Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2023 – 07:13 AM EDT

PDB ID	:	2R1A
Title	:	Crystal structure of the periplasmic lipopolysaccharide transport protein LptA (YhbN), trigonal form
Authors	:	Suits, M.D.L.; Polissi, A.; Jia, Z.; Montreal-Kingston Bacterial Structural Genomics Initiative (BSGI)
Deposited on	:	2007-08-22
Resolution	:	3.26 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:

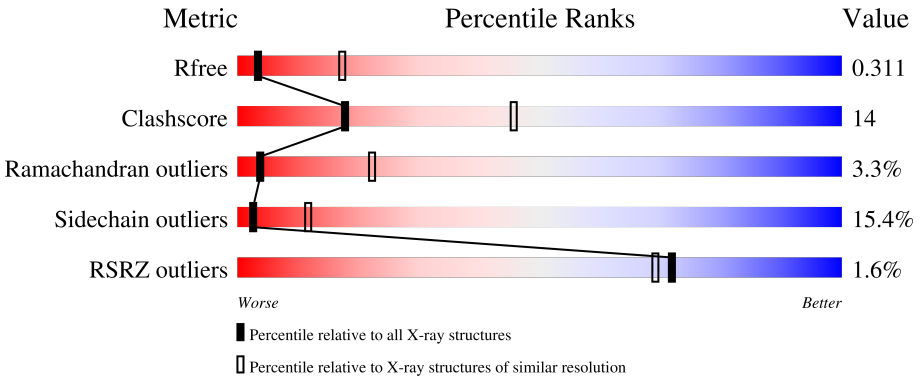
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.26 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	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

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	159	58% 22% 18%
1	B	159	47% 34% 16%
1	C	159	60% 20% 5% 15%
1	D	159	61% 21% 14%
1	E	159	55% 24% 17%

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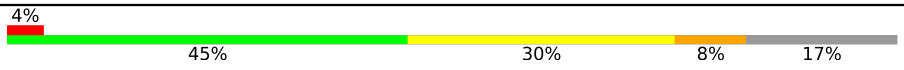
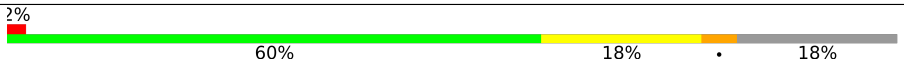
Mol	Chain	Length	Quality of chain
1	F	159	
1	G	159	
1	H	159	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7620 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 Protein yhbN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	131	Total	C	N	O	S	0	0	0
			927	578	154	191	4			
1	B	134	Total	C	N	O	S	0	0	0
			956	594	160	198	4			
1	C	135	Total	C	N	O	S	0	0	0
			989	617	163	206	3			
1	D	136	Total	C	N	O	S	0	0	0
			923	572	156	193	2			
1	E	132	Total	C	N	O	S	0	0	0
			918	569	155	192	2			
1	F	132	Total	C	N	O	S	0	0	0
			938	584	155	196	3			
1	G	135	Total	C	N	O	S	0	0	0
			980	609	165	203	3			
1	H	131	Total	C	N	O	S	0	0	0
			921	572	152	195	2			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	9	Total	O	0	0
			9	9		
2	B	8	Total	O	0	0
			8	8		
2	C	2	Total	O	0	0
			2	2		
2	D	8	Total	O	0	0
			8	8		
2	E	14	Total	O	0	0
			14	14		
2	F	9	Total	O	0	0
			9	9		

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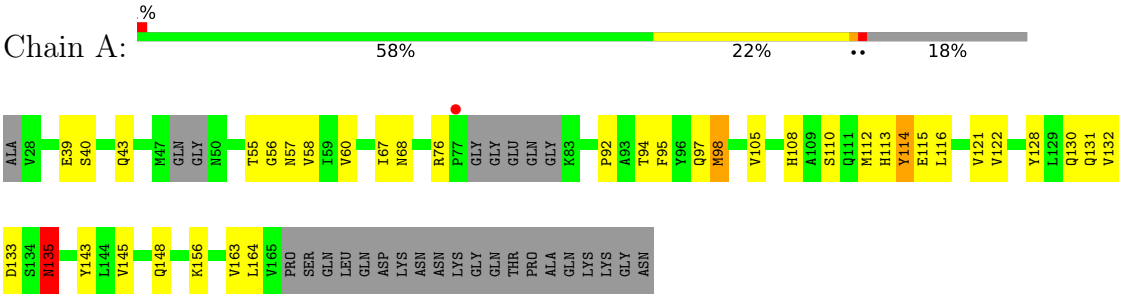
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	14	Total O 14 14	0	0
2	H	4	Total O 4 4	0	0

3 Residue-property plots

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.

