Full wwPDB X-ray Structure Validation Report (i)

Sep 27, 2023 – 12:16 PM EDT

PDB ID	:	1DEE
Title	:	Structure of S. aureus protein A bound to a human IgM Fab
Authors	:	Graille, M.; Stura, E.A.; Corper, A.L.; Sutton, B.J.; Taussig, M.J.; Charbonnier, J.B.; Silverman, G.J.
Deposited on	:	1999-11-15
Resolution	:	2.70 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 (i) 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 (1)) were used in the production of this report:

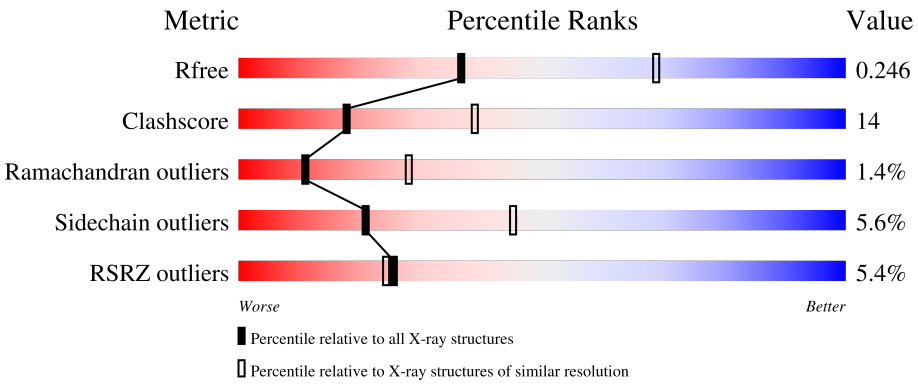
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	214	71% 25% ·
1	C	214	7% 66% 32% ·
1	E	214	64% 34% ·
2	B	223	5% 68% 30% ·
2	D	223	15% 63% 35% ·

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Mol	Chain	Length	Quality of chain
2	F	223	5% 67% 32%
3	G	54	6% 74% 19% 6%
3	H	54	6% 67% 28%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10859 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 IGM RF 2A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	214	1640	1021	276	337	6	0	0	0
1	C	214	1640	1021	276	337	6	0	0	0
1	E	214	1640	1021	276	337	6	0	0	0

- Molecule 2 is a protein called IGM RF 2A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	223	1701	1071	290	333	7	0	0	0
2	D	223	1701	1071	290	333	7	0	0	0
2	F	223	1701	1071	290	333	7	0	0	0

- Molecule 3 is a protein called IMMUNOGLOBULIN G BINDING PROTEIN A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	G	51	401	245	70	85	1	0	0	0
3	H	54	425	261	74	89	1	0	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	3	3	3	0	0
4	B	4	4	4	0	0

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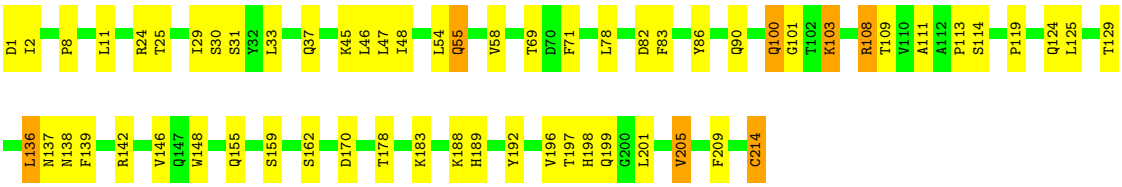
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	D	1	1	1	0	0
			Total	O		
4	F	2	2	2	0	0

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.

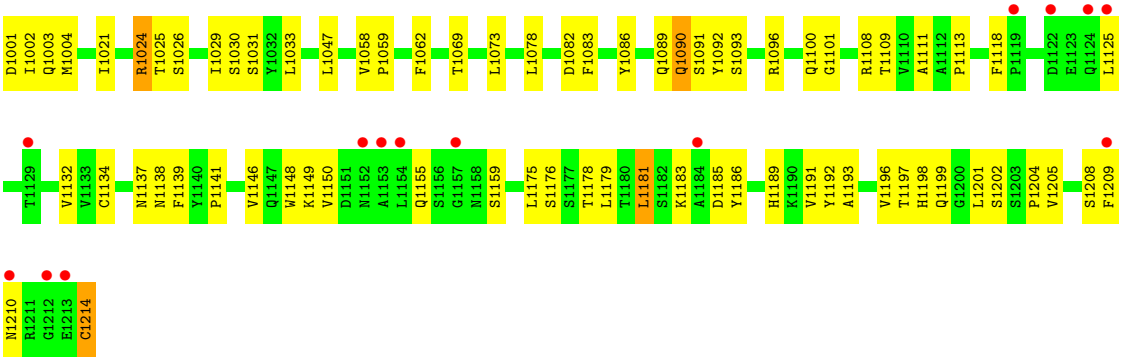
• Molecule 1: IGM RF 2A2

Chain A:



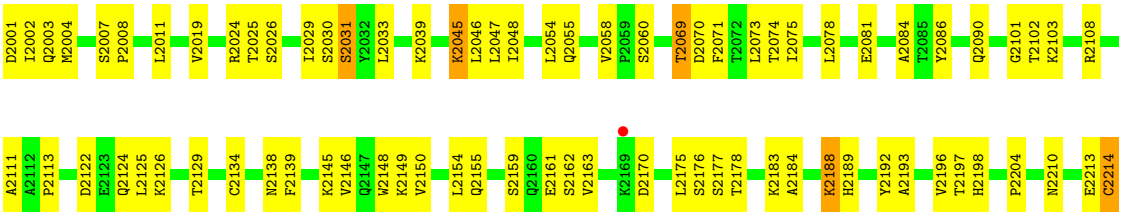
• Molecule 1: IGM RF 2A2

Chain C:



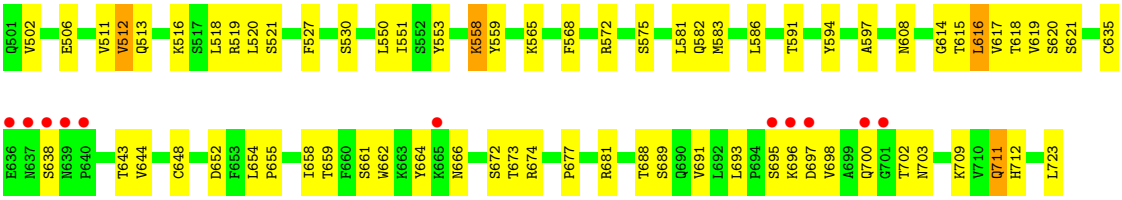
• Molecule 1: IGM RF 2A2

Chain E:



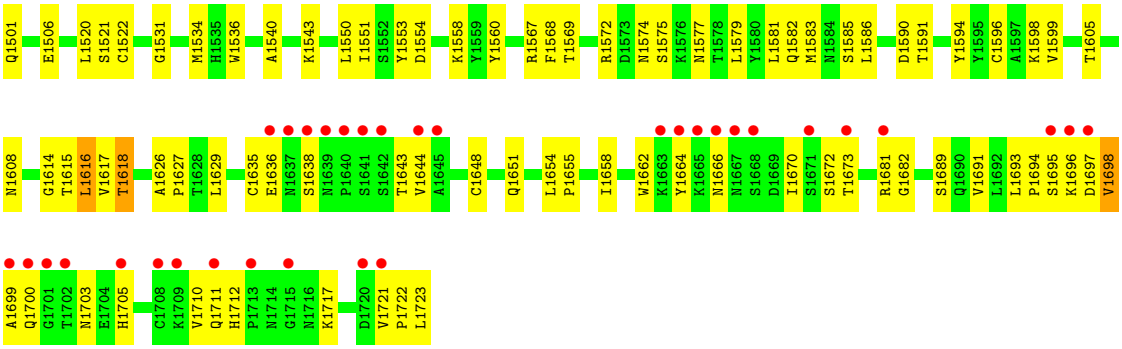
• Molecule 2: IGM RF 2A2

Chain B:



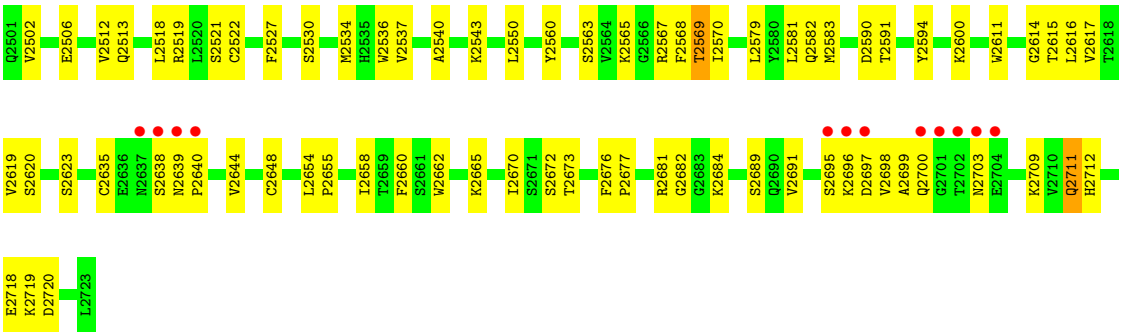
• Molecule 2: IGM RF 2A2

Chain D:



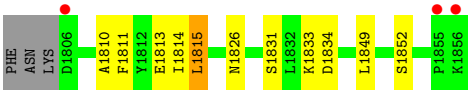
• Molecule 2: IGM RF 2A2

Chain F:



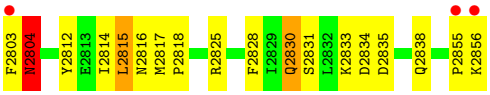
• Molecule 3: IMMUNOGLOBULIN G BINDING PROTEIN A

Chain G:



• Molecule 3: IMMUNOGLOBULIN G BINDING PROTEIN A

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	68.52Å 78.91Å 163.24Å 90.00° 100.71° 90.00°	Depositor
Resolution (Å)	10.00 – 2.70 19.96 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.70) 78.7 (19.96-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.25 (at 2.50Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.217 , 0.281 0.192 , 0.246	Depositor DCC
R_{free} test set	2328 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	51.4	Xtriage
Anisotropy	0.419	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 65.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.021 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10859	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% 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 (i)

5.1 Standard geometry (i)

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	0.44	0/1674	0.74	1/2270 (0.0%)
1	C	0.41	0/1674	0.69	0/2270
1	E	0.39	0/1674	0.70	1/2270 (0.0%)
2	B	0.41	0/1742	0.64	0/2367
2	D	0.40	0/1742	0.65	0/2367
2	F	0.37	0/1742	0.62	0/2367
3	G	0.34	0/406	0.55	0/545
3	H	0.36	0/431	0.61	0/579
All	All	0.40	0/11085	0.67	2/15035 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	11	LEU	CA-CB-CG	6.52	130.29	115.30
1	E	2011	LEU	CA-CB-CG	5.32	127.54	115.30

There are no chirality outliers.

There are no planarity outliers.

