



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:24 AM UTC

PDB ID : 6QNA / pdb_00006qna
Title : Structure of bovine anti-RSV hybrid Fab B13HC-B4LC
Authors : Ren, J.; Nettleship, J.E.; Harris, G.; Mwangi, W.; Rhaman, N.; Grant, C.;
Kotecha, A.; Fry, E.; Charleston, B.; Stuart, D.I.; Hammond, J.; Owens, R.J.
Deposited on : 2019-02-10
Resolution : 2.62 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

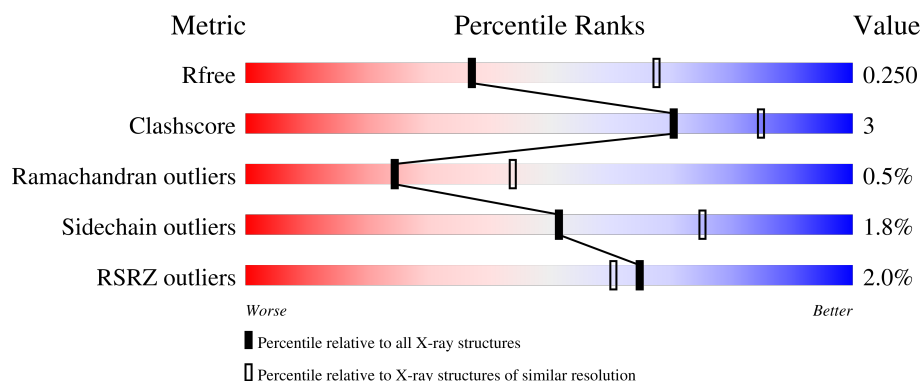
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.62 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.



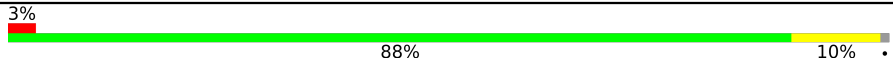
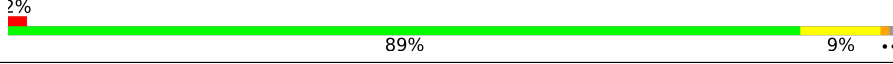
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (2.64-2.60)

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 $\leq 5\%$. 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	243	0.5% 86% 8% 6%
1	C	243	3% 83% 10% 7%
1	E	243	2% 86% 7% 6%
1	H	243	0.5% 84% 11% 5%
2	B	214	0.5% 90% 8% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	214	
2	F	214	
2	L	214	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13139 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 B13 Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	232	Total	C	N	O	S	0	0	0
			1727	1084	287	345	11			
1	A	229	Total	C	N	O	S	0	0	0
			1701	1069	280	341	11			
1	C	227	Total	C	N	O	S	0	0	0
			1684	1058	275	340	11			
1	E	228	Total	C	N	O	S	0	0	0
			1686	1059	276	340	11			

- Molecule 2 is a protein called B4 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	211	Total	C	N	O	S	0	0	0
			1571	976	263	326	6			
2	B	211	Total	C	N	O	S	0	0	0
			1571	976	263	326	6			
2	D	211	Total	C	N	O	S	0	0	0
			1571	976	263	326	6			
2	F	211	Total	C	N	O	S	0	0	0
			1571	976	263	326	6			

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		

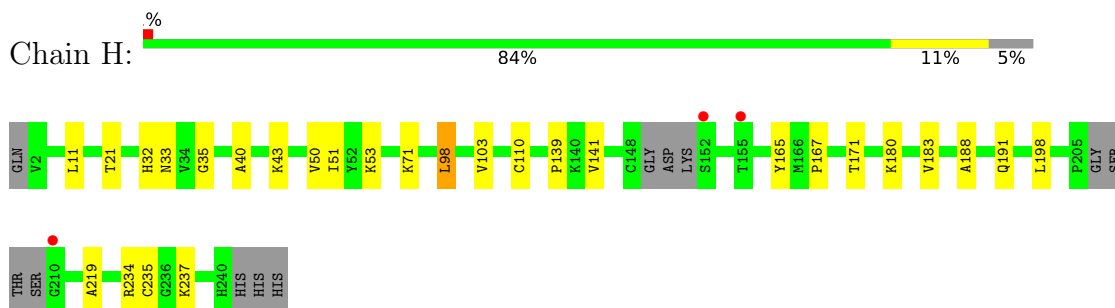
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	11	Total	O	0	0
			11	11		
4	L	9	Total	O	0	0
			9	9		
4	A	7	Total	O	0	0
			7	7		
4	B	2	Total	O	0	0
			2	2		
4	C	6	Total	O	0	0
			6	6		
4	D	5	Total	O	0	0
			5	5		
4	E	5	Total	O	0	0
			5	5		
4	F	6	Total	O	0	0
			6	6		