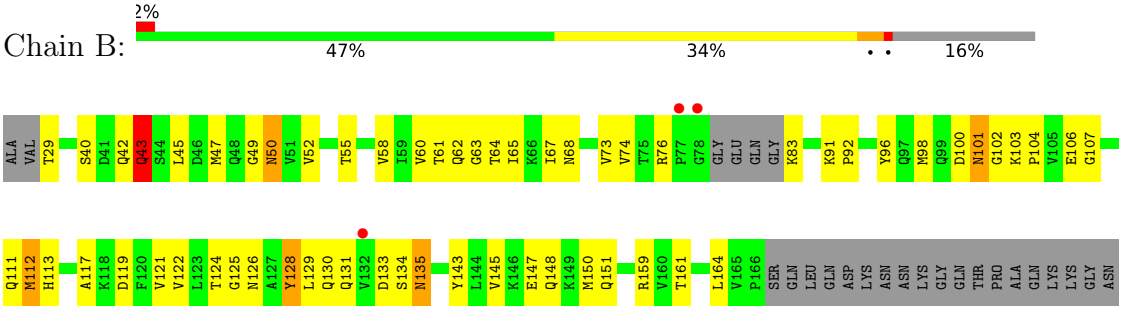
• Molecule 1: Protein yhbN

Chain A:



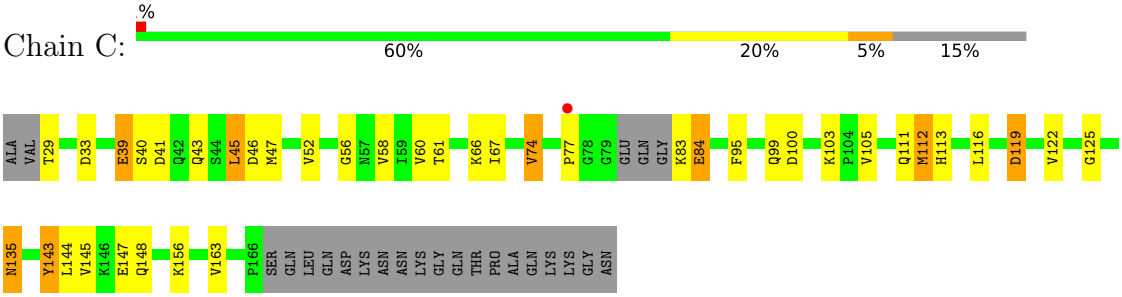
• Molecule 1: Protein yhbN

Chain B:



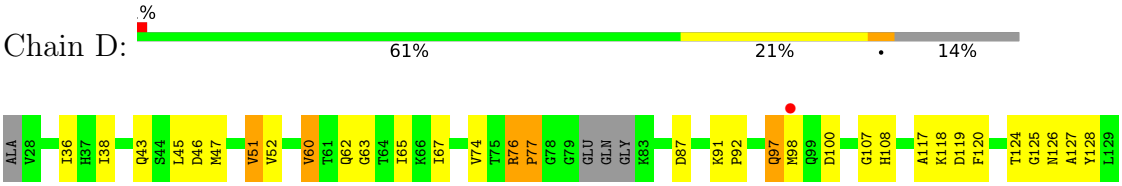
• Molecule 1: Protein yhbN

Chain C:



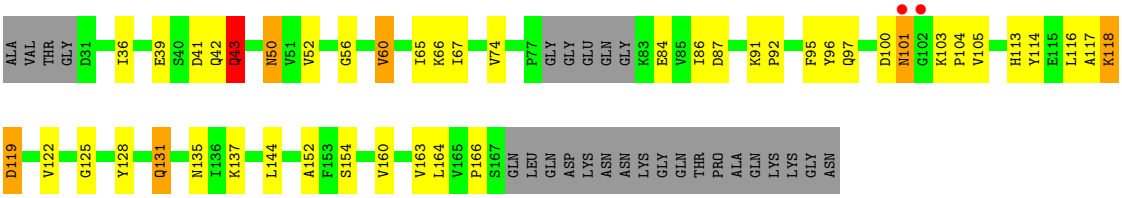
• Molecule 1: Protein yhbN

Chain D:



