Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:52 AM GMT

PDB ID	:	2J5L
Title	:	STRUCTURE OF A PLASMODIUM FALCIPARUM APICAL MEMBRANE ANTIGEN 1-FAB F8.12.19 COMPLEX
Authors	:	Igonet, S.; Vulliez-Le Normand, B.; Faure, G.; Riottot, M.M.; Kocken, C.H.M.; Thomas, A.W.; Bentley, G.A.
Deposited on	:	2006-09-18
Resolution	:	2.90 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

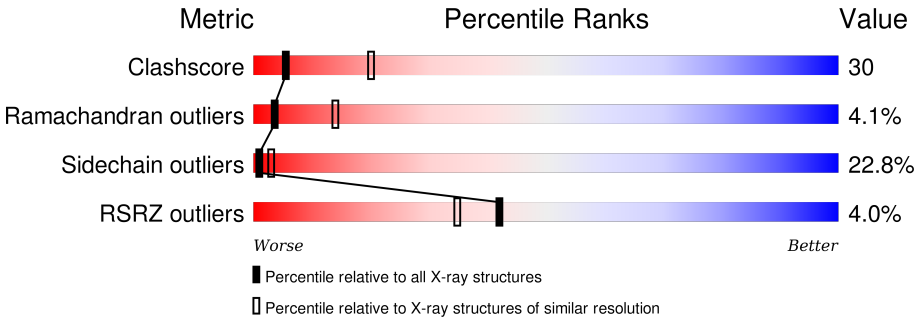
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance

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

The reported resolution of this entry is 2.90 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))
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	581	94%
2	B	213	39% 46% 12%
3	C	225	4% 44% 45% 9%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3605 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 APICAL MEMBRANE ANTIGEN 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	34	Total	C	N	O	S	0	0	0
			269	167	44	52	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	499	GLN	ASN	ENGINEERED MUTATION	UNP Q9GVB7

- Molecule 2 is a protein called FAB FRAGMENT OF MONOCLONAL ANTIBODY F8.12.19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	213	Total	C	N	O	S	0	0	0
			1635	1012	281	334	8			

- Molecule 3 is a protein called FAB FRAGMENT OF MONOCLONAL ANTIBODY F8.12.19.

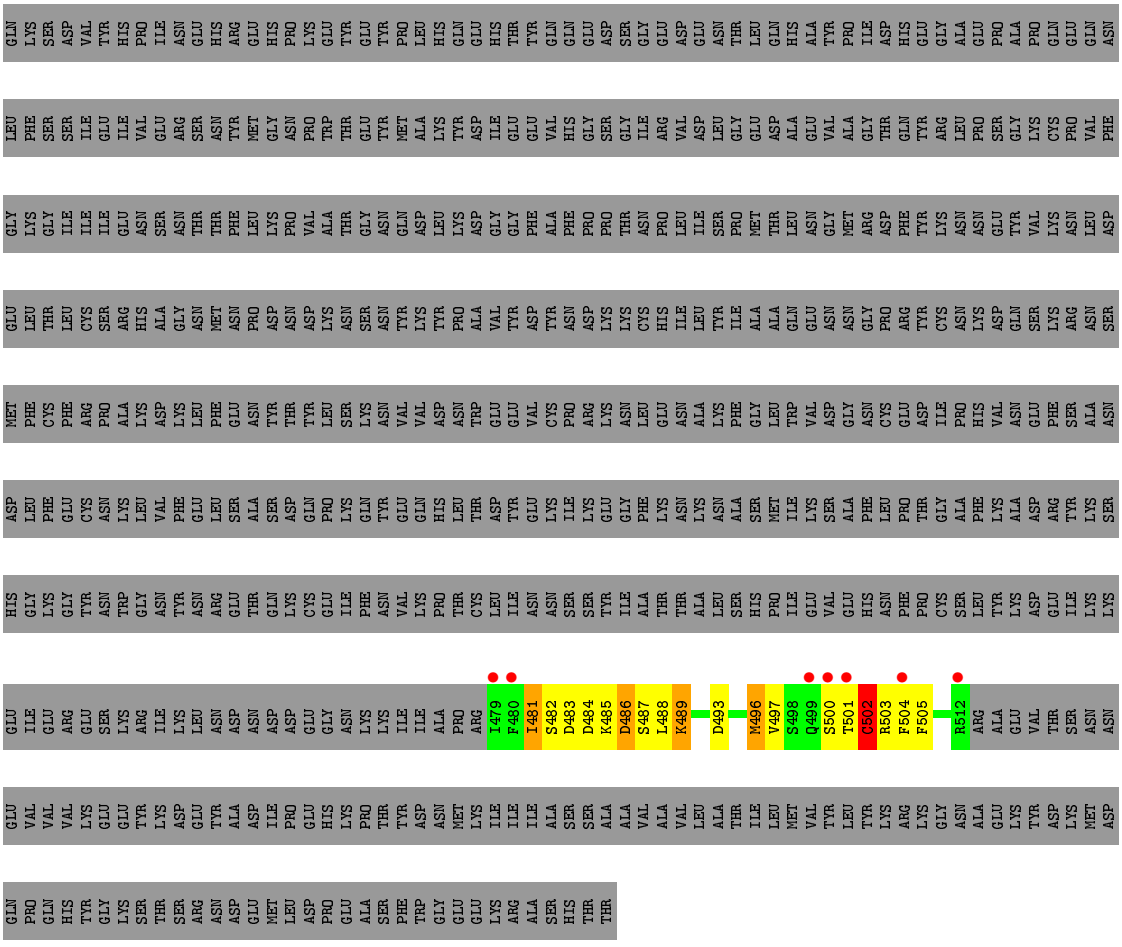
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	225	Total	C	N	O	S	0	0	0
			1701	1075	278	340	8			

