Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2023 – 10:03 PM JST

PDB ID	:	7XFF
Title	:	Polysaccharide export protein Wza
Authors	:	Zheng, J.; Wang, B.
Deposited on	:	2022-04-01
Resolution	:	2.30 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

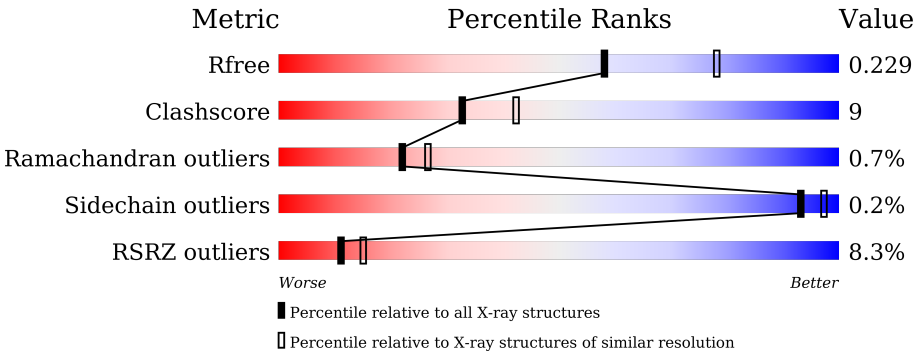
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	185	8% 80% 20%
1	B	185	5% 79% 16% 5%
1	C	185	8% 85% 14%
1	D	185	8% 86% 14%
1	E	185	7% 83% 15%
1	F	185	11% 80% 19%

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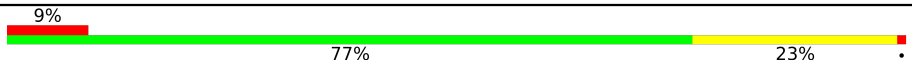
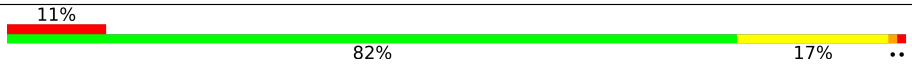
Mol	Chain	Length	Quality of chain
1	G	185	
1	H	185	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 12305 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 Polysaccharide export protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	185	Total	C	N	O	S	0	0	0
			1437	898	257	279	3			
1	B	176	Total	C	N	O	S	0	0	0
			1369	857	247	263	2			
1	C	185	Total	C	N	O	S	0	0	0
			1437	898	257	279	3			
1	D	185	Total	C	N	O	S	0	0	0
			1437	898	257	279	3			
1	E	185	Total	C	N	O	S	0	0	0
			1437	898	257	279	3			
1	F	185	Total	C	N	O	S	0	0	0
			1437	898	257	279	3			
1	G	185	Total	C	N	O	S	0	0	0
			1437	898	257	279	3			
1	H	185	Total	C	N	O	S	0	0	0
			1437	898	257	279	3			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	144	Total	O	0	0
			144	144		
2	B	119	Total	O	0	0
			119	119		
2	C	121	Total	O	0	0
			121	121		
2	D	113	Total	O	0	0
			113	113		
2	E	122	Total	O	0	0
			122	122		
2	F	92	Total	O	0	0
			92	92		

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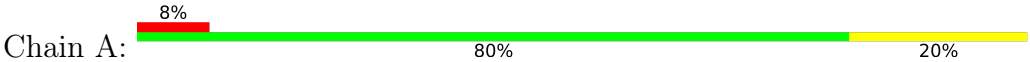
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	80	Total O 80 80	0	0
2	H	86	Total O 86 86	0	0

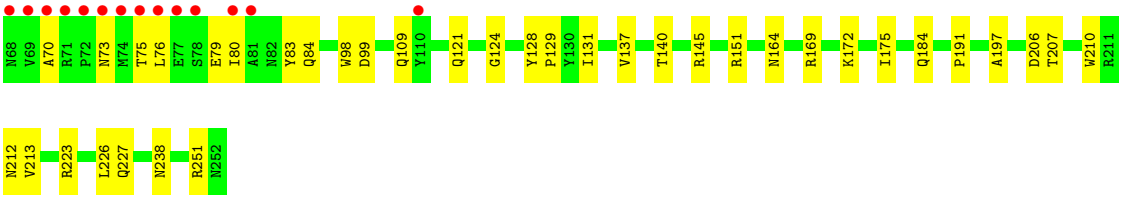
3 Residue-property plots (i)

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: Polysaccharide export protein

