Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2024 – 03:46 PM EDT

PDB ID	:	5C0N
Title	:	Development of a monoclonal antibody targeting secreted aP2 to treat diabetes and fatty liver disease
Authors	:	Doyle, C.
Deposited on	:	2015-06-12
Resolution	:	3.00 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:

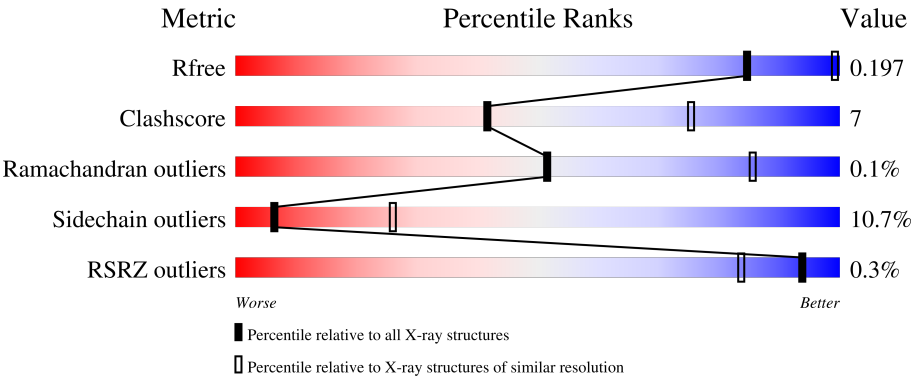
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	132	77% 22%
1	B	132	73% 23%
2	C	222	74% 21%
2	H	222	74% 20%
3	D	219	75% 21%

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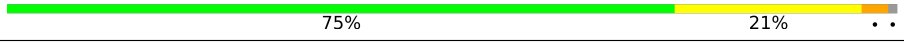
Mol	Chain	Length	Quality of chain
3	L	219	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8540 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 Fatty acid-binding protein, adipocyte.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	131	Total	C	N	O	S	0	0	0
			1017	639	174	198	6			
1	B	131	Total	C	N	O	S	0	0	0
			1017	639	174	198	6			

- Molecule 2 is a protein called Fab CA33 Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	214	Total	C	N	O	S	0	0	0
			1585	1009	253	316	7			
2	C	216	Total	C	N	O	S	0	0	0
			1599	1016	256	320	7			

- Molecule 3 is a protein called Fab CA33 light chain.

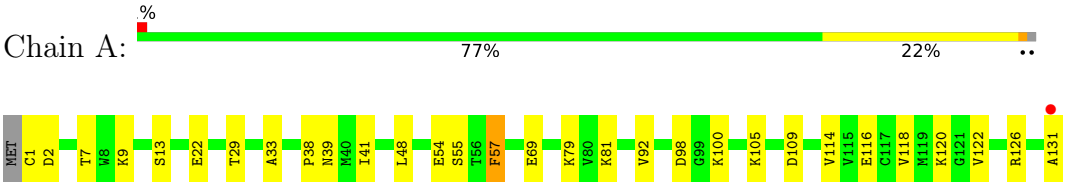
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	216	Total	C	N	O	S	0	0	0
			1661	1039	272	341	9			
3	D	216	Total	C	N	O	S	0	0	0
			1661	1039	272	341	9			

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.

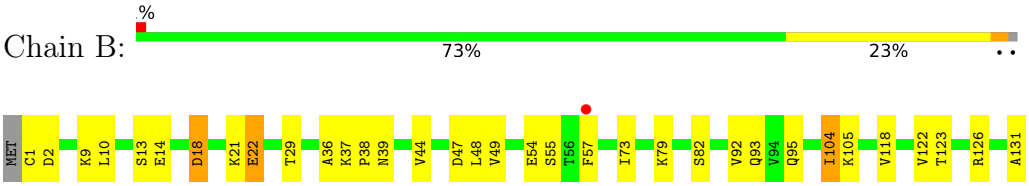
• Molecule 1: Fatty acid-binding protein, adipocyte

Chain A:



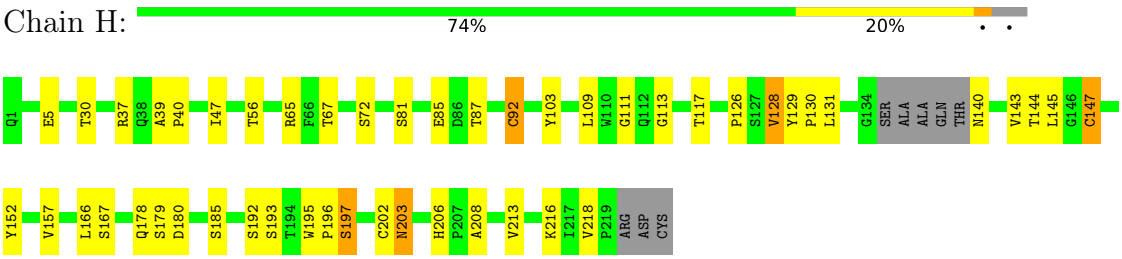
• Molecule 1: Fatty acid-binding protein, adipocyte

Chain B:



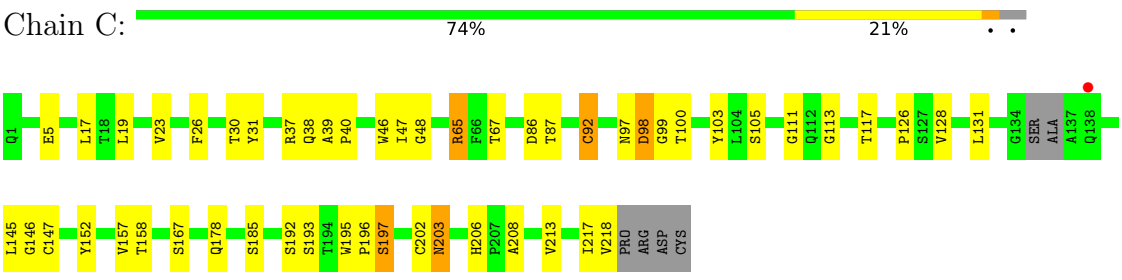
• Molecule 2: Fab CA33 Heavy chain

Chain H:



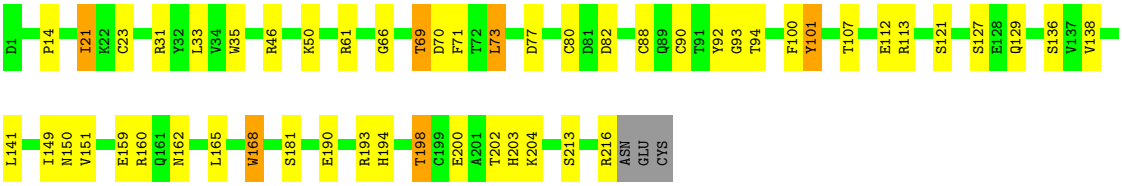
• Molecule 2: Fab CA33 Heavy chain

Chain C:



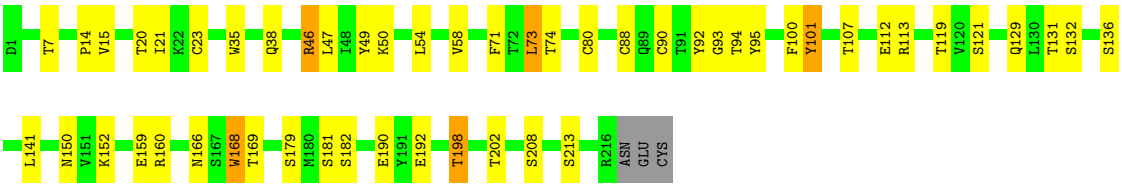
• Molecule 3: Fab CA33 light chain

Chain L:



• Molecule 3: Fab CA33 light chain

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	65.27Å 101.95Å 95.32Å 90.00° 90.03° 90.00°	Depositor
Resolution (Å)	54.97 – 3.00 54.97 – 2.95	Depositor EDS
% Data completeness (in resolution range)	98.9 (54.97-3.00) 98.8 (54.97-2.95)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.91 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.186 , 0.265 0.196 , 0.197	Depositor DCC
R_{free} test set	1333 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	57.5	Xtriage
Anisotropy	0.445	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 41.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.039 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	8540	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% 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	0.68	0/1029	0.78	0/1380
1	B	0.56	0/1029	0.79	0/1380
2	C	0.70	0/1642	0.84	1/2253 (0.0%)
2	H	0.68	0/1629	0.79	1/2236 (0.0%)
3	D	0.64	0/1700	0.81	0/2313
3	L	0.65	0/1700	0.79	0/2313
All	All	0.66	0/8729	0.80	2/11875 (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})
2	C	65	ARG	NE-CZ-NH2	-5.70	117.45	120.30
2	H	147	CYS	CA-CB-SG	-5.55	104.02	114.00

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	1017	0	1040	10	0
1	B	1017	0	1040	16	0
2	C	1599	0	1568	27	0
2	H	1585	0	1555	23	0
3	D	1661	0	1580	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	1661	0	1580	28	0
All	All	8540	0	8363	119	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 7.

