



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 6, 2024 – 05:44 PM EDT

PDB ID : 3B8O
Title : Structure of WzzE- Bacterial Polysaccharide Co-polymerase
Authors : Tocilj, A.; Matte, A.; Cygler, M.
Deposited on : 2007-11-01
Resolution : 2.40 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:

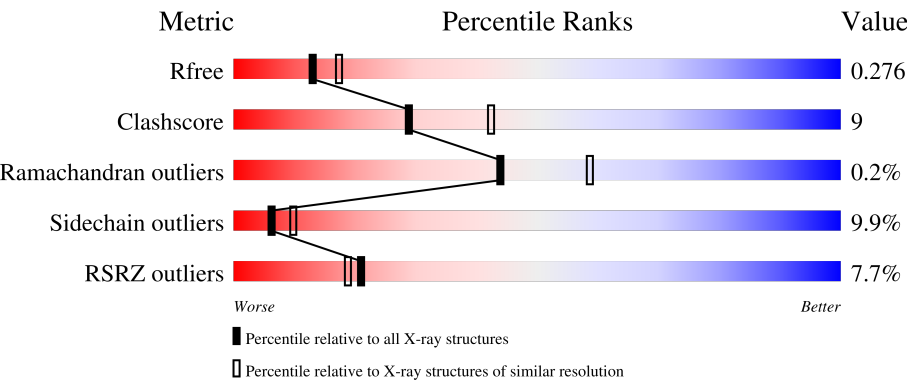
MolProbity : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.20.1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

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 2.40 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}	164625	4642 (2.40-2.40)
Clashscore	180529	5218 (2.40-2.40)
Ramachandran outliers	177936	5158 (2.40-2.40)
Sidechain outliers	177891	5159 (2.40-2.40)
RSRZ outliers	164620	4642 (2.40-2.40)

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	265	<div><div>5%</div><div><div></div><div>65%</div><div>17%</div><div>•</div><div>17%</div></div></div>
1	B	265	<div><div>5%</div><div><div></div><div>69%</div><div>13%</div><div>•</div><div>17%</div></div></div>
1	C	265	<div><div>8%</div><div><div></div><div>68%</div><div>13%</div><div>•</div><div>17%</div></div></div>
1	D	265	<div><div>9%</div><div><div></div><div>67%</div><div>13%</div><div>•</div><div>17%</div></div></div>
1	E	265	<div><div>5%</div><div><div></div><div>63%</div><div>17%</div><div>•</div><div>17%</div></div></div>

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Mol	Chain	Length	Quality of chain
1	F	265	<div><div></div><div>5%</div><div>63%</div><div>19%</div><div>•</div><div>17%</div></div>
1	G	265	<div><div></div><div>7%</div><div>66%</div><div>15%</div><div>•</div><div>17%</div></div>
1	H	265	<div><div></div><div>8%</div><div>66%</div><div>14%</div><div>•</div><div>17%</div></div>

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 14771 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 Lipopolysaccharide biosynthesis protein wzzE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	221	Total	C	N	O	Se	0	0	0
			1797	1124	321	344	8			
1	B	221	Total	C	N	O	Se	0	0	0
			1797	1124	321	344	8			
1	C	221	Total	C	N	O	Se	0	0	0
			1797	1124	321	344	8			
1	D	221	Total	C	N	O	Se	0	0	0
			1797	1124	321	344	8			
1	E	221	Total	C	N	O	Se	0	0	0
			1797	1124	321	344	8			
1	F	221	Total	C	N	O	Se	0	0	0
			1797	1124	321	344	8			
1	G	221	Total	C	N	O	Se	0	0	0
			1797	1124	321	344	8			
1	H	221	Total	C	N	O	Se	0	0	0
			1797	1124	321	344	8			

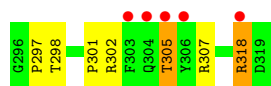
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	46	Total	O	0	0
			46	46		
2	B	48	Total	O	0	0
			48	48		
2	C	52	Total	O	0	0
			52	52		
2	D	48	Total	O	0	0
			48	48		
2	E	48	Total	O	0	0
			48	48		
2	F	58	Total	O	0	0
			58	58		

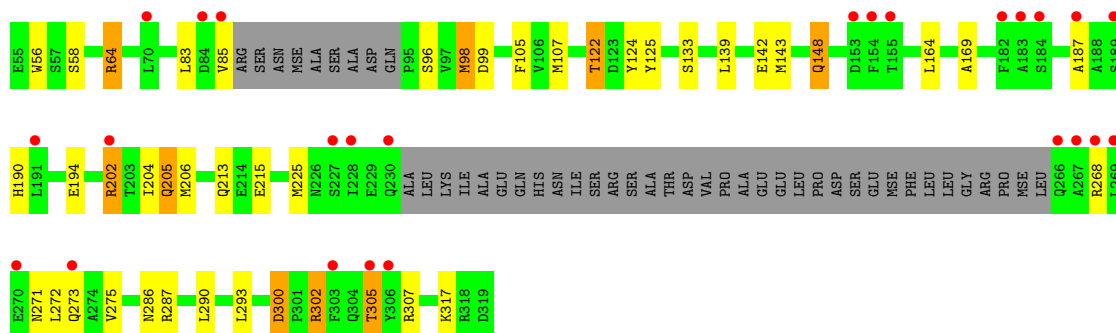
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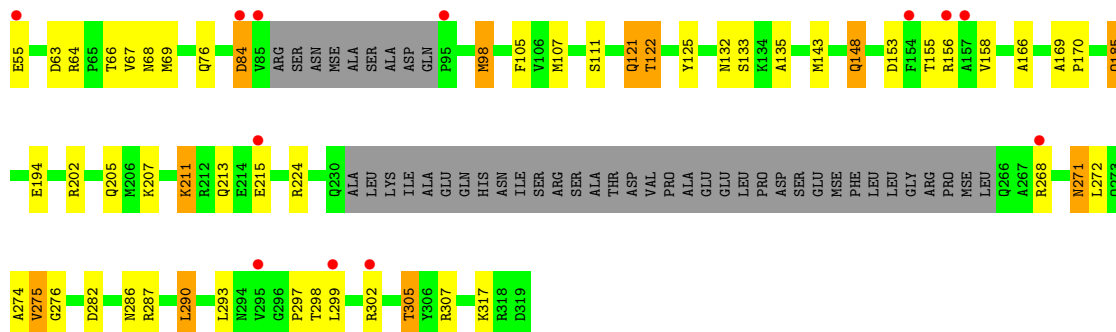
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	45	Total	O	0	0
			45	45		
2	H	50	Total	O	0	0
			50	50		



