Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:42 AM GMT

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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

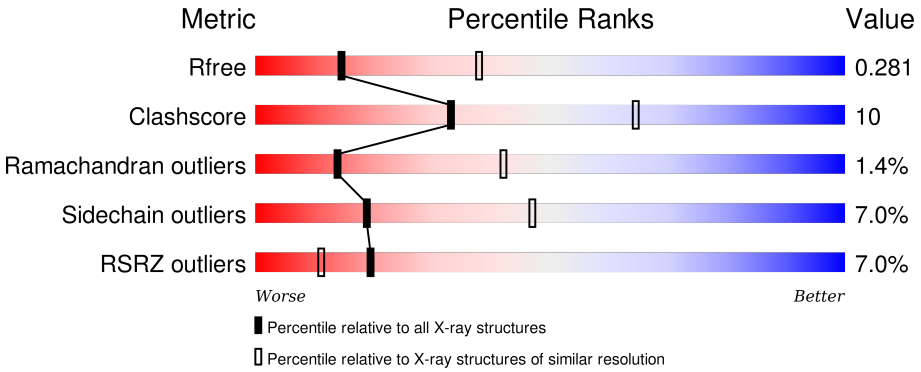
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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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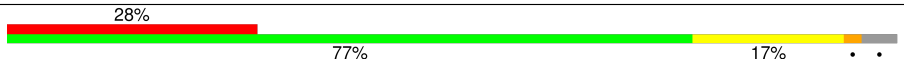
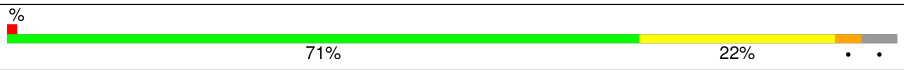
Mol	Chain	Length	Quality of chain
1	F	471	
1	G	471	
1	H	471	

2 Entry composition

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
1	A	454	Total	C	N	O	S	Se	0	0	0
			3520	2240	591	680	6	3			
1	B	454	Total	C	N	O	S	Se	0	0	0
			3520	2240	591	680	6	3			
1	C	454	Total	C	N	O	S	Se	0	0	0
			3520	2240	591	680	6	3			
1	D	454	Total	C	N	O	S	Se	0	0	0
			3520	2240	591	680	6	3			
1	E	454	Total	C	N	O	S	Se	0	0	0
			3520	2240	591	680	6	3			
1	F	454	Total	C	N	O	S	Se	0	0	0
			3520	2240	591	680	6	3			
1	G	454	Total	C	N	O	S	Se	0	0	0
			3520	2240	591	680	6	3			
1	H	454	Total	C	N	O	S	Se	0	0	0
			3520	2240	591	680	6	3			

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
2	A	12	Total O 12 12	0	0
2	B	19	Total O 19 19	0	0
2	C	2	Total O 2 2	0	0
2	D	6	Total O 6 6	0	0
2	E	11	Total O 11 11	0	0
2	F	5	Total O 5 5	0	0
2	G	1	Total O 1 1	0	0

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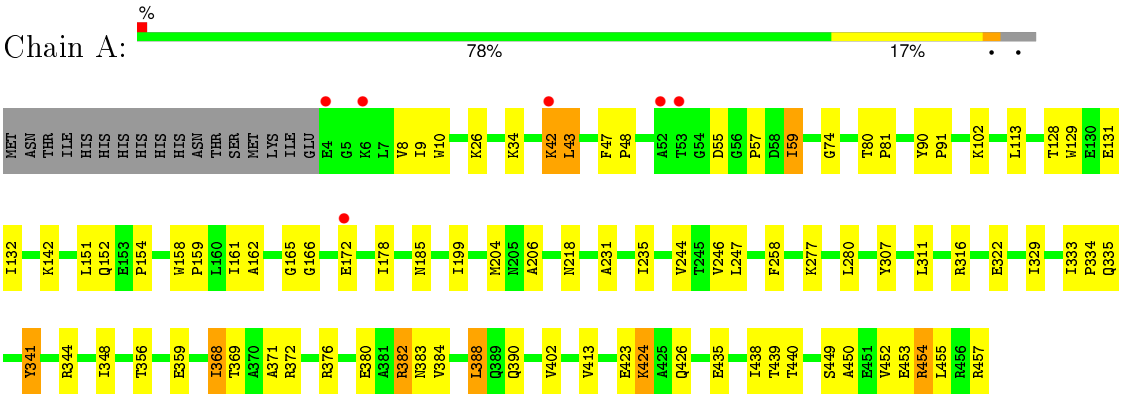
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	H	9	Total O 9 9	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

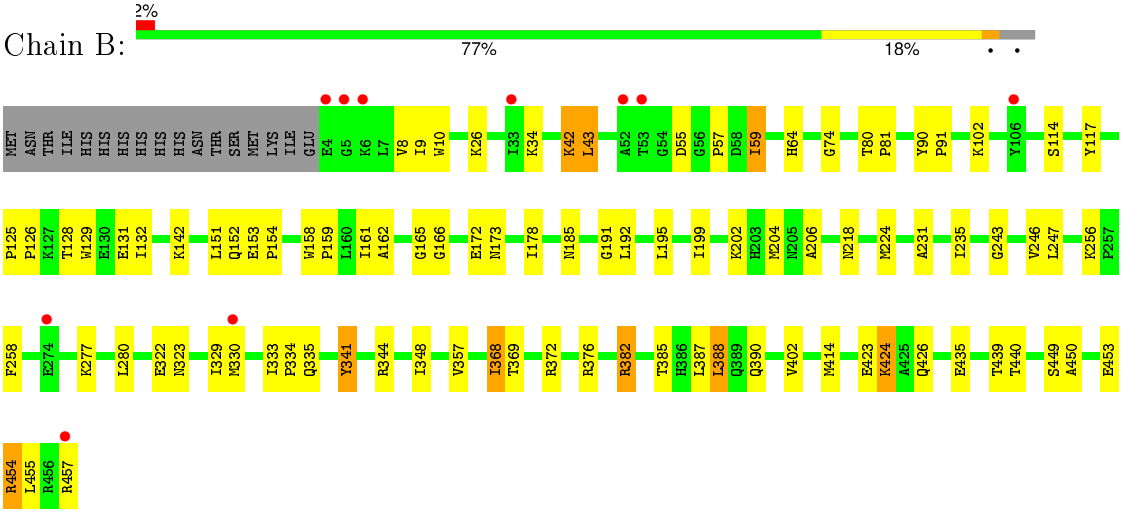
- Molecule 1: Bone marrow stromal antigen 2 fused to Maltose-binding periplasmic protein