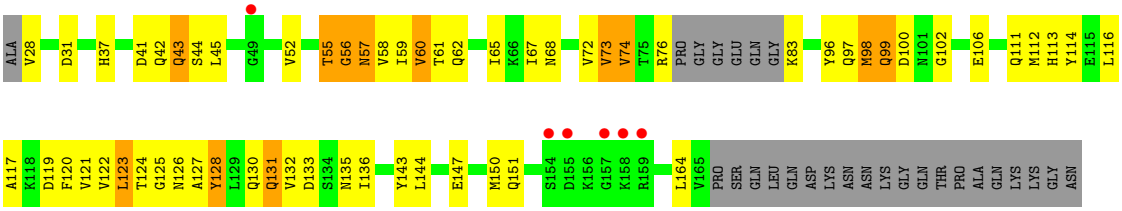
• Molecule 1: Protein yhbN

Chain E:



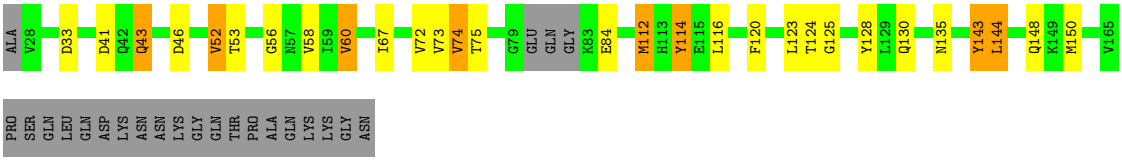
• Molecule 1: Protein yhbN

Chain F:



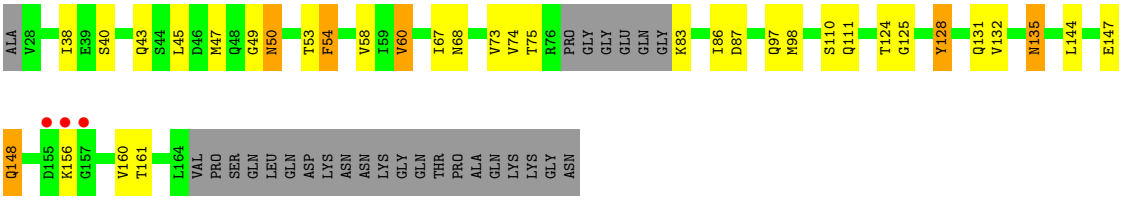
• Molecule 1: Protein yhbN

Chain G:



• Molecule 1: Protein yhbN

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	146.21Å 146.21Å 186.81Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.98 – 3.26 29.98 – 3.25	Depositor EDS
% Data completeness (in resolution range)	83.6 (29.98-3.26) 97.3 (29.98-3.25)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	3.55 (at 3.24Å)	Xtriage
Refinement program	REFMAC 5.4.0065, PHENIX	Depositor
R, R_{free}	0.298 , 0.361 0.306 , 0.311	Depositor DCC
R_{free} test set	1794 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	67.8	Xtriage
Anisotropy	0.935	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 62.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.033 for -h,-k,l	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	7620	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.40 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.4591e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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	0.34	0/940	0.52	0/1283
1	B	0.38	0/971	0.54	0/1327
1	C	0.36	0/1004	0.53	0/1371
1	D	0.36	0/937	0.51	0/1285
1	E	0.36	0/932	0.57	0/1280
1	F	0.39	1/951 (0.1%)	0.58	0/1301
1	G	0.34	0/994	0.52	0/1356
1	H	0.34	0/934	0.50	0/1281
All	All	0.36	1/7663 (0.0%)	0.53	0/10484

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	132	VAL	CB-CG1	-5.18	1.42	1.52

There are no bond angle outliers.

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	927	0	798	25	0
1	B	956	0	831	35	0
1	C	989	0	899	28	0
1	D	923	0	762	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	918	0	758	25	0
1	F	938	0	817	36	0
1	G	980	0	882	16	0
1	H	921	0	783	17	0
2	A	9	0	0	1	0
2	B	8	0	0	1	0
2	C	2	0	0	0	0
2	D	8	0	0	0	0
2	E	14	0	0	1	0
2	F	9	0	0	1	0
2	G	14	0	0	1	0
2	H	4	0	0	2	0
All	All	7620	0	6530	191	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 14.

