Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 09:03 pm BST

PDB ID	:	4ZFF
Title	:	Dual-acting Fab 5A12 in complex with VEGF
Authors	:	Harris, S.F.; Wu, P.
Deposited on	:	2015-04-21
Resolution	:	2.75 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 following versions of software and data (see references ⓘ) were used in the production of this report:

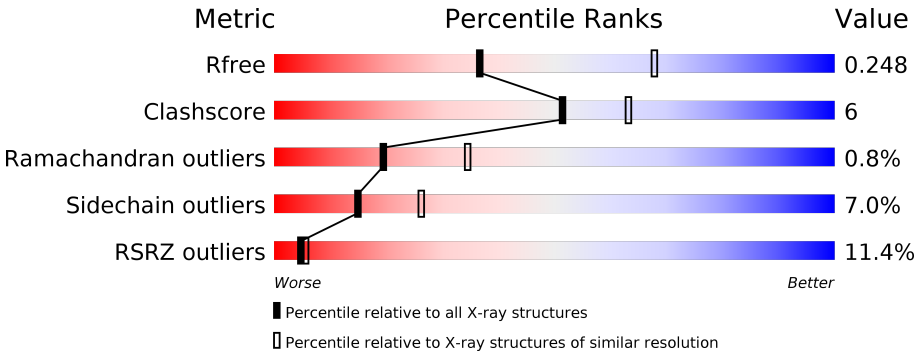
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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 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	228	25% 74% 15% • 10%
1	H	228	% 77% 14% • 7%
2	B	215	25% 80% 15% • •
2	L	215	% 82% 15% • •
3	C	99	85% 11% • •
3	D	99	2% 86% 14%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8374 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 Fragment antigen binding (Fab) 5A12 Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	206	Total	C	N	O	S	0	1	0
			1554	997	252	299	6			
1	H	211	Total	C	N	O	S	0	0	0
			1589	1019	259	305	6			

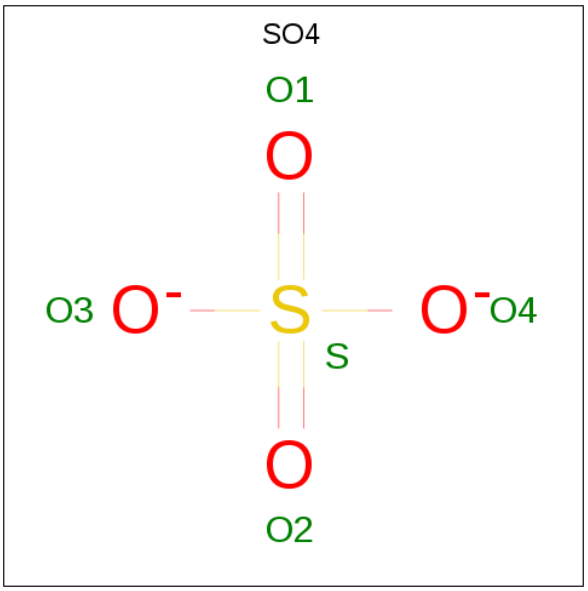
- Molecule 2 is a protein called Fragment antigen binding (Fab) 5A12 Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	210	Total	C	N	O	S	0	0	0
			1600	1006	266	323	5			
2	L	213	Total	C	N	O	S	0	0	0
			1622	1020	270	327	5			

- Molecule 3 is a protein called Vascular endothelial growth factor A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	96	Total	C	N	O	S	0	0	0
			775	486	130	146	13			
3	D	99	Total	C	N	O	S	0	0	0
			800	501	137	149	13			

