



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:07 PM UTC

PDB ID : 5Y9H / pdb_00005y9h
Title : Crystal structure of SafDAA-dsc complex
Authors : Zeng, L.H.; Zhang, L.; Wang, P.R.; Meng, G.
Deposited on : 2017-08-25
Resolution : 2.80 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

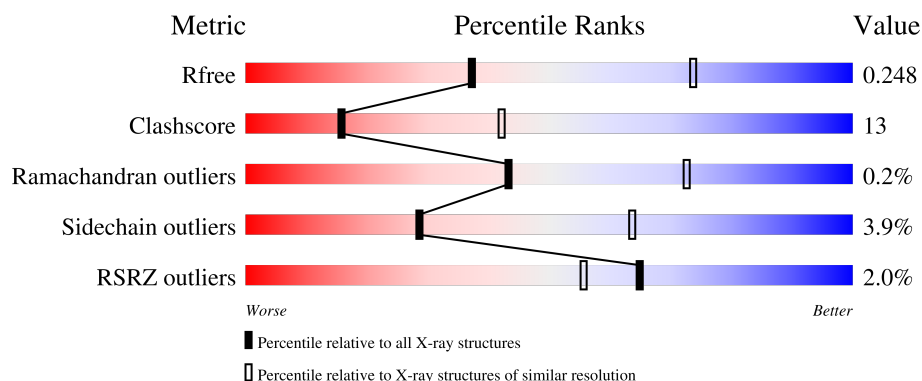
1 Overall quality at a glance

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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	466	70% 20% • 8%
1	B	466	3% 61% 29% • 9%
1	C	466	2% 65% 23% • 10%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18834 atoms, of which 9244 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 SafD,Putative outer membrane protein,Putative outer membrane protein,Putative outer membrane protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	430	Total	C	H	N	O	S	0	0	0
			6313	1999	3099	563	647	5			
1	B	424	Total	C	H	N	O	S	0	0	0
			6235	1969	3070	555	636	5			
1	C	421	Total	C	H	N	O	S	0	0	0
			6236	1965	3075	555	637	4			

There are 99 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP H9L4M7
A	2	GLY	-	expression tag	UNP H9L4M7
A	3	SER	-	expression tag	UNP H9L4M7
A	4	SER	-	expression tag	UNP H9L4M7
A	5	HIS	-	expression tag	UNP H9L4M7
A	6	HIS	-	expression tag	UNP H9L4M7
A	7	HIS	-	expression tag	UNP H9L4M7
A	8	HIS	-	expression tag	UNP H9L4M7
A	9	HIS	-	expression tag	UNP H9L4M7
A	10	HIS	-	expression tag	UNP H9L4M7
A	11	SER	-	expression tag	UNP H9L4M7
A	12	SER	-	expression tag	UNP H9L4M7
A	13	GLY	-	expression tag	UNP H9L4M7
A	14	LEU	-	expression tag	UNP H9L4M7
A	15	VAL	-	expression tag	UNP H9L4M7
A	16	PRO	-	expression tag	UNP H9L4M7
A	17	ARG	-	expression tag	UNP H9L4M7
A	18	GLY	-	expression tag	UNP H9L4M7
A	19	SER	-	expression tag	UNP H9L4M7
A	20	HIS	-	expression tag	UNP H9L4M7
A	21	MET	-	expression tag	UNP H9L4M7
A	148	ASP	-	linker	UNP H9L4M7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	149	ASN	-	linker	UNP H9L4M7
A	150	LYS	-	linker	UNP H9L4M7
A	151	GLN	-	linker	UNP H9L4M7
A	296	ASP	-	linker	UNP Q8ZRK4
A	297	ASN	-	linker	UNP Q8ZRK4
A	298	LYS	-	linker	UNP Q8ZRK4
A	299	GLN	-	linker	UNP Q8ZRK4
A	444	ASP	-	linker	UNP Q8ZRK4
A	445	ASN	-	linker	UNP Q8ZRK4
A	446	LYS	-	linker	UNP Q8ZRK4
A	447	GLN	-	linker	UNP Q8ZRK4
B	1	MET	-	initiating methionine	UNP H9L4M7
B	2	GLY	-	expression tag	UNP H9L4M7
B	3	SER	-	expression tag	UNP H9L4M7
B	4	SER	-	expression tag	UNP H9L4M7
B	5	HIS	-	expression tag	UNP H9L4M7
B	6	HIS	-	expression tag	UNP H9L4M7
B	7	HIS	-	expression tag	UNP H9L4M7
B	8	HIS	-	expression tag	UNP H9L4M7
B	9	HIS	-	expression tag	UNP H9L4M7
B	10	HIS	-	expression tag	UNP H9L4M7
B	11	SER	-	expression tag	UNP H9L4M7
B	12	SER	-	expression tag	UNP H9L4M7
B	13	GLY	-	expression tag	UNP H9L4M7
B	14	LEU	-	expression tag	UNP H9L4M7
B	15	VAL	-	expression tag	UNP H9L4M7
B	16	PRO	-	expression tag	UNP H9L4M7
B	17	ARG	-	expression tag	UNP H9L4M7
B	18	GLY	-	expression tag	UNP H9L4M7
B	19	SER	-	expression tag	UNP H9L4M7
B	20	HIS	-	expression tag	UNP H9L4M7
B	21	MET	-	expression tag	UNP H9L4M7
B	148	ASP	-	linker	UNP H9L4M7
B	149	ASN	-	linker	UNP H9L4M7
B	150	LYS	-	linker	UNP H9L4M7
B	151	GLN	-	linker	UNP H9L4M7
B	296	ASP	-	linker	UNP Q8ZRK4
B	297	ASN	-	linker	UNP Q8ZRK4
B	298	LYS	-	linker	UNP Q8ZRK4
B	299	GLN	-	linker	UNP Q8ZRK4
B	444	ASP	-	linker	UNP Q8ZRK4
B	445	ASN	-	linker	UNP Q8ZRK4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	446	LYS	-	linker	UNP Q8ZRK4
B	447	GLN	-	linker	UNP Q8ZRK4
C	1	MET	-	initiating methionine	UNP H9L4M7
C	2	GLY	-	expression tag	UNP H9L4M7
C	3	SER	-	expression tag	UNP H9L4M7
C	4	SER	-	expression tag	UNP H9L4M7
C	5	HIS	-	expression tag	UNP H9L4M7
C	6	HIS	-	expression tag	UNP H9L4M7
C	7	HIS	-	expression tag	UNP H9L4M7
C	8	HIS	-	expression tag	UNP H9L4M7
C	9	HIS	-	expression tag	UNP H9L4M7
C	10	HIS	-	expression tag	UNP H9L4M7
C	11	SER	-	expression tag	UNP H9L4M7
C	12	SER	-	expression tag	UNP H9L4M7
C	13	GLY	-	expression tag	UNP H9L4M7
C	14	LEU	-	expression tag	UNP H9L4M7
C	15	VAL	-	expression tag	UNP H9L4M7
C	16	PRO	-	expression tag	UNP H9L4M7
C	17	ARG	-	expression tag	UNP H9L4M7
C	18	GLY	-	expression tag	UNP H9L4M7
C	19	SER	-	expression tag	UNP H9L4M7
C	20	HIS	-	expression tag	UNP H9L4M7
C	21	MET	-	expression tag	UNP H9L4M7
C	148	ASP	-	linker	UNP H9L4M7
C	149	ASN	-	linker	UNP H9L4M7
C	150	LYS	-	linker	UNP H9L4M7
C	151	GLN	-	linker	UNP H9L4M7
C	296	ASP	-	linker	UNP Q8ZRK4
C	297	ASN	-	linker	UNP Q8ZRK4
C	298	LYS	-	linker	UNP Q8ZRK4
C	299	GLN	-	linker	UNP Q8ZRK4
C	444	ASP	-	linker	UNP Q8ZRK4
C	445	ASN	-	linker	UNP Q8ZRK4
C	446	LYS	-	linker	UNP Q8ZRK4
C	447	GLN	-	linker	UNP Q8ZRK4

