Full wwPDB X-ray Structure Validation Report ⓘ

Nov 7, 2023 – 12:09 AM JST

PDB ID	:	8HGF
Title	:	Human PKM2 mutant - C326S
Authors	:	Chen, Y.-C.; Lin, K.-T.; Cheng, H.-C.
Deposited on	:	2022-11-14
Resolution	:	3.10 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 ⓘ 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 ⓘ) were used in the production of this report:

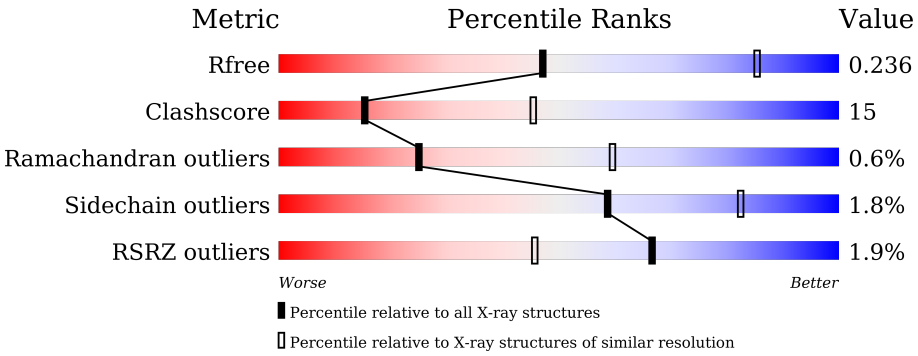
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	551	63% 27% 8%
1	B	551	61% 29% 8%
1	C	551	56% 17% 25%
1	D	551	62% 27% 8%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 30019 atoms, of which 15162 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 Pyruvate kinase PKM.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	508	Total	C	H	N	O	S	0	0	0
			7865	2447	3975	689	731	23			
1	B	508	Total	C	H	N	O	S	0	0	0
			7861	2447	3971	689	731	23			
1	D	508	Total	C	H	N	O	S	0	0	0
			7860	2447	3970	689	731	23			
1	C	414	Total	C	H	N	O	S	0	0	0
			6433	2002	3246	575	590	20			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP P14618
A	-18	GLY	-	expression tag	UNP P14618
A	-17	SER	-	expression tag	UNP P14618
A	-16	SER	-	expression tag	UNP P14618
A	-15	HIS	-	expression tag	UNP P14618
A	-14	HIS	-	expression tag	UNP P14618
A	-13	HIS	-	expression tag	UNP P14618
A	-12	ARG	-	expression tag	UNP P14618
A	-11	HIS	-	expression tag	UNP P14618
A	-10	HIS	-	expression tag	UNP P14618
A	-9	SER	-	expression tag	UNP P14618
A	-8	SER	-	expression tag	UNP P14618
A	-7	GLY	-	expression tag	UNP P14618
A	-6	LEU	-	expression tag	UNP P14618
A	-5	VAL	-	expression tag	UNP P14618
A	-4	PRO	-	expression tag	UNP P14618
A	-3	ARG	-	expression tag	UNP P14618
A	-2	GLY	-	expression tag	UNP P14618
A	-1	SER	-	expression tag	UNP P14618
A	0	HIS	-	expression tag	UNP P14618
A	326	SER	CYS	engineered mutation	UNP P14618

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	initiating methionine	UNP P14618
B	-18	GLY	-	expression tag	UNP P14618
B	-17	SER	-	expression tag	UNP P14618
B	-16	SER	-	expression tag	UNP P14618
B	-15	HIS	-	expression tag	UNP P14618
B	-14	HIS	-	expression tag	UNP P14618
B	-13	HIS	-	expression tag	UNP P14618
B	-12	ARG	-	expression tag	UNP P14618
B	-11	HIS	-	expression tag	UNP P14618
B	-10	HIS	-	expression tag	UNP P14618
B	-9	SER	-	expression tag	UNP P14618
B	-8	SER	-	expression tag	UNP P14618
B	-7	GLY	-	expression tag	UNP P14618
B	-6	LEU	-	expression tag	UNP P14618
B	-5	VAL	-	expression tag	UNP P14618
B	-4	PRO	-	expression tag	UNP P14618
B	-3	ARG	-	expression tag	UNP P14618
B	-2	GLY	-	expression tag	UNP P14618
B	-1	SER	-	expression tag	UNP P14618
B	0	HIS	-	expression tag	UNP P14618
B	326	SER	CYS	engineered mutation	UNP P14618
D	-19	MET	-	initiating methionine	UNP P14618
D	-18	GLY	-	expression tag	UNP P14618
D	-17	SER	-	expression tag	UNP P14618
D	-16	SER	-	expression tag	UNP P14618
D	-15	HIS	-	expression tag	UNP P14618
D	-14	HIS	-	expression tag	UNP P14618
D	-13	HIS	-	expression tag	UNP P14618
D	-12	ARG	-	expression tag	UNP P14618
D	-11	HIS	-	expression tag	UNP P14618
D	-10	HIS	-	expression tag	UNP P14618
D	-9	SER	-	expression tag	UNP P14618
D	-8	SER	-	expression tag	UNP P14618
D	-7	GLY	-	expression tag	UNP P14618
D	-6	LEU	-	expression tag	UNP P14618
D	-5	VAL	-	expression tag	UNP P14618
D	-4	PRO	-	expression tag	UNP P14618
D	-3	ARG	-	expression tag	UNP P14618
D	-2	GLY	-	expression tag	UNP P14618
D	-1	SER	-	expression tag	UNP P14618
D	0	HIS	-	expression tag	UNP P14618
D	326	SER	CYS	engineered mutation	UNP P14618

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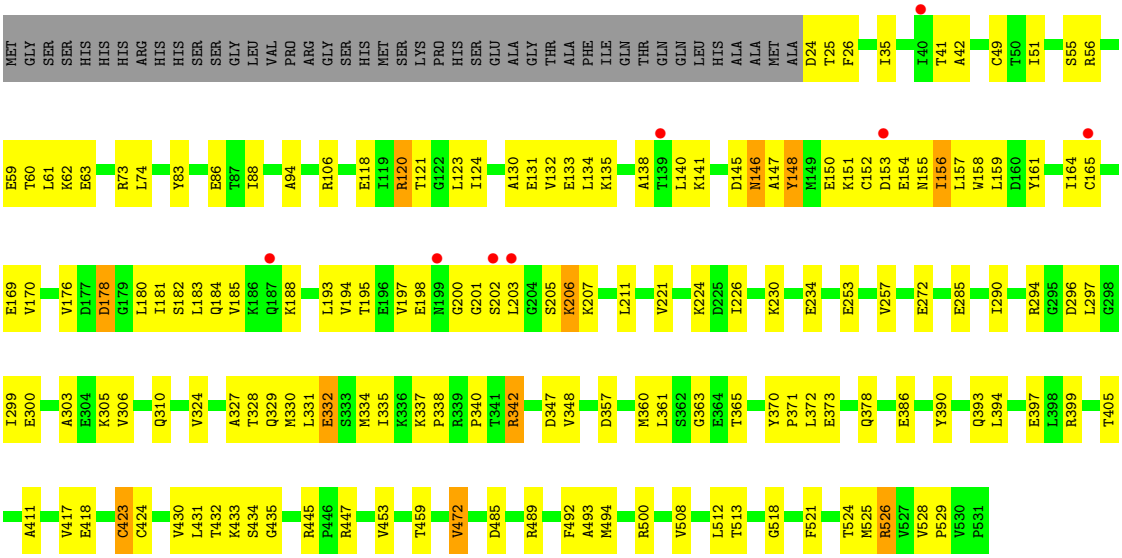
Chain	Residue	Modelled	Actual	Comment	Reference
C	-19	MET	-	initiating methionine	UNP P14618
C	-18	GLY	-	expression tag	UNP P14618
C	-17	SER	-	expression tag	UNP P14618
C	-16	SER	-	expression tag	UNP P14618
C	-15	HIS	-	expression tag	UNP P14618
C	-14	HIS	-	expression tag	UNP P14618
C	-13	HIS	-	expression tag	UNP P14618
C	-12	ARG	-	expression tag	UNP P14618
C	-11	HIS	-	expression tag	UNP P14618
C	-10	HIS	-	expression tag	UNP P14618
C	-9	SER	-	expression tag	UNP P14618
C	-8	SER	-	expression tag	UNP P14618
C	-7	GLY	-	expression tag	UNP P14618
C	-6	LEU	-	expression tag	UNP P14618
C	-5	VAL	-	expression tag	UNP P14618
C	-4	PRO	-	expression tag	UNP P14618
C	-3	ARG	-	expression tag	UNP P14618
C	-2	GLY	-	expression tag	UNP P14618
C	-1	SER	-	expression tag	UNP P14618
C	0	HIS	-	expression tag	UNP P14618
C	326	SER	CYS	engineered mutation	UNP P14618

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.

