Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2023 – 12:34 pm GMT

PDB ID	:	8C7L
Title	:	Serendipitous structure of OmpF contaminant in space group P21.
Authors	:	Bloch, Y.; Theunissen, S.; Savvides, S.N.
Deposited on	:	2023-01-16
Resolution	:	3.52 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:

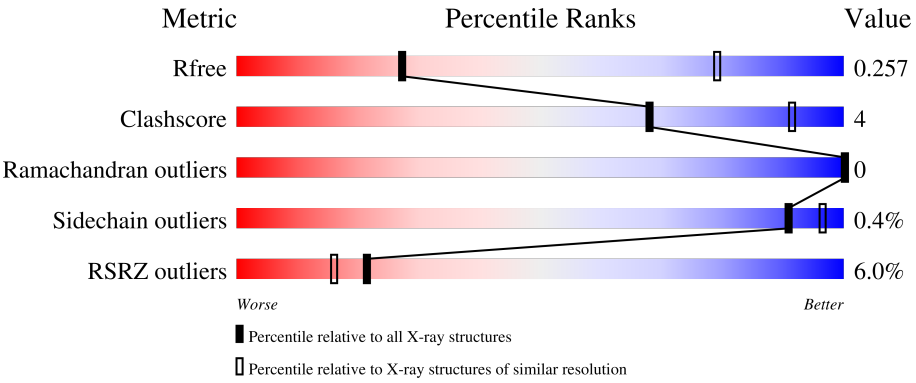
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.32.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

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 3.52 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	1161 (3.60-3.44)
Clashscore	141614	1244 (3.60-3.44)
Ramachandran outliers	138981	1206 (3.60-3.44)
Sidechain outliers	138945	1207 (3.60-3.44)
RSRZ outliers	127900	1080 (3.60-3.44)

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	362	8% 83% 11% 6%
1	B	362	5% 85% 9% 6%
1	C	362	3% 85% 9% 6%
1	D	362	7% 86% 8% 6%
1	E	362	6% 86% 8% 6%

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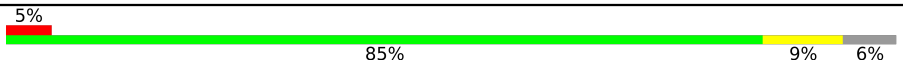
Mol	Chain	Length	Quality of chain
1	F	362	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 15894 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 Outer membrane porin F.

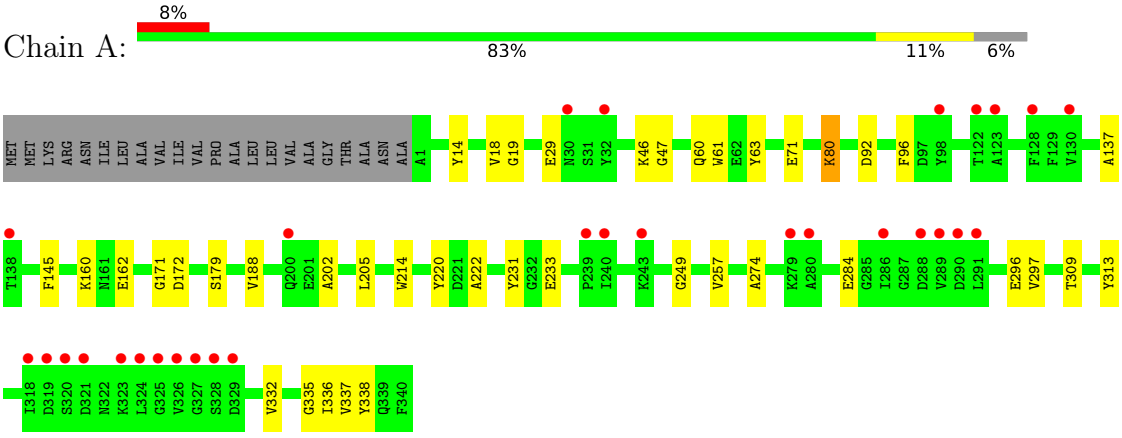
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	0	7	0
			2649	1671	438	537	3			
1	B	340	Total	C	N	O	S	0	7	0
			2649	1671	438	537	3			
1	C	340	Total	C	N	O	S	0	7	0
			2649	1671	438	537	3			
1	D	340	Total	C	N	O	S	0	7	0
			2649	1671	438	537	3			
1	E	340	Total	C	N	O	S	0	7	0
			2649	1671	438	537	3			
1	F	340	Total	C	N	O	S	0	7	0
			2649	1671	438	537	3			

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.