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	20	Total O 20 20	0	0
2	B	11	Total O 11 11	0	0

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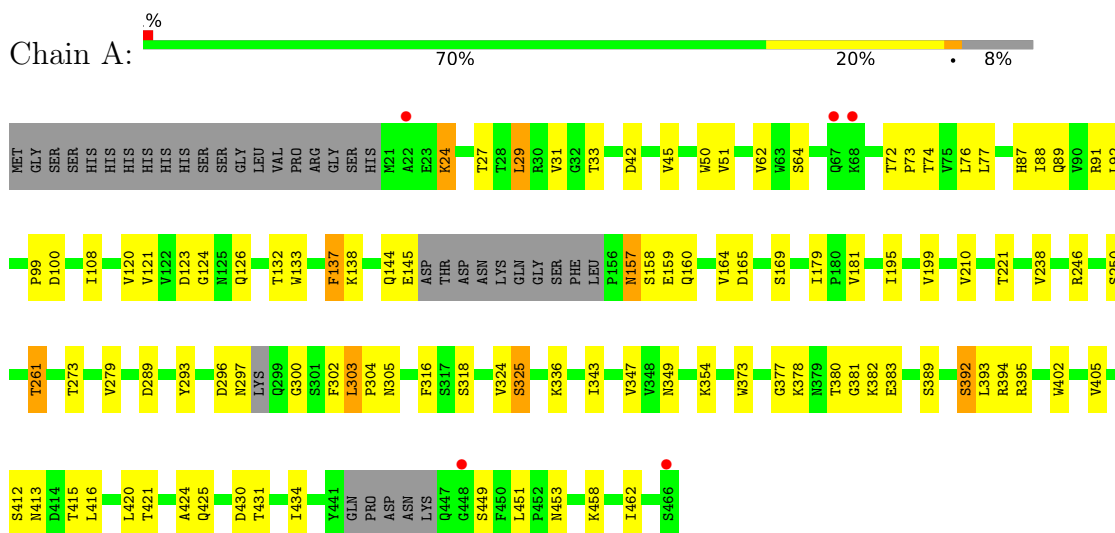
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	19	Total	O	0	0
			19	19		

