



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2017 – 05:30 AM EDT

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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

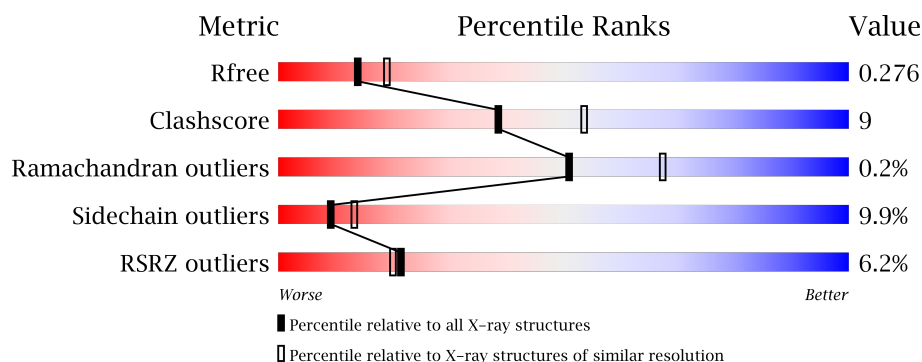
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	100719	3166 (2.40-2.40)
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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>7%</div> <div> <div></div> <div>65%</div> <div>17%</div> <div>•</div> <div>17%</div> </div> </div>
1	B	265	<div> <div>4%</div> <div> <div></div> <div>69%</div> <div>13%</div> <div>•</div> <div>17%</div> </div> </div>
1	C	265	<div> <div>5%</div> <div> <div></div> <div>68%</div> <div>13%</div> <div>•</div> <div>17%</div> </div> </div>
1	D	265	<div> <div>5%</div> <div> <div></div> <div>67%</div> <div>13%</div> <div>•</div> <div>17%</div> </div> </div>
1	E	265	<div> <div>4%</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	
1	G	265	
1	H	265	

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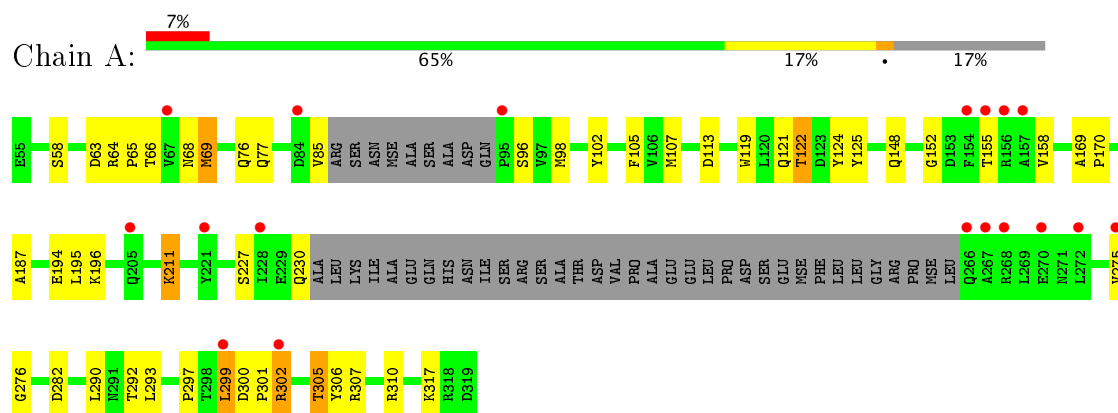
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	45	Total	O	0	0
			45	45		
2	H	50	Total	O	0	0
			50	50		

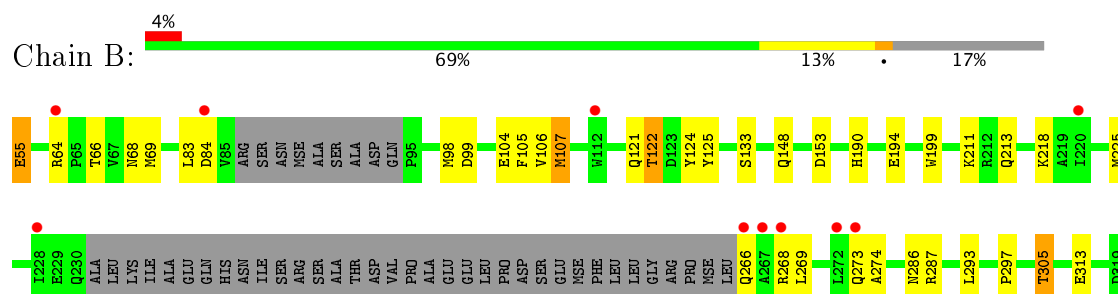
3 Residue-property plots [i](#)