Chain A:



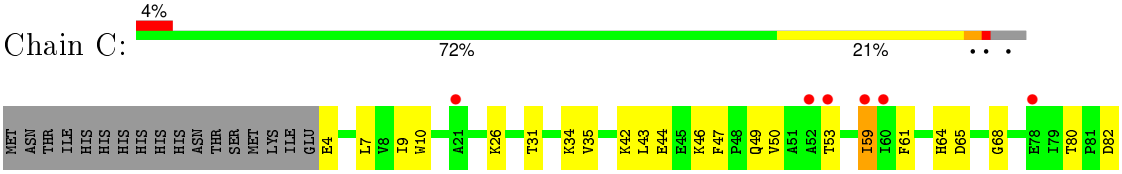
- Molecule 1: Bone marrow stromal antigen 2 fused to Maltose-binding periplasmic protein

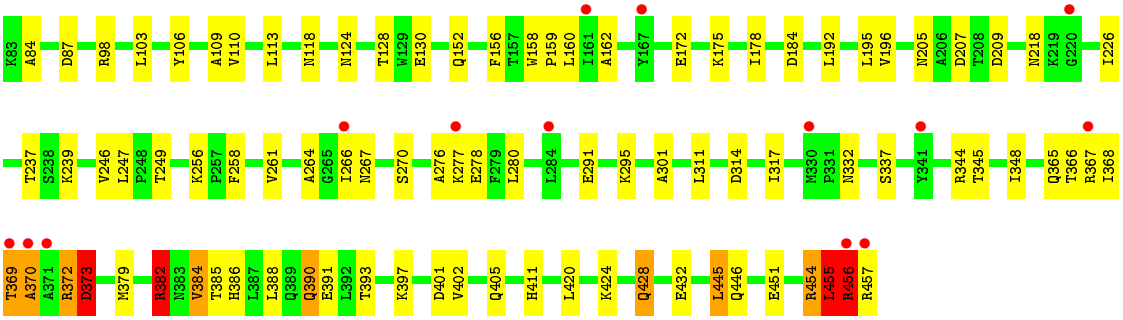
Chain B:



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

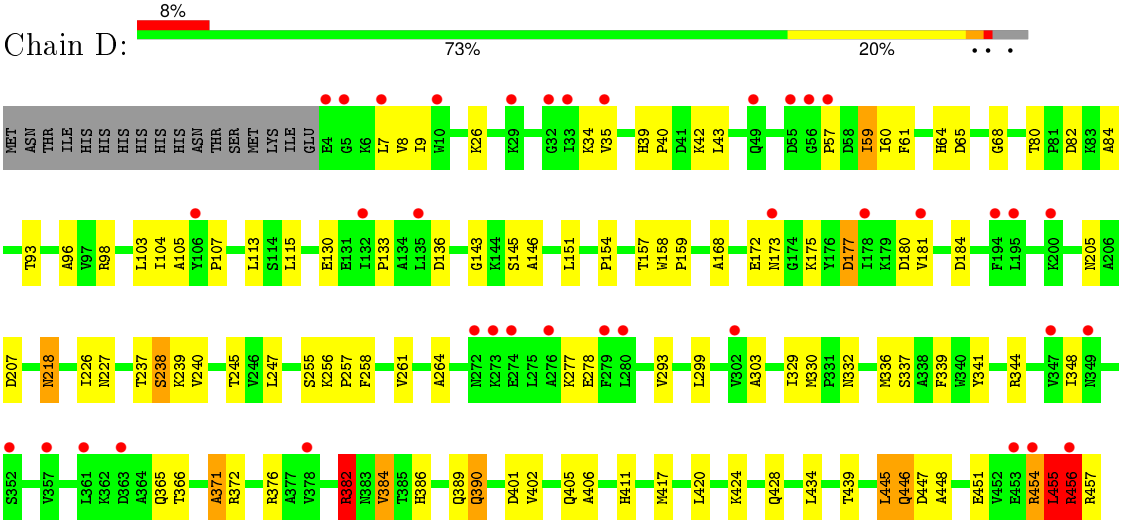
Chain C:





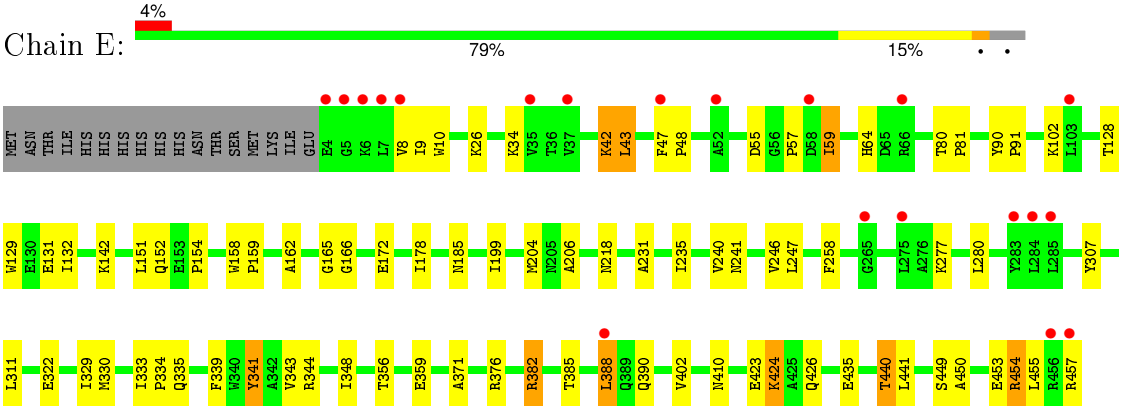
• Molecule 1: Bone marrow stromal antigen 2 fused to Maltose-binding periplasmic protein

Chain D:



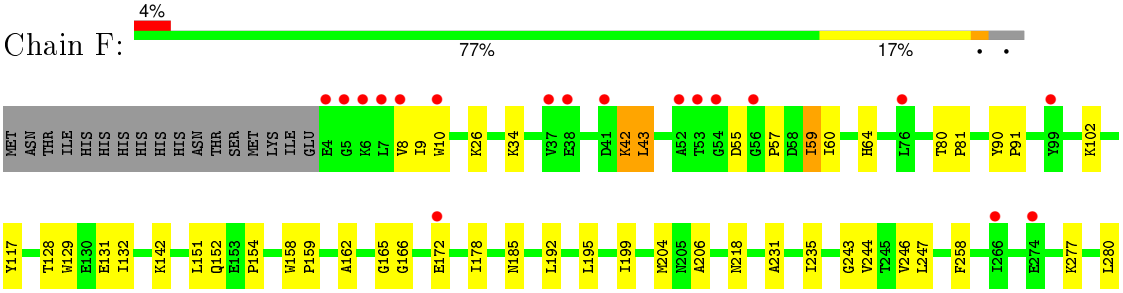
• Molecule 1: Bone marrow stromal antigen 2 fused to Maltose-binding periplasmic protein