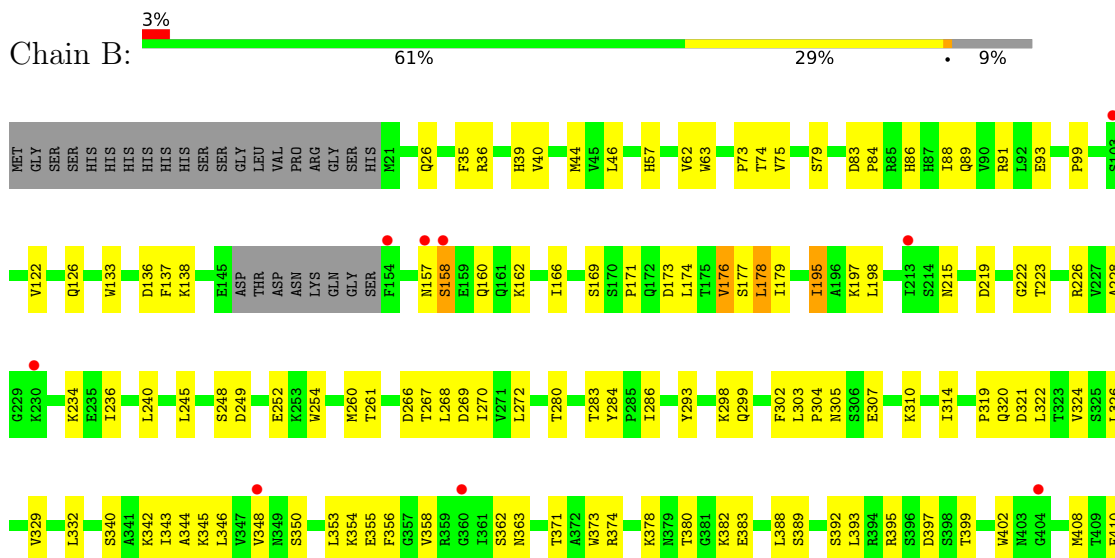
3 Residue-property plots [i](#)

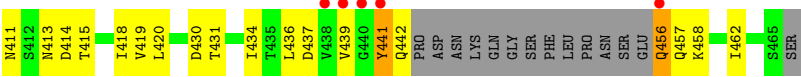
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: SafD,Putative outer membrane protein,Putative outer membrane protein,Putative outer membrane protein

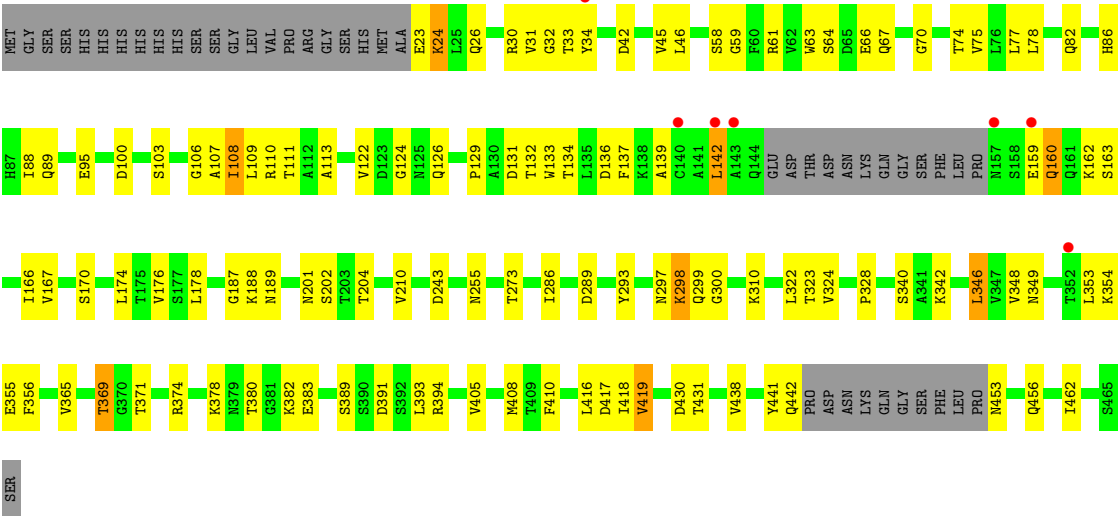


- Molecule 1: SafD,Putative outer membrane protein,Putative outer membrane protein,Putative outer membrane protein





● Molecule 1: SafD,Putative outer membrane protein,Putative outer membrane protein,Putative outer membrane protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	133.27Å 66.07Å 187.68Å 90.00° 96.22° 90.00°	Depositor
Resolution (Å)	93.29 – 2.80 93.29 – 2.80	Depositor EDS
% Data completeness (in resolution range)	95.6 (93.29-2.80) 95.7 (93.29-2.80)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 2.82Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, R_{free}	0.219 , 0.255 0.216 , 0.248	Depositor DCC
R_{free} test set	1895 reflections (4.68%)	wwPDB-VP
Wilson B-factor (Å ²)	71.7	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 99.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	18834	wwPDB-VP
Average B, all atoms (Å ²)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.20% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.41	3/3256 (0.1%)	0.56	0/4433
1	B	0.43	4/3209 (0.1%)	0.60	0/4373
1	C	0.26	0/3204	0.55	0/4364
All	All	0.37	7/9669 (0.1%)	0.57	0/13170

