



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 03:13 pm GMT

PDB ID : 2FJG
Title : Structure of the G6 Fab, a phage derived Fab fragment, in complex with VEGF
Authors : Wiesmann, C.
Deposited on : 2006-01-02
Resolution : 2.80 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

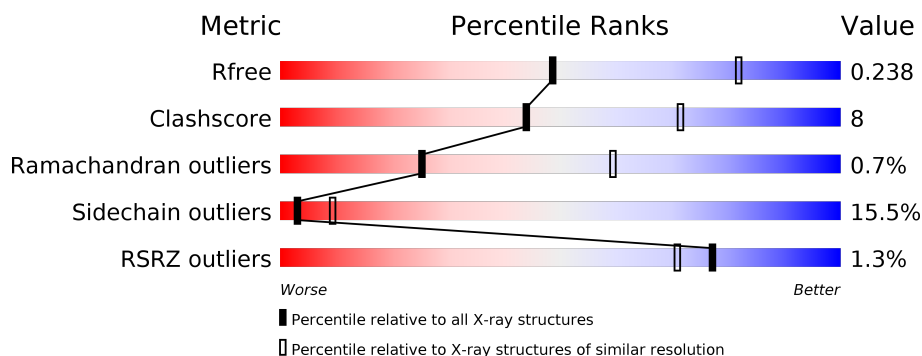
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

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 $\leq 5\%$. 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	V	102	<div> <div>69%</div> <div>16%</div> <div>8%</div> <div>7%</div> </div>
1	W	102	<div> <div>64%</div> <div>21%</div> <div>7%</div> <div>8%</div> </div>
2	A	214	<div> <div>71%</div> <div>22%</div> </div>
2	L	214	<div> <div>73%</div> <div>22%</div> </div>
3	B	227	<div> <div>72%</div> <div>22%</div> </div>
3	H	227	<div> <div>73%</div> <div>21%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	H	228	-	-	-	X
4	SO4	H	229	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8066 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 Vascular endothelial growth factor A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	V	95	Total	C	N	O	S	0	0	0
			770	484	130	143	13			
1	W	94	Total	C	N	O	S	0	0	0
			761	478	128	142	13			

- Molecule 2 is a protein called Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	211	Total	C	N	O	S	0	0	0
			1617	1014	268	330	5			
2	A	211	Total	C	N	O	S	0	0	0
			1617	1014	268	330	5			

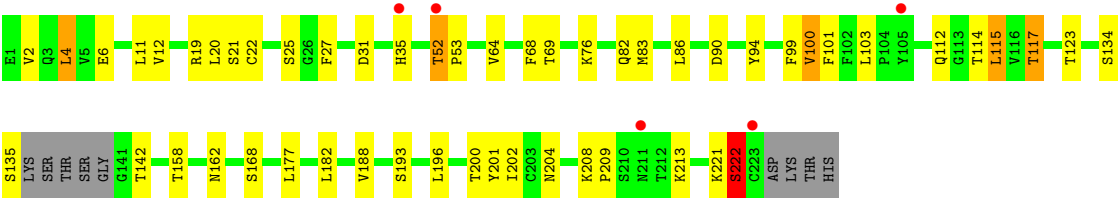
- Molecule 3 is a protein called Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	218	Total	C	N	O	S	0	0	0
			1633	1044	267	315	7			
3	B	218	Total	C	N	O	S	0	0	0
			1633	1044	267	315	7			

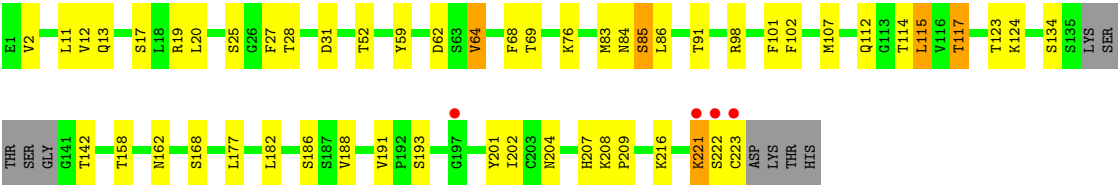
- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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



