



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 09:44 PM GMT

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 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/ValidationPDFNotes.html>

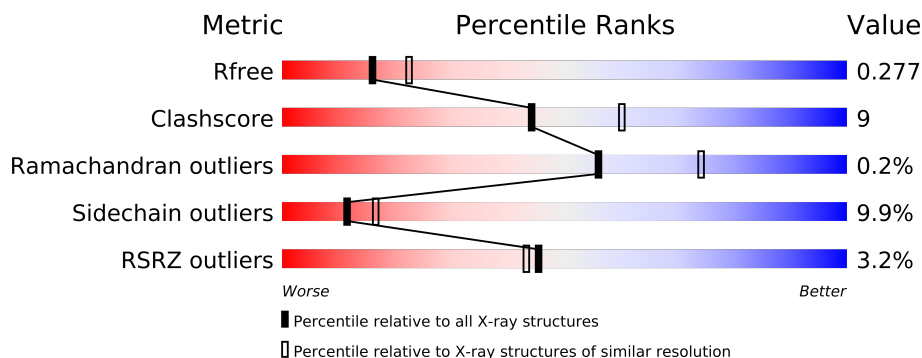
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	2207 (2.40-2.40)
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	265	
1	B	265	
1	C	265	
1	D	265	
1	E	265	
1	F	265	
1	G	265	
1	H	265	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14771 atoms, of which 0 are hydrogen and 0 are deuterium.

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			

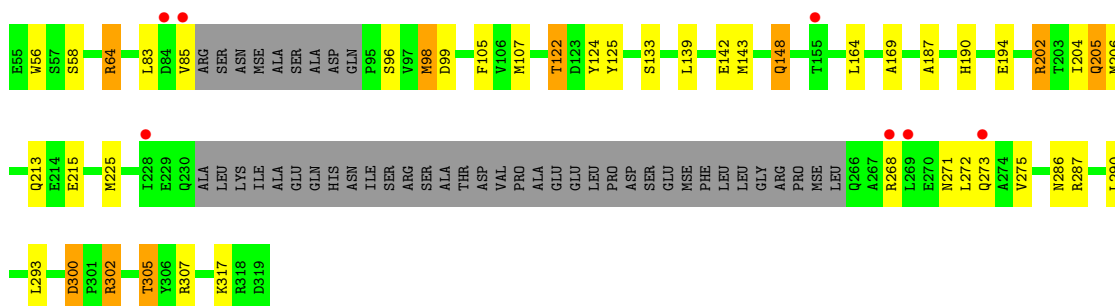
- Molecule 2 is water.

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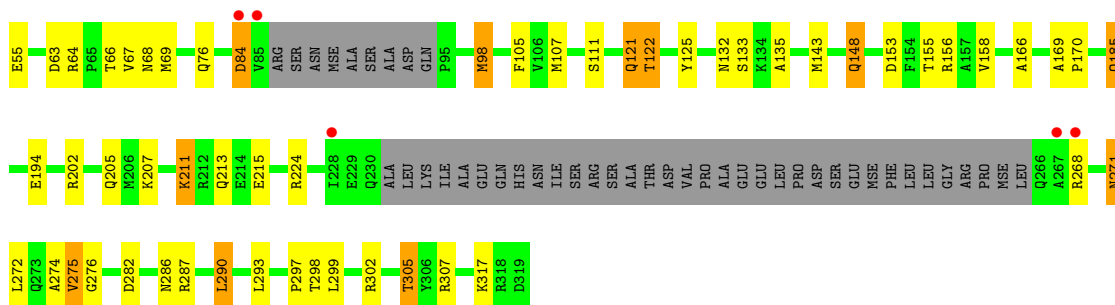
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	45	Total	O	0	0
			45	45		
2	H	50	Total	O	0	0
			50	50		