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

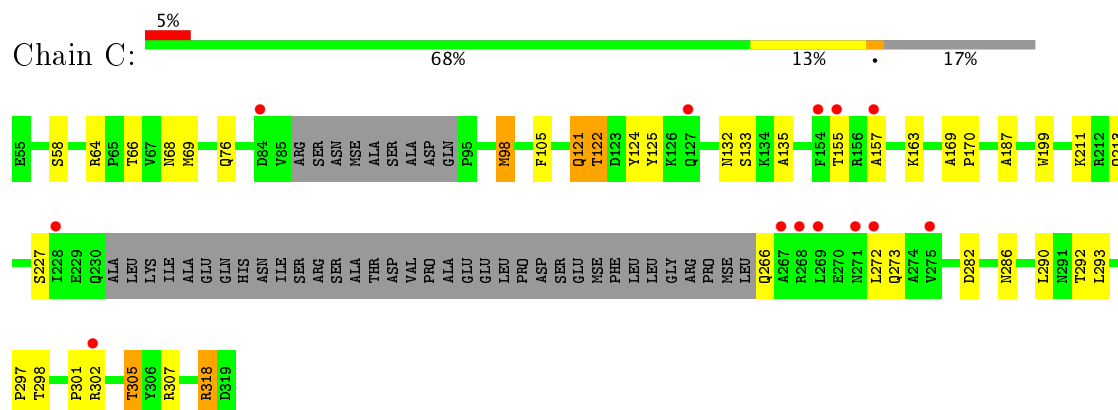
- Molecule 1: Lipopolysaccharide biosynthesis protein wzzE



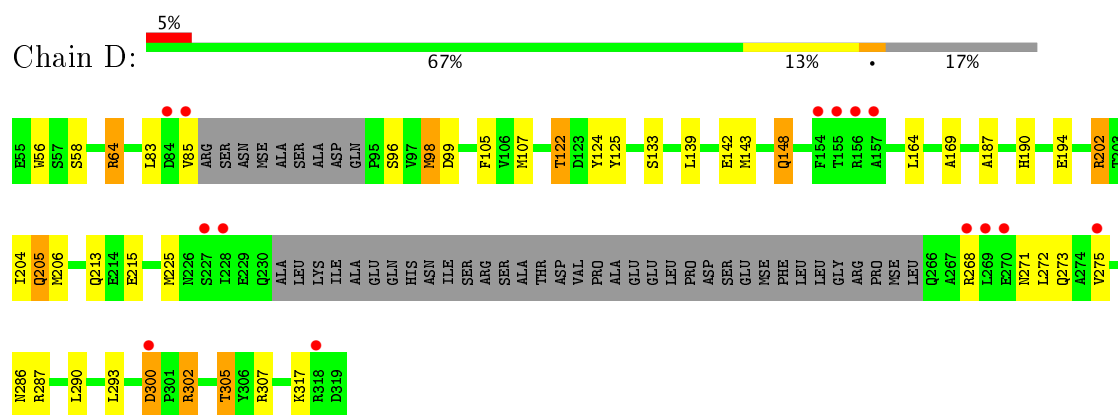
- Molecule 1: Lipopolysaccharide biosynthesis protein wzzE