All (191) 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:148:GLN:HG3	1:B:47:MET:HB2	1.48	0.95
1:F:98:MET:HA	1:F:99:GLN:CB	1.98	0.93
1:F:97:GLN:HG2	1:F:98:MET:H	1.43	0.83
1:B:148:GLN:HB3	1:C:47:MET:HB2	1.60	0.81
1:C:143:TYR:CE1	1:C:145:VAL:HA	2.15	0.81
1:A:115:GLU:HG3	2:A:205:HOH:O	1.82	0.78
1:C:148:GLN:HB3	1:D:47:MET:HB2	1.66	0.78
1:B:65:ILE:HA	1:B:96:TYR:O	1.84	0.77
1:B:42:GLN:HB2	1:B:55:THR:HG23	1.67	0.77
1:D:160:VAL:HG12	1:D:161:THR:H	1.54	0.73
1:G:84:GLU:HB2	1:G:116:LEU:HD12	1.70	0.72
1:C:143:TYR:HE1	1:C:145:VAL:HA	1.53	0.72
1:B:150:MET:HG2	1:B:151:GLN:H	1.54	0.72
1:B:106:GLU:HG3	1:B:107:GLY:H	1.54	0.71
1:F:130:GLN:HG2	1:F:131:GLN:H	1.55	0.71
1:E:118:LYS:O	1:E:119:ASP:HB2	1.92	0.70
1:G:46:ASP:HB2	2:G:201:HOH:O	1.91	0.70
1:C:41:ASP:HB2	1:C:56:GLY:HA3	1.72	0.70
1:B:125:GLY:HA3	1:B:126:ASN:C	2.12	0.69
1:C:135:ASN:O	1:C:135:ASN:ND2	2.24	0.69
1:B:42:GLN:O	1:B:43:GLN:HB3	1.91	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:VAL:HG13	1:C:67:ILE:HB	1.75	0.68
1:F:28:VAL:N	1:F:98:MET:O	2.27	0.68
1:F:136:ILE:HG12	1:G:43:GLN:HE21	1.59	0.68
1:B:29:THR:HB	1:B:100:ASP:HB3	1.77	0.67
1:D:160:VAL:HG12	1:D:161:THR:N	2.10	0.67
1:B:76:ARG:HB2	2:B:203:HOH:O	1.94	0.66
1:E:42:GLN:O	1:E:43:GLN:HB3	1.95	0.65
1:A:143:TYR:CE1	1:A:145:VAL:HA	2.32	0.64
1:A:143:TYR:HE1	1:A:145:VAL:HA	1.61	0.64
1:B:150:MET:HG2	1:B:151:GLN:N	2.11	0.63
1:E:131:GLN:HB2	2:E:209:HOH:O	1.96	0.63
1:E:86:ILE:HB	1:E:114:TYR:HB3	1.80	0.63
1:H:111:GLN:HB3	1:H:124:THR:HB	1.82	0.62
1:G:60:VAL:HG13	1:G:67:ILE:HB	1.82	0.62
1:C:95:PHE:HB2	1:C:112:MET:CE	2.31	0.61
1:F:98:MET:CA	1:F:99:GLN:CB	2.77	0.60
1:H:110:SER:HB2	1:H:125:GLY:HA3	1.83	0.60
1:G:112:MET:SD	1:G:123:LEU:HD22	2.42	0.60
1:G:58:VAL:HG11	1:G:72:VAL:HG21	1.84	0.59
1:F:52:VAL:HG13	1:F:74:VAL:HG13	1.83	0.59
1:A:92:PRO:HB2	1:A:108:HIS:HB2	1.85	0.58
1:E:154:SER:HB3	1:E:160:VAL:HG23	1.84	0.58
1:E:117:ALA:H	1:E:118:LYS:CB	2.17	0.57
1:F:136:ILE:HG12	1:G:43:GLN:NE2	2.18	0.57
1:A:98:MET:HA	1:A:98:MET:CE	2.35	0.56
1:A:132:VAL:HA	1:A:133:ASP:C	2.24	0.56
1:F:76:ARG:HG2	2:F:201:HOH:O	2.05	0.56
1:D:97:GLN:HE21	1:D:98:MET:H	1.53	0.56
1:F:65:ILE:HG12	1:F:97:GLN:HG3	1.86	0.56
1:F:111:GLN:HB3	1:F:124:THR:HB	1.87	0.56
1:F:59:ILE:O	1:F:59:ILE:HG22	2.06	0.56
1:B:106:GLU:HB3	1:B:130:GLN:HB3	1.87	0.56
1:A:60:VAL:HG13	1:A:67:ILE:HB	1.88	0.56
1:A:113:HIS:HB3	1:A:122:VAL:HB	1.89	0.55
1:G:128:TYR:HE2	1:G:130:GLN:HE21	1.54	0.54
1:H:40:SER:HB3	1:H:58:VAL:HG13	1.90	0.54
1:D:160:VAL:CG1	1:D:161:THR:H	2.19	0.54
1:E:101:ASN:N	1:E:101:ASN:HD22	2.06	0.54
1:E:152:ALA:HB3	1:F:43:GLN:HG3	1.89	0.54
1:C:29:THR:N	1:C:100:ASP:OD2	2.40	0.53
1:B:62:GLN:HE21	1:B:65:ILE:HD12	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:ASN:HD22	1:B:135:ASN:C	2.12	0.53
1:B:67:ILE:C	1:B:68:ASN:HD22	2.12	0.53
1:E:41:ASP:HB2	1:E:56:GLY:HA3	1.90	0.53
1:E:65:ILE:HG22	1:E:66:LYS:N	2.22	0.53