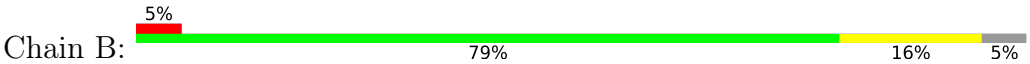
Chain A:





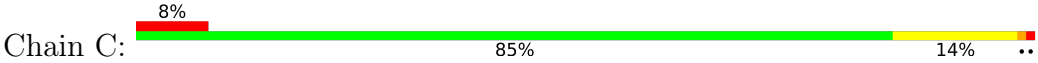
• Molecule 1: Polysaccharide export protein

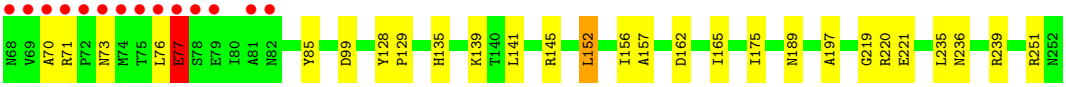
Chain B:



• Molecule 1: Polysaccharide export protein

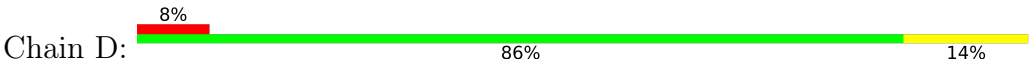
Chain C:





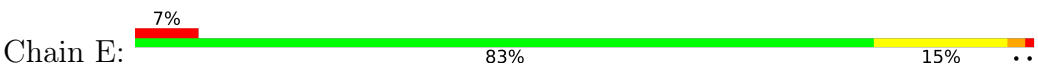
• Molecule 1: Polysaccharide export protein

Chain D:



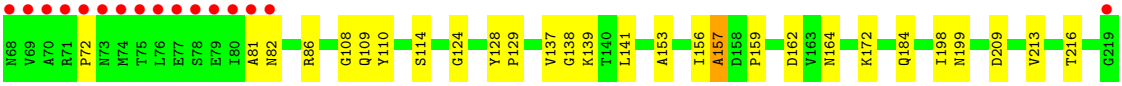
• Molecule 1: Polysaccharide export protein

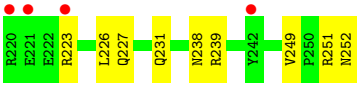
Chain E:



• Molecule 1: Polysaccharide export protein

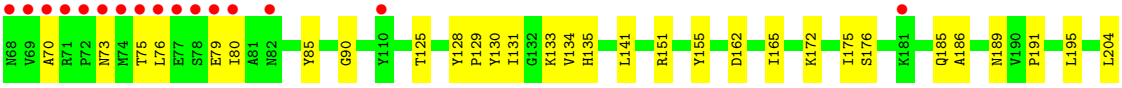
Chain F:

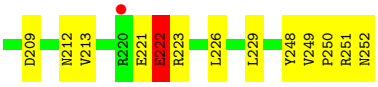




• Molecule 1: Polysaccharide export protein

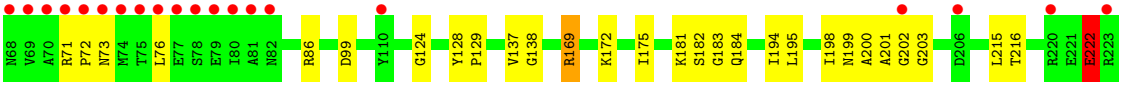
Chain G:





• Molecule 1: Polysaccharide export protein

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	185.77Å 193.04Å 106.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.63 – 2.30 26.63 – 2.30	Depositor EDS
% Data completeness (in resolution range)	83.8 (26.63-2.30) 83.1 (26.63-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.73 (at 2.31Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.184 , 0.229 0.184 , 0.229	Depositor DCC
R_{free} test set	2011 reflections (2.62%)	wwPDB-VP
Wilson B-factor (Å^2)	29.5	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 47.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.019 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12305	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.43	0/1466	0.65	0/2003
1	B	0.45	0/1397	0.70	1/1908 (0.1%)
1	C	0.48	1/1466 (0.1%)	0.70	3/2003 (0.1%)
1	D	0.44	0/1466	0.65	1/2003 (0.0%)
1	E	0.62	3/1466 (0.2%)	1.33	7/2003 (0.3%)
1	F	0.40	0/1466	0.64	0/2003
1	G	0.53	2/1466 (0.1%)	0.77	8/2003 (0.4%)
1	H	0.44	1/1466 (0.1%)	0.68	1/2003 (0.0%)
All	All	0.48	7/11659 (0.1%)	0.80	21/15929 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	1
All	All	0	5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	71	ARG	CG-CD	12.88	1.84	1.51
1	G	222	GLU	CD-OE1	8.52	1.35	1.25
1	C	77	GLU	CD-OE1	6.59	1.32	1.25
1	E	71	ARG	CB-CG	6.40	1.69	1.52
1	H	222	GLU	CD-OE1	6.28	1.32	1.25
1	G	222	GLU	CA-CB	5.66	1.66	1.53
1	E	71	ARG	CZ-NH2	5.47	1.40	1.33