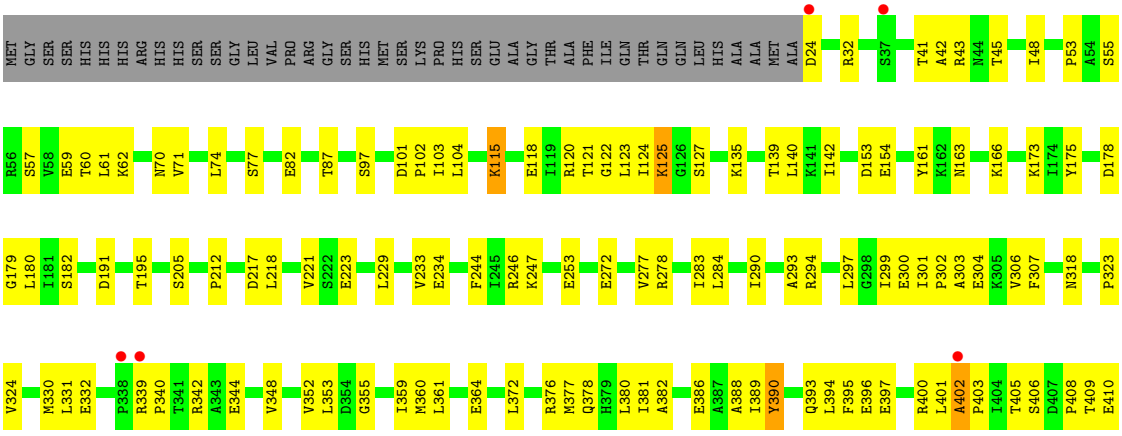
• Molecule 1: Pyruvate kinase PKM

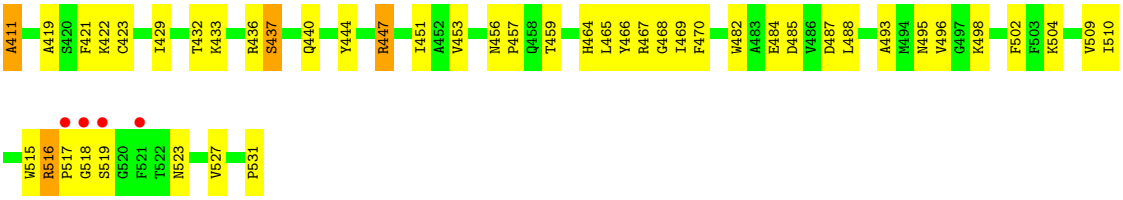
Chain A:



• Molecule 1: Pyruvate kinase PKM

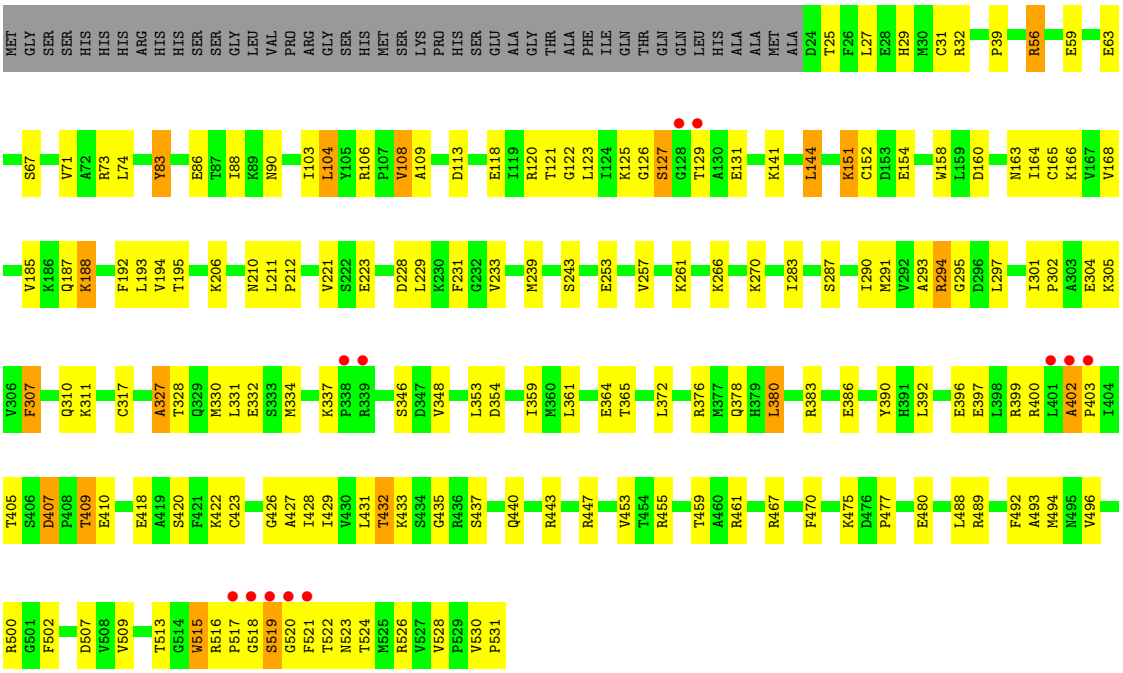
Chain B:





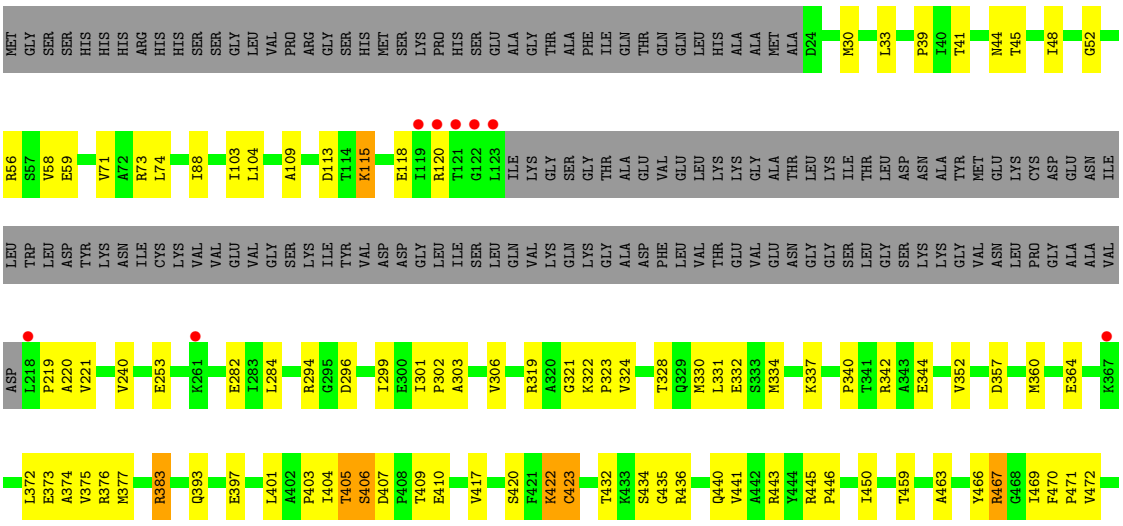
• Molecule 1: Pyruvate kinase PKM

Chain D:



• Molecule 1: Pyruvate kinase PKM

Chain C:




K475
W482
G497
K498
G514
W515
R516
P517
R526
V527
P531

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	181.51Å 156.37Å 121.59Å 90.00° 114.20° 90.00°	Depositor
Resolution (Å)	29.79 – 3.10 29.79 – 3.10	Depositor EDS
% Data completeness (in resolution range)	63.9 (29.79-3.10) 86.3 (29.79-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.86 (at 3.11Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.182 , 0.237 0.182 , 0.236	Depositor DCC
R_{free} test set	2000 reflections (4.00%)	wwPDB-VP
Wilson B-factor (Å^2)	53.6	Xtriage
Anisotropy	0.120	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 38.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	30019	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% 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