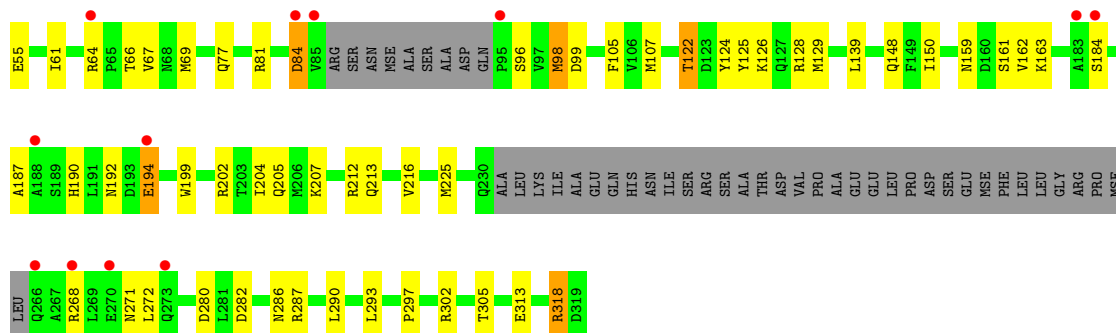
- Molecule 1: Lipopolysaccharide biosynthesis protein wzzE



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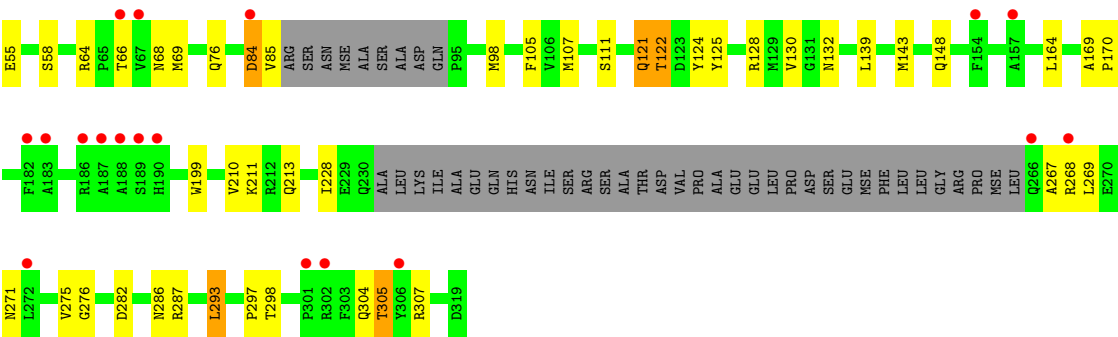


- Molecule 1: Lipopolysaccharide biosynthesis protein wzzE

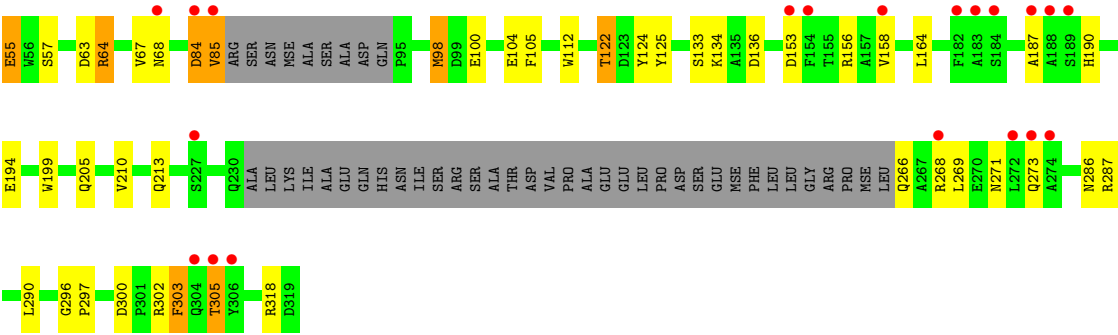


- Molecule 1: Lipopolysaccharide biosynthesis protein wzzE





● Molecule 1: Lipopolysaccharide biosynthesis protein wzzE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	107.44Å 108.30Å 122.57Å 90.00° 102.15° 90.00°	Depositor
Resolution (Å)	47.89 – 2.40 47.89 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.1 (47.89-2.40) 99.0 (47.89-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.78 (at 2.39Å)	Xtriage
Refinement program	REFMAC refmac_5.2.0019	Depositor
R, R_{free}	0.223 , 0.266 0.235 , 0.276	Depositor DCC
R_{free} test set	5290 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	37.2	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 43.6	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	0.90	EDS
Total number of atoms	14771	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.65% 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

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	0.69	0/1822	0.73	1/2451 (0.0%)
1	B	0.71	0/1822	0.77	1/2451 (0.0%)
1	C	0.73	1/1822 (0.1%)	0.77	0/2451
1	D	0.71	0/1822	0.76	1/2451 (0.0%)
1	E	0.79	0/1822	0.81	1/2451 (0.0%)
1	F	0.76	0/1822	0.75	0/2451
1	G	0.74	0/1822	0.78	2/2451 (0.1%)
1	H	0.67	0/1822	0.71	0/2451
All	All	0.73	1/14576 (0.0%)	0.76	6/19608 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	266	GLN	CD-NE2	5.16	1.45	1.32

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	113	ASP	CB-CG-OD1	5.48	123.23	118.30
1	G	121	GLN	CA-CB-CG	5.45	125.39	113.40
1	B	83	LEU	CA-CB-CG	5.39	127.70	115.30
1	D	307	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	G	293	LEU	CA-CB-CG	5.07	126.97	115.30
1	E	143	MSE	CB-CG-SE	-5.07	97.49	112.70

There are no chirality outliers.