● Molecule 3: Fab heavy chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	117.88Å 117.88Å 212.56Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.80 29.47 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (20.00-2.80) 99.7 (29.47-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.63 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.199 , 0.239 0.202 , 0.238	Depositor DCC
R_{free} test set	2158 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	64.0	Xtriage
Anisotropy	0.163	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 36.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.017 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8066	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	V	0.70	1/788 (0.1%)	0.94	3/1061 (0.3%)
1	W	0.68	0/779	0.93	4/1050 (0.4%)
2	A	0.64	0/1653	0.87	7/2248 (0.3%)
2	L	0.64	0/1653	0.84	6/2248 (0.3%)
3	B	0.64	0/1677	0.82	1/2290 (0.0%)
3	H	0.60	0/1677	0.81	2/2290 (0.1%)
All	All	0.64	1/8227 (0.0%)	0.85	23/11187 (0.2%)

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
1	V	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	V	63	ASP	CB-CG	5.39	1.63	1.51

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	V	63	ASP	CB-CG-OD2	8.91	126.32	118.30
2	A	28	ASP	CB-CG-OD2	7.85	125.37	118.30
1	W	63	ASP	CB-CG-OD2	7.01	124.61	118.30
2	A	108	ARG	NE-CZ-NH1	6.57	123.58	120.30
2	L	122	ASP	CB-CG-OD2	6.53	124.18	118.30
1	W	19	ASP	CB-CG-OD2	6.46	124.11	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	V	63	ASP	CB-CA-C	6.45	123.30	110.40
2	A	70	ASP	CB-CG-OD2	6.33	124.00	118.30
2	L	28	ASP	CB-CG-OD2	6.33	123.99	118.30
2	L	70	ASP	CB-CG-OD2	6.17	123.85	118.30
3	H	90	ASP	CB-CG-OD2	5.96	123.66	118.30
2	L	82	ASP	CB-CG-OD2	5.60	123.34	118.30
3	B	62	ASP	CB-CG-OD2	5.53	123.28	118.30
2	L	1	ASP	CB-CG-OD2	5.48	123.23	118.30
2	A	122	ASP	CB-CG-OD2	5.42	123.18	118.30
2	L	151	ASP	CB-CG-OD2	5.41	123.17	118.30
2	A	167	ASP	CB-CG-OD2	5.38	123.14	118.30
2	A	108	ARG	NE-CZ-NH2	-5.35	117.63	120.30
2	A	151	ASP	CB-CG-OD2	5.35	123.11	118.30
1	W	63	ASP	CB-CA-C	5.27	120.95	110.40
1	V	63	ASP	OD1-CG-OD2	-5.13	113.55	123.30
1	W	41	ASP	CB-CG-OD2	5.10	122.89	118.30
3	H	31	ASP	CB-CG-OD2	5.02	122.81	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	V	65	GLY	Peptide

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	V	770	0	739	23	0
1	W	761	0	726	22	0
2	A	1617	0	1573	29	0
2	L	1617	0	1573	17	0
3	B	1633	0	1592	26	0
3	H	1633	0	1592	17	0
4	B	20	0	0	2	0
4	H	15	0	0	0	0
All	All	8066	0	7795	120	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 8.