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	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	303	LEU	C-O	-7.67	1.17	1.24
1	B	305	ASN	C-O	-7.07	1.14	1.24
1	A	302	PHE	C-O	-7.05	1.15	1.23
1	A	303	LEU	C-O	-6.71	1.16	1.24
1	A	304	PRO	C-O	-5.81	1.16	1.24
1	B	305	ASN	CA-C	-5.66	1.44	1.52
1	B	304	PRO	C-O	-5.08	1.17	1.24

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	453	ASN	Peptide

5.2 Too-close contacts ⓘ

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	3214	3099	3101	65	0
1	B	3165	3070	3062	114	0
1	C	3161	3075	3070	75	0
2	A	20	0	0	3	0
2	B	11	0	0	5	0
2	C	19	0	0	2	0
All	All	9590	9244	9233	250	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (250) 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:C:442:GLN:NE2	2:C:501:HOH:O	1.82	1.11
1:B:248:SER:OG	1:B:249:ASP:OD1	1.83	0.96
1:B:442:GLN:NE2	2:B:501:HOH:O	1.93	0.93
1:B:26:GLN:NE2	2:B:502:HOH:O	2.06	0.88
1:B:458:LYS:CD	1:B:458:LYS:CB	2.56	0.83
1:B:388:LEU:HB2	1:B:393:LEU:HD11	1.62	0.81
1:A:144:GLN:NE2	1:A:145:GLU:OE1	2.15	0.80
1:C:58:SER:O	1:C:111:THR:N	2.14	0.80
1:B:293:TYR:HD1	1:B:302:PHE:CD1	2.00	0.79
1:B:215:ASN:OD1	1:B:215:ASN:ND2	2.15	0.79
1:A:221:THR:O	2:A:501:HOH:O	2.05	0.75
1:B:249:ASP:OD1	1:B:261:THR:N	2.21	0.73
1:B:293:TYR:CD1	1:B:302:PHE:CD1	2.78	0.72
1:C:160:GLN:OE1	1:C:162:LYS:NZ	2.23	0.71
1:C:243:ASP:OD2	1:C:243:ASP:CB	2.38	0.71
1:B:160:GLN:OE1	1:B:162:LYS:NZ	2.24	0.71
1:B:374:ARG:NH1	1:B:383:GLU:OE1	2.24	0.71
1:C:243:ASP:CB	1:C:243:ASP:OD1	2.39	0.70
1:C:33:THR:HA	2:C:503:HOH:O	1.93	0.68
1:C:67:GLN:HG2	1:C:75:VAL:O	1.93	0.68
1:A:24:LYS:HZ1	1:A:160:GLN:HG3	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:THR:O	1:B:284:TYR:OH	2.10	0.67
1:A:158:SER:O	2:A:502:HOH:O	2.13	0.67
1:B:348:VAL:HG21	1:B:356:PHE:CZ	2.30	0.66
1:B:176:VAL:O	1:B:177:SER:OG	2.10	0.65
1:C:89:GLN:O	1:C:126:GLN:NE2	2.30	0.65
1:B:380:THR:HG22	1:B:430:ASP:OD2	1.97	0.64
1:B:356:PHE:CZ	1:B:410:PHE:HB2	2.32	0.64
1:C:111:THR:HG22	1:C:113:ALA:H	1.62	0.64
1:C:348:VAL:HG21	1:C:356:PHE:CE2	2.32	0.63
1:B:46:LEU:HD11	1:B:122:VAL:HG13	1.81	0.62
1:B:380:THR:HG23	1:B:382:LYS:H	1.65	0.62
1:B:326:LEU:HD11	1:B:344:ALA:HB1	1.81	0.62
1:C:176:VAL:HG13	1:C:310:LYS:HE2	1.82	0.62
1:C:380:THR:HG23	1:C:382:LYS:H	1.63	0.62
1:B:178:LEU:HB2	1:B:198:LEU:HA	1.82	0.62
1:C:374:ARG:NH1	1:C:383:GLU:OE1	2.33	0.62
1:C:46:LEU:HD11	1:C:122:VAL:HG13	1.82	0.62
1:A:64:SER:CB	1:A:76:LEU:HD21	2.30	0.61
1:C:391:ASP:OD1	1:C:394:ARG:NH2	2.34	0.61
1:B:319:PRO:O	1:B:321:ASP:N	2.34	0.61
1:B:343:ILE:HD11	1:B:462:ILE:HG21	1.82	0.61
1:B:356:PHE:CE1	1:B:410:PHE:HB2	2.35	0.61
1:A:393:LEU:O	1:A:394:ARG:HG2	2.01	0.60
1:C:42:ASP:OD1	1:C:124:GLY:N	2.34	0.60
1:C:243:ASP:OD2	1:C:243:ASP:OD1	2.19	0.60
1:C:31:VAL:HG13	1:C:166:ILE:HD13	1.83	0.60
1:B:57:HIS:O	2:B:503:HOH:O	2.16	0.60
1:A:373:TRP:HZ2	1:A:434:ILE:HD11	1.66	0.59
1:C:100:ASP:OD2	1:C:103:SER:OG	2.20	0.59
1:C:453:ASN:O	1:C:453:ASN:ND2	2.35	0.59