All (119) 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:L:194:HIS:O	3:L:216:ARG:NH1	1.87	1.06
2:C:98:ASP:OD1	3:D:50:LYS:NZ	2.17	0.77
3:L:61:ARG:NH2	3:L:82:ASP:OD2	2.20	0.74
3:L:31:ARG:NH1	3:L:66:GLY:O	2.23	0.72
3:D:54:LEU:HD21	3:D:58:VAL:O	1.90	0.71
2:H:131:LEU:HD21	3:L:138:VAL:HG21	1.74	0.70
1:B:22:GLU:OE2	1:B:122:VAL:HG21	1.94	0.68
3:L:21:ILE:CG2	3:L:107:THR:HG21	2.25	0.67
2:C:65:ARG:NH2	2:C:86:ASP:OD2	2.28	0.67
2:H:206:HIS:CE1	2:H:208:ALA:HB3	2.31	0.65
3:D:159:GLU:HG3	3:D:160:ARG:N	2.12	0.65
3:L:198:THR:OG1	3:L:213:SER:HB3	1.97	0.65
1:B:82:SER:OG	1:B:95:GLN:HG2	1.96	0.65
2:C:206:HIS:CE1	2:C:208:ALA:HB3	2.33	0.64
1:B:37:LYS:O	1:B:37:LYS:HD3	1.99	0.61
2:H:144:THR:O	2:H:145:LEU:HD23	2.01	0.60
3:L:21:ILE:HG21	3:L:107:THR:HG21	1.85	0.58
1:B:92:VAL:HG22	1:B:105:LYS:HG2	1.84	0.58
1:A:22:GLU:HG3	1:A:122:VAL:HG21	1.87	0.57
3:D:92:TYR:O	3:D:100:PHE:O	2.24	0.56
1:A:92:VAL:HG22	1:A:105:LYS:HG2	1.87	0.56
3:D:159:GLU:HG3	3:D:160:ARG:H	1.71	0.56
2:H:5:GLU:OE2	2:H:113:GLY:N	2.35	0.56
2:C:103:TYR:CE1	3:D:93:GLY:HA3	2.41	0.56
1:B:36:ALA:HB2	1:B:57:PHE:CD2	2.41	0.55
1:B:38:PRO:HB3	1:B:55:SER:HB2	1.89	0.55
1:A:38:PRO:HB3	1:A:55:SER:HB2	1.88	0.55
3:L:92:TYR:O	3:L:100:PHE:O	2.25	0.54
3:D:169:THR:HG22	3:D:179:SER:H	1.73	0.54
1:A:98:ASP:O	1:A:100:LYS:HG3	2.07	0.54
2:C:5:GLU:OE2	2:C:113:GLY:N	2.38	0.54
3:L:21:ILE:HG22	3:L:107:THR:HG21	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:5:GLU:OE1	2:C:92:CYS:HB3	2.08	0.54
2:C:128:VAL:HG21	2:C:213:VAL:HG21	1.89	0.54
2:H:216:LYS:HG2	2:H:218:VAL:HG13	1.90	0.53
2:H:103:TYR:CE1	3:L:93:GLY:HA3	2.44	0.53
2:H:193:SER:O	2:H:197:SER:OG	2.16	0.52
3:D:14:PRO:HA	3:D:112:GLU:HB2	1.92	0.52
1:B:10:LEU:O	3:D:92:TYR:OH	2.26	0.52
2:C:38:GLN:HE22	3:D:38:GLN:HE22	1.58	0.51
1:B:22:GLU:CD	1:B:122:VAL:HG21	2.31	0.51
2:H:5:GLU:OE1	2:H:92:CYS:HB3	2.10	0.51
2:C:23:VAL:HG13	2:C:26:PHE:CZ	2.46	0.51
3:L:149:ILE:CD1	3:L:203:HIS:HB2	2.41	0.50
3:L:168:TRP:N	3:L:168:TRP:CD1	2.79	0.50
2:C:97:ASN:O	2:C:99:GLY:O	2.28	0.50
2:H:178:GLN:HE22	3:L:165:LEU:HD22	1.75	0.50
3:L:129:GLN:HE22	3:L:136:SER:HB2	1.76	0.50
1:B:118:VAL:HG22	1:B:123:THR:HB	1.93	0.50
3:L:21:ILE:HD11	3:L:73:LEU:HD12	1.92	0.50
1:A:69:GLU:OE2	1:A:81:LYS:HE2	2.11	0.50
3:D:168:TRP:N	3:D:168:TRP:CD1	2.80	0.49
2:H:128:VAL:CG1	2:H:213:VAL:HG11	2.43	0.49
1:A:33:ALA:HB2	1:A:57:PHE:CZ	2.48	0.49
3:D:141:LEU:HD12	3:D:141:LEU:N	2.28	0.48
3:D:49:TYR:HD1	3:D:50:LYS:HG2	1.78	0.48
2:H:128:VAL:HG13	2:H:213:VAL:HG11	1.96	0.48
1:A:39:ASN:OD1	1:A:54:GLU:N	2.38	0.48
3:L:14:PRO:HA	3:L:112:GLU:HB2	1.96	0.48
3:D:21:ILE:HG12	3:D:107:THR:HG21	1.96	0.48
3:D:35:TRP:CE2	3:D:73:LEU:HB2	2.48	0.47
2:C:145:LEU:HD23	2:C:217:ILE:HG21	1.95	0.47
3:L:69:THR:HG22	3:L:70:ASP:OD2	2.15	0.47
3:D:198:THR:HB	3:D:213:SER:HB3	1.96	0.47