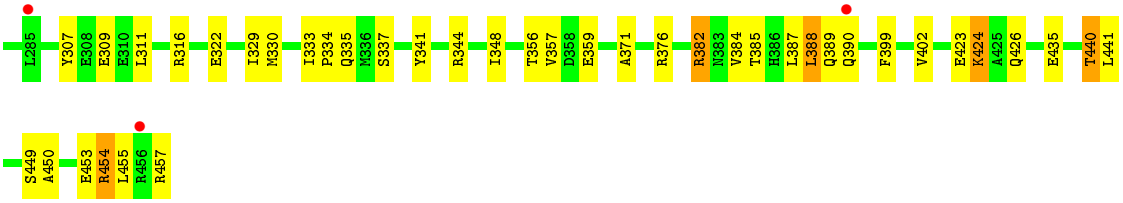
Chain E:



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

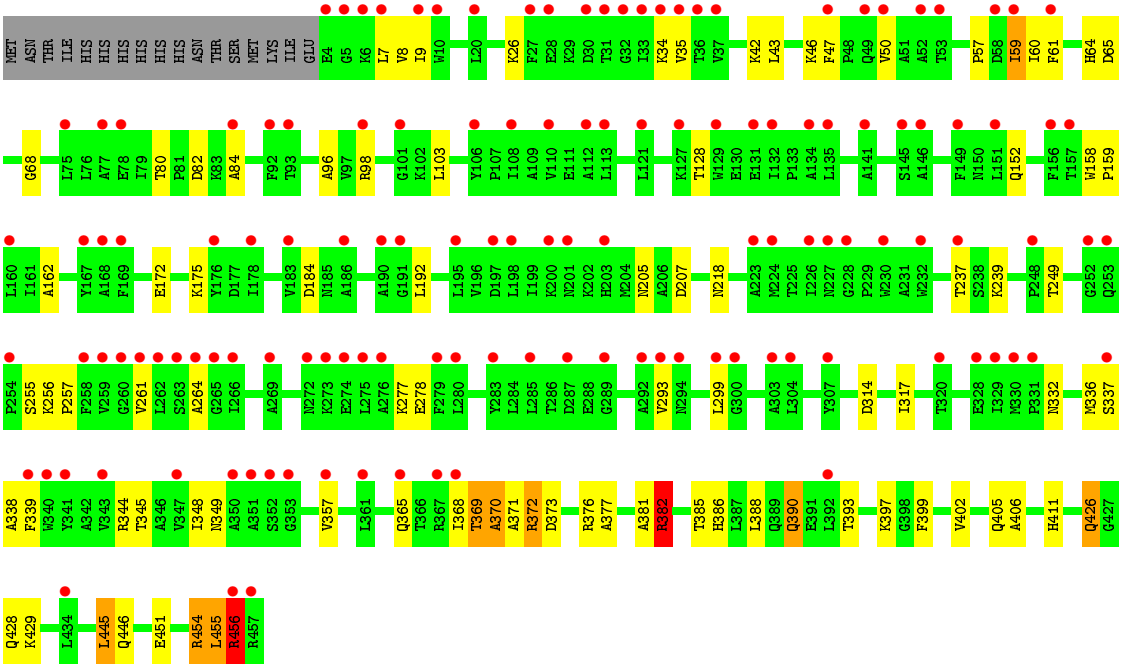
Chain F:





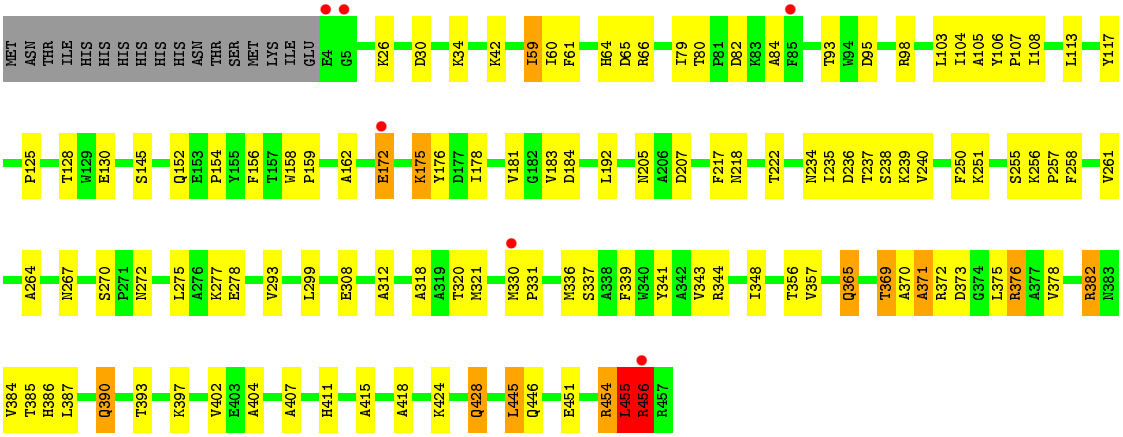
• Molecule 1: Bone marrow stromal antigen 2 fused to Maltose-binding periplasmic protein

Chain G:



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

Chain H:



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 (5.28%)	DCC
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
Estimated twinning fraction	0.066 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 94564 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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:NH1	1:D:456:ARG:HB3	1.25	1.49
1:D:456:ARG:CB	1:D:456:ARG:HH11	1.38	1.36
1:C:456:ARG:NH1	1:C:456:ARG:HB3	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:NH1	1:H:456:ARG:HB2	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:C:456:ARG:HB3	1:C:456:ARG:CZ	1.78	1.09
1:A:402:VAL:CG1	1:D:402:VAL:HG11	1.81	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:HB3	1:H:456:ARG:CZ	1.81	1.05
1:B:455:LEU:HD13	1:C:456:ARG:NH1	1.71	1.04
1:G:456:ARG:HB2	1:G:456:ARG:NH1	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:HB3	1:G:456:ARG:CZ	1.89	1.00
1:G:456:ARG:CB	1:G:456:ARG:CZ	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:H:370:ALA:CB	1:H:371:ALA:HB3	1.95	0.88
1:D:371:ALA:CB	1:D:372:ARG:HA	2.03	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: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:402:VAL:HG11	1:H:402:VAL:HG11	1.56	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:455:LEU:HD13	1:D:456:ARG:HH12	1.33	0.86
1:A:450:ALA:HB1	1:A:454:ARG:HH21	1.39	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:CB	1:H:456:ARG:NH1	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:CB	1:G:456:ARG:NH1	2.43	0.81
1:B:450:ALA:HB1	1:B:454:ARG:HH21	1.43	0.81
1:F:455:LEU:HD13	1:G:456:ARG:NH2	1.96	0.81
1:E:402:VAL:CG1	1:H:402:VAL:HG11	2.10	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:G:368:ILE:O	1:G:369:THR:HG22	1.87	0.74
1:C:382:ARG:HH11	1:C:382:ARG:HG2	1.53	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:H:371:ALA:HB3	1:H:376:ARG:NH1	2.04	0.73
1:F:455:LEU:HD13	1:G:456:ARG:HH22	1.53	0.73
1:A:9:ILE:HG12	1:A:59:ILE:HG23	1.71	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:HH11	1:D:382:ARG:HG2	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:HH11	1:C:456:ARG:CB	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:HG2	1:H:382:ARG:HH11	1.58	0.69
1:H:454:ARG:O	1:H:456:ARG:N	2.26	0.69
1:F:455:LEU:HD13	1:G:456:ARG:CZ	2.22	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:H:445:LEU:C	1:H:445:LEU:HD23	2.17	0.65
1:G:98:ARG:HG2	1:G:103:LEU:HD23	1.77	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:H:64:HIS:HD2	1:H:261:VAL:H	1.44	0.63
1:A:380:GLU:OE1	1:C:391:GLU:OE2	2.17	0.63
1:G:456:ARG:HB2	1:G:456:ARG:HH11	1.63	0.62
1:G:373:ASP:OD2	1:G:377:ALA:HB2	1.99	0.62
1:B:453:GLU:O	1:B:457:ARG:HG3	1.99	0.62
1:F:399:PHE:CE2	1:G:399:PHE:CE2	2.87	0.62
1:C:366:THR:O	1:C:368:ILE:N	2.32	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:D:64:HIS:HD2	1:D:261:VAL:H	1.47	0.61
1:C:428:GLN:O	1:C:432:GLU:HG2	2.00	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: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:A:344:ARG:O	1:A:348:ILE:HD13	2.00	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:B:246:VAL:CG2	1:B:322:GLU:OE1	2.51	0.59
1:A:383:ASN:HD21	1:C:53:THR:CG2	2.15	0.59
1:A:402:VAL:CG1	1:D:402:VAL:CG1	2.69	0.59
1:C:43:LEU:HD12	1:C:43:LEU:C	2.23	0.59
1:H:372:ARG:HA	1:H:376:ARG:HH21	1.66	0.59
1:G:454:ARG:O	1:G:456:ARG:N	2.35	0.59
1:H:370:ALA:CA	1:H:371:ALA:HB2	2.33	0.59
1:H:59:ILE:HD11	1:H:61:PHE:CE1	2.38	0.59
1:C:80:THR:O	1:C:277:LYS:NZ	2.36	0.59
1:H:158:TRP:CE2	1:H:162:ALA:HB2	2.37	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:E:329:ILE:H	1:E:329:ILE:HD12	1.68	0.58
1:A:129:TRP:HA	1:A:132:ILE:HD12	1.84	0.58
1:C:445:LEU:HD23	1:C:445:LEU:C	2.23	0.58
1:A:423:GLU:O	1:A:424:LYS:HB2	2.03	0.58
1:D:64:HIS:HE1	1:D:330:MET:O	1.87	0.58
1:C:82:ASP:OD1	1:C:84:ALA:HB3	2.03	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:D:371:ALA:HB1	1:D:372:ARG:HA	1.83	0.57
1:A:246:VAL:CG2	1:A:322:GLU:OE1	2.51	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:G:8:VAL:HG13	1:G:57:PRO:HA	1.86	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: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: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:D:104:ILE:HD12	1:D:105:ALA:N	2.21	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:H:128:THR:HB	1:H:130:GLU:OE1	2.07	0.55
1:F:158:TRP:CE2	1:F:162:ALA:HB2	2.41	0.55
1:E:341:TYR:CE2	1:G:406:ALA:HA	2.42	0.55
1:B:59:ILE:CD1	1:B:280:LEU:HD11	2.36	0.55
1:A:154:PRO:HG3	1:A:344:ARG:HA	1.89	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:D:177:ASP:OD1	1:D:180:ASP:CB	2.51	0.55
1:B:59:ILE:CD1	1:B:280:LEU:HD21	2.37	0.55
1:F:154:PRO:HG3	1:F:344:ARG:HA	1.89	0.55
1:F:8:VAL:HG13	1:F:57:PRO:HA	1.89	0.55
1:E:128:THR:OG1	1:E:131:GLU:HG2	2.07	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:G:128:THR:HG22	1:G:249:THR:OG1	2.07	0.54
1:E:246:VAL:CG2	1:E:322:GLU:OE1	2.55	0.54
1:E:59:ILE:HD11	1:E:280:LEU:HD21	1.90	0.54
1:A:10:TRP:HB3	1:A:43:LEU:HD13	1.89	0.54
1:F:246:VAL:CG2	1:F:322:GLU:OE1	2.55	0.54
1:B:129:TRP:HA	1:B:132:ILE:HD12	1.89	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:G:388:LEU:HD23	1:H:385:THR:HG21	1.90	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:B:423:GLU:O	1:B:424:LYS:HB2	2.07	0.54
1:G:59:ILE:HD11	1:G:61:PHE:CE1	2.43	0.53
1:D:82:ASP:OD1	1:D:84:ALA:HB3	2.08	0.53
1:B:388:LEU:HB2	1:D:384:VAL:HG11	1.90	0.53
1:F:59:ILE:HD11	1:F:280:LEU:HD21	1.89	0.53
1:B:402:VAL:CG1	1:C:402:VAL:HG11	2.37	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:F:59:ILE:CD1	1:F:280:LEU:HD21	2.39	0.53
1:B:335:GLN:OE1	1:B:335:GLN:N	2.41	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:C	1:G:445:LEU:HD23	2.29	0.53
1:G:372:ARG:O	1:G:373:ASP:C	2.46	0.53
1:B:246:VAL:HG12	1:B:247:LEU:O	2.08	0.53
1:B:59:ILE:HD11	1:B:280:LEU:HD21	1.89	0.53
1:D:130:GLU:N	1:D:130:GLU:OE1	2.38	0.53
1:E:455:LEU:HD12	1:H:456:ARG:NH1	2.24	0.53
1:E:199:ILE:HG21	1:E:206:ALA:HB2	1.91	0.53
1:G:393:THR:HG22	1:G:397:LYS:HE2	1.91	0.52
1:C:68:GLY:HA3	1:C:332:ASN:O	2.09	0.52
1:G:82:ASP:OD1	1:G:84:ALA:HB3	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:218:ASN:HD22	1:D:218:ASN:N	2.07	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: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:C:386:HIS:O	1:C:390:GLN:HG2	2.08	0.52
1:H:372:ARG:N	1:H:376:ARG:NH2	2.58	0.52
1:E:59:ILE:CD1	1:E:280:LEU:HD21	2.40	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:H:370:ALA:CA	1:H:371:ALA:CB	2.88	0.51
1:E:341:TYR:HE2	1:G:406:ALA:HB2	1.74	0.51
1:F:335:GLN:N	1:F:335:GLN:OE1	2.43	0.51
1:B:128:THR:OG1	1:B:131:GLU:HG2	2.10	0.51
1:E:423:GLU:O	1:E:424:LYS:HB2	2.09	0.51
1:E:246:VAL:HG12	1:E:247:LEU:O	2.09	0.51
1:D:136:ASP:HA	1:D:146:ALA:HB2	1.93	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: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:D:7:LEU:HB2	1:D:35:VAL:HG22	1.93	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:B:117:TYR:CZ	1:B:243:GLY:HA3	2.46	0.51
1:E:388:LEU:CD2	1:F:385:THR:HG21	2.40	0.51
