:HD3	1.94	0.49
1:G:95:ILE:HG13	1:G:136:PRO:O	2.12	0.49
1:I:289:LEU:HB3	1:I:290:PRO:HD3	1.94	0.49
1:P:11:PRO:HB2	1:P:14:ASN:HD21	1.78	0.49
1:C:98:THR:HG21	1:C:108:GLY:HA3	1.94	0.49
1:J:344:LEU:HB2	1:J:387:PHE:HA	1.94	0.49
1:K:151:THR:CG2	1:K:153:HIS:H	2.25	0.49
1:O:45:ARG:C	1:O:48:LYS:HB2	2.32	0.49
1:P:100:GLY:HA3	1:P:104:PRO:HG2	1.94	0.49
1:F:45:ARG:HA	1:F:52:VAL:HG21	1.95	0.48
1:I:333:ARG:NH2	1:R:322:ASP:OD1	2.46	0.48
1:K:144:ALA:H	1:K:187:LYS:NZ	2.11	0.48
1:K:291:HIS:CD2	3:K:1447:HOH:O	2.58	0.48
1:S:9:LEU:H	1:S:260:ASN:HD21	1.60	0.48
1:T:200:LEU:HG	1:T:227:ILE:HG21	1.94	0.48
1:H:171:ARG:CG	1:H:171:ARG:NH1	2.64	0.48
1:K:50:GLY:HA2	1:K:53:ASP:HB2	1.95	0.48
1:L:55:THR:O	1:L:59:LEU:HB2	2.13	0.48
1:L:273:LEU:HA	1:L:357:MET:HE1	1.95	0.48
1:S:50:GLY:HA3	3:S:1406:HOH:O	2.12	0.48
1:T:152:ARG:NH1	1:T:260:ASN:HD22	2.11	0.48
1:C:273:LEU:HA	1:C:357:MET:HE1	1.95	0.48
1:D:103:SER:HB2	1:D:104:PRO:HD3	1.95	0.48
1:I:375:ASN:ND2	1:I:378:GLU:H	2.12	0.48
1:P:113:ILE:HD11	1:P:172:ASN:HD21	1.79	0.48
1:R:203:ALA:HB1	1:R:224:ILE:HG13	1.95	0.48
1:S:151:THR:HG22	1:S:153:HIS:H	1.79	0.48
1:E:20:ALA:O	1:E:23:VAL:HG22	2.13	0.48
1:M:105:HIS:HE1	1:M:141:ASN:HD22	1.61	0.48
1:O:98:THR:OG1	1:O:105:HIS:HD2	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:PRO:HB2	1:A:283:VAL:HG22	1.94	0.48
1:H:230:ASN:OD1	1:H:246:TYR:CD2	2.66	0.48
1:L:11:PRO:HD2	1:L:150:VAL:HG22	1.96	0.48
1:P:290:PRO:CB	1:P:332:THR:HG22	2.44	0.48
1:S:89:ARG:HH11	1:S:89:ARG:HD2	1.77	0.48
1:A:146:THR:HG23	1:A:148:SER:H	1.78	0.48
1:J:21:ILE:HD11	1:J:55:THR:HB	1.96	0.48
1:N:55:THR:O	1:N:59:LEU:HB2	2.12	0.48
1:S:98:THR:OG1	1:S:105:HIS:HD2	1.96	0.48
1:A:152:ARG:H	1:A:259:ASN:HD21	1.61	0.48
1:G:213:ASN:C	1:G:213:ASN:HD22	2.17	0.48
1:I:298:ILE:HD11	1:I:372:ARG:CZ	2.44	0.48
1:C:13:VAL:HG22	1:F:9:LEU:HD22	1.94	0.48
3:H:1408:HOH:O	1:I:325:GLU:HG2	2.13	0.48
1:K:180:ASP:HB3	1:K:183:LEU:HD22	1.96	0.48
1:K:213:ASN:H	1:K:216:THR:HG22	1.79	0.48
1:K:241:LEU:HD22	1:K:245:GLU:HG3	1.96	0.48
1:O:55:THR:O	1:O:59:LEU:HB2	2.14	0.48
1:R:188:PRO:O	1:R:192:THR:HG23	2.13	0.48
1:C:39:VAL:HB	1:C:98:THR:HG22	1.96	0.48
1:I:142:THR:HG22	1:I:142:THR:O	2.13	0.48
1:N:233:GLN:HE21	1:N:233:GLN:N	1.97	0.48
1:Q:231:LEU:O	1:Q:235:VAL:HG13	2.14	0.48
1:F:375:ASN:HD22	1:F:375:ASN:C	2.16	0.48
1:G:13:VAL:HG22	1:R:9:LEU:HD22	1.94	0.48
1:G:266:VAL:HG12	1:G:285:ASN:HD22	1.79	0.48
1:O:154:CYS:SG	1:O:156:LEU:HD21	2.54	0.48
1:R:41:ASP:HB2	1:R:44:LEU:HD12	1.96	0.48
1:D:283:VAL:O	1:D:287:VAL:HG12	2.13	0.47
1:B:265:TYR:H	1:B:370:ASN:ND2	2.12	0.47
1:C:321:LEU:HD11	1:J:232:ARG:NH2	2.30	0.47
1:P:344:LEU:HB2	1:P:387:PHE:HA	1.95	0.47
1:R:38:LEU:HB3	1:R:68:ILE:HB	1.96	0.47
1:J:9:LEU:HB3	1:J:173:LEU:HD21	1.96	0.47
1:K:213:ASN:HD22	1:K:215:VAL:H	1.62	0.47
1:K:375:ASN:ND2	1:K:378:GLU:H	2.11	0.47
1:Q:152:ARG:H	1:Q:259:ASN:ND2	2.10	0.47
1:K:296:ASN:HD21	1:K:370:ASN:ND2	2.09	0.47
1:N:148:SER:HA	1:N:151:THR:HB	1.97	0.47
1:P:231:LEU:O	1:P:235:VAL:HG13	2.14	0.47
1:E:200:LEU:O	1:E:204:VAL:HG13	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:99:VAL:HB	1:N:140:VAL:HG13	1.97	0.47
1:T:222:GLN:HE21	1:T:222:GLN:HA	1.78	0.47
1:D:116:THR:HG21	1:D:133:PRO:O	2.15	0.47
1:F:38:LEU:HD11	1:F:99:VAL:CG1	2.44	0.47
1:N:21:ILE:O	1:N:24:VAL:HG22	2.15	0.47
1:B:222:GLN:HA	1:B:222:GLN:HE21	1.80	0.47
1:C:9:LEU:HD22	1:F:13:VAL:HG22	1.96	0.47
1:C:213:ASN:ND2	1:C:216:THR:H	2.13	0.47
1:H:368:PHE:HB2	3:H:1399:HOH:O	2.14	0.47
1:I:216:THR:HG21	1:I:261:ALA:HB2	1.95	0.47
1:L:39:VAL:HB	1:L:98:THR:HG22	1.97	0.47
1:M:21:ILE:O	1:M:24:VAL:HG22	2.14	0.47
1:N:152:ARG:H	1:N:259:ASN:ND2	2.12	0.47
1:Q:41:ASP:HB2	1:Q:44:LEU:HD12	1.96	0.47
1:S:118:GLU:O	1:S:120:ASP:N	2.47	0.47
1:F:265:TYR:H	1:F:370:ASN:ND2	2.12	0.47
1:S:50:GLY:HA2	1:S:53:ASP:HB2	1.97	0.47
1:M:13:VAL:HB	1:M:176:VAL:HG22	1.96	0.47
1:M:213:ASN:HD22	1:M:215:VAL:H	1.62	0.47
1:O:171:ARG:HG2	1:O:171:ARG:NH1	2.24	0.47
1:S:222:GLN:HE21	1:S:222:GLN:HA	1.79	0.47
1:T:152:ARG:H	1:T:259:ASN:ND2	2.08	0.47
1:H:78:ASP:N	1:H:78:ASP:OD1	2.48	0.47
1:K:121:LEU:HA	3:K:1398:HOH:O	2.14	0.47
1:P:200:LEU:HG	1:P:227:ILE:HG21	1.95	0.47
1:C:216:THR:CG2	1:C:261:ALA:HB2	2.40	0.46
1:D:274:GLY:O	1:D:278:ASP:HA	2.14	0.46
1:I:151:THR:HG23	1:I:153:HIS:H	1.80	0.46
1:K:45:ARG:HA	1:K:52:VAL:HG21	1.97	0.46
1:L:18:PRO:HD2	1:M:4:ARG:O	2.15	0.46
1:N:39:VAL:HB	1:N:98:THR:HG22	1.97	0.46
1:R:210:LYS:HE2	1:R:368:PHE:O	2.14	0.46
1:T:21:ILE:O	1:T:24:VAL:HG22	2.15	0.46
1:B:5:MET:HG3	1:O:20:ALA:HA	1.96	0.46
1:B:13:VAL:HB	1:B:176:VAL:HG22	1.97	0.46
1:J:151:THR:HG23	1:J:153:HIS:H	1.79	0.46
1:K:265:TYR:H	1:K:370:ASN:HD22	1.61	0.46
1:P:266:VAL:HG12	1:P:285:ASN:HD22	1.80	0.46
1:T:45:ARG:C	1:T:48:LYS:HB2	2.34	0.46
1:B:45:ARG:HA	1:B:52:VAL:HG21	1.98	0.46
1:D:328:ILE:O	1:D:332:THR:CG2	2.63	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:273:LEU:HD23	1:E:357:MET:HE1	1.97	0.46
1:H:27:ARG:HD3	3:H:1389:HOH:O	2.14	0.46
1:K:121:LEU:CG	1:K:122:TYR:H	2.28	0.46
1:O:103:SER:HB2	1:O:104:PRO:HD3	1.96	0.46
1:P:142:THR:O	1:P:142:THR:CG2	2.63	0.46
1:Q:49:ASP:N	1:Q:49:ASP:OD1	2.48	0.46
1:D:200:LEU:HG	1:D:227:ILE:HG21	1.97	0.46
1:P:99:VAL:HB	1:P:140:VAL:HG13	1.97	0.46
1:Q:375:ASN:ND2	1:Q:378:GLU:H	2.13	0.46
1:C:152:ARG:H	1:C:259:ASN:ND2	2.13	0.46
1:L:10:VAL:HG23	1:L:11:PRO:HD2	1.97	0.46
1:M:180:ASP:HB3	1:M:183:LEU:HD22	1.97	0.46
1:S:266:VAL:HG12	1:S:285:ASN:HD22	1.81	0.46
1:C:11:PRO:HD2	1:C:150:VAL:HG22	1.97	0.46
1:H:263:LEU:HD13	1:H:267:HIS:CG	2.51	0.46
1:J:100:GLY:HA3	1:J:104:PRO:HG2	1.96	0.46
1:N:117:HIS:HB3	1:N:124:TYR:CZ	2.50	0.46
1:A:230:ASN:OD1	1:A:246:TYR:HD2	1.98	0.46
1:H:152:ARG:HD2	1:H:259:ASN:ND2	2.31	0.46
1:E:151:THR:CG2	1:E:153:HIS:H	2.24	0.46
1:G:375:ASN:ND2	1:G:378:GLU:H	2.14	0.46
1:T:216:THR:HG21	1:T:261:ALA:CB	2.34	0.46
1:A:151:THR:CG2	1:A:153:HIS:H	2.24	0.46
1:D:233:GLN:HE21	1:D:233:GLN:N	1.98	0.46
1:E:155:VAL:HB	1:E:166:VAL:HG22	1.98	0.46
1:F:294:ARG:NH1	3:F:1395:HOH:O	2.49	0.46
1:M:55:THR:O	1:M:59:LEU:HB2	2.15	0.46
1:N:14:ASN:ND2	1:N:177:SER:OG	2.42	0.46
1:E:213:ASN:ND2	1:E:216:THR:H	2.14	0.46
1:F:230:ASN:OD1	1:F:246:TYR:HD2	1.99	0.46
1:K:45:ARG:C	1:K:48:LYS:HB2	2.37	0.46
1:L:21:ILE:HD11	1:L:55:THR:HB	1.98	0.46
1:M:78:ASP:HB3	1:M:121:LEU:HD13	1.97	0.46
1:N:180:ASP:HB3	1:N:183:LEU:HD22	1.96	0.46
1:T:11:PRO:HB2	1:T:14:ASN:HD21	1.81	0.46
1:T:200:LEU:O	1:T:204:VAL:HG13	2.16	0.46
1:D:39:VAL:HB	1:D:98:THR:HG22	1.97	0.45