1:B:388:LEU:CB	1:B:393:LEU:HD11	2.32	0.59
1:C:356:PHE:CE2	1:C:410:PHE:HB2	2.38	0.58
1:A:92:LEU:HD23	1:A:120:VAL:HG22	1.86	0.58
1:B:293:TYR:CD1	1:B:302:PHE:CE1	2.92	0.58
1:A:354:LYS:O	1:A:412:SER:N	2.31	0.57
1:A:343:ILE:HD11	1:A:420:LEU:HD23	1.86	0.57
1:B:373:TRP:HZ2	1:B:434:ILE:HD11	1.70	0.57
1:B:198:LEU:HB3	1:B:268:LEU:O	2.05	0.56
1:A:89:GLN:NE2	1:A:123:ASP:OD2	2.38	0.56
1:B:326:LEU:HD13	1:B:346:LEU:HB2	1.86	0.56
1:A:343:ILE:CG2	1:A:462:ILE:HG21	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:388:LEU:HD23	1:B:418:ILE:HD12	1.88	0.56
1:C:442:GLN:O	1:C:453:ASN:ND2	2.39	0.56
1:C:323:THR:HG23	1:C:349:ASN:HB2	1.88	0.55
1:C:110:ARG:O	1:C:111:THR:OG1	2.19	0.55
1:B:402:TRP:CZ3	1:B:439:VAL:HG21	2.42	0.55
1:B:176:VAL:HG13	1:B:310:LYS:HE2	1.88	0.55
1:B:176:VAL:O	1:B:310:LYS:HE3	2.06	0.54
1:B:343:ILE:HG13	1:B:462:ILE:HD13	1.90	0.54
1:A:157:ASN:OD1	1:A:157:ASN:N	2.39	0.53
1:B:197:LYS:HA	1:B:269:ASP:OD1	2.08	0.53
1:A:42:ASP:OD1	1:A:124:GLY:N	2.36	0.53
1:B:430:ASP:OD1	1:B:431:THR:N	2.33	0.53
1:B:298:LYS:HG3	1:B:299:GLN:H	1.74	0.53
1:C:31:VAL:CG1	1:C:166:ILE:HD13	2.39	0.53
1:A:380:THR:HG23	1:A:382:LYS:H	1.73	0.53
1:B:240:LEU:HB2	1:B:245:LEU:HD21	1.91	0.53
1:C:348:VAL:HG21	1:C:356:PHE:CD2	2.44	0.53
1:A:77:LEU:HD13	1:A:77:LEU:C	2.35	0.52
1:C:380:THR:HG22	1:C:430:ASP:OD2	2.09	0.52
1:A:393:LEU:C	1:A:395:ARG:H	2.17	0.52
1:C:139:ALA:O	1:C:159:GLU:HB2	2.09	0.52
1:B:46:LEU:HD23	1:B:166:ILE:HG21	1.92	0.52
1:A:421:THR:O	1:A:425:GLN:NE2	2.43	0.52
1:B:326:LEU:HD12	1:B:345:LYS:O	2.10	0.52
1:B:358:VAL:HG12	1:B:410:PHE:HE1	1.76	0.51
1:B:354:LYS:HD2	1:B:355:GLU:HG3	1.91	0.51
1:B:397:ASP:OD2	1:B:411:ASN:ND2	2.44	0.51
1:C:74:THR:HG22	1:C:107:ALA:HB2	1.92	0.51
1:B:348:VAL:HG22	1:B:414:ASP:O	2.11	0.51
1:B:395:ARG:NH1	1:B:415:THR:O	2.44	0.51
1:B:35:PHE:N	2:B:504:HOH:O	2.43	0.51
1:B:343:ILE:HG22	1:B:418:ILE:C	2.36	0.50
1:B:329:VAL:O	1:B:332:LEU:HD11	2.11	0.50
1:C:369:THR:OG1	1:C:408:MET:HG3	2.11	0.50
1:A:45:VAL:HA	1:A:121:VAL:HG22	1.94	0.50
1:B:136:ASP:OD1	1:B:136:ASP:O	2.30	0.50
1:A:389:SER:OG	1:A:392:SER:HB2	2.11	0.50
1:C:136:ASP:HA	1:C:163:SER:HA	1.94	0.50
1:A:73:PRO:HG2	1:A:99:PRO:HB3	1.94	0.49
1:A:380:THR:HG22	1:A:430:ASP:OD2	2.11	0.49
1:B:348:VAL:HG23	1:B:348:VAL:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:THR:HG22	1:A:51:VAL:HG12	1.94	0.49
1:A:29:LEU:HD11	1:A:137:PHE:CE1	2.47	0.49
1:B:157:ASN:O	1:B:158:SER:O	2.30	0.49
1:A:77:LEU:HD21	1:A:87:HIS:CD2	2.48	0.49
1:B:88:ILE:HG22	1:B:133:TRP:CD1	2.48	0.49
1:B:399:THR:HG22	1:B:408:MET:HG2	1.94	0.49
1:B:83:ASP:HB3	1:B:86:HIS:CD2	2.47	0.49
1:B:322:LEU:HD13	1:B:350:SER:HB2	1.95	0.49
1:A:77:LEU:HD11	1:A:87:HIS:CD2	2.47	0.48
1:B:215:ASN:N	1:C:26:GLN:OE1	2.45	0.48
1:A:100:ASP:HB2	1:A:108:ILE:HG23	1.95	0.48
1:C:353:LEU:HD12	1:C:354:LYS:HE2	1.95	0.48
1:C:328:PRO:HB3	1:C:462:ILE:HD13	1.96	0.48
1:B:254:TRP:HB2	1:B:302:PHE:CD2	2.48	0.48
1:B:393:LEU:C	1:B:395:ARG:H	2.21	0.48
1:A:246:ARG:O	1:A:246:ARG:HG3	2.12	0.48