1:E:60:VAL:HG13	1:E:67:ILE:HB	1.89	0.53
1:A:105:VAL:HG22	1:A:131:GLN:HG3	1.92	0.52
1:B:128:TYR:CD2	1:B:128:TYR:C	2.82	0.52
1:B:143:TYR:CZ	1:B:145:VAL:HA	2.45	0.52
1:C:135:ASN:HD22	1:C:135:ASN:C	2.14	0.51
1:D:36:ILE:HG23	1:D:62:GLN:HB2	1.90	0.51
1:C:143:TYR:C	1:C:143:TYR:CD1	2.84	0.51
1:F:143:TYR:HD1	1:F:150:MET:HG3	1.75	0.51
1:A:40:SER:HB3	1:A:58:VAL:HG13	1.93	0.51
1:C:45:LEU:HD23	1:C:46:ASP:H	1.76	0.51
1:F:123:LEU:HB3	1:F:127:ALA:HB1	1.92	0.51
1:A:121:VAL:HB	1:A:143:TYR:HB3	1.92	0.50
1:E:164:LEU:HD21	1:F:76:ARG:HH22	1.76	0.50
1:G:150:MET:HE3	1:H:47:MET:SD	2.51	0.50
1:D:130:GLN:HG2	1:D:131:GLN:H	1.76	0.50
1:H:131:GLN:HG3	1:H:132:VAL:H	1.77	0.50
1:D:60:VAL:HG13	1:D:67:ILE:HB	1.93	0.50
1:D:52:VAL:HB	1:D:74:VAL:HG13	1.94	0.50
1:B:106:GLU:HG3	1:B:107:GLY:N	2.26	0.49
1:B:159:ARG:HB2	1:B:159:ARG:HH21	1.77	0.49
1:B:159:ARG:HD3	1:C:39:GLU:HG3	1.93	0.49
1:F:41:ASP:HB2	1:F:56:GLY:HA3	1.94	0.49
1:F:113:HIS:HB3	1:F:122:VAL:HB	1.93	0.49
1:D:107:GLY:O	1:D:108:HIS:HB3	2.13	0.49
1:C:99:GLN:HB2	1:C:103:LYS:O	2.13	0.49
1:H:83:LYS:N	2:H:201:HOH:O	2.46	0.49
1:C:83:LYS:N	1:C:84:GLU:OE2	2.45	0.49
1:F:60:VAL:HG13	1:F:67:ILE:HB	1.93	0.49
1:H:147:GLU:O	1:H:148:GLN:HB2	2.13	0.48
1:F:120:PHE:HE1	1:F:122:VAL:HG23	1.79	0.48
1:B:83:LYS:HA	1:B:117:ALA:HB2	1.96	0.48
1:F:97:GLN:HG2	1:F:98:MET:N	2.22	0.48
1:C:163:VAL:HA	1:D:36:ILE:O	2.14	0.48
1:G:143:TYR:HD1	1:G:144:LEU:N	2.11	0.48
1:A:135:ASN:HB3	1:A:163:VAL:HG22	1.95	0.48
1:B:101:ASN:O	1:B:103:LYS:N	2.47	0.47
1:C:147:GLU:O	1:C:148:GLN:HB2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:TYR:CZ	1:A:130:GLN:HB2	2.49	0.47
1:D:125:GLY:O	1:D:127:ALA:N	2.47	0.47
1:F:55:THR:OG1	1:F:56:GLY:N	2.48	0.47
1:B:111:GLN:HB3	1:B:124:THR:HB	1.95	0.47
1:D:62:GLN:HE21	1:D:65:ILE:HD12	1.80	0.47
1:H:135:ASN:ND2	1:H:135:ASN:C	2.67	0.47
1:E:101:ASN:HD22	1:E:101:ASN:H	1.62	0.47
1:A:114:TYR:CD2	1:A:114:TYR:C	2.89	0.47
1:B:40:SER:HB2	1:B:58:VAL:HG12	1.97	0.47
1:C:143:TYR:C	1:C:143:TYR:HD1	2.17	0.47
1:D:76:ARG:N	1:D:77:PRO:HD3	2.30	0.47
1:G:53:THR:HG23	1:G:73:VAL:HG22	1.97	0.46
1:C:77:PRO:HD2	1:C:83:LYS:O	2.15	0.46
1:C:122:VAL:HG12	1:C:122:VAL:O	2.15	0.46
1:H:53:THR:HG23	1:H:73:VAL:HG12	1.97	0.46
1:G:41:ASP:HB2	1:G:56:GLY:HA3	1.96	0.46
1:B:52:VAL:HB	1:B:74:VAL:HG13	1.97	0.46
1:B:50:ASN:N	1:B:50:ASN:OD1	2.49	0.46
1:C:113:HIS:HB3	1:C:122:VAL:HB	1.97	0.46
1:D:128:TYR:CD2	1:D:128:TYR:C	2.89	0.46
1:F:72:VAL:HG12	1:F:73:VAL:N	2.31	0.46
1:E:117:ALA:N	1:E:118:LYS:CB	2.78	0.45
1:E:65:ILE:CG2	1:E:66:LYS:N	2.79	0.45
1:F:72:VAL:CG1	1:F:73:VAL:N	2.79	0.45
1:E:128:TYR:HA	1:E:137:LYS:HA	1.97	0.45
1:B:91:LYS:HA	1:B:92:PRO:HA	1.71	0.45
1:F:42:GLN:HB2	1:F:55:THR:HG23	1.99	0.45
1:F:128:TYR:HE2	1:F:135:ASN:HB2	1.82	0.45
1:G:143:TYR:HE1	1:G:148:GLN:HA	1.82	0.45
1:F:135:ASN:O	1:F:136:ILE:HG13	2.17	0.44
1:E:114:TYR:OH	1:E:116:LEU:HD13	2.17	0.44
1:B:113:HIS:HB3	1:B:122:VAL:HB	2.00	0.44