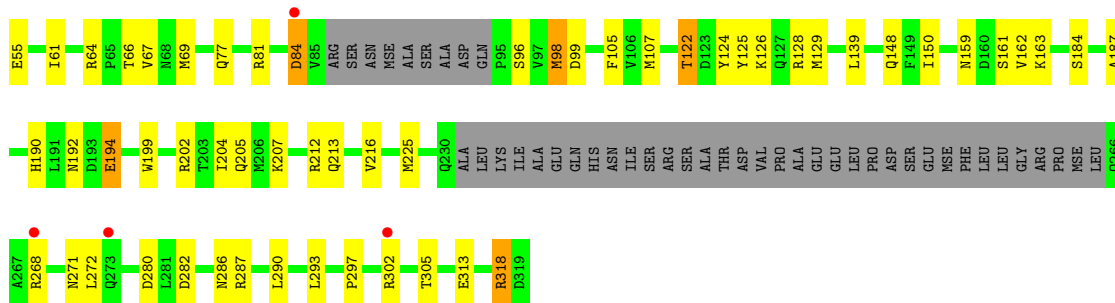
- Molecule 1: Lipopolysaccharide biosynthesis protein wzzE

Chain E:



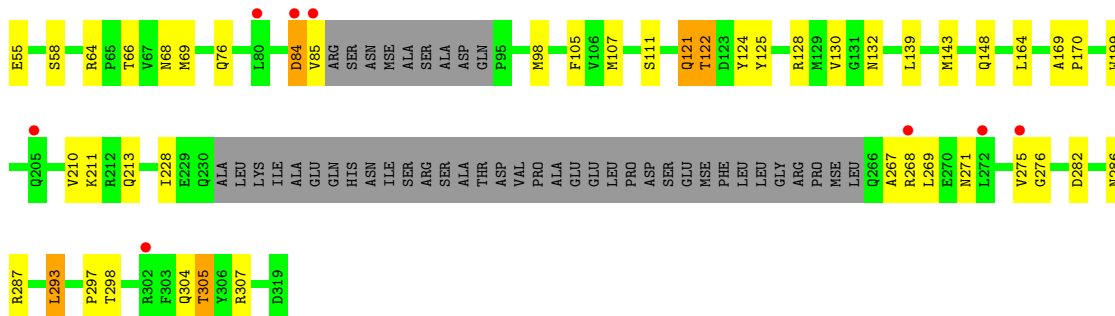
- Molecule 1: Lipopolysaccharide biosynthesis protein wzzE

Chain F:



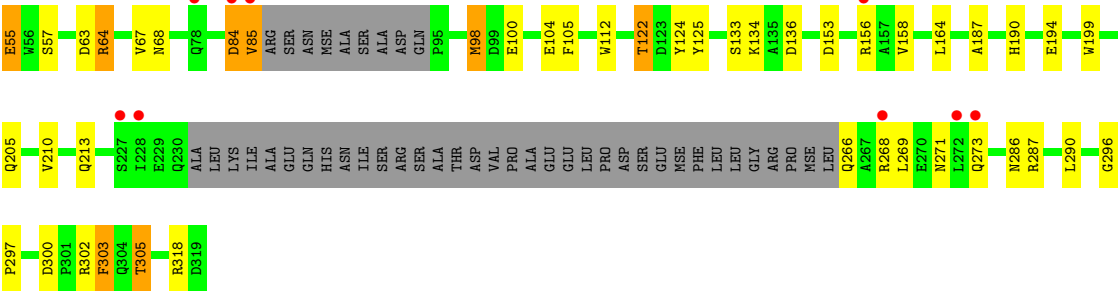
- Molecule 1: Lipopolysaccharide biosynthesis protein wzzE

Chain G:



- Molecule 1: Lipopolysaccharide biosynthesis protein wzzE

Chain H: 



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 5.2.0019	Depositor
R, R_{free}	0.223 , 0.266 0.236 , 0.277	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 , 41.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	8 of 106363 reflections (0.008%)	Xtriage
F_o, F_c correlation	0.91	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.

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 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 hydrogens

added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 9.