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

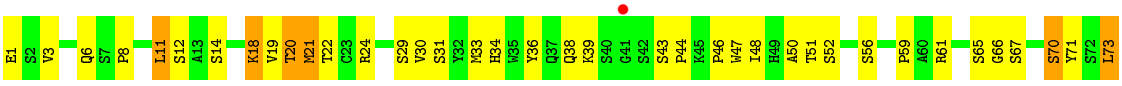
- Molecule 1: APICAL MEMBRANE ANTIGEN 1

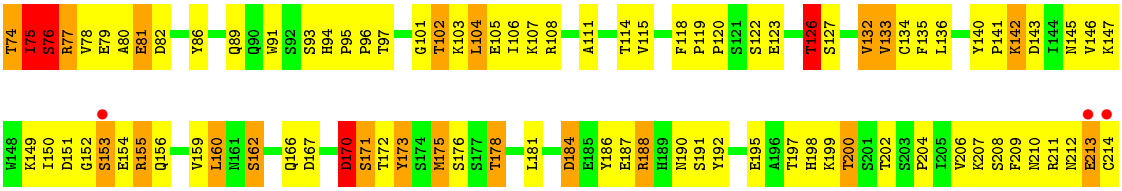
Chain A:



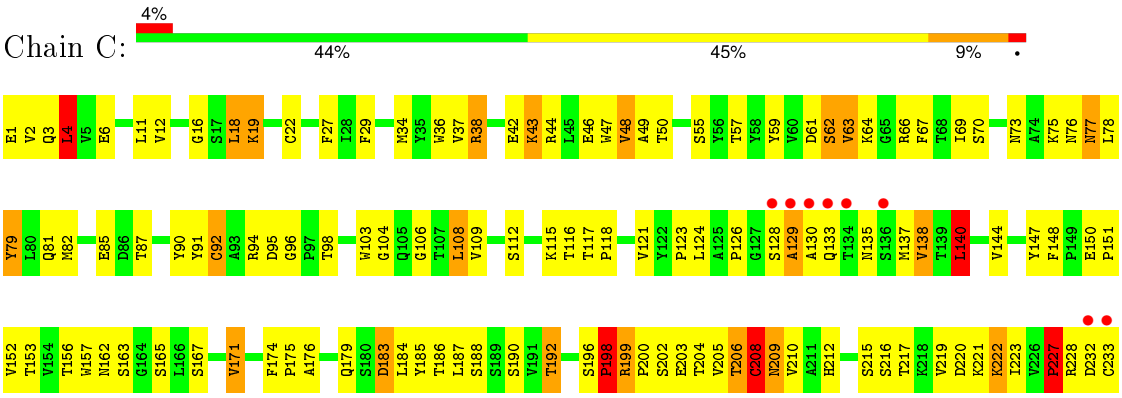
- Molecule 2: FAB FRAGMENT OF MONOCLONAL ANTIBODY F8.12.19