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	L	1	Total O S 5 4 1	0	0

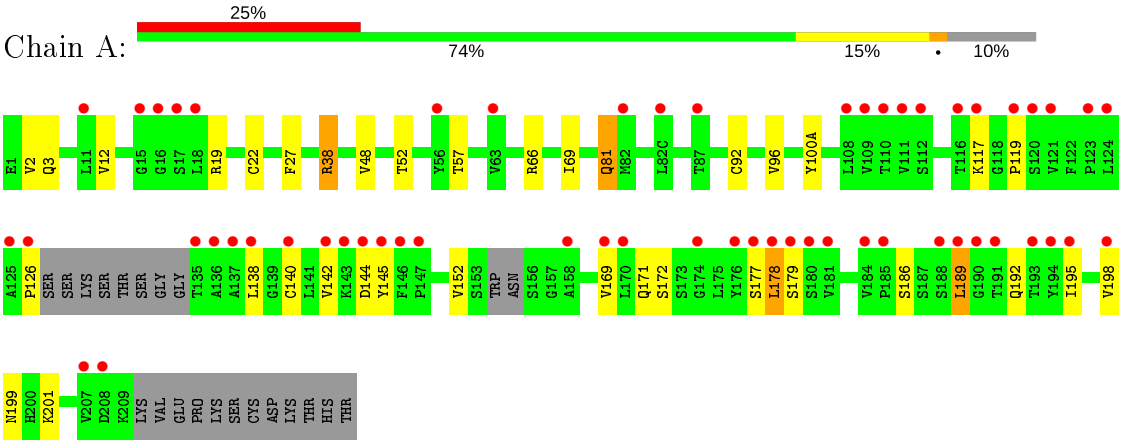
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	18	Total O 18 18	0	0
5	B	29	Total O 29 29	0	0
5	C	43	Total O 43 43	0	0
5	D	49	Total O 49 49	0	0
5	H	138	Total O 138 138	0	0
5	L	152	Total O 152 152	0	0

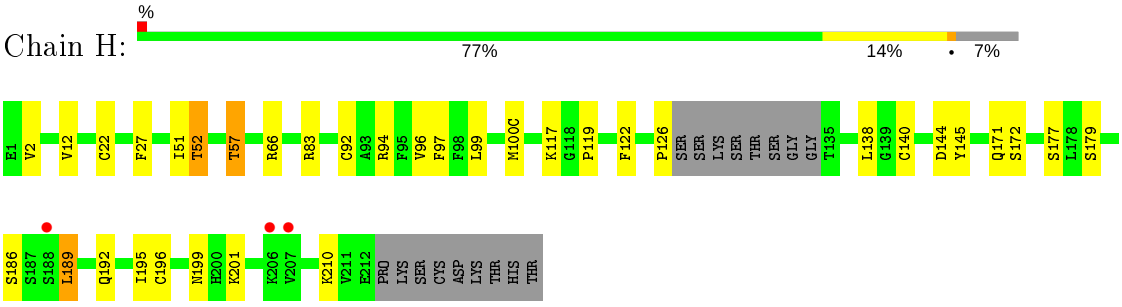
3 Residue-property plots (i)

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

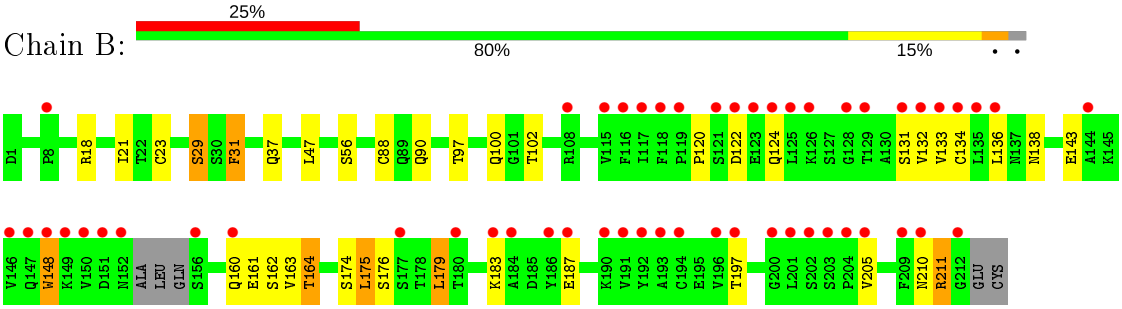
• Molecule 1: Fragment antigen binding (Fab) 5A12 Heavy chain