1:I:98:THR:HG21	1:I:108:GLY:HA3	1.98	0.45
1:I:105:HIS:HE1	1:I:141:ASN:ND2	2.13	0.45
1:O:151:THR:CG2	1:O:153:HIS:H	2.28	0.45
1:S:157:THR:HA	1:S:164:LYS:HA	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:PRO:O	1:A:75:ASN:HB2	2.16	0.45
1:D:296:ASN:HD21	1:D:370:ASN:HD21	1.64	0.45
1:L:127:ILE:O	1:L:129:THR:N	2.49	0.45
1:G:200:LEU:HG	1:G:227:ILE:HG21	1.99	0.45
1:H:296:ASN:HD21	1:H:370:ASN:ND2	2.08	0.45
1:I:328:ILE:O	1:I:332:THR:CG2	2.65	0.45
1:K:152:ARG:HG3	1:K:168:VAL:HG13	1.97	0.45
1:K:274:GLY:O	1:K:278:ASP:HA	2.17	0.45
1:L:116:THR:HG21	1:L:133:PRO:O	2.16	0.45
1:S:216:THR:HG21	1:S:261:ALA:HB2	1.98	0.45
1:A:344:LEU:HD22	1:A:349:VAL:HG21	1.99	0.45
1:D:203:ALA:HB1	1:D:224:ILE:HG13	1.97	0.45
1:H:375:ASN:HD22	1:H:378:GLU:H	1.65	0.45
1:I:246:TYR:HE1	3:I:1420:HOH:O	1.99	0.45
1:J:216:THR:HG22	3:J:1406:HOH:O	2.16	0.45
1:L:77:LYS:HD3	1:L:157:THR:HB	1.99	0.45
1:P:152:ARG:HG3	1:P:168:VAL:HG13	1.97	0.45
1:P:180:ASP:OD2	1:P:182:LEU:HB2	2.16	0.45
1:A:121:LEU:HD22	3:A:1409:HOH:O	2.15	0.45
1:A:227:ILE:HG13	1:A:250:ALA:HB1	1.99	0.45
1:E:153:HIS:HD2	1:E:168:VAL:HG22	1.80	0.45
1:E:213:ASN:HD22	1:E:215:VAL:H	1.63	0.45
1:L:328:ILE:O	1:L:332:THR:HG22	2.16	0.45
1:P:213:ASN:HD22	1:P:215:VAL:H	1.65	0.45
1:R:277:TYR:CZ	1:R:349:VAL:HA	2.51	0.45
1:S:117:HIS:CB	3:S:1390:HOH:O	2.54	0.45
1:T:273:LEU:HD23	1:T:357:MET:HE1	1.99	0.45
1:T:328:ILE:O	1:T:332:THR:CG2	2.64	0.45
1:B:280:PRO:HB2	1:B:283:VAL:HG13	1.99	0.45
1:F:119:GLY:O	1:F:120:ASP:HB2	2.16	0.45
1:R:180:ASP:HB3	1:R:183:LEU:HD22	1.99	0.45
1:B:51:ALA:HB3	3:B:1402:HOH:O	2.16	0.45
1:K:11:PRO:HD2	1:K:150:VAL:HG22	1.99	0.45
1:K:113:ILE:HA	1:K:134:LEU:HD22	1.98	0.45
1:Q:119:GLY:O	1:Q:120:ASP:HB2	2.17	0.45
1:F:78:ASP:HB2	1:F:121:LEU:HD13	1.98	0.45
1:F:88:PHE:CD1	1:F:93:CYS:HB2	2.52	0.45
1:G:222:GLN:HE21	1:G:222:GLN:HA	1.81	0.45
1:H:49:ASP:OD1	1:H:49:ASP:N	2.49	0.45
1:J:82:ARG:NH1	1:J:121:LEU:HD21	2.32	0.45
1:M:37:LEU:HD22	1:M:88:PHE:HB2	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:20:ALA:O	1:P:23:VAL:HG22	2.16	0.45
1:T:147:ALA:HB1	1:T:255:GLY:HA3	1.99	0.45
1:A:60:ARG:HB3	1:L:352:THR:HB	1.99	0.45
1:C:16:PHE:CE1	1:F:8:TYR:HB2	2.52	0.45
1:E:277:TYR:CE2	1:E:357:MET:HE3	2.52	0.45
1:I:20:ALA:O	1:I:23:VAL:HG22	2.17	0.45
1:L:95:ILE:HG13	1:L:136:PRO:O	2.17	0.45
1:P:48:LYS:O	1:P:49:ASP:OD1	2.35	0.45
1:T:11:PRO:HG3	1:T:174:PRO:HD2	1.99	0.45
1:E:315:ILE:HD13	1:E:315:ILE:HA	1.79	0.45
1:H:289:LEU:HB3	1:H:290:PRO:HD3	1.99	0.45
1:N:105:HIS:CE1	1:N:141:ASN:HD22	2.26	0.45
1:D:10:VAL:HG21	1:D:256:MET:HE2	1.97	0.44
1:B:188:PRO:O	1:B:192:THR:HG23	2.17	0.44
1:C:10:VAL:HG11	1:F:10:VAL:HG11	1.99	0.44
1:C:256:MET:HE3	3:C:1390:HOH:O	2.17	0.44
1:D:344:LEU:HB2	1:D:387:PHE:HA	1.98	0.44
1:I:204:VAL:O	1:I:208:ILE:HG12	2.17	0.44
1:L:134:LEU:HB3	1:L:135:PRO:HD2	1.99	0.44
1:N:266:VAL:HG22	1:N:292:VAL:HB	1.99	0.44
1:O:152:ARG:NH1	1:O:259:ASN:O	2.46	0.44
1:R:100:GLY:HA3	1:R:104:PRO:HG2	1.98	0.44
1:S:375:ASN:C	1:S:375:ASN:HD22	2.20	0.44
1:A:121:LEU:CG	1:A:122:TYR:H	2.31	0.44
1:F:187:LYS:HB2	1:F:244:ARG:HH22	1.82	0.44
1:H:95:ILE:HG13	1:H:136:PRO:O	2.16	0.44
1:N:142:THR:HG23	1:N:183:LEU:HB3	1.99	0.44
1:S:375:ASN:ND2	1:S:378:GLU:H	2.16	0.44
1:T:216:THR:CG2	1:T:261:ALA:HB2	2.34	0.44
1:C:26:GLU:HA	1:C:29:GLN:HE21	1.82	0.44
1:D:109:LYS:NZ	1:D:151:THR:HG22	2.32	0.44
1:G:328:ILE:O	1:G:332:THR:CG2	2.65	0.44
1:I:103:SER:HB2	1:I:104:PRO:HD3	1.98	0.44
1:O:375:ASN:C	1:O:375:ASN:HD22	2.21	0.44
1:P:98:THR:OG1	1:P:105:HIS:HD2	1.99	0.44
1:Q:290:PRO:HG3	1:Q:331:ILE:HG22	1.98	0.44
1:R:142:THR:O	1:R:142:THR:HG22	2.17	0.44
1:B:226:LEU:HD22	1:B:246:TYR:HB3	1.99	0.44
1:D:216:THR:CG2	3:D:1429:HOH:O	2.45	0.44
1:K:142:THR:HG22	1:K:142:THR:O	2.18	0.44
1:P:216:THR:HG22	1:P:217:ASP:N	2.33	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:85:LEU:HD13	1:S:115:ALA:HB2	1.98	0.44
1:A:210:LYS:HE2	1:A:368:PHE:O	2.18	0.44
1:C:280:PRO:HB2	1:C:283:VAL:HG22	2.00	0.44
1:F:11:PRO:HD2	1:F:150:VAL:HG22	1.99	0.44
1:F:21:ILE:HD11	1:F:55:THR:HB	1.99	0.44
1:G:216:THR:CG2	1:G:261:ALA:HB2	2.40	0.44
1:K:119:GLY:O	1:K:120:ASP:CB	2.65	0.44
1:M:216:THR:HG22	1:M:217:ASP:N	2.33	0.44
1:S:328:ILE:O	1:S:332:THR:HG23	2.18	0.44
1:A:18:PRO:HG2	1:D:4:ARG:HG3	1.99	0.44
1:C:96:ILE:HB	1:C:137:ILE:HG12	2.00	0.44
1:E:9:LEU:HD22	1:I:13:VAL:HG22	1.99	0.44
1:H:103:SER:HB2	1:H:104:PRO:HD3	2.00	0.44
1:O:74:PRO:O	1:O:75:ASN:HB2	2.18	0.44
1:P:95:ILE:HG13	1:P:136:PRO:O	2.18	0.44
1:P:127:ILE:O	1:P:129:THR:N	2.50	0.44
1:A:375:ASN:HD22	1:A:375:ASN:C	2.22	0.44
1:B:325:GLU:HG2	3:Q:1401:HOH:O	2.18	0.44
1:C:142:THR:O	1:C:142:THR:HG22	2.18	0.44
1:H:74:PRO:O	1:H:75:ASN:HB2	2.16	0.44
1:L:283:VAL:O	1:L:287:VAL:HG12	2.17	0.44
1:L:375:ASN:ND2	1:L:378:GLU:H	2.15	0.44
1:O:127:ILE:H	1:O:127:ILE:HG13	1.63	0.44
1:O:231:LEU:O	1:O:235:VAL:HG13	2.18	0.44
1:A:242:GLN:HG2	1:A:246:TYR:CE2	2.52	0.44
1:B:153:HIS:HD2	1:B:168:VAL:HG22	1.83	0.44
1:H:77:LYS:O	1:H:80:ASN:HB2	2.17	0.44
1:M:242:GLN:HE21	1:M:246:TYR:HE2	1.65	0.44
1:S:18:PRO:HG2	1:T:4:ARG:HB2	1.99	0.44
1:S:35:LYS:HG2	3:S:1396:HOH:O	2.17	0.44
1:T:68:ILE:H	1:T:68:ILE:HG13	1.64	0.44
1:B:231:LEU:O	1:B:235:VAL:HG13	2.17	0.43
1:J:13:VAL:HG22	1:N:9:LEU:HD22	2.00	0.43
1:M:231:LEU:O	1:M:235:VAL:HG13	2.18	0.43
1:O:45:ARG:O	1:O:48:LYS:HB2	2.18	0.43
1:Q:263:LEU:HD13	1:Q:267:HIS:CG	2.53	0.43
1:A:144:ALA:H	1:A:187:LYS:NZ	2.16	0.43
1:E:233:GLN:HE21	1:E:233:GLN:N	1.99	0.43
1:F:121:LEU:HG	1:F:122:TYR:N	2.27	0.43
1:J:213:ASN:HD22	1:J:215:VAL:H	1.66	0.43
1:N:263:LEU:HD13	1:N:267:HIS:CG	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:152:ARG:CD	1:S:259:ASN:HD21	2.31	0.43
1:B:119:GLY:O	1:B:120:ASP:CB	2.61	0.43
1:C:8:TYR:HB2	1:F:16:PHE:HE1	1.82	0.43
1:F:277:TYR:CE2	1:F:357:MET:HE3	2.53	0.43
1:I:98:THR:OG1	1:I:105:HIS:HD2	2.01	0.43
1:L:29:GLN:HG3	1:L:64:ILE:HD11	2.00	0.43
1:L:113:ILE:HA	1:L:134:LEU:HD22	2.00	0.43
1:Q:103:SER:HB2	1:Q:104:PRO:HD3	2.00	0.43
1:R:294:ARG:NH2	1:R:325:GLU:OE2	2.51	0.43
1:T:76:PRO:HB2	1:T:156:LEU:HD12	2.00	0.43
1:B:121:LEU:H	1:B:121:LEU:HG	1.53	0.43
1:E:180:ASP:HA	1:E:181:PRO:HD2	1.81	0.43
1:G:99:VAL:HG12	1:G:140:VAL:HG13	2.00	0.43
1:I:7:ASP:OD2	1:I:152:ARG:NH2	2.52	0.43
1:M:280:PRO:HB2	1:M:283:VAL:HG13	1.99	0.43
1:N:151:THR:CG2	1:N:153:HIS:H	2.24	0.43
1:O:328:ILE:O	1:O:332:THR:CG2	2.63	0.43
1:P:273:LEU:HA	1:P:357:MET:HE1	2.00	0.43
1:P:375:ASN:C	1:P:375:ASN:HD22	2.21	0.43
1:C:188:PRO:O	1:C:192:THR:HG23	2.18	0.43
1:M:152:ARG:NH1	1:M:260:ASN:HD22	2.16	0.43
