Full wwPDB X-ray Structure Validation Report (i)

Aug 29, 2023 – 03:15 AM EDT

PDB ID	:	3MQ9
Title	:	Crystal Structure of Ectodomain Mutant of BST-2/Tetherin/CD317 Fused to MBP
Authors	:	Xiong, Y.; Yang, H.; Wang, J.; Meng, W.
Deposited on	:	2010-04-27
Resolution	:	2.80 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:

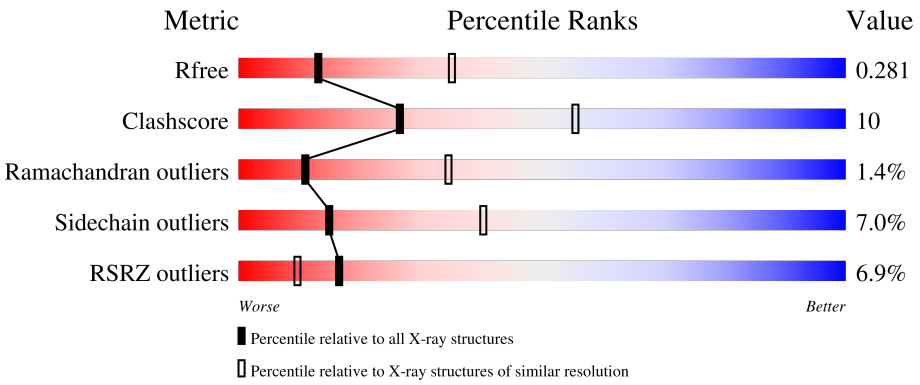
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	471	% 78% 17%
1	B	471	2% 77% 18%
1	C	471	4% 72% 21%
1	D	471	8% 73% 20%
1	E	471	4% 79% 15%

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Mol	Chain	Length	Quality of chain
1	F	471	4% 77% 17%
1	G	471	28% 77% 17%
1	H	471	% 71% 22%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 28225 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 Bone marrow stromal antigen 2 fused to Maltose-binding periplasmic protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	454	3520	2240	591	680	6	3	0	0	0
1	B	454	3520	2240	591	680	6	3	0	0	0
1	C	454	3520	2240	591	680	6	3	0	0	0
1	D	454	3520	2240	591	680	6	3	0	0	0
1	E	454	3520	2240	591	680	6	3	0	0	0
1	F	454	3520	2240	591	680	6	3	0	0	0
1	G	454	3520	2240	591	680	6	3	0	0	0
1	H	454	3520	2240	591	680	6	3	0	0	0

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	370	ALA	-	expression tag	UNP Q10589
A	371	ALA	-	expression tag	UNP Q10589
A	372	ARG	-	expression tag	UNP Q10589
A	373	ASP	-	expression tag	UNP Q10589
A	374	GLY	-	expression tag	UNP Q10589
A	375	LEU	-	expression tag	UNP Q10589
A	376	ARG	-	expression tag	UNP Q10589
A	377	ALA	-	expression tag	UNP Q10589
A	378	VAL	-	expression tag	UNP Q10589
A	379	MSE	-	expression tag	UNP Q10589
A	380	GLU	-	expression tag	UNP Q10589
A	381	ALA	-	expression tag	UNP Q10589

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Chain	Residue	Modelled	Actual	Comment	Reference
A	382	ARG	-	expression tag	UNP Q10589
A	383	ASN	-	expression tag	UNP Q10589
A	409	ALA	CYS	engineered mutation	UNP Q10589
B	370	ALA	-	expression tag	UNP Q10589
B	371	ALA	-	expression tag	UNP Q10589
B	372	ARG	-	expression tag	UNP Q10589
B	373	ASP	-	expression tag	UNP Q10589
B	374	GLY	-	expression tag	UNP Q10589
B	375	LEU	-	expression tag	UNP Q10589
B	376	ARG	-	expression tag	UNP Q10589
B	377	ALA	-	expression tag	UNP Q10589
B	378	VAL	-	expression tag	UNP Q10589
B	379	MSE	-	expression tag	UNP Q10589
B	380	GLU	-	expression tag	UNP Q10589
B	381	ALA	-	expression tag	UNP Q10589
B	382	ARG	-	expression tag	UNP Q10589
B	383	ASN	-	expression tag	UNP Q10589
B	409	ALA	CYS	engineered mutation	UNP Q10589
C	370	ALA	-	expression tag	UNP Q10589
C	371	ALA	-	expression tag	UNP Q10589
C	372	ARG	-	expression tag	UNP Q10589
C	373	ASP	-	expression tag	UNP Q10589
C	374	GLY	-	expression tag	UNP Q10589
C	375	LEU	-	expression tag	UNP Q10589
C	376	ARG	-	expression tag	UNP Q10589
C	377	ALA	-	expression tag	UNP Q10589
C	378	VAL	-	expression tag	UNP Q10589
C	379	MSE	-	expression tag	UNP Q10589
C	380	GLU	-	expression tag	UNP Q10589
C	381	ALA	-	expression tag	UNP Q10589
C	382	ARG	-	expression tag	UNP Q10589
C	383	ASN	-	expression tag	UNP Q10589
C	409	ALA	CYS	engineered mutation	UNP Q10589
D	370	ALA	-	expression tag	UNP Q10589
D	371	ALA	-	expression tag	UNP Q10589
D	372	ARG	-	expression tag	UNP Q10589
D	373	ASP	-	expression tag	UNP Q10589
D	374	GLY	-	expression tag	UNP Q10589
D	375	LEU	-	expression tag	UNP Q10589
D	376	ARG	-	expression tag	UNP Q10589
D	377	ALA	-	expression tag	UNP Q10589
D	378	VAL	-	expression tag	UNP Q10589

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Chain	Residue	Modelled	Actual	Comment	Reference
D	379	MSE	-	expression tag	UNP Q10589
D	380	GLU	-	expression tag	UNP Q10589
D	381	ALA	-	expression tag	UNP Q10589
D	382	ARG	-	expression tag	UNP Q10589
D	383	ASN	-	expression tag	UNP Q10589
D	409	ALA	CYS	engineered mutation	UNP Q10589
E	370	ALA	-	expression tag	UNP Q10589
E	371	ALA	-	expression tag	UNP Q10589
E	372	ARG	-	expression tag	UNP Q10589
E	373	ASP	-	expression tag	UNP Q10589
E	374	GLY	-	expression tag	UNP Q10589
E	375	LEU	-	expression tag	UNP Q10589
E	376	ARG	-	expression tag	UNP Q10589
E	377	ALA	-	expression tag	UNP Q10589
E	378	VAL	-	expression tag	UNP Q10589
E	379	MSE	-	expression tag	UNP Q10589
E	380	GLU	-	expression tag	UNP Q10589
E	381	ALA	-	expression tag	UNP Q10589
E	382	ARG	-	expression tag	UNP Q10589
E	383	ASN	-	expression tag	UNP Q10589
E	409	ALA	CYS	engineered mutation	UNP Q10589
F	370	ALA	-	expression tag	UNP Q10589
F	371	ALA	-	expression tag	UNP Q10589
F	372	ARG	-	expression tag	UNP Q10589
F	373	ASP	-	expression tag	UNP Q10589
F	374	GLY	-	expression tag	UNP Q10589
F	375	LEU	-	expression tag	UNP Q10589
F	376	ARG	-	expression tag	UNP Q10589
F	377	ALA	-	expression tag	UNP Q10589
F	378	VAL	-	expression tag	UNP Q10589
F	379	MSE	-	expression tag	UNP Q10589
F	380	GLU	-	expression tag	UNP Q10589
F	381	ALA	-	expression tag	UNP Q10589
F	382	ARG	-	expression tag	UNP Q10589
F	383	ASN	-	expression tag	UNP Q10589
F	409	ALA	CYS	engineered mutation	UNP Q10589
G	370	ALA	-	expression tag	UNP Q10589
G	371	ALA	-	expression tag	UNP Q10589
G	372	ARG	-	expression tag	UNP Q10589
G	373	ASP	-	expression tag	UNP Q10589
G	374	GLY	-	expression tag	UNP Q10589
G	375	LEU	-	expression tag	UNP Q10589

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Chain	Residue	Modelled	Actual	Comment	Reference
G	376	ARG	-	expression tag	UNP Q10589
G	377	ALA	-	expression tag	UNP Q10589
G	378	VAL	-	expression tag	UNP Q10589
G	379	MSE	-	expression tag	UNP Q10589
G	380	GLU	-	expression tag	UNP Q10589
G	381	ALA	-	expression tag	UNP Q10589
G	382	ARG	-	expression tag	UNP Q10589
G	383	ASN	-	expression tag	UNP Q10589
G	409	ALA	CYS	engineered mutation	UNP Q10589
H	370	ALA	-	expression tag	UNP Q10589
H	371	ALA	-	expression tag	UNP Q10589
H	372	ARG	-	expression tag	UNP Q10589
H	373	ASP	-	expression tag	UNP Q10589
H	374	GLY	-	expression tag	UNP Q10589
H	375	LEU	-	expression tag	UNP Q10589
H	376	ARG	-	expression tag	UNP Q10589
H	377	ALA	-	expression tag	UNP Q10589
H	378	VAL	-	expression tag	UNP Q10589
H	379	MSE	-	expression tag	UNP Q10589
H	380	GLU	-	expression tag	UNP Q10589
H	381	ALA	-	expression tag	UNP Q10589
H	382	ARG	-	expression tag	UNP Q10589
H	383	ASN	-	expression tag	UNP Q10589
H	409	ALA	CYS	engineered mutation	UNP Q10589

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	12	12	12	0	0
			Total	O		
2	B	19	19	19	0	0
			Total	O		
2	C	2	2	2	0	0
			Total	O		
2	D	6	6	6	0	0
			Total	O		
2	E	11	11	11	0	0
			Total	O		
2	F	5	5	5	0	0
			Total	O		
2	G	1	1	1	0	0

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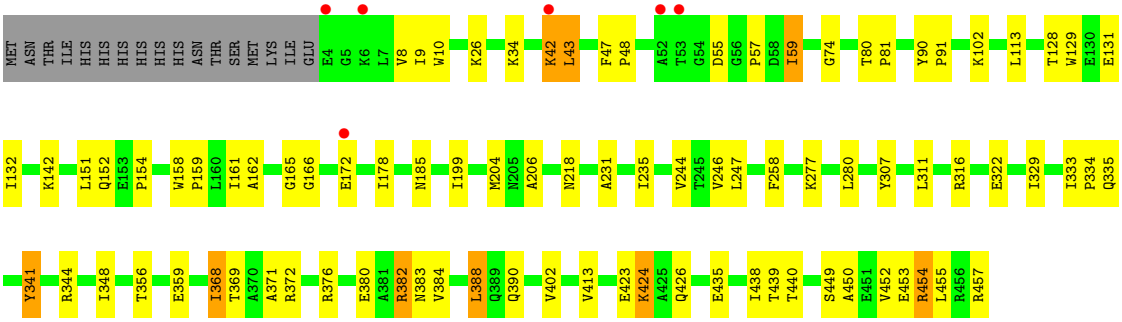
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	H	9	9	9	0	0

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.