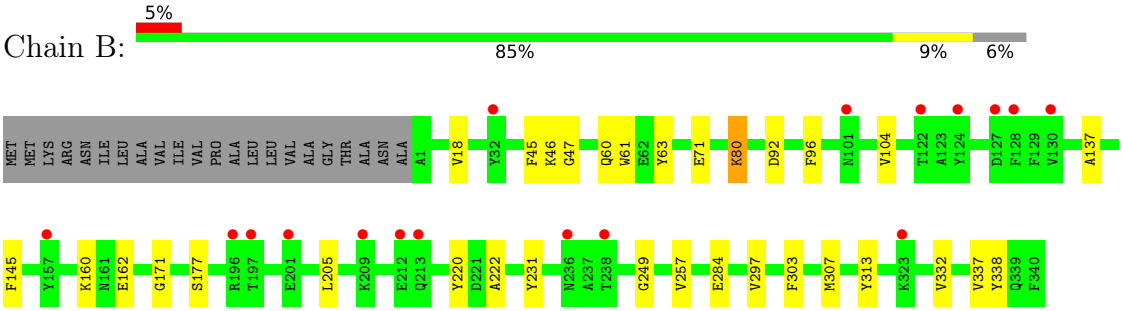
• Molecule 1: Outer membrane porin F

Chain A:



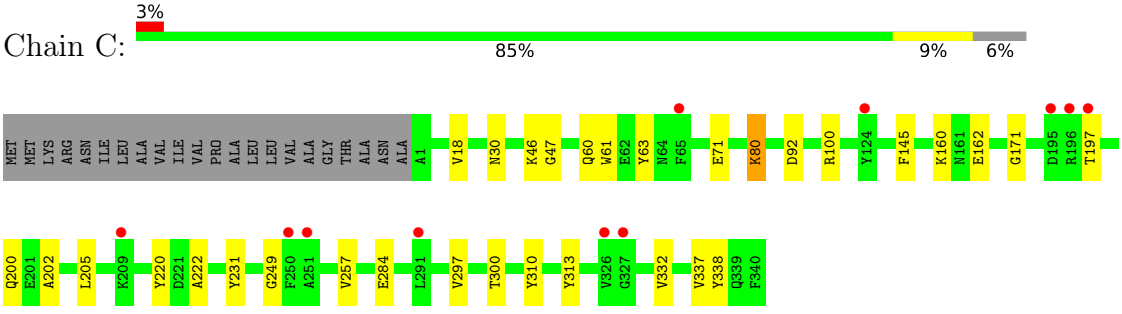
• Molecule 1: Outer membrane porin F

Chain B:



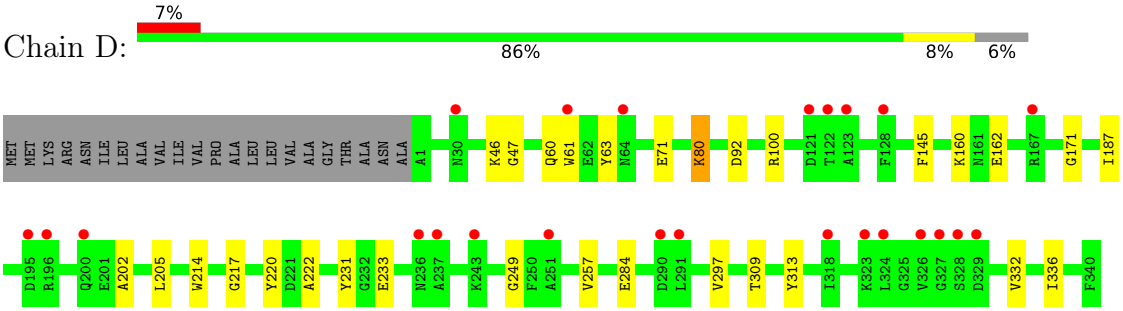
• Molecule 1: Outer membrane porin F

Chain C:



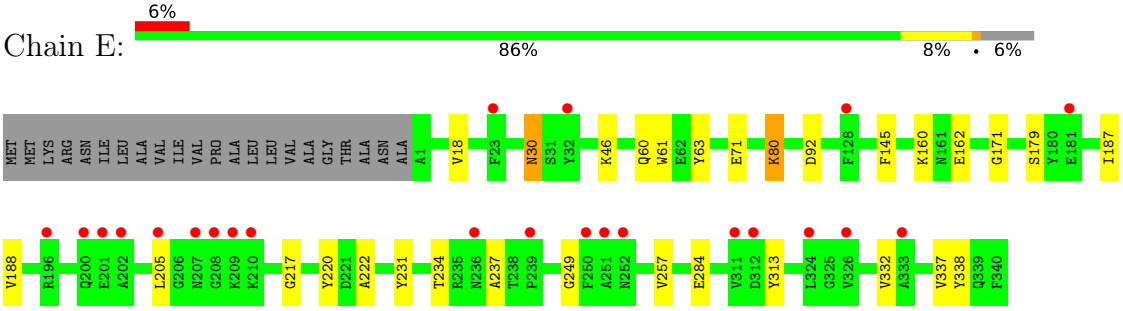
• Molecule 1: Outer membrane porin F

Chain D:



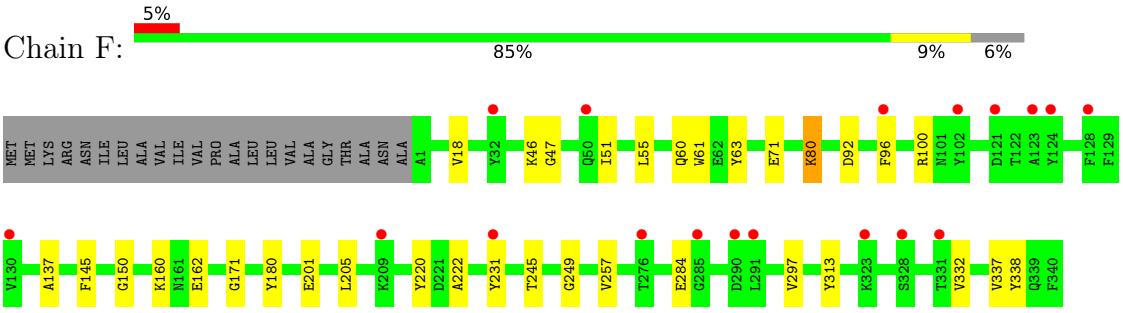
• Molecule 1: Outer membrane porin F

Chain E:



• Molecule 1: Outer membrane porin F

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	104.81Å 151.00Å 109.66Å 90.00° 117.94° 90.00°	Depositor
Resolution (Å)	92.60 – 3.52 92.60 – 3.51	Depositor EDS
% Data completeness (in resolution range)	98.6 (92.60-3.52) 99.4 (92.60-3.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.00 (at 3.49Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.234 , 0.255 0.235 , 0.257	Depositor DCC
R_{free} test set	1779 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å^2)	98.5	Xtriage
Anisotropy	0.388	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 37.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.053 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.83	EDS
Total number of atoms	15894	wwPDB-VP
Average B, all atoms (Å^2)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.74% 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	0.27	0/2733	0.56	0/3698
1	B	0.28	0/2733	0.55	0/3698
1	C	0.28	0/2733	0.56	0/3698
1	D	0.27	0/2733	0.56	0/3698
1	E	0.28	0/2733	0.55	0/3698
1	F	0.27	0/2733	0.55	0/3698
All	All	0.28	0/16398	0.55	0/22188

There are no bond length outliers.

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	2649	0	2468	27	0
1	B	2649	0	2468	21	0
1	C	2649	0	2468	21	0
1	D	2649	0	2468	21	0
1	E	2649	0	2468	20	0
1	F	2649	0	2468	26	0
All	All	15894	0	14808	117	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 4.