• Molecule 1: Fragment antigen binding (Fab) 5A12 Heavy chain

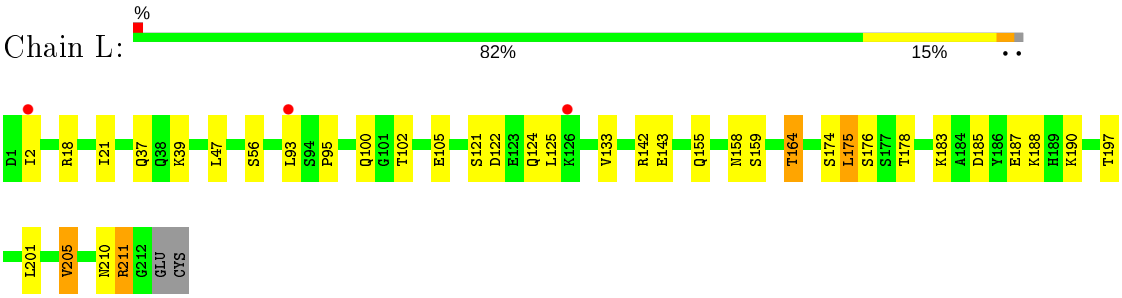


• Molecule 2: Fragment antigen binding (Fab) 5A12 Light chain



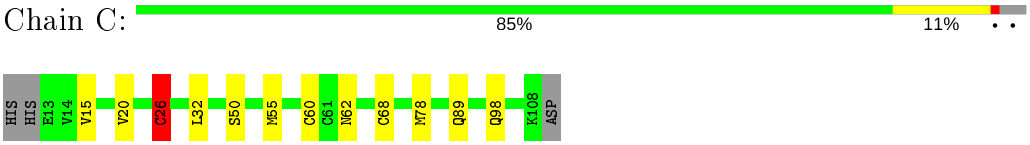
• Molecule 2: Fragment antigen binding (Fab) 5A12 Light chain

Chain L:



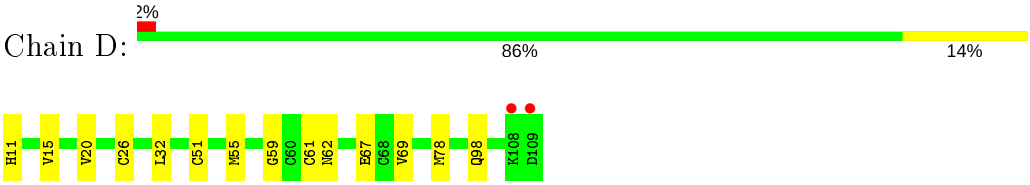
• Molecule 3: Vascular endothelial growth factor A

Chain C:



• Molecule 3: Vascular endothelial growth factor A

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	87.41Å 313.89Å 51.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.95 – 2.75 48.61 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.9 (26.95-2.75) 99.9 (48.61-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.53 (at 2.77Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.197 , 0.238 0.202 , 0.248	Depositor DCC
R_{free} test set	1934 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å^2)	51.1	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 85.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	8374	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% 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

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.41	0/1595	0.70	0/2178
1	H	0.51	0/1632	0.72	1/2230 (0.0%)
2	B	0.42	0/1634	0.68	0/2215
2	L	0.53	0/1657	0.75	1/2248 (0.0%)
3	C	0.48	0/793	0.68	0/1069
3	D	0.51	0/820	0.74	1/1106 (0.1%)
All	All	0.47	0/8131	0.71	3/11046 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	61	CYS	N-CA-C	-5.75	95.48	111.00
2	L	175	LEU	CA-CB-CG	5.50	127.95	115.30
1	H	99	LEU	N-CA-C	-5.06	97.34	111.00