1:B:393:LEU:C	1:B:395:ARG:N	2.71	0.48
1:C:63:TRP:HB3	1:C:106:GLY:HA3	1.95	0.48
1:C:67:GLN:OE1	1:C:70:GLY:HA2	2.14	0.48
1:B:89:GLN:O	1:B:126:GLN:NE2	2.47	0.48
1:B:355:GLU:HG2	2:B:501:HOH:O	2.14	0.48
1:B:195:ILE:HD11	1:B:272:LEU:HG	1.96	0.47
1:B:324:VAL:HG12	1:B:348:VAL:HA	1.97	0.47
1:B:437:ASP:HB2	1:B:457:GLN:HG2	1.95	0.47
1:B:219:ASP:OD1	1:B:222:GLY:N	2.47	0.47
1:B:348:VAL:O	1:B:413:ASN:HA	2.15	0.47
1:B:226:ARG:HA	1:B:236:ILE:O	2.15	0.47
1:C:132:THR:HG22	1:C:167:VAL:HG13	1.97	0.46
1:A:430:ASP:OD1	1:A:431:THR:N	2.42	0.46
1:B:178:LEU:HA	1:B:197:LYS:O	2.16	0.46
1:B:36:ARG:NH1	1:B:171:PRO:HD3	2.31	0.46
1:B:286:ILE:CG2	1:B:314:ILE:HD11	2.46	0.46
1:B:358:VAL:HG12	1:B:410:PHE:CE1	2.50	0.46
1:B:437:ASP:OD1	1:B:437:ASP:O	2.34	0.46
1:A:293:TYR:OH	1:A:300:GLY:HA3	2.16	0.45
1:B:179:ILE:HD12	1:B:179:ILE:O	2.16	0.45
1:C:389:SER:OG	1:C:417:ASP:HB2	2.16	0.45
1:A:378:LYS:HE2	1:A:431:THR:HB	1.98	0.45
1:B:46:LEU:N	1:B:46:LEU:HD12	2.31	0.45
1:C:324:VAL:HG11	1:C:438:VAL:HG21	1.98	0.45
1:A:74:THR:HG22	1:A:91:ARG:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:ILE:N	1:A:179:ILE:HD12	2.30	0.45
1:C:378:LYS:HG3	1:C:431:THR:O	2.17	0.45
1:B:254:TRP:HB2	1:B:302:PHE:CE2	2.52	0.45
1:B:434:ILE:HG21	1:B:462:ILE:HD11	1.98	0.45
1:C:371:THR:HG21	1:C:408:MET:HE2	1.99	0.44
1:A:181:VAL:HG13	1:A:195:ILE:C	2.43	0.44
1:A:324:VAL:HB	1:A:458:LYS:HD3	1.98	0.44
1:B:342:LYS:HA	1:B:419:VAL:HG12	1.98	0.44
1:C:178:LEU:HD21	1:C:286:ILE:CD1	2.48	0.44
1:A:132:THR:CG2	1:A:165:ASP:HB3	2.47	0.44
1:B:73:PRO:HG2	1:B:99:PRO:HB3	1.99	0.44
1:B:169:SER:HA	1:B:173:ASP:OD1	2.18	0.44
1:B:283:THR:HA	1:B:314:ILE:O	2.18	0.44
1:A:199:VAL:HG11	1:C:201:ASN:ND2	2.33	0.44
1:A:325:SER:HB2	1:A:347:VAL:HG22	1.99	0.44
1:B:393:LEU:N	1:B:393:LEU:HD12	2.32	0.44
1:C:322:LEU:O	1:C:456:GLN:NE2	2.49	0.44
1:A:349:ASN:OD1	1:A:413:ASN:HA	2.17	0.44
1:B:252:GLU:HG3	1:B:293:TYR:CZ	2.53	0.44
1:B:91:ARG:NE	1:B:93:GLU:OE2	2.40	0.44
1:A:402:TRP:HB2	1:A:451:LEU:HD13	2.00	0.44
1:B:254:TRP:CE3	1:B:302:PHE:CD2	3.06	0.44
1:B:44:MET:O	1:B:46:LEU:HD12	2.18	0.43
1:C:31:VAL:HG12	1:C:32:GLY:N	2.32	0.43
1:C:46:LEU:HB3	1:C:166:ILE:HD12	2.00	0.43
1:B:298:LYS:HG3	1:B:299:GLN:N	2.33	0.43
1:A:393:LEU:O	1:A:395:ARG:N	2.50	0.43
1:B:307:GLU:OE2	1:C:30:ARG:NE	2.51	0.43
1:C:299:GLN:HG3	1:C:299:GLN:O	2.19	0.43
1:C:59:GLY:HA3	1:C:109:LEU:O	2.19	0.43
1:B:340:SER:O	1:B:340:SER:OG	2.31	0.43
1:B:343:ILE:HG22	1:B:418:ILE:O	2.18	0.43
1:C:369:THR:OG1	1:C:371:THR:HG23	2.19	0.43
1:A:210:VAL:HA	1:A:289:ASP:O	2.19	0.43
1:B:223:THR:HG21	1:B:260:MET:SD	2.59	0.43
1:A:343:ILE:HG21	1:A:462:ILE:HD13	2.01	0.43
1:B:299:GLN:HG2	1:C:255:ASN:HA	2.01	0.43
1:B:62:VAL:HG13	1:B:137:PHE:CD2	2.54	0.42
1:B:63:TRP:CZ2	1:B:138:LYS:HD3	2.54	0.42
1:C:174:LEU:HD23	1:C:202:SER:HB2	2.00	0.42
1:C:441:TYR:O	1:C:442:GLN:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:GLY:O	1:A:126:GLN:HG3	2.18	0.42
1:A:169:SER:HB3	1:A:305:ASN:HB2	2.00	0.42