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	71	ARG	NE-CZ-NH1	-32.02	104.29	120.30
1	E	71	ARG	NE-CZ-NH2	29.28	134.94	120.30
1	E	71	ARG	CA-CB-CG	18.62	154.37	113.40
1	E	71	ARG	CD-NE-CZ	14.10	143.34	123.60
1	E	71	ARG	CB-CG-CD	11.47	141.43	111.60
1	G	222	GLU	CA-CB-CG	9.43	134.14	113.40
1	B	220	ARG	CG-CD-NE	-8.71	93.50	111.80
1	G	251	ARG	NE-CZ-NH1	6.63	123.61	120.30
1	G	172	LYS	CD-CE-NZ	-6.42	96.94	111.70
1	G	251	ARG	NE-CZ-NH2	6.41	123.50	120.30
1	E	71	ARG	CB-CA-C	6.40	123.19	110.40
1	G	222	GLU	OE1-CD-OE2	-6.08	116.01	123.30
1	G	251	ARG	NH1-CZ-NH2	-6.04	112.76	119.40
1	H	169	ARG	CG-CD-NE	5.98	124.35	111.80
1	G	222	GLU	CB-CA-C	5.92	122.25	110.40
1	D	251	ARG	NE-CZ-NH1	-5.50	117.55	120.30
1	C	251	ARG	CG-CD-NE	-5.42	100.42	111.80
1	C	251	ARG	NE-CZ-NH2	-5.33	117.63	120.30
1	G	222	GLU	N-CA-CB	-5.23	101.19	110.60
1	C	152	LEU	CB-CG-CD2	-5.17	102.22	111.00
1	E	109	GLN	CA-CB-CG	5.11	124.63	113.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	77	GLU	Sidechain
1	E	71	ARG	Sidechain
1	F	157	ALA	Peptide
1	G	222	GLU	Sidechain
1	H	222	GLU	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1437	0	1407	32	0
1	B	1369	0	1340	21	0
1	C	1437	0	1407	21	0
1	D	1437	0	1407	23	0
1	E	1437	0	1407	42	0
1	F	1437	0	1407	28	0
1	G	1437	0	1407	30	0
1	H	1437	0	1407	27	0
2	A	144	0	0	6	1
2	B	119	0	0	6	1
2	C	121	0	0	3	1
2	D	113	0	0	2	1
2	E	122	0	0	4	0
2	F	92	0	0	7	0
2	G	80	0	0	7	1
2	H	86	0	0	10	0
All	All	12305	0	11189	196	3