Chain B:





• Molecule 3: FAB FRAGMENT OF MONOCLONAL ANTIBODY F8.12.19



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	171.90Å 171.90Å 44.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.90 19.72 – 2.82	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-2.90) 97.9 (19.72-2.82)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.84 (at 2.83Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.212 , 0.278 0.214 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	50.4	Xtriage
Anisotropy	0.771	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 50.8	EDS
Estimated twinning fraction	0.066 for h,-h-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Outliers	2 of 18102 reflections (0.011%)	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	3605	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PCA

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	0.91	0/273	0.89	0/365
2	B	1.21	5/1669 (0.3%)	1.16	4/2269 (0.2%)
3	C	1.07	3/1745 (0.2%)	1.12	3/2381 (0.1%)
All	All	1.13	8/3687 (0.2%)	1.12	7/5015 (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
2	B	0	2
3	C	0	1
All	All	0	3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	173	TYR	CD1-CE1	10.93	1.55	1.39
3	C	208	CYS	CB-SG	-6.01	1.72	1.82
2	B	78	VAL	CA-CB	5.59	1.66	1.54
2	B	173	TYR	CD2-CE2	5.49	1.47	1.39
2	B	76	SER	CA-CB	-5.22	1.45	1.52
3	C	46	GLU	CG-CD	5.09	1.59	1.51
3	C	79	TYR	CZ-OH	-5.08	1.29	1.37
2	B	86	TYR	CD2-CE2	-5.04	1.31	1.39

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	11	LEU	CA-CB-CG	7.01	131.43	115.30
2	B	104	LEU	CB-CG-CD2	-6.51	99.92	111.00
3	C	140	LEU	CA-CB-CG	6.23	129.63	115.30
2	B	170	ASP	CB-CA-C	-5.36	99.67	110.40
3	C	4	LEU	CA-CB-CG	5.32	127.54	115.30
3	C	147	TYR	N-CA-C	5.30	125.32	111.00
2	B	143	ASP	CB-CG-OD1	-5.30	113.53	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	170	ASP	Peptide
2	B	75	ILE	Peptide
3	C	215	SER	Peptide

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	269	0	258	12	0
2	B	1635	0	1554	102	0
3	C	1701	0	1649	107	0
All	All	3605	0	3461	209	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 30.