1:A:50:TRP:NE1	2:A:504:HOH:O	2.29	0.42
1:B:39:HIS:CD2	1:B:40:VAL:N	2.88	0.42
1:B:178:LEU:HD11	1:B:270:ILE:HD12	2.00	0.42
1:B:441:TYR:CD1	1:B:441:TYR:N	2.85	0.42
1:A:62:VAL:HA	1:A:138:LYS:O	2.20	0.42
1:B:371:THR:HG21	1:B:408:MET:SD	2.59	0.42
1:A:250:SER:H	1:A:261:THR:HG22	1.83	0.42
1:C:88:ILE:HG22	1:C:133:TRP:CD1	2.55	0.42
1:A:88:ILE:HG22	1:A:133:TRP:CD1	2.55	0.42
1:C:124:GLY:O	1:C:126:GLN:HG3	2.19	0.42
1:B:79:SER:HB2	1:B:84:PRO:O	2.19	0.42
1:C:346:LEU:CD2	1:C:416:LEU:HB2	2.50	0.42
1:A:347:VAL:HG12	1:A:415:THR:HB	2.02	0.41
1:B:332:LEU:HD12	1:B:332:LEU:H	1.85	0.41
1:C:82:GLN:HG3	1:C:131:ASP:OD2	2.20	0.41
1:C:389:SER:O	1:C:393:LEU:HD12	2.19	0.41
1:C:23:GLU:HA	1:C:24:LYS:HG3	2.00	0.41
1:C:86:HIS:ND1	1:C:129:PRO:CG	2.83	0.41
1:C:187:GLY:O	1:C:189:ASN:ND2	2.52	0.41
1:C:328:PRO:HB3	1:C:462:ILE:CD1	2.50	0.41
1:A:62:VAL:HG23	1:A:92:LEU:HD13	2.02	0.41
1:B:286:ILE:HB	1:B:314:ILE:HD11	2.02	0.41
1:A:24:LYS:HE2	1:A:159:GLU:O	2.19	0.41
1:C:108:ILE:HG21	1:C:142:LEU:HD21	2.02	0.41
1:B:266:ASP:OD2	1:B:267:THR:N	2.44	0.41
1:C:355:GLU:HA	1:C:410:PHE:O	2.21	0.41
1:A:296:ASP:O	1:A:297:ASN:C	2.64	0.41
1:A:354:LYS:O	1:A:412:SER:CB	2.68	0.41
1:B:389:SER:OG	1:B:392:SER:HB3	2.21	0.41
1:C:293:TYR:OH	1:C:300:GLY:HA3	2.20	0.41
1:A:238:VAL:C	1:A:273:THR:HG23	2.46	0.41
1:A:392:SER:OG	1:A:416:LEU:HD22	2.20	0.41
1:B:389:SER:O	1:B:393:LEU:CD1	2.68	0.41
1:C:63:TRP:C	1:C:63:TRP:CD1	2.98	0.41
1:C:77:LEU:HA	1:C:89:GLN:HA	2.03	0.41
1:A:373:TRP:HZ2	1:A:434:ILE:CD1	2.32	0.41
1:A:377:GLY:O	1:A:381:GLY:HA2	2.19	0.41
1:C:66:GLU:OE1	1:C:78:LEU:HD21	2.20	0.41
1:C:297:ASN:O	1:C:298:LYS:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:VAL:HG11	1:A:316:PHE:CG	2.56	0.41
1:A:336:LYS:HE2	1:A:424:ALA:HB1	2.03	0.41
1:B:62:VAL:HG13	1:B:137:PHE:HD2	1.86	0.41
1:B:157:ASN:O	1:B:158:SER:C	2.64	0.41
1:B:358:VAL:HA	1:B:437:ASP:O	2.20	0.41
1:B:362:SER:OG	1:B:363:ASN:N	2.54	0.41
1:B:378:LYS:NZ	1:B:378:LYS:O	2.53	0.41
1:C:137:PHE:HE2	1:C:162:LYS:HB2	1.86	0.41
1:C:342:LYS:HA	1:C:419:VAL:HG23	2.03	0.41
1:C:353:LEU:HD12	1:C:354:LYS:H	1.85	0.41
1:B:456:GLN:HE21	1:B:456:GLN:N	2.18	0.41
1:A:434:ILE:HG21	1:A:462:ILE:HD11	2.02	0.40
1:C:210:VAL:HA	1:C:289:ASP:O	2.21	0.40
1:A:31:VAL:HG21	1:A:164:VAL:HG22	2.03	0.40
1:B:35:PHE:CD1	1:B:44:MET:HE3	2.57	0.40
1:B:340:SER:HA	1:B:420:LEU:O	2.22	0.40
1:B:353:LEU:HD12	1:B:354:LYS:H	1.86	0.40
1:C:61:ARG:NH2	1:C:100:ASP:OD1	2.55	0.40
1:A:303:LEU:HA	1:A:303:LEU:HD23	1.90	0.40
1:B:358:VAL:HG21	1:B:436:LEU:HD23	2.02	0.40
1:C:340:SER:C	1:C:419:VAL:HG22	2.47	0.40
1:A:343:ILE:CG2	1:A:462:ILE:HD13	2.52	0.40
1:A:347:VAL:O	1:A:347:VAL:HG23	2.22	0.40
1:B:228:ALA:HA	1:B:234:LYS:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	422/466 (91%)	404 (96%)	18 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	418/466 (90%)	402 (96%)	14 (3%)	2 (0%)	24	55
1	C	415/466 (89%)	389 (94%)	25 (6%)	1 (0%)	43	72
All	All	1255/1398 (90%)	1195 (95%)	57 (4%)	3 (0%)	43	72