All (245) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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	Distance(Å)	Clash(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:D:190:HIS:CE1	1:E:66:THR:HG21	2.27	0.68
1:C:318:ARG:H	1:C:318:ARG:HD2	1.58	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:E:275:VAL:CG1	1:E:276:GLY:H	2.02	0.67
1:C:132:ASN:ND2	1:C:135:ALA:H	1.93	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:G:76:GLN:NE2	1:G:298:THR:H	1.94	0.63
1:F:150:ILE:HD13	2:F:353:HOH:O	1.98	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:E:185:GLN:HE21	1:E:185:GLN:HA	1.67	0.59
1:A:63:ASP:OD2	1:A:64:ARG:HG2	2.02	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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:G:105:PHE:CB	1:G:305:THR:HG22	2.25	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: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:H:122:THR:HG22	1:H:125:TYR:H	1.73	0.52
1:D:96:SER:HB2	1:D:98:MSE:CE	2.39	0.52
1:F:64:ARG:HE	1:F:99:ASP:HA	1.73	0.52
2:E:335:HOH:O	1:F:313:GLU:HG3	2.08	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:307:ARG:NH2	1:H:104:GLU:OE1	2.38	0.51
1:A:77:GLN:HA	1:A:77:GLN:OE1	2.10	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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:F:122:THR:CG2	1:F:124:TYR:HB3	2.43	0.49
1:B:199:TRP:CD1	1:B:297:PRO:HD3	2.48	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:G:213:GLN:HE22	1:G:286:ASN:HD22	1.60	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: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:E:76:GLN:HE22	1:E:297:PRO:HA	1.79	0.47
1:D:96:SER:CB	1:D:98:MSE:HE2	2.44	0.47
1:H:100:GLU:HA	1:H:100:GLU:OE1	2.14	0.47
1:B:104:GLU:OE1	1:C:307:ARG:NH2	2.47	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:O	1:F:84:ASP:CG	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:B:122:THR:HG22	1:B:125:TYR:HB3	1.99	0.45
1:A:66:THR:HB	1:H:194:GLU:CD	2.36	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:G:213:GLN:NE2	1:G:286:ASN:HD22	2.16	0.44
1:D:139:LEU:HD12	1:D:142:GLU:OE2	2.18	0.44
1:F:225:MSE:CA	1:F:272:LEU:HD21	2.46	0.44
1:F:184:SER:OG	1:F:305:THR:HG22	2.18	0.44
1:D:205:GLN:HG3	1:D:206:MSE:N	2.31	0.44
1:H:67:VAL:HA	1:H:98:MSE:HE1	1.99	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: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:E:69:MSE:HE1	1:E:307:ARG:CB	2.42	0.44
1:B:68:ASN:ND2	1:B:68:ASN:H	2.15	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:E:272:LEU:HA	1:E:275:VAL:HG12	2.01	0.43
1:B:122:THR:HG23	1:B:125:TYR:H	1.81	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: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: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:H:302:ARG:O	1:H:303:PHE:O	2.37	0.42
1:G:199:TRP:CE2	1:G:297:PRO:HD3	2.54	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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:E:274:ALA:O	1:E:275:VAL:O	2.38	0.41
1:C:66:THR:H	1:C:69:MSE:SE	2.53	0.41
1:H:84:ASP:OD1	1:H:84:ASP:C	2.60	0.41
1:H:63:ASP:CG	1:H:64:ARG:H	2.24	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
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%)	38	53
1	F	215/265 (81%)	209 (97%)	5 (2%)	1 (0%)	38	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	215/265 (81%)	211 (98%)	4 (2%)	0	100	100
1	H	215/265 (81%)	212 (99%)	2 (1%)	1 (0%)	38	53
All	All	1720/2120 (81%)	1684 (98%)	33 (2%)	3 (0%)	56	74

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%)	9	12
1	B	190/216 (88%)	174 (92%)	16 (8%)	16	23
1	C	190/216 (88%)	172 (90%)	18 (10%)	12	18
1	D	190/216 (88%)	170 (90%)	20 (10%)	10	14
1	E	190/216 (88%)	163 (86%)	27 (14%)	5	5
1	F	190/216 (88%)	175 (92%)	15 (8%)	18	26
1	G	190/216 (88%)	172 (90%)	18 (10%)	12	18
1	H	190/216 (88%)	174 (92%)	16 (8%)	16	23
All	All	1520/1728 (88%)	1369 (90%)	151 (10%)	11	16