1:A:95:PHE:HB2	1:A:112:MET:HE1	2.00	0.44
1:C:40:SER:HB3	1:C:58:VAL:HG13	2.00	0.44
1:E:52:VAL:HB	1:E:74:VAL:HG23	2.00	0.44
1:F:67:ILE:C	1:F:68:ASN:HD22	2.21	0.44
1:A:98:MET:HA	1:A:98:MET:HE3	2.00	0.44
1:B:135:ASN:C	1:B:135:ASN:ND2	2.70	0.44
1:A:98:MET:HA	1:A:98:MET:HE2	2.00	0.44
1:F:62:GLN:HE22	1:F:116:LEU:HD21	1.83	0.44
1:C:99:GLN:HG2	1:C:105:VAL:HG23	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:ASN:O	1:A:135:ASN:ND2	2.44	0.43
1:A:114:TYR:C	1:A:114:TYR:HD2	2.22	0.43
1:G:52:VAL:HB	1:G:74:VAL:HG13	2.00	0.43
1:E:163:VAL:HG12	1:F:37:HIS:HA	2.01	0.43
1:C:52:VAL:HB	1:C:74:VAL:HG13	2.00	0.43
1:F:120:PHE:CE1	1:F:122:VAL:HG23	2.54	0.43
1:F:96:TYR:CD2	1:F:96:TYR:C	2.92	0.42
1:H:97:GLN:HG3	1:H:98:MET:N	2.34	0.42
1:G:114:TYR:CD2	1:G:114:TYR:C	2.93	0.42
1:A:95:PHE:HB2	1:A:112:MET:CE	2.49	0.42
1:H:128:TYR:HE2	1:H:135:ASN:HB2	1.85	0.42
1:D:38:ILE:N	1:D:38:ILE:HD12	2.34	0.42
1:D:97:GLN:HG3	1:D:98:MET:N	2.33	0.42
1:B:107:GLY:HA2	1:B:129:LEU:HA	2.00	0.42
1:A:135:ASN:CB	1:A:163:VAL:HG22	2.49	0.42
1:B:106:GLU:CG	1:B:107:GLY:H	2.20	0.42
1:C:119:ASP:O	1:C:145:VAL:HG23	2.20	0.42
1:A:68:ASN:HB2	1:A:94:THR:OG1	2.20	0.42
1:C:84:GLU:HB2	1:C:116:LEU:HD12	2.02	0.42
1:D:46:ASP:HB3	1:D:51:VAL:HB	2.02	0.42
1:B:64:THR:HG21	1:B:98:MET:HB3	2.02	0.42
1:C:29:THR:O	1:C:29:THR:HG23	2.19	0.42
1:E:36:ILE:H	1:E:36:ILE:HD12	1.85	0.42
1:F:150:MET:HG2	1:F:151:GLN:N	2.34	0.42
1:B:103:LYS:HA	1:B:104:PRO:HD3	1.84	0.41
1:D:91:LYS:HA	1:D:92:PRO:HA	1.91	0.41
1:E:103:LYS:HA	1:E:104:PRO:HD3	1.90	0.41
1:E:113:HIS:HB3	1:E:122:VAL:HB	2.02	0.41
1:H:54:PHE:CD1	1:H:54:PHE:N	2.87	0.41
1:A:143:TYR:HE1	1:A:145:VAL:CA	2.28	0.41
1:F:57:ASN:HD22	1:F:57:ASN:C	2.24	0.41
1:E:36:ILE:HD12	1:E:36:ILE:N	2.35	0.41
1:H:75:THR:HB	2:H:202:HOH:O	2.20	0.41
1:C:61:THR:HG22	1:C:66:LYS:HG3	2.03	0.41
1:E:95:PHE:CD2	1:E:96:TYR:N	2.89	0.41
1:H:49:GLY:O	1:H:50:ASN:HB2	2.20	0.41
1:H:60:VAL:HG13	1:H:67:ILE:HB	2.02	0.41
1:A:108:HIS:CE1	1:A:128:TYR:HD2	2.39	0.41
1:B:68:ASN:HD22	1:B:68:ASN:N	2.17	0.41
1:E:91:LYS:HA	1:E:92:PRO:HA	1.79	0.41
1:F:130:GLN:HG2	1:F:131:GLN:N	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:86:ILE:HG22	1:H:87:ASP:N	2.36	0.41
1:F:83:LYS:HA	1:F:117:ALA:HB2	2.02	0.40
1:H:160:VAL:HG12	1:H:161:THR:N	2.36	0.40
1:G:114:TYR:C	1:G:114:TYR:HD2	2.25	0.40
1:B:112:MET:SD	1:B:113:HIS:N	2.94	0.40
1:D:52:VAL:HB	1:D:74:VAL:CG1	2.52	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	125/159 (79%)	98 (78%)	23 (18%)	4 (3%)	4 23
1	B	130/159 (82%)	95 (73%)	31 (24%)	4 (3%)	4 24
1	C	131/159 (82%)	117 (89%)	12 (9%)	2 (2%)	10 39
1	D	132/159 (83%)	105 (80%)	19 (14%)	8 (6%)	1 10
1	E	128/159 (80%)	101 (79%)	19 (15%)	8 (6%)	1 9
1	F	128/159 (80%)	100 (78%)	24 (19%)	4 (3%)	4 24
1	G	131/159 (82%)	116 (88%)	14 (11%)	1 (1%)	19 52
1	H	127/159 (80%)	109 (86%)	15 (12%)	3 (2%)	6 28
All	All	1032/1272 (81%)	841 (82%)	157 (15%)	34 (3%)	4 22