3:L:141:LEU:HD12	3:L:141:LEU:N	2.30	0.47
2:C:5:GLU:OE1	2:C:111:GLY:HA3	2.15	0.47
3:L:61:ARG:HH22	3:L:82:ASP:CG	2.18	0.46
1:B:44:VAL:O	1:B:44:VAL:HG12	2.15	0.46
2:H:5:GLU:OE1	2:H:111:GLY:HA3	2.16	0.46
3:L:190:GLU:O	3:L:190:GLU:CG	2.64	0.46
3:L:129:GLN:HE22	3:L:136:SER:CB	2.29	0.46
3:L:90:CYS:O	3:L:101:TYR:HA	2.16	0.45
3:D:90:CYS:O	3:D:101:TYR:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:203:ASN:N	2:H:203:ASN:OD1	2.49	0.45
2:H:195:TRP:CG	2:H:196:PRO:HA	2.52	0.45
2:H:39:ALA:HB1	2:H:40:PRO:HD2	1.99	0.45
1:A:109:ASP:HB3	1:A:114:VAL:HG23	1.98	0.45
3:D:190:GLU:O	3:D:190:GLU:HG3	2.16	0.45
2:C:31:TYR:OH	2:C:100:THR:HG22	2.17	0.44
3:D:166:ASN:HD22	3:D:182:SER:HA	1.82	0.44
2:C:103:TYR:CZ	3:D:93:GLY:HA3	2.52	0.44
2:H:129:TYR:CE2	3:L:129:GLN:HG3	2.53	0.44
2:C:195:TRP:CG	2:C:196:PRO:HA	2.52	0.44
1:A:9:LYS:HB2	1:A:131:ALA:HB2	2.00	0.44
3:L:151:VAL:HA	3:L:200:GLU:O	2.18	0.44
1:B:9:LYS:HB2	1:B:131:ALA:HB2	2.00	0.44
2:C:39:ALA:HB1	2:C:40:PRO:HD2	2.00	0.43
2:C:203:ASN:OD1	2:C:203:ASN:N	2.51	0.43
3:D:20:THR:HG22	3:D:74:THR:OG1	2.19	0.43
2:C:105:SER:O	3:D:46:ARG:NH1	2.48	0.43
3:D:129:GLN:HE22	3:D:136:SER:HB2	1.83	0.43
1:B:44:VAL:HG22	1:B:49:VAL:HG22	2.01	0.43
3:D:15:VAL:HG23	3:D:112:GLU:O	2.19	0.43
2:H:192:SER:O	2:H:195:TRP:O	2.37	0.42
3:L:35:TRP:CE2	3:L:73:LEU:HB2	2.54	0.42
2:C:131:LEU:HB2	2:C:146:GLY:CA	2.49	0.42
2:H:37:ARG:HB3	2:H:47:ILE:HD11	2.00	0.42
2:C:128:VAL:HG21	2:C:213:VAL:CG2	2.49	0.42
2:C:37:ARG:HB3	2:C:47:ILE:HD11	2.00	0.42
3:L:160:ARG:HE	3:L:162:ASN:HB3	1.85	0.42
2:C:126:PRO:HB3	2:C:152:TYR:HB3	2.02	0.42
2:C:97:ASN:O	2:C:98:ASP:C	2.54	0.42
3:D:71:PHE:CD1	3:D:71:PHE:N	2.88	0.42
2:H:87:THR:HG23	2:H:117:THR:HA	2.01	0.41
1:B:47:ASP:OD1	1:B:47:ASP:C	2.58	0.41
1:B:39:ASN:OD1	1:B:54:GLU:N	2.37	0.41
2:C:87:THR:HG23	2:C:117:THR:HA	2.01	0.41
2:H:130:PRO:O	2:H:131:LEU:HD12	2.21	0.41
1:A:7:THR:HG23	1:A:41:ILE:HG12	2.02	0.41
1:B:18:ASP:HA	1:B:21:LYS:HE3	2.01	0.41
2:C:192:SER:O	2:C:195:TRP:O	2.39	0.41
1:B:93:GLN:HE21	1:B:104:ILE:HG13	1.84	0.41
2:H:81:SER:O	2:H:81:SER:OG	2.37	0.41
3:L:160:ARG:NE	3:L:162:ASN:HB3	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:193:SER:O	2:C:197:SER:OG	2.15	0.41
2:C:46:TRP:CZ2	2:C:48:GLY:HA2	2.56	0.40
2:H:109:LEU:HD12	2:H:109:LEU:HA	1.93	0.40
2:H:126:PRO:HB3	2:H:152:TYR:HB3	2.04	0.40
3:L:66:GLY:HA3	3:L:71:PHE:HA	2.04	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	129/132 (98%)	116 (90%)	13 (10%)	0	100	100
1	B	129/132 (98%)	116 (90%)	13 (10%)	0	100	100
2	C	212/222 (96%)	199 (94%)	13 (6%)	0	100	100
2	H	210/222 (95%)	195 (93%)	15 (7%)	0	100	100
3	D	214/219 (98%)	197 (92%)	17 (8%)	0	100	100
3	L	214/219 (98%)	198 (92%)	15 (7%)	1 (0%)	29	68
All	All	1108/1146 (97%)	1021 (92%)	86 (8%)	1 (0%)	51	85

