



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 20, 2023 – 09:47 PM EDT

PDB ID : 5JOF  
Title : Crystal structure of VRC03 gHVgLV antigen-binding fragment.  
Authors : Joyce, M.G.; Mascola, J.R.; Kwong, P.D.  
Deposited on : 2016-05-02  
Resolution : 3.21 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](mailto: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>.

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

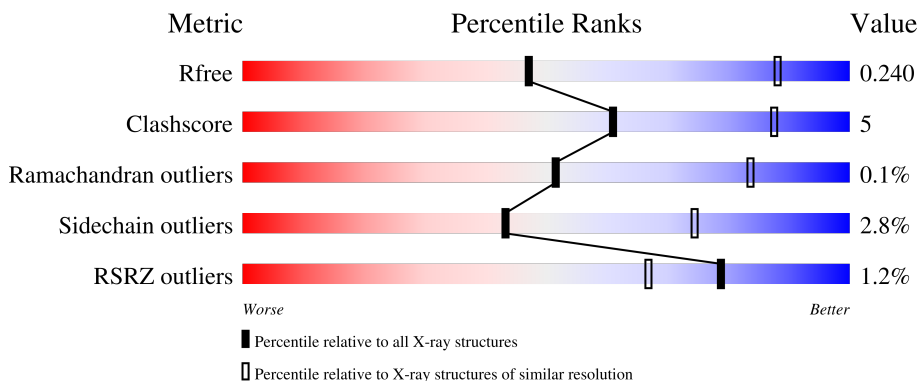
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.21 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.



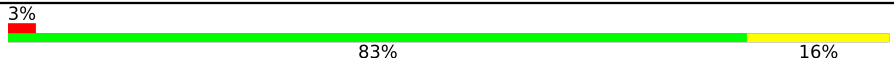
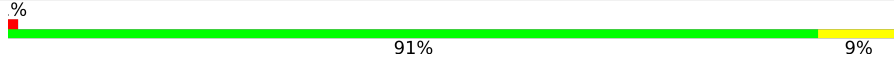

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	A	224	 82% 15% ..
1	C	224	 80% 16% ..
1	E	224	 88% 12%
1	H	224	 94% 6%
2	B	211	 88% 12%

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Mol	Chain	Length	Quality of chain
2	D	211	 3% 83% 16%
2	F	211	 % 91% 9%
2	L	211	 89% 11%

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 13238 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 VRC03 gHV heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	H	224	Total 1692	C 1067	N 288	O 327	S 10	0	0	0
1	A	220	Total 1664	C 1051	N 283	O 320	S 10	0	0	0
1	C	217	Total 1645	C 1040	N 280	O 315	S 10	0	0	0
1	E	224	Total 1692	C 1067	N 288	O 327	S 10	0	0	0

- Molecule 2 is a protein called VRC03 gLV light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	211	Total 1623	C 1016	N 273	O 329	S 5	0	0	0
2	B	210	Total 1617	C 1013	N 272	O 328	S 4	0	0	0
2	D	210	Total 1617	C 1013	N 272	O 328	S 4	0	0	0
2	F	210	Total 1617	C 1013	N 272	O 328	S 4	0	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	12	Total	O	0	0
			12	12		
4	L	10	Total	O	0	0
			10	10		
4	A	5	Total	O	0	0
			5	5		
4	B	9	Total	O	0	0
			9	9		
4	C	12	Total	O	0	0
			12	12		
4	D	3	Total	O	0	0
			3	3		
4	E	9	Total	O	0	0
			9	9		
4	F	6	Total	O	0	0
			6	6		