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	1.07	19/3953 (0.5%)	1.04	10/5338 (0.2%)
1	B	0.98	9/3953 (0.2%)	1.00	6/5338 (0.1%)
1	C	0.93	9/3242 (0.3%)	0.94	1/4379 (0.0%)
1	D	1.14	24/3953 (0.6%)	1.07	11/5338 (0.2%)
All	All	1.04	61/15101 (0.4%)	1.02	28/20393 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	1
1	C	0	2
1	D	0	2
All	All	0	8

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	434	SER	CB-OG	11.79	1.57	1.42
1	C	423	CYS	CB-SG	-11.21	1.63	1.82
1	D	31	CYS	CB-SG	-8.79	1.67	1.82
1	D	332	GLU	CG-CD	8.64	1.65	1.51
1	A	423	CYS	CB-SG	-8.58	1.67	1.82
1	B	154	GLU	CG-CD	8.34	1.64	1.51
1	D	386	GLU	CG-CD	-8.21	1.39	1.51
1	A	178	ASP	CB-CG	8.07	1.68	1.51
1	A	285	GLU	CG-CD	7.88	1.63	1.51
1	A	386	GLU	CD-OE2	7.87	1.34	1.25
1	A	49	CYS	CB-SG	-7.66	1.69	1.82
1	D	480	GLU	CB-CG	7.62	1.66	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	332	GLU	CG-CD	7.55	1.63	1.51
1	B	332	GLU	CB-CG	7.23	1.65	1.52
1	D	223	GLU	CG-CD	7.17	1.62	1.51
1	B	223	GLU	CG-CD	7.13	1.62	1.51
1	D	397	GLU	CG-CD	7.06	1.62	1.51
1	C	436	ARG	CG-CD	7.03	1.69	1.51
1	D	386	GLU	CB-CG	-6.94	1.39	1.52
1	B	437	SER	CB-OG	6.89	1.51	1.42
1	A	206	LYS	CD-CE	6.84	1.68	1.51
1	D	106	ARG	CG-CD	6.82	1.69	1.51
1	D	402	ALA	C-N	6.79	1.47	1.34
1	C	332	GLU	CG-CD	6.67	1.61	1.51
1	A	332	GLU	CB-CG	6.59	1.64	1.52
1	D	223	GLU	CB-CG	6.43	1.64	1.52
1	B	82	GLU	CB-CG	6.32	1.64	1.52
1	A	332	GLU	CG-CD	6.32	1.61	1.51
1	B	300	GLU	CG-CD	6.28	1.61	1.51
1	D	521	PHE	CB-CG	6.25	1.61	1.51
1	D	332	GLU	CB-CG	6.20	1.64	1.52
1	C	332	GLU	CB-CG	6.19	1.64	1.52
1	D	83	TYR	CB-CG	-5.98	1.42	1.51
1	D	307	PHE	CB-CG	-5.92	1.41	1.51
1	A	508	VAL	CB-CG2	-5.85	1.40	1.52
1	C	282	GLU	CG-CD	5.83	1.60	1.51
1	A	417	VAL	CB-CG2	-5.77	1.40	1.52
1	C	475	LYS	CE-NZ	5.64	1.63	1.49
1	D	151	LYS	CD-CE	5.62	1.65	1.51
1	A	472	VAL	CB-CG1	-5.54	1.41	1.52
1	D	432	THR	CA-CB	5.48	1.67	1.53
1	A	59	GLU	CG-CD	5.40	1.60	1.51
1	B	402	ALA	C-N	5.36	1.44	1.34
1	C	475	LYS	CD-CE	5.36	1.64	1.51
1	A	206	LYS	CG-CD	5.32	1.70	1.52
1	D	480	GLU	CG-CD	5.30	1.59	1.51
1	A	272	GLU	CG-CD	5.29	1.59	1.51
1	D	410	GLU	CG-CD	5.28	1.59	1.51
1	D	447	ARG	CG-CD	5.26	1.65	1.51
1	D	59	GLU	CG-CD	5.25	1.59	1.51
1	A	500	ARG	CB-CG	5.25	1.66	1.52
1	A	106	ARG	CB-CG	5.25	1.66	1.52
1	D	515	TRP	CB-CG	5.24	1.59	1.50
1	C	319	ARG	CG-CD	5.22	1.65	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	317	CYS	CB-SG	-5.19	1.73	1.81
1	A	206	LYS	CB-CG	5.17	1.66	1.52
1	D	108	VAL	CB-CG1	-5.15	1.42	1.52
1	D	475	LYS	CE-NZ	5.13	1.61	1.49
1	B	115	LYS	CD-CE	5.12	1.64	1.51
1	A	386	GLU	CD-OE1	5.08	1.31	1.25
1	C	472	VAL	CB-CG1	-5.08	1.42	1.52

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	386	GLU	OE1-CD-OE2	8.72	133.76	123.30
1	B	401	LEU	C-N-CA	7.84	141.30	121.70
1	A	386	GLU	OE1-CD-OE2	7.82	132.68	123.30
1	A	447	ARG	NE-CZ-NH1	6.65	123.62	120.30
1	D	500	ARG	O-C-N	-6.61	111.96	123.20
1	D	407	ASP	CB-CG-OD1	6.21	123.89	118.30
1	B	381	ILE	CG1-CB-CG2	-6.10	97.97	111.40
1	A	424	CYS	CA-CB-SG	-6.08	103.05	114.00
1	A	206	LYS	CD-CE-NZ	6.06	125.64	111.70
1	B	32	ARG	CG-CD-NE	-5.87	99.47	111.80
1	D	386	GLU	CA-CB-CG	-5.86	100.52	113.40
1	B	180	LEU	CB-CG-CD1	5.82	120.89	111.00
1	B	487	ASP	CB-CG-OD1	-5.79	113.09	118.30
1	D	141	LYS	CD-CE-NZ	5.77	124.98	111.70
1	A	494	MET	CG-SD-CE	-5.76	90.98	100.20
1	D	353	LEU	CB-CG-CD2	-5.64	101.41	111.00
1	A	180	LEU	CB-CG-CD1	5.59	120.50	111.00
1	A	224	LYS	CD-CE-NZ	5.45	124.24	111.70
1	D	432	THR	N-CA-CB	5.45	120.66	110.30
1	D	144	LEU	CA-CB-CG	-5.44	102.79	115.30
1	D	380	LEU	CB-CG-CD2	-5.42	101.79	111.00
1	A	297	LEU	CB-CG-CD2	-5.41	101.81	111.00
1	B	217	ASP	CB-CG-OD1	5.41	123.17	118.30
1	A	526	ARG	CG-CD-NE	-5.23	100.81	111.80
1	D	104	LEU	CA-CB-CG	-5.18	103.39	115.30
1	A	386	GLU	CA-CB-CG	-5.16	102.06	113.40
1	C	319	ARG	CG-CD-NE	5.12	122.55	111.80
1	D	409	THR	CA-CB-CG2	-5.00	105.40	112.40

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	423	CYS	Peptide
1	A	518	GLY	Peptide
1	A	526	ARG	Sidechain
1	B	447	ARG	Sidechain
1	C	405	THR	Peptide
1	C	467	ARG	Sidechain
1	D	327	ALA	Peptide
1	D	56	ARG	Sidechain

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	3890	3975	3976	121	1
1	B	3890	3971	3976	149	0
1	C	3187	3246	3249	79	0
1	D	3890	3970	3976	126	1
All	All	14857	15162	15177	448	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 15.