All (120) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:89:GLN:HE22	3:B:101:PHE:H	1.04	0.99
1:V:62:ASN:O	1:W:48:LYS:NZ	2.02	0.92
1:W:64:GLU:OE1	2:L:92:TYR:OH	1.92	0.87
1:V:64:GLU:OE1	2:A:92:TYR:OH	2.03	0.77
1:V:89:GLN:HE22	3:H:101:PHE:H	1.31	0.76
1:W:70:PRO:HB3	1:W:99:HIS:ND1	2.05	0.71
1:V:65:GLY:O	1:V:107:LYS:HB2	1.95	0.66
2:L:113:PRO:HD3	2:L:198:HIS:ND1	2.11	0.66
1:V:36:PHE:CE2	1:V:43:ILE:HG22	2.31	0.65
1:W:46:ILE:HD12	1:W:85:PRO:HG3	1.79	0.65
1:W:70:PRO:HG3	1:W:99:HIS:CE1	2.32	0.64
2:A:94:THR:OG1	3:B:52:THR:HG21	1.98	0.63
3:B:124:LYS:NZ	4:B:231:SO4:O1	2.32	0.62
2:L:90:GLN:NE2	2:L:93:THR:O	2.22	0.62
3:B:2:VAL:HG13	3:B:27:PHE:CD1	2.35	0.61
1:V:46:ILE:HD12	1:V:85:PRO:HG3	1.81	0.61
1:V:67:GLU:HB3	1:V:107:LYS:HD3	1.84	0.60
1:V:67:GLU:HG3	1:V:69:VAL:HG13	1.84	0.60
1:W:89:GLN:HE22	3:B:101:PHE:N	1.87	0.60
2:A:105:GLU:OE2	2:A:173:TYR:OH	2.17	0.59
3:B:91:THR:HG23	3:B:117:THR:HA	1.85	0.59
3:H:115:LEU:HD22	3:H:117:THR:HG22	1.86	0.58
2:A:42:LYS:HZ3	2:A:42:LYS:HA	1.68	0.58
1:W:63:ASP:O	1:W:64:GLU:CB	2.51	0.58
3:B:162:ASN:ND2	3:B:202:ILE:H	2.02	0.58
1:W:67:GLU:HG2	1:W:69:VAL:HG13	1.88	0.56
1:W:24:SER:OG	1:W:60:CYS:SG	2.64	0.55
3:B:2:VAL:HG13	3:B:27:PHE:HD1	1.72	0.54
2:A:40:PRO:HG2	2:A:165:GLU:HG2	1.88	0.54
3:H:162:ASN:ND2	3:H:202:ILE:H	2.05	0.53
2:L:90:GLN:HE21	2:L:93:THR:H	1.56	0.53
3:B:162:ASN:HD21	3:B:202:ILE:H	1.56	0.52
3:H:2:VAL:HG13	3:H:27:PHE:CD1	2.45	0.52
2:L:31:THR:O	2:L:50:SER:HA	2.10	0.50
2:L:32:ALA:CB	2:L:92:TYR:CG	2.94	0.50
2:A:94:THR:CG2	2:A:95:PRO:HA	2.41	0.50
1:W:70:PRO:HB3	1:W:99:HIS:HD1	1.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:90:GLN:NE2	2:A:92:TYR:H	2.10	0.50
2:A:108:ARG:HD3	2:A:109:THR:O	2.11	0.50
3:B:83:MET:HB3	3:B:86:LEU:HD21	1.92	0.49
1:W:106:PRO:HG2	2:L:28:ASP:HB3	1.95	0.49
2:A:189:HIS:N	2:A:189:HIS:CD2	2.80	0.49
3:B:115:LEU:HD13	3:B:117:THR:HG22	1.95	0.49
1:V:27:HIS:HB2	1:V:28:PRO:HD2	1.94	0.49
3:B:191:VAL:HG11	3:B:201:TYR:CE1	2.47	0.48
3:H:52:THR:HG23	3:H:53:PRO:HD2	1.95	0.48
2:L:32:ALA:HB1	2:L:92:TYR:HB2	1.96	0.48
3:H:68:PHE:HA	3:H:82:GLN:O	2.13	0.48
1:W:70:PRO:CG	1:W:99:HIS:CE1	2.97	0.48
2:A:40:PRO:HG2	2:A:165:GLU:CG	2.44	0.48
2:A:198:HIS:ND1	2:A:199:GLN:N	2.62	0.47
1:V:64:GLU:CD	1:V:64:GLU:N	2.67	0.47
1:V:27:HIS:HB2	1:V:28:PRO:CD	2.44	0.47
1:V:61:CYS:O	1:V:63:ASP:N	2.48	0.47
1:W:63:ASP:O	1:W:64:GLU:HB3	2.14	0.47
2:A:95:PRO:HB3	3:B:59:TYR:CE2	2.50	0.47
2:L:183:LYS:O	2:L:187:GLU:HG2	2.14	0.47
1:W:70:PRO:HG3	1:W:99:HIS:HE1	1.80	0.47
1:V:106:PRO:HG2	2:A:28:ASP:HB3	1.97	0.46
2:A:89:GLN:HG3	2:A:98:PHE:CE2	2.51	0.46
3:B:208:LYS:N	3:B:209:PRO:CD	2.79	0.46
3:H:162:ASN:HD21	3:H:202:ILE:H	1.62	0.46
3:B:64:VAL:HG13	3:B:68:PHE:HB2	1.95	0.46
2:L:40:PRO:HG2	2:L:165:GLU:CG	2.46	0.46