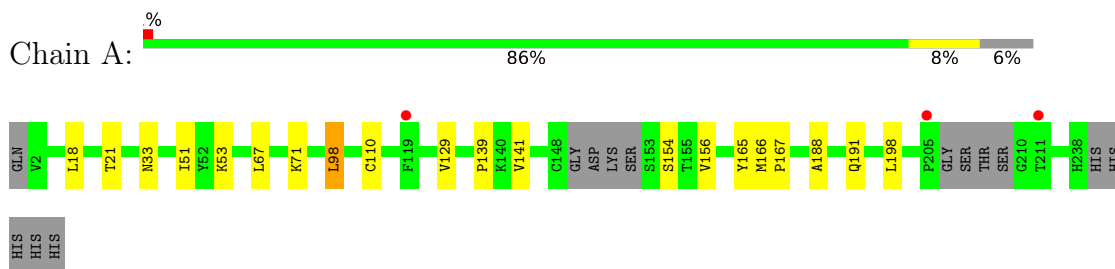
3 Residue-property plots [i](#)

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.

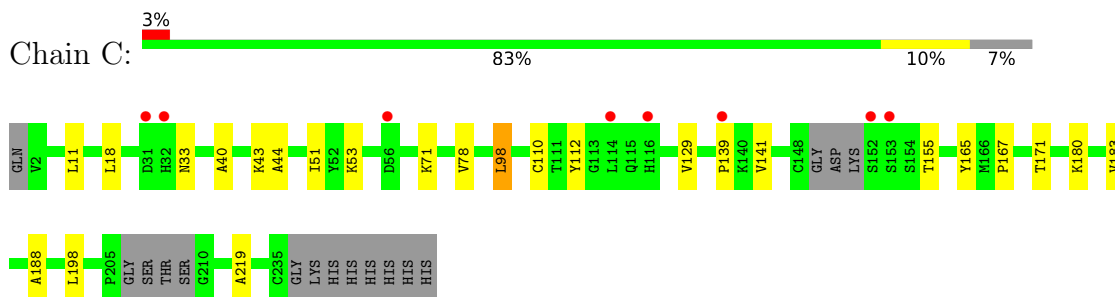
- Molecule 1: B13 Heavy chain



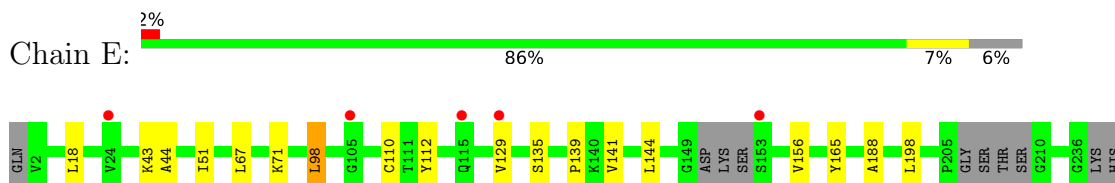
- Molecule 1: B13 Heavy chain



- Molecule 1: B13 Heavy chain

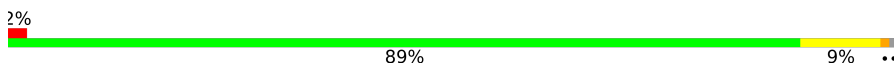


- Molecule 1: B13 Heavy chain



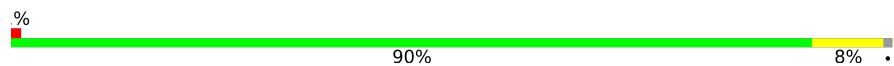
HIS
HIS
HIS
HIS
HIS

• Molecule 2: B4 light chain

Chain L:  2% 89% 9% ..