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 (196) 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:E:71:ARG:CD	1:E:71:ARG:CG	1.84	1.51
1:B:110:TYR:OH	2:B:301:HOH:O	1.88	0.91
1:E:162:ASP:OD1	2:E:301:HOH:O	1.87	0.90
1:G:90:GLY:O	2:G:301:HOH:O	1.96	0.83
1:D:109:GLN:HG2	1:F:108:GLY:HA3	1.61	0.83
1:A:172:LYS:HD3	1:A:184:GLN:HE21	1.46	0.79
1:H:200:ALA:O	2:H:301:HOH:O	2.00	0.78
1:H:222:GLU:OE1	1:H:239:ARG:NH1	2.16	0.78
1:E:70:ALA:HB1	1:E:72:PRO:HD3	1.68	0.76
1:F:209:ASP:HB2	1:F:252:ASN:HA	1.68	0.75
1:G:162:ASP:OD2	2:G:302:HOH:O	2.04	0.75
1:H:201:ALA:O	2:H:302:HOH:O	2.04	0.74
1:G:221:GLU:O	1:G:222:GLU:HB2	1.89	0.72
1:A:223:ARG:NH1	2:A:302:HOH:O	2.23	0.72
1:D:110:TYR:HD1	1:E:109:GLN:HB3	1.55	0.71
1:E:71:ARG:HD3	2:E:323:HOH:O	1.92	0.69
1:A:206:ASP:OD2	1:E:251:ARG:NH2	2.26	0.69
1:H:181:LYS:N	2:H:302:HOH:O	2.15	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:81:ALA:O	2:F:303:HOH:O	2.11	0.68
1:H:195:LEU:O	2:H:303:HOH:O	2.12	0.68
1:C:162:ASP:OD2	2:C:301:HOH:O	2.12	0.68
1:G:186:ALA:O	2:G:304:HOH:O	2.12	0.68
1:D:233:GLY:HA3	1:F:216:THR:HG21	1.76	0.67
1:B:214:VAL:HG22	1:B:223:ARG:HH12	1.58	0.67
1:F:114:SER:O	2:F:304:HOH:O	2.13	0.66
1:B:135:HIS:ND1	2:B:306:HOH:O	2.29	0.66
1:H:181:LYS:NZ	2:H:306:HOH:O	2.29	0.66
1:G:195:LEU:HD13	1:G:229:LEU:HD21	1.77	0.65
1:A:70:ALA:HB3	1:E:219:GLY:HA2	1.79	0.65
1:H:71:ARG:HG2	1:H:236:ASN:HD21	1.62	0.65
1:D:73:ASN:HD22	1:D:76:LEU:HB2	1.62	0.64
1:B:162:ASP:OD2	2:B:302:HOH:O	2.14	0.64
1:C:135:HIS:O	1:C:139:LYS:HE2	1.98	0.64
1:A:99:ASP:OD2	1:E:130:TYR:OH	2.15	0.64
1:D:108:GLY:HA3	1:E:109:GLN:CG	2.27	0.64
1:A:169:ARG:NH1	2:A:306:HOH:O	2.30	0.63
1:A:109:GLN:CG	1:E:108:GLY:HA3	2.28	0.62
1:A:109:GLN:HG2	1:E:108:GLY:HA3	1.82	0.61
1:G:130:TYR:OH	1:H:99:ASP:OD2	2.17	0.61
1:C:219:GLY:HA2	1:G:70:ALA:HB3	1.83	0.61
1:D:110:TYR:CD1	1:E:109:GLN:HB3	2.35	0.61
1:C:73:ASN:HD22	1:C:76:LEU:HD22	1.67	0.60
1:E:71:ARG:H	1:E:72:PRO:HD3	1.65	0.59
1:D:108:GLY:HA3	1:E:109:GLN:HG3	1.85	0.59
1:A:128:TYR:CG	1:A:129:PRO:HD2	2.38	0.59
1:D:172:LYS:HD3	1:D:184:GLN:NE2	2.18	0.59
1:F:82:ASN:ND2	2:F:309:HOH:O	2.36	0.58
1:C:145:ARG:NH1	2:C:302:HOH:O	2.12	0.58
1:D:76:LEU:HD22	1:D:238:ASN:HB3	1.85	0.58
1:F:251:ARG:NH1	2:F:301:HOH:O	2.08	0.58
1:E:71:ARG:HG3	1:E:234:ASP:CG	2.24	0.57
1:F:172:LYS:HD3	1:F:184:GLN:HE21	1.69	0.57
1:B:221:GLU:OE1	1:C:70:ALA:HB2	2.05	0.57
1:A:121:GLN:NE2	2:A:309:HOH:O	2.38	0.57
1:B:68:ASN:HB3	1:B:234:ASP:HB2	1.86	0.57
1:D:100:HIS:CE1	1:D:156:ILE:HD12	2.40	0.57
1:B:219:GLY:C	1:C:70:ALA:HB3	2.25	0.56
1:H:194:ILE:HD11	1:H:215:LEU:HD22	1.85	0.56
1:G:73:ASN:HB3	1:G:76:LEU:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:199:ASN:N	2:H:303:HOH:O	2.10	0.56
1:G:155:TYR:OH	2:G:303:HOH:O	2.10	0.56
1:B:210:TRP:CZ2	1:B:227:GLN:HG2	2.41	0.56
1:G:212:ASN:HB3	1:G:223:ARG:HH21	1.70	0.56
1:H:73:ASN:HD22	1:H:76:LEU:HB2	1.71	0.55
1:E:71:ARG:N	1:E:72:PRO:HD3	2.21	0.55