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	1640	0	1594	40	0
1	C	1640	0	1591	50	0
1	E	1640	0	1591	53	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1701	0	1648	49	0
2	D	1701	0	1648	51	0
2	F	1701	0	1648	47	0
3	G	401	0	385	8	0
3	H	425	0	402	14	0
4	A	3	0	0	0	0
4	B	4	0	0	0	0
4	D	1	0	0	0	0
4	F	2	0	0	0	0
All	All	10859	0	10507	288	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 (288) 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)
2:F:2569:THR:HG21	3:H:2831:SER:HA	1.53	0.89
1:C:1214:CYS:HG	2:D:1635:CYS:HG	1.10	0.86
1:E:2214:CYS:HG	2:F:2635:CYS:HG	1.21	0.85
2:F:2569:THR:HG22	2:F:2582:GLN:HB3	1.60	0.83
1:C:1146:VAL:HG12	1:C:1196:VAL:HG22	1.60	0.82
2:F:2654:LEU:HD12	2:F:2655:PRO:HA	1.64	0.80
1:E:2214:CYS:HB3	2:F:2635:CYS:SG	2.22	0.79
2:B:558:LYS:NZ	2:B:558:LYS:HB3	2.00	0.77
1:C:1209:PHE:HB2	2:D:1635:CYS:SG	2.25	0.77
1:A:214:CYS:CB	2:B:635:CYS:HG	1.99	0.76
1:A:214:CYS:HB3	2:B:635:CYS:SG	2.25	0.75
2:B:654:LEU:HD12	2:B:655:PRO:HA	1.68	0.75
2:D:1626:ALA:HA	2:D:1712:HIS:HD2	1.49	0.75
1:A:201:LEU:HD13	1:A:205:VAL:HG13	1.69	0.74
1:A:214:CYS:CB	2:B:635:CYS:SG	2.78	0.72
2:D:1520:LEU:HD12	2:D:1581:LEU:HD23	1.71	0.72
1:A:199:GLN:HA	2:D:1501:GLN:HA	1.70	0.72
1:C:1108:ARG:HG2	1:C:1109:THR:N	2.06	0.70
1:E:2003:GLN:HB2	1:E:2026:SER:HB3	1.73	0.70
2:B:558:LYS:HB3	2:B:558:LYS:HZ3	1.56	0.70
1:C:1047:LEU:HA	1:C:1058:VAL:HG21	1.74	0.69
1:C:1108:ARG:HG2	1:C:1109:THR:H	1.57	0.69
2:B:583:MET:HB3	2:B:586:LEU:HD21	1.73	0.69
2:F:2673:THR:HG22	2:F:2691:VAL:HG22	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2214:CYS:CB	2:F:2635:CYS:SG	2.82	0.68
2:D:1626:ALA:HA	2:D:1712:HIS:CD2	2.28	0.68
2:F:2519:ARG:HH11	2:F:2582:GLN:HE21	1.40	0.68
1:A:214:CYS:HG	2:B:635:CYS:HG	0.69	0.67
1:E:2108:ARG:NH2	1:E:2111:ALA:HB2	2.09	0.67
2:B:550:LEU:HD11	2:B:559:TYR:HD2	1.59	0.66
2:D:1662:TRP:HB3	2:D:1670:ILE:HD12	1.78	0.65
2:B:520:LEU:HG	2:B:583:MET:CE	2.27	0.65
1:E:2214:CYS:CB	2:F:2635:CYS:HG	2.09	0.65
2:F:2662:TRP:HB3	2:F:2670:ILE:HD12	1.79	0.65
2:B:655:PRO:O	2:B:712:HIS:HE1	1.81	0.64
1:E:2108:ARG:HD2	1:E:2170:ASP:O	1.98	0.64
1:E:2108:ARG:HH21	1:E:2111:ALA:HB2	1.63	0.64
2:D:1648:CYS:HB2	2:D:1662:TRP:CZ2	2.33	0.63
1:C:1090:GLN:HE21	1:C:1093:SER:H	1.46	0.63
1:A:124:GLN:HG2	1:A:129:THR:O	1.98	0.62
1:C:1004:MET:SD	1:C:1025:THR:HG22	2.41	0.61
1:C:1091:SER:O	2:D:1605:THR:HA	2.01	0.61
1:E:2048:ILE:HG12	1:E:2054:LEU:HD23	1.82	0.61
1:E:2197:THR:HG22	1:E:2204:PRO:HG3	1.83	0.61
2:B:594:TYR:O	2:B:614:GLY:HA2	2.00	0.60
1:E:2045:LYS:NZ	1:E:2045:LYS:HB3	2.16	0.60
1:E:2146:VAL:HG12	1:E:2196:VAL:HG22	1.83	0.60
3:H:2814:ILE:HD13	3:H:2828:PHE:HB3	1.83	0.60
1:C:1150:VAL:HG23	1:C:1155:GLN:HG3	1.85	0.59
1:C:1197:THR:HG22	1:C:1204:PRO:HB3	1.85	0.59
2:B:502:VAL:HG13	2:B:527:PHE:CD1	2.38	0.59
1:E:2046:LEU:HG	1:E:2055:GLN:HG3	1.85	0.59
1:C:1193:ALA:HA	1:C:1208:SER:HB3	1.84	0.59
2:B:551:ILE:HG13	2:B:558:LYS:HZ3	1.68	0.59
2:D:1703:ASN:O	2:D:1723:LEU:HD12	2.03	0.58
2:B:638:SER:HB2	2:B:644:VAL:HA	1.84	0.58
1:C:1078:LEU:HD22	1:C:1082:ASP:HB2	1.87	0.57
1:A:113:PRO:HB3	1:A:139:PHE:HB3	1.87	0.57
2:B:520:LEU:HD12	2:B:581:LEU:HD23	1.87	0.57
1:E:2055:GLN:HE21	2:F:2600:LYS:HD2	1.69	0.56
1:C:1141:PRO:O	1:C:1198:HIS:HE1	1.88	0.56
1:C:1132:VAL:HB	1:C:1179:LEU:HB3	1.87	0.56
2:B:553:TYR:HA	2:B:572:ARG:NH1	2.21	0.56
2:B:520:LEU:HG	2:B:583:MET:HE2	1.86	0.55
1:A:108:ARG:HD2	1:A:170:ASP:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:519:ARG:HD2	2:B:582:GLN:HE22	1.72	0.55
2:B:591:THR:HG23	2:B:618:THR:HA	1.88	0.55
1:C:1125:LEU:O	1:C:1183:LYS:HD2	2.06	0.55
1:C:1029:ILE:HG21	1:C:1090:GLN:HG3	1.89	0.55
2:B:550:LEU:HD11	2:B:559:TYR:CD2	2.40	0.55
1:E:2002:ILE:HD13	1:E:2029:ILE:HG22	1.88	0.55
3:G:1811:PHE:O	3:G:1815:LEU:HB2	2.07	0.55
1:E:2161:GLU:HB3	1:E:2175:LEU:HD21	1.87	0.55
2:F:2567:ARG:NH2	2:F:2590:ASP:OD2	2.40	0.55
1:C:1108:ARG:HH21	1:C:1111:ALA:HB2	1.72	0.54
1:E:2046:LEU:CD2	1:E:2055:GLN:HG3	2.38	0.54
1:C:1113:PRO:HB3	1:C:1139:PHE:HB3	1.89	0.54
2:D:1534:MET:HB3	2:D:1579:LEU:HD22	1.88	0.54
3:H:2830:GLN:HE22	3:H:2833:LYS:HD3	1.72	0.54
1:E:2031:SER:HA	1:E:2071:PHE:HE2	1.72	0.54
1:E:2189:HIS:HB2	1:E:2192:TYR:OH	2.08	0.53
1:A:2:ILE:HD13	1:A:29:ILE:HG22	1.91	0.53
2:B:648:CYS:HB2	2:B:662:TRP:CH2	2.43	0.53
2:D:1569:THR:HG22	3:G:1834:ASP:HB3	1.90	0.53
3:G:1826:ASN:HB3	3:H:2815:LEU:HD21	1.89	0.53
1:C:1090:GLN:HG2	1:C:1092:TYR:H	1.73	0.53
3:H:2830:GLN:HA	3:H:2830:GLN:NE2	2.24	0.53
1:C:1025:THR:HG21	1:C:1029:ILE:HD13	1.91	0.53
2:D:1567:ARG:HH22	2:D:1590:ASP:CG	2.11	0.53
1:C:1149:LYS:HB2	1:C:1193:ALA:HB3	1.90	0.53
2:B:506:GLU:HA	2:B:521:SER:O	2.09	0.53
1:A:159:SER:HA	1:A:178:THR:O	2.08	0.52
2:F:2502:VAL:HG13	2:F:2527:PHE:CD1	2.44	0.52