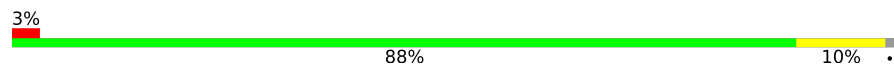
GLN ALA V3 L4 R17 N28 I29 W36 S43 G44 I49 Y50 Y51 V59 T91 Y94 M108 T147 V148 V149 W150 E162 K168 S172 L182 E196 V197 T198 C213 SER

• Molecule 2: B4 light chain

Chain B:  1% 90% 8% .

GLN ALA V3 L4 N28 I29 W36 I49 Y50 Y51 E52 E53 P56 V59 T91 Y94 T147 V148 V149 V161 E162 K168 S172 L182 E196 V197 T198 C213 SER

• Molecule 2: B4 light chain

Chain D:  3% 88% 10% .

GLN ALA V3 L4 S9 G12 N28 I29 V34 N35 W36 P41 I49 Y50 Y51 E52 E53 P56 V59 G65 T91 Y94 S101 V107 M108 V149 V161 K168 Q169 A175 L182 E196 C213 SER

• Molecule 2: B4 light chain

Chain F:  1% 86% 11% ..

GLN ALA V3 L4 T5 S11 Q16 N28 I29 Y51 R55 P56 V59 T91 Y94 N95 I96 M108 F120 P121 T147 V148 V149 D153 V161 K168 S172 L182 E196 V197 T198 V208 C213 SER

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	43.44Å 76.27Å 130.03Å 89.66° 87.35° 88.60°	Depositor
Resolution (Å)	65.62 – 2.62 65.62 – 2.62	Depositor EDS
% Data completeness (in resolution range)	98.2 (65.62-2.62) 98.2 (65.62-2.62)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 2.62Å)	Xtriage
Refinement program	PHENIX (dev_3386: ???)	Depositor
R, R_{free}	0.220 , 0.250 0.222 , 0.250	Depositor DCC
R_{free} test set	2230 reflections (4.53%)	wwPDB-VP
Wilson B-factor (Å ²)	71.4	Xtriage
Anisotropy	0.362	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 37.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.047 for h,-k,-l 0.066 for -h,k,-l 0.038 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13139	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.11% 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: GOL

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	0.09	0/1738	0.30	0/2372
1	C	0.09	0/1720	0.30	0/2349
1	E	0.08	0/1722	0.31	0/2351
1	H	0.11	0/1766	0.34	0/2410
2	B	0.09	0/1605	0.32	0/2187
2	D	0.09	0/1605	0.30	0/2187
2	F	0.09	0/1605	0.30	0/2187
2	L	0.09	0/1605	0.30	0/2187
All	All	0.09	0/13366	0.31	0/18230

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

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	1701	0	1664	12	0
1	C	1684	0	1646	13	0
1	E	1686	0	1647	12	0
1	H	1727	0	1683	17	0
2	B	1571	0	1522	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1571	0	1522	9	0
2	F	1571	0	1522	13	0
2	L	1571	0	1522	10	0
3	B	6	0	8	0	0
4	A	7	0	0	1	0
4	B	2	0	0	0	0
4	C	6	0	0	0	0
4	D	5	0	0	0	0
4	E	5	0	0	2	0
4	F	6	0	0	3	0
4	H	11	0	0	2	0
4	L	9	0	0	0	0
All	All	13139	0	12736	87	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 3.