1:D:293:VAL:CG1	1:D:299:LEU:HD21	2.41	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:B:195:LEU:HD12	1:B:195:LEU:C	2.31	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:ILE:HD12	1:A:329:ILE:H	1.75	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:382:ARG:CG	1:G:382:ARG:HH11	2.24	0.49
1:G:336:MET:O	1:G:339:PHE:HB3	2.12	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: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:B:382:ARG:CG	1:B:382:ARG:HH11	2.26	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:C:314:ASP:HB3	1:C:317: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:A:178:ILE:HG22	1:A:333:ILE:HD12	1.94	0.49
1:G:205:ASN:ND2	1:G:207:ASP:OD1	2.45	0.49
1:D:336:MET:O	1:D:339:PHE:HB3	2.12	0.49
1:A:128:THR:OG1	1:A:131:GLU:HG2	2.13	0.49
1:F:152:GLN:O	1:F:348:ILE:HD11	2.13	0.49
1:F:399:PHE:CD2	1:G:399:PHE:CZ	3.01	0.49
1:F:382:ARG:HH11	1:F:382:ARG:CG	2.26	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:E:344:ARG:O	1:E:348:ILE:CD1	2.59	0.48
1:A:388:LEU:HD21	1:B:385:THR:CG2	2.44	0.48
1:H:158:TRP:CD1	1:H:258:PHE:CE2	3.02	0.48
1:C:266:ILE:HD13	1:C:276:ALA:HB3	1.96	0.48
1:D:104:ILE:C	1:D:104:ILE:HD12	2.34	0.48
1:A:335:GLN:OE1	1:A:335:GLN:N	2.46	0.48
1:A:382:ARG:HH11	1:A:382:ARG:CG	2.26	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: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:A:158:TRP:N	1:A:159:PRO:HD2	2.29	0.48
1:B:348:ILE:N	1:B:348:ILE:HD12	2.30	0.47
1:B:158:TRP:CD1	1:B:258:PHE:CE2	3.02	0.47
1:H:293:VAL:CG1	1:H:299:LEU:HD21	2.44	0.47
1:F:384:VAL:CG2	1:H:387:LEU:HD23	2.44	0.47
1:C:393:THR:HG22	1:C:397:LYS:HE2	1.96	0.47
1:F:399:PHE:CE2	1:G:399:PHE:CZ	3.02	0.47
1:G:390:GLN:HA	1:G:390:GLN:HE21	1.79	0.47
1:B:80:THR:O	1:B:277:LYS:NZ	2.47	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:E:158:TRP:CE2	1:E:162:ALA:HB2	2.50	0.47
1:C:47:PHE:HA	1:C:50:VAL:HG22	1.97	0.47
1:B:455:LEU:HB3	1:C:456:ARG:NH1	2.29	0.47
1:E:385:THR:OG1	1:F:389:GLN:NE2	2.48	0.47
1:C:124:ASN:N	1:C:124:ASN:HD22	2.13	0.47
1:C:369:THR:HG23	1:C:373:ASP:OD1	2.15	0.47
1:G:59:ILE:HD13	1:G:264:ALA:HB1	1.96	0.47
1:C:420:LEU:HD11	1:C:424:LYS:HE3	1.95	0.47
1:B:152:GLN:O	1:B:348:ILE:HD11	2.15	0.47
1:A:158:TRP:CE2	1:A:162:ALA:HB2	2.50	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:A:80:THR:O	1:A:277:LYS:NZ	2.48	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:H:79:ILE:HD12	1:H:106:TYR:CE1	2.50	0.47
1:F:440:THR:HG22	1:F:441:LEU:N	2.30	0.47
1:G:388:LEU:HD23	1:H:385:THR:CG2	2.44	0.46
1:E:382:ARG:HH11	1:E:382:ARG:CG	2.27	0.46
1:C:205:ASN:ND2	1:C:207:ASP:OD1	2.45	0.46
1:E:341:TYR:CE2	1:G:406:ALA:CA	2.98	0.46
1:B:158:TRP:CE2	1:B:162:ALA:HB2	2.50	0.46
1:H:154:PRO:HB3	1:H:343:VAL:HG12	1.97	0.46
1:G:64:HIS:CD2	1:G:261:VAL:H	2.33	0.46
1:E:80:THR:O	1:E:277:LYS:NZ	2.49	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:G:426:GLN:NE2	1:G:426:GLN:HA	2.29	0.46
1:C:109:ALA:O	1:C:261:VAL:HA	2.15	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:387:LEU:HD22	1:H:341:TYR:CE2	2.51	0.46
1:F:80:THR:O	1:F:277:LYS:NZ	2.49	0.46
1:G:9:ILE:HG23	1:G:59:ILE:HG13	1.98	0.46
1:C:158:TRP:HB3	1:C:159:PRO:CD	2.46	0.46
1:H:336:MET:O	1:H:339:PHE:HB3	2.16	0.46
1:H:455:LEU:C	1:H:456:ARG:HG3	2.35	0.46
1:C:195:LEU:O	1:C:195:LEU:HD12	2.16	0.46
1:E:335:GLN:N	1:E:335:GLN:OE1	2.48	0.46
1:H:218:ASN:HD21	1:H:235:ILE:HG12	1.81	0.46
1:A:231:ALA:O	1:A:235:ILE:HG13	2.15	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:D:344:ARG:O	1:D:348:ILE:CD1	2.63	0.45
1:C:160:LEU:O	1:C:160:LEU:HD12	2.15	0.45
1:G:369:THR:O	1:G:370:ALA:HB2	2.15	0.45
1:C:59:ILE:HD11	1:C:61:PHE:CD1	2.52	0.45
1:H:415:ALA:O	1:H:418:ALA:HB3	2.16	0.45
1:H:344:ARG:O	1:H:348:ILE:HD12	2.15	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:H:371:ALA:O	1:H:372:ARG:HB2	2.15	0.45
1:H:376:ARG:HB3	1:H:376:ARG:HE	1.35	0.45
1:B:368:ILE:CG2	1:B:369:THR:HG23	2.46	0.45
1:A:244:VAL:HB	1:A:316:ARG:HG2	1.99	0.45
1:A:90:TYR:HA	1:A:91:PRO:HD2	1.79	0.45
1:F:166:GLY:HA2	1:F:185:ASN:HD21	1.81	0.45
1:D:371:ALA:C	1:D:376:ARG:NH2	2.60	0.45
1:A:158:TRP:HB3	1:A:159:PRO:HD3	1.98	0.45
1:F:59:ILE:CD1	1:F:280:LEU:HD11	2.46	0.45
1:H:445:LEU:HD23	1:H:446:GLN:N	2.31	0.45
1:E:246:VAL:HG21	1:E:322:GLU:OE1	2.17	0.45
1:G:59:ILE:HD12	1:G:60:ILE:N	2.32	0.45
1:C:118:ASN:OD1	1:C:118:ASN:C	2.55	0.45
1:G:393:THR:OG1	1:H:382:ARG:NH2	2.50	0.45
1:H:59:ILE:HD13	1:H:264:ALA:HB1	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:152:GLN:HE22	1:C:207:ASP:HA	1.82	0.45
1:E:450:ALA:CB	1:E:454:ARG:HH21	2.21	0.45
1:C:393:THR:HG23	1:D:382:ARG:NH2	2.32	0.45
1:G:345:THR:HG22	1:G:349:ASN:ND2	2.31	0.45
1:F:246:VAL:HG12	1:F:247:LEU:O	2.17	0.45
1:B:388:LEU:HD11	1:C:388:LEU:HD21	1.98	0.45
1:H:234:ASN:HA	1:H:234:ASN:HD22	1.61	0.45
1:A:402:VAL:HG13	1:D:402:VAL:CG1	2.43	0.44
1:H:382:ARG:CG	1:H:382:ARG:HH11	2.28	0.44
1:C:226:ILE:HD13	1:C:247:LEU:HD22	1.98	0.44
1:C:61:PHE:CE2	1:C:264:ALA:HB2	2.52	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: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:D:39:HIS:N	1:D:40:PRO:CD	2.80	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:C:291:GLU:O	1:C:295:LYS:HG3	2.17	0.44
1:H:152:GLN:HE22	1:H:207:ASP:HA	1.83	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:O	1:F:195:LEU:HD12	2.16	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:G:370:ALA:C	1:G:372:ARG:H	2.20	0.44
1:G:152:GLN:NE2	1:G:207:ASP:HA	2.33	0.44
1:C:158:TRP:CD1	1:C:258:PHE:CE2	3.06	0.44
1:A:438:ILE:CD1	1:D:434:LEU:HD22	2.48	0.44
1:D:456:ARG:HB3	1:D:456:ARG:HH11	0.45	0.44
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: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:A:388:LEU:CD2	1:B:385:THR:HG21	2.48	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
1:F:244:VAL:HB	1:F:316:ARG:HG2	2.00	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:E:158:TRP:N	1:E:159:PRO:HD2	2.34	0.43
1:F:117:TYR:CE1	1:F:243:GLY:HA3	2.53	0.43
1:D:154:PRO:HA	1:D:157:THR:OG1	2.19	0.43
1:F:64:HIS:CE1	1:F:330:MET:O	2.72	0.43
1:E:455:LEU:CD1	1:H:456:ARG:HH12	2.30	0.43
1:D:434:LEU:HD23	1:D:434:LEU:HA	1.82	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: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:B:117:TYR:CE2	1:B:125:PRO:HD3	2.54	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:A:307:TYR:CE2	1:A:311:LEU:HD11	2.53	0.43
1:C:113:LEU:HD11	1:C:156:PHE:HA	2.01	0.43
1:D:151:LEU:HD12	1:D:205:ASN:O	2.19	0.43
1:C:209:ASP:C	1:C:209:ASP:OD1	2.56	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:H:104:ILE:HD12	1:H:105:ALA:N	2.33	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: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:H:371:ALA:CB	1:H:376:ARG:CZ	2.97	0.42
1:G:59:ILE:HD11	1:G:61:PHE:CD1	2.54	0.42
1:A:199:ILE:HG21	1:A:206:ALA:HB2	2.02	0.42
1:H:424:LYS:O	1:H:428:GLN:HB3	2.19	0.42
1:E:455:LEU:CB	1:H:456:ARG:CZ	2.88	0.42
1:D:293:VAL:HG11	1:D:299:LEU:HD21	2.02	0.42
1:D:447:ASP:O	1:D:448:ALA:C	2.58	0.42
1:G:344:ARG:O	1:G:348:ILE:CD1	2.68	0.42
1:D:68:GLY:HA3	1:D:332:ASN:O	2.20	0.42