2:F:2655:PRO:O	2:F:2712:HIS:HE1	1.93	0.52
1:C:1021:ILE:HD12	1:C:1073:LEU:HD23	1.91	0.52
2:F:2623:SER:O	2:F:2684:LYS:HE2	2.09	0.52
1:E:2008:PRO:O	1:E:2102:THR:HG23	2.10	0.52
2:D:1664:TYR:HB2	2:D:1666:ASN:OD1	2.09	0.52
1:A:189:HIS:HB2	1:A:192:TYR:OH	2.09	0.52
1:A:78:LEU:HD23	1:A:82:ASP:HB2	1.92	0.52
2:B:695:SER:O	2:B:697:ASP:N	2.43	0.52
1:E:2025:THR:HG21	1:E:2029:ILE:HD13	1.92	0.52
1:C:1024:ARG:HA	1:C:1069:THR:O	2.10	0.51
2:D:1568:PHE:HA	2:D:1582:GLN:O	2.10	0.51
1:E:2113:PRO:HB3	1:E:2139:PHE:HB3	1.92	0.51
2:F:2594:TYR:O	2:F:2614:GLY:HA2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1695:SER:O	2:D:1697:ASP:N	2.43	0.51
1:A:47:LEU:HA	1:A:58:VAL:HG21	1.92	0.51
2:D:1594:TYR:O	2:D:1614:GLY:HA2	2.11	0.51
2:B:520:LEU:HG	2:B:583:MET:HE1	1.92	0.51
2:B:673:THR:HG22	2:B:691:VAL:HG22	1.93	0.51
2:F:2513:GLN:HA	2:F:2620:SER:O	2.11	0.51
1:C:1003:GLN:HB2	1:C:1026:SER:HB3	1.93	0.51
1:E:2086:TYR:O	1:E:2101:GLY:HA2	2.11	0.51
2:F:2537:VAL:HB	2:F:2611:TRP:HZ3	1.75	0.51
1:E:2210:ASN:O	1:E:2213:GLU:HG2	2.10	0.50
2:D:1553:TYR:CG	2:D:1554:ASP:N	2.79	0.50
2:D:1608:ASN:H	2:D:1608:ASN:HD22	1.59	0.50
1:C:1148:TRP:HB2	1:C:1155:GLN:HB2	1.93	0.50
2:D:1629:LEU:HD21	2:D:1710:VAL:HG21	1.93	0.50
1:E:2148:TRP:HB2	1:E:2155:GLN:HB2	1.94	0.50
1:A:119:PRO:HB3	1:A:209:PHE:CE1	2.46	0.50
1:A:162:SER:OG	2:B:677:PRO:HB2	2.10	0.50
2:B:591:THR:HA	2:B:617:VAL:O	2.12	0.50
1:E:2175:LEU:HD23	1:E:2176:SER:N	2.27	0.50
1:E:2046:LEU:HD23	1:E:2055:GLN:HG3	1.94	0.50
1:A:25:THR:HG21	1:A:29:ILE:HD13	1.94	0.50
1:A:46:LEU:HD23	1:A:55:GLN:CG	2.42	0.50
1:A:103:LYS:HD2	1:A:142:ARG:HH22	1.77	0.50
2:B:513:GLN:HA	2:B:620:SER:O	2.12	0.50
1:E:2149:LYS:HB2	1:E:2193:ALA:HB3	1.93	0.50
2:D:1567:ARG:NH2	2:D:1590:ASP:OD2	2.45	0.49
1:A:48:ILE:HG12	1:A:54:LEU:HD23	1.93	0.49
2:D:1558:LYS:NZ	3:G:1834:ASP:O	2.46	0.49
3:G:1833:LYS:HB2	3:H:2812:TYR:CE1	2.47	0.49
1:C:1002:ILE:HD13	1:C:1029:ILE:HG22	1.94	0.49
2:F:2519:ARG:HD2	2:F:2582:GLN:NE2	2.28	0.49
1:E:2046:LEU:CG	1:E:2055:GLN:HG3	2.42	0.49
1:C:1175:LEU:HD23	1:C:1176:SER:N	2.27	0.49
1:E:2134:CYS:HB2	1:E:2148:TRP:CH2	2.47	0.49
2:B:664:TYR:HB2	2:B:666:ASN:OD1	2.13	0.49
1:C:1159:SER:HA	1:C:1178:THR:O	2.11	0.49
1:E:2047:LEU:HA	1:E:2058:VAL:HG21	1.93	0.49
2:F:2665:LYS:HB3	2:F:2703:ASN:OD1	2.12	0.49
2:F:2648:CYS:HB2	2:F:2662:TRP:CH2	2.47	0.49
1:A:37:GLN:HB2	1:A:47:LEU:HD11	1.95	0.48
2:B:568:PHE:HA	2:B:582:GLN:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1179:LEU:HG	1:C:1181:LEU:HD21	1.95	0.48
2:D:1673:THR:HG22	2:D:1691:VAL:HG22	1.96	0.48
2:F:2518:LEU:HB3	2:F:2583:MET:HE3	1.94	0.48
1:E:2113:PRO:HD3	1:E:2198:HIS:CD2	2.48	0.48
2:B:658:ILE:HA	2:B:711:GLN:O	2.13	0.48
2:D:1658:ILE:HA	2:D:1711:GLN:O	2.13	0.48
1:A:136:LEU:HD11	1:A:146:VAL:CG1	2.44	0.48
2:F:2540:ALA:HB3	2:F:2543:LYS:HB2	1.96	0.48
1:A:100:GLN:CD	1:A:100:GLN:H	2.16	0.48
2:D:1694:PRO:O	2:D:1698:VAL:HG23	2.14	0.48
2:F:2658:ILE:HA	2:F:2711:GLN:O	2.13	0.47
3:G:1831:SER:HA	3:G:1834:ASP:HB2	1.96	0.47
1:A:108:ARG:HH21	1:A:111:ALA:HB2	1.79	0.47
2:F:2695:SER:HA	2:F:2699:ALA:HB2	1.95	0.47
1:A:78:LEU:HD13	1:A:83:PHE:CE1	2.49	0.47
3:H:2803:PHE:CD1	3:H:2804:ASN:HB2	2.49	0.47
2:B:511:VAL:HG21	2:B:655:PRO:HD3	1.96	0.47
2:B:703:ASN:O	2:B:723:LEU:HD12	2.13	0.47
2:B:672:SER:O	2:B:691:VAL:HA	2.15	0.47
1:C:1113:PRO:HD3	1:C:1198:HIS:CD2	2.50	0.47
1:C:1118:PHE:N	1:C:1118:PHE:CD2	2.82	0.47
2:D:1569:THR:CG2	3:G:1834:ASP:HB3	2.44	0.47
1:E:2145:LYS:HB3	1:E:2197:THR:OG1	2.14	0.47
2:F:2536:TRP:NE1	2:F:2581:LEU:HB2	2.30	0.47
2:F:2639:ASN:OD1	2:F:2640:PRO:HD3	2.14	0.47
1:E:2125:LEU:O	1:E:2183:LYS:HD2	2.15	0.47
2:D:1522:CYS:HB3	2:D:1579:LEU:HB3	1.95	0.47
2:F:2560:TYR:CE2	2:F:2570:ILE:HG22	2.50	0.47
3:H:2855:PRO:O	3:H:2856:LYS:HB3	2.15	0.47
1:A:8:PRO:HB3	2:D:1531:GLY:HA2	1.97	0.46
2:F:2534:MET:HB3	2:F:2579:LEU:HD22	1.96	0.46
2:F:2569:THR:HG23	3:H:2834:ASP:CB	2.45	0.46
1:A:103:LYS:HD2	1:A:142:ARG:NH2	2.30	0.46
1:A:24:ARG:HA	1:A:69:THR:O	2.15	0.46
2:F:2568:PHE:HA	2:F:2582:GLN:O	2.15	0.46
1:E:2124:GLN:HG2	1:E:2129:THR:O	2.15	0.46
1:A:113:PRO:HD3	1:A:198:HIS:CD2	2.50	0.46
2:B:659:THR:HB	2:B:711:GLN:HB2	1.98	0.46
2:D:1638:SER:HB2	2:D:1644:VAL:HA	1.96	0.46
2:D:1655:PRO:O	2:D:1712:HIS:HE1	1.99	0.46
2:B:673:THR:HG22	2:B:691:VAL:CG2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2004:MET:SD	1:E:2025:THR:HG22	2.56	0.46
1:E:2073:LEU:HD12	1:E:2074:THR:N	2.30	0.46
1:E:2159:SER:HA	1:E:2178:THR:O	2.15	0.46
2:F:2638:SER:HB2	2:F:2644:VAL:HA	1.98	0.46
3:H:2815:LEU:HA	3:H:2825:ARG:HD3	1.98	0.46
2:F:2591:THR:HA	2:F:2617:VAL:O	2.16	0.46
2:F:2709:LYS:HG2	2:F:2718:GLU:HB3	1.97	0.45
1:C:1192:TYR:HB2	1:C:1209:PHE:CE2	2.51	0.45