There are no planarity outliers.

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	1797	0	1748	42	0
1	B	1797	0	1748	29	0
1	C	1797	0	1748	30	0
1	D	1797	0	1748	27	0
1	E	1797	0	1748	43	0
1	F	1797	0	1748	38	0
1	G	1797	0	1748	26	0
1	H	1797	0	1748	35	0
2	A	46	0	0	2	0
2	B	48	0	0	1	0
2	C	52	0	0	4	0
2	D	48	0	0	0	0
2	E	48	0	0	3	0
2	F	58	0	0	1	0
2	G	45	0	0	1	0
2	H	50	0	0	1	0
All	All	14771	0	13984	245	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 9.

All (245) 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:A:105:PHE:HB2	1:A:305:THR:HG23	1.26	1.13
1:C:98:MSE:HG3	2:C:351:HOH:O	1.51	1.10
1:C:105:PHE:HB2	1:C:305:THR:HG23	1.29	1.09
1:A:65:PRO:HA	1:A:69:MSE:CE	1.82	1.09
1:E:105:PHE:HB2	1:E:305:THR:HG23	1.39	1.04
1:E:275:VAL:HG13	1:E:276:GLY:H	1.20	1.03
1:G:105:PHE:HB2	1:G:305:THR:CG2	1.90	1.02
1:G:105:PHE:HB2	1:G:305:THR:HG22	1.35	1.02
1:A:65:PRO:HA	1:A:69:MSE:HE2	1.48	0.96
1:A:105:PHE:HB2	1:A:305:THR:CG2	1.96	0.95
1:E:105:PHE:HB2	1:E:305:THR:CG2	1.99	0.93
1:B:105:PHE:HB2	1:B:305:THR:HG23	1.48	0.92
1:G:122:THR:HG22	1:G:125:TYR:H	1.36	0.91
1:A:65:PRO:HA	1:A:69:MSE:HE1	1.52	0.89
1:C:157:ALA:HA	2:C:334:HOH:O	1.74	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:PRO:CA	1:A:69:MSE:HE2	2.03	0.88
1:B:225:MSE:HE1	1:B:273:GLN:HG2	1.55	0.87
1:H:105:PHE:HB2	1:H:305:THR:HG23	1.57	0.86
1:G:76:GLN:HE21	1:G:298:THR:H	1.19	0.85
1:D:190:HIS:NE2	1:E:66:THR:HG21	1.91	0.84
1:B:122:THR:CG2	1:B:125:TYR:H	1.91	0.83
1:F:122:THR:HG22	1:F:125:TYR:H	1.43	0.83
1:C:132:ASN:HD22	1:C:135:ALA:H	1.24	0.81
1:A:122:THR:HG22	1:A:125:TYR:H	1.45	0.81
1:A:122:THR:CG2	1:A:125:TYR:H	1.93	0.81
1:A:69:MSE:HE1	1:A:307:ARG:HB3	1.64	0.80
1:D:105:PHE:HB2	1:D:305:THR:HG23	1.64	0.80
1:B:122:THR:HG22	1:B:125:TYR:H	1.47	0.79
1:A:69:MSE:HE3	1:A:306:TYR:O	1.83	0.78
1:C:105:PHE:HB2	1:C:305:THR:CG2	2.12	0.78
1:A:300:ASP:OD1	1:A:302:ARG:HB2	1.84	0.78
1:E:69:MSE:HE1	1:E:307:ARG:HB3	1.66	0.77
1:E:122:THR:CG2	1:E:125:TYR:H	1.97	0.77
1:A:65:PRO:CB	1:A:69:MSE:HE2	2.15	0.76
1:A:69:MSE:CE	1:A:307:ARG:HB3	2.15	0.76
1:C:301:PRO:HD2	1:C:302:ARG:CD	2.16	0.76
1:B:225:MSE:CE	1:B:273:GLN:HG2	2.15	0.75
1:D:107:MSE:HE1	1:E:63:ASP:OD2	1.87	0.74
1:C:122:THR:HG22	1:C:125:TYR:H	1.52	0.74
1:B:105:PHE:HB2	1:B:305:THR:CG2	2.17	0.73
1:C:76:GLN:HE22	1:C:298:THR:H	1.35	0.72
1:H:122:THR:CG2	1:H:125:TYR:H	2.04	0.70
1:A:66:THR:HB	1:H:194:GLU:OE2	1.90	0.70
1:C:76:GLN:HE22	1:C:298:THR:N	1.90	0.70
1:C:187:ALA:HB3	1:C:305:THR:HG21	1.72	0.70
1:F:122:THR:CG2	1:F:125:TYR:H	2.04	0.70
1:C:163:LYS:HG2	2:C:341:HOH:O	1.90	0.69
1:B:213:GLN:HE22	1:B:286:ASN:HD22	1.40	0.69
1:G:55:GLU:N	2:G:378:HOH:O	2.25	0.69
1:E:76:GLN:NE2	1:E:298:THR:H	1.91	0.69
2:A:335:HOH:O	1:B:313:GLU:HG3	1.91	0.68
1:C:318:ARG:HD2	1:C:318:ARG:H	1.58	0.68
1:D:190:HIS:CE1	1:E:66:THR:HG21	2.27	0.68
1:E:98:MSE:HG3	2:E:342:HOH:O	1.91	0.68
1:B:190:HIS:NE2	1:C:66:THR:HG21	2.09	0.68