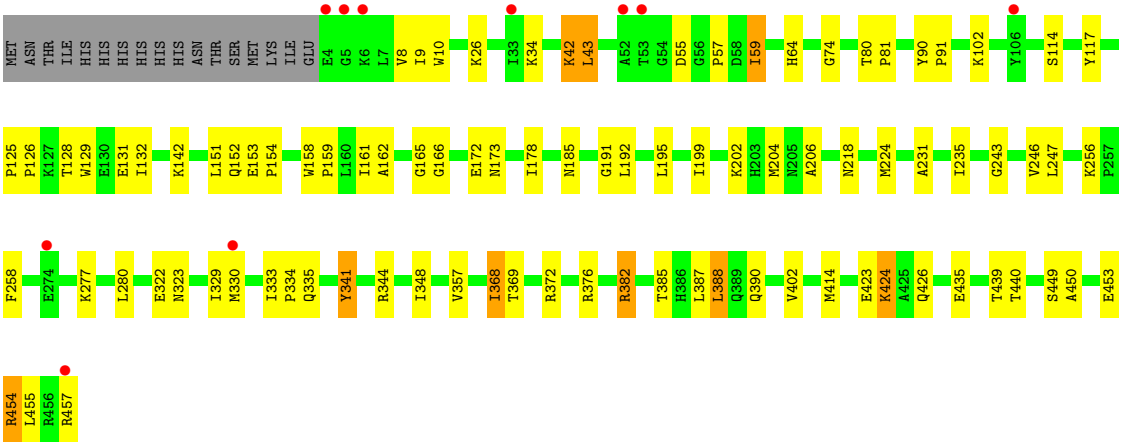
• Molecule 1: Bone marrow stromal antigen 2 fused to Maltose-binding periplasmic protein

Chain A:



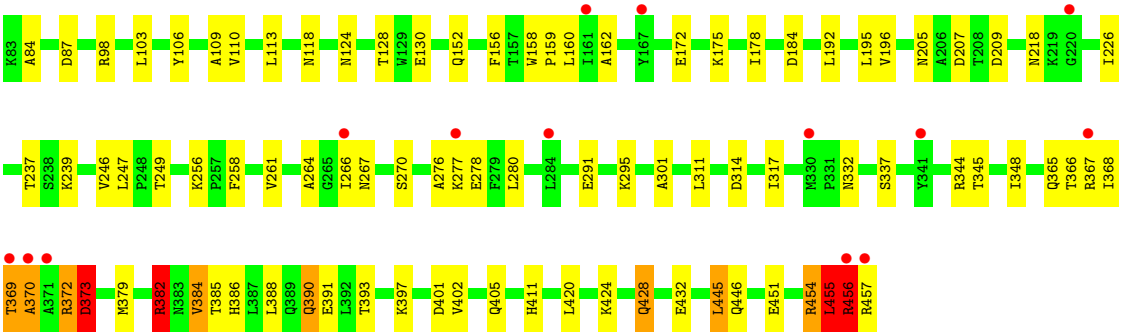
• Molecule 1: Bone marrow stromal antigen 2 fused to Maltose-binding periplasmic protein

Chain B:



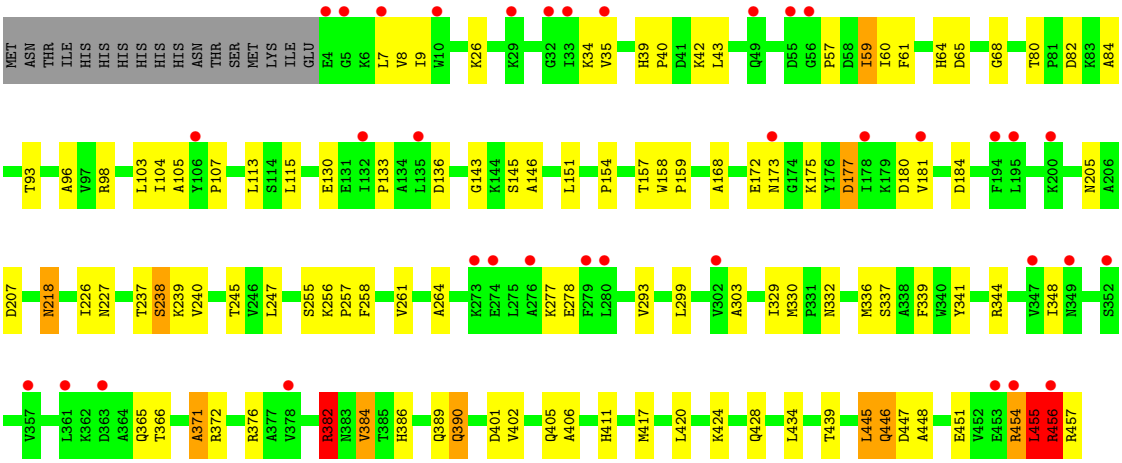
• Molecule 1: Bone marrow stromal antigen 2 fused to Maltose-binding periplasmic protein

Chain C:



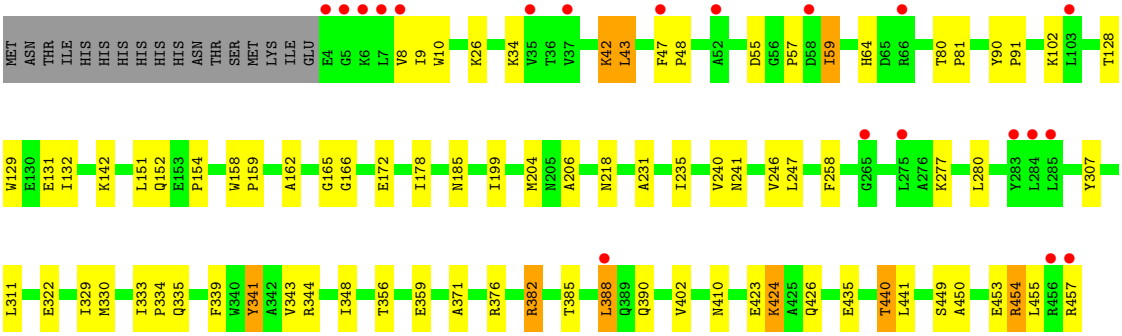
• Molecule 1: Bone marrow stromal antigen 2 fused to Maltose-binding periplasmic protein

Chain D:



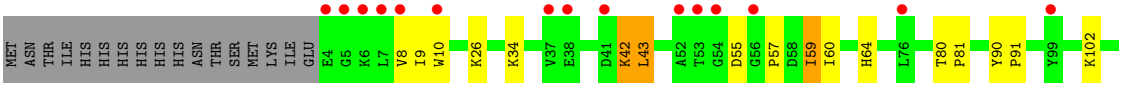
• Molecule 1: Bone marrow stromal antigen 2 fused to Maltose-binding periplasmic protein

Chain E:



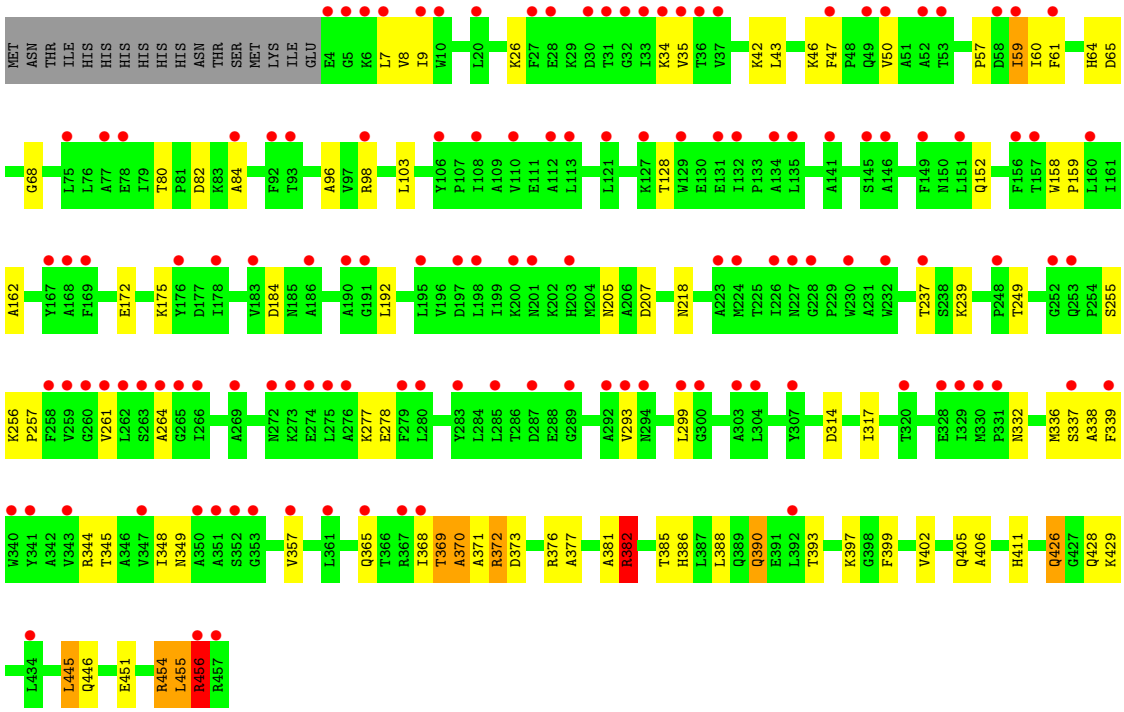
• Molecule 1: Bone marrow stromal antigen 2 fused to Maltose-binding periplasmic protein

Chain F:



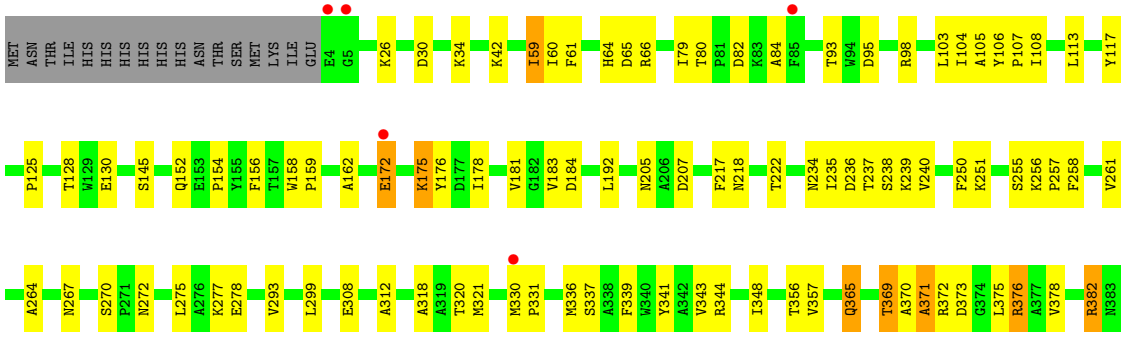
• Molecule 1: Bone marrow stromal antigen 2 fused to Maltose-binding periplasmic protein

Chain G:



• Molecule 1: Bone marrow stromal antigen 2 fused to Maltose-binding periplasmic protein

Chain H:



V384
T385
H386
L387
Q390
T393
K397
V402
E403
A404
A407
H411
A415
A418
K424
Q428
L445
Q446
E451
R454
L455
R456
R457

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	94.50Å 202.44Å 107.28Å 90.00° 90.41° 90.00°	Depositor
Resolution (Å)	42.47 – 2.80 42.47 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (42.47-2.80) 93.8 (42.47-2.80)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	1.70 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.231 , 0.279 0.230 , 0.281	Depositor DCC
R_{free} test set	4743 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	64.0	Xtriage
Anisotropy	0.380	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 31.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.066 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	28225	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% 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)

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	0.62	0/3590	0.65	0/4861
1	B	0.67	0/3590	0.70	0/4861
1	C	0.63	0/3590	0.69	1/4861 (0.0%)
1	D	0.55	0/3590	0.67	3/4861 (0.1%)
1	E	0.57	0/3590	0.63	0/4861
1	F	0.50	0/3590	0.63	0/4861
1	G	0.46	0/3590	0.58	1/4861 (0.0%)
1	H	0.61	0/3590	0.71	1/4861 (0.0%)
All	All	0.58	0/28720	0.66	6/38888 (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	C	0	1
1	H	0	1
All	All	0	2