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	158	SER
1	C	34	TYR
1	B	320	GLN

5.3.2 Protein sidechains ⓘ

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	347/395 (88%)	334 (96%)	13 (4%)	30	65
1	B	342/395 (87%)	334 (98%)	8 (2%)	44	78
1	C	344/395 (87%)	325 (94%)	19 (6%)	19	51
All	All	1033/1185 (87%)	993 (96%)	40 (4%)	28	64

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LYS
1	A	29	LEU
1	A	33	THR
1	A	72	THR
1	A	137	PHE
1	A	157	ASN
1	A	261	THR
1	A	318	SER
1	A	325	SER
1	A	383	GLU
1	A	392	SER

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Mol	Chain	Res	Type
1	A	405	VAL
1	A	449	SER
1	B	74	THR
1	B	75	VAL
1	B	174	LEU
1	B	176	VAL
1	B	178	LEU
1	B	195	ILE
1	B	441	TYR
1	B	456	GLN
1	C	24	LYS
1	C	45	VAL
1	C	64	SER
1	C	95	GLU
1	C	108	ILE
1	C	134	THR
1	C	142	LEU
1	C	160	GLN
1	C	170	SER
1	C	188	LYS
1	C	204	THR
1	C	273	THR
1	C	298	LYS
1	C	346	LEU
1	C	365	VAL
1	C	369	THR
1	C	405	VAL
1	C	418	ILE
1	C	419	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	HIS
1	A	115	ASN
1	A	379	ASN
1	B	39	HIS
1	B	115	ASN
1	B	258	ASN
1	B	265	ASN
1	B	349	ASN
1	B	456	GLN

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Mol	Chain	Res	Type
1	C	299	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	430/466 (92%)	0.07	5 (1%) 76 68	36, 82, 128, 178	1 (0%)
1	B	424/466 (90%)	0.50	14 (3%) 49 39	59, 122, 165, 198	0
1	C	421/466 (90%)	0.23	7 (1%) 69 60	43, 92, 179, 222	2 (0%)
All	All	1275/1398 (91%)	0.27	26 (2%) 65 56	36, 98, 165, 222	3 (0%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	441	TYR	3.5
1	B	230	LYS	3.4
1	B	440	GLY	3.3
1	B	157	ASN	3.1
1	A	67	GLN	2.9
1	B	158	SER	2.9
1	A	466	SER	2.8
1	B	348	VAL	2.7
1	C	142	LEU	2.7
1	A	68	LYS	2.7
1	C	157	ASN	2.6
1	B	439	VAL	2.5
1	B	213	ILE	2.4
1	C	140	CYS	2.4
1	B	360	GLY	2.3
1	C	34	TYR	2.3
1	B	103	SER	2.3
1	C	143	ALA	2.3
1	A	22	ALA	2.2
1	A	448	GLY	2.2
1	B	404	GLY	2.2
1	B	154	PHE	2.2
1	C	159	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	456	GLN	2.0
1	C	352	THR	2.0
1	B	438	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.