All (448) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:118:GLU:OE1	1:D:120:ARG:NH1	1.90	1.04
1:C:71:VAL:HG22	1:C:109:ALA:HB3	1.40	1.03
1:B:400:ARG:HG3	1:C:422:LYS:NZ	1.78	0.98
1:B:395:PHE:CZ	1:B:421:PHE:CE2	2.51	0.98
1:A:41:THR:HG22	1:A:42:ALA:O	1.64	0.98
1:B:400:ARG:HB2	1:C:422:LYS:HE2	1.46	0.96
1:A:140:LEU:HD11	1:A:157:LEU:HB2	1.51	0.93
1:D:402:ALA:HB1	1:D:443:ARG:NH1	1.87	0.89
1:D:56:ARG:NH1	1:D:83:TYR:CE1	2.43	0.87
1:C:303:ALA:HA	1:C:306:VAL:HG23	1.57	0.86
1:B:24:ASP:N	1:B:390:TYR:HH	1.76	0.84
1:C:410:GLU:OE1	1:C:440:GLN:NE2	2.11	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:LYS:O	1:A:459:THR:HG21	1.80	0.82
1:D:165:CYS:O	1:D:188:LYS:NZ	2.12	0.82
1:A:176:VAL:HB	1:A:181:ILE:HG23	1.61	0.81
1:B:395:PHE:CE1	1:B:421:PHE:CE2	2.69	0.80
1:B:395:PHE:CE1	1:B:421:PHE:CZ	2.72	0.78
1:B:400:ARG:HG3	1:C:422:LYS:CE	2.17	0.75
1:B:400:ARG:HG3	1:C:422:LYS:HZ3	1.50	0.75
1:A:165:CYS:O	1:A:188:LYS:NZ	2.18	0.74
1:A:183:LEU:HD13	1:A:195:THR:HG21	1.70	0.73
1:D:56:ARG:NH1	1:D:83:TYR:CZ	2.57	0.73
1:A:121:THR:HG22	1:A:207:LYS:H	1.52	0.73
1:C:405:THR:HG23	1:C:406:SER:HB3	1.71	0.72
1:A:133:GLU:HA	1:A:201:GLY:O	1.90	0.72
1:B:390:TYR:O	1:B:394:LEU:HD13	1.90	0.72
1:A:124:ILE:HA	1:A:152:CYS:HB2	1.70	0.71
1:B:77:SER:HA	1:B:115:LYS:HG3	1.71	0.71
1:B:400:ARG:CB	1:C:422:LYS:HE2	2.21	0.71
1:B:400:ARG:HD2	1:B:403:PRO:HB2	1.73	0.70
1:D:433:LYS:O	1:D:459:THR:HG21	1.91	0.70
1:A:361:LEU:HD21	1:A:378:GLN:NE2	2.07	0.70
1:D:295:GLY:H	1:D:328:THR:HG21	1.55	0.70
1:D:71:VAL:HG22	1:D:109:ALA:HB3	1.74	0.69
1:D:515:TRP:HE1	1:D:520:GLY:HA3	1.57	0.69
1:B:409:THR:HG21	1:B:440:GLN:NE2	2.06	0.69
1:A:361:LEU:HD21	1:A:378:GLN:HE21	1.56	0.69
1:D:103:ILE:HA	1:D:496:VAL:HG22	1.73	0.69
1:B:429:ILE:HD12	1:B:509:VAL:HG21	1.74	0.68
1:D:420:SER:HB3	1:D:428:ILE:HD11	1.74	0.68
1:C:405:THR:OG1	1:C:406:SER:N	2.25	0.68
1:B:244:PHE:CE2	1:B:246:ARG:HD3	2.29	0.67
1:A:197:VAL:O	1:A:197:VAL:HG13	1.92	0.67
1:B:244:PHE:N	1:B:272:GLU:OE2	2.27	0.67
1:A:121:THR:HG22	1:A:207:LYS:N	2.09	0.67
1:A:118:GLU:OE1	1:A:120:ARG:NH1	2.28	0.67
1:C:52:GLY:O	1:C:56:ARG:HG3	1.95	0.67
1:A:124:ILE:HD12	1:A:132:VAL:HG13	1.78	0.66
1:B:405:THR:HG22	1:C:422:LYS:HZ2	1.60	0.66
1:C:397:GLU:O	1:C:401:LEU:HD12	1.95	0.65
1:A:294:ARG:NH2	1:A:347:ASP:OD2	2.30	0.65
1:B:331:LEU:HD23	1:B:344:GLU:HB3	1.78	0.64
1:A:124:ILE:HD11	1:A:130:ALA:C	2.18	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:ALA:N	1:A:197:VAL:HG12	2.13	0.64
1:A:134:LEU:HD11	1:A:203:LEU:HB2	1.79	0.64
1:D:432:THR:HG23	1:D:435:GLY:H	1.62	0.64
1:B:218:LEU:O	1:B:246:ARG:NH1	2.31	0.63
1:A:348:VAL:HG11	1:A:378:GLN:OE1	1.98	0.63
1:B:330:MET:HE3	1:B:348:VAL:HG22	1.80	0.63
1:D:361:LEU:HD21	1:D:378:GLN:NE2	2.13	0.63
1:A:56:ARG:HD3	1:A:83:TYR:OH	1.98	0.63
1:A:185:VAL:HA	1:A:195:THR:OG1	1.99	0.63
1:D:402:ALA:HB1	1:D:443:ARG:CZ	2.28	0.63
1:D:526:ARG:HD2	1:D:528:VAL:HG12	1.80	0.63
1:D:185:VAL:HA	1:D:195:THR:HG22	1.81	0.62
1:A:334:MET:HA	1:A:337:LYS:O	1.99	0.62
1:D:327:ALA:O	1:D:328:THR:HG22	1.99	0.62
1:B:400:ARG:CG	1:C:422:LYS:HZ3	2.13	0.62
1:D:330:MET:HE3	1:D:359:ILE:CG2	2.30	0.61
1:A:330:MET:HG3	1:A:360:MET:O	2.00	0.61
1:D:144:LEU:HD11	1:D:164:ILE:HG22	1.82	0.61
1:D:331:LEU:HD23	1:D:334:MET:SD	2.40	0.61
1:D:402:ALA:HB1	1:D:443:ARG:HH12	1.66	0.61
1:B:518:GLY:O	1:B:519:SER:OG	2.07	0.61
1:D:429:ILE:HD12	1:D:509:VAL:HG21	1.81	0.61
1:B:411:ALA:HA	1:C:422:LYS:CD	2.31	0.61
1:D:103:ILE:HB	1:D:104:LEU:HD12	1.82	0.61
1:A:411:ALA:HB2	1:D:423:CYS:HB3	1.83	0.60
1:D:399:ARG:HE	1:D:400:ARG:HD2	1.66	0.60
1:D:86:GLU:O	1:D:90:ASN:OD1	2.19	0.60
1:B:45:THR:HG21	1:B:352:VAL:HG13	1.84	0.60
1:A:124:ILE:HD11	1:A:130:ALA:HB3	1.83	0.60
1:D:125:LYS:HE3	1:D:151:LYS:HD3	1.84	0.59
1:D:168:VAL:HG11	1:D:193:LEU:HD21	1.84	0.59
1:A:124:ILE:HD11	1:A:130:ALA:CB	2.32	0.59
1:D:126:GLY:O	1:D:127:SER:OG	2.17	0.59
1:A:337:LYS:HG3	1:A:338:PRO:HD2	1.84	0.59
1:B:411:ALA:HA	1:C:422:LYS:HD2	1.84	0.59
1:A:418:GLU:HG3	1:D:418:GLU:HG3	1.85	0.59
1:B:125:LYS:HE2	1:B:153:ASP:HB3	1.85	0.59
1:D:283:ILE:O	1:D:287:SER:OG	2.13	0.59
1:B:57:SER:O	1:B:61:LEU:HD12	2.03	0.58
1:A:290:ILE:O	1:A:324:VAL:HA	2.03	0.58
1:B:101:ASP:OD2	1:B:104:LEU:HD23	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:330:MET:HE3	1:D:359:ILE:HG23	1.86	0.58
1:A:489:ARG:O	1:A:492:PHE:HB3	2.04	0.58
1:D:294:ARG:N	1:D:328:THR:HG21	2.19	0.58
1:B:212:PRO:HB3	1:B:299:ILE:HG22	1.85	0.58
1:C:407:ASP:OD1	1:C:409:THR:N	2.35	0.58
1:D:330:MET:CE	1:D:359:ILE:HG23	2.34	0.58
1:A:157:LEU:HD23	1:A:203:LEU:HD11	1.86	0.58
1:D:523:ASN:N	1:D:523:ASN:OD1	2.35	0.57
1:B:24:ASP:N	1:B:390:TYR:OH	2.35	0.57
1:B:429:ILE:CD1	1:B:509:VAL:HG21	2.34	0.57
1:D:192:PHE:O	1:D:193:LEU:HD12	2.04	0.57
1:A:431:LEU:HD22	1:A:513:THR:HG22	1.84	0.57
1:A:123:LEU:O	1:A:124:ILE:HG12	2.04	0.57
1:B:229:LEU:O	1:B:233:VAL:HG23	2.04	0.57
1:A:130:ALA:O	1:A:131:GLU:HG3	2.05	0.57
1:A:157:LEU:HD13	1:A:158:TRP:N	2.20	0.57