1:N:77:LYS:HD3	1:N:157:THR:HB	1.98	0.43
1:Q:185:ILE:HD13	1:Q:244:ARG:HG2	2.00	0.43
1:A:51:ALA:HB3	3:A:1402:HOH:O	2.19	0.43
1:F:105:HIS:CD2	1:F:139:ALA:HB1	2.53	0.43
1:K:41:ASP:O	1:K:45:ARG:HB3	2.19	0.43
1:P:290:PRO:HG2	3:P:1408:HOH:O	2.19	0.43
1:R:204:VAL:O	1:R:208:ILE:HG12	2.18	0.43
1:D:144:ALA:H	1:D:187:LYS:HZ1	1.64	0.43
1:E:95:ILE:HG13	1:E:136:PRO:O	2.19	0.43
1:G:127:ILE:H	1:G:127:ILE:HG13	1.68	0.43
1:G:204:VAL:O	1:G:208:ILE:HG12	2.19	0.43
1:H:283:VAL:O	1:H:287:VAL:HG12	2.19	0.43
1:H:322:ASP:OD1	1:L:333:ARG:NH2	2.52	0.43
1:R:144:ALA:H	1:R:187:LYS:NZ	2.16	0.43
1:B:273:LEU:HA	1:B:357:MET:HE1	2.00	0.43
1:G:338:ILE:HG13	1:G:340:ILE:HG12	2.01	0.43
1:H:52:VAL:HG12	1:H:99:VAL:CG2	2.48	0.43
1:K:52:VAL:O	1:K:56:LEU:HB2	2.19	0.43
1:L:98:THR:OG1	1:L:105:HIS:HD2	2.02	0.43
1:N:121:LEU:HB2	1:N:165:PHE:CZ	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:38:LEU:HB3	1:S:68:ILE:HA	2.01	0.43
1:B:375:ASN:C	1:B:375:ASN:HD22	2.22	0.43
1:F:31:LEU:HD13	1:F:136:PRO:HB3	2.01	0.43
1:G:74:PRO:O	1:G:75:ASN:HB2	2.19	0.43
1:I:265:TYR:H	1:I:370:ASN:HD22	1.67	0.43
1:I:274:GLY:O	1:I:278:ASP:HA	2.18	0.43
1:S:98:THR:HG21	1:S:108:GLY:HA3	2.01	0.43
1:S:354:PHE:N	1:S:355:PRO:HD2	2.34	0.43
1:A:152:ARG:H	1:A:259:ASN:ND2	2.16	0.43
1:A:180:ASP:HA	1:A:181:PRO:HD2	1.95	0.43
1:B:76:PRO:HB2	1:B:156:LEU:HD12	2.01	0.43
1:H:203:ALA:HB1	1:H:224:ILE:HG13	2.01	0.43
1:B:17:GLY:O	1:B:181:PRO:HD2	2.19	0.42
1:C:184:MET:O	1:C:187:LYS:HG3	2.19	0.42
1:H:113:ILE:HD11	1:H:172:ASN:HD21	1.83	0.42
1:H:227:ILE:HG13	1:H:250:ALA:HB1	2.00	0.42
1:I:121:LEU:HD23	3:I:1406:HOH:O	2.19	0.42
1:I:294:ARG:NH1	3:I:1436:HOH:O	2.43	0.42
1:N:21:ILE:HD11	1:N:55:THR:HB	2.01	0.42
1:O:144:ALA:H	1:O:187:LYS:NZ	2.17	0.42
1:B:375:ASN:HD22	1:B:378:GLU:H	1.66	0.42
1:C:153:HIS:HD2	1:C:168:VAL:HG22	1.82	0.42
1:C:334:LEU:O	1:C:338:ILE:HG12	2.19	0.42
1:D:98:THR:HG21	1:D:108:GLY:HA3	2.01	0.42
1:F:103:SER:HB2	1:F:104:PRO:HD3	2.00	0.42
1:I:171:ARG:HG2	1:I:171:ARG:NH1	2.22	0.42
1:L:265:TYR:H	1:L:370:ASN:ND2	2.17	0.42
1:P:150:VAL:HG13	1:P:150:VAL:O	2.18	0.42
1:Q:9:LEU:HB3	1:Q:173:LEU:HD21	2.01	0.42
1:Q:181:PRO:HA	1:Q:184:MET:HG3	2.01	0.42
1:S:152:ARG:HD2	1:S:259:ASN:HD21	1.83	0.42
1:B:37:LEU:HD22	1:B:88:PHE:HB2	2.01	0.42
1:C:77:LYS:HD3	1:C:157:THR:HB	2.01	0.42
1:F:242:GLN:HG2	1:F:246:TYR:CE2	2.55	0.42
1:H:222:GLN:HE22	1:H:225:ARG:HE	1.66	0.42
1:K:134:LEU:HD11	1:K:172:ASN:HD22	1.84	0.42
1:L:142:THR:O	1:L:142:THR:CG2	2.68	0.42
1:N:109:LYS:NZ	1:N:151:THR:HG22	2.35	0.42
1:R:85:LEU:HD22	1:R:114:ALA:HB1	2.00	0.42
1:R:221:MET:HG2	1:R:310:LEU:HD21	2.01	0.42
1:S:37:LEU:HD22	1:S:88:PHE:HD1	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:253:LEU:HD11	1:T:215:VAL:HA	2.00	0.42
1:B:17:GLY:C	1:B:181:PRO:HD2	2.40	0.42
1:B:105:HIS:HE1	1:B:141:ASN:HD22	1.67	0.42
1:B:152:ARG:HD2	1:B:259:ASN:ND2	2.34	0.42
1:C:200:LEU:HG	1:C:227:ILE:HG21	1.99	0.42
1:G:39:VAL:HB	1:G:98:THR:HG22	2.01	0.42
1:H:375:ASN:ND2	1:H:378:GLU:H	2.17	0.42
1:L:152:ARG:HG3	1:L:168:VAL:HG13	2.02	0.42
1:A:95:ILE:HG13	1:A:136:PRO:O	2.18	0.42
1:I:152:ARG:HH12	1:I:260:ASN:HD22	1.66	0.42
1:J:127:ILE:H	1:J:127:ILE:HG13	1.67	0.42
1:M:95:ILE:HG13	1:M:136:PRO:O	2.19	0.42
1:M:121:LEU:HG	1:M:122:TYR:H	1.84	0.42
1:M:233:GLN:NE2	1:M:233:GLN:N	2.63	0.42
1:R:184:MET:HB3	1:R:187:LYS:HE2	2.01	0.42
1:S:152:ARG:H	1:S:259:ASN:HD21	1.67	0.42
1:T:187:LYS:HB2	1:T:244:ARG:HH22	1.83	0.42
1:A:145:GLY:HA2	1:A:199:ALA:HB2	2.01	0.42
1:I:21:ILE:HD11	1:I:55:THR:HG22	2.01	0.42
1:M:375:ASN:ND2	1:M:378:GLU:H	2.18	0.42
1:P:221:MET:HG2	1:P:310:LEU:HD21	2.02	0.42
1:Q:87:VAL:HG22	1:Q:90:ARG:HH22	1.84	0.42
1:Q:100:GLY:HA3	1:Q:104:PRO:HG2	2.01	0.42
1:R:76:PRO:HG3	1:R:103:SER:HA	2.02	0.42
1:S:39:VAL:HB	1:S:98:THR:HG22	2.02	0.42
1:A:375:ASN:ND2	1:A:378:GLU:H	2.17	0.42
1:M:222:GLN:HE21	1:M:222:GLN:HA	1.85	0.42
1:P:50:GLY:HA2	1:P:53:ASP:HB2	2.01	0.42
1:T:36:ALA:HA	1:T:95:ILE:O	2.20	0.42
1:T:181:PRO:HA	1:T:184:MET:HG3	2.02	0.42
1:E:82:ARG:HH22	1:E:121:LEU:HD21	1.83	0.42
1:F:82:ARG:NH2	1:F:121:LEU:HB3	2.34	0.42
1:K:121:LEU:HG	1:K:122:TYR:H	1.83	0.42
1:N:253:LEU:HD23	1:N:256:MET:HE2	2.02	0.42
1:P:375:ASN:ND2	1:P:378:GLU:H	2.17	0.42
1:R:113:ILE:HG12	1:R:130:LEU:HD21	2.02	0.42
1:R:375:ASN:HD22	1:R:375:ASN:C	2.23	0.42
1:S:45:ARG:HA	1:S:52:VAL:HG21	2.01	0.42
1:S:203:ALA:HB1	1:S:224:ILE:HG13	2.02	0.42
1:J:203:ALA:HB1	1:J:224:ILE:HG13	2.02	0.42
1:K:127:ILE:H	1:K:127:ILE:HG13	1.67	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:120:ASP:OD2	1:P:121:LEU:HG	2.20	0.42
1:Q:13:VAL:O	1:Q:176:VAL:HA	2.20	0.42
1:E:273:LEU:HA	1:E:357:MET:HE1	2.01	0.42
1:I:216:THR:HG22	1:I:217:ASP:N	2.34	0.42
1:L:232:ARG:NH1	1:L:337:ASP:OD2	2.43	0.42
1:Q:98:THR:OG1	1:Q:105:HIS:HD2	2.03	0.42
1:T:13:VAL:HB	1:T:176:VAL:HG22	2.01	0.42
1:T:113:ILE:HA	1:T:134:LEU:HD22	2.02	0.42
1:B:375:ASN:ND2	1:B:378:GLU:H	2.18	0.41
1:C:187:LYS:HB2	1:C:244:ARG:HH22	1.85	0.41
1:H:233:GLN:NE2	1:H:233:GLN:N	2.53	0.41
1:J:127:ILE:O	1:J:129:THR:N	2.53	0.41
1:R:294:ARG:HH11	1:R:328:ILE:HG21	1.85	0.41
1:A:121:LEU:HG	1:A:122:TYR:H	1.85	0.41
1:G:205:GLU:OE2	1:G:266:VAL:HG23	2.20	0.41
1:H:75:ASN:HD22	1:H:75:ASN:HA	1.65	0.41
1:H:151:THR:HG23	1:H:153:HIS:ND1	2.34	0.41
1:I:113:ILE:HA	1:I:134:LEU:HD22	2.01	0.41
1:M:334:LEU:O	1:M:338:ILE:HG12	2.20	0.41
1:Q:45:ARG:O	1:Q:48:LYS:HE2	2.19	0.41
1:R:233:GLN:H	1:R:233:GLN:NE2	2.09	0.41
1:G:109:LYS:HZ1	1:G:151:THR:HG22	1.85	0.41
1:Q:204:VAL:O	1:Q:208:ILE:HG12	2.20	0.41
1:S:95:ILE:HG13	1:S:136:PRO:O	2.21	0.41
1:B:266:VAL:HG22	1:B:292:VAL:HB	2.03	0.41
1:E:289:LEU:HD13	1:E:331:ILE:HG21	2.02	0.41
1:G:41:ASP:HB2	1:G:44:LEU:HD12	2.02	0.41
1:O:11:PRO:HD2	1:O:150:VAL:HG22	2.02	0.41
1:P:74:PRO:O	1:P:75:ASN:HB2	2.21	0.41
1:P:127:ILE:HB	1:P:128:GLU:H	1.63	0.41
1:P:210:LYS:HE2	1:P:368:PHE:O	2.20	0.41
1:S:350:LYS:HB2	3:S:1397:HOH:O	2.20	0.41
1:A:24:VAL:HG22	1:A:178:ILE:HD12	2.01	0.41
1:E:52:VAL:HG13	3:E:1396:HOH:O	2.19	0.41
1:G:334:LEU:O	1:G:338:ILE:HG12	2.21	0.41
1:H:222:GLN:NE2	1:H:225:ARG:HE	2.18	0.41
1:H:334:LEU:O	1:H:338:ILE:HG12	2.19	0.41
1:K:116:THR:HG21	1:K:133:PRO:O	2.20	0.41
1:L:221:MET:HG2	1:L:310:LEU:HD21	2.03	0.41
1:F:210:LYS:HE2	1:F:368:PHE:O	2.20	0.41
1:H:99:VAL:HB	1:H:140:VAL:HG22	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:152:ARG:NH1	1:H:259:ASN:O	2.54	0.41
1:N:48:LYS:HB3	1:N:49:ASP:H	1.65	0.41
1:P:6:PHE:HB2	1:Q:16:PHE:CE2	2.55	0.41