### 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.

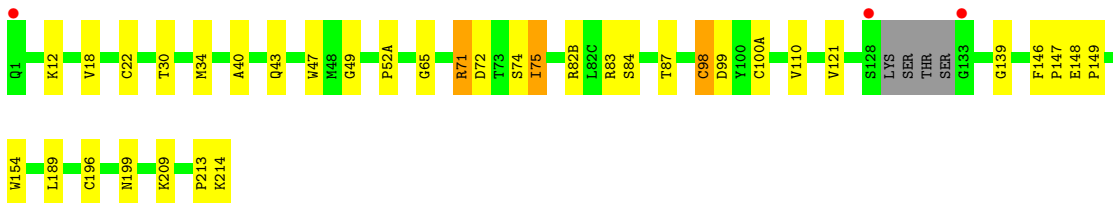
- Molecule 1: VRC03 gHV heavy chain

Chain H:  94% 6%




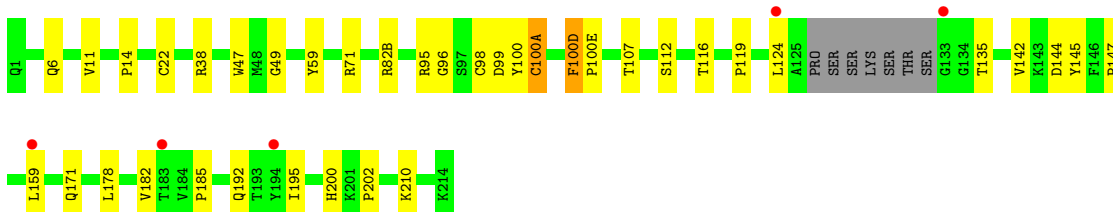
- Molecule 1: VRC03 gHV heavy chain

Chain A:  82% 15% ..




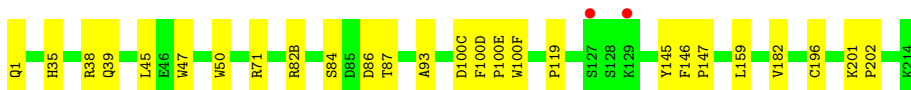
- Molecule 1: VRC03 gHV heavy chain

Chain C:  80% 16% ..




- Molecule 1: VRC03 gHV heavy chain

Chain E:  88% 12%




- Molecule 2: VRC03 gLV light chain

Chain L:  89% 11%




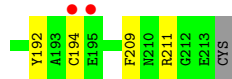
• Molecule 2: VRC03 gLV light chain

Chain B:  88% 12%

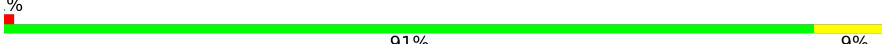


• Molecule 2: VRC03 gLV light chain

Chain D:  3% 83% 16%



• Molecule 2: VRC03 gLV light chain

Chain F:  0% 91% 9%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.92Å 132.90Å 188.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.46 – 3.21 45.46 – 3.21	Depositor EDS
% Data completeness (in resolution range)	95.0 (45.46-3.21) 95.0 (45.46-3.21)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.92 (at 3.19Å)	Xtrriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, $R_{free}$	0.195 , 0.241 0.196 , 0.240	Depositor DCC
$R_{free}$ test set	1813 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	59.6	Xtrriage
Anisotropy	0.067	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 49.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	13238	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

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	0.26	0/1708	0.46	0/2326
1	C	0.27	0/1688	0.45	0/2298
1	E	0.24	0/1737	0.46	0/2366
1	H	0.24	0/1737	0.45	0/2366
2	B	0.29	0/1653	0.45	0/2244
2	D	0.32	0/1653	0.48	0/2244
2	F	0.29	0/1653	0.46	0/2244
2	L	0.25	0/1659	0.46	0/2252
All	All	0.27	0/13488	0.46	0/18340

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1664	0	1613	19	0
1	C	1645	0	1596	20	0
1	E	1692	0	1644	14	0
1	H	1692	0	1644	7	0
2	B	1617	0	1558	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1617	0	1558	26	0
2	F	1617	0	1558	12	0
2	L	1623	0	1561	11	0
3	H	5	0	0	0	0
4	A	5	0	0	1	0
4	B	9	0	0	0	0
4	C	12	0	0	3	0
4	D	3	0	0	2	0
4	E	9	0	0	2	0
4	F	6	0	0	0	0
4	H	12	0	0	0	0
4	L	10	0	0	2	0
All	All	13238	0	12732	117	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 5.