2:A:29:VAL:O	2:A:32:ALA:HB3	2.16	0.46
3:H:162:ASN:HD21	3:H:201:TYR:HA	1.81	0.46
2:L:140:TYR:CG	2:L:141:PRO:HA	2.51	0.46
1:V:25:TYR:O	1:V:27:HIS:ND1	2.49	0.46
1:V:78:MET:HG2	1:W:15:VAL:HB	1.98	0.45
1:V:43:ILE:C	1:V:43:ILE:HD12	2.36	0.45
2:A:90:GLN:CD	2:A:90:GLN:C	2.74	0.45
2:L:110:VAL:HG21	2:L:199:GLN:NE2	2.31	0.45
2:A:140:TYR:CG	2:A:141:PRO:HA	2.52	0.45
2:A:136:LEU:HD11	2:A:196:VAL:HG22	1.99	0.45
3:H:2:VAL:HG13	3:H:27:PHE:HD1	1.82	0.45
1:W:19:ASP:O	1:W:23:ARG:HG3	2.17	0.45
2:A:175:LEU:HD23	2:A:175:LEU:C	2.38	0.45
1:W:86:HIS:CD2	1:W:86:HIS:N	2.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:6:GLU:HA	3:H:21:SER:O	2.17	0.44
2:A:90:GLN:O	2:A:96:PRO:HA	2.17	0.44
3:H:35:HIS:CE1	3:H:99:PHE:CB	3.00	0.44
3:B:207:HIS:HE1	3:B:209:PRO:HB2	1.82	0.44
3:H:83:MET:HE1	3:H:94:TYR:CZ	2.52	0.44
1:W:90:HIS:HD2	3:B:31:ASP:OD2	2.01	0.44
1:V:61:CYS:C	1:V:63:ASP:N	2.71	0.43
2:L:89:GLN:HB3	2:L:89:GLN:HE21	1.68	0.43
3:H:208:LYS:N	3:H:209:PRO:CD	2.82	0.43
2:A:141:PRO:HD2	2:A:198:HIS:HE1	1.84	0.43
2:A:132:VAL:HB	2:A:179:LEU:HB3	2.00	0.43
3:B:115:LEU:HD13	3:B:117:THR:CG2	2.49	0.42
2:L:37:GLN:HB2	2:L:47:LEU:HD11	2.00	0.42
2:L:42:LYS:HA	2:L:42:LYS:HE2	2.01	0.42
2:A:94:THR:HG23	2:A:95:PRO:HA	2.00	0.42
3:B:64:VAL:HG22	3:B:68:PHE:CD1	2.55	0.42
3:B:84:ASN:O	3:B:85:SER:C	2.57	0.42
3:B:28:THR:N	4:B:229:SO4:O3	2.53	0.42
1:V:72:GLU:HB2	1:V:101:LYS:HB2	2.01	0.42
1:W:89:GLN:HE21	3:B:102:PHE:HD2	1.68	0.42
1:V:61:CYS:C	1:V:63:ASP:H	2.22	0.42
1:V:67:GLU:CG	1:V:69:VAL:HG13	2.48	0.42
2:A:151:ASP:OD2	2:A:189:HIS:HB3	2.20	0.41
2:L:61:ARG:O	2:L:75:ILE:HA	2.20	0.41
2:A:95:PRO:HB3	3:B:59:TYR:CZ	2.55	0.41
2:A:188:LYS:C	2:A:189:HIS:HD2	2.23	0.41
1:V:27:HIS:ND1	1:V:27:HIS:N	2.68	0.41
1:V:36:PHE:CZ	1:V:43:ILE:HA	2.55	0.41
3:B:98:ARG:O	3:B:107:MET:HA	2.20	0.41
1:V:25:TYR:O	1:V:26:CYS:C	2.59	0.41
2:A:118:PHE:HA	2:A:119:PRO:HD3	1.92	0.41
3:H:4:LEU:HG	3:H:22:CYS:SG	2.61	0.41
2:A:113:PRO:HD3	2:A:198:HIS:CD2	2.55	0.41
3:B:221:LYS:O	3:B:223:CYS:N	2.53	0.40
2:A:108:ARG:HD3	2:A:109:THR:N	2.36	0.40
3:B:207:HIS:CE1	3:B:209:PRO:HB2	2.55	0.40
2:L:58:VAL:HA	2:L:59:PRO:HD3	1.94	0.40
1:W:45:TYR:N	1:W:45:TYR:CD1	2.90	0.40
3:H:221:LYS:O	3:H:222:SER:C	2.59	0.40
3:H:83:MET:HB3	3:H:86:LEU:HD21	2.03	0.40
3:H:100:VAL:CG1	3:H:103:LEU:H	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:66:LEU:HD13	1:W:104:CYS:HB3	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	V	93/102 (91%)	83 (89%)	8 (9%)	2 (2%)	8	26
1	W	92/102 (90%)	82 (89%)	8 (9%)	2 (2%)	8	26
2	A	209/214 (98%)	196 (94%)	13 (6%)	0	100	100
2	L	209/214 (98%)	200 (96%)	9 (4%)	0	100	100
3	B	214/227 (94%)	205 (96%)	7 (3%)	2 (1%)	20	52
3	H	214/227 (94%)	205 (96%)	8 (4%)	1 (0%)	32	67
All	All	1031/1086 (95%)	971 (94%)	53 (5%)	7 (1%)	25	59