1:C:132:ASN:ND2	1:C:135:ALA:H	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:275:VAL:CG1	1:E:276:GLY:H	2.02	0.67
1:F:64:ARG:HD3	1:F:99:ASP:OD1	1.94	0.67
1:C:301:PRO:HD2	1:C:302:ARG:HD3	1.76	0.67
1:E:275:VAL:HG13	1:E:276:GLY:N	2.01	0.67
1:G:122:THR:CG2	1:G:125:TYR:H	2.07	0.66
1:A:122:THR:HG23	1:A:124:TYR:HB3	1.78	0.66
1:C:122:THR:CG2	1:C:125:TYR:H	2.08	0.66
1:B:55:GLU:HB3	2:B:360:HOH:O	1.95	0.66
1:E:132:ASN:ND2	1:E:135:ALA:H	1.94	0.66
1:F:190:HIS:CE1	1:G:66:THR:HG21	2.31	0.66
1:B:269:LEU:O	1:B:273:GLN:HG3	1.95	0.65
1:F:122:THR:HG23	1:F:124:TYR:HB3	1.78	0.65
1:A:66:THR:HG21	1:H:190:HIS:CE1	2.32	0.65
1:F:64:ARG:NE	1:F:99:ASP:OD1	2.30	0.65
1:A:300:ASP:HB2	2:A:353:HOH:O	1.96	0.65
1:A:152:GLY:HA2	1:A:158:VAL:HG12	1.78	0.64
1:B:64:ARG:NE	1:B:99:ASP:OD1	2.26	0.64
1:F:150:ILE:HD13	2:F:353:HOH:O	1.98	0.63
1:G:76:GLN:NE2	1:G:298:THR:H	1.94	0.63
1:D:300:ASP:OD1	1:D:302:ARG:NH1	2.30	0.63
1:D:225:MSE:SE	1:D:272:LEU:HD23	2.49	0.63
1:C:213:GLN:HE22	1:C:286:ASN:HD22	1.47	0.62
1:D:213:GLN:HE22	1:D:286:ASN:HD22	1.47	0.62
1:D:64:ARG:NE	1:D:99:ASP:OD1	2.32	0.62
1:D:96:SER:HB2	1:D:98:MSE:HE2	1.82	0.61
1:F:225:MSE:HA	1:F:272:LEU:CD2	2.31	0.61
1:F:64:ARG:CD	1:F:99:ASP:OD1	2.48	0.61
1:G:275:VAL:HG13	1:G:276:GLY:O	2.01	0.61
1:D:122:THR:CG2	1:D:125:TYR:H	2.14	0.61
1:H:156:ARG:HG3	1:H:158:VAL:HG23	1.82	0.60
1:H:105:PHE:HB2	1:H:305:THR:CG2	2.32	0.59
1:E:132:ASN:HD22	1:E:135:ALA:H	1.49	0.59
1:A:63:ASP:OD2	1:A:64:ARG:HG2	2.02	0.59
1:E:185:GLN:HE21	1:E:185:GLN:HA	1.67	0.59
1:D:122:THR:HG22	1:D:125:TYR:H	1.68	0.58
1:D:187:ALA:HB3	1:D:305:THR:HG21	1.86	0.58
1:A:169:ALA:HB3	1:A:170:PRO:HD3	1.86	0.58
1:F:202:ARG:NH2	1:F:205:GLN:OE1	2.37	0.57
1:F:225:MSE:HA	1:F:272:LEU:HD21	1.86	0.57
1:E:84:ASP:C	1:E:84:ASP:OD1	2.43	0.57
1:C:301:PRO:HD2	1:C:302:ARG:HD2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:187:ALA:HB3	1:F:305:THR:HG21	1.87	0.56
1:F:105:PHE:HB2	1:F:305:THR:HG23	1.85	0.56
1:H:300:ASP:OD2	1:H:302:ARG:HB2	2.05	0.56
1:B:194:GLU:OE2	1:C:66:THR:HB	2.05	0.56
1:A:65:PRO:HB3	1:A:69:MSE:HE2	1.88	0.56
1:B:194:GLU:CD	1:C:66:THR:HB	2.27	0.55
1:H:55:GLU:OE2	1:H:318:ARG:NH1	2.38	0.55
1:D:194:GLU:OE2	1:E:66:THR:HB	2.06	0.55
1:F:190:HIS:HE1	1:G:66:THR:HG21	1.71	0.55
1:E:169:ALA:HB3	1:E:170:PRO:HD3	1.87	0.55
1:G:105:PHE:CB	1:G:305:THR:HG22	2.25	0.55
1:G:169:ALA:HB3	1:G:170:PRO:HD3	1.89	0.55
1:A:300:ASP:OD1	1:A:302:ARG:HD3	2.06	0.55
1:E:213:GLN:HE22	1:E:286:ASN:HD22	1.53	0.55
1:C:169:ALA:HB3	1:C:170:PRO:HD3	1.89	0.55
1:E:107:MSE:CE	1:F:159:ASN:HD21	2.20	0.54
1:G:84:ASP:O	1:G:85:VAL:HB	2.07	0.54
1:E:122:THR:HG23	1:E:125:TYR:H	1.72	0.54
1:G:210:VAL:HA	1:G:213:GLN:HE21	1.73	0.53
1:H:187:ALA:HB3	1:H:305:THR:HG21	1.91	0.52
1:H:210:VAL:HA	1:H:213:GLN:HE21	1.74	0.52
1:D:96:SER:HB2	1:D:98:MSE:CE	2.39	0.52
1:H:122:THR:HG22	1:H:125:TYR:H	1.73	0.52
2:E:335:HOH:O	1:F:313:GLU:HG3	2.08	0.52
1:F:64:ARG:HE	1:F:99:ASP:HA	1.73	0.52