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	236	ASP	CB-CG-OD2	-6.04	112.87	118.30
1	G	382	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	D	382	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	D	456	ARG	CG-CD-NE	5.47	123.28	111.80
1	D	456	ARG	NE-CZ-NH1	5.31	122.96	120.30
1	C	382	ARG	NE-CZ-NH1	5.23	122.91	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	372	ARG	Peptide
1	H	455	LEU	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	3520	0	3491	66	0
1	B	3520	0	3491	71	0
1	C	3520	0	3491	90	0
1	D	3520	0	3491	92	0
1	E	3520	0	3491	69	0
1	F	3520	0	3491	82	1
1	G	3520	0	3491	83	0
1	H	3520	0	3491	119	0
2	A	12	0	0	2	0
2	B	19	0	0	2	0
2	C	2	0	0	0	0
2	D	6	0	0	1	0
2	E	11	0	0	0	0
2	F	5	0	0	0	0
2	G	1	0	0	0	0
2	H	9	0	0	0	0
All	All	28225	0	27928	579	1

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 (579) 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:H:370:ALA:HB1	1:H:371:ALA:CB	1.36	1.50
1:D:456:ARG:HB3	1:D:456:ARG:NH1	1.25	1.49
1:D:456:ARG:HH11	1:D:456:ARG:CB	1.38	1.36
1:C:456:ARG:HB3	1:C:456:ARG:NH1	1.52	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:371:ALA:O	1:D:376:ARG:NH2	1.72	1.22
1:H:370:ALA:CB	1:H:371:ALA:CB	2.22	1.17
1:H:370:ALA:CB	1:H:371:ALA:HB2	1.75	1.15
1:H:456:ARG:HB2	1:H:456:ARG:NH1	1.61	1.14
1:H:456:ARG:CB	1:H:456:ARG:CZ	2.26	1.13
1:A:402:VAL:HG11	1:D:402:VAL:HG11	1.21	1.11
1:A:402:VAL:CG1	1:D:402:VAL:HG11	1.81	1.09
1:C:456:ARG:HB3	1:C:456:ARG:CZ	1.78	1.09
1:B:455:LEU:HD13	1:C:456:ARG:HH12	1.16	1.08
1:C:369:THR:HG22	1:C:370:ALA:H	1.09	1.07
1:A:455:LEU:HD13	1:D:456:ARG:NH1	1.69	1.06
1:H:456:ARG:CZ	1:H:456:ARG:HB3	1.81	1.05
1:B:455:LEU:HD13	1:C:456:ARG:NH1	1.71	1.04
1:G:456:ARG:NH1	1:G:456:ARG:HB2	1.72	1.04
1:H:370:ALA:HB1	1:H:371:ALA:HB3	1.38	1.03
1:E:455:LEU:HD13	1:H:456:ARG:NH2	1.74	1.02
1:G:456:ARG:CZ	1:G:456:ARG:HB3	1.89	1.00
1:G:456:ARG:CZ	1:G:456:ARG:CB	2.40	0.99
1:D:455:LEU:O	1:D:456:ARG:HB2	1.64	0.98
1:D:177:ASP:OD1	1:D:180:ASP:HB3	1.70	0.92
1:C:456:ARG:NH1	1:C:456:ARG:CB	2.33	0.90
1:E:450:ALA:HB1	1:E:454:ARG:HH21	1.38	0.89
1:D:371:ALA:CB	1:D:372:ARG:HA	2.03	0.88
1:H:370:ALA:CB	1:H:371:ALA:HB3	1.95	0.88
1:C:369:THR:CG2	1:C:370:ALA:H	1.87	0.88
1:H:456:ARG:HB2	1:H:456:ARG:CZ	1.99	0.88
1:H:370:ALA:HB1	1:H:371:ALA:HB2	0.87	0.86
1:E:402:VAL:HG11	1:H:402:VAL:HG11	1.56	0.86
1:F:387:LEU:HB2	1:H:341:TYR:CZ	2.10	0.86
1:H:82:ASP:OD1	1:H:84:ALA:HB3	1.76	0.86
1:E:455:LEU:HB3	1:H:456:ARG:CZ	2.06	0.86
1:F:450:ALA:HB1	1:F:454:ARG:HH21	1.40	0.86
1:A:450:ALA:HB1	1:A:454:ARG:HH21	1.39	0.86
1:A:455:LEU:HD13	1:D:456:ARG:HH12	1.33	0.86
1:E:455:LEU:HD13	1:H:456:ARG:HH22	1.40	0.85
1:C:369:THR:HG22	1:C:370:ALA:N	1.91	0.84
1:F:455:LEU:HB3	1:G:456:ARG:CZ	2.06	0.84
1:H:456:ARG:NH1	1:H:456:ARG:CB	2.39	0.83
1:D:371:ALA:HB3	1:D:372:ARG:HA	1.60	0.82
1:B:173:ASN:HD22	1:D:143:GLY:HA3	1.43	0.82
1:A:384:VAL:HG23	1:C:49:GLN:HG2	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:456:ARG:NH1	1:G:456:ARG:CB	2.43	0.81
1:B:450:ALA:HB1	1:B:454:ARG:HH21	1.43	0.81
1:E:402:VAL:CG1	1:H:402:VAL:HG11	2.10	0.81
1:F:455:LEU:HD13	1:G:456:ARG:NH2	1.96	0.81
1:B:256:LYS:HE3	2:B:473:HOH:O	1.80	0.81
1:F:402:VAL:HG11	1:G:402:VAL:HG11	1.63	0.80
1:D:455:LEU:O	1:D:456:ARG:CB	2.31	0.79
1:E:455:LEU:HD13	1:H:456:ARG:CZ	2.12	0.79
1:F:388:LEU:HB2	1:H:384:VAL:HG11	1.65	0.79
1:D:456:ARG:NH1	1:D:456:ARG:CB	2.16	0.79
1:D:445:LEU:C	1:D:445:LEU:HD23	2.03	0.79
1:F:387:LEU:HB2	1:H:341:TYR:CE2	2.18	0.78
1:A:341:TYR:HB3	1:C:405:GLN:HE21	1.49	0.78
1:C:455:LEU:O	1:C:456:ARG:HB2	1.83	0.77
1:F:402:VAL:CG1	1:G:402:VAL:HG11	2.14	0.77
1:E:344:ARG:O	1:E:348:ILE:HD13	1.84	0.77
1:B:344:ARG:O	1:B:348:ILE:HD13	1.85	0.76
1:B:59:ILE:HD12	1:B:280:LEU:HD11	1.67	0.76
1:B:173:ASN:ND2	1:D:143:GLY:HA3	2.02	0.75
1:E:9:ILE:HG12	1:E:59:ILE:HG23	1.69	0.75
1:B:9:ILE:HG12	1:B:59:ILE:HG23	1.68	0.74
1:C:382:ARG:HH11	1:C:382:ARG:HG2	1.53	0.74
1:G:368:ILE:O	1:G:369:THR:HG22	1.87	0.74
1:D:61:PHE:CE2	1:D:264:ALA:HB2	2.24	0.73
1:B:341:TYR:HB3	1:D:405:GLN:HE21	1.53	0.73
1:A:9:ILE:HG12	1:A:59:ILE:HG23	1.71	0.73
1:F:455:LEU:HD13	1:G:456:ARG:HH22	1.53	0.73
1:H:371:ALA:HB3	1:H:376:ARG:NH1	2.04	0.73
1:D:59:ILE:HD12	1:D:60:ILE:N	2.03	0.73
1:A:368:ILE:HG22	1:A:369:THR:HG23	1.71	0.72
1:G:338:ALA:HB3	1:G:368:ILE:HD12	1.71	0.72
1:D:382:ARG:HG2	1:D:382:ARG:HH11	1.55	0.72
1:E:59:ILE:HD12	1:E:280:LEU:HD11	1.72	0.71
1:B:455:LEU:CD1	1:C:456:ARG:NH1	2.51	0.71
1:A:59:ILE:HD12	1:A:280:LEU:HD11	1.73	0.71
1:D:113:LEU:HD13	1:D:226:ILE:HG22	1.71	0.71
1:D:366:THR:HG21	1:F:359:GLU:HB3	1.72	0.71
1:H:61:PHE:CE2	1:H:264:ALA:HB2	2.25	0.70
1:F:9:ILE:HG12	1:F:59:ILE:HG23	1.72	0.70
1:C:456:ARG:CB	1:C:456:ARG:HH11	2.04	0.70
1:E:455:LEU:HB3	1:H:456:ARG:NE	2.06	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:382:ARG:HH11	1:H:382:ARG:HG2	1.58	0.69
1:F:455:LEU:HD13	1:G:456:ARG:CZ	2.22	0.69
1:H:454:ARG:O	1:H:456:ARG:N	2.26	0.69
1:D:371:ALA:CB	1:D:372:ARG:CA	2.71	0.69
1:H:456:ARG:HB2	1:H:456:ARG:HH11	1.58	0.68
1:A:151:LEU:HD21	1:A:204:MET:HE1	1.75	0.68
1:F:455:LEU:HD13	1:G:456:ARG:NH1	2.08	0.68
1:D:454:ARG:O	1:D:456:ARG:N	2.26	0.68
1:C:128:THR:HG22	1:C:249:THR:OG1	1.93	0.68
1:F:453:GLU:O	1:F:457:ARG:HG3	1.94	0.68
1:G:382:ARG:HG2	1:G:382:ARG:HH11	1.59	0.68
1:F:344:ARG:O	1:F:348:ILE:HD13	1.95	0.67
1:D:9:ILE:HG23	1:D:59:ILE:HG13	1.75	0.67
1:E:151:LEU:HD21	1:E:204:MET:HE1	1.76	0.67
1:D:445:LEU:HD23	1:D:446:GLN:N	2.10	0.66
1:F:59:ILE:HD12	1:F:280:LEU:HD11	1.77	0.66
1:F:455:LEU:CD1	1:G:456:ARG:NH1	2.59	0.66
1:C:98:ARG:HG2	1:C:103:LEU:HD23	1.78	0.66
1:F:450:ALA:HB1	1:F:454:ARG:NH2	2.11	0.66
1:H:80:THR:O	1:H:277:LYS:NZ	2.30	0.65
1:G:98:ARG:HG2	1:G:103:LEU:HD23	1.77	0.65
1:H:445:LEU:C	1:H:445:LEU:HD23	2.17	0.65
1:F:387:LEU:HD22	1:H:341:TYR:CD2	2.32	0.65
1:A:450:ALA:HB1	1:A:454:ARG:NH2	2.11	0.64
1:E:450:ALA:HB1	1:E:454:ARG:NH2	2.11	0.64
1:C:455:LEU:O	1:C:456:ARG:CB	2.44	0.64
1:C:454:ARG:O	1:C:456:ARG:N	2.31	0.64
1:C:369:THR:CG2	1:C:370:ALA:N	2.55	0.64
1:E:453:GLU:O	1:E:457:ARG:HG3	1.97	0.63
1:D:113:LEU:HD13	1:D:226:ILE:CG2	2.27	0.63
1:H:64:HIS:CD2	1:H:261:VAL:H	2.17	0.63
1:E:455:LEU:CD1	1:H:456:ARG:NH1	2.62	0.63
1:A:380:GLU:OE1	1:C:391:GLU:OE2	2.17	0.63
1:H:64:HIS:HD2	1:H:261:VAL:H	1.44	0.63
1:B:453:GLU:O	1:B:457:ARG:HG3	1.99	0.62
1:G:373:ASP:OD2	1:G:377:ALA:HB2	1.99	0.62
1:G:456:ARG:HB2	1:G:456:ARG:HH11	1.63	0.62
1:C:366:THR:O	1:C:368:ILE:N	2.32	0.62
1:F:399:PHE:CE2	1:G:399:PHE:CE2	2.87	0.62
1:A:388:LEU:HB2	1:C:384:VAL:HG11	1.81	0.62
1:A:368:ILE:HG22	1:A:369:THR:CG2	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:104:ILE:HD12	1:H:104:ILE:C	2.20	0.62