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	156	LYS
1	D	77	PRO
1	D	119	ASP
1	E	118	LYS

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Mol	Chain	Res	Type
1	F	99	GLN
1	A	156	LYS
1	B	43	GLN
1	B	102	GLY
1	D	118	LYS
1	D	126	ASN
1	E	50	ASN
1	E	119	ASP
1	E	166	PRO
1	H	50	ASN
1	A	110	SER
1	A	135	ASN
1	B	63	GLY
1	D	117	ALA
1	E	43	GLN
1	H	156	LYS
1	D	76	ARG
1	E	84	GLU
1	F	102	GLY
1	H	148	GLN
1	D	63	GLY
1	F	56	GLY
1	F	125	GLY
1	B	49	GLY
1	D	51	VAL
1	A	56	GLY
1	E	105	VAL
1	E	125	GLY
1	G	125	GLY
1	C	125	GLY

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	88/135 (65%)	77 (88%)	11 (12%)	4 19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	91/135 (67%)	73 (80%)	18 (20%)	1 5
1	C	101/135 (75%)	89 (88%)	12 (12%)	5 20
1	D	82/135 (61%)	72 (88%)	10 (12%)	5 20
1	E	82/135 (61%)	71 (87%)	11 (13%)	4 16
1	F	91/135 (67%)	65 (71%)	26 (29%)	0 1
1	G	98/135 (73%)	85 (87%)	13 (13%)	4 16
1	H	87/135 (64%)	77 (88%)	10 (12%)	5 22
All	All	720/1080 (67%)	609 (85%)	111 (15%)	2 12

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	GLU
1	A	43	GLN
1	A	55	THR
1	A	57	ASN
1	A	76	ARG
1	A	97	GLN
1	A	98	MET
1	A	114	TYR
1	A	116	LEU
1	A	135	ASN
1	A	164	LEU
1	B	43	GLN
1	B	45	LEU
1	B	50	ASN
1	B	60	VAL
1	B	61	THR
1	B	73	VAL
1	B	101	ASN
1	B	112	MET
1	B	119	ASP
1	B	121	VAL
1	B	128	TYR
1	B	131	GLN
1	B	133	ASP
1	B	134	SER
1	B	135	ASN
1	B	147	GLU
1	B	161	THR