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	W	64	GLU
3	B	222	SER
1	V	64	GLU
3	B	85	SER
1	W	26	CYS
3	H	222	SER
1	V	26	CYS

5.3.2 Protein sidechains ⓘ

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	V	90/96 (94%)	80 (89%)	10 (11%)	7	21
1	W	89/96 (93%)	77 (86%)	12 (14%)	4	13
2	A	186/188 (99%)	155 (83%)	31 (17%)	2	7
2	L	186/188 (99%)	155 (83%)	31 (17%)	2	7
3	B	179/187 (96%)	152 (85%)	27 (15%)	3	10
3	H	179/187 (96%)	149 (83%)	30 (17%)	2	7
All	All	909/942 (96%)	768 (84%)	141 (16%)	3	9

All (141) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	V	27	HIS
1	V	36	PHE
1	V	60	CYS
1	V	64	GLU
1	V	67	GLU
1	V	81	MET
1	V	99	HIS
1	V	101	LYS
1	V	107	LYS
1	V	108	LYS
1	W	24	SER
1	W	27	HIS
1	W	30	GLU
1	W	36	PHE
1	W	45	TYR
1	W	60	CYS
1	W	64	GLU
1	W	66	LEU
1	W	67	GLU
1	W	74	SER
1	W	101	LYS
1	W	107	LYS

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Mol	Chain	Res	Type
2	L	11	LEU
2	L	18	ARG
2	L	20	THR
2	L	39	LYS
2	L	42	LYS
2	L	50	SER
2	L	56	SER
2	L	65	SER
2	L	73	LEU
2	L	74	THR
2	L	83	PHE
2	L	89	GLN
2	L	91	SER
2	L	93	THR
2	L	94	THR
2	L	105	GLU
2	L	108	ARG
2	L	122	ASP
2	L	123	GLU
2	L	125	LEU
2	L	127	SER
2	L	129	THR
2	L	135	LEU
2	L	143	GLU
2	L	154	LEU
2	L	164	THR
2	L	165	GLU
2	L	174	SER
2	L	176	SER
2	L	181	LEU
2	L	201	LEU
3	H	4	LEU
3	H	11	LEU
3	H	12	VAL
3	H	19	ARG
3	H	20	LEU
3	H	25	SER
3	H	52	THR
3	H	64	VAL
3	H	69	THR
3	H	76	LYS
3	H	100	VAL

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Mol	Chain	Res	Type
3	H	112	GLN
3	H	114	THR
3	H	115	LEU
3	H	117	THR
3	H	123	THR
3	H	134	SER
3	H	135	SER
3	H	142	THR
3	H	158	THR
3	H	168	SER
3	H	177	LEU
3	H	182	LEU
3	H	188	VAL
3	H	193	SER
3	H	196	LEU
3	H	200	THR
3	H	204	ASN
3	H	213	LYS
3	H	222	SER
2	A	1	ASP
2	A	9	SER
2	A	18	ARG
2	A	20	THR
2	A	27	GLN
2	A	39	LYS
2	A	42	LYS
2	A	50	SER
2	A	65	SER
2	A	73	LEU
2	A	83	PHE
2	A	89	GLN
2	A	105	GLU
2	A	108	ARG
2	A	125	LEU
2	A	129	THR
2	A	135	LEU
2	A	143	GLU
2	A	145	LYS
2	A	152	ASN
2	A	154	LEU
2	A	164	THR
2	A	165	GLU