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:388:LEU:HD11	1:G:388:LEU:HD21	2.02	0.41
1:A:383:ASN:ND2	1:C:53:THR:CG2	2.84	0.41
1:C:43:LEU:HD12	1:C:44:GLU:N	2.36	0.41
1:B:64:HIS:CE1	1:B:330:MET:O	2.74	0.41
1:A:47:PHE:N	1:A:48:PRO:HD2	2.36	0.41
1:F:90:TYR:HA	1:F:91:PRO:HD2	1.78	0.41
1:E:388:LEU:HD23	1:F:385:THR:HG21	2.03	0.41
1:D:158:TRP:N	1:D:159:PRO:HD2	2.35	0.41
1:C:64:HIS:CD2	1:C:261:VAL:H	2.38	0.41
1:H:393:THR:HG22	1:H:397:LYS:HE2	2.03	0.41
1:B:114:SER:HA	1:B:323:ASN:ND2	2.35	0.41
1:D:93:THR:HG21	1:D:303:ALA:CB	2.51	0.41
1:H:375:LEU:O	1:H:378:VAL:HB	2.21	0.41
1:C:7:LEU:HB2	1:C:35:VAL:HG22	2.03	0.41
1:D:456:ARG:O	1:D:457:ARG:HG3	2.21	0.40
1:C:382:ARG:NH1	1:C:382:ARG:HG2	2.30	0.40
1:H:238:SER:OG	1:H:240:VAL:HG23	2.21	0.40
1:H:176:TYR:CZ	1:H:331:PRO:HA	2.56	0.40
1:F:455:LEU:HD12	1:G:456:ARG:NH1	2.34	0.40
1:H:158:TRP:HB3	1:H:159:PRO:HD3	2.03	0.40
1:H:93:THR:O	1:H:107:PRO:HG3	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: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:C:152:GLN:NE2	1:C:207:ASP:HA	2.35	0.40
1:B:90:TYR:O	1:B:91:PRO:C	2.60	0.40
1:D:96:ALA:HB2	1:D:329:ILE:CG2	2.51	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:G:455:LEU:C	1:G:456:ARG:HG3	2.41	0.40
1:G:455:LEU:O	1:G:456:ARG:CB	2.68	0.40
1:G:344:ARG:O	1:G:348:ILE:HD12	2.21	0.40
1:A:413:VAL:HG11	1:B:153:GLU:OE2	2.22	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:G:369:THR:HG23	1:G:369:THR:O	2.21	0.40
1:A:388:LEU:CD2	1:B:385:THR:CG2	3.00	0.40
1:F:382:ARG:NH1	1:F:382:ARG:CG	2.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:293:VAL:CG1	1:G:299:LEU:HD21	2.52	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%)	13	40
1	B	452/471 (96%)	425 (94%)	21 (5%)	6 (1%)	15	44
1	C	452/471 (96%)	414 (92%)	30 (7%)	8 (2%)	11	34
1	D	452/471 (96%)	417 (92%)	30 (7%)	5 (1%)	17	50
1	E	452/471 (96%)	424 (94%)	22 (5%)	6 (1%)	15	44
1	F	452/471 (96%)	422 (93%)	24 (5%)	6 (1%)	15	44
1	G	452/471 (96%)	427 (94%)	20 (4%)	5 (1%)	17	50
1	H	452/471 (96%)	413 (91%)	33 (7%)	6 (1%)	15	44
All	All	3616/3768 (96%)	3361 (93%)	206 (6%)	49 (1%)	14	42