1:H:86:ARG:HD3	1:H:138:GLY:O	2.07	0.55
1:C:73:ASN:HB3	1:C:76:LEU:HB3	1.90	0.54
1:C:141:LEU:HD21	1:C:165:ILE:HG13	1.89	0.54
1:G:213:VAL:HG21	1:G:226:LEU:HG	1.90	0.54
1:G:133:LYS:NZ	2:G:308:HOH:O	2.41	0.54
1:E:71:ARG:N	1:E:72:PRO:CD	2.71	0.54
1:E:141:LEU:HD21	1:E:165:ILE:HG13	1.90	0.54
1:A:145:ARG:NH1	2:A:311:HOH:O	2.41	0.54
1:A:212:ASN:OD1	1:A:223:ARG:HD2	2.08	0.53
1:E:74:MET:O	1:E:77:GLU:HB2	2.08	0.53
1:G:212:ASN:HB3	1:G:223:ARG:NH2	2.24	0.53
1:F:128:TYR:CG	1:F:129:PRO:HD2	2.43	0.52
1:F:172:LYS:CD	1:F:184:GLN:HE21	2.22	0.52
1:D:110:TYR:CE2	1:F:110:TYR:CZ	2.97	0.52
1:E:180:ASN:ND2	2:E:303:HOH:O	2.17	0.52
1:B:214:VAL:CG2	1:B:223:ARG:HH12	2.20	0.52
1:C:220:ARG:HG3	1:C:220:ARG:HH11	1.73	0.52
1:D:108:GLY:HA3	1:E:109:GLN:HG2	1.91	0.52
1:E:71:ARG:HG3	1:E:234:ASP:OD2	2.09	0.52
1:E:73:ASN:N	1:E:235:LEU:HB2	2.25	0.52
1:F:162:ASP:OD2	2:F:305:HOH:O	2.19	0.51
1:G:128:TYR:CG	1:G:129:PRO:HD2	2.44	0.51
1:G:128:TYR:CD2	1:G:129:PRO:HD2	2.44	0.51
1:H:73:ASN:ND2	1:H:76:LEU:HB2	2.25	0.51
1:B:73:ASN:ND2	2:B:309:HOH:O	2.40	0.51
1:A:75:THR:O	1:A:79:GLU:HG3	2.11	0.51
1:F:139:LYS:NZ	2:F:311:HOH:O	2.44	0.51
1:F:157:ALA:HA	1:F:159:PRO:HD3	1.92	0.50
1:E:72:PRO:HB3	1:E:235:LEU:HD12	1.93	0.50
1:G:141:LEU:HD11	1:G:165:ILE:HD12	1.93	0.50
1:H:71:ARG:CG	1:H:236:ASN:HD21	2.25	0.50
1:H:201:ALA:O	1:H:203:GLY:N	2.44	0.50
1:H:216:THR:OG1	2:H:304:HOH:O	2.19	0.49
1:H:128:TYR:CG	1:H:129:PRO:HD2	2.48	0.49
1:A:80:ILE:HG23	1:A:191:PRO:HG2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:LEU:HD12	1:B:126:MET:SD	2.52	0.49
1:H:175:ILE:HG23	1:H:247:LEU:HD23	1.94	0.49
1:F:141:LEU:HD13	1:F:164:ASN:HA	1.94	0.49
1:D:213:VAL:HG21	1:D:226:LEU:HG	1.95	0.49
1:C:128:TYR:CG	1:C:129:PRO:HD2	2.47	0.49
1:B:252:ASN:OD1	1:B:252:ASN:N	2.44	0.48
1:A:172:LYS:HD3	1:A:184:GLN:NE2	2.22	0.48
1:E:175:ILE:HG12	1:E:197:ALA:HB1	1.94	0.48
1:B:130:TYR:OH	1:C:99:ASP:OD1	2.32	0.48
1:D:222:GLU:OE1	1:D:239:ARG:NH2	2.28	0.48
1:A:109:GLN:HG3	1:E:108:GLY:HA3	1.94	0.48
1:F:227:GLN:NE2	1:F:231:GLN:OE1	2.47	0.48
1:F:153:ALA:HA	1:F:156:ILE:O	2.14	0.48
1:C:157:ALA:O	2:C:303:HOH:O	2.20	0.48
1:F:86:ARG:HD3	1:F:138:GLY:O	2.13	0.48
1:H:169:ARG:HD3	2:H:305:HOH:O	2.12	0.47
1:A:175:ILE:HG12	1:A:197:ALA:HB1	1.95	0.47
1:D:110:TYR:CE2	1:E:110:TYR:CE1	3.03	0.47
1:E:69:VAL:O	1:E:232:ASN:HB3	2.14	0.47
1:E:70:ALA:HA	1:E:232:ASN:O	2.14	0.47
1:C:221:GLU:OE2	1:G:70:ALA:HB2	2.14	0.47
1:F:124:GLY:HA2	1:F:137:VAL:HG21	1.96	0.47
1:A:128:TYR:CD2	1:A:129:PRO:HD2	2.49	0.47
1:D:128:TYR:CG	1:D:129:PRO:HD2	2.49	0.47
1:E:70:ALA:O	1:E:71:ARG:HB2	2.14	0.47
1:G:209:ASP:HB2	1:G:252:ASN:HA	1.97	0.47
1:F:213:VAL:HG22	1:F:249:VAL:HG22	1.96	0.47
1:F:238:ASN:OD1	1:F:239:ARG:N	2.48	0.47
1:H:124:GLY:HA2	1:H:137:VAL:CG2	2.45	0.46
1:G:85:TYR:HB2	1:G:189:ASN:HA	1.97	0.46
1:H:238:ASN:O	1:H:239:ARG:HD3	2.16	0.46
1:B:128:TYR:CG	1:B:129:PRO:HD2	2.51	0.46
1:B:214:VAL:HG22	1:B:223:ARG:NH1	2.29	0.46