All (209) 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)
3:C:150:GLU:HG3	3:C:151:PRO:HA	1.19	1.09
3:C:123:PRO:HB2	3:C:223:ILE:HD13	1.37	1.06
3:C:123:PRO:HB2	3:C:223:ILE:CD1	1.88	1.02
2:B:123:GLU:O	2:B:126:THR:HB	1.66	0.94
3:C:34:MET:HB3	3:C:78:LEU:HD22	1.52	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:160:LEU:HD11	3:C:179:GLN:HE21	1.36	0.91
3:C:37:VAL:HG22	3:C:47:TRP:HA	1.53	0.90
2:B:8:PRO:O	2:B:102:THR:HG23	1.76	0.85
2:B:43:SER:HB3	3:C:91:TYR:CE1	2.12	0.84
3:C:156:THR:HG23	3:C:209:ASN:OD1	1.78	0.83
3:C:61:ASP:O	3:C:63:VAL:N	2.13	0.80
2:B:61:ARG:NH2	2:B:81:GLU:OE1	2.13	0.80
2:B:6:GLN:OE1	2:B:101:GLY:HA2	1.82	0.80
3:C:196:SER:O	3:C:202:SER:OG	2.00	0.79
2:B:147:LYS:HD3	2:B:155:ARG:HH11	1.48	0.79
2:B:160:LEU:HD21	3:C:179:GLN:HG3	1.66	0.78
3:C:6:GLU:OE1	3:C:106:GLY:N	2.17	0.76
3:C:176:ALA:HB1	3:C:185:TYR:HD1	1.49	0.76
3:C:217:THR:HG22	3:C:219:VAL:HG23	1.66	0.76
3:C:199:ARG:HD2	3:C:200:PRO:HA	1.70	0.74
2:B:1:PCA:HG2	2:B:95:PRO:HD2	1.69	0.73
2:B:147:LYS:HD3	2:B:155:ARG:NH1	2.03	0.73
2:B:160:LEU:HD21	3:C:179:GLN:CG	2.20	0.71
3:C:95:ASP:OD2	3:C:96:GLY:N	2.23	0.71
3:C:187:LEU:HD23	3:C:188:SER:N	2.06	0.70
2:B:20:THR:OG1	2:B:74:THR:HG23	1.91	0.70
3:C:38:ARG:HG2	3:C:48:VAL:CG1	2.22	0.69
2:B:21:MET:CE	2:B:102:THR:HB	2.23	0.69
3:C:200:PRO:HG3	3:C:227:PRO:HG3	1.76	0.68
2:B:186:TYR:O	2:B:211:ARG:HD2	1.94	0.68
3:C:123:PRO:HB2	3:C:223:ILE:HD11	1.75	0.67
3:C:167:SER:O	3:C:171:VAL:HG12	1.93	0.67
3:C:206:THR:HG23	3:C:222:LYS:HA	1.75	0.67
3:C:61:ASP:C	3:C:63:VAL:H	1.99	0.66
3:C:38:ARG:NH1	3:C:90:TYR:OH	2.28	0.66
3:C:150:GLU:CG	3:C:151:PRO:HA	2.13	0.66
3:C:209:ASN:HB3	3:C:220:ASP:OD1	1.96	0.65
1:A:496:MET:CE	1:A:503:ARG:HG2	2.27	0.65
2:B:140:TYR:CG	2:B:141:PRO:HA	2.31	0.65
1:A:501:THR:O	1:A:502:CYS:HB2	1.96	0.65
3:C:43:LYS:HD2	3:C:43:LYS:N	2.11	0.64
3:C:162:ASN:HB3	3:C:165:SER:OG	1.98	0.64
3:C:153:THR:O	3:C:210:VAL:HA	1.98	0.63
2:B:133:VAL:HG23	2:B:178:THR:HG23	1.80	0.63
2:B:170:ASP:HB3	2:B:172:THR:HG23	1.80	0.63
2:B:150:ILE:O	2:B:152:GLY:O	2.17	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:170:ASP:HB2	2:B:172:THR:H	1.65	0.62
2:B:108:ARG:NH2	2:B:111:ALA:HB2	2.16	0.61
3:C:34:MET:HB3	3:C:78:LEU:CD2	2.28	0.61
2:B:152:GLY:O	2:B:154:GLU:N	2.34	0.60
3:C:162:ASN:O	3:C:165:SER:OG	2.13	0.60
3:C:108:LEU:C	3:C:108:LEU:HD22	2.21	0.60
2:B:105:GLU:OE2	2:B:142:LYS:HE3	2.01	0.60
3:C:150:GLU:HG3	3:C:151:PRO:CA	2.12	0.59
2:B:149:LYS:HD3	2:B:153:SER:HB2	1.84	0.59
2:B:94:HIS:CD2	2:B:95:PRO:HA	2.38	0.59
3:C:117:THR:HG22	3:C:118:PRO:HD2	1.83	0.58
2:B:1:PCA:CG	2:B:95:PRO:HD2	2.34	0.58
2:B:151:ASP:N	2:B:191:SER:O	2.35	0.58
2:B:162:SER:HB3	3:C:174:PHE:HB3	1.84	0.58
3:C:156:THR:HG22	3:C:209:ASN:O	2.03	0.58
3:C:183:ASP:O	3:C:184:LEU:HD23	2.04	0.57
2:B:14:SER:HB3	2:B:107:LYS:HB2	1.85	0.57
2:B:21:MET:HE1	2:B:102:THR:HB	1.86	0.57
3:C:38:ARG:HG2	3:C:48:VAL:HG11	1.86	0.56
2:B:146:VAL:HA	2:B:195:GLU:O	2.05	0.56
2:B:211:ARG:HH11	2:B:211:ARG:HB3	1.69	0.56
2:B:170:ASP:CB	2:B:172:THR:H	2.18	0.56
3:C:157:TRP:CZ3	3:C:208:CYS:HB2	2.41	0.56