1:C:344:ARG:O	1:C:348:ILE:HD12	1.99	0.62
1:H:372:ARG:H	1:H:376:ARG:NH2	1.97	0.62
1:D:98:ARG:HG2	1:D:103:LEU:HD23	1.82	0.61
1:G:80:THR:O	1:G:277:LYS:NZ	2.33	0.61
1:D:439:THR:HG23	2:D:463:HOH:O	1.98	0.61
1:C:428:GLN:O	1:C:432:GLU:HG2	2.00	0.61
1:D:64:HIS:HD2	1:D:261:VAL:H	1.47	0.61
1:B:195:LEU:HD12	1:B:195:LEU:O	2.00	0.61
1:H:371:ALA:HB3	1:H:376:ARG:CZ	2.30	0.61
1:B:368:ILE:HG23	1:B:369:THR:HG23	1.83	0.61
1:A:402:VAL:HG13	1:D:402:VAL:HG11	1.81	0.60
1:A:344:ARG:O	1:A:348:ILE:HD13	2.00	0.60
1:A:453:GLU:O	1:A:457:ARG:HG3	2.01	0.60
1:B:192:LEU:HD23	1:B:357:VAL:HG13	1.82	0.60
1:H:59:ILE:HD11	1:H:61:PHE:CD1	2.36	0.60
1:C:246:VAL:HG12	1:C:247:LEU:O	2.02	0.60
1:F:455:LEU:CD1	1:G:456:ARG:HH12	2.15	0.60
1:H:370:ALA:HB3	1:H:376:ARG:NH1	2.17	0.59
1:A:383:ASN:HD21	1:C:53:THR:CG2	2.15	0.59
1:B:246:VAL:CG2	1:B:322:GLU:OE1	2.51	0.59
1:A:402:VAL:CG1	1:D:402:VAL:CG1	2.69	0.59
1:C:43:LEU:C	1:C:43:LEU:HD12	2.23	0.59
1:G:454:ARG:O	1:G:456:ARG:N	2.35	0.59
1:H:372:ARG:HA	1:H:376:ARG:HH21	1.66	0.59
1:C:80:THR:O	1:C:277:LYS:NZ	2.36	0.59
1:H:59:ILE:HD11	1:H:61:PHE:CE1	2.38	0.59
1:H:158:TRP:CE2	1:H:162:ALA:HB2	2.37	0.59
1:H:370:ALA:CA	1:H:371:ALA:HB2	2.33	0.59
1:C:372:ARG:HG2	1:C:372:ARG:HH11	1.68	0.59
1:C:456:ARG:CZ	1:C:456:ARG:CB	2.67	0.58
1:E:455:LEU:CD1	1:H:456:ARG:CZ	2.81	0.58
1:C:445:LEU:HD23	1:C:446:GLN:N	2.18	0.58
1:E:341:TYR:HB3	1:G:405:GLN:HE21	1.67	0.58
1:A:129:TRP:HA	1:A:132:ILE:HD12	1.84	0.58
1:E:329:ILE:HD12	1:E:329:ILE:H	1.68	0.58
1:A:423:GLU:O	1:A:424:LYS:HB2	2.03	0.58
1:C:445:LEU:HD23	1:C:445:LEU:C	2.23	0.58
1:C:82:ASP:OD1	1:C:84:ALA:HB3	2.03	0.58
1:D:64:HIS:HE1	1:D:330:MET:O	1.87	0.58
1:G:7:LEU:HB2	1:G:35:VAL:HG22	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:152:GLN:HE22	1:G:207:ASP:HA	1.69	0.58
1:G:158:TRP:CE2	1:G:162:ALA:HB2	2.39	0.57
1:A:246:VAL:CG2	1:A:322:GLU:OE1	2.51	0.57
1:D:371:ALA:HB1	1:D:372:ARG:HA	1.83	0.57
1:C:311:LEU:HB3	1:C:317:ILE:HD13	1.86	0.57
1:H:370:ALA:HB3	1:H:371:ALA:HB3	1.85	0.57
1:A:113:LEU:HG	2:A:460:HOH:O	2.05	0.57
1:F:151:LEU:HD21	1:F:204:MET:HE1	1.85	0.57
1:G:8:VAL:HG13	1:G:57:PRO:HA	1.86	0.57
1:F:384:VAL:HG21	1:H:387:LEU:HD23	1.86	0.57
1:B:329:ILE:H	1:B:329:ILE:HD12	1.68	0.57
1:B:387:LEU:HB2	1:D:341:TYR:CZ	2.39	0.57
1:B:151:LEU:HD21	1:B:204:MET:HE1	1.87	0.56
1:F:455:LEU:HD13	1:G:456:ARG:HH12	1.69	0.56
1:A:455:LEU:HB3	1:D:456:ARG:CZ	2.35	0.56
1:A:455:LEU:CD1	1:D:456:ARG:NH1	2.57	0.56
1:B:199:ILE:HG21	1:B:206:ALA:HB2	1.88	0.56
1:D:104:ILE:HD12	1:D:105:ALA:N	2.21	0.56
1:D:420:LEU:HD11	1:D:424:LYS:HE3	1.87	0.56
1:F:129:TRP:HA	1:F:132:ILE:HD12	1.88	0.56
1:H:370:ALA:CB	1:H:376:ARG:NH1	2.68	0.56
1:D:366:THR:CG2	1:F:359:GLU:HB3	2.35	0.56
1:G:445:LEU:HD23	1:G:446:GLN:N	2.21	0.56
1:B:450:ALA:HB1	1:B:454:ARG:NH2	2.16	0.56
1:A:59:ILE:HD11	1:A:280:LEU:HD21	1.88	0.56
1:A:356:THR:OG1	1:A:359:GLU:HG2	2.06	0.56
1:H:365:GLN:O	1:H:369:THR:OG1	2.24	0.56
1:H:372:ARG:H	1:H:376:ARG:CZ	2.19	0.55
1:B:8:VAL:HG13	1:B:57:PRO:HA	1.89	0.55
1:F:158:TRP:CE2	1:F:162:ALA:HB2	2.41	0.55
1:H:128:THR:HB	1:H:130:GLU:OE1	2.07	0.55
1:E:341:TYR:CE2	1:G:406:ALA:HA	2.42	0.55
1:A:154:PRO:HG3	1:A:344:ARG:HA	1.89	0.55
1:B:59:ILE:CD1	1:B:280:LEU:HD11	2.36	0.55
1:E:455:LEU:HD13	1:H:456:ARG:NH1	2.22	0.55
1:F:178:ILE:HG22	1:F:333:ILE:HD12	1.88	0.55
1:B:59:ILE:CD1	1:B:280:LEU:HD21	2.37	0.55
1:D:177:ASP:OD1	1:D:180:ASP:CB	2.51	0.55
1:E:128:THR:OG1	1:E:131:GLU:HG2	2.07	0.55
1:F:8:VAL:HG13	1:F:57:PRO:HA	1.89	0.55
1:F:154:PRO:HG3	1:F:344:ARG:HA	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:10:TRP:HB3	1:E:43:LEU:HD13	1.90	0.54
1:E:246:VAL:CG2	1:E:322:GLU:OE1	2.55	0.54
1:G:128:THR:HG22	1:G:249:THR:OG1	2.07	0.54
1:A:10:TRP:HB3	1:A:43:LEU:HD13	1.89	0.54
1:B:129:TRP:HA	1:B:132:ILE:HD12	1.89	0.54
1:E:59:ILE:HD11	1:E:280:LEU:HD21	1.90	0.54
1:F:246:VAL:CG2	1:F:322:GLU:OE1	2.55	0.54
1:H:59:ILE:HD12	1:H:60:ILE:N	2.22	0.54
1:H:255:SER:O	1:H:257:PRO:HD3	2.07	0.54
1:H:372:ARG:HA	1:H:376:ARG:NH2	2.22	0.54
1:D:371:ALA:HB1	1:D:372:ARG:CA	2.37	0.54
1:E:356:THR:OG1	1:E:359:GLU:HG2	2.07	0.54
1:E:9:ILE:CG1	1:E:59:ILE:HG23	2.38	0.54
1:C:366:THR:C	1:C:368:ILE:H	2.11	0.54
1:E:341:TYR:CZ	1:G:406:ALA:HA	2.41	0.54
1:G:61:PHE:CE2	1:G:264:ALA:HB2	2.43	0.54
1:G:388:LEU:HD23	1:H:385:THR:HG21	1.90	0.54
1:B:423:GLU:O	1:B:424:LYS:HB2	2.07	0.54
1:B:388:LEU:HB2	1:D:384:VAL:HG11	1.90	0.53
1:D:82:ASP:OD1	1:D:84:ALA:HB3	2.08	0.53
1:G:59:ILE:HD11	1:G:61:PHE:CE1	2.43	0.53
1:B:402:VAL:CG1	1:C:402:VAL:HG11	2.37	0.53
1:F:59:ILE:HD11	1:F:280:LEU:HD21	1.89	0.53
1:H:95:ASP:OD1	1:H:98:ARG:NH1	2.41	0.53
1:F:199:ILE:HG21	1:F:206:ALA:HB2	1.88	0.53
1:F:423:GLU:O	1:F:424:LYS:HB2	2.08	0.53
1:A:59:ILE:CD1	1:A:280:LEU:HD21	2.39	0.53
1:B:335:GLN:OE1	1:B:335:GLN:N	2.41	0.53
1:F:59:ILE:CD1	1:F:280:LEU:HD21	2.39	0.53
1:A:8:VAL:HG13	1:A:57:PRO:HA	1.90	0.53
1:C:59:ILE:HD11	1:C:61:PHE:CE1	2.44	0.53
1:G:445:LEU:HD23	1:G:445:LEU:C	2.29	0.53
1:B:246:VAL:HG12	1:B:247:LEU:O	2.08	0.53
1:G:372:ARG:O	1:G:373:ASP:C	2.46	0.53
1:B:59:ILE:HD11	1:B:280:LEU:HD21	1.89	0.53
1:D:130:GLU:OE1	1:D:130:GLU:N	2.38	0.53
1:E:199:ILE:HG21	1:E:206:ALA:HB2	1.91	0.53
1:E:455:LEU:HD12	1:H:456:ARG:NH1	2.24	0.53
1:C:68:GLY:HA3	1:C:332:ASN:O	2.09	0.52
1:G:393:THR:HG22	1:G:397:LYS:HE2	1.91	0.52
1:D:218:ASN:N	1:D:218:ASN:HD22	2.07	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:82:ASP:OD1	1:G:84:ALA:HB3	2.08	0.52
1:G:386:HIS:O	1:G:390:GLN:HG2	2.09	0.52
1:A:59:ILE:CD1	1:A:280:LEU:HD11	2.38	0.52
2:A:464:HOH:O	1:B:414:MSE:HE2	2.08	0.52
1:B:166:GLY:HA2	1:B:185:ASN:HD21	1.75	0.52
1:E:388:LEU:HD21	1:F:385:THR:CG2	2.39	0.52
1:H:205:ASN:ND2	1:H:207:ASP:OD1	2.39	0.52
1:B:9:ILE:CG1	1:B:59:ILE:HG23	2.37	0.52
1:B:154:PRO:HG3	1:B:344:ARG:HA	1.91	0.52
1:A:152:GLN:O	1:A:348:ILE:HD11	2.10	0.52
1:C:386:HIS:O	1:C:390:GLN:HG2	2.08	0.52
1:E:8:VAL:HG13	1:E:57:PRO:HA	1.91	0.52
1:E:129:TRP:HA	1:E:132:ILE:HD12	1.92	0.52
1:E:59:ILE:CD1	1:E:280:LEU:HD21	2.40	0.52
1:H:372:ARG:N	1:H:376:ARG:NH2	2.58	0.52
1:D:113:LEU:HD22	1:D:227:ASN:HA	1.92	0.52
1:H:64:HIS:HE1	1:H:330:MET:O	1.93	0.52
1:D:390:GLN:HA	1:D:390:GLN:HE21	1.74	0.52
1:B:128:THR:OG1	1:B:131:GLU:HG2	2.10	0.51
1:E:341:TYR:HE2	1:G:406:ALA:HB2	1.74	0.51
1:F:335:GLN:OE1	1:F:335:GLN:N	2.43	0.51
1:H:370:ALA:CA	1:H:371:ALA:CB	2.88	0.51
1:E:423:GLU:O	1:E:424:LYS:HB2	2.09	0.51
1:D:136:ASP:HA	1:D:146:ALA:HB2	1.93	0.51
1:E:246:VAL:HG12	1:E:247:LEU:O	2.09	0.51
1:D:371:ALA:O	1:D:376:ARG:CZ	2.50	0.51
1:F:128:THR:OG1	1:F:131:GLU:HG2	2.09	0.51
1:A:9:ILE:CG1	1:A:59:ILE:HG23	2.41	0.51
1:C:158:TRP:CE2	1:C:162:ALA:HB2	2.46	0.51