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

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Mol	Chain	Res	Type
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
1	C	122	THR
1	C	133	SER
1	C	155	THR
1	C	211	LYS
1	C	227	SER

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Mol	Chain	Res	Type
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
1	E	155	THR
1	E	156	ARG
1	E	185	GLN
1	E	202	ARG
1	E	205	GLN

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Mol	Chain	Res	Type
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
1	G	148	GLN
1	G	211	LYS
1	G	268	ARG
1	G	282	ASP
1	G	287	ARG

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Mol	Chain	Res	Type
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
1	B	148	GLN
1	B	192	ASN
1	B	205	GLN
1	B	213	GLN
1	B	291	ASN

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Mol	Chain	Res	Type
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
1	F	159	ASN
1	F	190	HIS
1	F	192	ASN
1	F	213	GLN
1	F	266	GLN

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Mol	Chain	Res	Type
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 chains 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	221/265 (83%)	0.13	6 (2%)	52	49	21, 30, 38, 44	0
1	B	221/265 (83%)	-0.02	10 (4%)	32	30	21, 30, 39, 44	0
1	C	221/265 (83%)	0.18	7 (3%)	45	43	22, 30, 38, 44	0
1	D	221/265 (83%)	0.11	7 (3%)	45	43	22, 30, 39, 44	0
1	E	221/265 (83%)	0.13	5 (2%)	57	55	22, 30, 39, 44	0
1	F	221/265 (83%)	-0.00	4 (1%)	65	63	21, 30, 38, 44	0
1	G	221/265 (83%)	0.21	8 (3%)	41	39	21, 30, 38, 44	0
1	H	221/265 (83%)	0.13	9 (4%)	35	33	21, 30, 38, 44	0
All	All	1768/2120 (83%)	0.11	56 (3%)	45	43	21, 30, 39, 44	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	228	ILE	6.2
1	H	84	ASP	4.9
1	C	154	PHE	4.2
1	F	268	ARG	4.1
1	D	228	ILE	4.1
1	H	273	GLN	3.9
1	G	268	ARG	3.9
1	E	84	ASP	3.8
1	G	84	ASP	3.8
1	E	268	ARG	3.6
1	D	268	ARG	3.6
1	G	85	VAL	3.5
1	G	272	LEU	3.5
1	H	85	VAL	3.4
1	H	227	SER	3.4
1	A	299	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	154	PHE	3.3
1	B	273	GLN	3.2
1	C	157	ALA	3.2
1	B	266	GLN	3.2
1	D	269	LEU	3.1
1	E	228	ILE	3.1
1	C	84	ASP	3.0
1	G	302	ARG	3.0
1	H	268	ARG	2.9
1	D	84	ASP	2.9
1	A	84	ASP	2.8
1	F	302	ARG	2.7
1	B	268	ARG	2.6
1	F	273	GLN	2.6
1	A	275	VAL	2.6
1	B	153	ASP	2.6
1	B	228	ILE	2.6
1	G	205	GLN	2.5
1	H	78	GLN	2.5
1	C	155	THR	2.4
1	E	267	ALA	2.4
1	B	64	ARG	2.4
1	D	155	THR	2.4
1	A	268	ARG	2.3
1	C	268	ARG	2.3
1	G	80	LEU	2.3
1	D	273	GLN	2.3
1	B	272	LEU	2.2
1	D	85	VAL	2.2
1	G	275	VAL	2.2
1	H	228	ILE	2.2
1	B	205	GLN	2.2
1	B	267	ALA	2.2
1	H	272	LEU	2.2
1	H	156	ARG	2.1
1	F	84	ASP	2.1
1	E	85	VAL	2.1
1	B	154	PHE	2.1
1	A	157	ALA	2.1
1	C	302	ARG	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.