All (117) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:61:ARG:NH1	2:F:82:ASP:OD2	1.97	0.96
2:D:32:TYR:HD2	2:D:91:PHE:CZ	1.95	0.84
2:D:32:TYR:CD2	2:D:91:PHE:CZ	2.69	0.80
2:D:32:TYR:O	2:D:90:GLN:NE2	2.20	0.74
1:A:98:CYS:SG	1:A:99:ASP:N	2.60	0.74
2:D:8:PRO:O	4:D:301:HOH:O	2.05	0.73
1:C:98:CYS:SG	1:C:100(A):CYS:N	2.60	0.72
2:F:14:SER:O	2:F:17:GLU:HG3	1.90	0.71
2:D:32:TYR:CD2	2:D:91:PHE:HZ	2.08	0.70
2:F:61:ARG:NH1	2:F:82:ASP:CG	2.44	0.70
1:C:82(B):ARG:NH2	4:C:303:HOH:O	2.24	0.70
2:F:59:PRO:HG2	2:F:62:PHE:CD1	2.28	0.69
1:C:59:TYR:O	4:C:301:HOH:O	2.11	0.68
1:C:98:CYS:SG	1:C:99:ASP:N	2.69	0.65
2:L:30:SER:HB3	2:L:51:ALA:HB2	1.78	0.65
2:L:127:SER:OG	4:L:301:HOH:O	2.09	0.65
2:F:59:PRO:HG2	2:F:62:PHE:HD1	1.62	0.64
2:B:54:ARG:HB2	2:B:58:ILE:HD11	1.80	0.64
2:B:50:GLY:O	2:B:51:ALA:HB3	1.98	0.63
2:D:123:GLU:HA	2:D:126:LYS:HE2	1.81	0.62
2:D:7:SER:OG	2:D:22:SER:OG	2.18	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:48:ILE:HA	2:D:54:ARG:HA	1.81	0.61
1:A:189:LEU:HD21	1:A:213:PRO:HG3	1.82	0.61
1:A:40:ALA:HB3	1:A:43:GLN:HB2	1.82	0.61
2:D:48:ILE:HG22	2:D:54:ARG:HB3	1.83	0.60
2:D:132:VAL:HG23	2:D:179:LEU:HB3	1.84	0.60
2:L:81:GLU:OE1	4:L:302:HOH:O	2.16	0.59
2:F:61:ARG:NH1	2:F:82:ASP:OD1	2.35	0.59
1:E:201:LYS:HG3	1:E:202:PRO:HD3	1.85	0.59
1:A:52(A):PRO:HA	1:A:71:ARG:HD2	1.86	0.58
1:C:159:LEU:HD13	1:C:182:VAL:HG21	1.86	0.57
1:C:192:GLN:NE2	4:C:304:HOH:O	2.28	0.57
1:H:119:PRO:HB3	1:H:145:TYR:HB3	1.88	0.55
2:D:33:LEU:HD12	2:D:90:GLN:HE21	1.72	0.55
1:C:142:VAL:HB	1:C:178:LEU:HD23	1.89	0.54
1:C:6:GLN:HE21	1:C:107:THR:HG23	1.72	0.54
1:A:148:GLU:HG2	1:A:149:PRO:HA	1.91	0.53
2:D:121:SER:OG	2:D:123:GLU:OE1	2.22	0.53
1:E:119:PRO:HB3	1:E:145:TYR:HB3	1.91	0.53
1:C:95:ARG:NH1	1:C:96:GLY:O	2.42	0.53
1:C:195:ILE:HG12	1:C:210:LYS:HA	1.91	0.53
1:E:100(D):PHE:H	1:E:100(E):PRO:HD2	1.75	0.52
2:F:37:GLN:HB2	2:F:47:LEU:HD11	1.91	0.51
1:C:135:THR:HG22	1:C:185:PRO:HA	1.91	0.51
2:B:167:ASP:OD1	2:B:168:SER:N	2.44	0.51
1:C:100(A):CYS:HB3	1:C:100(E):PRO:HG2	1.93	0.50
1:H:87:THR:HG23	1:H:110:VAL:HA	1.92	0.50
2:D:32:TYR:HD2	2:D:91:PHE:CE2	2.28	0.50
1:E:82(B):ARG:NH2	4:E:303:HOH:O	2.45	0.50
2:F:61:ARG:HH12	2:F:82:ASP:CG	2.08	0.50
2:D:155:GLN:NE2	4:D:302:HOH:O	2.44	0.50
2:L:155:GLN:OE1	2:L:158:ASN:ND2	2.42	0.49
2:L:12:SER:OG	2:L:105:GLU:OE1	2.28	0.49
1:A:87:THR:HG23	1:A:110:VAL:HA	1.94	0.49
1:A:47:TRP:CZ2	1:A:49:GLY:HA2	2.48	0.49
2:D:150:VAL:HG22	2:D:192:TYR:HD1	1.78	0.49
1:A:72:ASP:HB3	1:A:75:ILE:HG13	1.95	0.48
2:F:122:ASP:N	2:F:122:ASP:OD1	2.47	0.48
2:D:37:GLN:OE1	2:D:45:ARG:NH1	2.46	0.48
1:A:214:LYS:O	4:A:301:HOH:O	2.20	0.48
1:E:38:ARG:NH1	1:E:86:ASP:OD1	2.43	0.48
1:A:65:GLY:O	1:A:82(B):ARG:NH2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:GLY:HA2	1:A:154:TRP:CH2	2.50	0.47
2:L:186:TYR:O	2:L:192:TYR:OH	2.29	0.47