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%)	22	52
1	B	362/376 (96%)	339 (94%)	23 (6%)	22	52
1	C	362/376 (96%)	332 (92%)	30 (8%)	14	38
1	D	362/376 (96%)	330 (91%)	32 (9%)	12	35
1	E	362/376 (96%)	342 (94%)	20 (6%)	27	59
1	F	362/376 (96%)	342 (94%)	20 (6%)	27	59
1	G	362/376 (96%)	335 (92%)	27 (8%)	17	43
1	H	362/376 (96%)	335 (92%)	27 (8%)	17	43
All	All	2896/3008 (96%)	2694 (93%)	202 (7%)	19	47

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

Some 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

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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, 95^{th} 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%)	0.03	6 (1%) 79 71	2, 25, 60, 86	0
1	B	451/471 (95%)	-0.02	10 (2%) 65 54	2, 24, 60, 85	0
1	C	451/471 (95%)	0.17	20 (4%) 38 26	2, 38, 61, 80	0
1	D	451/471 (95%)	0.36	38 (8%) 14 6	2, 38, 62, 81	0
1	E	451/471 (95%)	0.17	20 (4%) 38 26	2, 25, 60, 85	0
1	F	451/471 (95%)	0.26	21 (4%) 35 24	2, 24, 60, 85	0
1	G	451/471 (95%)	1.51	133 (29%) 1 0	2, 37, 60, 79	0
1	H	451/471 (95%)	0.05	6 (1%) 79 71	2, 33, 59, 83	0
All	All	3608/3768 (95%)	0.32	254 (7%) 19 11	2, 31, 60, 86	0

All (254) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	52	ALA	18.6
1	G	53	THR	16.4
1	G	266	ILE	11.6
1	E	5	GLY	10.9
1	C	370	ALA	9.9
1	G	330	MET	9.4
1	G	265	GLY	9.2
1	E	457	ARG	9.2
1	G	6	LYS	7.2
1	E	4	GLU	7.1
1	A	53	THR	7.1
1	G	264	ALA	6.7
1	G	135	LEU	6.6
1	G	190	ALA	6.4
1	C	53	THR	6.4
1	G	7	LEU	6.3

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Mol	Chain	Res	Type	RSRZ
1	G	9	ILE	6.2
1	G	156	PHE	6.1
1	G	276	ALA	6.1
1	G	198	LEU	5.8
1	G	4	GLU	5.8
1	G	289	GLY	5.8
1	E	6	LYS	5.8
1	G	134	ALA	5.6
1	G	110	VAL	5.6
1	A	52	ALA	5.6
1	F	4	GLU	5.5
1	G	201	ASN	5.5
1	G	262	LEU	5.4
1	G	228	GLY	5.3
1	G	106	TYR	5.3
1	G	33	ILE	5.3
1	D	357	VAL	5.2
1	G	197	ASP	5.2
1	G	35	VAL	5.2
1	G	299	LEU	5.1
1	F	285	LEU	5.1
1	G	347	VAL	4.9
1	G	59	ILE	4.8
1	G	169	PHE	4.8
1	G	456	ARG	4.8
1	G	30	ASP	4.8
1	G	28	GLU	4.7
1	D	7	LEU	4.7
1	G	20	LEU	4.7
1	G	457	ARG	4.7
1	G	34	LYS	4.7
1	C	52	ALA	4.7
1	D	347	VAL	4.7
1	H	4	GLU	4.6
1	E	7	LEU	4.6
1	G	31	THR	4.6
1	G	365	GLN	4.5
1	F	274	GLU	4.5
1	B	5	GLY	4.4
1	F	41	ASP	4.3
1	D	4	GLU	4.3
1	G	341	TYR	4.3