1:H:199:TRP:CG	1:H:297:PRO:HD3	2.44	0.52
1:A:122:THR:CG2	1:A:124:TYR:HB3	2.40	0.52
1:E:122:THR:HG22	1:E:125:TYR:HB3	1.91	0.52
1:F:61:ILE:HG12	1:F:161:SER:HB3	1.92	0.52
1:E:122:THR:HG22	1:E:125:TYR:H	1.74	0.51
1:A:77:GLN:OE1	1:A:77:GLN:HA	2.10	0.51
1:A:307:ARG:NH2	1:H:104:GLU:OE1	2.38	0.51
1:A:66:THR:HG21	1:H:190:HIS:NE2	2.26	0.51
1:A:76:GLN:HE22	1:A:297:PRO:HA	1.75	0.50
1:B:68:ASN:H	1:B:68:ASN:HD22	1.59	0.50
1:H:84:ASP:OD1	1:H:85:VAL:N	2.43	0.50
1:A:301:PRO:HD2	1:A:302:ARG:HD3	1.93	0.50
1:H:213:GLN:HE22	1:H:286:ASN:HD22	1.59	0.50
1:E:121:GLN:O	1:E:121:GLN:HG2	2.12	0.50
1:D:83:LEU:HB3	1:D:202:ARG:HH11	1.75	0.50
1:D:164:LEU:C	1:D:164:LEU:HD23	2.31	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:122:THR:HG23	1:D:124:TYR:HB3	1.94	0.49
1:G:76:GLN:OE1	1:G:76:GLN:HA	2.12	0.49
1:H:122:THR:HG23	1:H:125:TYR:H	1.77	0.49
1:B:66:THR:OG1	1:B:69:MSE:HG3	2.12	0.49
1:G:267:ALA:O	1:G:271:ASN:HB2	2.12	0.49
1:H:122:THR:HG23	1:H:124:TYR:HB3	1.94	0.49
1:H:199:TRP:CD1	1:H:297:PRO:HD3	2.47	0.49
1:B:199:TRP:CD1	1:B:297:PRO:HD3	2.48	0.49
1:F:122:THR:CG2	1:F:124:TYR:HB3	2.43	0.49
1:E:207:LYS:HG3	1:E:290:LEU:HD21	1.95	0.49
1:F:66:THR:OG1	1:F:69:MSE:HG3	2.13	0.49
1:D:139:LEU:HD11	1:D:143:MSE:HE2	1.95	0.48
1:B:190:HIS:CE1	1:C:66:THR:HG21	2.48	0.48
1:A:194:GLU:OE2	1:B:66:THR:HB	2.13	0.48
1:A:196:LYS:HD2	1:A:299:LEU:HD21	1.95	0.48
1:G:213:GLN:HE22	1:G:286:ASN:HD22	1.60	0.48
1:F:287:ARG:HG2	1:F:287:ARG:HH11	1.78	0.48
1:A:77:GLN:OE1	1:A:195:LEU:HD13	2.14	0.48
1:B:107:MSE:HB3	1:B:107:MSE:HE2	1.52	0.48
1:E:67:VAL:HG22	1:E:98:MSE:SE	2.64	0.48
1:H:269:LEU:O	1:H:273:GLN:HG3	2.14	0.47
1:A:119:TRP:O	1:A:122:THR:HB	2.14	0.47
1:E:213:GLN:NE2	1:E:286:ASN:HD22	2.12	0.47
1:F:268:ARG:HA	1:F:271:ASN:HB2	1.94	0.47
1:G:128:ARG:HB3	1:G:139:LEU:HD21	1.97	0.47
1:C:121:GLN:HG3	2:C:348:HOH:O	2.15	0.47
1:B:225:MSE:HE1	1:B:273:GLN:CG	2.34	0.47
1:B:104:GLU:OE1	1:C:307:ARG:NH2	2.47	0.47
1:D:96:SER:CB	1:D:98:MSE:HE2	2.44	0.47
1:E:76:GLN:HE22	1:E:297:PRO:HA	1.79	0.47
1:H:100:GLU:OE1	1:H:100:GLU:HA	2.14	0.47
1:C:122:THR:HG23	1:C:124:TYR:HB3	1.97	0.47
1:A:65:PRO:CA	1:A:69:MSE:CE	2.66	0.46
1:A:211:LYS:HA	1:A:211:LYS:HE3	1.97	0.46
1:G:228:ILE:HG22	1:G:269:LEU:HD13	1.97	0.46
1:F:128:ARG:HB3	1:F:139:LEU:HD21	1.97	0.46
1:B:122:THR:HG23	1:B:124:TYR:HB3	1.98	0.46
1:F:84:ASP:CG	1:F:84:ASP:O	2.54	0.46
1:F:280:ASP:OD1	1:F:282:ASP:HB3	2.15	0.45
1:A:230:GLN:OE1	1:B:274:ALA:HB1	2.17	0.45
1:A:66:THR:HB	1:H:194:GLU:CD	2.36	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:THR:HG22	1:B:125:TYR:HB3	1.99	0.45
1:F:199:TRP:O	1:F:199:TRP:CD1	2.70	0.45
1:E:148:GLN:HG3	2:E:334:HOH:O	2.17	0.44
1:F:77:GLN:O	1:F:81:ARG:HG3	2.17	0.44
1:H:67:VAL:HA	1:H:98:MSE:CE	2.47	0.44
1:A:187:ALA:HB3	1:A:305:THR:HG21	1.98	0.44
1:D:139:LEU:HD12	1:D:142:GLU:OE2	2.18	0.44
1:G:213:GLN:NE2	1:G:286:ASN:HD22	2.16	0.44
1:D:205:GLN:HG3	1:D:206:MSE:N	2.31	0.44
1:F:184:SER:OG	1:F:305:THR:HG22	2.18	0.44