1:A:253:GLU:O	1:A:257:VAL:HG23	2.04	0.57
1:D:331:LEU:O	1:D:364:GLU:HG2	2.05	0.56
1:B:393:GLN:HA	1:B:393:GLN:OE1	2.05	0.56
1:D:405:THR:O	1:D:405:THR:HG22	2.05	0.56
1:A:55:SER:HA	1:A:60:THR:HG21	1.87	0.56
1:B:331:LEU:O	1:B:364:GLU:HG2	2.06	0.56
1:A:132:VAL:HG21	1:A:153:ASP:O	2.05	0.56
1:B:118:GLU:OE2	1:B:120:ARG:HD3	2.05	0.56
1:D:63:GLU:HB3	1:D:372:LEU:HD21	1.87	0.56
1:C:301:ILE:HG22	1:C:302:PRO:HD2	1.88	0.56
1:A:56:ARG:NH2	1:A:86:GLU:OE1	2.30	0.56
1:A:294:ARG:HD2	1:A:310:GLN:OE1	2.06	0.56
1:B:175:TYR:CE1	1:B:182:SER:HB3	2.41	0.56
1:B:400:ARG:HD2	1:B:403:PRO:CB	2.36	0.56
1:A:169:GLU:O	1:A:185:VAL:HG21	2.06	0.56
1:D:420:SER:CB	1:D:428:ILE:HD11	2.36	0.56
1:A:51:ILE:HD12	1:A:61:LEU:HD21	1.88	0.55
1:C:303:ALA:HA	1:C:306:VAL:CG2	2.33	0.55
1:A:150:GLU:O	1:A:151:LYS:HG3	2.06	0.55
1:B:330:MET:CE	1:B:348:VAL:HG22	2.36	0.55
1:C:432:THR:OG1	1:C:435:GLY:HA2	2.07	0.55
1:D:25:THR:HG22	1:D:27:LEU:H	1.70	0.55
1:D:361:LEU:CD2	1:D:378:GLN:NE2	2.69	0.55
1:D:513:THR:OG1	1:D:524:THR:HB	2.07	0.55
1:A:152:CYS:O	1:A:156:ILE:O	2.25	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:400:ARG:CD	1:B:403:PRO:HG2	2.36	0.55
1:D:295:GLY:N	1:D:328:THR:HG21	2.21	0.55
1:A:453:VAL:HG21	1:A:493:ALA:HB2	1.89	0.55
1:B:396:GLU:HG2	1:B:396:GLU:O	2.06	0.55
1:A:296:ASP:O	1:A:300:GLU:HG2	2.07	0.54
1:A:25:THR:HG22	1:A:26:PHE:N	2.22	0.54
1:A:141:LYS:HB3	1:A:194:VAL:HG22	1.90	0.54
1:A:157:LEU:CD2	1:A:203:LEU:HD11	2.37	0.54
1:B:101:ASP:OD1	1:B:102:PRO:HD2	2.08	0.54
1:D:453:VAL:HG21	1:D:493:ALA:HB2	1.88	0.54
1:B:24:ASP:CA	1:B:390:TYR:OH	2.56	0.54
1:B:59:GLU:O	1:B:59:GLU:HG2	2.06	0.54
1:B:221:VAL:HG21	1:B:253:GLU:CG	2.38	0.54
1:B:453:VAL:HG21	1:B:493:ALA:HB2	1.89	0.54
1:D:302:PRO:HB2	1:D:305:LYS:HD2	1.90	0.54
1:A:327:ALA:HB1	1:A:360:MET:HE2	1.89	0.54
1:B:515:TRP:HB2	1:B:523:ASN:HB2	1.89	0.53
1:B:244:PHE:HE2	1:B:246:ARG:HD3	1.70	0.53
1:A:159:LEU:HD12	1:A:164:ILE:HD13	1.91	0.53
1:B:432:THR:HB	1:B:437:SER:HB2	1.91	0.53
1:D:121:THR:HG22	1:D:122:GLY:O	2.09	0.53
1:A:152:CYS:O	1:A:155:ASN:O	2.27	0.53
1:D:392:LEU:O	1:D:396:GLU:OE1	2.27	0.53
1:C:372:LEU:O	1:C:373:GLU:C	2.48	0.53
1:B:432:THR:HB	1:B:437:SER:CB	2.38	0.53
1:C:463:ALA:HB3	1:C:471:PRO:HB3	1.91	0.53
1:B:55:SER:HA	1:B:60:THR:HG21	1.92	0.52
1:D:144:LEU:HD11	1:D:164:ILE:CG2	2.39	0.52
1:D:372:LEU:HD23	1:D:376:ARG:NH1	2.23	0.52
1:A:73:ARG:HD3	1:A:360:MET:SD	2.49	0.52
1:C:323:PRO:HD3	1:C:466:TYR:CE2	2.45	0.52
1:B:59:GLU:O	1:B:59:GLU:CG	2.58	0.52
1:A:135:LYS:O	1:A:197:VAL:HG11	2.09	0.52
1:C:434:SER:HA	1:C:459:THR:HG21	1.91	0.52
1:B:139:THR:HG22	1:B:140:LEU:N	2.23	0.52
1:B:411:ALA:HB2	1:C:422:LYS:HD3	1.92	0.52
1:B:142:ILE:HD12	1:B:195:THR:HG21	1.91	0.52
1:B:330:MET:HG3	1:B:360:MET:O	2.08	0.52
1:D:513:THR:O	1:D:522:THR:HG23	2.10	0.52
1:D:304:GLU:HG2	1:D:305:LYS:N	2.24	0.52
1:D:187:GLN:HB2	1:D:194:VAL:HB	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:482:TRP:HH2	1:C:514:GLY:O	1.93	0.52
1:A:159:LEU:HD12	1:A:164:ILE:CD1	2.40	0.52
1:B:361:LEU:HD21	1:B:378:GLN:CG	2.40	0.52
1:A:170:VAL:O	1:A:185:VAL:HG23	2.09	0.51
1:D:399:ARG:HE	1:D:400:ARG:CD	2.22	0.51
1:A:178:ASP:O	1:A:299:ILE:HD11	2.10	0.51
1:B:353:LEU:HD21	1:B:388:ALA:HB3	1.91	0.51
1:B:432:THR:OG1	1:B:437:SER:OG	2.19	0.51
1:A:134:LEU:HD11	1:A:203:LEU:CB	2.39	0.51
1:B:400:ARG:CG	1:C:422:LYS:CE	2.89	0.51
1:D:118:GLU:CD	1:D:120:ARG:NH1	2.64	0.51
1:D:307:PHE:O	1:D:311:LYS:HG3	2.11	0.51
1:D:399:ARG:NH2	1:D:400:ARG:HH11	2.09	0.51
1:A:154:GLU:HG2	1:A:155:ASN:H	1.75	0.51
1:A:335:ILE:HD11	1:A:363:GLY:HA3	1.92	0.51
1:B:429:ILE:HD12	1:B:509:VAL:CG2	2.40	0.51
1:B:386:GLU:OE1	1:B:467:ARG:NH2	2.44	0.51
1:B:323:PRO:HB3	1:B:465:LEU:O	2.11	0.50
1:C:115:LYS:HG2	1:C:118:GLU:OE1	2.12	0.50
1:B:103:ILE:HD13	1:B:495:ASN:HB3	1.94	0.50
1:B:498:LYS:HE2	1:B:531:PRO:O	2.12	0.50
1:B:43:ARG:NH2	1:B:70:ASN:OD1	2.44	0.50
1:C:48:ILE:HG12	1:C:71:VAL:HB	1.94	0.50
1:A:176:VAL:HB	1:A:181:ILE:CG2	2.38	0.50
1:A:74:LEU:HD11	1:A:88:ILE:HG13	1.94	0.50
1:D:74:LEU:HD11	1:D:88:ILE:HG13	1.93	0.50
1:C:463:ALA:HB1	1:C:469:ILE:HG21	1.93	0.50
1:A:176:VAL:O	1:A:181:ILE:HG22	2.11	0.49
1:D:293:ALA:O	1:D:297:LEU:HB2	2.12	0.49
1:B:470:PHE:N	1:B:470:PHE:CD1	2.80	0.49
1:A:453:VAL:CG2	1:A:493:ALA:HB2	2.42	0.49
1:B:361:LEU:HD21	1:B:378:GLN:HG3	1.93	0.49
1:B:510:ILE:CD1	1:B:527:VAL:HG22	2.42	0.49
1:A:170:VAL:C	1:A:185:VAL:HG23	2.32	0.49
1:D:210:ASN:O	1:D:212:PRO:HD3	2.12	0.49
1:D:297:LEU:O	1:D:301:ILE:HB	2.12	0.49
1:D:123:LEU:O	1:D:152:CYS:HB2	2.13	0.49
1:D:334:MET:HA	1:D:337:LYS:O	2.11	0.49
1:C:321:GLY:CA	1:C:443:ARG:HD2	2.42	0.49
1:B:293:ALA:O	1:B:297:LEU:HB2	2.13	0.49
1:C:240:VAL:HG12	1:C:240:VAL:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:THR:O	1:D:423:CYS:HA	2.13	0.49
1:C:301:ILE:CG2	1:C:302:PRO:HD2	2.43	0.49
1:B:406:SER:O	1:B:408:PRO:HD3	2.13	0.48
1:A:331:LEU:HD22	1:A:340:PRO:CB	2.43	0.48
1:B:24:ASP:HA	1:B:390:TYR:OH	2.14	0.48
1:D:109:ALA:HB1	1:D:239:MET:HE3	1.94	0.48