All (117) 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:71:GLU:HG2	1:C:80:LYS:HG3	1.64	0.78
1:E:30:ASN:O	1:E:30:ASN:ND2	2.19	0.76
1:E:71:GLU:HG2	1:F:80:LYS:HG3	1.67	0.75
1:A:160:LYS:HG3	1:A:171:GLY:HA2	1.69	0.75
1:B:80:LYS:HG3	1:C:71:GLU:HG2	1.71	0.73
1:D:80:LYS:HG3	1:F:71:GLU:HG2	1.70	0.73
1:B:160:LYS:HG3	1:B:171:GLY:HA2	1.70	0.72
1:A:80:LYS:HG3	1:B:71:GLU:HG2	1.70	0.72
1:D:71:GLU:HG2	1:E:80:LYS:HG3	1.73	0.71
1:F:160:LYS:HG3	1:F:171:GLY:HA2	1.73	0.70
1:B:160:LYS:HE2	1:B:162:GLU:HG3	1.78	0.65
1:D:160:LYS:HG3	1:D:171:GLY:HA2	1.78	0.65
1:E:160:LYS:HG3	1:E:171:GLY:HA2	1.82	0.62
1:E:160:LYS:HE2	1:E:162:GLU:HG3	1.83	0.60
1:F:160:LYS:HE2	1:F:162:GLU:HG3	1.85	0.59
1:C:160:LYS:HE2	1:C:162:GLU:HG3	1.85	0.58
1:C:313:TYR:CD1	1:C:332:VAL:HG22	2.39	0.57
1:D:313:TYR:CD1	1:D:332:VAL:HG22	2.40	0.57
1:A:202:ALA:HB2	1:D:202:ALA:HB2	1.86	0.57
1:D:160:LYS:HE2	1:D:162:GLU:HG3	1.87	0.57
1:A:284:GLU:H	1:A:284:GLU:CD	2.08	0.56
1:C:160:LYS:HG3	1:C:171:GLY:HA2	1.86	0.56
1:B:313:TYR:CD1	1:B:332:VAL:HG22	2.40	0.56
1:F:313:TYR:CD1	1:F:332:VAL:HG22	2.40	0.56
1:F:284:GLU:H	1:F:284:GLU:CD	2.08	0.56
1:E:313:TYR:CD1	1:E:332:VAL:HG22	2.40	0.56
1:F:205:LEU:HB2	1:F:249:GLY:HA3	1.88	0.54
1:A:205:LEU:HB2	1:A:249:GLY:HA3	1.90	0.54
1:A:160:LYS:HE2	1:A:162:GLU:HG3	1.90	0.54
1:E:284:GLU:H	1:E:284:GLU:CD	2.11	0.54
1:B:284:GLU:H	1:B:284:GLU:CD	2.11	0.54
1:A:220:TYR:CZ	1:A:222:ALA:HB3	2.44	0.52
1:C:18:VAL:HG22	1:C:337:VAL:HG22	1.90	0.52
1:C:61:TRP:CZ2	1:C:63:TYR:HB2	2.45	0.52
1:E:18:VAL:HG22	1:E:337:VAL:HG22	1.92	0.52
1:D:205:LEU:HB2	1:D:249:GLY:HA3	1.92	0.52
1:D:309[A]:THR:HG22	1:D:336:ILE:HG13	1.90	0.52
1:B:205:LEU:HB2	1:B:249:GLY:HA3	1.91	0.51
1:B:61:TRP:CZ2	1:B:63:TYR:HB2	2.45	0.51
1:A:313:TYR:CD1	1:A:332:VAL:HG22	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:284:GLU:H	1:C:284:GLU:CD	2.14	0.51
1:D:220:TYR:CZ	1:D:222:ALA:HB3	2.45	0.50
1:A:46:LYS:HG2	1:A:60:GLN:HG3	1.94	0.50