1:A:485:LYS:O	1:A:488:LEU:HB2	2.06	0.56
2:B:186:TYR:CZ	2:B:211:ARG:HG3	2.41	0.56
2:B:149:LYS:HD3	2:B:153:SER:CB	2.36	0.56
2:B:66:GLY:HA3	2:B:70:SER:O	2.05	0.56
2:B:166:GLN:HA	2:B:172:THR:O	2.06	0.55
3:C:126:PRO:O	3:C:228:ARG:HD2	2.06	0.55
2:B:43:SER:CB	3:C:91:TYR:CE1	2.87	0.55
1:A:496:MET:HE2	1:A:503:ARG:HG2	1.88	0.55
1:A:496:MET:HB2	1:A:505:PHE:CE2	2.41	0.55
2:B:120:PRO:O	3:C:228:ARG:NH2	2.33	0.55
3:C:11:LEU:HD12	3:C:12:VAL:H	1.72	0.55
3:C:108:LEU:HD22	3:C:109:VAL:N	2.22	0.54
2:B:135:PHE:CD2	3:C:190:SER:HB3	2.42	0.54
3:C:117:THR:CG2	3:C:118:PRO:HD2	2.37	0.54
3:C:2:VAL:HG12	3:C:3:GLN:N	2.21	0.54
3:C:223:ILE:O	3:C:223:ILE:HG22	2.07	0.54
3:C:19:LYS:HE3	3:C:79:TYR:CD1	2.43	0.53
2:B:59:PRO:HB3	2:B:61:ARG:NH1	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:191:SER:HB2	2:B:210:ASN:HD22	1.73	0.53
2:B:135:PHE:CE2	3:C:190:SER:HB3	2.43	0.53
3:C:157:TRP:CH2	3:C:208:CYS:HB2	2.44	0.53
2:B:187:GLU:O	2:B:211:ARG:CZ	2.57	0.53
3:C:6:GLU:OE2	3:C:91:TYR:HA	2.09	0.52
2:B:106:ILE:O	2:B:166:GLN:NE2	2.42	0.52
2:B:210:ASN:O	2:B:213:GLU:HB2	2.09	0.52
3:C:217:THR:HG22	3:C:219:VAL:CG2	2.40	0.52
3:C:200:PRO:CG	3:C:227:PRO:HG3	2.40	0.52
3:C:187:LEU:C	3:C:187:LEU:HD23	2.30	0.51
3:C:48:VAL:O	3:C:49:ALA:HB2	2.11	0.51
2:B:141:PRO:O	2:B:198:HIS:HE1	1.93	0.51
2:B:191:SER:CB	2:B:210:ASN:HD22	2.23	0.51
3:C:198:PRO:HA	3:C:203:GLU:HG3	1.92	0.51
2:B:21:MET:HE2	2:B:102:THR:HG21	1.94	0.50
2:B:191:SER:CB	2:B:210:ASN:ND2	2.75	0.50
2:B:211:ARG:NH1	2:B:211:ARG:HB3	2.26	0.50
2:B:211:ARG:HG2	2:B:211:ARG:O	2.12	0.50
2:B:36:TYR:HD2	2:B:46:PRO:HA	1.77	0.50
2:B:209:PHE:C	2:B:209:PHE:CD1	2.84	0.50
3:C:140:LEU:HG	3:C:223:ILE:HG21	1.94	0.50
2:B:43:SER:HB3	3:C:91:TYR:HE1	1.71	0.50
2:B:136:LEU:N	2:B:136:LEU:HD12	2.26	0.50
3:C:129:ALA:O	3:C:130:ALA:HB3	2.11	0.49
2:B:186:TYR:O	2:B:211:ARG:CD	2.60	0.49
1:A:488:LEU:O	1:A:489:LYS:C	2.50	0.49
3:C:34:MET:CB	3:C:78:LEU:HD22	2.31	0.49
2:B:191:SER:HB2	2:B:210:ASN:ND2	2.27	0.49
3:C:63:VAL:HA	3:C:66:ARG:NH1	2.28	0.49
2:B:166:GLN:HG3	2:B:173:TYR:CZ	2.48	0.49
2:B:187:GLU:HA	2:B:211:ARG:NE	2.27	0.49
2:B:80:ALA:C	2:B:82:ASP:H	2.15	0.49
3:C:18:LEU:O	3:C:82:MET:HG3	2.12	0.48
2:B:66:GLY:CA	2:B:70:SER:O	2.61	0.48
2:B:21:MET:HE2	2:B:102:THR:CB	2.43	0.48
2:B:184:ASP:HB2	2:B:188:ARG:HH21	1.79	0.48
2:B:11:LEU:HD21	2:B:19:VAL:HB	1.96	0.48
3:C:138:VAL:O	3:C:192:THR:HA	2.14	0.48
2:B:48:ILE:CD1	2:B:73:LEU:HD12	2.44	0.47
2:B:21:MET:HE2	2:B:102:THR:HB	1.97	0.47
3:C:186:THR:HG22	3:C:187:LEU:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:67:PHE:HA	3:C:81:GLN:O	2.15	0.47
3:C:144:VAL:O	3:C:144:VAL:HG12	2.14	0.47
3:C:103:TRP:N	3:C:103:TRP:CD1	2.81	0.47
3:C:121:VAL:HG21	3:C:210:VAL:HG11	1.97	0.47
2:B:18:LYS:HA	2:B:75:ILE:O	2.14	0.47
1:A:481:ILE:HG13	1:A:482:SER:N	2.30	0.46
2:B:118:PHE:HA	2:B:119:PRO:HD3	1.64	0.46
3:C:85:GLU:H	3:C:85:GLU:CD	2.18	0.46
2:B:167:ASP:O	2:B:171:SER:HA	2.15	0.46
2:B:115:VAL:HA	2:B:135:PHE:O	2.15	0.46
1:A:489:LYS:HB3	1:A:489:LYS:HE3	1.63	0.46
3:C:87:THR:HA	3:C:109:VAL:O	2.16	0.46
3:C:77:ASN:HD22	3:C:77:ASN:HA	1.52	0.46