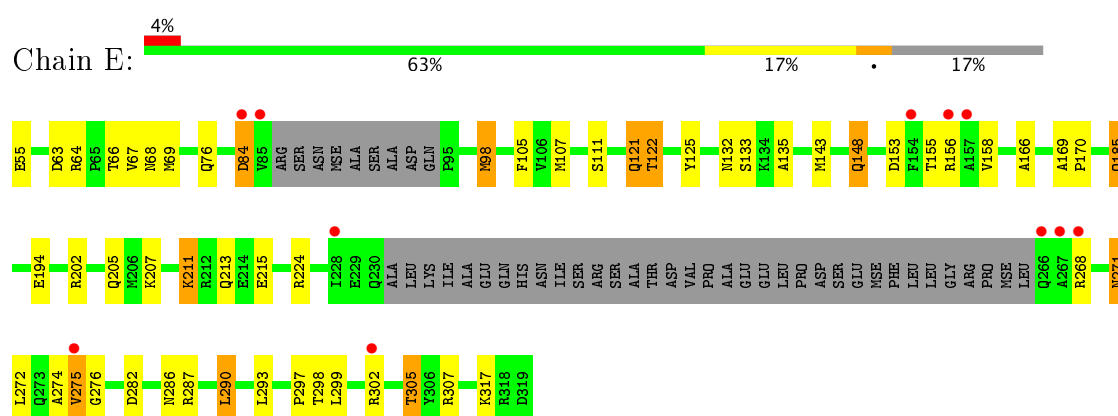
- Molecule 1: Lipopolysaccharide biosynthesis protein wzzE



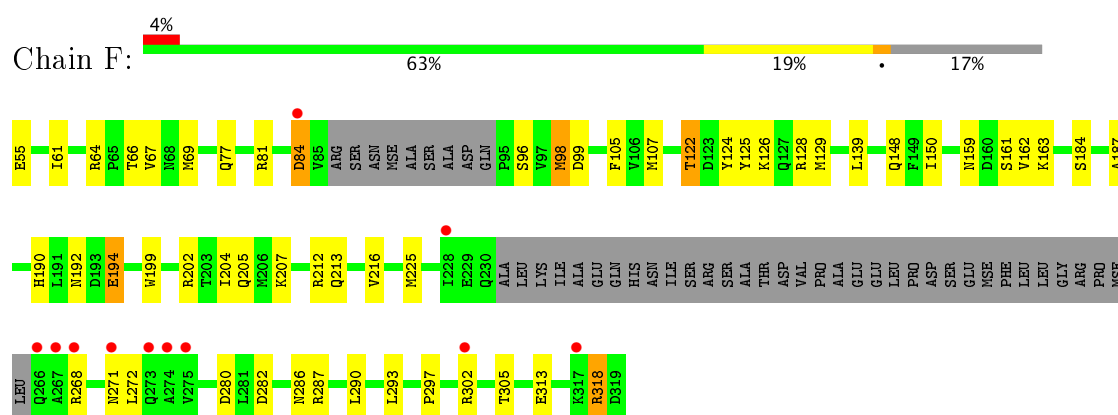
- Molecule 1: Lipopolysaccharide biosynthesis protein wzzE



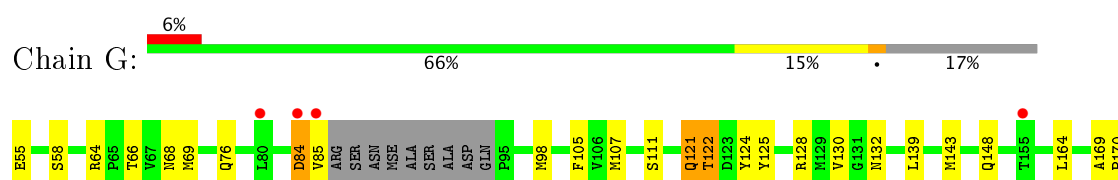
- Molecule 1: Lipopolysaccharide biosynthesis protein wzzE