1:D:253:GLU:O	1:D:257:VAL:HG23	2.14	0.48
1:D:407:ASP:OD1	1:D:407:ASP:O	2.31	0.48
1:C:422:LYS:HG2	1:C:423:CYS:N	2.28	0.48
1:A:185:VAL:HG12	1:A:193:LEU:HD21	1.95	0.48
1:B:410:GLU:O	1:B:411:ALA:HB2	2.14	0.48
1:B:484:GLU:O	1:B:485:ASP:C	2.52	0.48
1:D:67:SER:HB3	1:D:376:ARG:HG3	1.95	0.48
1:A:145:ASP:C	1:A:147:ALA:H	2.17	0.48
1:B:376:ARG:O	1:B:380:LEU:HD13	2.14	0.48
1:A:140:LEU:O	1:A:195:THR:HG22	2.13	0.48
1:D:221:VAL:HG21	1:D:253:GLU:HG3	1.96	0.48
1:B:103:ILE:HG22	1:B:104:LEU:HD22	1.95	0.47
1:B:488:LEU:HD13	1:D:488:LEU:CD1	2.44	0.47
1:B:62:LYS:HE2	1:B:97:SER:CB	2.44	0.47
1:A:399:ARG:NH1	1:A:418:GLU:OE2	2.46	0.47
1:B:246:ARG:HH21	1:B:247:LYS:NZ	2.13	0.47
1:B:400:ARG:HD3	1:B:403:PRO:HG2	1.96	0.47
1:B:402:ALA:HB3	1:B:403:PRO:HD3	1.96	0.47
1:B:74:LEU:HD11	1:B:87:THR:HB	1.96	0.47
1:C:73:ARG:NH1	1:C:113:ASP:OD2	2.47	0.47
1:A:405:THR:HG23	1:D:422:LYS:NZ	2.29	0.47
1:B:419:ALA:C	1:B:421:PHE:H	2.17	0.47
1:D:399:ARG:NE	1:D:400:ARG:HD2	2.30	0.47
1:D:429:ILE:CD1	1:D:509:VAL:HG21	2.45	0.47
1:C:466:TYR:HB2	1:C:469:ILE:HD12	1.96	0.47
1:A:184:GLN:OE1	1:A:198:GLU:OE2	2.33	0.47
1:B:395:PHE:O	1:B:396:GLU:C	2.51	0.47
1:C:30:MET:O	1:C:33:LEU:HG	2.15	0.47
1:D:331:LEU:O	1:D:364:GLU:CG	2.63	0.47
1:D:470:PHE:CD2	1:D:502:PHE:HZ	2.33	0.47
1:D:294:ARG:HD2	1:D:310:GLN:OE1	2.14	0.47
1:A:148:TYR:HB3	1:A:151:LYS:O	2.15	0.47
1:B:173:LYS:HD2	1:B:175:TYR:OH	2.16	0.47
1:D:403:PRO:HD2	1:D:443:ARG:HH22	1.78	0.47
1:D:432:THR:HG21	1:D:437:SER:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:VAL:HG12	1:A:226:ILE:HG13	1.98	0.46
1:A:399:ARG:NH2	1:D:399:ARG:NH1	2.64	0.46
1:C:321:GLY:HA3	1:C:443:ARG:HD2	1.96	0.46
1:C:324:VAL:O	1:C:357:ASP:HB2	2.15	0.46
1:A:134:LEU:HD12	1:A:134:LEU:H	1.80	0.46
1:B:103:ILE:HD11	1:D:477:PRO:HG3	1.98	0.46
1:B:301:ILE:HG22	1:B:302:PRO:O	2.15	0.46
1:B:395:PHE:CB	1:B:444:TYR:O	2.63	0.46
1:A:365:THR:HA	1:A:371:PRO:HB3	1.98	0.46
1:C:331:LEU:HA	1:C:344:GLU:OE2	2.15	0.46
1:A:24:ASP:N	1:A:390:TYR:HH	2.13	0.46
1:A:329:GLN:HA	1:A:332:GLU:CG	2.46	0.46
1:B:221:VAL:HG21	1:B:253:GLU:HG3	1.98	0.46
1:B:467:ARG:HG2	1:B:468:GLY:N	2.31	0.46
1:D:302:PRO:HG2	1:D:305:LYS:HD2	1.98	0.46
1:A:155:ASN:O	1:A:156:ILE:O	2.34	0.46
1:A:303:ALA:C	1:A:305:LYS:H	2.18	0.46
1:B:303:ALA:HA	1:B:306:VAL:HG23	1.97	0.46
1:A:56:ARG:HD3	1:A:83:TYR:CZ	2.51	0.46
1:B:397:GLU:OE1	1:B:397:GLU:HA	2.15	0.46
1:D:431:LEU:HD22	1:D:513:THR:HG22	1.97	0.46
1:D:516:ARG:HB3	1:D:517:PRO:CD	2.46	0.46
1:B:123:LEU:HD23	1:B:205:SER:HB3	1.98	0.46
1:B:359:ILE:HG21	1:B:378:GLN:OE1	2.15	0.46
1:B:400:ARG:CD	1:B:403:PRO:HB2	2.45	0.46
1:D:494:MET:HG2	1:D:531:PRO:HD2	1.97	0.46
1:B:433:LYS:O	1:B:459:THR:HG21	2.15	0.45
1:B:125:LYS:HE2	1:B:153:ASP:CB	2.47	0.45
1:D:158:TRP:CH2	1:D:160:ASP:HB3	2.52	0.45
1:C:372:LEU:O	1:C:375:VAL:N	2.49	0.45
1:C:482:TRP:CH2	1:C:514:GLY:O	2.68	0.45
1:A:205:SER:O	1:A:207:LYS:HE2	2.17	0.45
1:D:507:ASP:O	1:D:530:VAL:HG23	2.16	0.45
1:B:163:ASN:HB3	1:B:166:LYS:HD2	1.99	0.45
1:D:290:ILE:CG2	1:D:291:MET:N	2.79	0.45
1:D:123:LEU:HD11	1:D:206:LYS:HE2	1.98	0.45
1:A:62:LYS:HG3	1:A:94:ALA:HB1	1.99	0.45
1:A:331:LEU:HD22	1:A:340:PRO:HB3	1.99	0.45
1:B:142:ILE:CD1	1:B:195:THR:HG21	2.46	0.45
1:B:405:THR:HG22	1:C:422:LYS:NZ	2.30	0.45
1:B:516:ARG:HB3	1:B:517:PRO:CD	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:372:LEU:HD13	1:C:376:ARG:NH2	2.31	0.45
1:C:470:PHE:CD1	1:C:470:PHE:N	2.84	0.45
1:A:120:ARG:HD3	1:A:206:LYS:O	2.16	0.45
1:C:410:GLU:OE2	1:C:440:GLN:HG2	2.16	0.45
1:A:181:ILE:HD13	1:A:200:GLY:HA2	1.99	0.45
1:B:124:ILE:HD12	1:B:124:ILE:N	2.32	0.45
1:B:421:PHE:HE1	1:B:447:ARG:HD2	1.82	0.45
1:A:393:GLN:O	1:A:397:GLU:HG3	2.17	0.45
1:D:243:SER:HA	1:D:270:LYS:HB2	1.99	0.44
1:D:426:GLY:O	1:D:427:ALA:HB2	2.16	0.44
1:D:515:TRP:O	1:D:516:ARG:HG2	2.17	0.44
1:B:135:LYS:HB2	1:B:135:LYS:HE2	1.80	0.44
1:B:482:TRP:CH2	1:B:515:TRP:CE3	3.04	0.44
1:A:472:VAL:CG1	1:A:492:PHE:CE2	3.01	0.44
1:B:372:LEU:HD23	1:B:376:ARG:NH2	2.33	0.44
1:C:334:MET:HA	1:C:337:LYS:O	2.16	0.44
1:B:175:TYR:CE2	1:B:212:PRO:HG3	2.52	0.44
1:B:400:ARG:CB	1:C:422:LYS:CE	2.93	0.44
1:B:411:ALA:CB	1:C:422:LYS:HD3	2.47	0.44
1:D:301:ILE:HG21	1:D:301:ILE:HD13	1.57	0.44
1:D:330:MET:HE3	1:D:348:VAL:HG22	2.00	0.44
1:C:294:ARG:NH2	1:C:330:MET:SD	2.91	0.44
1:C:48:ILE:HG22	1:C:360:MET:HG3	1.99	0.44
1:C:284:LEU:CD1	1:C:322:LYS:HD2	2.48	0.44
1:C:342:ARG:HD2	1:C:342:ARG:C	2.38	0.44
1:B:488:LEU:HD13	1:D:488:LEU:HD13	2.00	0.44
1:D:380:LEU:HD12	1:D:380:LEU:HA	1.72	0.44
1:D:489:ARG:O	1:D:492:PHE:HB3	2.18	0.44
1:D:39:PRO:HB2	1:D:383:ARG:HE	1.81	0.44
1:D:164:ILE:HD11	1:D:211:LEU:HD21	1.99	0.44
1:C:103:ILE:HG22	1:C:104:LEU:HD23	2.00	0.44
1:B:175:TYR:HB3	1:B:179:GLY:HA2	1.98	0.43
1:B:340:PRO:HG3	1:B:377:MET:HG2	2.00	0.43
1:B:466:TYR:HB2	1:B:469:ILE:HD12	2.00	0.43
1:D:327:ALA:C	1:D:328:THR:HG22	2.38	0.43
1:D:518:GLY:O	1:D:519:SER:OG	2.29	0.43
1:B:103:ILE:HG23	1:B:496:VAL:HA	2.00	0.43