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Mol	Chain	Res	Type
1	B	164	LEU
1	C	33	ASP
1	C	39	GLU
1	C	43	GLN
1	C	45	LEU
1	C	74	VAL
1	C	84	GLU
1	C	111	GLN
1	C	112	MET
1	C	119	ASP
1	C	135	ASN
1	C	143	TYR
1	C	144	LEU
1	D	43	GLN
1	D	45	LEU
1	D	60	VAL
1	D	87	ASP
1	D	97	GLN
1	D	100	ASP
1	D	120	PHE
1	D	124	THR
1	D	135	ASN
1	D	144	LEU
1	E	39	GLU
1	E	43	GLN
1	E	50	ASN
1	E	60	VAL
1	E	87	ASP
1	E	97	GLN
1	E	100	ASP
1	E	101	ASN
1	E	131	GLN
1	E	135	ASN
1	E	144	LEU
1	F	31	ASP
1	F	43	GLN
1	F	44	SER
1	F	45	LEU
1	F	55	THR
1	F	57	ASN
1	F	58	VAL
1	F	60	VAL

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Mol	Chain	Res	Type
1	F	61	THR
1	F	73	VAL
1	F	74	VAL
1	F	98	MET
1	F	100	ASP
1	F	106	GLU
1	F	112	MET
1	F	114	TYR
1	F	119	ASP
1	F	121	VAL
1	F	123	LEU
1	F	126	ASN
1	F	128	TYR
1	F	131	GLN
1	F	133	ASP
1	F	144	LEU
1	F	147	GLU
1	F	164	LEU
1	G	33	ASP
1	G	43	GLN
1	G	52	VAL
1	G	60	VAL
1	G	74	VAL
1	G	75	THR
1	G	112	MET
1	G	114	TYR
1	G	120	PHE
1	G	124	THR
1	G	135	ASN
1	G	143	TYR
1	G	144	LEU
1	H	38	ILE
1	H	43	GLN
1	H	45	LEU
1	H	54	PHE
1	H	60	VAL
1	H	68	ASN
1	H	74	VAL
1	H	128	TYR
1	H	135	ASN
1	H	144	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	A	68	ASN
1	A	101	ASN
1	A	108	HIS
1	A	131	GLN
1	B	42	GLN
1	B	62	GLN
1	B	68	ASN
1	B	130	GLN
1	B	135	ASN
1	B	148	GLN
1	C	42	GLN
1	C	50	ASN
1	C	57	ASN
1	C	62	GLN
1	C	108	HIS
1	C	113	HIS
1	C	148	GLN
1	D	62	GLN
1	D	97	GLN
1	D	101	ASN
1	D	130	GLN
1	E	62	GLN
1	E	68	ASN
1	E	101	ASN
1	F	57	ASN
1	F	62	GLN
1	F	68	ASN
1	F	108	HIS
1	G	42	GLN
1	G	62	GLN
1	G	130	GLN
1	G	135	ASN
1	H	50	ASN
1	H	62	GLN
1	H	68	ASN
1	H	130	GLN
1	H	131	GLN

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

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	131/159 (82%)	-0.06	1 (0%)	86	86	44, 64, 75, 77	0
1	B	134/159 (84%)	0.08	3 (2%)	62	59	54, 63, 74, 80	0
1	C	135/159 (84%)	-0.21	1 (0%)	87	88	32, 41, 61, 65	0
1	D	136/159 (85%)	-0.03	1 (0%)	87	88	46, 69, 76, 78	0
1	E	132/159 (83%)	0.11	2 (1%)	73	71	63, 71, 77, 80	0
1	F	132/159 (83%)	0.03	6 (4%)	33	31	46, 58, 68, 70	0
1	G	135/159 (84%)	-0.20	0	100	100	34, 46, 58, 60	0
1	H	131/159 (82%)	-0.09	3 (2%)	60	58	35, 54, 68, 71	0
All	All	1066/1272 (83%)	-0.05	17 (1%)	72	69	32, 60, 75, 80	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	77	PRO	3.6
1	F	49	GLY	2.6
1	H	155	ASP	2.6
1	F	155	ASP	2.5
1	B	77	PRO	2.4
1	H	156	LYS	2.3
1	E	101	ASN	2.3
1	F	154	SER	2.3
1	F	157	GLY	2.2
1	F	158	LYS	2.1
1	F	159	ARG	2.1
1	C	77	PRO	2.1
1	H	157	GLY	2.1
1	B	78	GLY	2.0
1	D	98	MET	2.0
1	E	102	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	132	VAL	2.0

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

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

6.3 Carbohydrates (i)

There are no 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.