1:P:184:MET:O	1:P:187:LYS:HG3	2.20	0.41
1:R:88:PHE:CD1	1:R:93:CYS:CB	3.03	0.41
1:D:145:GLY:HA2	1:D:199:ALA:HB2	2.03	0.41
1:I:151:THR:HG22	1:I:153:HIS:H	1.85	0.41
1:N:216:THR:HG21	1:N:261:ALA:HB2	2.03	0.41
1:O:24:VAL:HG13	1:O:178:ILE:HD13	2.01	0.41
1:S:127:ILE:HB	1:S:128:GLU:H	1.62	0.41
1:D:148:SER:C	1:D:150:VAL:H	2.24	0.41
1:E:216:THR:HG22	1:E:217:ASP:N	2.35	0.41
1:H:113:ILE:HG12	1:H:130:LEU:HD21	2.02	0.41
1:P:10:VAL:HG11	1:Q:10:VAL:HG11	2.02	0.41
1:P:11:PRO:HD2	1:P:150:VAL:HG22	2.02	0.41
1:T:15:PHE:O	1:T:178:ILE:HA	2.21	0.41
1:B:213:ASN:HB2	1:B:214:PRO:HD2	2.03	0.41
1:J:7:ASP:HB3	1:N:15:PHE:CE2	2.55	0.41
1:K:302:GLU:HG3	1:K:320:THR:HG21	2.02	0.41
1:L:103:SER:CB	1:L:104:PRO:HD3	2.47	0.41
1:L:375:ASN:HD22	1:L:378:GLU:H	1.69	0.41
1:M:298:ILE:HD11	1:M:372:ARG:CZ	2.50	0.41
1:N:200:LEU:O	1:N:204:VAL:HG13	2.21	0.41
1:N:273:LEU:HD23	1:N:357:MET:HE1	2.02	0.41
1:N:278:ASP:O	1:N:278:ASP:CG	2.59	0.41
1:Q:11:PRO:HD2	1:Q:150:VAL:HG22	2.02	0.41
1:S:152:ARG:H	1:S:259:ASN:ND2	2.19	0.41
1:T:127:ILE:HB	1:T:128:GLU:H	1.67	0.41
1:T:188:PRO:O	1:T:192:THR:HG22	2.21	0.41
1:T:264:GLY:HA3	1:T:370:ASN:HD22	1.86	0.41
1:A:75:ASN:HD22	1:A:75:ASN:HA	1.70	0.41
1:B:77:LYS:O	1:B:80:ASN:HB2	2.21	0.41
1:G:382:ILE:HA	1:G:385:GLN:HE21	1.86	0.41
1:H:11:PRO:HD2	1:H:150:VAL:HG22	2.03	0.41
1:H:204:VAL:O	1:H:208:ILE:HG12	2.21	0.41
1:M:13:VAL:O	1:M:176:VAL:HA	2.21	0.41
1:R:265:TYR:H	1:R:370:ASN:HD22	1.68	0.41
1:T:121:LEU:HD23	1:T:121:LEU:H	1.86	0.41
1:B:12:ASN:OD1	1:O:173:LEU:HD23	2.21	0.40
1:D:21:ILE:HD11	1:D:55:THR:HB	2.03	0.40
1:F:21:ILE:O	1:F:24:VAL:HG22	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:95:ILE:HG13	1:K:136:PRO:O	2.20	0.40
1:K:127:ILE:O	1:K:129:THR:N	2.53	0.40
1:L:21:ILE:O	1:L:24:VAL:HG22	2.21	0.40
1:N:49:ASP:OD1	1:N:49:ASP:N	2.41	0.40
1:O:21:ILE:HD11	1:O:55:THR:HB	2.03	0.40
1:Q:184:MET:O	1:Q:187:LYS:HG3	2.21	0.40
1:S:280:PRO:O	1:S:282:GLY:N	2.55	0.40
1:T:298:ILE:HG23	3:T:1411:HOH:O	2.20	0.40
1:C:7:ASP:OD2	1:C:152:ARG:NH2	2.52	0.40
1:E:40:THR:O	1:E:70:ASP:HA	2.21	0.40
1:E:152:ARG:N	1:E:259:ASN:HD21	2.12	0.40
1:G:9:LEU:HB3	1:G:173:LEU:HD21	2.04	0.40
1:M:117:HIS:O	1:M:119:GLY:N	2.44	0.40
1:A:103:SER:HB2	1:A:104:PRO:HD3	2.03	0.40
1:E:354:PHE:HB2	1:E:355:PRO:HD3	2.03	0.40
1:G:113:ILE:HG12	1:G:130:LEU:HD21	2.03	0.40
1:I:263:LEU:HD13	1:I:267:HIS:CG	2.57	0.40
1:J:45:ARG:C	1:J:48:LYS:N	2.75	0.40
1:Q:20:ALA:HB3	1:Q:180:ASP:HB2	2.03	0.40
1:S:277:TYR:CE2	1:S:357:MET:HE1	2.57	0.40
1:B:150:VAL:O	1:B:150:VAL:HG13	2.21	0.40
1:B:334:LEU:O	1:B:338:ILE:HG12	2.22	0.40
1:C:152:ARG:HG3	1:C:168:VAL:HG13	2.03	0.40
1:H:232:ARG:NH2	1:I:321:LEU:HD11	2.35	0.40
1:J:152:ARG:HG3	1:J:168:VAL:HG13	2.03	0.40
1:O:13:VAL:O	1:O:176:VAL:HA	2.21	0.40
1:P:382:ILE:HA	1:P:385:GLN:HE21	1.86	0.40
1:A:127:ILE:HD12	1:A:128:GLU:H	1.85	0.40
1:D:60:ARG:NE	3:D:1413:HOH:O	2.54	0.40
1:E:360:MET:HA	1:E:360:MET:HE2	2.03	0.40
1:G:121:LEU:H	1:G:121:LEU:CD2	2.30	0.40
1:G:152:ARG:NH1	1:G:259:ASN:O	2.55	0.40
1:H:119:GLY:O	1:H:120:ASP:CB	2.69	0.40
1:H:152:ARG:HH12	1:H:260:ASN:ND2	2.19	0.40
1:J:213:ASN:HD22	1:J:215:VAL:N	2.19	0.40
1:K:74:PRO:O	1:K:75:ASN:HB2	2.21	0.40
1:L:68:ILE:H	1:L:68:ILE:HG13	1.60	0.40
1:L:338:ILE:HG13	1:L:340:ILE:HG12	2.02	0.40
1:R:152:ARG:NH1	1:R:259:ASN:O	2.50	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	378/387 (98%)	361 (96%)	10 (3%)	7 (2%)	8	20
1	B	378/387 (98%)	356 (94%)	15 (4%)	7 (2%)	8	20
1	C	378/387 (98%)	357 (94%)	15 (4%)	6 (2%)	9	24
1	D	378/387 (98%)	357 (94%)	15 (4%)	6 (2%)	9	24
1	E	378/387 (98%)	359 (95%)	12 (3%)	7 (2%)	8	20
1	F	378/387 (98%)	358 (95%)	14 (4%)	6 (2%)	9	24
1	G	378/387 (98%)	356 (94%)	16 (4%)	6 (2%)	9	24
1	H	378/387 (98%)	359 (95%)	13 (3%)	6 (2%)	9	24
1	I	378/387 (98%)	356 (94%)	15 (4%)	7 (2%)	8	20
1	J	378/387 (98%)	352 (93%)	19 (5%)	7 (2%)	8	20
1	K	378/387 (98%)	358 (95%)	12 (3%)	8 (2%)	7	18
1	L	378/387 (98%)	360 (95%)	11 (3%)	7 (2%)	8	20
1	M	378/387 (98%)	363 (96%)	9 (2%)	6 (2%)	9	24
1	N	378/387 (98%)	359 (95%)	13 (3%)	6 (2%)	9	24
1	O	378/387 (98%)	360 (95%)	12 (3%)	6 (2%)	9	24
1	P	378/387 (98%)	354 (94%)	19 (5%)	5 (1%)	12	30
1	Q	378/387 (98%)	358 (95%)	16 (4%)	4 (1%)	14	34
1	R	378/387 (98%)	363 (96%)	11 (3%)	4 (1%)	14	34
1	S	378/387 (98%)	352 (93%)	15 (4%)	11 (3%)	4	10
1	T	378/387 (98%)	356 (94%)	18 (5%)	4 (1%)	14	34
All	All	7560/7740 (98%)	7154 (95%)	280 (4%)	126 (2%)	9	23

All (126) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	120	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	127	ILE
1	B	120	ASP
1	B	127	ILE
1	D	120	ASP
1	D	127	ILE
1	E	120	ASP
1	E	127	ILE
1	F	127	ILE
1	H	75	ASN
1	H	120	ASP
1	H	121	LEU
1	I	120	ASP
1	J	119	GLY
1	K	49	ASP
1	K	120	ASP
1	K	121	LEU
1	K	127	ILE
1	L	119	GLY
1	L	128	GLU
1	M	118	GLU
1	M	120	ASP
1	M	121	LEU
1	N	127	ILE
1	O	119	GLY
1	O	127	ILE
1	P	127	ILE
1	Q	119	GLY
1	Q	127	ILE
1	R	127	ILE
1	S	119	GLY
1	S	281	HIS
1	T	127	ILE
1	B	50	GLY
1	B	145	GLY
1	C	50	GLY
1	C	119	GLY
1	C	128	GLU
1	C	316	THR
1	D	119	GLY
1	E	119	GLY
1	E	278	ASP
1	G	50	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	119	GLY
1	G	127	ILE
1	G	145	GLY
1	H	145	GLY
1	H	278	ASP
1	I	127	ILE
1	I	128	GLU
1	I	145	GLY
1	J	127	ILE
1	J	128	GLU
1	J	145	GLY
1	L	50	GLY
1	L	127	ILE
1	M	119	GLY
1	N	118	GLU
1	O	145	GLY
1	Q	51	ALA
1	R	49	ASP
1	A	119	GLY
1	B	119	GLY
1	C	92	GLN
1	C	145	GLY
1	D	50	GLY
1	E	51	ALA
1	E	145	GLY
1	F	145	GLY
1	I	119	GLY
1	J	49	ASP
1	L	121	LEU
1	L	145	GLY
1	M	145	GLY
1	N	145	GLY
1	P	145	GLY
1	R	50	GLY
1	R	145	GLY
1	S	49	ASP
1	S	118	GLU
1	S	278	ASP
1	T	50	GLY
1	A	121	LEU
1	A	145	GLY
1	D	145	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	50	GLY
1	F	119	GLY
1	G	128	GLU
1	H	50	GLY
1	K	50	GLY
1	K	128	GLU
1	L	120	ASP
1	N	119	GLY
1	N	120	ASP
1	O	50	GLY
1	O	278	ASP
1	P	51	ALA
1	P	120	ASP
1	Q	145	GLY
1	S	127	ILE
1	T	145	GLY
1	B	49	ASP
1	D	51	ALA
1	F	120	ASP
1	F	278	ASP
1	I	162	LYS
1	K	145	GLY
1	M	50	GLY
1	S	50	GLY
1	S	128	GLU
1	S	145	GLY
1	S	353	ASP
1	A	50	GLY
1	A	316	THR
1	G	75	ASN
1	N	50	GLY
1	B	75	ASN
1	J	50	GLY
1	P	50	GLY
1	S	75	ASN
1	T	75	ASN
1	J	75	ASN
1	E	75	ASN
1	K	75	ASN
1	O	75	ASN
1	I	50	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	296/302 (98%)	260 (88%)	36 (12%)	5	11
1	B	296/302 (98%)	257 (87%)	39 (13%)	4	9
1	C	296/302 (98%)	267 (90%)	29 (10%)	8	18
1	D	296/302 (98%)	253 (86%)	43 (14%)	3	8
1	E	296/302 (98%)	253 (86%)	43 (14%)	3	8
1	F	296/302 (98%)	261 (88%)	35 (12%)	5	12