2:B:38:GLN:HG2	2:B:39:LYS:N	2.31	0.45
1:A:484:ASP:O	1:A:487:SER:OG	2.33	0.45
2:B:21:MET:HE2	2:B:102:THR:CG2	2.47	0.45
2:B:36:TYR:CD2	2:B:46:PRO:HA	2.51	0.45
3:C:206:THR:HG23	3:C:222:LYS:CA	2.46	0.45
3:C:47:TRP:HE1	3:C:50:THR:HG1	1.63	0.45
2:B:59:PRO:CB	2:B:61:ARG:NH1	2.79	0.45
2:B:198:HIS:O	2:B:199:LYS:C	2.54	0.45
2:B:19:VAL:HG23	2:B:19:VAL:O	2.17	0.45
3:C:11:LEU:CD2	3:C:148:PHE:HE2	2.30	0.44
3:C:64:LYS:HE3	3:C:64:LYS:HB2	1.71	0.44
3:C:121:VAL:HG21	3:C:210:VAL:CG1	2.47	0.44
2:B:151:ASP:OD1	2:B:190:ASN:N	2.49	0.44
2:B:160:LEU:CD1	3:C:179:GLN:HE21	2.17	0.44
2:B:66:GLY:HA3	2:B:71:TYR:HA	1.98	0.44
3:C:123:PRO:CB	3:C:223:ILE:HD11	2.45	0.44
3:C:174:PHE:HA	3:C:175:PRO:HD3	1.66	0.44
3:C:38:ARG:HG2	3:C:48:VAL:HG12	1.96	0.43
3:C:222:LYS:HE2	3:C:223:ILE:N	2.33	0.43
3:C:82:MET:HE2	3:C:82:MET:HB3	1.75	0.43
2:B:91:TRP:CG	2:B:96:PRO:HB3	2.52	0.43
3:C:176:ALA:HB1	3:C:185:TYR:CD1	2.41	0.43
3:C:42:GLU:O	3:C:43:LYS:HB2	2.17	0.43
2:B:94:HIS:CG	2:B:95:PRO:HA	2.54	0.43
3:C:67:PHE:N	3:C:67:PHE:CD1	2.84	0.43
3:C:108:LEU:C	3:C:108:LEU:CD2	2.84	0.43
2:B:159:VAL:CG2	2:B:160:LEU:N	2.81	0.43
2:B:198:HIS:HD2	2:B:200:THR:OG1	2.02	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:62:SER:O	3:C:66:ARG:NH1	2.51	0.43
2:B:79:GLU:HB3	2:B:80:ALA:H	1.71	0.43
3:C:103:TRP:C	3:C:104:GLY:O	2.57	0.43
2:B:33:MET:O	2:B:51:THR:N	2.35	0.43
2:B:43:SER:O	2:B:44:PRO:C	2.55	0.43
1:A:486:ASP:C	1:A:488:LEU:H	2.21	0.43
2:B:132:VAL:O	2:B:178:THR:HA	2.20	0.42
2:B:162:SER:OG	3:C:175:PRO:O	2.35	0.42
3:C:61:ASP:C	3:C:63:VAL:N	2.63	0.42
2:B:155:ARG:HE	2:B:155:ARG:HB2	1.27	0.42
2:B:93:SER:O	2:B:95:PRO:O	2.38	0.42
1:A:501:THR:O	1:A:502:CYS:CB	2.67	0.42
2:B:166:GLN:HG3	2:B:173:TYR:CE2	2.55	0.42
3:C:18:LEU:HA	3:C:18:LEU:HD23	1.77	0.42
2:B:175:MET:HE2	2:B:176:SER:N	2.35	0.42
3:C:75:LYS:O	3:C:76:ASN:C	2.57	0.42
3:C:2:VAL:CG1	3:C:3:GLN:N	2.82	0.42
2:B:136:LEU:HD13	2:B:175:MET:HG3	2.02	0.42
3:C:4:LEU:HG	3:C:92:CYS:SG	2.60	0.42
3:C:29:PHE:HE2	3:C:73:ASN:OD1	2.03	0.42
3:C:36:TRP:HD1	3:C:69:ILE:HD12	1.85	0.41
2:B:175:MET:O	2:B:175:MET:HG3	2.20	0.41
3:C:70:SER:O	3:C:78:LEU:HD12	2.20	0.41
1:A:486:ASP:OD1	1:A:486:ASP:N	2.54	0.41
2:B:159:VAL:HG22	2:B:160:LEU:N	2.35	0.41
3:C:2:VAL:O	3:C:3:GLN:HG2	2.21	0.41
2:B:192:TYR:O	2:B:208:SER:HA	2.20	0.41
3:C:117:THR:HG22	3:C:118:PRO:CD	2.50	0.41
2:B:106:ILE:H	2:B:166:GLN:NE2	2.19	0.41
2:B:76:SER:OG	2:B:77:ARG:N	2.54	0.41
2:B:106:ILE:H	2:B:166:GLN:HE22	1.69	0.41
2:B:34:HIS:HB2	2:B:89:GLN:HB3	2.03	0.41
2:B:50:ALA:O	2:B:52:SER:N	2.54	0.41
3:C:135:ASN:N	3:C:135:ASN:HD22	2.19	0.41
3:C:27:PHE:CD1	3:C:27:PHE:N	2.89	0.41
2:B:159:VAL:O	2:B:160:LEU:HD13	2.20	0.40
3:C:11:LEU:C	3:C:12:VAL:CG2	2.89	0.40
3:C:69:ILE:HD11	3:C:78:LEU:HD11	2.03	0.40
3:C:57:THR:HG1	3:C:59:TYR:HE1	1.70	0.40
3:C:152:VAL:HG12	3:C:212:HIS:HD2	1.87	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	32/581 (6%)	25 (78%)	4 (12%)	3 (9%)	1 2
2	B	211/213 (99%)	181 (86%)	23 (11%)	7 (3%)	5 20
3	C	223/225 (99%)	190 (85%)	24 (11%)	9 (4%)	4 15
All	All	466/1019 (46%)	396 (85%)	51 (11%)	19 (4%)	3 14