1:F:225:MSE:CA	1:F:272:LEU:HD21	2.46	0.44
1:B:266:GLN:O	1:B:266:GLN:HG2	2.17	0.44
1:D:148:GLN:HE21	1:D:148:GLN:HB2	1.61	0.44
1:H:67:VAL:HA	1:H:98:MSE:HE1	1.99	0.44
1:A:301:PRO:HD2	1:A:302:ARG:CD	2.48	0.44
1:E:194:GLU:OE2	1:F:66:THR:HB	2.18	0.44
1:B:68:ASN:H	1:B:68:ASN:ND2	2.15	0.44
1:E:69:MSE:HE1	1:E:307:ARG:CB	2.42	0.44
1:C:213:GLN:NE2	1:C:286:ASN:HD22	2.13	0.44
1:D:271:ASN:O	1:D:275:VAL:HG12	2.17	0.43
1:D:194:GLU:CD	1:E:66:THR:HB	2.39	0.43
1:F:192:ASN:HD22	1:F:192:ASN:HA	1.60	0.43
1:H:156:ARG:HG3	1:H:156:ARG:O	2.19	0.43
1:E:305:THR:HG23	1:E:305:THR:O	2.19	0.43
1:E:76:GLN:HE22	1:E:298:THR:H	1.64	0.43
1:B:122:THR:HG23	1:B:125:TYR:H	1.81	0.43
1:E:272:LEU:HA	1:E:275:VAL:HG12	2.01	0.43
1:E:55:GLU:HB2	1:E:166:ALA:O	2.19	0.43
1:E:153:ASP:H	1:E:158:VAL:HB	1.84	0.43
1:F:67:VAL:HG22	1:F:98:MSE:SE	2.68	0.43
1:F:213:GLN:HE22	1:F:286:ASN:HD22	1.67	0.43
1:H:156:ARG:CG	1:H:158:VAL:HG23	2.46	0.43
1:F:162:VAL:HG13	1:F:162:VAL:O	2.18	0.43
1:E:121:GLN:O	1:E:121:GLN:CG	2.66	0.42
1:E:271:ASN:O	1:E:275:VAL:HG12	2.18	0.42
1:H:136:ASP:OD2	2:H:333:HOH:O	2.22	0.42
1:G:199:TRP:CE2	1:G:297:PRO:HD3	2.54	0.42
1:H:302:ARG:O	1:H:303:PHE:O	2.37	0.42
1:E:76:GLN:NE2	1:E:298:THR:N	2.65	0.42
1:F:126:LYS:O	1:F:129:MSE:HE2	2.20	0.42
1:F:194:GLU:HA	1:G:68:ASN:OD1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:GLU:OE2	1:C:66:THR:CB	2.67	0.42
1:H:199:TRP:NE1	1:H:296:GLY:HA2	2.34	0.42
1:C:76:GLN:NE2	1:C:298:THR:N	2.64	0.42
1:F:212:ARG:O	1:F:216:VAL:HG23	2.20	0.41
1:A:64:ARG:HA	1:A:102:TYR:CD1	2.55	0.41
1:D:56:TRP:CE3	1:D:169:ALA:HB2	2.54	0.41
1:A:275:VAL:HG13	1:A:276:GLY:O	2.20	0.41
1:A:307:ARG:HH22	1:H:104:GLU:CD	2.23	0.41
1:G:122:THR:HG23	1:G:124:TYR:HB3	2.01	0.41
1:G:164:LEU:C	1:G:164:LEU:HD23	2.40	0.41
1:D:202:ARG:HH21	1:D:205:GLN:CD	2.24	0.41
1:G:139:LEU:O	1:G:143:MSE:HG3	2.20	0.41
1:C:199:TRP:CD1	1:C:297:PRO:HD3	2.56	0.41
1:H:57:SER:HA	1:H:164:LEU:O	2.20	0.41
1:C:66:THR:H	1:C:69:MSE:SE	2.53	0.41
1:E:274:ALA:O	1:E:275:VAL:O	2.38	0.41
1:H:63:ASP:CG	1:H:64:ARG:H	2.24	0.41
1:H:84:ASP:OD1	1:H:84:ASP:C	2.60	0.41
1:F:199:TRP:CD1	1:F:297:PRO:HD3	2.55	0.41
1:G:130:VAL:HG23	1:G:132:ASN:HB3	2.03	0.41
1:D:139:LEU:HD11	1:D:143:MSE:CE	2.50	0.40
1:E:132:ASN:HD22	1:E:135:ALA:CB	2.34	0.40
1:H:266:GLN:HG2	1:H:266:GLN:O	2.21	0.40
1:A:310:ARG:HB2	1:H:112:TRP:HB3	2.04	0.40
1:E:211:LYS:HE3	1:E:211:LYS:HA	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	215/265 (81%)	208 (97%)	7 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	215/265 (81%)	212 (99%)	3 (1%)	0	100	100
1	C	215/265 (81%)	212 (99%)	3 (1%)	0	100	100
1	D	215/265 (81%)	210 (98%)	5 (2%)	0	100	100
1	E	215/265 (81%)	210 (98%)	4 (2%)	1 (0%)	25	38
1	F	215/265 (81%)	209 (97%)	5 (2%)	1 (0%)	25	38
1	G	215/265 (81%)	211 (98%)	4 (2%)	0	100	100
1	H	215/265 (81%)	212 (99%)	2 (1%)	1 (0%)	25	38
All	All	1720/2120 (81%)	1684 (98%)	33 (2%)	3 (0%)	44	59