All (87) 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:A:21:THR:OG1	4:A:301:HOH:O	2.07	0.72
1:C:11:LEU:HB2	1:C:167:PRO:HG3	1.74	0.69
1:H:11:LEU:HB2	1:H:167:PRO:HG3	1.74	0.68
1:H:21:THR:OG1	4:H:301:HOH:O	2.14	0.64
2:F:153:ASP:N	4:F:301:HOH:O	2.30	0.61
2:L:147:THR:OG1	2:L:198:THR:OG1	2.15	0.60
1:A:139:PRO:HB3	1:A:165:TYR:HB3	1.83	0.60
2:B:147:THR:HG1	2:B:198:THR:HG1	1.50	0.59
2:L:149:VAL:HG23	2:L:196:GLU:HB2	1.86	0.56
1:H:139:PRO:HB3	1:H:165:TYR:HB3	1.86	0.56
2:L:4:LEU:HD11	2:L:91:THR:HG22	1.87	0.56
1:C:139:PRO:HB3	1:C:165:TYR:HB3	1.87	0.56
2:F:55:ARG:NH2	4:F:303:HOH:O	2.35	0.55
2:B:4:LEU:HD11	2:B:91:THR:HG22	1.87	0.55
1:E:139:PRO:HB3	1:E:165:TYR:HB3	1.87	0.54
2:D:4:LEU:HD11	2:D:91:THR:HG22	1.89	0.54
1:A:51:ILE:HD13	1:A:71:LYS:HB3	1.89	0.54
2:F:4:LEU:HD11	2:F:91:THR:HG22	1.90	0.53
1:C:51:ILE:HD13	1:C:71:LYS:HB3	1.92	0.52
2:B:149:VAL:HG23	2:B:196:GLU:HB2	1.90	0.52
1:A:191:GLN:HA	2:B:162:GLU:HG3	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:149:VAL:HG23	2:F:196:GLU:HB2	1.90	0.52
2:D:149:VAL:HG23	2:D:196:GLU:HB2	1.91	0.52
2:F:147:THR:HG1	2:F:198:THR:HG1	1.55	0.51
1:H:234:ARG:NH1	1:H:237:LYS:HE3	2.26	0.51
1:H:51:ILE:HD13	1:H:71:LYS:HB3	1.93	0.51
2:D:41:PRO:HG2	2:D:168:LYS:HD2	1.93	0.51
1:E:44:ALA:N	4:E:301:HOH:O	2.21	0.50
1:C:44:ALA:HB2	2:D:101:SER:HA	1.92	0.50
1:C:188:ALA:HA	1:C:198:LEU:HB3	1.94	0.49
1:E:98:LEU:HD22	1:E:110:CYS:HB3	1.94	0.49
1:C:40:ALA:HB3	1:C:43:LYS:HB2	1.94	0.49
2:D:53:SER:OG	2:D:65:GLY:O	2.30	0.48
1:E:18:LEU:HD13	1:E:129:VAL:HG11	1.95	0.48
2:B:168:LYS:NZ	2:B:172:SER:OG	2.46	0.48
1:C:98:LEU:HD22	1:C:110:CYS:HB3	1.96	0.47
1:A:18:LEU:HD13	1:A:129:VAL:HG11	1.96	0.47
1:C:18:LEU:HD13	1:C:129:VAL:HG21	1.98	0.46
2:B:28:ASN:OD1	2:B:29:ILE:N	2.41	0.46
1:C:71:LYS:HB2	1:C:78:VAL:HG22	1.98	0.46
2:F:28:ASN:OD1	2:F:29:ILE:N	2.42	0.45
1:A:53:LYS:O	1:A:71:LYS:NZ	2.49	0.45
2:F:168:LYS:NZ	2:F:172:SER:OG	2.49	0.45
2:F:16:GLN:NE2	4:F:304:HOH:O	2.49	0.45
2:L:36:TRP:CD1	2:L:49:ILE:HD11	2.52	0.45
2:D:28:ASN:OD1	2:D:29:ILE:N	2.41	0.45
2:F:11:SER:HB3	2:F:108:MET:HE2	1.99	0.44
1:H:32:HIS:ND1	4:H:302:HOH:O	2.35	0.44
1:A:154:SER:HB3	1:E:135:SER:OG	2.18	0.44
1:E:51:ILE:HD13	1:E:71:LYS:HB3	1.99	0.43
1:A:98:LEU:HD22	1:A:110:CYS:HB3	1.99	0.43
1:E:188:ALA:HA	1:E:198:LEU:HB3	2.00	0.43
1:H:103:VAL:HG21	2:L:51:TYR:CZ	2.54	0.43
1:H:188:ALA:HA	1:H:198:LEU:HB3	2.01	0.43
2:L:43:SER:OG	2:L:44:GLY:N	2.51	0.43
1:A:188:ALA:HA	1:A:198:LEU:HB3	2.01	0.43
2:L:168:LYS:NZ	2:L:172:SER:OG	2.52	0.43
2:B:56:PRO:O	2:B:59:VAL:HG13	2.19	0.43
1:H:180:LYS:O	1:H:183:VAL:HG12	2.19	0.42