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Mol	Chain	Res	Type
2	A	176	SER
2	A	181	LEU
2	A	188	LYS
2	A	189	HIS
2	A	190	LYS
2	A	199	GLN
2	A	201	LEU
2	A	202	SER
3	B	11	LEU
3	B	12	VAL
3	B	13	GLN
3	B	17	SER
3	B	19	ARG
3	B	20	LEU
3	B	25	SER
3	B	64	VAL
3	B	69	THR
3	B	76	LYS
3	B	112	GLN
3	B	114	THR
3	B	115	LEU
3	B	117	THR
3	B	123	THR
3	B	134	SER
3	B	142	THR
3	B	158	THR
3	B	168	SER
3	B	177	LEU
3	B	182	LEU
3	B	186	SER
3	B	188	VAL
3	B	193	SER
3	B	204	ASN
3	B	216	LYS
3	B	221	LYS

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

Mol	Chain	Res	Type
1	V	22	GLN
1	V	89	GLN
1	V	100	ASN

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Mol	Chain	Res	Type
1	W	22	GLN
1	W	86	HIS
1	W	89	GLN
1	W	90	HIS
1	W	100	ASN
2	L	89	GLN
2	L	138	ASN
2	L	160	GLN
2	L	199	GLN
2	L	210	ASN
3	H	35	HIS
3	H	162	ASN
3	H	171	HIS
2	A	89	GLN
2	A	90	GLN
2	A	138	ASN
2	A	147	GLN
2	A	152	ASN
2	A	160	GLN
2	A	210	ASN
3	B	35	HIS
3	B	162	ASN
3	B	199	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 ⓘ

7 ligands are 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	B	228	-	4,4,4	0.36	0	6,6,6	0.32	0
4	SO4	B	229	-	4,4,4	0.26	0	6,6,6	0.33	0
4	SO4	B	230	-	4,4,4	0.13	0	6,6,6	0.30	0
4	SO4	B	231	-	4,4,4	0.07	0	6,6,6	0.63	0
4	SO4	H	228	-	4,4,4	0.21	0	6,6,6	0.54	0
4	SO4	H	229	-	4,4,4	0.26	0	6,6,6	0.44	0
4	SO4	H	230	-	4,4,4	0.16	0	6,6,6	0.29	0

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
4	SO4	B	228	-	-	0/0/0/0	0/0/0/0
4	SO4	B	229	-	-	0/0/0/0	0/0/0/0
4	SO4	B	230	-	-	0/0/0/0	0/0/0/0
4	SO4	B	231	-	-	0/0/0/0	0/0/0/0
4	SO4	H	228	-	-	0/0/0/0	0/0/0/0
4	SO4	H	229	-	-	0/0/0/0	0/0/0/0
4	SO4	H	230	-	-	0/0/0/0	0/0/0/0

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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	229	SO4	1	0
4	B	231	SO4	1	0

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 [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	V	95/102 (93%)	-0.25	0 100 100	18, 34, 63, 69	0
1	W	94/102 (92%)	-0.24	1 (1%) 80 74	18, 35, 61, 67	0
2	A	211/214 (98%)	-0.24	3 (1%) 75 69	25, 37, 49, 60	0
2	L	211/214 (98%)	-0.25	1 (0%) 90 88	23, 37, 48, 57	0
3	B	218/227 (96%)	-0.22	4 (1%) 69 60	25, 37, 48, 73	0
3	H	218/227 (96%)	-0.07	5 (2%) 61 51	22, 36, 48, 75	0
All	All	1047/1086 (96%)	-0.20	14 (1%) 77 71	18, 37, 51, 75	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	223	CYS	5.6
3	B	221	LYS	4.0
3	B	222	SER	3.7
2	A	154	LEU	3.1
3	H	223	CYS	2.7
2	L	91	SER	2.7
3	H	211	ASN	2.7
2	A	91	SER	2.6
1	W	72	GLU	2.6
3	H	52	THR	2.5
3	B	197	GLY	2.4
3	H	35	HIS	2.3
2	A	152	ASN	2.1
3	H	105	TYR	2.1

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. 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, 95th 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(\AA^2)	Q<0.9
4	SO4	H	229	5/5	0.86	0.25	3.35	47,52,56,56	0
4	SO4	H	228	5/5	0.87	0.25	2.41	48,50,52,55	0
4	SO4	B	229	5/5	0.93	0.19	1.90	52,54,56,57	0
4	SO4	B	228	5/5	0.90	0.19	0.28	32,40,40,40	0
4	SO4	B	231	5/5	0.96	0.12	-1.28	31,32,38,41	5
4	SO4	H	230	5/5	0.90	0.19	-	82,83,86,87	5
4	SO4	B	230	5/5	0.92	0.18	-	61,63,64,70	5

6.5 Other polymers [i](#)

There are no such residues in this entry.