1:D:7:LEU:HB2	1:D:35:VAL:HG22	1.93	0.51
1:E:178:ILE:HG22	1:E:333:ILE:HD12	1.92	0.51
1:F:329:ILE:HD12	1:F:329:ILE:H	1.75	0.51
1:B:117:TYR:CZ	1:B:243:GLY:HA3	2.46	0.51
1:E:152:GLN:O	1:E:348:ILE:HD11	2.11	0.51
1:E:231:ALA:O	1:E:235:ILE:HG13	2.10	0.51
1:D:293:VAL:CG1	1:D:299:LEU:HD21	2.41	0.51
1:E:388:LEU:CD2	1:F:385:THR:HG21	2.40	0.51
1:D:115:LEU:HB2	1:D:247:LEU:HD23	1.93	0.50
1:E:59:ILE:CD1	1:E:280:LEU:HD11	2.41	0.50
1:E:307:TYR:CE2	1:E:311:LEU:HD11	2.46	0.50
1:A:329:ILE:HD12	1:A:329:ILE:H	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:LEU:HD12	1:B:195:LEU:C	2.31	0.50
1:D:80:THR:O	1:D:277:LYS:NZ	2.45	0.50
1:H:181:VAL:HG13	1:H:183:VAL:HG23	1.93	0.50
1:D:205:ASN:ND2	1:D:207:ASP:OD1	2.42	0.50
1:D:238:SER:OG	1:D:240:VAL:HG23	2.12	0.50
1:F:10:TRP:HB3	1:F:43:LEU:HD13	1.94	0.49
1:G:336:MET:O	1:G:339:PHE:HB3	2.12	0.49
1:G:382:ARG:HH11	1:G:382:ARG:CG	2.24	0.49
1:D:158:TRP:CD1	1:D:258:PHE:CE2	3.00	0.49
1:H:98:ARG:HG2	1:H:103:LEU:HD23	1.95	0.49
1:B:382:ARG:HH11	1:B:382:ARG:CG	2.26	0.49
1:E:154:PRO:HG3	1:E:344:ARG:HA	1.93	0.49
1:F:9:ILE:CG1	1:F:59:ILE:HG23	2.40	0.49
1:H:107:PRO:O	1:H:108:ILE:HD13	2.13	0.49
1:B:178:ILE:HG22	1:B:333:ILE:HD12	1.94	0.49
1:A:178:ILE:HG22	1:A:333:ILE:HD12	1.94	0.49
1:B:10:TRP:HB3	1:B:43:LEU:HD13	1.94	0.49
1:C:267:ASN:HB3	1:C:270:SER:HB2	1.95	0.49
1:C:314:ASP:HB3	1:C:317:ILE:HD12	1.94	0.49
1:A:128:THR:OG1	1:A:131:GLU:HG2	2.13	0.49
1:D:336:MET:O	1:D:339:PHE:HB3	2.12	0.49
1:G:205:ASN:ND2	1:G:207:ASP:OD1	2.45	0.49
1:F:152:GLN:O	1:F:348:ILE:HD11	2.13	0.49
1:F:382:ARG:CG	1:F:382:ARG:HH11	2.26	0.49
1:F:399:PHE:CD2	1:G:399:PHE:CZ	3.01	0.49
1:C:369:THR:O	1:C:370:ALA:HB3	2.13	0.48
1:F:455:LEU:HB3	1:G:456:ARG:NE	2.27	0.48
1:G:381:ALA:O	1:G:385:THR:HG23	2.13	0.48
1:B:158:TRP:N	1:B:159:PRO:HD2	2.28	0.48
1:B:158:TRP:HB3	1:B:159:PRO:HD3	1.94	0.48
1:D:344:ARG:O	1:D:348:ILE:HD12	2.14	0.48
1:A:388:LEU:HD21	1:B:385:THR:CG2	2.44	0.48
1:C:266:ILE:HD13	1:C:276:ALA:HB3	1.96	0.48
1:E:344:ARG:O	1:E:348:ILE:CD1	2.59	0.48
1:H:158:TRP:CD1	1:H:258:PHE:CE2	3.02	0.48
1:A:335:GLN:OE1	1:A:335:GLN:N	2.46	0.48
1:A:382:ARG:CG	1:A:382:ARG:HH11	2.26	0.48
1:D:104:ILE:HD12	1:D:104:ILE:C	2.34	0.48
1:C:128:THR:HB	1:C:130:GLU:OE1	2.14	0.48
1:H:404:ALA:O	1:H:407:ALA:HB3	2.14	0.48
1:B:117:TYR:CE1	1:B:125:PRO:HG3	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:267:ASN:HB3	1:H:270:SER:HB2	1.96	0.48
1:A:158:TRP:N	1:A:159:PRO:HD2	2.29	0.48
1:F:158:TRP:CD1	1:F:258:PHE:CE2	3.02	0.48
1:H:192:LEU:HD23	1:H:357:VAL:HG13	1.95	0.48
1:B:158:TRP:CD1	1:B:258:PHE:CE2	3.02	0.47
1:B:348:ILE:HD12	1:B:348:ILE:N	2.30	0.47
1:H:293:VAL:CG1	1:H:299:LEU:HD21	2.44	0.47
1:B:80:THR:O	1:B:277:LYS:NZ	2.47	0.47
1:C:393:THR:HG22	1:C:397:LYS:HE2	1.96	0.47
1:F:384:VAL:CG2	1:H:387:LEU:HD23	2.44	0.47
1:F:399:PHE:CE2	1:G:399:PHE:CZ	3.02	0.47
1:G:390:GLN:HE21	1:G:390:GLN:HA	1.79	0.47
1:D:401:ASP:O	1:D:405:GLN:HG2	2.14	0.47
1:B:341:TYR:CE2	1:D:406:ALA:HA	2.50	0.47
1:C:47:PHE:HA	1:C:50:VAL:HG22	1.97	0.47
1:E:158:TRP:CE2	1:E:162:ALA:HB2	2.50	0.47
1:B:455:LEU:HB3	1:C:456:ARG:NH1	2.29	0.47
1:C:124:ASN:HD22	1:C:124:ASN:N	2.13	0.47
1:E:385:THR:OG1	1:F:389:GLN:NE2	2.48	0.47
1:C:369:THR:HG23	1:C:373:ASP:OD1	2.15	0.47
1:C:420:LEU:HD11	1:C:424:LYS:HE3	1.95	0.47
1:G:59:ILE:HD13	1:G:264:ALA:HB1	1.96	0.47
1:A:158:TRP:CE2	1:A:162:ALA:HB2	2.50	0.47
1:B:152:GLN:O	1:B:348:ILE:HD11	2.15	0.47
1:A:80:THR:O	1:A:277:LYS:NZ	2.48	0.47
1:D:454:ARG:O	1:D:455:LEU:C	2.53	0.47
1:H:113:LEU:HD11	1:H:156:PHE:HA	1.96	0.47
1:H:386:HIS:O	1:H:390:GLN:HG2	2.15	0.47
1:B:231:ALA:O	1:B:235:ILE:HG13	2.15	0.47
1:F:440:THR:HG22	1:F:441:LEU:N	2.30	0.47
1:H:79:ILE:HD12	1:H:106:TYR:CE1	2.50	0.47
1:C:205:ASN:ND2	1:C:207:ASP:OD1	2.45	0.46
1:E:382:ARG:HH11	1:E:382:ARG:CG	2.27	0.46
1:G:388:LEU:HD23	1:H:385:THR:CG2	2.44	0.46
1:B:158:TRP:CE2	1:B:162:ALA:HB2	2.50	0.46
1:E:80:THR:O	1:E:277:LYS:NZ	2.49	0.46
1:E:341:TYR:CE2	1:G:406:ALA:CA	2.98	0.46
1:G:64:HIS:CD2	1:G:261:VAL:H	2.33	0.46
1:H:154:PRO:HB3	1:H:343:VAL:HG12	1.97	0.46
1:F:384:VAL:HG13	1:H:384:VAL:HG13	1.96	0.46
1:A:246:VAL:HG21	1:A:322:GLU:OE1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:109:ALA:O	1:C:261:VAL:HA	2.15	0.46
1:G:426:GLN:HA	1:G:426:GLN:NE2	2.29	0.46
1:A:246:VAL:HG22	1:A:322:GLU:HG2	1.98	0.46
1:E:388:LEU:CD2	1:F:385:THR:CG2	2.94	0.46
1:G:314:ASP:HB3	1:G:317:ILE:HD12	1.98	0.46
1:F:80:THR:O	1:F:277:LYS:NZ	2.49	0.46
1:F:387:LEU:HD22	1:H:341:TYR:CE2	2.51	0.46
1:C:158:TRP:HB3	1:C:159:PRO:CD	2.46	0.46
1:G:9:ILE:HG23	1:G:59:ILE:HG13	1.98	0.46
1:H:336:MET:O	1:H:339:PHE:HB3	2.16	0.46
1:A:231:ALA:O	1:A:235:ILE:HG13	2.15	0.46
1:C:195:LEU:HD12	1:C:195:LEU:O	2.16	0.46
1:E:335:GLN:OE1	1:E:335:GLN:N	2.48	0.46
1:H:218:ASN:HD21	1:H:235:ILE:HG12	1.81	0.46
1:H:455:LEU:C	1:H:456:ARG:HG3	2.35	0.46
1:B:455:LEU:HB3	1:C:456:ARG:CZ	2.46	0.46
1:E:166:GLY:HA2	1:E:185:ASN:HD21	1.81	0.46
1:C:160:LEU:O	1:C:160:LEU:HD12	2.15	0.45
1:D:344:ARG:O	1:D:348:ILE:CD1	2.63	0.45
1:C:59:ILE:HD11	1:C:61:PHE:CD1	2.52	0.45
1:G:369:THR:O	1:G:370:ALA:HB2	2.15	0.45
1:H:344:ARG:O	1:H:348:ILE:HD12	2.15	0.45
1:H:415:ALA:O	1:H:418:ALA:HB3	2.16	0.45
1:A:158:TRP:CD1	1:A:258:PHE:CE2	3.04	0.45
1:A:166:GLY:HA2	1:A:185:ASN:HD21	1.81	0.45
1:H:217:PHE:HA	1:H:222:THR:HG22	1.98	0.45
1:A:90:TYR:HA	1:A:91:PRO:HD2	1.79	0.45
1:A:244:VAL:HB	1:A:316:ARG:HG2	1.99	0.45
1:B:368:ILE:CG2	1:B:369:THR:HG23	2.46	0.45
1:F:166:GLY:HA2	1:F:185:ASN:HD21	1.81	0.45
1:H:371:ALA:O	1:H:372:ARG:HB2	2.15	0.45
1:H:376:ARG:HE	1:H:376:ARG:HB3	1.35	0.45
1:A:158:TRP:HB3	1:A:159:PRO:HD3	1.98	0.45
1:D:371:ALA:C	1:D:376:ARG:NH2	2.60	0.45
1:C:118:ASN:C	1:C:118:ASN:OD1	2.55	0.45
1:E:246:VAL:HG21	1:E:322:GLU:OE1	2.17	0.45
1:F:59:ILE:CD1	1:F:280:LEU:HD11	2.46	0.45
1:G:59:ILE:HD12	1:G:60:ILE:N	2.32	0.45
1:H:445:LEU:HD23	1:H:446:GLN:N	2.31	0.45
1:G:393:THR:OG1	1:H:382:ARG:NH2	2.50	0.45
1:C:152:GLN:HE22	1:C:207:ASP:HA	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:59:ILE:HD13	1:H:264:ALA:HB1	1.99	0.45
1:C:393:THR:HG23	1:D:382:ARG:NH2	2.32	0.45
1:E:450:ALA:CB	1:E:454:ARG:HH21	2.21	0.45
1:G:345:THR:HG22	1:G:349:ASN:ND2	2.31	0.45
1:B:388:LEU:HD11	1:C:388:LEU:HD21	1.98	0.45
1:F:246:VAL:HG12	1:F:247:LEU:O	2.17	0.45
1:H:234:ASN:HD22	1:H:234:ASN:HA	1.61	0.45
1:A:402:VAL:HG13	1:D:402:VAL:CG1	2.43	0.44
1:C:61:PHE:CE2	1:C:264:ALA:HB2	2.52	0.44
1:C:226:ILE:HD13	1:C:247:LEU:HD22	1.98	0.44
1:E:339:PHE:CZ	1:E:343:VAL:HG21	2.52	0.44
1:H:308:GLU:OE2	1:H:321:MET:HE2	2.17	0.44
1:H:382:ARG:HH11	1:H:382:ARG:CG	2.28	0.44
1:D:39:HIS:N	1:D:40:PRO:CD	2.80	0.44
1:E:64:HIS:CE1	1:E:330:MET:O	2.70	0.44