1:C:220:TYR:CZ	1:C:222:ALA:HB3	2.47	0.50
1:B:220:TYR:CZ	1:B:222:ALA:HB3	2.47	0.50
1:D:284:GLU:CD	1:D:284:GLU:H	2.13	0.50
1:E:205:LEU:HB2	1:E:249:GLY:HA3	1.93	0.49
1:B:303:PHE:HB2	1:B:307:MET:HB3	1.95	0.49
1:A:92:ASP:O	1:A:145:PHE:HA	2.12	0.49
1:C:92:ASP:O	1:C:145:PHE:HA	2.12	0.49
1:E:220:TYR:CZ	1:E:222:ALA:HB3	2.48	0.49
1:F:220:TYR:CZ	1:F:222:ALA:HB3	2.48	0.49
1:E:179:SER:HB3	1:E:188:VAL:HG23	1.95	0.49
1:C:46:LYS:HG2	1:C:60:GLN:HG3	1.95	0.48
1:E:338:TYR:CE2	1:F:47:GLY:HA3	2.48	0.48
1:E:92:ASP:O	1:E:145:PHE:HA	2.12	0.48
1:B:92:ASP:O	1:B:145:PHE:HA	2.14	0.47
1:D:100:ARG:NH2	1:F:71:GLU:HG3	2.29	0.47
1:A:29:GLU:OE1	1:F:245:THR:HG22	2.14	0.47
1:C:231:TYR:HD1	1:C:257[A]:VAL:HG22	1.80	0.47
1:E:71:GLU:HG3	1:F:100:ARG:NH2	2.30	0.47
1:F:96:PHE:CE1	1:F:137:ALA:HB1	2.50	0.47
1:B:46:LYS:HG2	1:B:60:GLN:HG3	1.97	0.47
1:C:30:ASN:OD1	1:C:30:ASN:O	2.32	0.47
1:D:46:LYS:HG2	1:D:60:GLN:HG3	1.97	0.47
1:E:61:TRP:CZ2	1:E:63:TYR:HB2	2.50	0.47
1:B:96:PHE:CE1	1:B:137:ALA:HB1	2.50	0.46
1:F:92:ASP:O	1:F:145:PHE:HA	2.16	0.46
1:C:202:ALA:HB1	1:F:201:GLU:O	2.15	0.46
1:C:205:LEU:HB2	1:C:249:GLY:HA3	1.96	0.46
1:A:309[A]:THR:HG22	1:A:336:ILE:HG13	1.98	0.46
1:B:18:VAL:HG22	1:B:337:VAL:HG22	1.98	0.46
1:D:92:ASP:O	1:D:145:PHE:HA	2.16	0.46
1:F:46:LYS:HG2	1:F:60:GLN:HG3	1.98	0.46
1:B:297[B]:VAL:HG13	1:B:313:TYR:HB3	1.98	0.45
1:E:338:TYR:CZ	1:F:47:GLY:HA3	2.51	0.45
1:C:197:THR:OG1	1:C:200:GLN:HG3	2.16	0.45
1:A:61:TRP:CZ2	1:A:63:TYR:HB2	2.52	0.45
1:A:231:TYR:HD1	1:A:257[A]:VAL:HG22	1.82	0.45
1:A:338:TYR:CZ	1:C:47:GLY:HA3	2.52	0.45
1:B:47:GLY:HA3	1:C:338:TYR:CE2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:231:TYR:HD1	1:E:257[A]:VAL:HG22	1.83	0.44
1:D:231:TYR:HD1	1:D:257[A]:VAL:HG22	1.82	0.44
1:C:300:THR:HG23	1:C:310:TYR:HB3	1.99	0.44
1:F:18:VAL:HG22	1:F:337:VAL:HG22	2.00	0.44
1:D:61:TRP:CZ2	1:D:63:TYR:HB2	2.53	0.43
1:A:179:SER:HB3	1:A:188:VAL:HG23	2.00	0.43
1:C:297[B]:VAL:HG13	1:C:313:TYR:HB3	1.99	0.43