2:D:1643:THR:HA	2:D:1693:LEU:O	2.16	0.45
3:H:2830:GLN:NE2	3:H:2833:LYS:HD3	2.31	0.45
1:C:1086:TYR:O	1:C:1101:GLY:HA2	2.17	0.45
1:A:114:SER:HB2	1:A:137:ASN:HB2	1.97	0.45
2:B:688:THR:HG22	2:B:689:SER:N	2.32	0.45
2:F:2506:GLU:HA	2:F:2521:SER:O	2.17	0.45
2:F:2695:SER:O	2:F:2697:ASP:N	2.50	0.45
1:A:108:ARG:HG2	1:A:109:THR:H	1.82	0.45
1:A:136:LEU:HD11	1:A:146:VAL:HG12	1.98	0.45
1:E:2029:ILE:HD11	1:E:2033:LEU:HB2	1.98	0.45
1:C:1134:CYS:HB2	1:C:1148:TRP:CH2	2.52	0.45
2:D:1572:ARG:HG3	2:D:1574:ASN:OD1	2.16	0.45
2:D:1591:THR:HA	2:D:1617:VAL:O	2.16	0.45
2:B:558:LYS:NZ	2:B:558:LYS:CB	2.78	0.44
1:C:1078:LEU:HD13	1:C:1083:PHE:CE1	2.52	0.44
2:F:2660:PHE:CD2	2:F:2689:SER:HB2	2.53	0.44
2:D:1506:GLU:HA	2:D:1521:SER:O	2.17	0.44
2:D:1568:PHE:CD1	2:D:1568:PHE:N	2.86	0.44
1:E:2024:ARG:HA	1:E:2069:THR:O	2.16	0.44
2:B:512:VAL:HG21	2:B:518:LEU:HD13	1.98	0.44
1:C:1186:TYR:HA	1:C:1192:TYR:OH	2.18	0.44
1:E:2045:LYS:HB3	1:E:2045:LYS:HZ2	1.80	0.44
1:A:31:SER:HA	1:A:71:PHE:HE2	1.82	0.44
2:F:2672:SER:O	2:F:2691:VAL:HA	2.17	0.44
2:F:2719:LYS:HG3	2:F:2720:ASP:N	2.33	0.44
2:B:597:ALA:HB1	2:B:608:ASN:HB3	1.99	0.43
2:D:1506:GLU:HG3	2:D:1596:CYS:SG	2.58	0.43
1:E:2146:VAL:HG21	1:E:2177:SER:HB2	2.00	0.43
1:A:45:LYS:HE3	1:A:45:LYS:HB2	1.81	0.43
2:B:661:SER:HB3	2:B:709:LYS:HB2	2.00	0.43
1:A:48:ILE:CG1	1:A:54:LEU:HD23	2.49	0.43
1:C:1058:VAL:HA	1:C:1059:PRO:HD3	1.87	0.43
1:E:2149:LYS:HG2	1:E:2154:LEU:HD22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1695:SER:HA	2:D:1699:ALA:HB2	2.00	0.43
1:E:2039:LYS:HG2	1:E:2084:ALA:HB2	2.01	0.43
2:F:2567:ARG:HH22	2:F:2590:ASP:CG	2.21	0.43
3:H:2817:MET:HA	3:H:2818:PRO:HD2	1.76	0.43
1:A:46:LEU:HD23	1:A:55:GLN:HG2	1.99	0.43
1:A:148:TRP:HB2	1:A:155:GLN:HB2	1.99	0.43
2:B:643:THR:HA	2:B:693:LEU:O	2.18	0.43
2:D:1536:TRP:CE2	2:D:1581:LEU:HB2	2.53	0.43
2:B:551:ILE:HG13	2:B:558:LYS:NZ	2.32	0.43
1:E:2019:VAL:HG23	1:E:2078:LEU:HG	2.01	0.43
2:F:2550:LEU:HD12	2:F:2550:LEU:C	2.39	0.43
2:D:1705:HIS:HA	2:D:1723:LEU:HG	2.00	0.43
1:C:1185:ASP:O	1:C:1189:HIS:HD2	2.01	0.43
2:D:1648:CYS:HB3	2:D:1689:SER:HB3	2.00	0.43
2:B:616:LEU:HD13	2:B:618:THR:OG1	2.19	0.43
2:D:1560:TYR:CE2	2:D:1569:THR:HA	2.54	0.43
3:H:2835:ASP:OD2	3:H:2838:GLN:HG3	2.19	0.43
1:C:1191:VAL:HG22	1:C:1210:ASN:OD1	2.18	0.42
1:C:1199:GLN:O	1:C:1199:GLN:HG2	2.19	0.42
2:D:1540:ALA:HB3	2:D:1543:LYS:HB2	2.00	0.42
2:F:2522:CYS:HB3	2:F:2579:LEU:HB3	2.01	0.42
2:B:530:SER:O	2:B:553:TYR:HB2	2.19	0.42
1:C:1025:THR:OG1	1:C:1069:THR:HA	2.19	0.42
3:G:1810:ALA:O	3:G:1814:ILE:HG13	2.19	0.42
1:E:2075:ILE:HG21	1:E:2078:LEU:HD23	2.02	0.42
1:E:2122:ASP:O	1:E:2126:LYS:HG3	2.19	0.42
2:D:1627:PRO:O	2:D:1717:LYS:HD2	2.19	0.42
2:D:1672:SER:O	2:D:1691:VAL:HA	2.20	0.42
2:B:620:SER:HB3	2:B:654:LEU:HD21	2.01	0.42
1:A:86:TYR:O	1:A:101:GLY:HA2	2.19	0.42
2:B:565:LYS:HE2	2:B:565:LYS:HB3	1.77	0.42
2:D:1654:LEU:HD12	2:D:1655:PRO:HA	2.01	0.42
1:E:2025:THR:OG1	1:E:2069:THR:HA	2.20	0.42
1:A:146:VAL:HG12	1:A:196:VAL:HG22	2.02	0.41
1:C:1096:ARG:HH11	2:D:1608:ASN:HD21	1.66	0.41
2:D:1583:MET:HB3	2:D:1586:LEU:HD21	2.02	0.41
2:D:1721:VAL:HA	2:D:1722:PRO:HD3	1.88	0.41
1:E:2150:VAL:HG23	1:E:2155:GLN:HG3	2.02	0.41
2:F:2512:VAL:O	2:F:2619:VAL:HA	2.20	0.41
2:F:2648:CYS:HB2	2:F:2662:TRP:CZ2	2.55	0.41
1:C:1090:GLN:NE2	1:C:1093:SER:H	2.16	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1616:LEU:HD12	2:D:1618:THR:OG1	2.20	0.41
1:C:1201:LEU:HD13	1:C:1205:VAL:HG13	2.03	0.41
2:F:2563:SER:O	2:F:2567:ARG:NH1	2.52	0.41
1:C:1029:ILE:CG2	1:C:1090:GLN:HG3	2.49	0.41
1:C:1047:LEU:HD13	1:C:1062:PHE:CE2	2.56	0.41
1:E:2163:VAL:HG22	1:E:2175:LEU:HG	2.03	0.41
1:E:2184:ALA:O	1:E:2188:LYS:HG2	2.20	0.41
1:A:125:LEU:O	1:A:183:LYS:HD3	2.21	0.41
2:D:1551:ILE:HG13	2:D:1558:LYS:HG2	2.03	0.41
2:B:512:VAL:O	2:B:619:VAL:HA	2.21	0.40
2:F:2676:PHE:HA	2:F:2677:PRO:HD3	1.90	0.40
2:D:1598:LYS:HG2	2:D:1599:VAL:O	2.21	0.40
1:E:2103:LYS:HB2	1:E:2103:LYS:HE3	1.81	0.40
1:C:1150:VAL:HG23	1:C:1155:GLN:CG	2.51	0.40
1:E:2197:THR:HG22	1:E:2204:PRO:CG	2.51	0.40
1:C:1089:GLN:HG2	1:C:1090:GLN:N	2.35	0.40
1:C:1137:ASN:HB3	1:C:1138:ASN:HD22	1.85	0.40
2:F:2569:THR:CG2	3:H:2834:ASP:HB2	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	212/214 (99%)	201 (95%)	9 (4%)	2 (1%)	17 40
1	C	212/214 (99%)	197 (93%)	13 (6%)	2 (1%)	17 40
1	E	212/214 (99%)	199 (94%)	10 (5%)	3 (1%)	11 28
2	B	221/223 (99%)	202 (91%)	16 (7%)	3 (1%)	11 28
2	D	221/223 (99%)	201 (91%)	16 (7%)	4 (2%)	8 21
2	F	221/223 (99%)	204 (92%)	13 (6%)	4 (2%)	8 21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	G	49/54 (91%)	48 (98%)	1 (2%)	0	100	100
3	H	52/54 (96%)	49 (94%)	2 (4%)	1 (2%)	8	20
All	All	1400/1419 (99%)	1301 (93%)	80 (6%)	19 (1%)	11	28