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	502	CYS
2	B	126	THR
2	B	153	SER
3	C	62	SER
3	C	128	SER
3	C	183	ASP
1	A	504	PHE
2	B	76	SER
2	B	188	ARG
3	C	216	SER
2	B	67	SER
3	C	98	THR
3	C	129	ALA
3	C	227	PRO
1	A	500	SER
3	C	16	GLY
2	B	204	PRO
3	C	198	PRO
2	B	3	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	34/521 (6%)	26 (76%)	8 (24%)	1 2
2	B	186/186 (100%)	138 (74%)	48 (26%)	0 2
3	C	192/192 (100%)	154 (80%)	38 (20%)	1 5
All	All	412/899 (46%)	318 (77%)	94 (23%)	1 3

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	481	ILE
1	A	483	ASP
1	A	486	ASP
1	A	489	LYS
1	A	493	ASP
1	A	496	MET
1	A	497	VAL
1	A	502	CYS
2	B	12	SER
2	B	18	LYS
2	B	20	THR
2	B	21	MET
2	B	22	THR
2	B	24	ARG
2	B	29	SER
2	B	30	VAL
2	B	31	SER
2	B	47	TRP
2	B	56	SER
2	B	65	SER
2	B	70	SER
2	B	73	LEU
2	B	74	THR
2	B	75	ILE
2	B	77	ARG
2	B	81	GLU

