Full wwPDB X-ray Structure Validation Report (i)

Aug 22, 2023 – 07:20 AM EDT

PDB ID	:	2QLR
Title	:	Crystal structure of human kynurenine aminotransferase II
Authors	:	Han, Q.; Robinson, R.; Li, J.
Deposited on	:	2007-07-13
Resolution	:	2.30 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 (i)) were used in the production of this report:

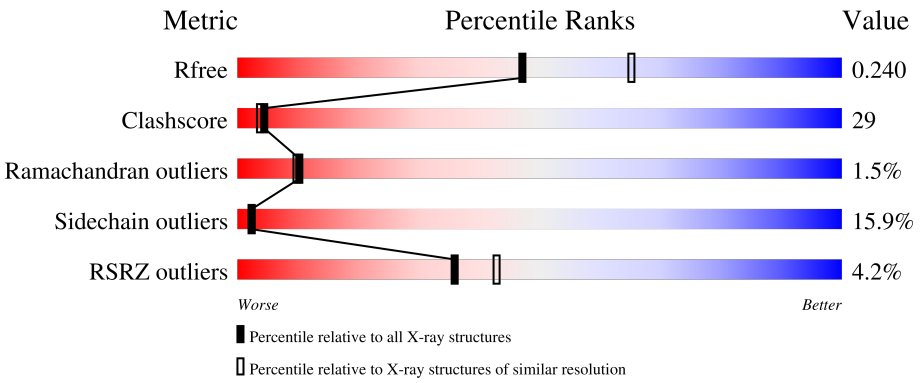
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	425	4% 54% 34% 10% •
1	B	425	4% 54% 32% 13% •
1	C	425	5% 51% 38% 10% •
1	D	425	3% 49% 37% 12% •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	C	429	-	-	-	X
2	GOL	D	427	-	-	X	X
2	GOL	D	428	-	-	X	-
2	GOL	D	429	-	X	X	X

2 Entry composition (i)

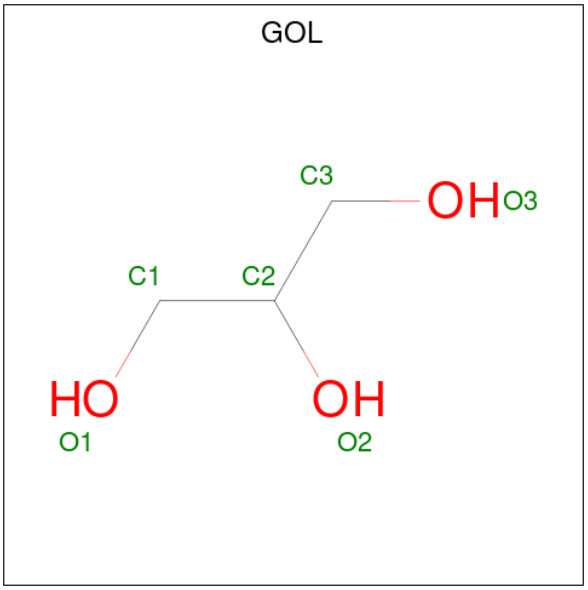
There are 3 unique types of molecules in this entry. The entry contains 14176 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Kynurenine/alpha-aminoadipate aminotransferase mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	425	3347	2147	560	621	1	18	0	0	0
1	B	425	3348	2147	560	622	1	18	0	0	0
1	C	425	3347	2147	560	621	1	18	0	0	0
1	D	425	3348	2147	560	622	1	18	0	0	0

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	6	3	3	0	0
2	A	1	6	3	3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	B	1	6	3	3	0	0
2	C	1	6	3	3	0	0
2	C	1	6	3	3	0	0
2	C	1	6	3	3	0	0
2	C	1	6	3	3	0	0
2	C	1	6	3	3	0	0
2	D	1	6	3	3	0	0
2	D	1	6	3	3	0	0
2	D	1	6	3	3	0	0
2	D	1	6	3	3	0	0

- Molecule 3 is water.

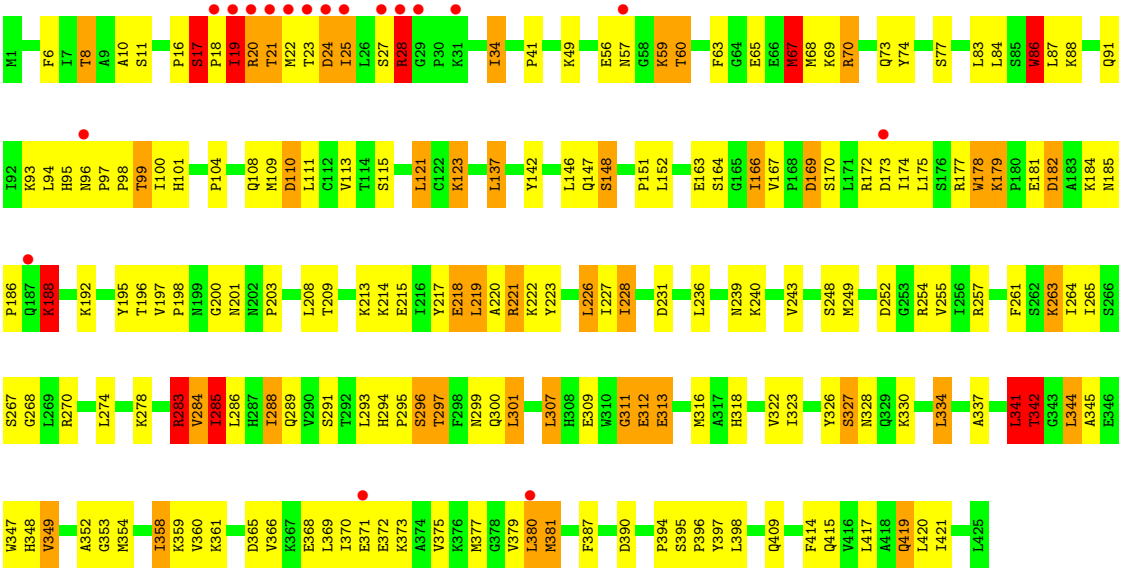
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	166	166	166	0	0
3	B	199	199	199	0	0
3	C	166	166	166	0	0
3	D	183	183	183	0	0

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.

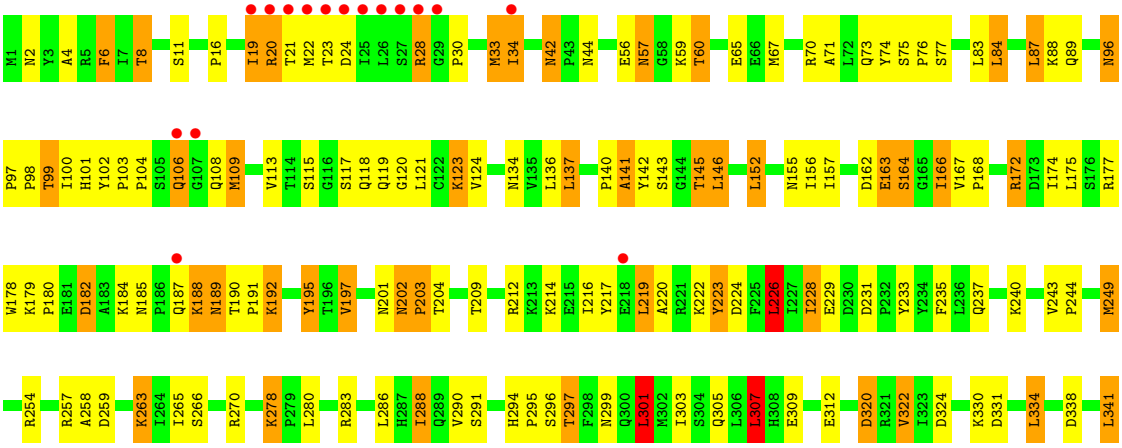
• Molecule 1: Kynurenine/alpha-aminoadipate aminotransferase mitochondrial

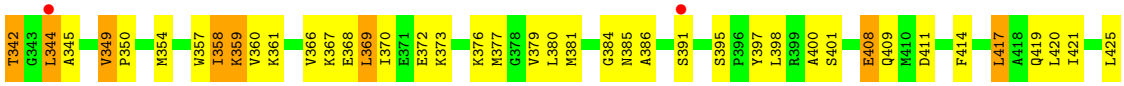
Chain A:



• Molecule 1: Kynurenine/alpha-aminoadipate aminotransferase mitochondrial

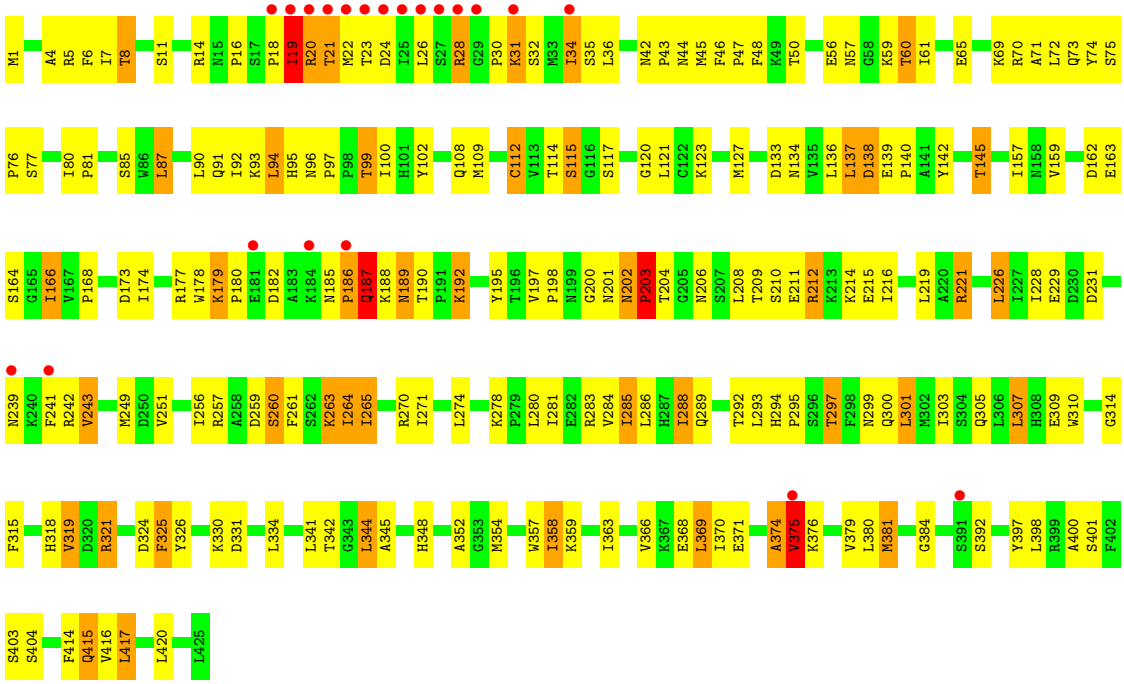
Chain B:





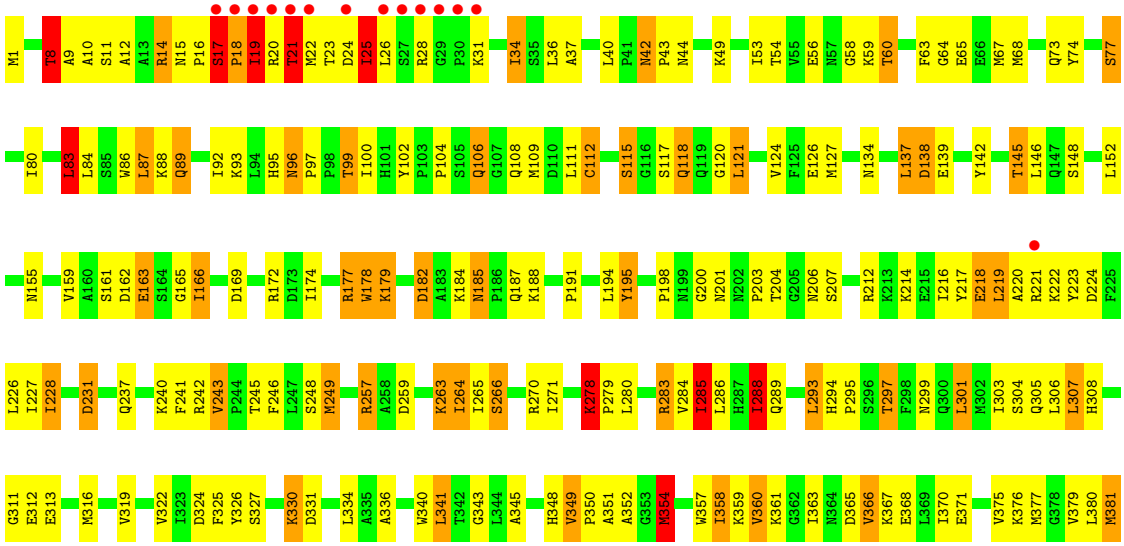
• Molecule 1: Kynurenine/alpha-aminoadipate aminotransferase mitochondrial

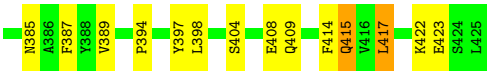
Chain C:



• Molecule 1: Kynurenine/alpha-aminoadipate aminotransferase mitochondrial

Chain D:




N385
A386
F387
Y388
V389
P394
Y397
L398
S404
E408
Q409
F414
Q415
V416
L417
K422
E423
S424
L425

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	109.50Å 70.97Å 121.13Å 90.00° 101.10° 90.00°	Depositor
Resolution (Å)	30.11 – 2.30 30.10 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.3 (30.11-2.30) 96.3 (30.10-2.30)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.87 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.242 , 0.256 0.226 , 0.240	Depositor DCC
R_{free} test set	3883 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	37.7	Xtriage
Anisotropy	0.137	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 50.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.56$, $< L^2 > = 0.40$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	14176	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 51.65 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.4387e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: GOL, LLP