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	696	LYS
2	D	1696	LYS
2	F	2696	LYS
1	C	1031	SER
1	A	30	SER
1	C	1030	SER
1	E	2030	SER
1	A	138	ASN
2	B	700	GLN
2	D	1700	GLN
2	F	2700	GLN
1	E	2031	SER
3	H	2804	ASN
1	E	2138	ASN
2	F	2698	VAL
2	D	1698	VAL
2	F	2682	GLY
2	B	698	VAL
2	D	1682	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	189/189 (100%)	177 (94%)	12 (6%)	18	40
1	C	189/189 (100%)	181 (96%)	8 (4%)	30	58
1	E	189/189 (100%)	178 (94%)	11 (6%)	20	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	188/188 (100%)	176 (94%)	12 (6%)	17	39
2	D	188/188 (100%)	178 (95%)	10 (5%)	22	48
2	F	188/188 (100%)	181 (96%)	7 (4%)	34	63
3	G	45/48 (94%)	41 (91%)	4 (9%)	9	22
3	H	47/48 (98%)	43 (92%)	4 (8%)	10	24
All	All	1223/1227 (100%)	1155 (94%)	68 (6%)	21	45

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	ASP
1	A	33	LEU
1	A	55	GLN
1	A	90	GLN
1	A	100	GLN
1	A	103	LYS
1	A	108	ARG
1	A	136	LEU
1	A	188	LYS
1	A	197	THR
1	A	205	VAL
1	A	214	CYS
2	B	512	VAL
2	B	516	LYS
2	B	558	LYS
2	B	575	SER
2	B	615	THR
2	B	616	LEU
2	B	621	SER
2	B	652	ASP
2	B	674	ARG
2	B	681	ARG
2	B	702	THR
2	B	711	GLN
1	C	1001	ASP
1	C	1024	ARG
1	C	1033	LEU
1	C	1090	GLN
1	C	1100	GLN
1	C	1181	LEU