1:G:192:LEU:HD23	1:G:357:VAL:HG13	1.98	0.44
1:C:291:GLU:O	1:C:295:LYS:HG3	2.17	0.44
1:D:445:LEU:C	1:D:445:LEU:CD2	2.78	0.44
1:F:158:TRP:HB3	1:F:159:PRO:HD3	1.98	0.44
1:B:117:TYR:CE1	1:B:243:GLY:HA3	2.52	0.44
1:E:158:TRP:HB3	1:E:159:PRO:HD3	1.99	0.44
1:F:195:LEU:HD12	1:F:195:LEU:O	2.16	0.44
1:H:152:GLN:HE22	1:H:207:ASP:HA	1.83	0.44
1:E:410:ASN:HD22	1:F:337:SER:HB2	1.83	0.44
1:D:386:HIS:O	1:D:390:GLN:HG2	2.18	0.44
1:E:90:TYR:HA	1:E:91:PRO:HD2	1.80	0.44
1:E:158:TRP:CD1	1:E:258:PHE:CE2	3.05	0.44
1:A:438:ILE:CD1	1:D:434:LEU:HD22	2.48	0.44
1:C:158:TRP:CD1	1:C:258:PHE:CE2	3.06	0.44
1:G:152:GLN:NE2	1:G:207:ASP:HA	2.33	0.44
1:G:370:ALA:C	1:G:372:ARG:H	2.20	0.44
1:D:456:ARG:HB3	1:D:456:ARG:HH11	0.45	0.44
1:B:202:LYS:HE3	2:B:476:HOH:O	2.17	0.43
1:D:173:ASN:HD21	1:H:356:THR:HG21	1.83	0.43
1:F:356:THR:OG1	1:F:359:GLU:HG2	2.18	0.43
1:G:64:HIS:ND1	1:G:96:ALA:HB1	2.33	0.43
1:H:172:GLU:HG3	1:H:175:LYS:O	2.18	0.43
1:A:388:LEU:CD2	1:B:385:THR:HG21	2.48	0.43
1:F:244:VAL:HB	1:F:316:ARG:HG2	2.00	0.43
1:F:246:VAL:HG22	1:F:322:GLU:HG2	2.00	0.43
1:G:43:LEU:HA	1:G:46:LYS:HB2	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:VAL:HG12	1:A:247:LEU:O	2.18	0.43
1:H:372:ARG:O	1:H:373:ASP:C	2.56	0.43
1:D:154:PRO:HA	1:D:157:THR:OG1	2.19	0.43
1:E:158:TRP:N	1:E:159:PRO:HD2	2.34	0.43
1:F:64:HIS:CE1	1:F:330:MET:O	2.72	0.43
1:F:117:TYR:CE1	1:F:243:GLY:HA3	2.53	0.43
1:D:434:LEU:HD23	1:D:434:LEU:HA	1.82	0.43
1:E:455:LEU:CD1	1:H:456:ARG:HH12	2.30	0.43
1:G:255:SER:O	1:G:257:PRO:HD3	2.19	0.43
1:C:382:ARG:HH11	1:C:382:ARG:CG	2.25	0.43
1:E:246:VAL:HG22	1:E:322:GLU:HG2	2.01	0.43
1:A:307:TYR:CE2	1:A:311:LEU:HD11	2.53	0.43
1:B:117:TYR:CE2	1:B:125:PRO:HD3	2.54	0.43
1:B:348:ILE:HD12	1:B:348:ILE:H	1.84	0.43
1:C:9:ILE:HG12	1:C:59:ILE:HG13	2.01	0.43
1:C:113:LEU:HD11	1:C:156:PHE:HA	2.01	0.43
1:D:115:LEU:HD23	1:D:245:THR:CG2	2.48	0.43
1:H:390:GLN:HE21	1:H:390:GLN:HA	1.83	0.43
1:C:209:ASP:OD1	1:C:209:ASP:C	2.56	0.43
1:D:151:LEU:HD12	1:D:205:ASN:O	2.19	0.43
1:F:60:ILE:HG23	1:F:60:ILE:O	2.19	0.43
1:F:388:LEU:HD12	1:H:384:VAL:CG1	2.49	0.43
1:G:370:ALA:C	1:G:372:ARG:N	2.72	0.43
1:H:272:ASN:HB3	1:H:275:LEU:HB2	2.00	0.43
1:A:450:ALA:CB	1:A:454:ARG:HH21	2.20	0.42
1:A:452:VAL:HG23	1:A:453:GLU:N	2.34	0.42
1:C:192:LEU:O	1:C:196:VAL:HG23	2.19	0.42
1:D:255:SER:O	1:D:257:PRO:HD3	2.19	0.42
1:G:68:GLY:HA3	1:G:332:ASN:O	2.19	0.42
1:H:104:ILE:HD12	1:H:105:ALA:N	2.33	0.42
1:B:246:VAL:HG21	1:B:322:GLU:OE1	2.20	0.42
1:C:43:LEU:HA	1:C:46:LYS:HB2	2.00	0.42
1:A:199:ILE:HG21	1:A:206:ALA:HB2	2.02	0.42
1:G:59:ILE:HD11	1:G:61:PHE:CD1	2.54	0.42
1:H:371:ALA:CB	1:H:376:ARG:CZ	2.97	0.42
1:H:424:LYS:O	1:H:428:GLN:HB3	2.19	0.42
1:D:293:VAL:HG11	1:D:299:LEU:HD21	2.02	0.42
1:E:455:LEU:CB	1:H:456:ARG:CZ	2.88	0.42
1:D:447:ASP:O	1:D:448:ALA:C	2.58	0.42
1:D:68:GLY:HA3	1:D:332:ASN:O	2.20	0.42
1:G:344:ARG:O	1:G:348:ILE:CD1	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:VAL:HG22	1:B:322:GLU:HG2	2.01	0.42
1:C:110:VAL:O	1:C:301:ALA:HB3	2.19	0.42
1:C:372:ARG:HH11	1:C:372:ARG:CG	2.33	0.42
1:G:455:LEU:O	1:G:456:ARG:HG3	2.20	0.42
1:H:117:TYR:CE1	1:H:125:PRO:HG3	2.55	0.42
1:H:293:VAL:HG12	1:H:299:LEU:HD21	2.01	0.42
1:D:158:TRP:HB3	1:D:159:PRO:HD3	2.02	0.42
1:F:246:VAL:HG21	1:F:322:GLU:OE1	2.20	0.42
1:A:341:TYR:HB3	1:C:405:GLN:NE2	2.28	0.42
1:B:126:PRO:HD2	1:B:224:MET:SD	2.60	0.42
1:E:440:THR:HG22	1:E:441:LEU:N	2.35	0.42
1:F:402:VAL:CG1	1:G:402:VAL:CG1	2.93	0.42
1:C:158:TRP:HB3	1:C:159:PRO:HD3	2.00	0.41
1:C:384:VAL:HG12	1:C:385:THR:N	2.35	0.41
1:F:195:LEU:HD12	1:F:195:LEU:C	2.40	0.41
1:H:158:TRP:O	1:H:159:PRO:C	2.58	0.41
1:D:64:HIS:CE1	1:D:330:MET:O	2.71	0.41
1:H:455:LEU:C	1:H:456:ARG:CG	2.88	0.41
1:A:158:TRP:O	1:A:161:ILE:N	2.53	0.41
1:C:454:ARG:O	1:C:455:LEU:C	2.54	0.41
1:F:450:ALA:CB	1:F:454:ARG:HH21	2.20	0.41
1:G:158:TRP:HB3	1:G:159:PRO:CD	2.50	0.41
1:H:183:VAL:HG12	1:H:183:VAL:O	2.21	0.41
1:B:450:ALA:CB	1:B:454:ARG:HH21	2.25	0.41
1:C:10:TRP:CH2	1:C:50:VAL:HG21	2.55	0.41
1:C:192:LEU:O	1:C:192:LEU:HD12	2.19	0.41
1:D:8:VAL:HG13	1:D:57:PRO:HA	2.02	0.41
1:D:158:TRP:HB3	1:D:159:PRO:CD	2.50	0.41
1:F:402:VAL:HG11	1:G:402:VAL:CG1	2.41	0.41
1:H:344:ARG:O	1:H:348:ILE:CD1	2.68	0.41
1:C:207:ASP:OD1	1:C:207:ASP:N	2.47	0.41
1:D:43:LEU:HD12	1:D:43:LEU:C	2.40	0.41
1:C:372:ARG:NH2	1:C:379:MSE:CE	2.84	0.41
1:C:456:ARG:O	1:C:457:ARG:HB2	2.20	0.41
1:E:341:TYR:CE2	1:G:406:ALA:HB2	2.54	0.41
1:F:158:TRP:N	1:F:159:PRO:HD2	2.35	0.41
1:G:47:PHE:HA	1:G:50:VAL:HG22	2.02	0.41
1:H:158:TRP:N	1:H:159:PRO:HD2	2.35	0.41
1:E:240:VAL:HG12	1:E:241:ASN:N	2.35	0.41
1:F:307:TYR:CE2	1:F:311:LEU:HD11	2.55	0.41
1:H:117:TYR:CZ	1:H:125:PRO:HG3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:PHE:N	1:A:48:PRO:HD2	2.36	0.41
1:A:383:ASN:ND2	1:C:53:THR:CG2	2.84	0.41
1:B:64:HIS:CE1	1:B:330:MET:O	2.74	0.41
1:C:43:LEU:HD12	1:C:44:GLU:N	2.36	0.41
1:F:90:TYR:HA	1:F:91:PRO:HD2	1.78	0.41
1:F:388:LEU:HD11	1:G:388:LEU:HD21	2.02	0.41
1:B:114:SER:HA	1:B:323:ASN:ND2	2.35	0.41
1:C:7:LEU:HB2	1:C:35:VAL:HG22	2.03	0.41
1:C:64:HIS:CD2	1:C:261:VAL:H	2.38	0.41
1:D:93:THR:HG21	1:D:303:ALA:CB	2.51	0.41
1:D:158:TRP:N	1:D:159:PRO:HD2	2.35	0.41
1:E:388:LEU:HD23	1:F:385:THR:HG21	2.03	0.41
1:H:375:LEU:O	1:H:378:VAL:HB	2.21	0.41
1:H:393:THR:HG22	1:H:397:LYS:HE2	2.03	0.41
1:C:382:ARG:HG2	1:C:382:ARG:NH1	2.30	0.40
1:D:456:ARG:O	1:D:457:ARG:HG3	2.21	0.40
1:H:176:TYR:CZ	1:H:331:PRO:HA	2.56	0.40
1:H:238:SER:OG	1:H:240:VAL:HG23	2.21	0.40
1:E:47:PHE:N	1:E:48:PRO:HD2	2.37	0.40
1:F:192:LEU:HD23	1:F:357:VAL:HG13	2.03	0.40
1:F:455:LEU:HD12	1:G:456:ARG:NH1	2.34	0.40
1:H:93:THR:O	1:H:107:PRO:HG3	2.21	0.40
1:H:158:TRP:HB3	1:H:159:PRO:HD3	2.03	0.40
1:B:90:TYR:O	1:B:91:PRO:C	2.60	0.40
1:B:161:ILE:HA	1:B:191:GLY:HA3	2.03	0.40
1:C:106:TYR:CD2	1:C:280:LEU:HD13	2.56	0.40
1:C:152:GLN:NE2	1:C:207:ASP:HA	2.35	0.40
1:D:96:ALA:HB2	1:D:329:ILE:CG2	2.51	0.40
1:D:456:ARG:NH1	1:D:456:ARG:CA	2.82	0.40
1:H:455:LEU:O	1:H:456:ARG:HG3	2.21	0.40
1:A:413:VAL:HG11	1:B:153:GLU:OE2	2.22	0.40
1:G:344:ARG:O	1:G:348:ILE:HD12	2.21	0.40
1:G:455:LEU:O	1:G:456:ARG:CB	2.68	0.40
1:G:455:LEU:C	1:G:456:ARG:HG3	2.41	0.40
1:H:250:PHE:CE2	1:H:251:LYS:HD2	2.56	0.40
1:H:312:ALA:HB1	1:H:318:ALA:HB2	2.03	0.40
1:A:388:LEU:CD2	1:B:385:THR:CG2	3.00	0.40
1:D:93:THR:HB	1:D:107:PRO:HB3	2.03	0.40
1:F:231:ALA:O	1:F:235:ILE:HG13	2.21	0.40
1:F:382:ARG:CG	1:F:382:ARG:NH1	2.84	0.40
1:G:293:VAL:CG1	1:G:299:LEU:HD21	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:369:THR:O	1:G:369:THR:HG23	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:309:GLU:O	1:F:440:THR:OG1[1_454]	2.15	0.05