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	1.26	6/3404 (0.2%)	1.24	20/4620 (0.4%)
1	B	1.33	14/3405 (0.4%)	1.17	17/4620 (0.4%)
1	C	1.33	8/3404 (0.2%)	1.23	25/4620 (0.5%)
1	D	1.34	17/3405 (0.5%)	1.21	19/4620 (0.4%)
All	All	1.32	45/13618 (0.3%)	1.21	81/18480 (0.4%)

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	A	0	5
1	B	0	4
1	C	0	5
1	D	1	4
All	All	1	18

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	195	TYR	CD1-CE1	10.56	1.55	1.39
1	C	112	CYS	CB-SG	-9.87	1.65	1.82
1	D	12	ALA	CA-CB	8.14	1.69	1.52
1	A	86	TRP	CB-CG	8.11	1.64	1.50
1	B	312	GLU	CB-CG	7.82	1.67	1.52
1	B	312	GLU	CG-CD	7.47	1.63	1.51
1	B	401	SER	CB-OG	7.45	1.51	1.42
1	D	182	ASP	CB-CG	7.32	1.67	1.51
1	D	278	LYS	CE-NZ	6.73	1.65	1.49
1	A	182	ASP	CB-CG	6.52	1.65	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	322	VAL	CB-CG1	-6.34	1.39	1.52
1	C	4	ALA	CA-CB	6.25	1.65	1.52
1	B	235	PHE	CE1-CZ	6.17	1.49	1.37
1	B	359	LYS	CE-NZ	6.15	1.64	1.49
1	B	312	GLU	CD-OE1	6.00	1.32	1.25
1	C	278	LYS	CE-NZ	5.96	1.64	1.49
1	C	325	PHE	CE2-CZ	5.95	1.48	1.37
1	D	231	ASP	CB-CG	5.88	1.64	1.51
1	D	312	GLU	CD-OE1	5.84	1.32	1.25
1	B	309	GLU	CB-CG	5.83	1.63	1.52
1	B	141	ALA	CA-CB	5.76	1.64	1.52
1	C	229	GLU	CB-CG	-5.67	1.41	1.52
1	A	173	ASP	CB-CG	5.63	1.63	1.51
1	C	260	SER	CB-OG	-5.63	1.34	1.42
1	A	371	GLU	CG-CD	5.56	1.60	1.51
1	D	118	GLN	CB-CG	-5.48	1.37	1.52
1	A	347	TRP	CG-CD1	5.44	1.44	1.36
1	C	278	LYS	CD-CE	5.44	1.64	1.51
1	D	278	LYS	CD-CE	5.42	1.64	1.51
1	D	14	ARG	C-O	5.41	1.33	1.23
1	B	197	VAL	CB-CG2	5.40	1.64	1.52
1	B	123	LYS	CD-CE	5.40	1.64	1.51
1	B	195	TYR	CG-CD1	5.35	1.46	1.39
1	C	374	ALA	CA-CB	5.34	1.63	1.52
1	D	422	LYS	CE-NZ	5.32	1.62	1.49
1	D	285	ILE	CB-CG2	5.24	1.69	1.52
1	A	285	ILE	CA-CB	5.23	1.66	1.54
1	D	115	SER	CB-OG	5.20	1.49	1.42
1	B	223	TYR	CE2-CZ	5.12	1.45	1.38
1	D	288	ILE	CA-CB	5.10	1.66	1.54
1	D	257	ARG	CG-CD	5.10	1.64	1.51
1	D	9	ALA	C-O	-5.06	1.13	1.23
1	B	320	ASP	CB-CG	5.06	1.62	1.51
1	D	351	ALA	CA-CB	-5.03	1.41	1.52
1	D	195	TYR	CG-CD1	5.01	1.45	1.39

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	283	ARG	NE-CZ-NH1	15.51	128.06	120.30
1	A	283	ARG	NE-CZ-NH2	-12.25	114.18	120.30
1	C	14	ARG	NE-CZ-NH2	9.75	125.18	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	257	ARG	NE-CZ-NH1	9.66	125.13	120.30
1	C	321	ARG	NE-CZ-NH2	-8.95	115.82	120.30
1	D	257	ARG	NE-CZ-NH2	-8.76	115.92	120.30
1	A	257	ARG	NE-CZ-NH2	-8.46	116.07	120.30
1	C	242	ARG	NE-CZ-NH1	-7.77	116.42	120.30
1	D	242	ARG	NE-CZ-NH2	-7.41	116.60	120.30
1	D	231	ASP	CB-CG-OD1	7.34	124.91	118.30
1	A	254	ARG	NE-CZ-NH2	-7.17	116.72	120.30
1	C	321	ARG	NE-CZ-NH1	7.05	123.83	120.30
1	D	324	ASP	CB-CG-OD2	6.84	124.46	118.30
1	B	361	LYS	C-N-CA	-6.83	107.97	122.30
1	C	212	ARG	NE-CZ-NH2	-6.81	116.89	120.30
1	D	106	GLN	C-N-CA	-6.64	108.35	122.30
1	D	83	LEU	CB-CG-CD2	6.64	122.29	111.00
1	B	320	ASP	CB-CG-OD1	6.58	124.22	118.30
1	A	231	ASP	CB-CG-OD1	6.51	124.16	118.30
1	C	342	THR	C-N-CA	-6.49	108.67	122.30
1	C	14	ARG	NE-CZ-NH1	-6.47	117.06	120.30
1	A	307	LEU	CB-CG-CD1	6.44	121.94	111.00
1	A	70	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	C	380	LEU	CA-CB-CG	6.33	129.86	115.30
1	C	226	LEU	CA-CB-CG	6.27	129.71	115.30
1	B	87	LEU	CA-CB-CG	6.25	129.66	115.30
1	A	252	ASP	CB-CG-OD1	6.21	123.89	118.30
1	C	70	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	C	173	ASP	CB-CG-OD1	6.12	123.81	118.30
1	C	375	VAL	CB-CA-C	-6.11	99.79	111.40
1	A	110	ASP	CB-CG-OD2	-6.08	112.83	118.30
1	B	312	GLU	CB-CA-C	6.02	122.44	110.40
1	D	354	MET	CA-CB-CG	5.93	123.38	113.30
1	A	169	ASP	CB-CG-OD2	-5.91	112.98	118.30
1	D	354	MET	CG-SD-CE	-5.82	90.89	100.20
1	C	115	SER	CB-CA-C	5.79	121.10	110.10
1	C	417	LEU	CA-CB-CG	5.78	128.60	115.30
1	B	226	LEU	CB-CG-CD1	5.72	120.72	111.00
1	D	194	LEU	CB-CG-CD1	5.71	120.71	111.00
1	A	270	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	B	307	LEU	CB-CG-CD2	5.66	120.62	111.00
1	B	87	LEU	CB-CG-CD1	5.63	120.57	111.00
1	A	121	LEU	CB-CG-CD1	-5.53	101.59	111.00
1	D	8	THR	N-CA-CB	-5.51	99.83	110.30
1	A	327	SER	N-CA-CB	5.44	118.66	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	283	ARG	CD-NE-CZ	5.43	131.20	123.60
1	B	417	LEU	CA-CB-CG	5.43	127.78	115.30
1	A	285	ILE	CA-CB-CG2	5.42	121.73	110.90
1	B	152	LEU	CB-CG-CD1	5.42	120.20	111.00
1	A	342	THR	C-N-CA	-5.41	110.95	122.30
1	C	226	LEU	CB-CG-CD1	5.37	120.12	111.00
1	B	254	ARG	NE-CZ-NH1	-5.36	117.62	120.30
1	D	417	LEU	CA-CB-CG	5.33	127.56	115.30
1	A	173	ASP	CB-CA-C	5.32	121.04	110.40
1	C	344	LEU	CA-CB-CG	5.31	127.51	115.30
1	D	138	ASP	CB-CG-OD2	5.29	123.06	118.30
1	D	285	ILE	CA-CB-CG2	5.29	121.48	110.90
1	D	324	ASP	CB-CG-OD1	-5.28	113.55	118.30
1	C	36	LEU	CB-CG-CD1	-5.28	102.02	111.00
1	C	138	ASP	CB-CG-OD2	5.28	123.05	118.30
1	D	283	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	B	189	ASN	CB-CA-C	-5.26	99.87	110.40
1	C	331	ASP	CB-CG-OD1	5.24	123.02	118.30
1	A	137	LEU	CA-CB-CG	5.21	127.29	115.30
1	C	212	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	D	146	LEU	CB-CG-CD1	5.21	119.86	111.00
1	D	257	ARG	CD-NE-CZ	5.17	130.84	123.60
1	B	146	LEU	CA-CB-CG	-5.16	103.44	115.30
1	C	26	LEU	CA-CB-CG	5.14	127.11	115.30
1	A	285	ILE	N-CA-CB	5.12	122.58	110.80
1	B	226	LEU	CA-CB-CG	5.12	127.08	115.30
1	C	417	LEU	CB-CG-CD1	5.12	119.70	111.00
1	B	401	SER	N-CA-CB	5.10	118.14	110.50
1	B	70	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	D	227	ILE	C-N-CA	-5.09	108.97	121.70
1	B	249	MET	CG-SD-CE	-5.06	92.10	100.20
1	B	301	LEU	CB-CG-CD1	5.05	119.58	111.00
1	C	319	VAL	CG1-CB-CG2	5.04	118.96	110.90
1	C	401	SER	N-CA-CB	-5.02	102.98	110.50
1	A	257	ARG	NE-CZ-NH1	5.01	122.81	120.30
1	C	375	VAL	CG1-CB-CG2	5.01	118.92	110.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	D	188	LYS	CA

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	17	SER	Peptide
1	A	188	LYS	Peptide
1	A	19	ILE	Peptide
1	A	341	LEU	Peptide
1	A	342	THR	Peptide
1	B	106	GLN	Peptide
1	B	19	ILE	Peptide
1	B	202	ASN	Peptide
1	B	98	PRO	Peptide
1	C	187	GLN	Peptide
1	C	19	ILE	Peptide
1	C	202	ASN	Peptide
1	C	203	PRO	Peptide
1	C	21	THR	Peptide
1	D	17	SER	Peptide
1	D	19	ILE	Peptide
1	D	23	THR	Peptide
1	D	240	LYS	Peptide

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	3347	0	3356	205	0
1	B	3348	0	3356	200	0
1	C	3347	0	3356	208	0
1	D	3348	0	3356	205	0
2	A	12	0	16	1	0
2	B	6	0	8	0	0
2	C	30	0	40	6	0
2	D	24	0	32	24	0
3	A	166	0	0	25	0
3	B	199	0	0	27	0
3	C	166	0	0	17	0
3	D	183	0	0	34	0
All	All	14176	0	13520	777	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 29.