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	1554	0	1516	14	0
1	H	1589	0	1553	16	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1600	0	1567	18	0
2	L	1622	0	1590	16	0
3	C	775	0	742	13	0
3	D	800	0	758	11	0
4	L	5	0	0	0	0
5	A	18	0	0	0	0
5	B	29	0	0	0	0
5	C	43	0	0	0	0
5	D	49	0	0	1	0
5	H	138	0	0	2	0
5	L	152	0	0	2	0
All	All	8374	0	7726	76	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 6.

All (76) 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:60:CYS:HG	3:D:51:CYS:HG	0.88	0.85
3:C:89:GLN:HE22	1:H:97:PHE:H	1.28	0.78
1:H:195:ILE:HG22	1:H:210:LYS:HA	1.68	0.74
3:C:50:SER:H	3:D:62:ASN:ND2	1.90	0.69
2:B:148:TRP:CE3	2:B:179:LEU:HD11	2.30	0.66
3:C:15:VAL:HB	3:D:78:MET:HG2	1.79	0.62
1:H:140:CYS:HG	1:H:196:CYS:CB	2.11	0.62
2:B:148:TRP:CE2	2:B:179:LEU:HD21	2.35	0.61
3:C:60:CYS:CB	3:D:51:CYS:HG	2.17	0.58
2:L:183:LYS:O	2:L:187:GLU:HG2	2.04	0.57
3:C:78:MET:HG2	3:D:15:VAL:HB	1.86	0.57
2:B:183:LYS:O	2:B:187:GLU:HG2	2.05	0.57
2:B:120:PRO:HD3	2:B:132:VAL:HG22	1.87	0.57
1:H:22:CYS:CB	1:H:92:CYS:HG	2.18	0.56
2:L:105:GLU:HG2	5:L:471:HOH:O	2.05	0.56
2:L:164:THR:HG22	2:L:174:SER:H	1.71	0.55
2:B:134:CYS:HB2	2:B:148:TRP:CH2	2.41	0.55
2:L:37:GLN:HB2	2:L:47:LEU:HD11	1.89	0.55
2:L:185:ASP:HA	2:L:188:LYS:HE2	1.90	0.53
2:B:23:CYS:CB	2:B:88:CYS:HG	2.20	0.52
1:A:22:CYS:CB	1:A:92:CYS:HG	2.22	0.52
2:L:155:GLN:HE21	2:L:158:ASN:HD21	1.58	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:179:LEU:H	2:B:179:LEU:HD22	1.76	0.50
2:B:37:GLN:HB2	2:B:47:LEU:HD11	1.93	0.50
3:C:26:CYS:CB	3:C:68:CYS:HG	2.17	0.50
1:H:119:PRO:HB3	1:H:145:TYR:HB3	1.95	0.49
1:A:119:PRO:HB3	1:A:145:TYR:HB3	1.94	0.49
1:A:152:VAL:HG23	1:A:198:VAL:HG22	1.95	0.48
1:A:199:ASN:HD21	1:A:201:LYS:HE2	1.77	0.48
2:L:201:LEU:HD13	2:L:205:VAL:HG13	1.95	0.48
1:H:199:ASN:HD21	1:H:201:LYS:HE2	1.78	0.48
3:C:50:SER:H	3:D:62:ASN:HD22	1.60	0.48
1:H:195:ILE:HD11	5:H:326:HOH:O	2.13	0.47
2:L:95:PRO:HB2	5:L:405:HOH:O	2.15	0.47
1:A:19:ARG:HG3	1:A:81:GLN:HG2	1.97	0.47
1:H:51:ILE:HG12	1:H:57:THR:HG22	1.97	0.47
3:D:55:MET:H	3:D:98:GLN:NE2	2.13	0.47