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Mol	Chain	Res	Type
2	B	97	THR
2	B	102	THR
2	B	103	LYS
2	B	104	LEU
2	B	114	THR
2	B	122	SER
2	B	126	THR
2	B	127	SER
2	B	132	VAL
2	B	133	VAL
2	B	134	CYS
2	B	142	LYS
2	B	145	ASN
2	B	155	ARG
2	B	156	GLN
2	B	160	LEU
2	B	162	SER
2	B	171	SER
2	B	175	MET
2	B	178	THR
2	B	181	LEU
2	B	184	ASP
2	B	197	THR
2	B	200	THR
2	B	202	THR
2	B	206	VAL
2	B	207	LYS
2	B	212	ASN
2	B	213	GLU
2	B	214	CYS
3	C	1	GLU
3	C	4	LEU
3	C	18	LEU
3	C	19	LYS
3	C	22	CYS
3	C	38	ARG
3	C	43	LYS
3	C	44	ARG
3	C	48	VAL
3	C	55	SER
3	C	63	VAL
3	C	77	ASN

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Mol	Chain	Res	Type
3	C	92	CYS
3	C	94	ARG
3	C	108	LEU
3	C	112	SER
3	C	115	LYS
3	C	116	THR
3	C	124	LEU
3	C	133	GLN
3	C	137	MET
3	C	138	VAL
3	C	140	LEU
3	C	163	SER
3	C	171	VAL
3	C	192	THR
3	C	198	PRO
3	C	199	ARG
3	C	204	THR
3	C	205	VAL
3	C	206	THR
3	C	208	CYS
3	C	209	ASN
3	C	221	LYS
3	C	222	LYS
3	C	227	PRO
3	C	232	ASP
3	C	233	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	190	ASN
2	B	198	HIS
2	B	210	ASN
2	B	212	ASN
3	C	77	ASN
3	C	135	ASN
3	C	179	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	PCA	B	1	2	7,8,9	1.43	1 (14%)	9,10,12	2.59	4 (44%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PCA	B	1	2	-	0/0/11/13	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	PCA	CD-N	3.48	1.45	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1	PCA	CA-N-CD	-5.76	94.51	113.81
2	B	1	PCA	CB-CA-C	-3.30	108.24	112.76
2	B	1	PCA	O-C-CA	-2.08	119.95	125.44
2	B	1	PCA	CB-CA-N	2.38	110.15	103.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	PCA	2	0

5.5 Carbohydrates (i)

There are no carbohydrates 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

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	34/581 (5%)	0.62	7 (20%) 1 1	59, 81, 113, 114	0
2	B	212/213 (99%)	-0.31	4 (1%) 70 66	16, 55, 88, 125	2 (0%)
3	C	225/225 (100%)	-0.29	8 (3%) 46 38	33, 56, 86, 125	0
All	All	471/1019 (46%)	-0.24	19 (4%) 42 35	16, 57, 97, 125	2 (0%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	233	CYS	7.2
2	B	214	CYS	6.8
1	A	500	SER	5.4
2	B	213	GLU	4.6
3	C	232	ASP	4.6
3	C	130	ALA	4.1
1	A	480	PHE	3.3
3	C	134	THR	3.1
1	A	512	ARG	3.1
3	C	136	SER	2.7
2	B	153	SER	2.7
3	C	128	SER	2.6
3	C	129	ALA	2.6
1	A	504	PHE	2.5
1	A	499	GLN	2.3
1	A	501	THR	2.2
3	C	133	GLN	2.1
2	B	41	GLY	2.1
1	A	479	ILE	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	PCA	B	1	8/9	0.85	0.27	-	85,86,87,87	0

6.3 Carbohydrates (i)

There are no carbohydrates 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.