1	G	296/302 (98%)	258 (87%)	38 (13%)	4	10
1	H	296/302 (98%)	256 (86%)	40 (14%)	4	9
1	I	296/302 (98%)	262 (88%)	34 (12%)	5	13
1	J	296/302 (98%)	264 (89%)	32 (11%)	6	15
1	K	296/302 (98%)	253 (86%)	43 (14%)	3	8
1	L	296/302 (98%)	262 (88%)	34 (12%)	5	13
1	M	296/302 (98%)	258 (87%)	38 (13%)	4	10
1	N	296/302 (98%)	262 (88%)	34 (12%)	5	13
1	O	296/302 (98%)	257 (87%)	39 (13%)	4	9
1	P	296/302 (98%)	249 (84%)	47 (16%)	2	6
1	Q	296/302 (98%)	253 (86%)	43 (14%)	3	8
1	R	296/302 (98%)	263 (89%)	33 (11%)	6	14
1	S	296/302 (98%)	265 (90%)	31 (10%)	7	16
1	T	296/302 (98%)	271 (92%)	25 (8%)	11	25
All	All	5920/6040 (98%)	5184 (88%)	736 (12%)	4	11

All (736) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	LEU
1	A	49	ASP
1	A	56	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	59	LEU
1	A	66	VAL
1	A	68	ILE
1	A	94	ASP
1	A	116	THR
1	A	121	LEU
1	A	131	THR
1	A	140	VAL
1	A	146	THR
1	A	150	VAL
1	A	151	THR
1	A	152	ARG
1	A	156	LEU
1	A	160	GLU
1	A	171	ARG
1	A	173	LEU
1	A	191	LEU
1	A	192	THR
1	A	200	LEU
1	A	204	VAL
1	A	213	ASN
1	A	216	THR
1	A	222	GLN
1	A	233	GLN
1	A	244	ARG
1	A	258	PHE
1	A	288	LEU
1	A	289	LEU
1	A	310	LEU
1	A	332	THR
1	A	333	ARG
1	A	362	LEU
1	A	375	ASN
1	B	24	VAL
1	B	38	LEU
1	B	49	ASP
1	B	56	LEU
1	B	59	LEU
1	B	65	GLU
1	B	68	ILE
1	B	99	VAL
1	B	116	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	120	ASP
1	B	121	LEU
1	B	128	GLU
1	B	140	VAL
1	B	143	THR
1	B	148	SER
1	B	150	VAL
1	B	151	THR
1	B	152	ARG
1	B	155	VAL
1	B	173	LEU
1	B	182	LEU
1	B	191	LEU
1	B	192	THR
1	B	200	LEU
1	B	213	ASN
1	B	216	THR
1	B	222	GLN
1	B	233	GLN
1	B	235	VAL
1	B	241	LEU
1	B	244	ARG
1	B	258	PHE
1	B	288	LEU
1	B	289	LEU
1	B	310	LEU
1	B	332	THR
1	B	333	ARG
1	B	375	ASN
1	B	377	GLN
1	C	49	ASP
1	C	68	ILE
1	C	116	THR
1	C	118	GLU
1	C	120	ASP
1	C	128	GLU
1	C	131	THR
1	C	140	VAL
1	C	150	VAL
1	C	152	ARG
1	C	173	LEU
1	C	182	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	191	LEU
1	C	192	THR
1	C	200	LEU
1	C	213	ASN
1	C	216	THR
1	C	222	GLN
1	C	233	GLN
1	C	241	LEU
1	C	244	ARG
1	C	258	PHE
1	C	288	LEU
1	C	289	LEU
1	C	310	LEU
1	C	332	THR
1	C	333	ARG
1	C	362	LEU
1	C	375	ASN
1	D	24	VAL
1	D	38	LEU
1	D	45	ARG
1	D	48	LYS
1	D	49	ASP
1	D	55	THR
1	D	56	LEU
1	D	60	ARG
1	D	61	GLU
1	D	68	ILE
1	D	116	THR
1	D	121	LEU
1	D	131	THR
1	D	140	VAL
1	D	150	VAL
1	D	151	THR
1	D	152	ARG
1	D	156	LEU
1	D	173	LEU
1	D	175	SER
1	D	182	LEU
1	D	183	LEU
1	D	191	LEU
1	D	192	THR
1	D	200	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	204	VAL
1	D	213	ASN
1	D	222	GLN
1	D	233	GLN
1	D	235	VAL
1	D	241	LEU
1	D	244	ARG
1	D	258	PHE
1	D	283	VAL
1	D	288	LEU
1	D	289	LEU
1	D	310	LEU
1	D	332	THR
1	D	333	ARG
1	D	347	LEU
1	D	362	LEU
1	D	375	ASN
1	D	377	GLN
1	E	38	LEU
1	E	45	ARG
1	E	55	THR
1	E	56	LEU
1	E	59	LEU
1	E	65	GLU
1	E	68	ILE
1	E	99	VAL
1	E	116	THR
1	E	120	ASP
1	E	121	LEU
1	E	128	GLU
1	E	130	LEU
1	E	140	VAL
1	E	142	THR
1	E	143	THR
1	E	150	VAL
1	E	151	THR
1	E	152	ARG
1	E	155	VAL
1	E	173	LEU
1	E	182	LEU
1	E	183	LEU
1	E	191	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	192	THR
1	E	200	LEU
1	E	204	VAL
1	E	213	ASN
1	E	216	THR
1	E	222	GLN
1	E	233	GLN
1	E	235	VAL
1	E	241	LEU
1	E	244	ARG
1	E	258	PHE
1	E	283	VAL
1	E	288	LEU
1	E	289	LEU
1	E	310	LEU
1	E	332	THR
1	E	347	LEU
1	E	362	LEU
1	E	375	ASN
1	F	38	LEU
1	F	41	ASP
1	F	49	ASP
1	F	55	THR
1	F	56	LEU
1	F	68	ILE
1	F	82	ARG
1	F	116	THR
1	F	121	LEU
1	F	130	LEU
1	F	131	THR
1	F	140	VAL
1	F	143	THR
1	F	150	VAL
1	F	151	THR
1	F	152	ARG
1	F	155	VAL
1	F	173	LEU
1	F	191	LEU
1	F	192	THR
1	F	200	LEU
1	F	204	VAL
1	F	213	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	216	THR
1	F	222	GLN
1	F	233	GLN
1	F	241	LEU
1	F	244	ARG
1	F	258	PHE
1	F	288	LEU
1	F	289	LEU
1	F	310	LEU
1	F	347	LEU
1	F	368	PHE
1	F	375	ASN
1	G	4	ARG
1	G	24	VAL
1	G	38	LEU
1	G	49	ASP
1	G	55	THR
1	G	65	GLU
1	G	68	ILE
1	G	99	VAL
1	G	106	ASP
1	G	116	THR
1	G	128	GLU
1	G	140	VAL
1	G	143	THR
1	G	150	VAL
1	G	151	THR
1	G	152	ARG
1	G	159	THR
1	G	173	LEU
1	G	182	LEU
1	G	191	LEU
1	G	192	THR
1	G	200	LEU
1	G	204	VAL
1	G	213	ASN
1	G	216	THR
1	G	222	GLN
1	G	233	GLN
1	G	235	VAL
1	G	241	LEU
1	G	244	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	258	PHE
1	G	288	LEU
1	G	289	LEU
1	G	310	LEU
1	G	332	THR
1	G	362	LEU
1	G	375	ASN
1	G	377	GLN
1	H	38	LEU
1	H	45	ARG
1	H	49	ASP
1	H	55	THR
1	H	56	LEU
1	H	68	ILE
1	H	75	ASN
1	H	99	VAL
1	H	121	LEU
1	H	128	GLU
1	H	131	THR
1	H	140	VAL
1	H	143	THR
1	H	150	VAL
1	H	152	ARG
1	H	155	VAL
1	H	156	LEU
1	H	171	ARG
1	H	173	LEU
1	H	182	LEU
1	H	183	LEU
1	H	191	LEU
1	H	192	THR
1	H	200	LEU
1	H	204	VAL
1	H	213	ASN
1	H	216	THR
1	H	222	GLN
1	H	233	GLN
1	H	235	VAL
1	H	241	LEU
1	H	244	ARG
1	H	258	PHE
1	H	288	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	289	LEU
1	H	310	LEU
1	H	332	THR
1	H	333	ARG
1	H	362	LEU
1	H	375	ASN
1	I	55	THR
1	I	56	LEU
1	I	116	THR
1	I	120	ASP
1	I	121	LEU
1	I	128	GLU
1	I	140	VAL
1	I	150	VAL
1	I	151	THR
1	I	152	ARG
1	I	173	LEU
1	I	182	LEU
1	I	183	LEU
1	I	192	THR
1	I	200	LEU
1	I	204	VAL
1	I	213	ASN
1	I	216	THR
1	I	222	GLN
1	I	233	GLN
1	I	235	VAL
1	I	241	LEU
1	I	242	GLN
1	I	244	ARG
1	I	258	PHE
1	I	278	ASP
1	I	288	LEU
1	I	289	LEU
1	I	310	LEU
1	I	332	THR
1	I	333	ARG
1	I	359	GLU
1	I	362	LEU
1	I	375	ASN
1	J	24	VAL
1	J	45	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	49	ASP
1	J	55	THR
1	J	68	ILE
1	J	116	THR
1	J	121	LEU
1	J	128	GLU
1	J	132	ASN
1	J	140	VAL
1	J	142	THR
1	J	143	THR
1	J	150	VAL
1	J	173	LEU
1	J	182	LEU
1	J	191	LEU
1	J	192	THR
1	J	200	LEU
1	J	213	ASN
1	J	222	GLN
1	J	233	GLN
1	J	235	VAL
1	J	241	LEU
1	J	244	ARG
1	J	258	PHE
1	J	289	LEU
1	J	310	LEU
1	J	332	THR
1	J	333	ARG
1	J	347	LEU
1	J	368	PHE
1	J	375	ASN
1	K	24	VAL
1	K	45	ARG
1	K	55	THR
1	K	56	LEU
1	K	68	ILE
1	K	94	ASP
1	K	99	VAL
1	K	116	THR
1	K	121	LEU
1	K	128	GLU
1	K	131	THR
1	K	140	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	143	THR
1	K	150	VAL
1	K	151	THR
1	K	152	ARG
1	K	156	LEU
1	K	173	LEU
1	K	182	LEU
1	K	183	LEU
1	K	191	LEU
1	K	192	THR
1	K	200	LEU
1	K	204	VAL
1	K	213	ASN
1	K	216	THR
1	K	222	GLN
1	K	233	GLN
1	K	235	VAL
1	K	241	LEU
1	K	242	GLN
1	K	244	ARG
1	K	258	PHE
1	K	283	VAL
1	K	287	VAL
1	K	288	LEU
1	K	289	LEU
1	K	310	LEU
1	K	332	THR
1	K	333	ARG
1	K	347	LEU
1	K	362	LEU
1	K	375	ASN
1	L	12	ASN
1	L	41	ASP
1	L	49	ASP
1	L	55	THR
1	L	65	GLU
1	L	116	THR
1	L	121	LEU
1	L	128	GLU
1	L	131	THR
1	L	140	VAL
1	L	143	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	150	VAL