1:F:231:GLN:HG2	1:H:248:TYR:CE1	2.51	0.45
1:E:236:ASN:O	1:E:239:ARG:NH1	2.49	0.45
1:A:131:ILE:O	1:A:151:ARG:NH2	2.50	0.45
1:B:123:ASP:OD2	2:B:303:HOH:O	2.21	0.45
1:A:124:GLY:HA2	1:A:137:VAL:CG2	2.47	0.45
1:C:152:LEU:HD22	1:C:156:ILE:HD12	1.99	0.45
1:G:80:ILE:HG23	1:G:191:PRO:HG2	1.99	0.45
1:D:219:GLY:HA2	1:E:72:PRO:HG3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:71:ARG:H	1:E:72:PRO:CD	2.30	0.45
1:H:172:LYS:HD3	1:H:184:GLN:OE1	2.17	0.44
1:F:198:ILE:HG13	1:F:226:LEU:HD11	1.98	0.44
1:G:175:ILE:HG13	1:G:185:GLN:NE2	2.31	0.44
1:D:121:GLN:NE2	2:D:314:HOH:O	2.50	0.44
1:A:124:GLY:HA2	1:A:137:VAL:HG21	1.99	0.44
1:C:128:TYR:CD2	1:C:129:PRO:HD2	2.53	0.44
1:E:195:LEU:HD13	1:E:229:LEU:HD21	1.99	0.43
1:F:199:ASN:HB3	1:H:183:GLY:HA2	2.00	0.43
1:G:176:SER:O	1:G:248:TYR:HA	2.17	0.43
1:D:76:LEU:CD2	1:D:235:LEU:HD12	2.48	0.43
1:A:73:ASN:ND2	1:A:76:LEU:HB2	2.33	0.43
1:H:201:ALA:HA	2:H:301:HOH:O	2.18	0.43
1:D:221:GLU:OE1	1:E:70:ALA:HB2	2.19	0.43
1:C:85:TYR:HB2	1:C:189:ASN:HA	2.01	0.43
1:C:71:ARG:O	1:C:235:LEU:HB2	2.18	0.43
1:D:178:GLN:HB2	1:D:249:VAL:HG12	2.01	0.43
1:A:164:ASN:ND2	2:A:307:HOH:O	2.36	0.43
1:E:222:GLU:OE1	1:E:239:ARG:NE	2.46	0.43
1:D:151:ARG:NH2	2:D:315:HOH:O	2.51	0.42
1:A:80:ILE:HA	1:A:83:TYR:HB2	2.00	0.42
1:B:236:ASN:O	1:B:239:ARG:NH1	2.52	0.42
1:G:75:THR:O	1:G:79:GLU:N	2.46	0.42
1:A:207:THR:O	1:A:251:ARG:HA	2.19	0.42
1:F:109:GLN:NE2	2:F:315:HOH:O	2.52	0.42
1:A:210:TRP:CZ2	1:A:227:GLN:HG2	2.55	0.42
1:B:111:ARG:NH1	2:B:312:HOH:O	2.43	0.42
1:G:125:THR:HA	1:G:134:VAL:O	2.20	0.42
1:A:84:GLN:HG2	1:A:140:THR:HG22	2.01	0.42
1:E:71:ARG:CD	1:E:71:ARG:HG2	2.24	0.42
1:E:145:ARG:HG3	1:E:162:ASP:HA	2.02	0.42
1:H:198:ILE:N	2:H:303:HOH:O	2.52	0.42
1:C:219:GLY:HA2	1:G:70:ALA:CB	2.48	0.42
1:G:204:LEU:HD22	1:G:249:VAL:HG11	2.02	0.42
1:G:248:TYR:CE1	1:G:250:PRO:HA	2.55	0.42
1:A:98:TRP:O	2:A:301:HOH:O	2.22	0.41
1:C:175:ILE:HG12	1:C:197:ALA:HB1	2.00	0.41
1:B:175:ILE:HG12	1:B:197:ALA:HB1	2.01	0.41
1:B:214:VAL:HG22	1:B:223:ARG:HH22	1.85	0.41
1:G:85:TYR:O	2:G:305:HOH:O	2.21	0.41
1:A:76:LEU:HD22	1:A:238:ASN:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:TRP:CZ3	1:A:227:GLN:HA	2.55	0.41
1:E:111:ARG:NH1	2:E:305:HOH:O	2.27	0.41
1:F:124:GLY:HA2	1:F:137:VAL:CG2	2.50	0.41
1:B:85:TYR:HB2	1:B:189:ASN:HA	2.03	0.41
1:D:128:TYR:CD2	1:D:129:PRO:HD2	2.56	0.41
1:E:72:PRO:HA	1:E:235:LEU:HB2	2.02	0.41
1:C:236:ASN:O	1:C:239:ARG:NH1	2.54	0.41
1:G:131:ILE:O	1:G:151:ARG:NH2	2.54	0.41
1:E:128:TYR:CG	1:E:129:PRO:HD2	2.56	0.41
1:G:135:HIS:HB3	2:G:360:HOH:O	2.21	0.41
1:A:109:GLN:HB3	1:E:110:TYR:HD2	1.86	0.40
1:F:199:ASN:HD22	1:H:183:GLY:HA2	1.87	0.40
1:F:223:ARG:H	1:F:223:ARG:HG2	1.64	0.40
1:A:213:VAL:HG21	1:A:226:LEU:CD1	2.51	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:436:HOH:O	2:B:354:HOH:O[4_555]	2.07	0.13
2:D:383:HOH:O	2:G:331:HOH:O[6_554]	2.10	0.10
2:C:372:HOH:O	2:C:415:HOH:O[4_556]	2.12	0.08