1:B:231:TYR:HD1	1:B:257[A]:VAL:HG22	1.84	0.43
1:D:47:GLY:HA3	1:F:338:TYR:CE2	2.54	0.42
1:F:231:TYR:HD1	1:F:257[A]:VAL:HG22	1.85	0.42
1:A:274:ALA:HB3	1:A:296:GLU:HB3	2.01	0.42
1:F:61:TRP:CZ2	1:F:63:TYR:HB2	2.53	0.42
1:B:160:LYS:HE2	1:B:162:GLU:CG	2.47	0.42
1:F:160:LYS:HE2	1:F:162:GLU:CG	2.49	0.42
1:D:214:TRP:NE1	1:D:233:GLU:HB2	2.35	0.42
1:D:187:ILE:HA	1:D:217:GLY:O	2.20	0.42
1:A:19:GLY:O	1:A:335:GLY:HA2	2.20	0.42
1:A:18:VAL:HG22	1:A:337:VAL:HG22	2.01	0.41
1:E:46:LYS:HG2	1:E:60:GLN:HG3	2.00	0.41
1:A:160:LYS:N	1:A:172:ASP:OD1	2.53	0.41
1:A:297[B]:VAL:HG13	1:A:313:TYR:HB3	2.01	0.41
1:D:297[B]:VAL:HG13	1:D:313:TYR:HB3	2.02	0.41
1:D:47:GLY:HA3	1:F:338:TYR:CZ	2.55	0.41
1:E:187:ILE:HA	1:E:217:GLY:O	2.21	0.41
1:A:214:TRP:NE1	1:A:233:GLU:HB2	2.35	0.41
1:E:234:THR:HB	1:E:237:ALA:HB3	2.01	0.41
1:B:104:VAL:HG22	1:B:177:SER:HB3	2.03	0.41
1:D:160:LYS:HE2	1:D:162:GLU:CG	2.51	0.41
1:A:47:GLY:HA3	1:B:338:TYR:CZ	2.56	0.40
1:F:297[B]:VAL:HG13	1:F:313:TYR:HB3	2.03	0.40
1:A:71:GLU:HG3	1:C:100:ARG:NH2	2.37	0.40
1:F:150:GLY:O	1:F:180:TYR:HA	2.21	0.40
1:A:96:PHE:CE1	1:A:137:ALA:HB1	2.57	0.40
1:A:14:TYR:CE1	1:A:46:LYS:HG3	2.56	0.40
1:F:51:ILE:HD12	1:F:55:LEU:HG	2.03	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	345/362 (95%)	328 (95%)	17 (5%)	0	100	100
1	B	345/362 (95%)	328 (95%)	17 (5%)	0	100	100
1	C	345/362 (95%)	328 (95%)	17 (5%)	0	100	100
1	D	345/362 (95%)	328 (95%)	17 (5%)	0	100	100
1	E	345/362 (95%)	328 (95%)	17 (5%)	0	100	100
1	F	345/362 (95%)	328 (95%)	17 (5%)	0	100	100
All	All	2070/2172 (95%)	1968 (95%)	102 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	270/279 (97%)	269 (100%)	1 (0%)	91	96
1	B	270/279 (97%)	269 (100%)	1 (0%)	91	96
1	C	270/279 (97%)	269 (100%)	1 (0%)	91	96
1	D	270/279 (97%)	269 (100%)	1 (0%)	91	96
1	E	270/279 (97%)	268 (99%)	2 (1%)	84	93
1	F	270/279 (97%)	269 (100%)	1 (0%)	91	96
All	All	1620/1674 (97%)	1613 (100%)	7 (0%)	91	96