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	275	VAL
1	H	303	PHE
1	F	318	ARG

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	190/216 (88%)	169 (89%)	21 (11%)	5	7
1	B	190/216 (88%)	174 (92%)	16 (8%)	9	14
1	C	190/216 (88%)	172 (90%)	18 (10%)	7	11
1	D	190/216 (88%)	170 (90%)	20 (10%)	5	8
1	E	190/216 (88%)	163 (86%)	27 (14%)	2	3
1	F	190/216 (88%)	175 (92%)	15 (8%)	10	16
1	G	190/216 (88%)	172 (90%)	18 (10%)	7	11
1	H	190/216 (88%)	174 (92%)	16 (8%)	9	14
All	All	1520/1728 (88%)	1369 (90%)	151 (10%)	6	10

All (151) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	SER
1	A	68	ASN
1	A	69	MSE
1	A	85	VAL
1	A	96	SER
1	A	98	MSE
1	A	107	MSE
1	A	121	GLN
1	A	122	THR
1	A	148	GLN
1	A	155	THR
1	A	211	LYS
1	A	227	SER
1	A	282	ASP
1	A	290	LEU
1	A	292	THR
1	A	293	LEU
1	A	299	LEU
1	A	302	ARG
1	A	305	THR
1	A	317	LYS
1	B	55	GLU
1	B	84	ASP
1	B	98	MSE
1	B	106	VAL
1	B	107	MSE
1	B	121	GLN
1	B	122	THR
1	B	133	SER
1	B	148	GLN
1	B	153	ASP
1	B	211	LYS
1	B	218	LYS
1	B	268	ARG
1	B	287	ARG
1	B	293	LEU
1	B	305	THR
1	C	58	SER
1	C	64	ARG
1	C	68	ASN
1	C	98	MSE
1	C	121	GLN

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Mol	Chain	Res	Type
1	C	122	THR
1	C	133	SER
1	C	155	THR
1	C	211	LYS
1	C	227	SER
1	C	272	LEU
1	C	273	GLN
1	C	282	ASP
1	C	290	LEU
1	C	292	THR
1	C	293	LEU
1	C	305	THR
1	C	318	ARG
1	D	58	SER
1	D	64	ARG
1	D	85	VAL
1	D	98	MSE
1	D	122	THR
1	D	133	SER
1	D	148	GLN
1	D	202	ARG
1	D	204	ILE
1	D	205	GLN
1	D	215	GLU
1	D	268	ARG
1	D	273	GLN
1	D	287	ARG
1	D	290	LEU
1	D	293	LEU
1	D	300	ASP
1	D	302	ARG
1	D	305	THR
1	D	317	LYS
1	E	64	ARG
1	E	68	ASN
1	E	84	ASP
1	E	98	MSE
1	E	111	SER
1	E	121	GLN
1	E	122	THR
1	E	133	SER
1	E	148	GLN

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Mol	Chain	Res	Type
1	E	155	THR
1	E	156	ARG
1	E	185	GLN
1	E	202	ARG
1	E	205	GLN
1	E	211	LYS
1	E	215	GLU
1	E	224	ARG
1	E	268	ARG
1	E	271	ASN
1	E	282	ASP
1	E	287	ARG
1	E	290	LEU
1	E	293	LEU
1	E	299	LEU
1	E	302	ARG
1	E	305	THR
1	E	317	LYS
1	F	55	GLU
1	F	84	ASP
1	F	96	SER
1	F	98	MSE
1	F	107	MSE
1	F	122	THR
1	F	148	GLN
1	F	163	LYS
1	F	194	GLU
1	F	204	ILE
1	F	207	LYS
1	F	290	LEU
1	F	293	LEU
1	F	302	ARG
1	F	318	ARG
1	G	58	SER
1	G	64	ARG
1	G	69	MSE
1	G	84	ASP
1	G	98	MSE
1	G	107	MSE
1	G	111	SER
1	G	121	GLN
1	G	122	THR

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Mol	Chain	Res	Type
1	G	148	GLN
1	G	211	LYS
1	G	268	ARG
1	G	282	ASP
1	G	287	ARG
1	G	293	LEU
1	G	304	GLN
1	G	305	THR
1	G	307	ARG
1	H	55	GLU
1	H	64	ARG
1	H	68	ASN
1	H	84	ASP
1	H	85	VAL
1	H	98	MSE
1	H	122	THR
1	H	133	SER
1	H	134	LYS
1	H	153	ASP
1	H	205	GLN
1	H	268	ARG
1	H	271	ASN
1	H	287	ARG
1	H	290	LEU
1	H	305	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	GLN
1	A	82	ASN
1	A	127	GLN
1	A	146	ASN
1	A	148	GLN
1	A	185	GLN
1	A	192	ASN
1	A	213	GLN
1	A	291	ASN
1	A	294	ASN
1	B	68	ASN
1	B	127	GLN
1	B	146	ASN

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Mol	Chain	Res	Type
1	B	148	GLN
1	B	192	ASN
1	B	205	GLN
1	B	213	GLN
1	B	291	ASN
1	B	294	ASN
1	C	76	GLN
1	C	82	ASN
1	C	132	ASN
1	C	146	ASN
1	C	148	GLN
1	C	192	ASN
1	C	205	GLN
1	C	213	GLN
1	C	271	ASN
1	C	273	GLN
1	C	291	ASN
1	C	294	ASN
1	D	68	ASN
1	D	82	ASN
1	D	146	ASN
1	D	148	GLN
1	D	192	ASN
1	D	213	GLN
1	D	294	ASN
1	E	76	GLN
1	E	82	ASN
1	E	127	GLN
1	E	132	ASN
1	E	146	ASN
1	E	148	GLN
1	E	185	GLN
1	E	192	ASN
1	E	209	GLN
1	E	213	GLN
1	E	291	ASN
1	E	294	ASN
1	E	304	GLN
1	F	78	GLN
1	F	82	ASN
1	F	146	ASN
1	F	148	GLN