All (777) 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:D:60:THR:HG22	3:D:555:HOH:O	1.38	1.22
1:D:182:ASP:HB2	3:D:568:HOH:O	1.40	1.22
1:D:137:LEU:C	1:D:137:LEU:HD23	1.61	1.20
1:C:166:ILE:HD11	1:C:216:ILE:CD1	1.71	1.18
1:C:166:ILE:HD11	1:C:216:ILE:HD11	1.24	1.16
1:B:344:LEU:HB2	3:B:571:HOH:O	1.43	1.16
1:A:182:ASP:HB2	3:A:537:HOH:O	1.43	1.15
1:D:22:MET:O	1:D:25:ILE:HB	1.46	1.15
1:A:17:SER:HB2	1:A:18:PRO:HD3	1.25	1.11
1:A:41:PRO:HB3	1:B:354:MET:HE1	1.30	1.11
1:A:342:THR:HB	1:A:344:LEU:HD22	1.33	1.10
1:D:201:ASN:HB2	2:D:428:GOL:H11	1.24	1.10
1:C:179:LYS:HG3	1:C:180:PRO:HD2	1.28	1.09
1:C:137:LEU:C	1:C:137:LEU:HD23	1.72	1.07
1:C:99:THR:HG21	3:C:531:HOH:O	1.52	1.07
1:B:67:MET:HG2	3:B:591:HOH:O	1.53	1.07
1:B:30:PRO:HD2	1:B:33:MET:HE3	1.33	1.06
1:B:8:THR:HG22	1:B:11:SER:H	1.19	1.06
1:B:60:THR:HG22	3:B:540:HOH:O	1.56	1.05
1:C:192:LYS:HE2	1:C:192:LYS:H	1.21	1.05
1:A:121:LEU:CD2	1:A:228:ILE:HD11	1.87	1.04
1:D:288:ILE:HD12	1:D:288:ILE:C	1.75	1.04
1:C:137:LEU:HD23	1:C:137:LEU:O	1.56	1.04
1:A:342:THR:O	1:A:342:THR:CG2	2.06	1.04
1:D:21:THR:HA	3:D:597:HOH:O	1.58	1.03
1:D:83:LEU:HD22	1:D:87:LEU:HD22	1.40	1.03
1:A:65:GLU:HG2	3:A:437:HOH:O	1.57	1.01
1:D:112:CYS:HB3	3:D:591:HOH:O	1.61	1.01
1:C:415:GLN:HG3	1:C:416:VAL:N	1.77	1.00
2:D:429:GOL:H31	3:D:480:HOH:O	1.62	1.00
1:C:370:ILE:HD11	1:C:398:LEU:HD21	1.43	0.99
1:D:137:LEU:C	1:D:137:LEU:CD2	2.31	0.98
1:B:121:LEU:CD1	1:B:228:ILE:HD11	1.94	0.98
1:B:96:ASN:HB3	3:B:572:HOH:O	1.62	0.98
1:A:22:MET:HG3	1:A:23:THR:H	1.27	0.97
1:C:261:PHE:HB3	1:C:265:ILE:CD1	1.95	0.96
1:A:121:LEU:HD21	1:A:228:ILE:HD11	1.47	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:LYS:CD	1:D:188:LYS:HD3	1.97	0.95
1:C:345:ALA:HB1	1:C:358:ILE:CD1	1.97	0.95
1:A:8:THR:HG22	1:A:11:SER:H	1.28	0.95
1:A:8:THR:HG21	3:A:561:HOH:O	1.65	0.94
1:B:56:GLU:O	1:B:57:ASN:HB2	1.66	0.94
1:B:243:VAL:HG13	3:B:534:HOH:O	1.68	0.94
1:D:126:GLU:HB3	2:D:429:GOL:O2	1.66	0.94
1:C:192:LYS:HE2	1:C:192:LYS:N	1.84	0.93
1:A:59:LYS:CB	1:A:59:LYS:NZ	2.30	0.93
1:D:137:LEU:HD23	1:D:137:LEU:O	1.68	0.93
1:D:16:PRO:O	1:D:17:SER:HB3	1.69	0.92
1:B:73:GLN:O	1:B:297:THR:HG21	1.70	0.91
1:B:121:LEU:HD12	1:B:228:ILE:HD11	1.52	0.90
1:A:342:THR:O	1:A:342:THR:HG22	1.69	0.89
1:B:301:LEU:O	1:B:305:GLN:HG3	1.70	0.89
1:D:201:ASN:HB2	2:D:428:GOL:C1	2.02	0.89
1:B:155:ASN:HB3	3:B:583:HOH:O	1.72	0.89
1:D:11:SER:HB2	2:D:429:GOL:H12	1.53	0.89
1:C:45:MET:HE2	1:D:322:VAL:HG22	1.52	0.89
1:A:409:GLN:HB3	1:B:34:ILE:HD13	1.52	0.89
1:B:377:MET:HG3	1:B:420:LEU:HD11	1.54	0.88
1:C:257:ARG:HD3	1:C:259:ASP:OD2	1.74	0.87
1:B:341:LEU:HD22	1:B:414:PHE:CD2	2.09	0.87
1:A:170:SER:O	1:A:174:ILE:HG12	1.74	0.87
1:A:17:SER:HB2	1:A:18:PRO:CD	2.05	0.87
1:C:420:LEU:HG	3:C:499:HOH:O	1.73	0.87
1:C:8:THR:HG22	1:C:11:SER:H	1.38	0.86
1:B:28:ARG:HH11	1:B:28:ARG:HB3	1.39	0.86
1:D:325:PHE:HD1	3:D:546:HOH:O	1.57	0.86
1:C:214:LYS:HA	1:C:249:MET:HE1	1.57	0.86
1:B:30:PRO:HD2	1:B:33:MET:CE	2.04	0.86
1:B:345:ALA:HB1	1:B:358:ILE:CD1	2.05	0.85
1:D:343:GLY:O	1:D:361:LYS:HE2	1.76	0.85
1:A:41:PRO:CB	1:B:354:MET:HE1	2.07	0.85
1:C:345:ALA:HB1	1:C:358:ILE:HD13	1.57	0.85
1:D:257:ARG:HD3	1:D:259:ASP:OD2	1.77	0.84
1:C:261:PHE:HB3	1:C:265:ILE:HD12	1.60	0.84
1:A:409:GLN:HB3	1:B:34:ILE:CD1	2.06	0.83
1:A:59:LYS:HD3	1:D:188:LYS:HD3	1.58	0.83
1:B:341:LEU:HD22	1:B:414:PHE:HD2	1.43	0.83
1:A:239:ASN:HB3	3:A:495:HOH:O	1.78	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:LYS:NZ	1:A:59:LYS:HB3	1.92	0.83
1:A:214:LYS:HA	1:A:249:MET:HE1	1.61	0.83
1:A:148:SER:HB2	1:B:290:VAL:HB	1.61	0.83
1:C:18:PRO:HG2	1:C:20:ARG:HB3	1.60	0.82
1:A:93:LYS:HG3	1:A:312:GLU:OE1	1.79	0.82
1:D:16:PRO:O	1:D:17:SER:CB	2.24	0.82
1:D:20:ARG:C	1:D:22:MET:H	1.82	0.82
1:C:81:PRO:HG3	3:C:514:HOH:O	1.79	0.82
1:D:148:SER:O	1:D:152:LEU:HD13	1.80	0.81
1:C:137:LEU:C	1:C:137:LEU:CD2	2.44	0.81
1:D:179:LYS:HG3	3:D:559:HOH:O	1.79	0.80
1:A:17:SER:CB	1:A:18:PRO:HD3	2.08	0.80
1:D:42:ASN:HD22	1:D:44:ASN:H	1.30	0.80
1:C:8:THR:HB	1:C:127:MET:O	1.82	0.80
1:C:166:ILE:CD1	1:C:216:ILE:HD11	2.07	0.80
1:C:134:ASN:H	1:C:192:LYS:HZ1	1.30	0.80
1:C:179:LYS:HG3	1:C:180:PRO:CD	2.11	0.80
1:C:99:THR:HG22	1:C:109:MET:HB2	1.65	0.79
1:A:59:LYS:HD2	1:D:188:LYS:HD3	1.63	0.79
1:C:137:LEU:O	1:C:137:LEU:CD2	2.31	0.79
1:D:11:SER:HB2	2:D:429:GOL:C1	2.12	0.79
1:C:197:VAL:HB	1:C:201:ASN:HD22	1.45	0.79
1:C:310:TRP:NE1	2:C:427:GOL:H12	1.98	0.79
2:C:430:GOL:H32	1:D:56:GLU:OE2	1.81	0.79
1:D:8:THR:HG21	2:D:429:GOL:O1	1.83	0.78
1:A:342:THR:CB	1:A:344:LEU:HD22	2.12	0.78
1:D:8:THR:HG22	1:D:11:SER:H	1.47	0.78
1:A:56:GLU:O	1:A:57:ASN:HB2	1.82	0.78
1:A:220:ALA:CB	1:A:227:ILE:HD11	2.14	0.78
1:A:264:ILE:O	1:A:318:HIS:HE1	1.67	0.78
1:B:121:LEU:HD11	1:B:228:ILE:HD11	1.66	0.77
1:B:182:ASP:OD2	1:B:188:LYS:HB3	1.84	0.77
1:C:303:ILE:HG22	1:C:307:LEU:HD22	1.65	0.77
1:D:370:ILE:HG13	1:D:398:LEU:HD21	1.66	0.77
1:D:368:GLU:HB3	3:D:573:HOH:O	1.85	0.77
1:A:142:TYR:CG	1:A:263:LLP:H2'3	2.20	0.77
1:B:217:TYR:HB2	1:B:249:MET:CE	2.15	0.77
1:A:283:ARG:HD3	3:A:461:HOH:O	1.84	0.76
1:B:344:LEU:HB2	3:B:627:HOH:O	1.86	0.76
1:A:294:HIS:HD2	1:A:295:PRO:O	1.68	0.76
1:C:261:PHE:HB3	1:C:265:ILE:HD13	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:18:PRO:HB3	1:D:20:ARG:HG2	1.67	0.76
1:B:345:ALA:HB1	1:B:358:ILE:HD13	1.67	0.76
1:A:84:LEU:O	1:A:88:LYS:HG3	1.86	0.75
1:C:345:ALA:CB	1:C:358:ILE:HD13	2.16	0.75
1:C:134:ASN:H	1:C:192:LYS:NZ	1.84	0.75
1:B:212:ARG:O	1:B:216:ILE:HD12	1.86	0.75
1:B:243:VAL:HG11	3:B:581:HOH:O	1.87	0.75
1:A:163:GLU:HG3	1:A:348:HIS:CE1	2.22	0.74
1:A:121:LEU:CD2	1:A:228:ILE:CD1	2.65	0.74
1:D:137:LEU:CD2	1:D:137:LEU:O	2.33	0.74
1:D:368:GLU:HB2	3:D:581:HOH:O	1.88	0.74
1:B:366:VAL:HG23	1:B:369:LEU:HD23	1.70	0.74
1:B:8:THR:HG22	1:B:11:SER:N	1.99	0.73
1:B:102:TYR:O	1:B:108:GLN:HG3	1.88	0.73
1:D:325:PHE:HB3	3:D:546:HOH:O	1.87	0.73
1:A:365:ASP:HB2	1:A:394:PRO:HB3	1.69	0.73
1:B:8:THR:CG2	1:B:11:SER:H	1.99	0.73
1:A:285:ILE:HG12	1:A:285:ILE:O	1.87	0.73
1:D:325:PHE:CD1	3:D:546:HOH:O	2.34	0.73
1:B:182:ASP:HB2	3:B:451:HOH:O	1.88	0.72
1:D:326:TYR:CD2	3:D:546:HOH:O	2.43	0.72
1:A:142:TYR:CD1	1:A:263:LLP:H2'3	2.23	0.72
1:C:370:ILE:HD11	1:C:398:LEU:CD2	2.17	0.72
1:D:370:ILE:HG13	1:D:398:LEU:CD2	2.20	0.72
1:A:41:PRO:HB3	1:B:354:MET:CE	2.14	0.72
1:A:342:THR:H	1:A:344:LEU:H	1.38	0.72
1:B:214:LYS:HA	1:B:249:MET:HE1	1.72	0.72
1:A:172:ARG:NH2	1:A:215:GLU:OE2	2.22	0.71
1:A:60:THR:HG22	3:A:531:HOH:O	1.90	0.71
1:B:338:ASP:O	1:B:342:THR:HG23	1.91	0.71
1:A:17:SER:CB	1:A:18:PRO:CD	2.67	0.71
1:C:73:GLN:O	1:C:297:THR:HG21	1.89	0.71
1:A:59:LYS:CB	1:A:59:LYS:HZ1	2.02	0.71
1:C:179:LYS:HE3	1:C:180:PRO:HD3	1.72	0.71
1:C:221:ARG:HH21	1:C:251:VAL:CG1	2.03	0.71
1:C:8:THR:CG2	1:C:11:SER:H	2.04	0.70
1:C:284:VAL:O	1:C:288:ILE:HG23	1.90	0.70
1:D:366:VAL:HG11	1:D:398:LEU:CD2	2.21	0.70
1:B:288:ILE:HD13	3:B:537:HOH:O	1.90	0.70
1:A:97:PRO:O	1:A:99:THR:N	2.23	0.70
1:A:22:MET:HG3	1:A:23:THR:N	2.03	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:303:ILE:HG22	1:D:307:LEU:HD22	1.71	0.70
1:D:285:ILE:HD13	1:D:285:ILE:C	2.12	0.69
1:A:19:ILE:HD12	3:A:549:HOH:O	1.93	0.69
1:C:404:SER:O	2:C:428:GOL:H2	1.92	0.69
1:B:257:ARG:NH1	1:B:259:ASP:OD1	2.26	0.69
1:C:186:PRO:O	1:C:187:GLN:HG2	1.93	0.69
1:D:294:HIS:HD2	1:D:295:PRO:O	1.75	0.69
1:B:134:ASN:ND2	1:B:178:TRP:CH2	2.61	0.69
1:D:1:MET:N	3:D:431:HOH:O	2.22	0.69
1:D:169:ASP:HA	1:D:172:ARG:NH1	2.08	0.68
1:B:283:ARG:HD3	3:B:553:HOH:O	1.93	0.68
1:C:140:PRO:HB2	1:C:203:PRO:HG3	1.76	0.68
1:A:59:LYS:NZ	1:A:59:LYS:HB2	2.08	0.67
1:B:231:ASP:OD2	1:B:257:ARG:NH2	2.26	0.67
1:A:59:LYS:HB3	1:A:59:LYS:HZ2	1.59	0.67
1:C:185:ASN:O	1:C:186:PRO:C	2.33	0.67
1:C:345:ALA:CB	1:C:358:ILE:CD1	2.68	0.67
1:B:75:SER:HB2	1:B:76:PRO:CD	2.25	0.67
1:C:163:GLU:HG2	1:C:348:HIS:CE1	2.30	0.67
1:D:142:TYR:CD2	1:D:263:LLP:H2'3	2.28	0.67
1:C:16:PRO:HA	1:C:286:LEU:HD22	1.77	0.67
1:D:73:GLN:O	1:D:297:THR:HG21	1.95	0.67
1:C:214:LYS:HA	1:C:249:MET:CE	2.24	0.67
1:D:89:GLN:HA	1:D:89:GLN:NE2	2.10	0.67
1:B:217:TYR:HB2	1:B:249:MET:HE2	1.76	0.67
1:C:96:ASN:N	1:C:97:PRO:HD3	2.10	0.67
1:D:86:TRP:HZ2	3:D:583:HOH:O	1.76	0.67
1:D:358:ILE:O	1:D:358:ILE:HG13	1.95	0.67
1:D:366:VAL:CG1	1:D:398:LEU:HD21	2.25	0.67
1:D:370:ILE:CG1	1:D:398:LEU:HD21	2.25	0.66
1:A:27:SER:O	1:A:28:ARG:HB3	1.95	0.66
1:C:185:ASN:O	1:C:187:GLN:N	2.28	0.66
1:A:361:LYS:HD3	3:A:560:HOH:O	1.95	0.66
1:D:24:ASP:CB	3:D:584:HOH:O	2.44	0.66
1:D:163:GLU:O	1:D:206:ASN:HB3	1.95	0.66
1:A:375:VAL:HG12	1:A:380:LEU:HD22	1.76	0.66