1:D:409:THR:HB	1:D:440:GLN:HE22	1.84	0.43
1:C:393:GLN:O	1:C:397:GLU:HG3	2.18	0.43
1:C:515:TRP:O	1:C:516:ARG:HB2	2.18	0.43
1:B:48:ILE:HB	1:B:360:MET:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:470:PHE:CD1	1:D:470:PHE:N	2.86	0.43
1:C:515:TRP:O	1:C:516:ARG:O	2.36	0.43
1:A:197:VAL:O	1:A:197:VAL:CG1	2.64	0.43
1:B:121:THR:HG22	1:B:122:GLY:N	2.34	0.43
1:B:432:THR:CB	1:B:437:SER:OG	2.67	0.43
1:B:456:ASN:O	1:B:457:PRO:C	2.56	0.43
1:B:516:ARG:HB3	1:B:517:PRO:HD2	2.01	0.43
1:D:311:LYS:NZ	1:D:354:ASP:OD1	2.28	0.43
1:A:157:LEU:HD23	1:A:203:LEU:CD1	2.47	0.43
1:B:400:ARG:HD2	1:B:403:PRO:O	2.18	0.43
1:C:406:SER:OG	1:C:407:ASP:N	2.51	0.43
1:A:370:TYR:HB3	1:A:373:GLU:HB2	2.01	0.43
1:D:109:ALA:HB1	1:D:239:MET:CE	2.49	0.43
1:D:433:LYS:HE3	1:D:455:ARG:H	1.84	0.43
1:D:519:SER:OG	1:D:520:GLY:N	2.49	0.43
1:B:395:PHE:HB3	1:B:444:TYR:O	2.18	0.43
1:D:108:VAL:O	1:D:461:ARG:HD2	2.18	0.43
1:A:211:LEU:HD12	1:A:211:LEU:N	2.33	0.43
1:A:230:LYS:HD2	1:A:234:GLU:OE2	2.19	0.43
1:A:430:VAL:HG22	1:A:512:LEU:HB2	2.00	0.43
1:B:359:ILE:HG21	1:B:378:GLN:CD	2.39	0.43
1:D:290:ILE:HG22	1:D:291:MET:N	2.32	0.43
1:A:51:ILE:HD12	1:A:61:LEU:CD2	2.48	0.43
1:A:63:GLU:HB3	1:A:372:LEU:HD21	2.01	0.43
1:A:329:GLN:HA	1:A:332:GLU:HG2	2.00	0.43
1:B:124:ILE:O	1:B:125:LYS:O	2.37	0.43
1:B:432:THR:HB	1:B:437:SER:OG	2.18	0.43
1:A:485:ASP:OD2	1:A:489:ARG:NH2	2.52	0.42
1:B:139:THR:CG2	1:B:140:LEU:N	2.82	0.42
1:C:45:THR:HG21	1:C:352:VAL:HG22	2.01	0.42
1:C:482:TRP:CD1	1:C:517:PRO:HB3	2.54	0.42
1:A:432:THR:HG21	1:A:435:GLY:HA2	2.00	0.42
1:A:431:LEU:N	1:A:431:LEU:CD1	2.81	0.42
1:B:104:LEU:HD13	1:B:104:LEU:HA	1.96	0.42
1:B:233:VAL:O	1:B:234:GLU:C	2.58	0.42
1:A:183:LEU:O	1:A:183:LEU:HD12	2.20	0.42
1:A:472:VAL:HG12	1:A:492:PHE:CE2	2.53	0.42
1:D:163:ASN:O	1:D:164:ILE:C	2.58	0.42
1:C:417:VAL:HG13	1:C:446:PRO:HB3	2.00	0.42
1:B:386:GLU:HA	1:B:389:ILE:HD12	2.00	0.42
1:C:74:LEU:HD11	1:C:88:ILE:HG13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:ASP:C	1:A:147:ALA:N	2.73	0.42
1:B:221:VAL:HG21	1:B:253:GLU:HG2	2.01	0.42
1:A:25:THR:HG22	1:A:26:PHE:H	1.85	0.42
1:B:161:TYR:CD1	1:B:161:TYR:C	2.93	0.42
1:B:277:VAL:O	1:B:278:ARG:C	2.57	0.42
1:B:421:PHE:HE1	1:B:447:ARG:CD	2.32	0.42
1:A:157:LEU:HD13	1:A:157:LEU:C	2.39	0.42
1:A:394:LEU:HD13	1:A:445:ARG:HG3	2.01	0.42
1:D:229:LEU:O	1:D:233:VAL:HG23	2.19	0.42
1:C:331:LEU:O	1:C:364:GLU:HG2	2.20	0.42
1:B:382:ALA:O	1:B:386:GLU:HG2	2.20	0.41
1:D:163:ASN:HB3	1:D:166:LYS:CG	2.49	0.41
1:D:361:LEU:HB3	1:D:365:THR:HG23	2.01	0.41
1:A:305:LYS:O	1:A:306:VAL:C	2.58	0.41
1:A:342:ARG:HD3	1:A:342:ARG:C	2.41	0.41
1:B:395:PHE:CZ	1:B:421:PHE:CD2	3.07	0.41
1:C:58:VAL:O	1:C:59:GLU:C	2.57	0.41
1:B:400:ARG:HA	1:B:403:PRO:HD2	2.03	0.41
1:B:408:PRO:HB3	1:C:527:VAL:HG12	2.02	0.41
1:D:129:THR:O	1:D:131:GLU:N	2.53	0.41
1:A:182:SER:O	1:A:183:LEU:HB3	2.20	0.41
1:B:290:ILE:O	1:B:324:VAL:HA	2.20	0.41
1:B:318:ASN:HD21	1:B:355:GLY:HA3	1.85	0.41
1:B:395:PHE:CZ	1:B:421:PHE:HE2	2.26	0.41
1:D:103:ILE:HG23	1:D:496:VAL:HA	2.02	0.41
1:D:407:ASP:OD1	1:D:407:ASP:C	2.58	0.41
1:C:219:PRO:O	1:C:220:ALA:HB3	2.20	0.41
1:D:302:PRO:HG2	1:D:305:LYS:CD	2.51	0.41
1:C:441:VAL:HG11	1:C:450:ILE:HG12	2.02	0.41
1:B:422:LYS:O	1:C:404:ILE:HB	2.20	0.41
1:B:451:ILE:HD11	1:B:502:PHE:HD2	1.85	0.41
1:D:73:ARG:NH1	1:D:113:ASP:OD2	2.54	0.41
1:D:168:VAL:CG1	1:D:193:LEU:HD21	2.49	0.41
1:C:41:THR:O	1:C:383:ARG:NH2	2.54	0.41
1:C:340:PRO:HG3	1:C:377:MET:HG2	2.02	0.41
1:A:512:LEU:HD23	1:A:525:MET:HA	2.03	0.41
1:A:528:VAL:CG2	1:A:529:PRO:HD2	2.50	0.41
1:B:41:THR:HG22	1:B:42:ALA:N	2.35	0.41
1:B:510:ILE:HD13	1:B:527:VAL:HG22	2.01	0.41
1:C:221:VAL:HG22	1:C:253:GLU:OE1	2.21	0.41
1:A:138:ALA:H	1:A:197:VAL:CG1	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:ASN:H	1:A:158:TRP:HE1	1.69	0.41
1:B:41:THR:HG22	1:B:42:ALA:H	1.86	0.41
1:D:239:MET:HA	1:D:266:LYS:O	2.21	0.41
1:D:297:LEU:HG	1:D:301:ILE:HD12	2.03	0.41
1:C:372:LEU:C	1:C:374:ALA:N	2.74	0.41
1:A:133:GLU:HA	1:A:202:SER:HA	2.01	0.41
1:A:418:GLU:HG3	1:D:418:GLU:CG	2.51	0.41
1:A:418:GLU:CG	1:D:418:GLU:HG3	2.51	0.41
1:A:512:LEU:HA	1:A:524:THR:O	2.20	0.41
1:B:175:TYR:CD1	1:B:182:SER:HB3	2.55	0.41
1:B:283:ILE:O	1:B:284:LEU:C	2.59	0.41
1:D:494:MET:CG	1:D:531:PRO:HD2	2.51	0.41
1:C:44:ASN:O	1:C:467:ARG:HG3	2.21	0.41
1:C:296:ASP:O	1:C:299:ILE:HG12	2.21	0.41
1:C:497:GLY:O	1:C:498:LYS:C	2.59	0.41
1:B:48:ILE:HG23	1:B:71:VAL:HB	2.02	0.40
1:B:304:GLU:O	1:B:307:PHE:CE1	2.74	0.40
1:B:423:CYS:HA	1:C:405:THR:HA	2.02	0.40
1:C:39:PRO:HB2	1:C:383:ARG:HH11	1.86	0.40
1:B:70:ASN:HB3	1:B:464:HIS:CG	2.56	0.40
1:D:29:HIS:ND1	1:D:32:ARG:NH2	2.70	0.40
1:D:228:ASP:O	1:D:231:PHE:HB3	2.21	0.40
1:A:123:LEU:HD12	1:A:150:GLU:HB3	2.04	0.40
1:C:372:LEU:O	1:C:374:ALA:N	2.55	0.40
1:D:261:LYS:HD3	1:D:261:LYS:N	2.37	0.40
1:C:39:PRO:HB2	1:C:383:ARG:NH1	2.37	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:A:35:ILE:O	1:D:305:LYS:NZ[2_556]	1.90	0.30