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Mol	Chain	Res	Type
1	F	159	ASN
1	F	190	HIS
1	F	192	ASN
1	F	213	GLN
1	F	266	GLN
1	F	271	ASN
1	F	291	ASN
1	F	294	ASN
1	G	76	GLN
1	G	82	ASN
1	G	127	GLN
1	G	146	ASN
1	G	148	GLN
1	G	192	ASN
1	G	209	GLN
1	G	213	GLN
1	G	294	ASN
1	G	304	GLN
1	H	68	ASN
1	H	82	ASN
1	H	146	ASN
1	H	148	GLN
1	H	192	ASN
1	H	213	GLN
1	H	291	ASN
1	H	294	ASN

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 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	213/265 (80%)	0.57	12 (5%)	31	28	21, 30, 39, 44	0
1	B	213/265 (80%)	0.35	13 (6%)	28	26	21, 30, 39, 44	0
1	C	213/265 (80%)	0.41	20 (9%)	15	14	22, 30, 39, 44	0
1	D	213/265 (80%)	0.51	25 (11%)	10	9	22, 30, 39, 44	0
1	E	213/265 (80%)	0.36	12 (5%)	31	28	22, 30, 39, 44	0
1	F	213/265 (80%)	0.32	12 (5%)	31	28	21, 30, 39, 44	0
1	G	213/265 (80%)	0.50	18 (8%)	18	17	21, 30, 38, 44	0
1	H	213/265 (80%)	0.47	20 (9%)	15	14	21, 30, 38, 44	0
All	All	1704/2120 (80%)	0.44	132 (7%)	21	19	21, 30, 39, 44	0

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	273	GLN	5.6
1	C	228	ILE	4.9
1	A	95	PRO	4.7
1	A	157	ALA	4.4
1	H	227	SER	4.2
1	G	84	ASP	4.0
1	A	84	ASP	4.0
1	B	267	ALA	3.9
1	H	273	GLN	3.9
1	F	273	GLN	3.8
1	A	299	LEU	3.7
1	G	183	ALA	3.7
1	E	85	VAL	3.7
1	A	154	PHE	3.6
1	G	268	ARG	3.6
1	D	305	THR	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	266	GLN	3.5
1	C	154	PHE	3.5
1	H	184	SER	3.4
1	H	268	ARG	3.4
1	D	154	PHE	3.4
1	F	268	ARG	3.3
1	B	64	ARG	3.3
1	D	183	ALA	3.3
1	D	268	ARG	3.2
1	A	155	THR	3.2
1	C	95	PRO	3.2
1	C	183	ALA	3.1
1	E	55	GLU	3.1
1	D	266	GLN	3.1
1	H	84	ASP	3.1
1	A	85	VAL	3.1
1	C	85	VAL	3.1
1	H	183	ALA	3.1
1	B	85	VAL	3.0
1	D	85	VAL	3.0
1	G	187	ALA	3.0
1	H	182	PHE	3.0
1	F	184	SER	3.0
1	G	188	ALA	3.0
1	D	155	THR	3.0
1	F	64	ARG	2.9
1	C	70	LEU	2.9
1	D	267	ALA	2.9
1	H	306	TYR	2.9
1	C	304	GLN	2.9
1	C	188	ALA	2.9
1	B	153	ASP	2.8
1	C	157	ALA	2.8
1	H	153	ASP	2.8
1	G	189	SER	2.8
1	E	84	ASP	2.8
1	G	302	ARG	2.8
1	G	182	PHE	2.8
1	C	66	THR	2.8
1	D	182	PHE	2.8
1	G	154	PHE	2.8
1	B	228	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	268	ARG	2.7
1	F	85	VAL	2.7
1	H	85	VAL	2.7
1	E	268	ARG	2.7
1	H	187	ALA	2.7
1	A	156	ARG	2.6
1	C	306	TYR	2.6
1	E	95	PRO	2.6
1	D	202	ARG	2.6
1	D	184	SER	2.6
1	G	272	LEU	2.6
1	A	64	ARG	2.6
1	G	157	ALA	2.6
1	F	183	ALA	2.6
1	F	95	PRO	2.6
1	E	154	PHE	2.6
1	G	186	ARG	2.6
1	C	305	THR	2.5
1	H	305	THR	2.5
1	H	68	ASN	2.5
1	E	302	ARG	2.5
1	E	157	ALA	2.5
1	H	188	ALA	2.5
1	F	194	GLU	2.4
1	D	230	GLN	2.4
1	C	84	ASP	2.4
1	D	306	TYR	2.4
1	D	227	SER	2.4
1	D	84	ASP	2.4
1	D	228	ILE	2.4
1	C	67	VAL	2.4
1	F	270	GLU	2.3
1	E	295	VAL	2.3
1	G	266	GLN	2.3
1	C	271	ASN	2.3
1	B	268	ARG	2.3
1	G	301	PRO	2.3
1	B	230	GLN	2.3
1	H	304	GLN	2.3
1	G	66	THR	2.3
1	D	153	ASP	2.3
1	D	273	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	297	PRO	2.2
1	F	266	GLN	2.2
1	A	187	ALA	2.2
1	B	154	PHE	2.2
1	G	306	TYR	2.2
1	D	269	LEU	2.2
1	H	272	LEU	2.2
1	D	189	SER	2.2
1	E	156	ARG	2.2
1	G	67	VAL	2.2
1	G	190	HIS	2.2
1	E	299	LEU	2.2
1	B	270	GLU	2.2
1	H	189	SER	2.1
1	F	84	ASP	2.1
1	D	70	LEU	2.1
1	D	187	ALA	2.1
1	F	188	ALA	2.1
1	B	272	LEU	2.1
1	D	191	LEU	2.1
1	H	274	ALA	2.1
1	C	318	ARG	2.1
1	H	154	PHE	2.1
1	E	215	GLU	2.1
1	D	303	PHE	2.1
1	C	68	ASN	2.1
1	C	215	GLU	2.0
1	A	275	VAL	2.0
1	C	295	VAL	2.0
1	H	158	VAL	2.0
1	C	303	PHE	2.0
1	D	270	GLU	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.