1:A:97:PRO:C	1:A:99:THR:H	1.99	0.66
1:D:231:ASP:OD2	1:D:257:ARG:NH2	2.28	0.66
1:A:67:MET:O	1:A:70:ARG:N	2.27	0.66
1:A:59:LYS:HE2	1:D:178:TRP:CZ3	2.30	0.66
1:D:96:ASN:HB3	3:D:547:HOH:O	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:166:ILE:HD11	1:C:216:ILE:HD12	1.72	0.65
1:D:278:LYS:HB3	1:D:279:PRO:HD3	1.78	0.65
1:A:342:THR:O	1:A:342:THR:HG23	1.94	0.65
1:B:172:ARG:HG2	1:B:219:LEU:HD11	1.79	0.65
1:B:345:ALA:CB	1:B:358:ILE:CD1	2.75	0.65
1:C:34:ILE:HD12	1:D:409:GLN:HB3	1.78	0.65
1:B:143:SER:HB3	1:B:386:ALA:O	1.96	0.65
1:D:126:GLU:CB	2:D:429:GOL:O2	2.42	0.65
1:A:179:LYS:HB3	1:A:181:GLU:OE2	1.97	0.65
1:B:137:LEU:HD21	1:B:156:ILE:CG2	2.26	0.65
1:B:99:THR:HG23	1:B:109:MET:H	1.62	0.65
1:B:344:LEU:CB	3:B:627:HOH:O	2.43	0.65
1:D:163:GLU:HG2	1:D:348:HIS:CE1	2.32	0.65
1:A:86:TRP:HZ3	3:A:558:HOH:O	1.79	0.65
1:C:221:ARG:NH2	1:C:251:VAL:HG13	2.11	0.65
1:D:137:LEU:HD23	1:D:138:ASP:N	2.12	0.65
1:D:14:ARG:HH21	2:D:429:GOL:H2	1.61	0.65
1:D:120:GLY:O	1:D:124:VAL:HG23	1.97	0.65
1:B:345:ALA:CB	1:B:358:ILE:HD13	2.26	0.64
1:A:299:ASN:HD21	1:B:299:ASN:HD21	1.45	0.64
1:C:22:MET:HA	3:C:540:HOH:O	1.96	0.64
1:C:264:ILE:O	1:C:318:HIS:HE1	1.81	0.64
1:D:340:TRP:CE2	1:D:415:GLN:HB2	2.32	0.64
1:B:137:LEU:CD2	1:B:156:ILE:HG23	2.28	0.64
1:D:112:CYS:SG	3:D:591:HOH:O	2.55	0.64
1:A:220:ALA:HB2	1:A:227:ILE:HD11	1.78	0.63
1:B:344:LEU:HD12	1:B:421:ILE:CG2	2.27	0.63
1:B:408:GLU:H	1:B:408:GLU:CD	2.00	0.63
1:C:303:ILE:CG2	1:C:307:LEU:HD22	2.28	0.63
1:C:415:GLN:CG	1:C:416:VAL:N	2.59	0.63
1:B:56:GLU:O	1:B:57:ASN:CB	2.43	0.63
1:A:288:ILE:HD11	1:A:293:LEU:O	1.99	0.63
1:C:239:ASN:ND2	1:C:241:PHE:O	2.32	0.63
1:D:99:THR:HG23	1:D:109:MET:HB2	1.78	0.63
1:C:133:ASP:OD2	1:C:192:LYS:HD2	1.98	0.63
1:C:310:TRP:CD1	2:C:427:GOL:H12	2.34	0.63
1:C:117:SER:HB3	1:C:260:SER:HB3	1.79	0.63
1:C:221:ARG:HH21	1:C:251:VAL:HG13	1.63	0.63
1:B:2:ASN:HD21	1:B:4:ALA:HB3	1.64	0.63
1:A:115:SER:O	1:A:115:SER:OG	2.16	0.62
1:C:294:HIS:HD2	1:C:295:PRO:O	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:42:ASN:ND2	1:D:44:ASN:HB2	2.14	0.62
1:A:300:GLN:NE2	3:A:478:HOH:O	2.25	0.62
1:C:192:LYS:CD	3:C:446:HOH:O	2.47	0.62
1:A:195:TYR:HD1	1:A:228:ILE:HG12	1.64	0.62
1:D:126:GLU:HB3	2:D:429:GOL:HO2	1.60	0.62
1:A:381:MET:HE2	1:A:398:LEU:HD13	1.82	0.62
1:A:196:THR:HG23	3:A:568:HOH:O	1.99	0.62
1:A:100:ILE:HD12	1:A:101:HIS:CE1	2.34	0.62
1:B:369:LEU:O	1:B:373:LYS:HB2	1.99	0.62
1:C:142:TYR:CG	1:C:263:LLP:H2'3	2.35	0.62
1:C:192:LYS:HD2	3:C:446:HOH:O	2.00	0.61
1:A:345:ALA:HB1	1:A:358:ILE:HD12	1.81	0.61
1:C:370:ILE:CD1	1:C:398:LEU:HD21	2.27	0.61
1:A:8:THR:CG2	1:A:10:ALA:HB3	2.31	0.61
1:A:41:PRO:HA	1:B:354:MET:HE2	1.82	0.61
1:B:99:THR:HG21	3:B:577:HOH:O	2.01	0.61
1:B:222:LYS:HE2	1:B:223:TYR:CE2	2.34	0.61
1:A:73:GLN:O	1:A:297:THR:HG21	2.01	0.61
1:D:83:LEU:HD22	1:D:87:LEU:CD2	2.22	0.60
1:A:34:ILE:CD1	1:B:409:GLN:HB3	2.31	0.60
1:C:231:ASP:OD2	1:C:257:ARG:NH2	2.34	0.60
1:C:261:PHE:CB	1:C:265:ILE:HD12	2.29	0.60
1:A:59:LYS:HZ1	1:A:59:LYS:HB2	1.66	0.60
1:D:288:ILE:C	1:D:288:ILE:CD1	2.60	0.60
1:D:142:TYR:CG	1:D:263:LLP:H2'3	2.36	0.60
1:B:179:LYS:CG	1:B:180:PRO:HD2	2.32	0.60
1:C:73:GLN:O	1:C:297:THR:CG2	2.49	0.60
1:C:288:ILE:HD11	1:C:293:LEU:O	2.02	0.60
1:B:84:LEU:HD13	1:B:113:VAL:HG23	1.85	0.59
1:A:41:PRO:CB	1:B:354:MET:CE	2.77	0.59
1:C:326:TYR:CE1	1:C:354:MET:HE2	2.38	0.59
1:D:285:ILE:HD13	1:D:286:LEU:N	2.17	0.59
1:A:147:GLN:HG3	3:A:544:HOH:O	2.03	0.59
1:D:265:ILE:O	1:D:266:SER:HB2	2.03	0.59
1:D:42:ASN:HD21	1:D:44:ASN:HB2	1.68	0.59
1:B:187:GLN:O	1:B:188:LYS:HB2	2.03	0.59
1:C:197:VAL:HB	1:C:201:ASN:ND2	2.18	0.59
1:C:34:ILE:HD13	1:D:409:GLN:O	2.03	0.58
1:C:142:TYR:CD1	1:C:263:LLP:H2'3	2.38	0.58
1:B:190:THR:O	1:B:192:LYS:NZ	2.34	0.58
1:C:384:GLY:N	1:C:397:TYR:O	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:LYS:HB3	1:A:59:LYS:HZ1	1.65	0.58
1:C:178:TRP:HZ3	1:C:188:LYS:O	1.85	0.58
1:D:24:ASP:HB2	3:D:584:HOH:O	2.01	0.58
1:B:338:ASP:O	1:B:342:THR:CG2	2.51	0.58
1:D:10:ALA:HB2	3:D:469:HOH:O	2.02	0.58
1:B:42:ASN:HD22	1:B:44:ASN:H	1.51	0.58
1:D:99:THR:HG21	3:D:552:HOH:O	2.04	0.58
1:C:92:ILE:HG12	1:C:100:ILE:HG21	1.86	0.58
1:C:102:TYR:O	1:C:108:GLN:HB2	2.03	0.58
1:B:345:ALA:HB1	1:B:358:ILE:HD12	1.85	0.58
1:C:16:PRO:HA	1:C:286:LEU:CD2	2.32	0.58
1:C:261:PHE:CG	1:C:265:ILE:HD12	2.39	0.58
1:D:304:SER:O	1:D:308:HIS:HD2	1.87	0.58
1:C:99:THR:HG23	1:C:99:THR:O	2.04	0.57
1:C:163:GLU:CG	1:C:348:HIS:CE1	2.87	0.57
1:A:123:LYS:HB3	1:A:284:VAL:HB	1.85	0.57
1:B:134:ASN:ND2	1:B:178:TRP:HH2	2.02	0.57
1:B:341:LEU:CD2	1:B:414:PHE:HD2	2.16	0.57
1:D:96:ASN:CB	3:D:547:HOH:O	2.50	0.57
1:D:237:GLN:HE22	1:D:243:VAL:H	1.53	0.57
1:B:142:TYR:CD2	1:B:263:LLP:H2'3	2.40	0.56
1:D:201:ASN:HB2	2:D:428:GOL:H2	1.87	0.56
1:D:365:ASP:HB2	1:D:394:PRO:HB2	1.86	0.56
1:A:34:ILE:HD13	1:B:409:GLN:HB3	1.87	0.56
1:C:139:GLU:HA	1:C:140:PRO:C	2.26	0.56
1:D:86:TRP:CZ2	3:D:583:HOH:O	2.52	0.56
1:A:188:LYS:O	1:A:188:LYS:HD3	2.05	0.56
1:B:113:VAL:HG12	1:B:295:PRO:HG2	1.87	0.56
1:C:21:THR:HB	1:C:24:ASP:HB2	1.86	0.56
1:D:366:VAL:CG1	1:D:366:VAL:O	2.52	0.56
1:C:114:THR:HG21	1:C:120:GLY:HA3	1.87	0.56
1:C:133:ASP:HB3	1:C:192:LYS:HE3	1.88	0.56
1:A:203:PRO:HG3	1:A:387:PHE:CG	2.40	0.56
1:D:16:PRO:O	1:D:289:GLN:OE1	2.24	0.56
1:A:370:ILE:HG21	1:A:381:MET:O	2.06	0.56
1:D:177:ARG:HB3	1:D:177:ARG:HH11	1.71	0.56
1:D:201:ASN:HB2	2:D:428:GOL:C2	2.35	0.56
1:A:163:GLU:HG2	3:A:550:HOH:O	2.06	0.55
1:A:197:VAL:HB	1:A:201:ASN:HD22	1.71	0.55
1:C:221:ARG:NH2	1:C:251:VAL:CG1	2.69	0.55
1:D:102:TYR:O	1:D:108:GLN:HB2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:231:ASP:HA	3:D:487:HOH:O	2.07	0.55
1:B:341:LEU:CD2	1:B:414:PHE:CD2	2.85	0.55
1:C:34:ILE:CD1	1:D:409:GLN:HB3	2.35	0.55
1:D:20:ARG:C	1:D:22:MET:N	2.58	0.55
1:D:288:ILE:HD12	1:D:289:GLN:N	2.21	0.55
1:D:67:MET:H	2:D:427:GOL:H11	1.71	0.55
1:D:95:HIS:O	1:D:96:ASN:C	2.43	0.55
1:D:201:ASN:CB	2:D:428:GOL:H11	2.17	0.55
1:A:261:PHE:CD1	1:A:265:ILE:HD12	2.42	0.55
1:B:108:GLN:NE2	1:B:278:LYS:NZ	2.54	0.55
1:C:8:THR:HG22	1:C:11:SER:HB3	1.89	0.55
1:C:271:ILE:HD12	1:C:300:GLN:HG2	1.87	0.55
1:A:169:ASP:OD1	1:A:172:ARG:NH1	2.40	0.55
1:A:197:VAL:C	3:A:568:HOH:O	2.45	0.55
1:D:366:VAL:CG1	1:D:398:LEU:CD2	2.85	0.55
1:A:179:LYS:HD2	1:A:179:LYS:N	2.22	0.55
1:B:142:TYR:CG	1:B:263:LLP:H2'3	2.42	0.55
1:B:217:TYR:CB	1:B:249:MET:CE	2.84	0.55
1:B:243:VAL:CG1	3:B:534:HOH:O	2.39	0.55
1:D:241:PHE:HD1	3:D:479:HOH:O	1.89	0.55
1:B:330:LYS:HG2	1:B:334:LEU:HD22	1.89	0.54
1:D:204:THR:OG1	2:D:428:GOL:H32	2.07	0.54
1:D:316:MET:O	1:D:319:VAL:HG22	2.07	0.54
1:A:200:GLY:N	1:A:352:ALA:HB3	2.22	0.54
1:C:20:ARG:HD3	1:C:21:THR:N	2.22	0.54
1:A:163:GLU:CG	1:A:348:HIS:CE1	2.89	0.54
1:A:166:ILE:HD12	1:A:167:VAL:C	2.28	0.54
1:B:137:LEU:HD21	1:B:156:ILE:HG23	1.87	0.54
1:B:237:GLN:HE22	1:B:243:VAL:H	1.55	0.54
1:B:303:ILE:HG22	1:B:307:LEU:HD22	1.90	0.54
1:C:288:ILE:O	1:C:288:ILE:HD12	2.08	0.54
1:A:59:LYS:CB	1:A:59:LYS:HZ2	2.15	0.54
1:B:197:VAL:HB	1:B:201:ASN:HD22	1.73	0.54
1:C:22:MET:HG3	1:C:23:THR:HG23	1.90	0.53
1:B:368:GLU:O	1:B:372:GLU:HB2	2.08	0.53
1:C:99:THR:CG2	1:C:109:MET:HB2	2.37	0.53
1:C:261:PHE:CB	1:C:265:ILE:CD1	2.80	0.53
1:C:363:ILE:HD13	3:C:564:HOH:O	2.08	0.53
1:D:341:LEU:HD22	1:D:414:PHE:CD2	2.44	0.53
1:A:377:MET:HG3	1:A:420:LEU:HD11	1.90	0.53
1:C:100:ILE:O	1:C:108:GLN:HG3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:GLN:O	1:B:297:THR:CG2	2.52	0.53
1:C:145:THR:HG21	1:C:195:TYR:OH	2.08	0.53
1:A:6:PHE:CE2	1:A:226:LEU:HD13	2.44	0.53
1:A:18:PRO:CD	1:A:289:GLN:HB3	2.38	0.53
1:B:179:LYS:HG3	1:B:180:PRO:HD2	1.91	0.53
1:D:359:LYS:HB2	1:D:397:TYR:CE1	2.43	0.53
1:C:99:THR:CG2	1:C:109:MET:N	2.72	0.53
1:D:288:ILE:HD12	1:D:288:ILE:O	2.06	0.53
1:A:59:LYS:NZ	1:D:177:ARG:HD3	2.24	0.52
2:D:428:GOL:H31	3:D:572:HOH:O	2.09	0.52
1:A:108:GLN:HE21	1:A:278:LYS:HD3	1.74	0.52
1:C:294:HIS:HB2	1:C:295:PRO:CD	2.40	0.52
1:D:203:PRO:HG3	1:D:387:PHE:CG	2.45	0.52
1:A:264:ILE:O	1:A:318:HIS:CE1	2.56	0.52
1:A:334:LEU:HD21	1:A:349:VAL:HB	1.91	0.52
1:D:24:ASP:HB3	3:D:584:HOH:O	2.06	0.52
1:D:341:LEU:HD22	1:D:414:PHE:HD2	1.74	0.52
1:A:24:ASP:OD2	1:A:25:ILE:N	2.42	0.52
1:B:178:TRP:CZ3	1:B:188:LYS:O	2.62	0.52
1:B:178:TRP:HZ3	1:B:188:LYS:O	1.92	0.52
1:B:303:ILE:O	1:B:307:LEU:HB2	2.09	0.52
1:D:366:VAL:O	1:D:366:VAL:HG13	2.08	0.52
1:B:301:LEU:O	1:B:305:GLN:CG	2.51	0.52
1:C:74:TYR:HD1	1:C:294:HIS:HE1	1.58	0.52
1:D:198:PRO:O	1:D:207:SER:HA	2.09	0.52
1:A:86:TRP:CZ3	3:A:558:HOH:O	2.54	0.52