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	452/471 (96%)	419 (93%)	26 (6%)	7 (2%)	10	33
1	B	452/471 (96%)	425 (94%)	21 (5%)	6 (1%)	12	36
1	C	452/471 (96%)	414 (92%)	30 (7%)	8 (2%)	8	28
1	D	452/471 (96%)	417 (92%)	30 (7%)	5 (1%)	14	41
1	E	452/471 (96%)	424 (94%)	22 (5%)	6 (1%)	12	36
1	F	452/471 (96%)	422 (93%)	24 (5%)	6 (1%)	12	36
1	G	452/471 (96%)	427 (94%)	20 (4%)	5 (1%)	14	41
1	H	452/471 (96%)	413 (91%)	33 (7%)	6 (1%)	12	36
All	All	3616/3768 (96%)	3361 (93%)	206 (6%)	49 (1%)	11	34

All (49) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	371	ALA
1	A	424	LYS
1	B	424	LYS
1	C	367	ARG

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Mol	Chain	Res	Type
1	C	370	ALA
1	C	456	ARG
1	D	371	ALA
1	D	456	ARG
1	E	424	LYS
1	F	424	LYS
1	G	370	ALA
1	G	456	ARG
1	H	371	ALA
1	H	456	ARG
1	C	454	ARG
1	C	455	LEU
1	D	455	LEU
1	F	371	ALA
1	G	455	LEU
1	H	178	ILE
1	H	455	LEU
1	A	42	LYS
1	A	165	GLY
1	B	165	GLY
1	C	178	ILE
1	D	454	ARG
1	E	165	GLY
1	E	371	ALA
1	F	165	GLY
1	G	371	ALA
1	G	454	ARG
1	H	66	ARG
1	H	454	ARG
1	B	42	LYS
1	C	369	THR
1	C	373	ASP
1	B	334	PRO
1	D	168	ALA
1	E	42	LYS
1	E	334	PRO
1	F	42	LYS
1	F	334	PRO
1	A	334	PRO
1	B	74	GLY
1	A	81	PRO
1	E	81	PRO

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Mol	Chain	Res	Type
1	A	74	GLY
1	B	81	PRO
1	F	81	PRO

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	362/376 (96%)	339 (94%)	23 (6%)	17	45
1	B	362/376 (96%)	339 (94%)	23 (6%)	17	45
1	C	362/376 (96%)	332 (92%)	30 (8%)	11	32
1	D	362/376 (96%)	330 (91%)	32 (9%)	10	29
1	E	362/376 (96%)	342 (94%)	20 (6%)	21	52
1	F	362/376 (96%)	342 (94%)	20 (6%)	21	52
1	G	362/376 (96%)	335 (92%)	27 (8%)	13	37
1	H	362/376 (96%)	335 (92%)	27 (8%)	13	37
All	All	2896/3008 (96%)	2694 (93%)	202 (7%)	15	40

All (202) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	LYS
1	A	34	LYS
1	A	42	LYS
1	A	43	LEU
1	A	55	ASP
1	A	59	ILE
1	A	102	LYS
1	A	142	LYS
1	A	172	GLU
1	A	218	ASN
1	A	341	TYR
1	A	368	ILE

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Mol	Chain	Res	Type
1	A	372	ARG
1	A	376	ARG
1	A	382	ARG
1	A	388	LEU
1	A	390	GLN
1	A	426	GLN
1	A	435	GLU
1	A	439	THR
1	A	440	THR
1	A	449	SER
1	A	454	ARG
1	B	26	LYS
1	B	34	LYS
1	B	42	LYS
1	B	43	LEU
1	B	55	ASP
1	B	59	ILE
1	B	102	LYS
1	B	142	LYS
1	B	172	GLU
1	B	218	ASN
1	B	341	TYR
1	B	368	ILE
1	B	372	ARG
1	B	376	ARG
1	B	382	ARG
1	B	388	LEU
1	B	390	GLN
1	B	426	GLN
1	B	435	GLU
1	B	439	THR
1	B	440	THR
1	B	449	SER
1	B	454	ARG
1	C	4	GLU
1	C	26	LYS
1	C	31	THR
1	C	34	LYS
1	C	42	LYS
1	C	59	ILE
1	C	65	ASP
1	C	87	ASP

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Mol	Chain	Res	Type
1	C	172	GLU
1	C	175	LYS
1	C	184	ASP
1	C	218	ASN
1	C	237	THR
1	C	239	LYS
1	C	256	LYS
1	C	278	GLU
1	C	337	SER
1	C	345	THR
1	C	365	GLN
1	C	373	ASP
1	C	382	ARG
1	C	384	VAL
1	C	390	GLN
1	C	401	ASP
1	C	411	HIS
1	C	428	GLN
1	C	445	LEU
1	C	451	GLU
1	C	455	LEU
1	C	456	ARG
1	D	26	LYS
1	D	34	LYS
1	D	42	LYS
1	D	59	ILE
1	D	65	ASP
1	D	133	PRO
1	D	145	SER
1	D	172	GLU
1	D	175	LYS
1	D	177	ASP
1	D	181	VAL
1	D	184	ASP
1	D	218	ASN
1	D	237	THR
1	D	238	SER
1	D	239	LYS
1	D	256	LYS
1	D	278	GLU
1	D	337	SER
1	D	365	GLN

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Mol	Chain	Res	Type
1	D	382	ARG
1	D	384	VAL
1	D	389	GLN
1	D	390	GLN
1	D	411	HIS
1	D	417	MSE
1	D	428	GLN
1	D	445	LEU
1	D	446	GLN
1	D	451	GLU
1	D	455	LEU
1	D	456	ARG
1	E	26	LYS
1	E	34	LYS
1	E	42	LYS
1	E	43	LEU
1	E	55	ASP
1	E	59	ILE
1	E	102	LYS
1	E	142	LYS
1	E	172	GLU
1	E	218	ASN
1	E	341	TYR
1	E	376	ARG
1	E	382	ARG
1	E	388	LEU
1	E	390	GLN
1	E	426	GLN
1	E	435	GLU
1	E	440	THR
1	E	449	SER
1	E	454	ARG
1	F	26	LYS
1	F	34	LYS
1	F	42	LYS
1	F	43	LEU
1	F	55	ASP
1	F	59	ILE
1	F	102	LYS
1	F	142	LYS
1	F	172	GLU
1	F	218	ASN

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Mol	Chain	Res	Type
1	F	341	TYR
1	F	376	ARG
1	F	382	ARG
1	F	388	LEU
1	F	390	GLN
1	F	426	GLN
1	F	435	GLU
1	F	440	THR
1	F	449	SER
1	F	454	ARG
1	G	26	LYS
1	G	34	LYS
1	G	42	LYS
1	G	59	ILE
1	G	65	ASP
1	G	172	GLU
1	G	175	LYS
1	G	184	ASP
1	G	218	ASN
1	G	237	THR
1	G	239	LYS
1	G	256	LYS
1	G	278	GLU
1	G	337	SER
1	G	365	GLN
1	G	369	THR
1	G	372	ARG
1	G	376	ARG
1	G	382	ARG
1	G	390	GLN
1	G	411	HIS
1	G	426	GLN
1	G	428	GLN
1	G	429	LYS
1	G	445	LEU
1	G	451	GLU
1	G	456	ARG
1	H	26	LYS
1	H	30	ASP
1	H	34	LYS
1	H	42	LYS
1	H	59	ILE