3:C:55:MET:H	3:C:98:GLN:NE2	2.14	0.46
1:A:38:ARG:HG2	1:A:48:VAL:CG2	2.46	0.46
3:C:55:MET:H	3:C:98:GLN:HE21	1.63	0.45
2:L:155:GLN:HE21	2:L:158:ASN:ND2	2.14	0.45
3:D:67:GLU:HG3	3:D:69:VAL:HG13	1.99	0.45
1:A:142:VAL:HB	1:A:178:LEU:HB3	1.98	0.45
3:D:55:MET:H	3:D:98:GLN:HE21	1.64	0.45
1:H:195:ILE:HG22	1:H:210:LYS:CA	2.42	0.45
1:H:186:SER:HA	1:H:189:LEU:HD12	1.98	0.45
2:L:159:SER:HA	2:L:178:THR:O	2.18	0.44
1:H:126:PRO:HD3	1:H:138:LEU:HB3	2.00	0.44
2:L:190:LYS:O	2:L:210:ASN:HA	2.18	0.43
1:A:186:SER:HA	1:A:189:LEU:HD12	1.99	0.43
1:A:169:VAL:HG22	2:B:162:SER:HB2	2.00	0.43
1:H:52:THR:HG22	5:H:309:HOH:O	2.17	0.43
1:H:171:GLN:NE2	1:H:177:SER:HB2	2.33	0.43
2:B:29:SER:HB2	2:B:31:PHE:CZ	2.54	0.43
3:D:51:CYS:HB3	5:D:218:HOH:O	2.18	0.42
1:A:100(A):TYR:OH	3:C:62:ASN:HB3	2.18	0.42
3:C:26:CYS:CB	3:C:68:CYS:SG	3.05	0.42
2:B:136:LEU:HD22	2:B:175:LEU:HD23	2.01	0.42
1:H:2:VAL:HG13	1:H:27:PHE:CD1	2.55	0.42
2:B:21:ILE:HG12	2:B:102:THR:HG21	2.00	0.42
2:L:21:ILE:HG12	2:L:102:THR:HG21	2.01	0.42
1:H:94:ARG:O	1:H:100(C):MET:HA	2.19	0.42
1:A:126:PRO:HD3	1:A:138:LEU:HB3	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:2:ILE:HD11	2:L:93:LEU:HD22	2.02	0.41
2:B:163:VAL:HG22	2:B:175:LEU:HD13	2.01	0.41
2:B:210:ASN:O	2:B:211:ARG:HB2	2.21	0.41
2:B:164:THR:HG22	2:B:174:SER:H	1.85	0.41
1:H:122:PHE:CE2	2:L:124:GLN:HG3	2.55	0.41
1:A:171:GLN:NE2	1:A:177:SER:HB2	2.36	0.41
1:A:2:VAL:HG13	1:A:27:PHE:CD1	2.55	0.41
3:C:32:LEU:HD13	3:D:59:GLY:CA	2.51	0.41
2:B:90:GLN:HG3	2:B:97:THR:HG22	2.03	0.41
1:A:169:VAL:CG2	2:B:162:SER:HB2	2.52	0.40
2:L:121:SER:O	2:L:125:LEU:HD23	2.20	0.40
2:B:124:GLN:HE22	2:B:131:SER:H	1.70	0.40
2:L:210:ASN:O	2:L:211:ARG:HB2	2.22	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	201/228 (88%)	194 (96%)	6 (3%)	1 (0%)	29	47
1	H	207/228 (91%)	201 (97%)	5 (2%)	1 (0%)	29	47
2	B	206/215 (96%)	195 (95%)	8 (4%)	3 (2%)	10	18
2	L	211/215 (98%)	204 (97%)	6 (3%)	1 (0%)	29	47
3	C	94/99 (95%)	93 (99%)	0	1 (1%)	14	25
3	D	97/99 (98%)	92 (95%)	4 (4%)	1 (1%)	15	27
All	All	1016/1084 (94%)	979 (96%)	29 (3%)	8 (1%)	19	34