1:A:366:VAL:O	1:A:366:VAL:HG22	2.10	0.52
1:A:369:LEU:HD23	1:A:370:ILE:HD13	1.91	0.52
1:B:344:LEU:HD11	1:B:425:LEU:HD21	1.92	0.52
1:C:200:GLY:N	1:C:352:ALA:HB3	2.25	0.52
1:C:159:VAL:HG11	1:C:166:ILE:HD13	1.92	0.52
1:D:34:ILE:HD11	1:D:36:LEU:HD21	1.92	0.52
1:C:1:MET:HA	3:C:550:HOH:O	2.08	0.51
1:C:142:TYR:HD1	1:C:145:THR:CG2	2.23	0.51
1:D:159:VAL:HG11	1:D:166:ILE:HD13	1.91	0.51
1:A:74:TYR:HD1	1:A:294:HIS:HE1	1.57	0.51
1:A:97:PRO:HG2	1:A:109:MET:SD	2.51	0.51
1:A:217:TYR:O	1:A:220:ALA:HB3	2.10	0.51
1:A:366:VAL:O	1:A:370:ILE:HG12	2.11	0.51
1:B:142:TYR:CD2	1:B:145:THR:HG22	2.46	0.51
1:B:174:ILE:O	1:B:177:ARG:HD3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:264:ILE:HG22	1:D:322:VAL:HG11	1.91	0.51
1:B:204:THR:HA	1:B:357:TRP:HB2	1.91	0.51
1:C:345:ALA:HB1	1:C:358:ILE:HD12	1.87	0.51
1:A:152:LEU:HD12	1:A:152:LEU:N	2.25	0.51
1:A:278:LYS:HD2	3:A:552:HOH:O	2.10	0.51
1:A:294:HIS:HB2	1:A:295:PRO:CD	2.40	0.51
1:A:345:ALA:HB1	1:A:358:ILE:CD1	2.40	0.51
1:C:138:ASP:HB3	1:C:166:ILE:HG22	1.92	0.51
1:D:8:THR:HG23	1:D:10:ALA:H	1.75	0.51
1:B:134:ASN:HD21	1:B:178:TRP:HH2	1.56	0.51
1:D:92:ILE:HG12	1:D:100:ILE:HG21	1.93	0.51
1:C:61:ILE:HG23	1:C:305:GLN:HE21	1.76	0.51
1:C:345:ALA:HA	1:C:359:LYS:O	2.10	0.51
1:A:8:THR:HG22	1:A:11:SER:N	2.12	0.51
1:C:99:THR:HG23	1:C:109:MET:N	2.25	0.51
1:C:285:ILE:O	1:C:289:GLN:HG3	2.10	0.51
1:D:345:ALA:HB1	1:D:358:ILE:HD12	1.93	0.51
1:B:174:ILE:HD12	1:B:175:LEU:N	2.26	0.50
1:A:227:ILE:HB	1:A:255:VAL:HG22	1.92	0.50
1:B:42:ASN:ND2	1:B:44:ASN:H	2.09	0.50
1:B:137:LEU:HD22	1:B:156:ILE:HG23	1.93	0.50
1:B:385:ASN:O	1:B:391:SER:HA	2.11	0.50
1:C:142:TYR:HD1	1:C:145:THR:HG22	1.76	0.50
1:B:96:ASN:CB	3:B:572:HOH:O	2.38	0.50
1:B:142:TYR:HD2	1:B:145:THR:HG22	1.76	0.50
1:B:283:ARG:CD	3:B:553:HOH:O	2.56	0.50
1:C:123:LYS:HD2	1:C:288:ILE:HG22	1.92	0.50
1:A:209:THR:O	1:A:213:LYS:HG3	2.10	0.50
1:B:172:ARG:HG3	1:B:172:ARG:NH1	2.25	0.50
1:C:341:LEU:HD11	1:C:414:PHE:CE2	2.46	0.50
1:A:164:SER:O	1:A:208:LEU:HA	2.12	0.50
1:A:337:ALA:O	1:A:341:LEU:HB2	2.11	0.50
1:B:344:LEU:CB	3:B:571:HOH:O	2.24	0.50
1:B:344:LEU:HD12	1:B:421:ILE:HG23	1.93	0.50
1:C:24:ASP:O	1:C:28:ARG:HD2	2.11	0.50
1:C:99:THR:O	1:C:100:ILE:C	2.47	0.50
1:C:99:THR:O	1:C:99:THR:CG2	2.58	0.50
1:B:233:TYR:CE1	1:B:263:LLP:HD3	2.47	0.50
1:C:71:ALA:HB2	1:C:301:LEU:HD23	1.94	0.50
1:D:311:GLY:C	1:D:313:GLU:N	2.63	0.50
1:A:18:PRO:HD3	1:A:289:GLN:HB3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:366:VAL:HG12	1:B:395:SER:O	2.11	0.50
1:D:20:ARG:NH2	3:D:449:HOH:O	2.45	0.50
1:B:222:LYS:HE2	1:B:223:TYR:CZ	2.47	0.50
1:A:151:PRO:HG2	1:A:152:LEU:CD1	2.42	0.50
1:B:408:GLU:OE1	1:B:408:GLU:N	2.27	0.50
1:B:381:MET:HE3	1:B:400:ALA:HB2	1.93	0.49
1:C:256:ILE:HD11	1:C:280:LEU:HD13	1.94	0.49
1:D:80:ILE:HD13	1:D:301:LEU:HD13	1.93	0.49
1:A:73:GLN:O	1:A:297:THR:CG2	2.59	0.49
1:B:97:PRO:C	1:B:99:THR:H	2.16	0.49
1:C:381:MET:HE3	1:C:398:LEU:HB3	1.94	0.49
1:D:270:ARG:O	1:D:271:ILE:HD13	2.12	0.49
1:D:366:VAL:HG11	1:D:398:LEU:HD21	1.89	0.49
1:A:299:ASN:HD21	1:B:299:ASN:ND2	2.09	0.49
1:C:60:THR:HG22	3:C:487:HOH:O	2.10	0.49
1:D:177:ARG:O	1:D:177:ARG:HG2	2.11	0.49
1:D:228:ILE:HG13	1:D:228:ILE:O	2.13	0.49
1:A:25:ILE:HG13	2:A:426:GOL:H12	1.92	0.49
1:A:342:THR:N	1:A:344:LEU:H	2.07	0.49
1:C:35:SER:HB2	1:D:380:LEU:HD12	1.93	0.49
1:A:104:PRO:HG3	1:A:108:GLN:NE2	2.28	0.49
1:C:7:ILE:HD13	1:C:283:ARG:HD3	1.93	0.49
1:B:89:GLN:HA	1:B:89:GLN:NE2	2.28	0.49
1:C:1:MET:N	3:C:548:HOH:O	2.28	0.49
1:C:97:PRO:HG2	1:C:109:MET:SD	2.53	0.49
1:D:214:LYS:HA	1:D:249:MET:HE1	1.95	0.49
1:A:59:LYS:HZ3	1:D:177:ARG:HG2	1.77	0.49
1:A:366:VAL:CG2	1:A:398:LEU:HD21	2.42	0.49
1:A:415:GLN:O	1:A:419:GLN:NE2	2.45	0.49
1:B:99:THR:HG23	1:B:109:MET:N	2.26	0.49
1:A:218:GLU:HG2	1:A:219:LEU:N	2.24	0.49
1:B:104:PRO:O	1:B:106:GLN:O	2.31	0.49
1:A:34:ILE:O	1:B:379:VAL:HA	2.13	0.48
1:A:174:ILE:O	1:A:177:ARG:HD3	2.13	0.48
1:A:236:LEU:HD23	1:A:353:GLY:HA2	1.94	0.48
1:D:145:THR:HG21	1:D:195:TYR:OH	2.12	0.48
1:A:195:TYR:CD1	1:A:228:ILE:HG12	2.47	0.48
1:B:108:GLN:NE2	1:B:278:LYS:HZ3	2.11	0.48
1:C:95:HIS:HD2	3:C:458:HOH:O	1.95	0.48
1:C:163:GLU:HG2	1:C:348:HIS:ND1	2.28	0.48
1:D:220:ALA:O	1:D:224:ASP:HA	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:HIS:NE2	1:B:270:ARG:HD3	2.28	0.48
1:A:341:LEU:CD2	1:A:414:PHE:CE2	2.96	0.48
1:C:190:THR:O	1:C:192:LYS:NZ	2.42	0.48
1:B:2:ASN:ND2	1:B:4:ALA:HB3	2.29	0.48
1:A:97:PRO:C	1:A:99:THR:N	2.65	0.48
1:B:370:ILE:HG13	1:B:398:LEU:HD21	1.96	0.48
1:D:42:ASN:ND2	1:D:44:ASN:H	2.05	0.48
1:C:87:LEU:O	1:C:91:GLN:HG2	2.14	0.48
1:C:204:THR:HA	1:C:357:TRP:HB2	1.95	0.48
1:A:91:GLN:O	1:A:95:HIS:N	2.38	0.48
1:A:366:VAL:HG21	1:A:398:LEU:HD21	1.95	0.48
1:D:99:THR:CG2	1:D:109:MET:HB2	2.44	0.48
1:D:200:GLY:N	1:D:352:ALA:HB3	2.29	0.48
1:A:95:HIS:O	1:A:248:SER:HA	2.14	0.48
1:D:127:MET:HA	2:D:429:GOL:H32	1.94	0.48
1:B:411:ASP:OD1	3:B:456:HOH:O	2.20	0.47
1:D:19:ILE:HG23	3:D:553:HOH:O	2.13	0.47
1:B:42:ASN:HD21	1:B:44:ASN:HD22	1.63	0.47
1:D:245:THR:O	1:D:248:SER:OG	2.30	0.47
1:A:196:THR:CB	3:A:568:HOH:O	2.62	0.47
1:D:42:ASN:HD21	1:D:44:ASN:HD22	1.62	0.47
1:D:117:SER:O	1:D:121:LEU:HD12	2.14	0.47
1:D:294:HIS:CD2	1:D:295:PRO:O	2.63	0.47
1:A:86:TRP:CD1	1:A:86:TRP:C	2.87	0.47
1:C:162:ASP:OD1	1:C:212:ARG:NH1	2.35	0.47
1:A:121:LEU:HD23	1:A:228:ILE:CD1	2.44	0.47
1:B:344:LEU:HG	3:B:571:HOH:O	2.14	0.47
1:C:21:THR:CB	1:C:24:ASP:HB2	2.43	0.47
1:D:349:VAL:HA	1:D:350:PRO:HD3	1.70	0.47
1:B:42:ASN:ND2	1:B:44:ASN:HB2	2.29	0.47
1:B:121:LEU:HD23	3:B:568:HOH:O	2.14	0.47
1:B:295:PRO:O	1:B:296:SER:C	2.53	0.47
1:C:221:ARG:HH21	1:C:251:VAL:HG11	1.79	0.47
1:A:198:PRO:N	3:A:568:HOH:O	2.48	0.47
1:A:359:LYS:HB2	1:A:397:TYR:CE2	2.49	0.47
1:B:16:PRO:HA	1:B:286:LEU:HD22	1.97	0.47
1:B:84:LEU:O	1:B:88:LYS:HG3	2.15	0.47
1:B:263:LLP:H5'2	1:B:263:LLP:NZ	2.30	0.47
1:C:80:ILE:CD1	1:C:301:LEU:HD13	2.45	0.47
1:C:264:ILE:O	1:C:318:HIS:CE1	2.66	0.47
1:C:374:ALA:HA	1:C:420:LEU:CD1	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:LEU:N	1:A:152:LEU:CD1	2.78	0.47
1:A:341:LEU:HD22	1:A:414:PHE:CD2	2.49	0.47
1:C:243:VAL:HG13	3:C:544:HOH:O	2.15	0.47
1:A:63:PHE:HD2	1:A:68:MET:HE1	1.79	0.47
1:A:192:LYS:HD3	3:A:492:HOH:O	2.14	0.47
1:A:341:LEU:CD2	1:A:414:PHE:CD2	2.98	0.47
1:B:163:GLU:HG2	3:B:561:HOH:O	2.15	0.47
1:A:342:THR:HB	1:A:344:LEU:CD2	2.24	0.46
1:B:185:ASN:O	1:B:187:GLN:O	2.33	0.46
1:D:336:ALA:HA	3:D:519:HOH:O	2.13	0.46
1:A:326:TYR:CE1	1:A:354:MET:HE2	2.50	0.46
1:D:218:GLU:HG2	1:D:219:LEU:N	2.29	0.46
1:A:296:SER:O	1:A:300:GLN:HG3	2.15	0.46
1:B:136:LEU:CD2	1:B:174:ILE:HD13	2.44	0.46
1:B:334:LEU:HD21	1:B:349:VAL:HB	1.97	0.46
1:D:11:SER:HB2	2:D:429:GOL:H11	1.96	0.46
1:B:324:ASP:HB3	3:B:458:HOH:O	2.15	0.46
1:D:104:PRO:O	1:D:106:GLN:O	2.33	0.46
1:A:111:LEU:HA	1:A:274:LEU:O	2.14	0.46
1:C:203:PRO:HB2	1:C:357:TRP:CE3	2.51	0.46
1:C:292:THR:HG22	1:D:115:SER:HB2	1.96	0.46
1:A:59:LYS:NZ	1:D:177:ARG:HG2	2.31	0.46
1:A:223:TYR:N	1:A:223:TYR:CD2	2.83	0.46
1:A:293:LEU:HD21	1:B:118:GLN:NE2	2.31	0.46
1:C:168:PRO:HG2	1:C:215:GLU:OE1	2.16	0.46
1:D:408:GLU:OE1	1:D:408:GLU:N	2.33	0.46
1:A:221:ARG:O	1:A:222:LYS:C	2.54	0.46
1:A:360:VAL:HG13	1:A:421:ILE:HD13	1.96	0.46
1:C:30:PRO:C	1:C:32:SER:H	2.20	0.46
1:A:147:GLN:NE2	3:A:544:HOH:O	2.49	0.46
1:A:285:ILE:O	1:A:285:ILE:CG1	2.61	0.46
1:A:409:GLN:HB3	1:B:34:ILE:HD12	1.94	0.46
1:B:187:GLN:O	1:B:188:LYS:CB	2.63	0.46
1:C:299:ASN:HD21	1:D:299:ASN:HD21	1.63	0.46
1:D:185:ASN:C	1:D:185:ASN:HD22	2.18	0.46
1:D:360:VAL:HG23	1:D:363:ILE:HB	1.97	0.45
1:A:59:LYS:HD2	1:D:188:LYS:CD	2.40	0.45
1:B:220:ALA:O	1:B:224:ASP:HA	2.16	0.45
1:C:8:THR:HG22	1:C:11:SER:N	2.18	0.45
1:C:303:ILE:O	1:C:307:LEU:HB2	2.16	0.45
1:A:263:LLP:NZ	1:A:263:LLP:C5'	2.77	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:ILE:HD11	1:B:216:ILE:HG12	1.97	0.45
1:C:134:ASN:N	1:C:192:LYS:HZ1	2.07	0.45
1:C:179:LYS:HE3	1:C:180:PRO:CD	2.45	0.45
1:D:16:PRO:HA	1:D:286:LEU:HD22	1.98	0.45
1:D:203:PRO:HB2	1:D:357:TRP:CE3	2.51	0.45
1:A:16:PRO:HA	1:A:286:LEU:HD22	1.98	0.45
1:A:146:LEU:HD23	1:A:146:LEU:HA	1.47	0.45
1:A:196:THR:CG2	3:A:568:HOH:O	2.59	0.45
1:D:11:SER:O	1:D:283:ARG:NH2	2.24	0.45
1:A:83:LEU:HD23	1:A:113:VAL:HG21	1.99	0.45
1:B:344:LEU:CG	3:B:571:HOH:O	2.63	0.45
1:C:371:GLU:O	1:C:375:VAL:CG2	2.65	0.45
1:A:68:MET:O	1:A:69:LYS:C	2.55	0.45
1:A:268:GLY:O	1:B:296:SER:HA	2.17	0.45
1:C:45:MET:CE	1:D:322:VAL:HG22	2.37	0.45
1:C:203:PRO:HG2	1:C:204:THR:HG23	1.98	0.45
1:C:209:THR:HB	1:C:211:GLU:OE1	2.16	0.45