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Mol	Chain	Res	Type	RSRZ
1	G	146	ALA	4.2
1	D	56	GLY	4.2
1	G	58	ASP	4.2
1	G	339	PHE	4.1
1	F	5	GLY	4.1
1	G	108	ILE	4.1
1	G	357	VAL	4.1
1	A	6	LYS	4.1
1	G	78	GLU	4.0
1	D	135	LEU	4.0
1	G	260	GLY	4.0
1	G	151	LEU	4.0
1	G	279	PHE	4.0
1	G	343	VAL	3.9
1	D	454	ARG	3.9
1	G	263	SER	3.9
1	G	176	TYR	3.9
1	G	350	ALA	3.8
1	G	36	THR	3.8
1	G	92	PHE	3.8
1	G	351	ALA	3.8
1	C	59	ILE	3.8
1	G	352	SER	3.8
1	G	224	MET	3.8
1	C	341	TYR	3.7
1	G	5	GLY	3.7
1	C	60	ILE	3.7
1	G	292	ALA	3.7
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	B	52	ALA	3.6
1	G	329	ILE	3.6
1	D	352	SER	3.6
1	G	252	GLY	3.6
1	D	55	ASP	3.5
1	G	248	PRO	3.5
1	F	52	ALA	3.5
1	C	371	ALA	3.5
1	G	274	GLU	3.5
1	G	337	SER	3.5

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Mol	Chain	Res	Type	RSRZ
1	G	84	ALA	3.5
1	A	172	GLU	3.4
1	G	157	THR	3.3
1	G	258	PHE	3.3
1	D	49	GLN	3.3
1	G	280	LEU	3.3
1	G	303	ALA	3.3
1	B	457	ARG	3.3
1	G	285	LEU	3.3
1	D	200	LYS	3.3
1	D	132	ILE	3.3
1	C	330	MET	3.2
1	C	457	ARG	3.2
1	G	47	PHE	3.2
1	E	275	LEU	3.2
1	G	320	THR	3.2
1	G	10	TRP	3.2
1	G	367	ARG	3.1
1	E	8	VAL	3.1
1	G	253	GLN	3.1
1	F	390	GLN	3.1
1	C	284	LEU	3.1
1	G	304	LEU	3.1
1	D	106	TYR	3.0
1	E	283	TYR	3.0
1	D	453	GLU	3.0
1	G	77	ALA	3.0
1	G	230	TRP	3.0
1	F	37	VAL	3.0
1	G	269	ALA	3.0
1	G	328	GLU	3.0
1	B	6	LYS	3.0
1	C	21	ALA	3.0
1	G	293	VAL	3.0
1	H	330	MET	2.9
1	E	37	VAL	2.9
1	F	456	ARG	2.9
1	G	237	THR	2.9
1	G	27	PHE	2.9
1	G	272	ASN	2.9
1	F	266	ILE	2.8
1	F	10	TRP	2.8

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Mol	Chain	Res	Type	RSRZ
1	H	456	ARG	2.8
1	G	141	ALA	2.8
1	D	456	ARG	2.8
1	F	53	THR	2.8
1	G	178	ILE	2.8
1	D	280	LEU	2.8
1	G	232	TRP	2.8
1	G	227	ASN	2.8
1	G	275	LEU	2.8
1	F	6	LYS	2.7
1	G	37	VAL	2.7
1	G	307	TYR	2.7
1	F	76	LEU	2.7
1	D	194	PHE	2.7
1	A	4	GLU	2.7
1	F	99	TYR	2.7
1	D	274	GLU	2.7
1	B	274	GLU	2.7
1	G	183	VAL	2.7
1	G	331	PRO	2.7
1	G	160	LEU	2.6
1	F	54	GLY	2.6
1	D	378	VAL	2.6
1	D	361	LEU	2.6
1	G	294	ASN	2.6
1	G	167	TYR	2.6
1	G	353	GLY	2.6
1	F	56	GLY	2.6
1	D	178	ILE	2.6
1	G	49	GLN	2.6
1	G	340	TRP	2.6
1	D	276	ALA	2.5
1	E	52	ALA	2.5
1	G	168	ALA	2.5
1	D	35	VAL	2.5
1	G	121	LEU	2.5
1	G	434	LEU	2.5
1	G	61	PHE	2.5
1	E	285	LEU	2.5
1	C	369	THR	2.5
1	G	195	LEU	2.5
1	G	287	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	G	259	VAL	2.5
1	G	273	LYS	2.5
1	B	33	ILE	2.5
1	G	112	ALA	2.5
1	G	129	TRP	2.5
1	G	132	ILE	2.4
1	D	181	VAL	2.4
1	B	4	GLU	2.4
1	D	349	ASN	2.4
1	E	456	ARG	2.4
1	F	7	LEU	2.4
1	C	266	ILE	2.4
1	D	10	TRP	2.4
1	G	200	LYS	2.4
1	G	300	GLY	2.3
1	D	29	LYS	2.3
1	G	186	ALA	2.3
1	H	5	GLY	2.3
1	E	47	PHE	2.3
1	E	58	ASP	2.3
1	H	172	GLU	2.3
1	G	113	LEU	2.3
1	D	173	ASN	2.3
1	D	33	ILE	2.3
1	C	78	GLU	2.3
1	D	273	LYS	2.3
1	G	127	LYS	2.3
1	B	53	THR	2.3
1	C	220	GLY	2.3
1	G	145	SER	2.3
1	G	203	HIS	2.3
1	G	93	THR	2.3
1	C	456	ARG	2.3
1	B	106	TYR	2.3
1	G	226	ILE	2.3
1	D	363	ASP	2.2
1	A	42	LYS	2.2
1	F	8	VAL	2.2
1	G	392	LEU	2.2
1	G	131	GLU	2.2
1	G	223	ALA	2.2
1	G	149	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	368	ILE	2.2
1	C	167	TYR	2.2
1	G	283	TYR	2.2
1	G	98	ARG	2.2
1	B	330	MET	2.2
1	D	5	GLY	2.1
1	G	361	LEU	2.1
1	C	161	ILE	2.1
1	C	277	LYS	2.1
1	E	284	LEU	2.1
1	D	279	PHE	2.1
1	E	35	VAL	2.1
1	F	38	GLU	2.1
1	E	103	LEU	2.1
1	E	265	GLY	2.1
1	G	261	VAL	2.1
1	G	191	GLY	2.1
1	D	272	ASN	2.1
1	E	388	LEU	2.1
1	H	85	PHE	2.0
1	E	66	ARG	2.0
1	D	302	VAL	2.0
1	G	50	VAL	2.0
1	D	57	PRO	2.0
1	F	172	GLU	2.0
1	C	367	ARG	2.0
1	G	101	GLY	2.0
1	G	254	PRO	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 carbohydrates 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.