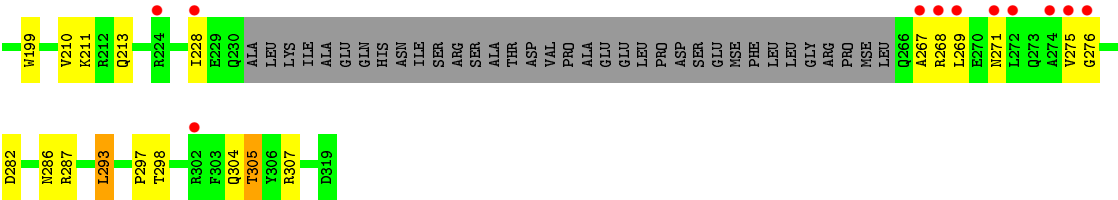


- Molecule 1: Lipopolysaccharide biosynthesis protein wzzE

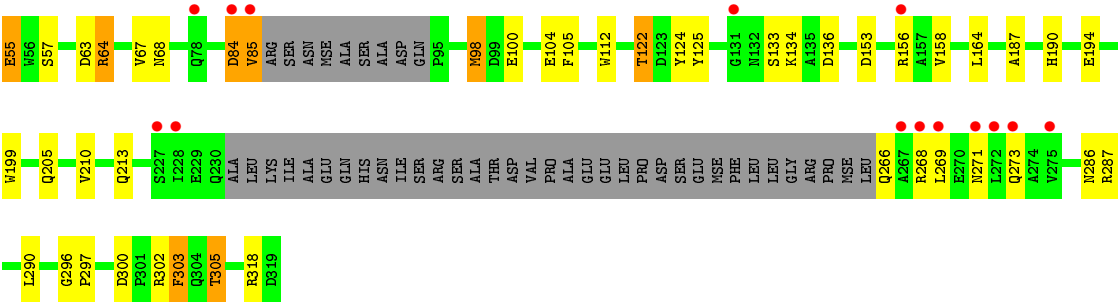


- Molecule 1: Lipopolysaccharide biosynthesis protein wzzE





● 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 46.23 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.1 (47.89-2.40) 99.1 (46.23-2.40)	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 (5.23%)	DCC
Wilson B-factor (Å ²)	37.2	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 32.9	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	0.88	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:C:76:GLN:HE22	1:C:298:THR:N	1.90	0.70
1:A:66:THR:HB	1:H:194:GLU:OE2	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:H	1:C:318:ARG:HD2	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:F:64:ARG:NE	1:F:99:ASP:OD1	2.30	0.65
1:A:66:THR:HG21	1:H:190:HIS:CE1	2.32	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:169:ALA:HB3	1:G:170:PRO:HD3	1.89	0.55
1:G:105:PHE:CB	1:G:305:THR:HG22	2.25	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:HA	1:A:77:GLN:OE1	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:HD23	1:D:164:LEU:C	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:HA	1:G:76:GLN:OE1	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:196:LYS:HD2	1:A:299:LEU:HD21	1.95	0.48
1:A:194:GLU:OE2	1:B:66:THR:HB	2.13	0.48
1:G:213:GLN:HE22	1:G:286:ASN:HD22	1.60	0.48
1:F:287:ARG:HH11	1:F:287:ARG:HG2	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:HA	1:H:100:GLU:OE1	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:HG2	1:B:266:GLN:O	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:ND2	1:B:68:ASN:H	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:153:ASP:H	1:E:158:VAL:HB	1.84	0.43
1:E:55:GLU:HB2	1:E:166:ALA:O	2.19	0.43
1:F:213:GLN:HE22	1:F:286:ASN:HD22	1.67	0.43
1:F:67:VAL:HG22	1:F:98:MSE:SE	2.68	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:HD23	1:G:164:LEU:C	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:E:211:LYS:HA	1:E:211:LYS:HE3	2.04	0.40
1:A:310:ARG:HB2	1:H:112:TRP:HB3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	32	46
1	F	215/265 (81%)	209 (97%)	5 (2%)	1 (0%)	32	46
1	G	215/265 (81%)	211 (98%)	4 (2%)	0	100	100
1	H	215/265 (81%)	212 (99%)	2 (1%)	1 (0%)	32	46
All	All	1720/2120 (81%)	1684 (98%)	33 (2%)	3 (0%)	51	67

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%)	7	10
1	B	190/216 (88%)	174 (92%)	16 (8%)	13	19
1	C	190/216 (88%)	172 (90%)	18 (10%)	10	14
1	D	190/216 (88%)	170 (90%)	20 (10%)	8	11
1	E	190/216 (88%)	163 (86%)	27 (14%)	4	4
1	F	190/216 (88%)	175 (92%)	15 (8%)	14	22
1	G	190/216 (88%)	172 (90%)	18 (10%)	10	14
1	H	190/216 (88%)	174 (92%)	16 (8%)	13	19
All	All	1520/1728 (88%)	1369 (90%)	151 (10%)	9	13