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	26	CYS
1	A	144	ASP
2	B	211	ARG
2	L	211	ARG
2	B	138	ASN
1	H	144	ASP
2	B	31	PHE
3	C	26	CYS

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	169/188 (90%)	152 (90%)	17 (10%)	7 12
1	H	173/188 (92%)	162 (94%)	11 (6%)	17 31
2	B	183/187 (98%)	167 (91%)	16 (9%)	10 18
2	L	185/187 (99%)	172 (93%)	13 (7%)	15 26
3	C	90/94 (96%)	88 (98%)	2 (2%)	52 70
3	D	92/94 (98%)	89 (97%)	3 (3%)	38 58
All	All	892/938 (95%)	830 (93%)	62 (7%)	15 26

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	12	VAL
1	A	38	ARG
1	A	52	THR
1	A	57	THR
1	A	66	ARG
1	A	69	ILE
1	A	81	GLN
1	A	96	VAL
1	A	117	LYS
1	A	140	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	172	SER
1	A	178	LEU
1	A	179	SER
1	A	189	LEU
1	A	192	GLN
1	A	195	ILE
2	B	18	ARG
2	B	29	SER
2	B	56	SER
2	B	100	GLN
2	B	122	ASP
2	B	133	VAL
2	B	143	GLU
2	B	148	TRP
2	B	160	GLN
2	B	161	GLU
2	B	164	THR
2	B	175	LEU
2	B	176	SER
2	B	179	LEU
2	B	197	THR
2	B	205	VAL
3	C	20	VAL
3	C	26	CYS
3	D	11	HIS
3	D	20	VAL
3	D	32	LEU
1	H	12	VAL
1	H	52	THR
1	H	57	THR
1	H	66	ARG
1	H	83	ARG
1	H	96	VAL
1	H	117	LYS
1	H	172	SER
1	H	179	SER
1	H	189	LEU
1	H	192	GLN
2	L	18	ARG
2	L	39	LYS
2	L	56	SER
2	L	100	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L	122	ASP
2	L	133	VAL
2	L	142	ARG
2	L	143	GLU
2	L	164	THR
2	L	175	LEU
2	L	176	SER
2	L	197	THR
2	L	205	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	197	ASN
1	A	199	ASN
2	B	124	GLN
3	C	22	GLN
3	C	89	GLN
3	C	98	GLN
3	D	22	GLN
3	D	62	ASN
3	D	98	GLN
1	H	199	ASN
2	L	155	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

1 ligand 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	$\#\|Z\| > 2$
4	SO4	L	301	-	4,4,4	0.34	0	6,6,6	0.20	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	206/228 (90%)	1.28	57 (27%) 0 0	54, 111, 146, 158	0
1	H	211/228 (92%)	0.01	3 (1%) 75 82	24, 42, 80, 101	0
2	B	210/215 (97%)	1.41	53 (25%) 0 0	56, 101, 143, 150	0
2	L	213/215 (99%)	-0.10	3 (1%) 75 82	24, 38, 68, 85	0
3	C	96/99 (96%)	-0.08	0 100 100	30, 49, 89, 100	0
3	D	99/99 (100%)	0.15	2 (2%) 65 73	31, 47, 79, 105	0
All	All	1035/1084 (95%)	0.53	118 (11%) 5 5	24, 59, 140, 158	0