1	L	151	THR
1	L	152	ARG
1	L	173	LEU
1	L	182	LEU
1	L	191	LEU
1	L	192	THR
1	L	200	LEU
1	L	213	ASN
1	L	216	THR
1	L	222	GLN
1	L	233	GLN
1	L	241	LEU
1	L	244	ARG
1	L	258	PHE
1	L	288	LEU
1	L	289	LEU
1	L	310	LEU
1	L	332	THR
1	L	333	ARG
1	L	352	THR
1	L	362	LEU
1	L	375	ASN
1	M	24	VAL
1	M	38	LEU
1	M	41	ASP
1	M	45	ARG
1	M	49	ASP
1	M	55	THR
1	M	59	LEU
1	M	68	ILE
1	M	99	VAL
1	M	118	GLU
1	M	121	LEU
1	M	128	GLU
1	M	140	VAL
1	M	143	THR
1	M	152	ARG
1	M	155	VAL
1	M	173	LEU
1	M	183	LEU
1	M	191	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	M	192	THR
1	M	200	LEU
1	M	213	ASN
1	M	216	THR
1	M	222	GLN
1	M	233	GLN
1	M	235	VAL
1	M	241	LEU
1	M	244	ARG
1	M	258	PHE
1	M	283	VAL
1	M	288	LEU
1	M	289	LEU
1	M	310	LEU
1	M	332	THR
1	M	333	ARG
1	M	347	LEU
1	M	362	LEU
1	M	375	ASN
1	N	38	LEU
1	N	41	ASP
1	N	48	LYS
1	N	49	ASP
1	N	55	THR
1	N	120	ASP
1	N	121	LEU
1	N	122	TYR
1	N	140	VAL
1	N	142	THR
1	N	143	THR
1	N	150	VAL
1	N	151	THR
1	N	152	ARG
1	N	173	LEU
1	N	191	LEU
1	N	192	THR
1	N	200	LEU
1	N	204	VAL
1	N	213	ASN
1	N	216	THR
1	N	222	GLN
1	N	233	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	N	235	VAL
1	N	241	LEU
1	N	244	ARG
1	N	258	PHE
1	N	278	ASP
1	N	289	LEU
1	N	310	LEU
1	N	332	THR
1	N	333	ARG
1	N	362	LEU
1	N	375	ASN
1	O	24	VAL
1	O	38	LEU
1	O	48	LYS
1	O	49	ASP
1	O	55	THR
1	O	82	ARG
1	O	118	GLU
1	O	128	GLU
1	O	130	LEU
1	O	131	THR
1	O	140	VAL
1	O	143	THR
1	O	150	VAL
1	O	151	THR
1	O	152	ARG
1	O	171	ARG
1	O	173	LEU
1	O	182	LEU
1	O	191	LEU
1	O	192	THR
1	O	200	LEU
1	O	204	VAL
1	O	213	ASN
1	O	216	THR
1	O	222	GLN
1	O	233	GLN
1	O	235	VAL
1	O	241	LEU
1	O	244	ARG
1	O	258	PHE
1	O	288	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	O	289	LEU
1	O	310	LEU
1	O	332	THR
1	O	333	ARG
1	O	347	LEU
1	O	352	THR
1	O	362	LEU
1	O	375	ASN
1	P	24	VAL
1	P	38	LEU
1	P	45	ARG
1	P	48	LYS
1	P	52	VAL
1	P	55	THR
1	P	56	LEU
1	P	59	LEU
1	P	66	VAL
1	P	68	ILE
1	P	94	ASP
1	P	99	VAL
1	P	116	THR
1	P	120	ASP
1	P	121	LEU
1	P	128	GLU
1	P	130	LEU
1	P	131	THR
1	P	140	VAL
1	P	143	THR
1	P	150	VAL
1	P	151	THR
1	P	155	VAL
1	P	173	LEU
1	P	182	LEU
1	P	183	LEU
1	P	191	LEU
1	P	192	THR
1	P	200	LEU
1	P	204	VAL
1	P	213	ASN
1	P	216	THR
1	P	222	GLN
1	P	233	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	P	235	VAL
1	P	241	LEU
1	P	244	ARG
1	P	258	PHE
1	P	278	ASP
1	P	283	VAL
1	P	288	LEU
1	P	289	LEU
1	P	310	LEU
1	P	332	THR
1	P	333	ARG
1	P	347	LEU
1	P	375	ASN
1	Q	24	VAL
1	Q	38	LEU
1	Q	41	ASP
1	Q	45	ARG
1	Q	52	VAL
1	Q	55	THR
1	Q	56	LEU
1	Q	59	LEU
1	Q	68	ILE
1	Q	99	VAL
1	Q	121	LEU
1	Q	123	GLN
1	Q	128	GLU
1	Q	130	LEU
1	Q	131	THR
1	Q	140	VAL
1	Q	143	THR
1	Q	148	SER
1	Q	150	VAL
1	Q	151	THR
1	Q	152	ARG
1	Q	156	LEU
1	Q	173	LEU
1	Q	175	SER
1	Q	183	LEU
1	Q	192	THR
1	Q	200	LEU
1	Q	204	VAL
1	Q	213	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	Q	216	THR
1	Q	222	GLN
1	Q	233	GLN
1	Q	235	VAL
1	Q	241	LEU
1	Q	244	ARG
1	Q	258	PHE
1	Q	288	LEU
1	Q	289	LEU
1	Q	310	LEU
1	Q	332	THR
1	Q	333	ARG
1	Q	362	LEU
1	Q	375	ASN
1	R	38	LEU
1	R	45	ARG
1	R	49	ASP
1	R	55	THR
1	R	68	ILE
1	R	116	THR
1	R	131	THR
1	R	143	THR
1	R	150	VAL
1	R	152	ARG
1	R	173	LEU
1	R	182	LEU
1	R	183	LEU
1	R	191	LEU
1	R	200	LEU
1	R	204	VAL
1	R	213	ASN
1	R	216	THR
1	R	222	GLN
1	R	233	GLN
1	R	235	VAL
1	R	241	LEU
1	R	244	ARG
1	R	258	PHE
1	R	288	LEU
1	R	289	LEU
1	R	294	ARG
1	R	310	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	R	325	GLU
1	R	332	THR
1	R	333	ARG
1	R	362	LEU
1	R	375	ASN
1	S	24	VAL
1	S	38	LEU
1	S	56	LEU
1	S	70	ASP
1	S	79	THR
1	S	99	VAL
1	S	116	THR
1	S	121	LEU
1	S	128	GLU
1	S	130	LEU
1	S	140	VAL
1	S	143	THR
1	S	151	THR
1	S	152	ARG
1	S	191	LEU
1	S	200	LEU
1	S	213	ASN
1	S	216	THR
1	S	222	GLN
1	S	233	GLN
1	S	241	LEU
1	S	244	ARG
1	S	258	PHE
1	S	288	LEU
1	S	289	LEU
1	S	310	LEU
1	S	315	ILE
1	S	332	THR
1	S	362	LEU
1	S	368	PHE
1	S	375	ASN
1	T	24	VAL
1	T	38	LEU
1	T	49	ASP
1	T	116	THR
1	T	121	LEU
1	T	122	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	T	140	VAL
1	T	191	LEU
1	T	192	THR
1	T	200	LEU
1	T	204	VAL
1	T	213	ASN
1	T	222	GLN
1	T	233	GLN
1	T	235	VAL
1	T	241	LEU
1	T	258	PHE
1	T	288	LEU
1	T	289	LEU
1	T	310	LEU
1	T	332	THR
1	T	333	ARG
1	T	362	LEU
1	T	375	ASN
1	T	384	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (322) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	29	GLN
1	A	75	ASN
1	A	105	HIS
1	A	123	GLN
1	A	141	ASN
1	A	172	ASN
1	A	213	ASN
1	A	222	GLN
1	A	233	GLN
1	A	242	GLN
1	A	259	ASN
1	A	260	ASN
1	A	285	ASN
1	A	342	GLN
1	A	370	ASN
1	A	375	ASN
1	A	385	GLN
1	B	29	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	75	ASN
1	B	105	HIS
1	B	141	ASN
1	B	153	HIS
1	B	172	ASN
1	B	213	ASN
1	B	222	GLN
1	B	233	GLN
1	B	259	ASN
1	B	260	ASN
1	B	285	ASN
1	B	291	HIS
1	B	370	ASN
1	B	375	ASN
1	B	385	GLN
1	C	14	ASN
1	C	29	GLN
1	C	75	ASN
1	C	105	HIS
1	C	141	ASN
1	C	153	HIS
1	C	172	ASN
1	C	213	ASN
1	C	222	GLN
1	C	233	GLN
1	C	259	ASN
1	C	260	ASN
1	C	285	ASN
1	C	370	ASN
1	C	375	ASN
1	C	385	GLN
1	D	14	ASN
1	D	29	GLN
1	D	75	ASN
1	D	105	HIS
1	D	141	ASN
1	D	172	ASN
1	D	213	ASN
1	D	222	GLN
1	D	233	GLN
1	D	259	ASN
1	D	260	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	285	ASN
1	D	291	HIS
1	D	366	ASN
1	D	370	ASN
1	D	375	ASN
1	D	385	GLN
1	E	29	GLN
1	E	75	ASN
1	E	92	GLN
1	E	105	HIS
1	E	123	GLN
1	E	141	ASN
1	E	153	HIS
1	E	172	ASN
1	E	213	ASN
1	E	222	GLN
1	E	233	GLN
1	E	259	ASN
1	E	260	ASN
1	E	285	ASN
1	E	370	ASN
1	E	375	ASN
1	F	141	ASN
1	F	172	ASN
1	F	213	ASN
1	F	222	GLN
1	F	233	GLN
1	F	242	GLN
1	F	259	ASN
1	F	260	ASN
1	F	285	ASN
1	F	370	ASN
1	F	375	ASN
1	F	385	GLN
1	G	14	ASN
1	G	29	GLN
1	G	75	ASN
1	G	105	HIS
1	G	141	ASN
1	G	153	HIS
1	G	158	ASN
1	G	172	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	213	ASN
1	G	222	GLN
1	G	233	GLN
1	G	259	ASN
1	G	260	ASN
1	G	285	ASN
1	G	370	ASN
1	G	375	ASN
1	G	385	GLN
1	H	14	ASN
1	H	29	GLN
1	H	75	ASN
1	H	92	GLN
1	H	105	HIS
1	H	123	GLN
1	H	141	ASN
1	H	172	ASN
1	H	213	ASN
1	H	222	GLN
1	H	233	GLN
1	H	242	GLN
1	H	259	ASN
1	H	260	ASN
1	H	285	ASN
1	H	370	ASN
1	H	375	ASN
1	H	385	GLN
1	I	14	ASN
1	I	29	GLN
1	I	105	HIS
1	I	123	GLN
1	I	141	ASN
1	I	172	ASN
1	I	213	ASN
1	I	222	GLN
1	I	233	GLN
1	I	259	ASN
1	I	260	ASN
1	I	271	HIS
1	I	285	ASN
1	I	291	HIS
1	I	366	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	370	ASN
1	I	375	ASN
1	J	14	ASN
1	J	29	GLN
1	J	75	ASN
1	J	105	HIS
1	J	123	GLN
1	J	141	ASN
1	J	172	ASN
1	J	213	ASN
1	J	222	GLN
1	J	233	GLN
1	J	242	GLN
1	J	259	ASN
1	J	260	ASN