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	159	GLU

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	113/114 (99%)	102 (90%)	11 (10%)	8 31
1	B	113/114 (99%)	101 (89%)	12 (11%)	6 26
2	C	184/189 (97%)	168 (91%)	16 (9%)	10 37
2	H	183/189 (97%)	163 (89%)	20 (11%)	6 25
3	D	189/192 (98%)	166 (88%)	23 (12%)	5 21
3	L	189/192 (98%)	167 (88%)	22 (12%)	5 23
All	All	971/990 (98%)	867 (89%)	104 (11%)	6 26

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	CYS
1	A	2	ASP
1	A	13	SER
1	A	29	THR
1	A	48	LEU
1	A	57	PHE
1	A	79	LYS
1	A	116	GLU
1	A	118	VAL
1	A	120	LYS
1	A	126	ARG
2	H	30	THR
2	H	56	THR
2	H	65	ARG
2	H	67	THR
2	H	72	SER
2	H	85	GLU
2	H	92	CYS
2	H	128	VAL
2	H	140	ASN
2	H	143	VAL
2	H	147	CYS
2	H	157	VAL
2	H	166	LEU
2	H	167	SER
2	H	179	SER
2	H	180	ASP

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Mol	Chain	Res	Type
2	H	185	SER
2	H	197	SER
2	H	202	CYS
2	H	203	ASN
3	L	21	ILE
3	L	23	CYS
3	L	33	LEU
3	L	46	ARG
3	L	50	LYS
3	L	69	THR
3	L	73	LEU
3	L	77	ASP
3	L	80	CYS
3	L	88	CYS
3	L	94	THR
3	L	101	TYR
3	L	113	ARG
3	L	121	SER
3	L	127	SER
3	L	150	ASN
3	L	168	TRP
3	L	181	SER
3	L	193	ARG
3	L	198	THR
3	L	202	THR
3	L	204	LYS
1	B	1	CYS
1	B	2	ASP
1	B	13	SER
1	B	14	GLU
1	B	18	ASP
1	B	22	GLU
1	B	29	THR
1	B	48	LEU
1	B	73	ILE
1	B	79	LYS
1	B	104	ILE
1	B	126	ARG
2	C	17	LEU
2	C	19	LEU
2	C	30	THR
2	C	67	THR

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Mol	Chain	Res	Type
2	C	92	CYS
2	C	98	ASP
2	C	147	CYS
2	C	157	VAL
2	C	158	THR
2	C	167	SER
2	C	178	GLN
2	C	185	SER
2	C	197	SER
2	C	202	CYS
2	C	203	ASN
2	C	218	VAL
3	D	7	THR
3	D	23	CYS
3	D	46	ARG
3	D	47	LEU
3	D	73	LEU
3	D	80	CYS
3	D	88	CYS
3	D	94	THR
3	D	95	TYR
3	D	101	TYR
3	D	113	ARG
3	D	119	THR
3	D	121	SER
3	D	131	THR
3	D	132	SER
3	D	150	ASN
3	D	152	LYS
3	D	168	TRP
3	D	181	SER
3	D	192	GLU
3	D	198	THR
3	D	202	THR
3	D	208	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	140	ASN
2	H	162	ASN
2	H	178	GLN

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Mol	Chain	Res	Type
3	L	150	ASN
3	L	166	ASN
1	B	93	GLN
2	C	162	ASN
3	D	38	GLN
3	D	166	ASN
3	D	171	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	131/132 (99%)	-0.47	1 (0%)	86	65	35, 55, 75, 98	0
1	B	131/132 (99%)	-0.18	1 (0%)	86	65	45, 83, 125, 170	0
2	C	216/222 (97%)	-0.41	1 (0%)	91	75	20, 50, 87, 123	0
2	H	214/222 (96%)	-0.51	0	100	100	27, 54, 82, 93	0
3	D	216/219 (98%)	-0.45	0	100	100	33, 61, 84, 98	0
3	L	216/219 (98%)	-0.46	0	100	100	34, 61, 98, 110	0
All	All	1124/1146 (98%)	-0.43	3 (0%)	94	84	20, 58, 99, 170	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	57	PHE	3.3
2	C	138	GLN	2.3
1	A	131	ALA	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.