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	196	VAL	8.7
2	B	148	TRP	7.6
2	B	209	PHE	7.2
1	A	119	PRO	7.0
1	A	174	GLY	6.8
2	B	135	LEU	6.7
2	B	193	ALA	6.4
1	A	138	LEU	6.2
2	B	191	VAL	5.9
1	A	194	TYR	5.8
1	A	207	VAL	5.7
1	A	112	SER	5.6
2	B	201	LEU	5.2
2	B	194	CYS	5.1
1	A	184	VAL	5.1
2	B	115	VAL	5.1
1	A	142	VAL	4.9
2	B	136	LEU	4.8
1	A	145	TYR	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	147	GLN	4.6
1	A	147	PRO	4.6
3	D	109	ASP	4.5
1	A	185	PRO	4.5
2	B	117	ILE	4.3
1	A	11	LEU	4.3
1	A	125	ALA	4.3
2	B	152	ASN	4.3
2	B	205	VAL	4.2
2	B	116	PHE	4.2
1	A	146	PHE	4.1
1	A	136	ALA	4.0
2	B	192	TYR	3.9
1	A	121	VAL	3.9
2	B	108	ARG	3.9
2	B	126	LYS	3.8
1	A	124	LEU	3.7
2	B	180	THR	3.7
2	B	132	VAL	3.7
2	B	160	GLN	3.6
2	B	200	GLY	3.6
1	A	191	THR	3.6
1	A	120	SER	3.5
2	B	149	LYS	3.5
2	B	133	VAL	3.5
1	A	188	SER	3.4
1	A	109	VAL	3.4
2	L	93	LEU	3.4
1	A	169	VAL	3.4
2	B	186	TYR	3.3
2	B	128	GLY	3.3
2	B	134	CYS	3.2
1	A	110	THR	3.1
1	A	18	LEU	3.1
2	B	146	VAL	3.1
1	A	16	GLY	3.1
2	B	197	THR	3.0
2	B	150	VAL	3.0
2	B	202	SER	3.0
2	B	184	ALA	2.9
1	A	87	THR	2.9
1	A	116	THR	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	170	LEU	2.8
2	B	122	ASP	2.8
1	A	63	VAL	2.8
1	A	135	THR	2.8
2	B	183	LYS	2.8
2	B	156	SER	2.7
1	A	190	GLY	2.7
1	A	208	ASP	2.7
1	A	177	SER	2.7
1	A	126	PRO	2.6
2	B	119	PRO	2.6
2	B	125	LEU	2.6
1	A	17	SER	2.6
2	B	8	PRO	2.6
2	B	129	THR	2.6
1	H	188	SER	2.6
2	B	204	PRO	2.5
2	L	126	LYS	2.5
1	A	180	SER	2.5
2	B	118	PHE	2.5
1	A	176	TYR	2.5
2	B	210	ASN	2.5
1	A	189	LEU	2.5
1	A	198	VAL	2.4
2	B	212	GLY	2.4
1	A	140	CYS	2.4
2	B	203	SER	2.4
2	L	2	ILE	2.4
1	A	178	LEU	2.4
1	A	111	VAL	2.4
1	A	195	ILE	2.3
2	B	151	ASP	2.3
1	H	207	VAL	2.3
2	B	131	SER	2.3
1	A	193	THR	2.2
2	B	123	GLU	2.2
1	A	108	LEU	2.2
1	A	144	ASP	2.2
1	H	206	LYS	2.2
1	A	143	LYS	2.2
1	A	179	SER	2.2
1	A	15	GLY	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	144	ALA	2.1
3	D	108	LYS	2.1
1	A	82(C)	LEU	2.1
1	A	123	PRO	2.1
1	A	181	VAL	2.1
1	A	82	MET	2.1
2	B	177	SER	2.1
1	A	56[A]	TYR	2.1
1	A	158	ALA	2.1
2	B	187	GLU	2.1
2	B	124	GLN	2.0
2	B	121	SER	2.0
1	A	117	LYS	2.0
1	A	137	ALA	2.0
2	B	190	LYS	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 carbohydrates in this entry.

6.4 Ligands (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. 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	B-factors(Å^2)	Q<0.9
4	SO4	L	301	5/5	0.98	0.15	47,49,51,52	0

6.5 Other polymers (i)

There are no such residues in this entry.