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Mol	Chain	Res	Type
1	C	1202	SER
1	C	1214	CYS
2	D	1550	LEU
2	D	1575	SER
2	D	1577	ASN
2	D	1585	SER
2	D	1615	THR
2	D	1616	LEU
2	D	1618	THR
2	D	1636	GLU
2	D	1651	GLN
2	D	1681	ARG
1	E	2001	ASP
1	E	2007	SER
1	E	2045	LYS
1	E	2060	SER
1	E	2069	THR
1	E	2070	ASP
1	E	2081	GLU
1	E	2090	GLN
1	E	2162	SER
1	E	2188	LYS
1	E	2214	CYS
2	F	2530	SER
2	F	2565	LYS
2	F	2569	THR
2	F	2615	THR
2	F	2616	LEU
2	F	2681	ARG
2	F	2711	GLN
3	G	1813	GLU
3	G	1815	LEU
3	G	1849	LEU
3	G	1852	SER
3	H	2804	ASN
3	H	2815	LEU
3	H	2816	ASN
3	H	2830	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	GLN
1	A	147	GLN
2	B	513	GLN
2	B	557	ASN
2	B	577	ASN
2	B	582	GLN
2	B	651	GLN
2	B	700	GLN
2	B	705	HIS
2	B	712	HIS
1	C	1100	GLN
1	C	1138	ASN
1	C	1198	HIS
2	D	1577	ASN
2	D	1608	ASN
2	D	1700	GLN
2	D	1705	HIS
1	E	2055	GLN
1	E	2124	GLN
2	F	2577	ASN
2	F	2582	GLN
2	F	2700	GLN
2	F	2712	HIS
3	H	2804	ASN
3	H	2808	GLN
3	H	2816	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	214/214 (100%)	-0.68	0 100 100	11, 30, 70, 91	0
1	C	214/214 (100%)	-0.13	14 (6%) 18 17	12, 40, 96, 109	0
1	E	214/214 (100%)	-0.54	1 (0%) 91 92	19, 45, 72, 99	0
2	B	223/223 (100%)	-0.30	11 (4%) 29 28	11, 31, 132, 163	0
2	D	223/223 (100%)	0.27	33 (14%) 2 1	12, 46, 135, 156	0
2	F	223/223 (100%)	-0.24	12 (5%) 25 24	17, 45, 124, 153	0
3	G	51/54 (94%)	-0.30	3 (5%) 22 21	17, 42, 113, 156	0
3	H	54/54 (100%)	-0.18	3 (5%) 24 23	27, 51, 80, 110	0
All	All	1416/1419 (99%)	-0.26	77 (5%) 25 24	11, 40, 106, 163	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	2638	SER	9.9
3	G	1856	LYS	9.5
2	D	1638	SER	8.0
2	B	696	LYS	7.7
2	D	1699	ALA	7.4
2	F	2696	LYS	7.3
2	D	1664	TYR	6.6
1	C	1184	ALA	6.2
3	H	2856	LYS	5.9
2	B	638	SER	5.8
2	B	697	ASP	5.8
2	B	639	ASN	5.4
2	D	1637	ASN	5.2
3	H	2803	PHE	5.2
2	F	2697	ASP	4.9
1	C	1152	ASN	4.7