1	J	271	HIS
1	J	285	ASN
1	J	342	GLN
1	J	366	ASN
1	J	370	ASN
1	J	375	ASN
1	J	385	GLN
1	K	29	GLN
1	K	105	HIS
1	K	123	GLN
1	K	141	ASN
1	K	172	ASN
1	K	213	ASN
1	K	222	GLN
1	K	233	GLN
1	K	242	GLN
1	K	259	ASN
1	K	260	ASN
1	K	271	HIS
1	K	285	ASN
1	K	291	HIS
1	K	343	HIS
1	K	370	ASN
1	K	375	ASN
1	K	385	GLN
1	L	14	ASN
1	L	29	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	75	ASN
1	L	105	HIS
1	L	141	ASN
1	L	153	HIS
1	L	158	ASN
1	L	172	ASN
1	L	213	ASN
1	L	222	GLN
1	L	233	GLN
1	L	259	ASN
1	L	260	ASN
1	L	285	ASN
1	L	370	ASN
1	L	375	ASN
1	L	385	GLN
1	M	29	GLN
1	M	105	HIS
1	M	123	GLN
1	M	141	ASN
1	M	172	ASN
1	M	213	ASN
1	M	222	GLN
1	M	233	GLN
1	M	242	GLN
1	M	259	ASN
1	M	260	ASN
1	M	285	ASN
1	M	370	ASN
1	M	375	ASN
1	M	385	GLN
1	N	14	ASN
1	N	29	GLN
1	N	75	ASN
1	N	105	HIS
1	N	141	ASN
1	N	172	ASN
1	N	213	ASN
1	N	222	GLN
1	N	233	GLN
1	N	259	ASN
1	N	260	ASN
1	N	285	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	N	370	ASN
1	N	375	ASN
1	N	385	GLN
1	O	14	ASN
1	O	29	GLN
1	O	75	ASN
1	O	105	HIS
1	O	141	ASN
1	O	153	HIS
1	O	172	ASN
1	O	213	ASN
1	O	222	GLN
1	O	233	GLN
1	O	259	ASN
1	O	260	ASN
1	O	285	ASN
1	O	366	ASN
1	O	370	ASN
1	O	375	ASN
1	P	14	ASN
1	P	29	GLN
1	P	75	ASN
1	P	105	HIS
1	P	123	GLN
1	P	141	ASN
1	P	153	HIS
1	P	172	ASN
1	P	213	ASN
1	P	222	GLN
1	P	233	GLN
1	P	259	ASN
1	P	260	ASN
1	P	285	ASN
1	P	370	ASN
1	P	375	ASN
1	P	385	GLN
1	Q	14	ASN
1	Q	29	GLN
1	Q	105	HIS
1	Q	123	GLN
1	Q	141	ASN
1	Q	153	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	Q	172	ASN
1	Q	213	ASN
1	Q	222	GLN
1	Q	233	GLN
1	Q	259	ASN
1	Q	260	ASN
1	Q	285	ASN
1	Q	370	ASN
1	Q	375	ASN
1	R	14	ASN
1	R	29	GLN
1	R	105	HIS
1	R	141	ASN
1	R	172	ASN
1	R	213	ASN
1	R	222	GLN
1	R	233	GLN
1	R	259	ASN
1	R	260	ASN
1	R	285	ASN
1	R	342	GLN
1	R	370	ASN
1	R	375	ASN
1	S	29	GLN
1	S	75	ASN
1	S	105	HIS
1	S	123	GLN
1	S	141	ASN
1	S	202	HIS
1	S	213	ASN
1	S	222	GLN
1	S	233	GLN
1	S	259	ASN
1	S	260	ASN
1	S	285	ASN
1	S	370	ASN
1	S	375	ASN
1	S	385	GLN
1	T	14	ASN
1	T	141	ASN
1	T	172	ASN
1	T	213	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	T	222	GLN
1	T	233	GLN
1	T	259	ASN
1	T	260	ASN
1	T	285	ASN
1	T	366	ASN
1	T	370	ASN
1	T	375	ASN
1	T	385	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 20 ligands modelled in this entry, 20 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	382/387 (98%)	0.31	17 (4%)	33	31	41, 46, 51, 57	0
1	B	382/387 (98%)	0.32	18 (4%)	31	30	39, 45, 51, 56	0
1	C	382/387 (98%)	0.44	30 (7%)	12	10	41, 46, 51, 55	0
1	D	382/387 (98%)	0.38	25 (6%)	18	17	39, 46, 51, 56	0
1	E	382/387 (98%)	0.20	12 (3%)	49	49	40, 45, 51, 56	0
1	F	382/387 (98%)	0.53	39 (10%)	6	5	41, 46, 51, 56	0
1	G	382/387 (98%)	0.41	28 (7%)	15	13	41, 45, 51, 57	0
1	H	382/387 (98%)	0.20	15 (3%)	39	38	39, 45, 51, 58	0
1	I	382/387 (98%)	0.41	21 (5%)	25	24	40, 46, 51, 55	0
1	J	382/387 (98%)	0.37	20 (5%)	27	25	41, 46, 51, 56	0
1	K	382/387 (98%)	0.23	17 (4%)	33	31	39, 45, 51, 59	0
1	L	382/387 (98%)	0.40	25 (6%)	18	17	41, 46, 51, 58	0
1	M	382/387 (98%)	0.26	18 (4%)	31	30	39, 45, 50, 57	0
1	N	382/387 (98%)	0.37	17 (4%)	33	31	41, 46, 51, 55	0
1	O	382/387 (98%)	0.29	14 (3%)	41	41	40, 45, 51, 58	0
1	P	382/387 (98%)	0.20	8 (2%)	63	65	40, 45, 50, 56	0
1	Q	382/387 (98%)	0.32	22 (5%)	23	22	39, 46, 50, 55	0
1	R	382/387 (98%)	0.43	21 (5%)	25	24	41, 46, 50, 57	0
1	S	382/387 (98%)	0.71	47 (12%)	4	3	41, 46, 51, 58	0
1	T	382/387 (98%)	0.84	64 (16%)	1	1	40, 46, 50, 55	0
All	All	7640/7740 (98%)	0.38	478 (6%)	20	19	39, 46, 51, 59	0

All (478) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	S	160	GLU	6.1
1	S	48	LYS	6.1
1	T	72	VAL	5.9
1	Q	160	GLU	5.8
1	T	121	LEU	5.5
1	K	118	GLU	5.5
1	D	352	THR	5.4
1	T	32	GLY	5.2
1	T	110	GLY	5.1
1	I	278	ASP	4.9
1	M	49	ASP	4.9
1	B	368	PHE	4.9
1	T	127	ILE	4.9
1	L	48	LYS	4.9
1	S	119	GLY	4.9
1	N	118	GLU	4.8
1	T	74	PRO	4.7
1	I	48	LYS	4.7
1	M	48	LYS	4.6
1	F	43	GLY	4.6
1	G	160	GLU	4.6
1	O	352	THR	4.5
1	T	91	GLU	4.5
1	C	160	GLU	4.5
1	F	352	THR	4.5
1	L	161	THR	4.4
1	T	161	THR	4.4
1	E	278	ASP	4.4
1	I	49	ASP	4.4
1	T	157	THR	4.3
1	J	278	ASP	4.3
1	N	368	PHE	4.3
1	O	74	PRO	4.2
1	S	352	THR	4.2
1	L	160	GLU	4.2
1	T	160	GLU	4.2
1	S	118	GLU	4.1
1	H	118	GLU	4.1
1	T	278	ASP	4.1
1	P	48	LYS	4.1
1	T	90	ARG	4.0
1	F	118	GLU	4.0
1	S	122	TYR	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	161	THR	4.0
1	C	120	ASP	4.0
1	H	160	GLU	4.0
1	M	119	GLY	4.0
1	A	352	THR	4.0
1	O	48	LYS	4.0
1	D	278	ASP	4.0
1	T	119	GLY	3.9
1	M	118	GLU	3.9
1	P	368	PHE	3.9
1	T	116	THR	3.9
1	B	278	ASP	3.9
1	T	81	VAL	3.9
1	D	127	ILE	3.9
1	F	89	ARG	3.8
1	Q	119	GLY	3.8
1	T	352	THR	3.8
1	T	89	ARG	3.8
1	J	127	ILE	3.8
1	T	156	LEU	3.8
1	T	368	PHE	3.8
1	F	81	VAL	3.8
1	D	118	GLU	3.7
1	N	275	GLY	3.7
1	L	368	PHE	3.7
1	Q	48	LYS	3.7
1	T	94	ASP	3.7
1	G	90	ARG	3.7
1	F	49	ASP	3.7
1	D	160	GLU	3.7
1	T	48	LYS	3.7
1	J	159	THR	3.6
1	B	123	GLN	3.6
1	T	96	ILE	3.6
1	F	4	ARG	3.6
1	S	278	ASP	3.6
1	A	383	PHE	3.6
1	G	110	GLY	3.6
1	S	65	GLU	3.6
1	D	161	THR	3.6
1	Q	352	THR	3.5
1	C	127	ILE	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	278	ASP	3.5
1	J	160	GLU	3.5
1	K	81	VAL	3.5
1	I	86	ALA	3.4
1	F	50	GLY	3.4
1	A	161	THR	3.4
1	R	160	GLU	3.4
1	T	97	VAL	3.4
1	S	368	PHE	3.4
1	B	118	GLU	3.4
1	S	123	GLN	3.4
1	M	161	THR	3.4
1	C	41	ASP	3.4
1	N	161	THR	3.4
1	T	61	GLU	3.4
1	G	123	GLN	3.3
1	I	90	ARG	3.3
1	O	160	GLU	3.3
1	L	93	CYS	3.3
1	C	111	ILE	3.3
1	F	74	PRO	3.3
1	C	82	ARG	3.3
1	D	368	PHE	3.2
1	C	164	LYS	3.2
1	O	161	THR	3.2
1	H	246	TYR	3.2
1	I	121	LEU	3.2
1	A	81	VAL	3.2
1	C	96	ILE	3.2
1	G	48	LYS	3.2
1	H	48	LYS	3.2
1	K	160	GLU	3.2
1	T	118	GLU	3.2
1	T	246	TYR	3.2
1	C	74	PRO	3.2
1	J	118	GLU	3.2
1	R	127	ILE	3.2
1	L	90	ARG	3.2
1	N	160	GLU	3.1
1	L	120	ASP	3.1
1	G	86	ALA	3.1
1	S	94	ASP	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	131	THR	3.1
1	C	163	VAL	3.1
1	J	119	GLY	3.1
1	F	114	ALA	3.1
1	T	31	LEU	3.1
1	Q	74	PRO	3.1
1	C	161	THR	3.1
1	J	74	PRO	3.1
1	J	368	PHE	3.1
1	Q	161	THR	3.1
1	T	158	ASN	3.1
1	K	48	LYS	3.1
1	R	110	GLY	3.1
1	S	157	THR	3.0
1	I	118	GLU	3.0
1	T	82	ARG	3.0
1	S	127	ILE	3.0
1	L	74	PRO	3.0
1	R	97	VAL	3.0
1	B	160	GLU	3.0
1	D	122	TYR	3.0
1	H	161	THR	3.0
1	A	110	GLY	3.0
1	C	368	PHE	3.0
1	S	246	TYR	3.0
1	G	118	GLU	3.0
1	T	60	ARG	3.0
1	T	122	TYR	3.0
1	L	360	MET	3.0
1	E	160	GLU	3.0
1	H	49	ASP	3.0
1	O	246	TYR	3.0
1	I	92	GLN	2.9
1	F	110	GLY	2.9
1	B	48	LYS	2.9
1	I	160	GLU	2.9
1	B	110	GLY	2.9
1	T	68	ILE	2.9
1	T	95	ILE	2.9
1	J	246	TYR	2.9