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	183/185 (99%)	178 (97%)	5 (3%)	0	100 100
1	B	172/185 (93%)	165 (96%)	5 (3%)	2 (1%)	13 14
1	C	183/185 (99%)	177 (97%)	6 (3%)	0	100 100
1	D	183/185 (99%)	179 (98%)	3 (2%)	1 (0%)	29 35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	E	183/185 (99%)	177 (97%)	4 (2%)	2 (1%)	14 15
1	F	183/185 (99%)	175 (96%)	7 (4%)	1 (0%)	29 35
1	G	183/185 (99%)	176 (96%)	6 (3%)	1 (0%)	29 35
1	H	183/185 (99%)	173 (94%)	7 (4%)	3 (2%)	9 9
All	All	1453/1480 (98%)	1400 (96%)	43 (3%)	10 (1%)	22 26

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	69	VAL
1	F	72	PRO
1	H	72	PRO
1	G	222	GLU
1	B	72	PRO
1	D	72	PRO
1	E	72	PRO
1	H	182	SER
1	H	202	GLY
1	E	69	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	155/155 (100%)	155 (100%)	0	100 100
1	B	147/155 (95%)	147 (100%)	0	100 100
1	C	155/155 (100%)	154 (99%)	1 (1%)	86 94
1	D	155/155 (100%)	155 (100%)	0	100 100
1	E	155/155 (100%)	154 (99%)	1 (1%)	86 94
1	F	155/155 (100%)	155 (100%)	0	100 100
1	G	155/155 (100%)	155 (100%)	0	100 100
1	H	155/155 (100%)	155 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1232/1240 (99%)	1230 (100%)	2 (0%)	93 97