1:D:88:LYS:HE3	1:D:111:LEU:HB3	1.99	0.45
1:A:67:MET:O	1:A:68:MET:C	2.54	0.45
1:A:110:ASP:CG	1:A:278:LYS:HE2	2.36	0.45
1:A:263:LLP:NZ	1:A:263:LLP:H5'2	2.31	0.45
1:B:119:GLN:O	1:B:123:LYS:HG3	2.17	0.45
1:C:164:SER:O	1:C:208:LEU:HA	2.17	0.45
1:C:381:MET:HA	1:D:37:ALA:HB2	1.99	0.45
1:A:175:LEU:O	1:A:178:TRP:HD1	2.00	0.45
1:D:15:ASN:HB3	1:D:16:PRO:HD2	1.99	0.45
1:D:58:GLY:HA2	3:D:571:HOH:O	2.16	0.45
1:D:325:PHE:CB	3:D:546:HOH:O	2.58	0.45
1:A:8:THR:HG23	1:A:10:ALA:H	1.81	0.44
1:A:184:LYS:HD2	1:A:184:LYS:N	2.32	0.44
1:C:270:ARG:C	1:C:271:ILE:HG12	2.38	0.44
1:B:338:ASP:HA	1:B:342:THR:HG22	1.99	0.44
1:C:75:SER:HB2	1:C:76:PRO:CD	2.47	0.44
1:C:270:ARG:HD3	1:D:294:HIS:CE1	2.52	0.44
1:C:310:TRP:HB3	1:C:314:GLY:HA3	1.99	0.44
1:D:97:PRO:C	1:D:99:THR:H	2.21	0.44
1:A:19:ILE:HA	1:A:22:MET:CE	2.47	0.44
1:A:330:LYS:HG2	1:A:334:LEU:HD22	1.99	0.44
1:B:115:SER:HA	1:B:270:ARG:O	2.18	0.44
1:C:197:VAL:HA	1:C:198:PRO:HD3	1.79	0.44
1:A:358:ILE:HG13	1:A:358:ILE:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:MET:HG3	1:B:23:THR:HG23	1.98	0.44
1:B:42:ASN:HD21	1:B:44:ASN:HB2	1.83	0.44
1:B:146:LEU:HA	1:B:146:LEU:HD23	1.66	0.44
1:D:204:THR:HG1	2:D:428:GOL:H32	1.81	0.44
1:D:305:GLN:NE2	3:D:596:HOH:O	2.46	0.44
1:A:63:PHE:CD2	1:A:68:MET:HE1	2.53	0.44
1:A:381:MET:HE2	1:A:398:LEU:CD1	2.47	0.44
1:B:42:ASN:HD22	1:B:44:ASN:N	2.16	0.44
1:C:257:ARG:CD	1:C:259:ASP:OD2	2.56	0.44
1:D:139:GLU:OE1	1:D:389:VAL:HG23	2.17	0.44
1:A:166:ILE:HD12	1:A:167:VAL:N	2.33	0.44
1:A:240:LYS:HE2	1:A:323:ILE:CG2	2.47	0.44
1:B:243:VAL:HA	1:B:244:PRO:HD2	1.47	0.44
1:C:42:ASN:OD1	1:C:44:ASN:HB2	2.17	0.44
1:C:45:MET:HE3	1:C:45:MET:HA	2.00	0.44
1:C:288:ILE:HD11	1:C:293:LEU:C	2.37	0.44
1:D:201:ASN:CB	2:D:428:GOL:H2	2.48	0.44
1:C:43:PRO:HA	1:C:46:PHE:CD2	2.53	0.44
1:A:311:GLY:C	1:A:313:GLU:N	2.71	0.44
1:B:345:ALA:HA	1:B:359:LYS:O	2.18	0.44
1:A:21:THR:HA	1:A:24:ASP:CG	2.38	0.43
1:A:63:PHE:CZ	1:A:301:LEU:HB3	2.53	0.43
1:D:80:ILE:CD1	1:D:301:LEU:HD13	2.48	0.43
1:A:285:ILE:O	1:A:289:GLN:HG3	2.19	0.43
1:B:237:GLN:NE2	1:B:243:VAL:HG12	2.33	0.43
1:B:366:VAL:HG11	1:B:397:TYR:O	2.18	0.43
1:D:95:HIS:CE1	1:D:245:THR:HG21	2.52	0.43
1:D:134:ASN:ND2	1:D:178:TRP:HH2	2.16	0.43
1:D:365:ASP:HB2	1:D:394:PRO:CB	2.49	0.43
1:B:288:ILE:HA	1:B:291:SER:HB2	1.99	0.43
1:C:50:THR:O	1:D:53:ILE:HA	2.19	0.43
1:D:67:MET:HB2	2:D:427:GOL:O1	2.17	0.43
1:D:285:ILE:O	1:D:289:GLN:HG3	2.17	0.43
1:B:167:VAL:HA	1:B:168:PRO:HD3	1.87	0.43
1:C:90:LEU:HG	1:C:94:LEU:HD22	2.00	0.43
1:C:94:LEU:HD12	1:C:94:LEU:HA	1.78	0.43
1:C:133:ASP:CG	1:C:192:LYS:HD2	2.37	0.43
1:B:121:LEU:HD12	1:B:228:ILE:CD1	2.37	0.43
1:B:172:ARG:HG3	1:B:172:ARG:HH11	1.82	0.43
1:C:59:LYS:HD3	1:C:309:GLU:HG2	2.00	0.43
1:D:64:GLY:HA3	2:D:427:GOL:H2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:ILE:CG2	1:B:380:LEU:HD11	2.49	0.43
1:B:195:TYR:CD2	1:B:195:TYR:C	2.92	0.43
1:C:206:ASN:ND2	3:C:555:HOH:O	2.31	0.43
1:D:177:ARG:HD2	1:D:178:TRP:CE2	2.53	0.43
1:B:108:GLN:O	1:B:109:MET:C	2.56	0.43
1:B:134:ASN:HB3	1:B:157:ILE:HD11	2.00	0.43
1:B:155:ASN:CB	3:B:583:HOH:O	2.43	0.43
1:C:99:THR:HG23	1:C:109:MET:H	1.83	0.43
1:C:133:ASP:CB	1:C:192:LYS:HE3	2.48	0.43
1:D:301:LEU:HD12	1:D:301:LEU:HA	1.82	0.43
1:A:6:PHE:CZ	1:A:226:LEU:HD13	2.53	0.42
1:A:163:GLU:HG3	1:A:348:HIS:NE2	2.33	0.42
1:A:390:ASP:C	1:A:390:ASP:OD2	2.58	0.42
1:B:240:LYS:HZ1	1:B:320:ASP:HB3	1.83	0.42
1:C:179:LYS:O	1:C:182:ASP:HB2	2.18	0.42
1:A:299:ASN:ND2	1:B:299:ASN:HD21	2.12	0.42
1:A:311:GLY:C	1:A:313:GLU:H	2.23	0.42
1:A:354:MET:HE2	1:A:354:MET:HB3	1.90	0.42
1:B:217:TYR:CB	1:B:249:MET:HE3	2.50	0.42
1:C:56:GLU:HB2	1:D:49:LYS:HE3	2.01	0.42
1:A:278:LYS:CD	3:A:552:HOH:O	2.65	0.42
1:A:373:LYS:NZ	3:A:516:HOH:O	2.53	0.42
1:B:140:PRO:HB2	1:B:203:PRO:CG	2.49	0.42
1:D:49:LYS:C	1:D:68:MET:HG2	2.39	0.42
1:C:48:PHE:HB2	1:C:72:LEU:HD11	2.00	0.42
1:C:97:PRO:C	1:C:99:THR:H	2.22	0.42
1:A:366:VAL:HG22	1:A:370:ILE:HG12	2.01	0.42
1:B:240:LYS:NZ	1:B:320:ASP:HB3	2.34	0.42
1:D:17:SER:HA	1:D:18:PRO:HD3	1.79	0.42
1:D:134:ASN:O	1:D:191:PRO:HA	2.20	0.42
1:D:368:GLU:HA	3:D:592:HOH:O	2.20	0.42
1:A:197:VAL:N	3:A:568:HOH:O	2.52	0.42
1:B:117:SER:HB2	1:B:258:ALA:HB1	2.01	0.42
1:B:120:GLY:O	1:B:124:VAL:HG23	2.19	0.42
1:C:46:PHE:HA	1:C:47:PRO:HD3	1.94	0.42
1:D:20:ARG:O	1:D:22:MET:N	2.51	0.42
1:B:172:ARG:CG	1:B:219:LEU:HD11	2.49	0.42
1:C:69:LYS:HE2	3:C:560:HOH:O	2.20	0.42
1:C:186:PRO:C	1:C:187:GLN:HG2	2.39	0.42
1:C:315:PHE:O	1:C:319:VAL:HG13	2.19	0.42
1:A:59:LYS:HG2	1:A:309:GLU:HG2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:ILE:CD1	1:B:101:HIS:CE1	3.02	0.42
1:A:396:PRO:HG3	3:A:497:HOH:O	2.20	0.42
1:B:99:THR:O	1:B:108:GLN:HA	2.20	0.42
1:B:178:TRP:CE2	1:B:191:PRO:HD3	2.54	0.42
1:B:229:GLU:OE2	3:B:500:HOH:O	2.22	0.42
1:D:162:ASP:CG	1:D:212:ARG:HH22	2.24	0.42
1:D:354:MET:HE3	1:D:354:MET:HB3	1.44	0.42
1:A:185:ASN:HA	1:A:186:PRO:HD3	1.89	0.42
1:B:349:VAL:HA	1:B:350:PRO:HD3	1.83	0.42
1:B:359:LYS:NZ	3:B:490:HOH:O	2.52	0.42
1:C:99:THR:CG2	1:C:109:MET:H	2.33	0.42
1:D:375:VAL:CG2	1:D:376:LYS:N	2.82	0.42
1:A:41:PRO:HA	1:B:354:MET:CE	2.49	0.41
1:B:172:ARG:HH11	1:B:172:ARG:CG	2.33	0.41
1:D:161:SER:HA	1:D:165:GLY:O	2.19	0.41
1:D:367:LYS:HB3	1:D:367:LYS:HE3	1.89	0.41
1:D:370:ILE:HG21	1:D:381:MET:O	2.20	0.41
1:A:288:ILE:HG13	1:A:289:GLN:N	2.34	0.41
1:B:243:VAL:CG1	3:B:581:HOH:O	2.56	0.41
1:C:140:PRO:HB2	1:C:203:PRO:CG	2.47	0.41
1:A:148:SER:O	1:A:152:LEU:HD13	2.20	0.41
1:B:71:ALA:HB2	1:B:301:LEU:HD23	2.02	0.41
1:B:190:THR:O	1:B:191:PRO:C	2.55	0.41
1:C:381:MET:CE	1:C:400:ALA:HB2	2.51	0.41
2:C:430:GOL:H32	1:D:56:GLU:CD	2.40	0.41
1:D:217:TYR:HB3	1:D:249:MET:HE1	2.01	0.41
1:C:50:THR:OG1	1:D:54:THR:OG1	2.19	0.41
1:C:200:GLY:O	1:C:201:ASN:C	2.57	0.41
1:C:341:LEU:HD11	1:C:414:PHE:HE2	1.86	0.41
1:B:162:ASP:C	1:B:162:ASP:OD1	2.59	0.41
1:B:179:LYS:HG2	1:B:180:PRO:HD2	2.02	0.41
1:B:384:GLY:N	1:B:397:TYR:O	2.49	0.41
1:C:57:ASN:HD22	1:C:321:ARG:NH1	2.18	0.41
1:D:222:LYS:HG2	1:D:223:TYR:CE2	2.56	0.41
1:A:220:ALA:HB1	1:A:227:ILE:HD11	2.00	0.41
1:B:20:ARG:O	1:B:22:MET:HG2	2.21	0.41
1:C:314:GLY:CA	3:C:562:HOH:O	2.68	0.41
1:A:366:VAL:HG11	1:A:398:LEU:CD2	2.51	0.41
1:B:204:THR:HA	1:B:357:TRP:CG	2.56	0.41
1:B:294:HIS:HD2	1:B:295:PRO:O	2.03	0.41
1:C:288:ILE:CD1	1:C:293:LEU:C	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:325:PHE:C	1:C:325:PHE:CD2	2.93	0.41
1:D:288:ILE:HD11	1:D:293:LEU:O	2.20	0.41
1:C:7:ILE:HD13	1:C:7:ILE:HG21	1.91	0.41
1:C:45:MET:CE	1:C:45:MET:HA	2.51	0.41
1:C:209:THR:O	1:C:210:SER:C	2.59	0.41
1:C:283:ARG:HD2	3:C:486:HOH:O	2.21	0.41
1:C:403:SER:O	1:D:42:ASN:HB2	2.20	0.41
1:B:6:PHE:CD2	1:B:226:LEU:HD22	2.56	0.41
1:B:74:TYR:HD1	1:B:294:HIS:HE1	1.69	0.41
1:B:141:ALA:HB3	1:B:146:LEU:HD11	2.03	0.41
1:B:265:ILE:O	1:B:266:SER:HB2	2.20	0.41
1:C:19:ILE:HG22	1:C:22:MET:SD	2.60	0.41
1:C:65:GLU:HB3	3:C:557:HOH:O	2.20	0.41
1:C:80:ILE:HD13	1:C:80:ILE:HG21	1.82	0.41
1:C:97:PRO:C	1:C:99:THR:N	2.74	0.41
1:C:114:THR:HG21	1:C:120:GLY:CA	2.49	0.41
1:C:204:THR:HA	1:C:357:TRP:CB	2.51	0.41
1:C:404:SER:O	2:C:428:GOL:C2	2.65	0.41
1:D:63:PHE:N	1:D:63:PHE:CD1	2.86	0.41
1:B:204:THR:HA	1:B:357:TRP:CB	2.51	0.41
1:D:20:ARG:HD2	1:D:21:THR:H	1.85	0.41
1:D:142:TYR:HD2	1:D:145:THR:HG22	1.84	0.41
1:D:166:ILE:HG13	1:D:216:ILE:HD11	2.02	0.41
1:D:330:LYS:O	1:D:331:ASP:C	2.59	0.41
2:D:429:GOL:C3	3:D:480:HOH:O	2.41	0.41
1:C:157:ILE:HG21	1:C:174:ILE:HG21	2.02	0.40
1:C:293:LEU:HD21	1:D:118:GLN:HG2	2.03	0.40
1:D:200:GLY:O	1:D:201:ASN:C	2.59	0.40
1:D:311:GLY:C	1:D:313:GLU:H	2.24	0.40
1:A:49:LYS:HE3	1:B:56:GLU:OE1	2.20	0.40
1:B:164:SER:HB3	1:B:209:THR:HG23	2.03	0.40
1:D:246:PHE:HA	1:D:249:MET:HG3	2.02	0.40
1:B:28:ARG:HB3	1:B:28:ARG:NH1	2.19	0.40
1:B:103:PRO:HD2	1:B:106:GLN:NE2	2.35	0.40
1:C:257:ARG:O	1:C:274:LEU:HA	2.22	0.40
1:B:22:MET:HG2	1:B:22:MET:H	1.67	0.40
1:C:204:THR:HG22	1:C:357:TRP:CD1	2.57	0.40
1:C:212:ARG:O	1:C:216:ILE:HG12	2.21	0.40
1:C:281:ILE:O	1:C:285:ILE:HG23	2.22	0.40
1:C:369:LEU:O	1:C:374:ALA:N	2.48	0.40
1:D:65:GLU:N	2:D:427:GOL:H2	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:77:SER:HA	1:D:294:HIS:HB3	2.04	0.40
1:D:83:LEU:HG	1:D:304:SER:HB2	2.04	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	422/425 (99%)	381 (90%)	33 (8%)	8 (2%)	8	7
1	B	422/425 (99%)	391 (93%)	26 (6%)	5 (1%)	13	14
1	C	422/425 (99%)	393 (93%)	24 (6%)	5 (1%)	13	14
1	D	422/425 (99%)	381 (90%)	33 (8%)	8 (2%)	8	7
All	All	1688/1700 (99%)	1546 (92%)	116 (7%)	26 (2%)	10	10