1	L	92	GLN	2.9
1	S	161	THR	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	T	269	MET	2.9
1	G	75	ASN	2.9
1	K	133	PRO	2.9
1	T	114	ALA	2.9
1	O	75	ASN	2.9
1	O	278	ASP	2.9
1	A	74	PRO	2.9
1	F	90	ARG	2.9
1	L	50	GLY	2.9
1	B	352	THR	2.9
1	L	97	VAL	2.9
1	Q	51	ALA	2.9
1	E	368	PHE	2.8
1	S	51	ALA	2.8
1	L	387	PHE	2.8
1	L	118	GLU	2.8
1	N	48	LYS	2.8
1	T	73	GLU	2.8
1	A	119	GLY	2.8
1	F	275	GLY	2.8
1	M	121	LEU	2.8
1	Q	269	MET	2.8
1	B	246	TYR	2.8
1	S	345	ARG	2.8
1	F	368	PHE	2.8
1	P	160	GLU	2.8
1	C	116	THR	2.8
1	F	133	PRO	2.8
1	I	110	GLY	2.8
1	F	48	LYS	2.8
1	G	127	ILE	2.8
1	S	74	PRO	2.7
1	S	120	ASP	2.7
1	B	288	LEU	2.7
1	G	50	GLY	2.7
1	G	126	GLY	2.7
1	I	111	ILE	2.7
1	K	119	GLY	2.7
1	P	278	ASP	2.7
1	N	60	ARG	2.7
1	F	61	GLU	2.7
1	R	352	THR	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	49	ASP	2.7
1	T	120	ASP	2.7
1	J	61	GLU	2.7
1	D	50	GLY	2.7
1	T	100	GLY	2.7
1	G	246	TYR	2.7
1	P	246	TYR	2.7
1	F	345	ARG	2.7
1	S	363	LYS	2.7
1	F	316	THR	2.7
1	B	49	ASP	2.7
1	Q	62	ALA	2.7
1	S	376	GLU	2.7
1	I	352	THR	2.7
1	M	50	GLY	2.7
1	T	57	HIS	2.7
1	A	246	TYR	2.7
1	B	111	ILE	2.7
1	E	127	ILE	2.7
1	R	65	GLU	2.6
1	K	90	ARG	2.6
1	C	352	THR	2.6
1	I	97	VAL	2.6
1	R	49	ASP	2.6
1	F	161	THR	2.6
1	T	159	THR	2.6
1	T	53	ASP	2.6
1	E	161	THR	2.6
1	H	352	THR	2.6
1	F	160	GLU	2.6
1	T	144	ALA	2.6
1	G	278	ASP	2.6
1	M	246	TYR	2.6
1	S	62	ALA	2.6
1	T	377	GLN	2.6
1	R	368	PHE	2.6
1	D	82	ARG	2.6
1	T	86	ALA	2.6
1	G	273	LEU	2.6
1	R	344	LEU	2.6
1	H	132	ASN	2.6
1	F	127	ILE	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	N	316	THR	2.5
1	R	51	ALA	2.5
1	S	97	VAL	2.5
1	Q	97	VAL	2.5
1	S	279	MET	2.5
1	S	377	GLN	2.5
1	N	278	ASP	2.5
1	Q	278	ASP	2.5
1	F	45	ARG	2.5
1	E	118	GLU	2.5
1	L	68	ILE	2.5
1	G	60	ARG	2.5
1	O	50	GLY	2.5
1	D	246	TYR	2.5
1	D	92	GLN	2.5
1	C	159	THR	2.5
1	G	82	ARG	2.5
1	I	82	ARG	2.5
1	L	345	ARG	2.5
1	N	274	GLY	2.5
1	R	242	GLN	2.5
1	C	42	LYS	2.5
1	K	74	PRO	2.5
1	S	317	GLY	2.5
1	E	242	GLN	2.5
1	I	344	LEU	2.5
1	M	383	PHE	2.5
1	P	4	ARG	2.5
1	B	50	GLY	2.4
1	T	25	GLY	2.4
1	D	74	PRO	2.4
1	Q	108	GLY	2.4
1	G	161	THR	2.4
1	C	37	LEU	2.4
1	I	127	ILE	2.4
1	T	85	LEU	2.4
1	T	22	SER	2.4
1	J	29	GLN	2.4
1	N	246	TYR	2.4
1	Q	316	THR	2.4
1	A	90	ARG	2.4
1	J	163	VAL	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	T	39	VAL	2.4
1	J	158	ASN	2.4
1	Q	368	PHE	2.4
1	O	82	ARG	2.4
1	J	48	LYS	2.4
1	M	19	ASN	2.4
1	C	110	GLY	2.4
1	T	45	ARG	2.4
1	E	352	THR	2.4
1	K	121	LEU	2.4
1	K	159	THR	2.4
1	T	131	THR	2.4
1	L	278	ASP	2.4
1	M	160	GLU	2.4
1	S	350	LYS	2.4
1	H	74	PRO	2.4
1	T	29	GLN	2.4
1	C	278	ASP	2.4
1	R	111	ILE	2.4
1	T	49	ASP	2.4
1	T	24	VAL	2.4
1	T	4	ARG	2.4
1	G	108	GLY	2.4
1	Q	107	CYS	2.4
1	Q	345	ARG	2.4
1	R	82	ARG	2.4
1	C	34	LYS	2.3
1	T	111	ILE	2.3
1	Q	246	TYR	2.3
1	I	94	ASP	2.3
1	S	200	LEU	2.3
1	T	106	ASP	2.3
1	F	32	GLY	2.3
1	H	50	GLY	2.3
1	F	60	ARG	2.3
1	M	368	PHE	2.3
1	G	377	GLN	2.3
1	F	158	ASN	2.3
1	G	352	THR	2.3
1	N	86	ALA	2.3
1	N	34	LYS	2.3
1	N	377	GLN	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	M	74	PRO	2.3
1	L	38	LEU	2.3
1	E	48	LYS	2.3
1	F	42	LYS	2.3
1	K	127	ILE	2.3
1	S	280	PRO	2.3
1	J	377	GLN	2.3
1	S	131	THR	2.3
1	K	111	ILE	2.3
1	E	61	GLU	2.3
1	Q	376	GLU	2.3
1	T	59	LEU	2.3
1	F	115	ALA	2.3
1	G	316	THR	2.3
1	Q	60	ARG	2.3
1	S	33	GLY	2.3
1	S	35	LYS	2.3
1	S	348	GLY	2.3
1	F	276	LEU	2.3
1	G	92	GLN	2.3
1	S	37	LEU	2.3
1	T	76	PRO	2.3
1	B	107	CYS	2.3
1	R	246	TYR	2.3
1	M	60	ARG	2.3
1	G	94	ASP	2.3
1	B	119	GLY	2.2
1	D	145	GLY	2.2
1	T	115	ALA	2.2
1	R	4	ARG	2.2
1	S	53	ASP	2.2
1	C	108	GLY	2.2
1	T	130	LEU	2.2
1	F	51	ALA	2.2
1	S	86	ALA	2.2
1	M	131	THR	2.2
1	I	368	PHE	2.2
1	J	120	ASP	2.2
1	K	92	GLN	2.2
1	O	68	ILE	2.2
1	S	154	CYS	2.2
1	S	385	GLN	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	J	75	ASN	2.2
1	T	18	PRO	2.2
1	S	159	THR	2.2
1	J	91	GLU	2.2
1	P	127	ILE	2.2
1	B	132	ASN	2.2
1	H	90	ARG	2.2
1	C	53	ASP	2.2
1	K	352	THR	2.2
1	F	123	GLN	2.2
1	T	112	GLY	2.2
1	C	246	TYR	2.2
1	L	124	TYR	2.2
1	L	39	VAL	2.2
1	D	133	PRO	2.2
1	C	118	GLU	2.2
1	D	65	GLU	2.2
1	L	356	TYR	2.2
1	C	60	ARG	2.2
1	B	19	ASN	2.2
1	F	111	ILE	2.2
1	L	140	VAL	2.2
1	Q	39	VAL	2.2
1	K	107	CYS	2.2
1	R	118	GLU	2.2
1	A	50	GLY	2.2
1	C	126	GLY	2.2
1	L	86	ALA	2.2
1	F	159	THR	2.2
1	N	356	TYR	2.2
1	A	127	ILE	2.2
1	A	108	GLY	2.2
1	M	352	THR	2.2
1	N	352	THR	2.2
1	D	4	ARG	2.2
1	S	4	ARG	2.2
1	F	97	VAL	2.1
1	I	61	GLU	2.1
1	D	274	GLY	2.1
1	O	70	ASP	2.1
1	F	157	THR	2.1
1	R	60	ARG	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	S	75	ASN	2.1
1	O	127	ILE	2.1
1	D	121	LEU	2.1
1	Q	90	ARG	2.1
1	C	113	ILE	2.1
1	O	356	TYR	2.1
1	D	288	LEU	2.1
1	H	82	ARG	2.1
1	G	368	PHE	2.1
1	G	89	ARG	2.1
1	I	345	ARG	2.1
1	K	246	TYR	2.1
1	H	51	ALA	2.1
1	H	159	THR	2.1
1	S	383	PHE	2.1
1	C	45	ARG	2.1
1	M	110	GLY	2.1
1	F	277	TYR	2.1
1	Q	191	LEU	2.1
1	R	161	THR	2.1
1	F	82	ARG	2.1
1	R	89	ARG	2.1
1	J	49	ASP	2.1
1	L	60	ARG	2.1
1	M	89	ARG	2.1
1	A	111	ILE	2.1
1	K	96	ILE	2.1
1	S	68	ILE	2.1
1	P	350	LYS	2.1
1	T	107	CYS	2.1
1	S	158	ASN	2.1
1	A	351	GLU	2.1
1	R	336	MET	2.1
1	R	121	LEU	2.0
1	T	44	LEU	2.0
1	G	74	PRO	2.0
1	D	356	TYR	2.0
1	A	269	MET	2.0
1	F	92	GLN	2.0
1	G	345	ARG	2.0
1	L	246	TYR	2.0
1	E	131	THR	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	123	GLN	2.0
1	D	377	GLN	2.0
1	N	92	GLN	2.0
1	B	90	ARG	2.0
1	D	111	ILE	2.0
1	A	122	TYR	2.0
1	C	94	ASP	2.0
1	D	110	GLY	2.0
1	H	108	GLY	2.0
1	J	383	PHE	2.0
1	S	93	CYS	2.0
1	E	60	ARG	2.0
1	S	60	ARG	2.0
1	S	61	GLU	2.0
1	G	140	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FE2	A	1388	1/1	0.98	0.13	41,41,41,41	0
2	FE2	B	1388	1/1	0.98	0.11	40,40,40,40	0
2	FE2	C	1388	1/1	0.98	0.14	43,43,43,43	0
2	FE2	F	1388	1/1	0.98	0.14	51,51,51,51	0
2	FE2	G	1388	1/1	0.98	0.12	43,43,43,43	0
2	FE2	I	1388	1/1	0.98	0.14	36,36,36,36	0
2	FE2	L	1388	1/1	0.98	0.14	39,39,39,39	0
2	FE2	D	1388	1/1	0.99	0.16	38,38,38,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FE2	J	1388	1/1	0.99	0.12	43,43,43,43	0
2	FE2	K	1388	1/1	0.99	0.13	27,27,27,27	0
2	FE2	H	1388	1/1	0.99	0.14	31,31,31,31	0
2	FE2	N	1388	1/1	0.99	0.16	44,44,44,44	0
2	FE2	O	1388	1/1	0.99	0.16	33,33,33,33	0
2	FE2	P	1388	1/1	0.99	0.14	36,36,36,36	0
2	FE2	Q	1388	1/1	0.99	0.15	42,42,42,42	0
2	FE2	R	1388	1/1	0.99	0.14	49,49,49,49	0
2	FE2	S	1388	1/1	0.99	0.06	64,64,64,64	0
2	FE2	T	1388	1/1	0.99	0.11	65,65,65,65	0
2	FE2	M	1388	1/1	1.00	0.16	30,30,30,30	0
2	FE2	E	1388	1/1	1.00	0.15	30,30,30,30	0

6.5 Other polymers (i)

There are no such residues in this entry.