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Mol	Chain	Res	Type
1	H	65	ASP
1	H	145	SER
1	H	172	GLU
1	H	175	LYS
1	H	184	ASP
1	H	237	THR
1	H	239	LYS
1	H	256	LYS
1	H	278	GLU
1	H	320	THR
1	H	337	SER
1	H	365	GLN
1	H	369	THR
1	H	376	ARG
1	H	382	ARG
1	H	390	GLN
1	H	411	HIS
1	H	428	GLN
1	H	445	LEU
1	H	451	GLU
1	H	455	LEU
1	H	456	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	GLN
1	A	86	GLN
1	A	218	ASN
1	A	383	ASN
1	A	390	GLN
1	A	411	HIS
1	B	49	GLN
1	B	64	HIS
1	B	86	GLN
1	B	173	ASN
1	B	218	ASN
1	B	389	GLN
1	B	390	GLN
1	C	64	HIS
1	C	72	GLN
1	C	86	GLN

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Mol	Chain	Res	Type
1	C	124	ASN
1	C	152	GLN
1	C	218	ASN
1	C	234	ASN
1	C	390	GLN
1	C	405	GLN
1	D	64	HIS
1	D	72	GLN
1	D	152	GLN
1	D	173	ASN
1	D	218	ASN
1	D	234	ASN
1	D	389	GLN
1	D	390	GLN
1	D	405	GLN
1	D	446	GLN
1	E	49	GLN
1	E	64	HIS
1	E	86	GLN
1	E	218	ASN
1	E	390	GLN
1	F	49	GLN
1	F	64	HIS
1	F	86	GLN
1	F	218	ASN
1	F	386	HIS
1	F	389	GLN
1	F	390	GLN
1	G	64	HIS
1	G	72	GLN
1	G	124	ASN
1	G	152	GLN
1	G	218	ASN
1	G	234	ASN
1	G	390	GLN
1	G	405	GLN
1	G	426	GLN
1	H	18	ASN
1	H	64	HIS
1	H	86	GLN
1	H	124	ASN
1	H	152	GLN

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Mol	Chain	Res	Type
1	H	218	ASN
1	H	234	ASN
1	H	390	GLN
1	H	428	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)

There are no ligands in this entry.

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	451/471 (95%)	0.02	6 (1%)	77	72	2, 25, 60, 86	0
1	B	451/471 (95%)	-0.03	10 (2%)	62	52	2, 24, 60, 85	0
1	C	451/471 (95%)	0.16	20 (4%)	34	24	2, 38, 61, 80	0
1	D	451/471 (95%)	0.34	36 (7%)	12	6	2, 38, 62, 81	0
1	E	451/471 (95%)	0.16	20 (4%)	34	24	2, 25, 60, 85	0
1	F	451/471 (95%)	0.24	20 (4%)	34	24	2, 24, 60, 85	0
1	G	451/471 (95%)	1.48	131 (29%)	0	0	2, 37, 60, 79	0
1	H	451/471 (95%)	0.04	6 (1%)	77	72	2, 33, 59, 83	0
All	All	3608/3768 (95%)	0.30	249 (6%)	16	10	2, 31, 60, 86	0

All (249) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	52	ALA	18.7
1	G	53	THR	16.0
1	G	266	ILE	11.4
1	E	5	GLY	10.8
1	C	370	ALA	10.0
1	E	457	ARG	9.6
1	G	330	MET	9.2
1	G	265	GLY	9.1
1	G	6	LYS	7.1
1	E	4	GLU	7.0
1	A	53	THR	6.9
1	G	264	ALA	6.7
1	G	135	LEU	6.5
1	G	190	ALA	6.5
1	G	7	LEU	6.2
1	C	53	THR	6.2

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Mol	Chain	Res	Type	RSRZ
1	G	276	ALA	6.1
1	G	9	ILE	6.1
1	G	156	PHE	6.0
1	G	289	GLY	5.7
1	G	198	LEU	5.7
1	G	4	GLU	5.7
1	E	6	LYS	5.7
1	G	134	ALA	5.7
1	A	52	ALA	5.6
1	G	110	VAL	5.5
1	F	4	GLU	5.4
1	G	262	LEU	5.3
1	G	228	GLY	5.3
1	G	201	ASN	5.3
1	G	106	TYR	5.2
1	G	33	ILE	5.2
1	D	357	VAL	5.2
1	G	35	VAL	5.1
1	G	197	ASP	5.0
1	G	299	LEU	5.0
1	F	285	LEU	5.0
1	G	456	ARG	5.0
1	G	457	ARG	4.9
1	G	347	VAL	4.8
1	G	59	ILE	4.8
1	G	169	PHE	4.7
1	C	52	ALA	4.7
1	D	7	LEU	4.7
1	G	20	LEU	4.6
1	G	28	GLU	4.6
1	D	347	VAL	4.6
1	G	30	ASP	4.6
1	G	34	LYS	4.6
1	E	7	LEU	4.5
1	H	4	GLU	4.5
1	G	31	THR	4.5
1	G	365	GLN	4.4
1	F	274	GLU	4.4
1	B	5	GLY	4.3
1	G	146	ALA	4.2
1	D	4	GLU	4.2
1	F	41	ASP	4.2

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Mol	Chain	Res	Type	RSRZ
1	G	341	TYR	4.2
1	D	56	GLY	4.1
1	D	454	ARG	4.1
1	F	5	GLY	4.1
1	G	339	PHE	4.1
1	G	357	VAL	4.1
1	G	108	ILE	4.0
1	G	58	ASP	4.0
1	A	6	LYS	4.0
1	D	135	LEU	4.0
1	G	260	GLY	4.0
1	G	151	LEU	3.9
1	G	78	GLU	3.9
1	G	343	VAL	3.9
1	G	279	PHE	3.9
1	G	350	ALA	3.8
1	G	351	ALA	3.8
1	G	263	SER	3.8
1	G	176	TYR	3.8
1	G	92	PHE	3.7
1	C	59	ILE	3.7
1	G	36	THR	3.7
1	G	292	ALA	3.7
1	G	352	SER	3.7
1	C	341	TYR	3.7
1	G	224	MET	3.6
1	B	52	ALA	3.6
1	G	5	GLY	3.6
1	C	60	ILE	3.6
1	D	32	GLY	3.6
1	G	32	GLY	3.6
1	D	195	LEU	3.6
1	G	75	LEU	3.6
1	F	52	ALA	3.6
1	G	329	ILE	3.5
1	G	252	GLY	3.5
1	D	352	SER	3.5
1	C	371	ALA	3.5
1	G	84	ALA	3.5
1	D	55	ASP	3.4
1	G	248	PRO	3.4
1	B	457	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
1	G	337	SER	3.4
1	G	274	GLU	3.4
1	C	457	ARG	3.4
1	A	172	GLU	3.4
1	G	303	ALA	3.3
1	G	258	PHE	3.3
1	G	367	ARG	3.3
1	G	280	LEU	3.2
1	G	157	THR	3.2
1	D	132	ILE	3.2
1	G	285	LEU	3.2
1	D	49	GLN	3.2
1	D	200	LYS	3.2
1	E	275	LEU	3.2
1	G	47	PHE	3.2
1	C	330	MET	3.1
1	E	8	VAL	3.1
1	G	320	THR	3.1
1	G	10	TRP	3.1
1	C	284	LEU	3.1
1	G	304	LEU	3.1
1	G	77	ALA	3.0
1	G	253	GLN	3.0
1	F	456	ARG	3.0
1	G	269	ALA	3.0
1	F	390	GLN	3.0
1	C	21	ALA	3.0
1	F	37	VAL	3.0
1	D	106	TYR	3.0
1	E	283	TYR	2.9
1	G	293	VAL	2.9
1	H	456	ARG	2.9
1	D	453	GLU	2.9
1	D	456	ARG	2.9
1	B	6	LYS	2.9
1	G	230	TRP	2.9
1	G	328	GLU	2.9
1	E	37	VAL	2.9
1	G	141	ALA	2.8
1	H	330	MET	2.8
1	G	27	PHE	2.8
1	F	266	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	G	237	THR	2.8
1	G	272	ASN	2.8
1	F	10	TRP	2.7
1	G	178	ILE	2.7
1	D	280	LEU	2.7
1	G	37	VAL	2.7
1	G	275	LEU	2.7
1	F	53	THR	2.7
1	G	232	TRP	2.7
1	F	76	LEU	2.7
1	F	6	LYS	2.7
1	D	194	PHE	2.7
1	G	307	TYR	2.7
1	G	227	ASN	2.7
1	G	183	VAL	2.6
1	A	4	GLU	2.6
1	F	99	TYR	2.6
1	D	378	VAL	2.6
1	F	54	GLY	2.6
1	D	274	GLU	2.6
1	G	160	LEU	2.6
1	B	274	GLU	2.6
1	D	361	LEU	2.6
1	G	353	GLY	2.6
1	G	331	PRO	2.6
1	F	56	GLY	2.6
1	D	276	ALA	2.6
1	E	52	ALA	2.6
1	G	168	ALA	2.6
1	D	178	ILE	2.6
1	G	167	TYR	2.6
1	G	294	ASN	2.5
1	D	35	VAL	2.5
1	G	112	ALA	2.5
1	G	434	LEU	2.5
1	E	456	ARG	2.5
1	G	121	LEU	2.5
1	E	285	LEU	2.5
1	G	61	PHE	2.5
1	G	340	TRP	2.5
1	G	49	GLN	2.5
1	G	259	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	G	195	LEU	2.5
1	B	33	ILE	2.4
1	G	132	ILE	2.4
1	G	273	LYS	2.4
1	D	181	VAL	2.4
1	C	369	THR	2.4
1	G	287	ASP	2.4
1	G	129	TRP	2.4
1	B	4	GLU	2.4
1	G	186	ALA	2.4
1	C	266	ILE	2.4
1	C	456	ARG	2.4
1	F	7	LEU	2.4
1	D	349	ASN	2.3
1	G	300	GLY	2.3
1	G	200	LYS	2.3
1	H	5	GLY	2.3
1	D	10	TRP	2.3
1	E	47	PHE	2.3
1	G	98	ARG	2.3
1	D	29	LYS	2.3
1	G	113	LEU	2.3
1	D	33	ILE	2.3
1	H	172	GLU	2.3
1	C	220	GLY	2.2
1	G	223	ALA	2.2
1	D	273	LYS	2.2
1	E	58	ASP	2.2
1	G	127	LYS	2.2
1	G	203	HIS	2.2
1	B	53	THR	2.2
1	C	78	GLU	2.2
1	G	226	ILE	2.2
1	B	106	TYR	2.2
1	F	8	VAL	2.2
1	D	173	ASN	2.2
1	G	392	LEU	2.2
1	G	93	THR	2.2
1	G	145	SER	2.2
1	G	368	ILE	2.2
1	A	42	LYS	2.2
1	G	149	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	167	TYR	2.2
1	G	283	TYR	2.2
1	D	363	ASP	2.2
1	G	131	GLU	2.2
1	B	330	MET	2.1
1	E	66	ARG	2.1
1	D	5	GLY	2.1
1	G	361	LEU	2.1
1	C	161	ILE	2.1
1	E	35	VAL	2.1
1	C	367	ARG	2.1
1	D	279	PHE	2.1
1	E	284	LEU	2.1
1	E	103	LEU	2.1
1	C	277	LYS	2.1
1	G	261	VAL	2.1
1	E	265	GLY	2.0
1	F	38	GLU	2.0
1	G	191	GLY	2.0
1	E	388	LEU	2.0
1	D	302	VAL	2.0
1	H	85	PHE	2.0
1	G	50	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.