2:B:108:ARG:HG2	2:B:109:THR:N	2.30	0.47
2:L:47:LEU:HA	2:L:58:ILE:HG12	1.96	0.47
1:E:82(B):ARG:NH1	4:E:302:HOH:O	2.42	0.46
2:B:108:ARG:NH1	2:B:170:ASP:O	2.47	0.46
1:E:93:ALA:HB1	1:E:100(F):TRP:HB3	1.96	0.46
2:D:192:TYR:HB2	2:D:209:PHE:CE1	2.51	0.46
1:H:82(B):ARG:O	1:H:83:ARG:NH1	2.49	0.46
2:D:108:ARG:HG2	2:D:109:THR:N	2.30	0.46
1:A:121:VAL:HB	1:A:209:LYS:HG3	1.97	0.45
2:B:2:ILE:HD13	2:B:28:VAL:HG12	1.98	0.45
1:C:200:HIS:CD2	1:C:202:PRO:HD2	2.51	0.45
1:E:84:SER:O	1:E:87:THR:HG22	2.16	0.45
1:E:146:PHE:HA	1:E:147:PRO:HA	1.78	0.45
1:A:30:THR:HA	1:A:52(A):PRO:HB2	1.99	0.45
1:C:124:LEU:HB3	2:D:118:PHE:CD1	2.51	0.45
1:A:22:CYS:SG	1:A:34:MET:HE1	2.58	0.44
1:A:98:CYS:SG	1:A:100(A):CYS:N	2.87	0.44
2:D:187:GLU:HG3	2:D:211:ARG:NH2	2.33	0.44
1:C:47:TRP:CZ2	1:C:49:GLY:HA2	2.53	0.44
1:H:38:ARG:NH2	1:H:46:GLU:OE1	2.39	0.44
1:C:11:VAL:HG21	1:C:147:PRO:HG3	1.99	0.43
2:F:21:LEU:HD13	2:F:102:SER:HB2	1.99	0.43
1:H:47:TRP:CZ2	1:H:49:GLY:HA2	2.53	0.43
1:A:146:PHE:HA	1:A:147:PRO:HA	1.80	0.43
2:D:35:TRP:CD1	2:D:48:ILE:HD11	2.53	0.43
1:E:159:LEU:HD13	1:E:182:VAL:HG21	2.01	0.43
2:F:59:PRO:HG2	2:F:62:PHE:CE1	2.54	0.43
2:B:18:ARG:NH2	2:B:76:SER:OG	2.52	0.42
1:E:159:LEU:HD23	1:E:159:LEU:HA	1.82	0.42
1:C:116:THR:HG22	1:C:147:PRO:HD3	2.01	0.42
1:H:171:GLN:HA	2:L:160:GLN:HE22	1.84	0.42
2:L:120:PRO:HD3	2:L:132:VAL:HG22	2.02	0.42
2:L:189:HIS:N	2:L:211:ARG:NH2	2.66	0.42
2:B:50:GLY:O	2:B:51:ALA:CB	2.64	0.42
1:A:12:LYS:HD2	1:A:18:VAL:HB	2.02	0.42
2:B:89:GLN:HG2	2:B:90:GLN:N	2.35	0.42
2:F:39:LYS:HG3	2:F:84:ALA:HB2	2.02	0.42
1:E:39:GLN:HB2	1:E:45:LEU:HD23	2.01	0.42
1:C:14:PRO:HD3	1:C:112:SER:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:134:CYS:HB2	2:D:148:TRP:CZ2	2.55	0.41
2:D:33:LEU:HD12	2:D:90:GLN:NE2	2.34	0.41
1:A:83:ARG:HG2	1:A:84:SER:H	1.85	0.41
2:B:150:VAL:HB	2:B:155:GLN:HE21	1.85	0.41
1:A:139:GLY:HA2	1:A:154:TRP:HH2	1.85	0.41
2:D:150:VAL:HG22	2:D:192:TYR:CD1	2.56	0.41
1:E:47:TRP:HZ2	1:E:50:TRP:CD1	2.39	0.41
1:H:30:THR:HA	1:H:52(A):PRO:HB2	2.03	0.41
2:L:148:TRP:HE1	2:L:159:SER:HG	1.66	0.41
1:C:144:ASP:OD1	1:C:171:GLN:OE1	2.39	0.41
2:D:169:LYS:HG3	2:D:170:ASP:N	2.36	0.41
1:C:119:PRO:HB3	1:C:145:TYR:HB3	2.03	0.41
1:E:35:HIS:CE1	1:E:50:TRP:HB3	2.56	0.41
2:D:32:TYR:CE2	2:D:91:PHE:HZ	2.40	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	216/224 (96%)	203 (94%)	13 (6%)	0	100	100
1	C	213/224 (95%)	202 (95%)	10 (5%)	1 (0%)	29	67
1	E	222/224 (99%)	210 (95%)	12 (5%)	0	100	100
1	H	222/224 (99%)	213 (96%)	9 (4%)	0	100	100
2	B	208/211 (99%)	199 (96%)	9 (4%)	0	100	100
2	D	208/211 (99%)	195 (94%)	13 (6%)	0	100	100
2	F	208/211 (99%)	195 (94%)	13 (6%)	0	100	100
2	L	209/211 (99%)	203 (97%)	6 (3%)	0	100	100
All	All	1706/1740 (98%)	1620 (95%)	85 (5%)	1 (0%)	51	83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	100(D)	PHE