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	77	GLU
1	E	71	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	184	GLN
1	D	73	ASN
1	D	184	GLN
1	F	184	GLN
1	H	236	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 monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	185/185 (100%)	0.16	14 (7%) 13 18	17, 26, 76, 105	0
1	B	176/185 (95%)	-0.10	9 (5%) 28 35	16, 27, 49, 75	0
1	C	185/185 (100%)	0.18	14 (7%) 13 18	18, 29, 78, 103	0
1	D	185/185 (100%)	0.30	15 (8%) 12 16	19, 29, 92, 107	0
1	E	185/185 (100%)	0.14	13 (7%) 16 21	18, 29, 63, 84	0
1	F	185/185 (100%)	0.72	20 (10%) 5 8	19, 36, 105, 128	0
1	G	185/185 (100%)	0.39	17 (9%) 9 12	21, 38, 72, 97	0
1	H	185/185 (100%)	0.65	20 (10%) 5 8	21, 40, 95, 117	0
All	All	1471/1480 (99%)	0.31	122 (8%) 11 15	16, 31, 78, 128	0

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	69	VAL	16.4
1	F	69	VAL	13.7
1	D	69	VAL	13.6
1	C	74	MET	12.2
1	E	72	PRO	12.1
1	H	74	MET	11.9
1	D	75	THR	11.8
1	G	74	MET	11.7
1	H	75	THR	11.4
1	C	72	PRO	11.1
1	H	72	PRO	11.1
1	F	68	ASN	11.1
1	F	74	MET	10.6
1	F	75	THR	10.4
1	C	69	VAL	10.3
1	F	81	ALA	10.2

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Mol	Chain	Res	Type	RSRZ
1	H	70	ALA	10.2
1	F	77	GLU	10.0
1	F	73	ASN	9.9
1	A	72	PRO	9.8
1	F	72	PRO	9.6
1	F	76	LEU	9.5
1	H	73	ASN	9.4
1	B	70	ALA	9.1
1	F	71	ARG	8.7
1	A	70	ALA	8.6
1	C	75	THR	8.3
1	C	73	ASN	8.2
1	H	76	LEU	8.2
1	H	71	ARG	8.2
1	A	74	MET	8.2
1	D	78	SER	8.0
1	D	81	ALA	7.9
1	A	73	ASN	7.9
1	G	75	THR	7.9
1	E	73	ASN	7.8
1	H	78	SER	7.8
1	D	68	ASN	7.8
1	E	75	THR	7.8
1	D	72	PRO	7.7
1	A	75	THR	7.5
1	C	78	SER	7.4
1	G	72	PRO	7.3
1	F	70	ALA	7.3
1	C	70	ALA	7.3
1	C	68	ASN	7.2
1	G	73	ASN	7.2
1	B	69	VAL	7.2
1	E	78	SER	7.2
1	G	78	SER	7.1
1	B	72	PRO	7.1
1	D	74	MET	7.1
1	H	81	ALA	6.9
1	H	68	ASN	6.8
1	C	76	LEU	6.8
1	A	71	ARG	6.8
1	E	68	ASN	6.8
1	G	76	LEU	6.8

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Mol	Chain	Res	Type	RSRZ
1	D	76	LEU	6.8
1	A	69	VAL	6.6
1	H	77	GLU	6.5
1	D	73	ASN	6.4
1	G	77	GLU	6.4
1	A	76	LEU	6.3
1	G	70	ALA	6.2
1	G	69	VAL	6.2
1	G	71	ARG	6.1
1	E	71	ARG	6.1
1	G	68	ASN	6.0
1	E	69	VAL	5.9
1	E	74	MET	5.9
1	D	77	GLU	5.8
1	D	80	ILE	5.7
1	D	70	ALA	5.7
1	E	79	GLU	5.6
1	D	71	ARG	5.5
1	A	81	ALA	5.5
1	A	78	SER	5.4
1	E	76	LEU	5.4
1	C	77	GLU	5.4
1	A	68	ASN	5.2
1	F	78	SER	5.1
1	B	68	ASN	5.1
1	C	71	ARG	5.0
1	A	77	GLU	5.0
1	B	71	ARG	4.9
1	F	80	ILE	4.7
1	F	79	GLU	4.7
1	A	80	ILE	4.6
1	H	80	ILE	4.1
1	D	82	ASN	4.1
1	H	202	GLY	4.0
1	C	81	ALA	4.0
1	H	79	GLU	3.9
1	F	223	ARG	3.9
1	B	220	ARG	3.9
1	H	82	ASN	3.6
1	F	220	ARG	3.4
1	G	220	ARG	3.4
1	H	206	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	79	GLU	3.2
1	G	80	ILE	3.1
1	E	70	ALA	3.0
1	F	82	ASN	2.9
1	H	220	ARG	2.9
1	G	181	LYS	2.9
1	E	220	ARG	2.8
1	C	79	GLU	2.8
1	H	223	ARG	2.8
1	B	73	ASN	2.7
1	E	77	GLU	2.6
1	G	110	TYR	2.5
1	G	79	GLU	2.5
1	G	82	ASN	2.5
1	F	219	GLY	2.4
1	B	110	TYR	2.3
1	A	110	TYR	2.1
1	H	110	TYR	2.1
1	F	221	GLU	2.1
1	F	242	TYR	2.1
1	C	82	ASN	2.1
1	B	223	ARG	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.