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	LYS
1	B	80	LYS
1	C	80	LYS
1	D	80	LYS
1	E	30	ASN
1	E	80	LYS
1	F	80	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	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

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	340/362 (93%)	0.45	30 (8%) 10 8	41, 82, 124, 181	0
1	B	340/362 (93%)	0.33	17 (5%) 28 21	43, 88, 119, 145	0
1	C	340/362 (93%)	0.29	11 (3%) 47 36	42, 73, 104, 134	0
1	D	340/362 (93%)	0.39	24 (7%) 16 13	40, 81, 113, 179	0
1	E	340/362 (93%)	0.41	23 (6%) 17 14	40, 76, 111, 158	0
1	F	340/362 (93%)	0.38	18 (5%) 26 20	43, 84, 114, 150	0
All	All	2040/2172 (93%)	0.38	123 (6%) 21 16	40, 81, 115, 181	0

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	290	ASP	9.2
1	E	196	ARG	5.3
1	A	319	ASP	4.9
1	A	291	LEU	4.7
1	B	209	LYS	4.5
1	A	327	GLY	4.4
1	A	289	VAL	4.3
1	A	243	LYS	4.3
1	D	243	LYS	4.2
1	A	320	SER	4.0
1	C	326	VAL	4.0
1	F	291	LEU	3.8
1	D	291	LEU	3.8
1	D	329	ASP	3.8
1	E	312	ASP	3.7
1	A	318	ILE	3.7
1	E	209	LYS	3.6
1	E	236	ASN	3.6
1	D	122	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	E	205	LEU	3.4
1	A	128	PHE	3.4
1	F	124	TYR	3.4
1	A	122	THR	3.3
1	F	121	ASP	3.3
1	B	101	ASN	3.3
1	B	130	VAL	3.3
1	D	327	GLY	3.2
1	D	237	ALA	3.2
1	B	213	GLN	3.2
1	C	291	LEU	3.1
1	C	327	GLY	3.1
1	D	326	VAL	3.1
1	E	250	PHE	3.1
1	A	321	ASP	3.1
1	A	326	VAL	3.0
1	E	181	GLU	3.0
1	A	32	TYR	2.9
1	B	212	GLU	2.9
1	A	324	LEU	2.9
1	E	251	ALA	2.9
1	F	276	THR	2.8
1	A	288	ASP	2.8
1	E	32	TYR	2.8
1	C	196	ARG	2.7
1	D	318	ILE	2.7
1	E	207	ASN	2.7
1	E	128	PHE	2.7
1	C	124	TYR	2.7
1	D	128	PHE	2.7
1	B	122	THR	2.7
1	F	128	PHE	2.7
1	E	200	GLN	2.7
1	E	208	GLY	2.7
1	D	251	ALA	2.6
1	C	197	THR	2.6
1	E	202	ALA	2.6
1	F	123	ALA	2.6
1	D	324	LEU	2.6
1	A	323	LYS	2.6
1	C	251	ALA	2.6
1	F	290	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	236	ASN	2.6
1	D	236	ASN	2.6
1	D	195	ASP	2.6
1	D	323	LYS	2.6
1	B	196	ARG	2.6
1	D	328	SER	2.6
1	E	201	GLU	2.5
1	A	328	SER	2.5
1	F	32	TYR	2.5
1	F	130	VAL	2.5
1	B	157	TYR	2.5
1	E	23	PHE	2.5
1	F	231	TYR	2.5
1	F	209	LYS	2.5
1	F	50	GLN	2.5
1	E	210	LYS	2.5
1	D	200	GLN	2.4
1	D	196	ARG	2.4
1	B	128	PHE	2.4
1	A	280	ALA	2.4
1	A	138	THR	2.4
1	A	30	ASN	2.3
1	F	328	SER	2.3
1	B	238	THR	2.3
1	E	311	VAL	2.3
1	A	240	ILE	2.3
1	D	30	ASN	2.3
1	D	123	ALA	2.3
1	D	61	TRP	2.3
1	B	127	ASP	2.3
1	A	325	GLY	2.2
1	A	329	ASP	2.2
1	D	290	ASP	2.2
1	A	200	GLN	2.2
1	F	331	THR	2.2
1	E	252	ASN	2.2
1	C	195	ASP	2.2
1	D	64	ASN	2.2
1	B	323	LYS	2.2
1	C	250	PHE	2.2
1	B	32	TYR	2.1
1	F	323	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	279	LYS	2.1
1	A	286	ILE	2.1
1	D	167	ARG	2.1
1	A	130	VAL	2.1
1	B	197	THR	2.1
1	E	333	ALA	2.1
1	F	102	TYR	2.1
1	E	326	VAL	2.1
1	D	121	ASP	2.1
1	C	65	PHE	2.1
1	B	124	TYR	2.1
1	F	285	GLY	2.0
1	F	96	PHE	2.0
1	A	98	TYR	2.0
1	B	201	GLU	2.0
1	A	123	ALA	2.0
1	A	239	PRO	2.0
1	E	239	PRO	2.0
1	C	209	LYS	2.0
1	E	324	LEU	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.