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

Some 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 carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.64	18 (8%) 11 10	21, 30, 39, 44	0
1	B	213/265 (80%)	0.41	10 (4%) 32 30	21, 30, 39, 44	0
1	C	213/265 (80%)	0.58	13 (6%) 22 20	22, 30, 39, 44	0
1	D	213/265 (80%)	0.61	14 (6%) 19 17	22, 30, 39, 44	0
1	E	213/265 (80%)	0.57	11 (5%) 28 26	22, 30, 39, 44	0
1	F	213/265 (80%)	0.52	11 (5%) 28 26	21, 30, 39, 44	0
1	G	213/265 (80%)	0.58	15 (7%) 17 15	21, 30, 38, 44	0
1	H	213/265 (80%)	0.53	14 (6%) 19 17	21, 30, 38, 44	0
All	All	1704/2120 (80%)	0.56	106 (6%) 21 20	21, 30, 39, 44	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	228	ILE	7.3
1	H	84	ASP	5.4
1	G	268	ARG	5.3
1	F	268	ARG	5.0
1	G	272	LEU	5.0
1	A	84	ASP	4.9
1	H	85	VAL	4.8
1	G	228	ILE	4.8
1	D	228	ILE	4.6
1	E	84	ASP	4.3
1	B	228	ILE	4.2
1	E	268	ARG	4.1
1	D	268	ARG	4.1
1	D	85	VAL	4.0
1	A	267	ALA	4.0
1	E	267	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
1	G	267	ALA	4.0
1	D	84	ASP	3.9
1	H	273	GLN	3.9
1	D	269	LEU	3.8
1	C	157	ALA	3.7
1	C	267	ALA	3.7
1	D	155	THR	3.7
1	A	268	ARG	3.7
1	A	154	PHE	3.7
1	B	266	GLN	3.6
1	F	273	GLN	3.6
1	E	228	ILE	3.6
1	B	267	ALA	3.5
1	A	275	VAL	3.5
1	G	84	ASP	3.5
1	B	273	GLN	3.5
1	H	275	VAL	3.5
1	B	268	ARG	3.4
1	E	302	ARG	3.4
1	G	85	VAL	3.4
1	C	268	ARG	3.4
1	C	269	LEU	3.3
1	F	84	ASP	3.3
1	D	154	PHE	3.3
1	H	268	ARG	3.3
1	G	271	ASN	3.3
1	H	227	SER	3.2
1	E	275	VAL	3.2
1	A	95	PRO	3.1
1	A	156	ARG	3.1
1	C	84	ASP	3.1
1	A	157	ALA	3.0
1	G	275	VAL	3.0
1	C	271	ASN	3.0
1	A	228	ILE	2.9
1	C	154	PHE	2.9
1	G	302	ARG	2.8
1	F	317	LYS	2.8
1	F	267	ALA	2.8
1	C	302	ARG	2.8
1	H	269	LEU	2.8
1	A	270	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	H	272	LEU	2.6
1	B	64	ARG	2.6
1	A	155	THR	2.6
1	F	302	ARG	2.6
1	G	80	LEU	2.6
1	H	228	ILE	2.6
1	C	272	LEU	2.5
1	B	272	LEU	2.5
1	D	227	SER	2.5
1	F	266	GLN	2.4
1	B	84	ASP	2.4
1	D	275	VAL	2.4
1	F	275	VAL	2.4
1	D	270	GLU	2.4
1	H	78	GLN	2.4
1	C	275	VAL	2.4
1	D	156	ARG	2.4
1	G	274	ALA	2.4
1	A	67	VAL	2.4
1	E	85	VAL	2.4
1	H	156	ARG	2.4
1	E	156	ARG	2.3
1	F	271	ASN	2.3
1	A	272	LEU	2.3
1	G	269	LEU	2.3
1	D	300	ASP	2.2
1	A	302	ARG	2.2
1	D	157	ALA	2.2
1	C	127	GLN	2.2
1	G	224	ARG	2.2
1	F	274	ALA	2.2
1	A	221	TYR	2.2
1	E	266	GLN	2.1
1	E	157	ALA	2.1
1	H	267	ALA	2.1
1	C	155	THR	2.1
1	G	276	GLY	2.1
1	G	155	THR	2.1
1	D	318	ARG	2.1
1	E	154	PHE	2.1
1	H	131	GLY	2.1
1	F	228	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	299	LEU	2.1
1	A	266	GLN	2.1
1	B	220	ILE	2.0
1	H	271	ASN	2.0
1	A	205	GLN	2.0
1	B	112	TRP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.