### 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	184/188 (98%)	178 (97%)	6 (3%)	38	71
1	C	181/188 (96%)	175 (97%)	6 (3%)	38	71
1	E	188/188 (100%)	184 (98%)	4 (2%)	53	79
1	H	188/188 (100%)	187 (100%)	1 (0%)	88	95
2	B	182/183 (100%)	174 (96%)	8 (4%)	28	64
2	D	182/183 (100%)	177 (97%)	5 (3%)	44	75
2	F	182/183 (100%)	177 (97%)	5 (3%)	44	75
2	L	183/183 (100%)	177 (97%)	6 (3%)	38	71
All	All	1470/1484 (99%)	1429 (97%)	41 (3%)	43	74

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	95	ARG
2	L	24	ARG
2	L	33	LEU
2	L	60	ASP
2	L	77	ARG
2	L	179	LEU
2	L	211	ARG
1	A	71	ARG
1	A	74	SER
1	A	75	ILE
1	A	98	CYS
1	A	196	CYS
1	A	199	ASN

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Mol	Chain	Res	Type
2	B	1	GLU
2	B	24	ARG
2	B	45	ARG
2	B	52	SER
2	B	96	GLU
2	B	137	ASN
2	B	152	ASN
2	B	160	GLN
1	C	22	CYS
1	C	38	ARG
1	C	71	ARG
1	C	100	TYR
1	C	100(A)	CYS
1	C	100(D)	PHE
2	D	13	LEU
2	D	30	SER
2	D	31	SER
2	D	33	LEU
2	D	194	CYS
1	E	1	GLN
1	E	71	ARG
1	E	100(C)	ASP
1	E	196	CYS
2	F	11	LEU
2	F	33	LEU
2	F	60	ASP
2	F	151	ASP
2	F	179	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	GLN
1	C	171	GLN
2	D	90	GLN

### 5.3.3 RNA

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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	$\# Z  > 2$
3	SO4	H	301	-	4,4,4	0.14	0	6,6,6	0.04	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	220/224 (98%)	0.10	3 (1%) 75 63	28, 63, 106, 117	0
1	C	217/224 (96%)	0.07	5 (2%) 60 47	25, 54, 115, 128	0
1	E	224/224 (100%)	-0.05	2 (0%) 84 75	26, 51, 74, 118	0
1	H	224/224 (100%)	-0.15	0 100 100	23, 39, 61, 85	0
2	B	210/211 (99%)	0.14	1 (0%) 91 86	31, 66, 94, 110	0
2	D	210/211 (99%)	0.41	7 (3%) 46 30	43, 79, 122, 136	0
2	F	210/211 (99%)	-0.05	3 (1%) 75 63	24, 49, 98, 122	0
2	L	211/211 (100%)	-0.11	0 100 100	21, 43, 72, 109	0
All	All	1726/1740 (99%)	0.04	21 (1%) 79 67	21, 54, 104, 136	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	133	GLY	5.1
2	D	156	SER	3.8
2	D	157	GLY	3.2
2	D	185	ASP	2.9
2	F	152	ASN	2.9
2	D	194	CYS	2.8
1	A	128	SER	2.7
1	E	127	SER	2.6
2	D	128	GLY	2.5
2	D	155	GLN	2.4
1	A	133	GLY	2.3
1	A	1	GLN	2.3
2	F	213	GLU	2.3
2	D	195	GLU	2.2
1	C	124	LEU	2.2
2	F	151	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	159	LEU	2.2
1	C	183	THR	2.1
1	C	194	TYR	2.1
1	E	129	LYS	2.0
2	B	212	GLY	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	SO4	H	301	5/5	0.63	0.40	159,159,160,161	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.