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	SER
1	A	28	ARG
1	B	203	PRO
1	C	203	PRO
1	D	19	ILE
1	A	21	THR
1	B	331	ASP
1	D	21	THR
1	D	25	ILE
1	D	293	LEU
1	B	57	ASN
1	C	186	PRO
1	C	189	ASN

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Mol	Chain	Res	Type
1	D	18	PRO
1	A	20	ARG
1	A	67	MET
1	A	98	PRO
1	B	21	THR
1	B	202	ASN
1	C	31	LYS
1	D	17	SER
1	D	74	TYR
1	D	266	SER
1	A	19	ILE
1	C	202	ASN
1	A	311	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	369/369 (100%)	312 (85%)	57 (15%)	2 2
1	B	369/369 (100%)	315 (85%)	54 (15%)	3 3
1	C	369/369 (100%)	315 (85%)	54 (15%)	3 3
1	D	369/369 (100%)	300 (81%)	69 (19%)	1 1
All	All	1476/1476 (100%)	1242 (84%)	234 (16%)	2 2

All (234) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	THR
1	A	20	ARG
1	A	24	ASP
1	A	25	ILE
1	A	28	ARG
1	A	34	ILE
1	A	59	LYS
1	A	60	THR

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Mol	Chain	Res	Type
1	A	67	MET
1	A	77	SER
1	A	86	TRP
1	A	87	LEU
1	A	94	LEU
1	A	96	ASN
1	A	99	THR
1	A	123	LYS
1	A	137	LEU
1	A	148	SER
1	A	166	ILE
1	A	178	TRP
1	A	179	LYS
1	A	188	LYS
1	A	218	GLU
1	A	219	LEU
1	A	221	ARG
1	A	226	LEU
1	A	228	ILE
1	A	243	VAL
1	A	267	SER
1	A	283	ARG
1	A	284	VAL
1	A	285	ILE
1	A	288	ILE
1	A	291	SER
1	A	296	SER
1	A	297	THR
1	A	301	LEU
1	A	307	LEU
1	A	312	GLU
1	A	313	GLU
1	A	316	MET
1	A	322	VAL
1	A	327	SER
1	A	328	ASN
1	A	334	LEU
1	A	341	LEU
1	A	344	LEU
1	A	349	VAL
1	A	358	ILE
1	A	368	GLU

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Mol	Chain	Res	Type
1	A	372	GLU
1	A	379	VAL
1	A	380	LEU
1	A	381	MET
1	A	395	SER
1	A	417	LEU
1	A	419	GLN
1	B	6	PHE
1	B	8	THR
1	B	19	ILE
1	B	20	ARG
1	B	24	ASP
1	B	28	ARG
1	B	33	MET
1	B	34	ILE
1	B	42	ASN
1	B	59	LYS
1	B	60	THR
1	B	65	GLU
1	B	77	SER
1	B	83	LEU
1	B	84	LEU
1	B	87	LEU
1	B	96	ASN
1	B	99	THR
1	B	109	MET
1	B	137	LEU
1	B	145	THR
1	B	152	LEU
1	B	163	GLU
1	B	164	SER
1	B	166	ILE
1	B	172	ARG
1	B	182	ASP
1	B	184	LYS
1	B	188	LYS
1	B	189	ASN
1	B	192	LYS
1	B	219	LEU
1	B	226	LEU
1	B	228	ILE
1	B	278	LYS

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Mol	Chain	Res	Type
1	B	280	LEU
1	B	288	ILE
1	B	297	THR
1	B	301	LEU
1	B	307	LEU
1	B	322	VAL
1	B	334	LEU
1	B	341	LEU
1	B	342	THR
1	B	344	LEU
1	B	349	VAL
1	B	358	ILE
1	B	360	VAL
1	B	367	LYS
1	B	369	LEU
1	B	376	LYS
1	B	408	GLU
1	B	417	LEU
1	B	419	GLN
1	C	5	ARG
1	C	6	PHE
1	C	8	THR
1	C	19	ILE
1	C	20	ARG
1	C	28	ARG
1	C	31	LYS
1	C	34	ILE
1	C	60	THR
1	C	77	SER
1	C	85	SER
1	C	87	LEU
1	C	93	LYS
1	C	94	LEU
1	C	99	THR
1	C	112	CYS
1	C	115	SER
1	C	121	LEU
1	C	136	LEU
1	C	137	LEU
1	C	145	THR
1	C	166	ILE
1	C	177	ARG

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Mol	Chain	Res	Type
1	C	179	LYS
1	C	187	GLN
1	C	189	ASN
1	C	192	LYS
1	C	219	LEU
1	C	221	ARG
1	C	226	LEU
1	C	228	ILE
1	C	243	VAL
1	C	264	ILE
1	C	265	ILE
1	C	285	ILE
1	C	288	ILE
1	C	297	THR
1	C	301	LEU
1	C	307	LEU
1	C	324	ASP
1	C	330	LYS
1	C	334	LEU
1	C	344	LEU
1	C	358	ILE
1	C	366	VAL
1	C	368	GLU
1	C	369	LEU
1	C	375	VAL
1	C	376	LYS
1	C	379	VAL
1	C	381	MET
1	C	392	SER
1	C	415	GLN
1	C	417	LEU
1	D	8	THR
1	D	21	THR
1	D	25	ILE
1	D	26	LEU
1	D	28	ARG
1	D	31	LYS
1	D	34	ILE
1	D	40	LEU
1	D	42	ASN
1	D	43	PRO
1	D	59	LYS

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Mol	Chain	Res	Type
1	D	60	THR
1	D	77	SER
1	D	83	LEU
1	D	84	LEU
1	D	87	LEU
1	D	89	GLN
1	D	93	LYS
1	D	96	ASN
1	D	99	THR
1	D	112	CYS
1	D	121	LEU
1	D	137	LEU
1	D	145	THR
1	D	155	ASN
1	D	163	GLU
1	D	166	ILE
1	D	174	ILE
1	D	177	ARG
1	D	178	TRP
1	D	179	LYS
1	D	184	LYS
1	D	185	ASN
1	D	187	GLN
1	D	218	GLU
1	D	219	LEU
1	D	221	ARG
1	D	226	LEU
1	D	228	ILE
1	D	243	VAL
1	D	249	MET
1	D	264	ILE
1	D	278	LYS
1	D	280	LEU
1	D	284	VAL
1	D	285	ILE
1	D	288	ILE
1	D	297	THR
1	D	301	LEU
1	D	306	LEU
1	D	307	LEU
1	D	327	SER
1	D	330	LYS

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Mol	Chain	Res	Type
1	D	334	LEU
1	D	341	LEU
1	D	349	VAL
1	D	354	MET
1	D	358	ILE
1	D	360	VAL
1	D	366	VAL
1	D	371	GLU
1	D	377	MET
1	D	379	VAL
1	D	381	MET
1	D	385	ASN
1	D	404	SER
1	D	415	GLN
1	D	417	LEU
1	D	423	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	A	95	HIS
1	A	96	ASN
1	A	101	HIS
1	A	108	GLN
1	A	187	GLN
1	A	201	ASN
1	A	206	ASN
1	A	237	GLN
1	A	294	HIS
1	A	299	ASN
1	A	305	GLN
1	A	318	HIS
1	A	328	ASN
1	A	419	GLN
1	B	2	ASN
1	B	42	ASN
1	B	89	GLN
1	B	96	ASN
1	B	101	HIS
1	B	106	GLN
1	B	108	GLN

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Mol	Chain	Res	Type
1	B	118	GLN
1	B	134	ASN
1	B	185	ASN
1	B	189	ASN
1	B	201	ASN
1	B	237	GLN
1	B	294	HIS
1	B	305	GLN
1	B	419	GLN
1	C	57	ASN
1	C	91	GLN
1	C	95	HIS
1	C	96	ASN
1	C	108	GLN
1	C	118	GLN
1	C	150	HIS
1	C	201	ASN
1	C	294	HIS
1	C	299	ASN
1	C	305	GLN
1	C	318	HIS
1	D	2	ASN
1	D	42	ASN
1	D	57	ASN
1	D	89	GLN
1	D	106	GLN
1	D	108	GLN
1	D	150	HIS
1	D	185	ASN
1	D	201	ASN
1	D	237	GLN
1	D	294	HIS
1	D	305	GLN
1	D	308	HIS
1	D	328	ASN
1	D	385	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	LLP	A	263	1	23,24,25	1.68	5 (21%)	25,32,34	1.86	7 (28%)
1	LLP	C	263	1	23,24,25	2.02	7 (30%)	25,32,34	1.97	7 (28%)
1	LLP	B	263	1	23,24,25	2.33	8 (34%)	25,32,34	1.76	10 (40%)
1	LLP	D	263	1	23,24,25	1.84	5 (21%)	25,32,34	2.05	9 (36%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LLP	A	263	1	-	3/16/17/19	0/1/1/1
1	LLP	C	263	1	-	5/16/17/19	0/1/1/1
1	LLP	B	263	1	-	5/16/17/19	0/1/1/1
1	LLP	D	263	1	-	5/16/17/19	0/1/1/1