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	506/551 (92%)	456 (90%)	48 (10%)	2 (0%)	34	69
1	B	506/551 (92%)	452 (89%)	50 (10%)	4 (1%)	19	54
1	C	410/551 (74%)	369 (90%)	37 (9%)	4 (1%)	15	49
1	D	506/551 (92%)	456 (90%)	48 (10%)	2 (0%)	34	69
All	All	1928/2204 (88%)	1733 (90%)	183 (10%)	12 (1%)	25	59

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	125	LYS
1	B	411	ALA
1	B	516	ARG
1	C	406	SER
1	A	156	ILE
1	D	127	SER
1	D	519	SER
1	C	328	THR
1	B	127	SER
1	A	328	THR
1	C	403	PRO
1	C	516	ARG

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	419/453 (92%)	412 (98%)	7 (2%)	60	83
1	B	419/453 (92%)	410 (98%)	9 (2%)	53	79
1	C	342/453 (76%)	335 (98%)	7 (2%)	55	80
1	D	419/453 (92%)	413 (99%)	6 (1%)	67	86
All	All	1599/1812 (88%)	1570 (98%)	29 (2%)	59	82

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	120	ARG
1	A	146	ASN
1	A	148	TYR
1	A	161	TYR
1	A	342	ARG
1	A	357	ASP
1	A	521	PHE
1	B	53	PRO
1	B	178	ASP
1	B	191	ASP
1	B	294	ARG
1	B	339	ARG
1	B	342	ARG
1	B	390	TYR
1	B	436	ARG
1	B	504	LYS
1	D	154	GLU
1	D	188	LYS
1	D	294	ARG
1	D	346	SER
1	D	390	TYR
1	D	467	ARG
1	C	115	LYS
1	C	120	ARG
1	C	383	ARG
1	C	420	SER
1	C	422	LYS
1	C	445	ARG
1	C	526	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	378	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 monosaccharides 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	508/551 (92%)	-0.14	8 (1%)	72	51	23, 49, 102, 113	0
1	B	508/551 (92%)	-0.10	9 (1%)	68	47	36, 55, 84, 116	0
1	C	414/551 (75%)	-0.03	8 (1%)	66	46	35, 60, 87, 120	0
1	D	508/551 (92%)	-0.11	12 (2%)	59	37	25, 46, 73, 99	0
All	All	1938/2204 (87%)	-0.10	37 (1%)	66	46	23, 53, 90, 120	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	402	ALA	6.9
1	D	402	ALA	4.5
1	D	519	SER	4.5
1	D	517	PRO	4.4
1	D	403	PRO	4.3
1	D	518	GLY	4.2
1	B	521	PHE	3.5
1	B	517	PRO	3.5
1	D	401	LEU	3.2
1	C	123	LEU	3.2
1	C	121	THR	3.1
1	B	24	ASP	3.1
1	C	120	ARG	2.9
1	B	519	SER	2.9
1	D	521	PHE	2.8
1	D	128	GLY	2.7
1	D	339	ARG	2.6
1	B	518	GLY	2.6
1	A	203	LEU	2.5
1	A	199	ASN	2.5
1	C	122	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	119	ILE	2.4
1	A	165	CYS	2.4
1	A	202	SER	2.4
1	A	139	THR	2.4
1	A	40	ILE	2.4
1	B	338	PRO	2.3
1	C	218	LEU	2.2
1	D	129	THR	2.2
1	D	520	GLY	2.2
1	A	187	GLN	2.2
1	C	261	LYS	2.1
1	A	153	ASP	2.1
1	B	339	ARG	2.1
1	B	37	SER	2.0
1	D	338	PRO	2.0
1	C	367	LYS	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.