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Mol	Chain	Res	Type	RSRZ
1	C	1154	LEU	4.6
2	D	1700	GLN	4.5
2	F	2639	ASN	4.4
2	D	1702	THR	4.4
2	D	1696	LYS	4.3
1	C	1119	PRO	4.1
2	D	1711	GLN	4.0
2	B	640	PRO	3.9
2	D	1636	GLU	3.9
2	D	1644	VAL	3.9
2	D	1668	SER	3.7
2	B	637	ASN	3.7
2	D	1640	PRO	3.7
2	B	636	GLU	3.6
2	D	1645	ALA	3.6
2	D	1709	LYS	3.6
2	D	1642	SER	3.6
2	D	1705	HIS	3.5
2	F	2637	ASN	3.4
2	D	1671	SER	3.2
2	B	695	SER	3.1
1	C	1122	ASP	3.0
2	F	2695	SER	3.0
2	D	1639	ASN	3.0
3	G	1806	ASP	3.0
2	D	1715	GLY	2.9
2	D	1666	ASN	2.9
1	C	1125	LEU	2.9
2	D	1665	LYS	2.8
2	D	1667	ASN	2.8
1	C	1153	ALA	2.8
1	C	1157	GLY	2.8
2	B	700	GLN	2.7
1	C	1124	GLN	2.7
2	D	1697	ASP	2.7
1	C	1209	PHE	2.7
2	D	1695	SER	2.7
1	C	1213	GLU	2.6
2	F	2640	PRO	2.6
2	F	2703	ASN	2.5
3	G	1855	PRO	2.5
2	F	2701	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
2	D	1681	ARG	2.4
2	D	1641	SER	2.4
1	C	1212	GLY	2.4
2	D	1721	VAL	2.4
2	D	1708	CYS	2.3
2	F	2700	GLN	2.3
2	D	1663	LYS	2.3
2	B	665	LYS	2.3
1	C	1210	ASN	2.2
3	H	2855	PRO	2.2
2	D	1701	GLY	2.2
2	F	2702	THR	2.2
1	E	2169	LYS	2.1
1	C	1129	THR	2.1
2	B	701	GLY	2.1
2	D	1713	PRO	2.1
2	F	2704	GLU	2.0
2	D	1720	ASP	2.0
2	D	1673	THR	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.