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	263	LLP	O3-C3	-6.19	1.22	1.37
1	B	263	LLP	CE-NZ	5.42	1.58	1.46
1	B	263	LLP	C4-C4'	4.85	1.55	1.46
1	D	263	LLP	O3-C3	-4.69	1.26	1.37
1	A	263	LLP	O3-C3	-4.69	1.26	1.37
1	B	263	LLP	O3-C3	-4.22	1.27	1.37
1	D	263	LLP	CE-NZ	3.85	1.55	1.46
1	B	263	LLP	C3-C2	-3.51	1.37	1.40
1	C	263	LLP	C2-N1	3.43	1.40	1.33
1	D	263	LLP	C2-N1	3.16	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	263	LLP	C4'-NZ	2.93	1.37	1.27
1	B	263	LLP	C4-C5	-2.84	1.38	1.42
1	A	263	LLP	C6-N1	2.83	1.40	1.34
1	A	263	LLP	C2-N1	2.79	1.39	1.33
1	D	263	LLP	C4-C4'	2.74	1.51	1.46
1	D	263	LLP	C6-C5	2.53	1.43	1.37
1	C	263	LLP	P-OP3	-2.51	1.45	1.54
1	C	263	LLP	CB-CA	2.41	1.56	1.53
1	C	263	LLP	C6-N1	2.39	1.39	1.34
1	C	263	LLP	CE-NZ	2.33	1.51	1.46
1	A	263	LLP	C4-C4'	2.32	1.51	1.46
1	B	263	LLP	C6-N1	2.32	1.39	1.34
1	A	263	LLP	CE-NZ	2.14	1.51	1.46
1	C	263	LLP	CD-CE	2.05	1.58	1.51
1	B	263	LLP	CB-CA	2.04	1.56	1.53

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	263	LLP	CE-NZ-C4'	-4.74	104.33	118.90
1	C	263	LLP	OP2-P-OP4	-4.48	94.80	106.73
1	D	263	LLP	CD-CE-NZ	4.41	121.74	110.93
1	D	263	LLP	C5'-C5-C6	-4.30	112.29	119.37
1	D	263	LLP	C4-C4'-NZ	-4.10	105.48	124.31
1	A	263	LLP	C3-C4-C5	4.05	121.37	118.26
1	A	263	LLP	CE-NZ-C4'	-3.62	107.79	118.90
1	C	263	LLP	C3-C4-C5	3.56	120.99	118.26
1	B	263	LLP	C5'-C5-C6	-3.36	113.84	119.37
1	A	263	LLP	C4-C4'-NZ	-3.31	109.10	124.31
1	D	263	LLP	OP2-P-OP4	-3.25	98.08	106.73
1	A	263	LLP	OP4-P-OP1	-3.21	97.48	106.47
1	D	263	LLP	C5-C6-N1	-2.95	118.90	123.82
1	B	263	LLP	OP2-P-OP4	-2.78	99.32	106.73
1	C	263	LLP	C5-C6-N1	-2.71	119.30	123.82
1	C	263	LLP	C5-C4-C4'	-2.64	117.21	121.56
1	C	263	LLP	C2'-C2-N1	2.57	122.69	117.67
1	B	263	LLP	OP3-P-OP2	2.51	117.24	107.64
1	B	263	LLP	O3-C3-C2	-2.46	112.13	117.49
1	A	263	LLP	C5-C6-N1	-2.45	119.74	123.82
1	B	263	LLP	C4-C3-C2	2.44	121.70	120.19
1	B	263	LLP	O3-C3-C4	2.44	126.14	119.60
1	D	263	LLP	OP3-P-OP2	2.41	116.86	107.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	263	LLP	C4-C3-C2	-2.35	118.73	120.19
1	D	263	LLP	OP3-P-OP4	-2.34	100.50	106.73
1	B	263	LLP	C5-C6-N1	-2.21	120.14	123.82
1	C	263	LLP	C2'-C2-C3	-2.20	118.17	120.89
1	B	263	LLP	OP4-P-OP1	2.16	112.54	106.47
1	B	263	LLP	CD-CE-NZ	2.14	116.18	110.93
1	A	263	LLP	OP2-P-OP4	-2.12	101.09	106.73
1	D	263	LLP	OP4-C5'-C5	2.09	113.34	109.35
1	D	263	LLP	C6-C5-C4	2.07	121.96	118.15
1	B	263	LLP	C4-C4'-NZ	-2.07	114.83	124.31

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	263	LLP	N-CA-CB-CG
1	B	263	LLP	C-CA-CB-CG
1	C	263	LLP	C5-C4-C4'-NZ
1	C	263	LLP	CG-CD-CE-NZ
1	C	263	LLP	C4-C4'-NZ-CE
1	B	263	LLP	CA-CB-CG-CD
1	D	263	LLP	CE-CD-CG-CB
1	C	263	LLP	C3-C4-C4'-NZ
1	B	263	LLP	CE-CD-CG-CB
1	B	263	LLP	CG-CD-CE-NZ
1	A	263	LLP	CD-CE-NZ-C4'
1	D	263	LLP	N-CA-CB-CG
1	D	263	LLP	C5-C4-C4'-NZ
1	C	263	LLP	CE-CD-CG-CB
1	A	263	LLP	C3-C4-C4'-NZ
1	D	263	LLP	CG-CD-CE-NZ
1	D	263	LLP	C3-C4-C4'-NZ
1	A	263	LLP	C4-C4'-NZ-CE

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	263	LLP	4	0
1	C	263	LLP	2	0
1	B	263	LLP	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	263	LLP	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	GOL	D	426	-	5,5,5	0.72	0	5,5,5	0.99	0
2	GOL	A	427	-	5,5,5	0.38	0	5,5,5	0.58	0
2	GOL	C	426	-	5,5,5	0.51	0	5,5,5	0.65	0
2	GOL	C	427	-	5,5,5	0.56	0	5,5,5	1.08	0
2	GOL	A	426	-	5,5,5	0.31	0	5,5,5	0.91	0
2	GOL	D	428	-	5,5,5	0.91	0	5,5,5	1.64	1 (20%)
2	GOL	C	430	-	5,5,5	0.61	0	5,5,5	0.81	0
2	GOL	D	429	-	5,5,5	1.11	0	5,5,5	2.19	3 (60%)
2	GOL	D	427	-	5,5,5	0.39	0	5,5,5	0.53	0
2	GOL	C	428	-	5,5,5	0.54	0	5,5,5	1.26	0
2	GOL	C	429	-	5,5,5	0.51	0	5,5,5	0.53	0
2	GOL	B	426	-	5,5,5	0.52	0	5,5,5	1.02	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	D	426	-	-	4/4/4/4	-
2	GOL	A	427	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	C	426	-	-	2/4/4/4	-
2	GOL	C	427	-	-	2/4/4/4	-
2	GOL	A	426	-	-	2/4/4/4	-
2	GOL	D	428	-	-	3/4/4/4	-
2	GOL	C	430	-	-	4/4/4/4	-
2	GOL	D	429	-	-	4/4/4/4	-
2	GOL	D	427	-	-	1/4/4/4	-
2	GOL	C	428	-	-	4/4/4/4	-
2	GOL	C	429	-	-	2/4/4/4	-
2	GOL	B	426	-	-	3/4/4/4	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	429	GOL	O1-C1-C2	3.31	126.09	110.20
2	D	429	GOL	O2-C2-C3	-2.81	96.75	109.12
2	D	428	GOL	O3-C3-C2	2.45	121.97	110.20
2	D	429	GOL	O3-C3-C2	2.27	121.10	110.20

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	426	GOL	O2-C2-C3-O3
2	C	426	GOL	C1-C2-C3-O3
2	C	426	GOL	O2-C2-C3-O3
2	C	427	GOL	C1-C2-C3-O3
2	C	428	GOL	O1-C1-C2-C3
2	C	428	GOL	C1-C2-C3-O3
2	C	429	GOL	C1-C2-C3-O3
2	C	430	GOL	O1-C1-C2-O2
2	C	430	GOL	C1-C2-C3-O3
2	D	426	GOL	O1-C1-C2-C3
2	D	428	GOL	O1-C1-C2-C3
2	D	429	GOL	O1-C1-C2-C3
2	D	426	GOL	O1-C1-C2-O2
2	A	426	GOL	C1-C2-C3-O3
2	A	427	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
2	A	427	GOL	C1-C2-C3-O3
2	B	426	GOL	C1-C2-C3-O3
2	C	430	GOL	O1-C1-C2-C3
2	D	426	GOL	C1-C2-C3-O3
2	D	428	GOL	C1-C2-C3-O3
2	C	427	GOL	O2-C2-C3-O3
2	C	428	GOL	O2-C2-C3-O3
2	D	426	GOL	O2-C2-C3-O3
2	D	428	GOL	O1-C1-C2-O2
2	A	427	GOL	O1-C1-C2-O2
2	A	427	GOL	O2-C2-C3-O3
2	C	428	GOL	O1-C1-C2-O2
2	C	429	GOL	O2-C2-C3-O3
2	C	430	GOL	O2-C2-C3-O3
2	A	426	GOL	O2-C2-C3-O3
2	D	429	GOL	O1-C1-C2-O2
2	B	426	GOL	O1-C1-C2-C3
2	D	429	GOL	C1-C2-C3-O3
2	D	427	GOL	O1-C1-C2-O2
2	D	429	GOL	O2-C2-C3-O3

There are no ring outliers.

7 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	427	GOL	2	0
2	A	426	GOL	1	0
2	D	428	GOL	9	0
2	C	430	GOL	2	0
2	D	429	GOL	11	0
2	D	427	GOL	4	0
2	C	428	GOL	2	0

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	424/425 (99%)	0.20	18 (4%)	36	43	24, 36, 54, 78	0
1	B	424/425 (99%)	0.19	18 (4%)	36	43	23, 34, 51, 92	0
1	C	424/425 (99%)	0.22	21 (4%)	28	35	23, 35, 52, 77	0
1	D	424/425 (99%)	0.18	14 (3%)	46	53	23, 35, 52, 84	0
All	All	1696/1700 (99%)	0.20	71 (4%)	36	43	23, 35, 53, 92	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	27	SER	10.0
1	C	29	GLY	9.4
1	B	28	ARG	8.0
1	B	26	LEU	6.9
1	C	27	SER	6.7
1	D	28	ARG	6.6
1	B	24	ASP	6.0
1	A	27	SER	5.8
1	D	19	ILE	5.7
1	D	18	PRO	5.5
1	B	25	ILE	5.2
1	D	26	LEU	5.1
1	C	28	ARG	4.9
1	D	21	THR	4.9
1	A	28	ARG	4.8
1	A	18	PRO	4.8
1	A	57	ASN	4.7
1	D	27	SER	4.2
1	C	26	LEU	4.2
1	C	186	PRO	4.2
1	D	30	PRO	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	29	GLY	4.0
1	B	29	GLY	3.9
1	A	20	ARG	3.9
1	A	25	ILE	3.7
1	C	23	THR	3.7
1	C	21	THR	3.7
1	D	22	MET	3.5
1	A	380	LEU	3.5
1	D	24	ASP	3.4
1	A	19	ILE	3.4
1	C	241	PHE	3.3
1	B	20	ARG	3.3
1	A	371	GLU	3.1
1	C	375	VAL	3.1
1	B	107	GLY	3.1
1	B	22	MET	3.1
1	C	22	MET	3.0
1	D	29	GLY	2.9
1	C	25	ILE	2.9
1	C	19	ILE	2.8
1	D	17	SER	2.8
1	C	184	LYS	2.8
1	A	23	THR	2.8
1	A	21	THR	2.8
1	A	96	ASN	2.8
1	B	23	THR	2.8
1	C	239	ASN	2.6
1	C	34	ILE	2.6
1	A	24	ASP	2.5
1	C	24	ASP	2.5
1	B	21	THR	2.5
1	D	31	LYS	2.5
1	B	19	ILE	2.4
1	A	31	LYS	2.3
1	A	187	GLN	2.3
1	B	187	GLN	2.3
1	D	20	ARG	2.3
1	B	344	LEU	2.3
1	D	221	ARG	2.3
1	C	181	GLU	2.2
1	C	20	ARG	2.2
1	A	173	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	31	LYS	2.2
1	B	391	SER	2.2
1	B	34	ILE	2.1
1	B	218	GLU	2.1
1	C	391	SER	2.1
1	C	18	PRO	2.1
1	A	22	MET	2.0
1	B	106	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	LLP	D	263	24/25	0.95	0.17	23,32,35,35	0
1	LLP	B	263	24/25	0.96	0.18	23,30,33,34	0
1	LLP	A	263	24/25	0.96	0.14	23,33,36,36	0
1	LLP	C	263	24/25	0.97	0.15	27,30,34,37	0

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	GOL	C	428	6/6	0.55	0.34	54,56,58,60	0
2	GOL	C	430	6/6	0.61	0.21	48,53,56,57	0
2	GOL	C	429	6/6	0.64	0.48	63,66,68,69	0
2	GOL	D	427	6/6	0.68	0.44	55,56,59,62	0
2	GOL	C	426	6/6	0.69	0.32	59,64,65,65	0
2	GOL	D	428	6/6	0.73	0.39	46,51,52,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GOL	A	426	6/6	0.75	0.22	68,70,71,72	0
2	GOL	D	429	6/6	0.75	0.45	23,30,40,43	0
2	GOL	B	426	6/6	0.80	0.30	63,64,66,66	0
2	GOL	A	427	6/6	0.80	0.27	58,61,62,63	0
2	GOL	D	426	6/6	0.83	0.23	44,52,55,59	0
2	GOL	C	427	6/6	0.83	0.35	34,47,53,54	0

6.5 Other polymers (i)

There are no such residues in this entry.