1:H:33:ASN:OD1	1:H:53:LYS:HG3	2.19	0.42
1:E:43:LYS:HB3	4:E:301:HOH:O	2.19	0.42
1:H:33:ASN:HB2	1:H:98:LEU:HB3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:234:ARG:CZ	1:H:237:LYS:HE3	2.49	0.42
1:A:33:ASN:OD1	1:A:53:LYS:HG3	2.19	0.42
2:D:36:TRP:CD1	2:D:49:ILE:HD11	2.54	0.42
2:D:169:GLN:HE21	2:D:175:ALA:HB2	1.84	0.42
1:E:98:LEU:HG	1:E:112:TYR:CE2	2.55	0.42
1:E:67:LEU:HD23	1:E:67:LEU:HA	1.86	0.42
2:L:17:ARG:HD3	2:F:5:THR:HG23	2.01	0.42
1:H:40:ALA:HB3	1:H:43:LYS:HB2	2.02	0.42
1:A:67:LEU:HD23	1:A:67:LEU:HA	1.88	0.42
2:D:56:PRO:O	2:D:59:VAL:HG13	2.20	0.42
1:C:180:LYS:O	1:C:183:VAL:HG12	2.20	0.41
1:H:171:THR:HG23	1:H:219:ALA:HB3	2.02	0.41
1:H:98:LEU:HD22	1:H:110:CYS:HB3	2.01	0.41
2:L:28:ASN:OD1	2:L:29:ILE:N	2.42	0.41
1:C:33:ASN:OD1	1:C:53:LYS:HG3	2.20	0.41
2:F:56:PRO:O	2:F:59:VAL:HG13	2.21	0.41
1:C:98:LEU:HG	1:C:112:TYR:CE2	2.55	0.41
1:H:191:GLN:HA	2:L:162:GLU:HG3	2.02	0.41
1:E:144:LEU:HB3	2:F:120:PHE:CD1	2.55	0.41
1:E:98:LEU:HD23	1:E:98:LEU:HA	1.96	0.40
1:A:166:MET:HA	1:A:167:PRO:HA	1.84	0.40
2:F:121:PRO:HB3	2:F:208:VAL:HG21	2.03	0.40
1:H:35:GLY:HA2	1:H:50:VAL:HA	2.02	0.40
2:B:36:TRP:CD1	2:B:49:ILE:HD11	2.57	0.40
1:C:171:THR:HG23	1:C:219:ALA:HB3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	223/243 (92%)	211 (95%)	12 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	221/243 (91%)	211 (96%)	9 (4%)	1 (0%)	24	44
1	E	222/243 (91%)	213 (96%)	9 (4%)	0	100	100
1	H	226/243 (93%)	217 (96%)	9 (4%)	0	100	100
2	B	209/214 (98%)	203 (97%)	5 (2%)	1 (0%)	24	44
2	D	209/214 (98%)	202 (97%)	5 (2%)	2 (1%)	12	26
2	F	209/214 (98%)	203 (97%)	4 (2%)	2 (1%)	12	26
2	L	209/214 (98%)	198 (95%)	9 (4%)	2 (1%)	12	26
All	All	1728/1828 (94%)	1658 (96%)	62 (4%)	8 (0%)	24	44

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	51	TYR
2	B	51	TYR
2	L	94	TYR
1	C	155	THR
2	D	51	TYR
2	D	94	TYR
2	F	51	TYR
2	F	94	TYR

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	A	198/210 (94%)	195 (98%)	3 (2%)	57	79
1	C	197/210 (94%)	195 (99%)	2 (1%)	68	85
1	E	196/210 (93%)	193 (98%)	3 (2%)	57	79
1	H	201/210 (96%)	198 (98%)	3 (2%)	57	79
2	B	182/184 (99%)	178 (98%)	4 (2%)	45	70
2	D	182/184 (99%)	178 (98%)	4 (2%)	45	70

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	182/184 (99%)	177 (97%)	5 (3%)	39	65
2	L	182/184 (99%)	178 (98%)	4 (2%)	45	70
All	All	1520/1576 (96%)	1492 (98%)	28 (2%)	51	75

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	98	LEU
1	H	141	VAL
1	H	235	CYS
2	L	59	VAL
2	L	94	TYR
2	L	182	LEU
2	L	213	CYS
1	A	98	LEU
1	A	141	VAL
1	A	156	VAL
2	B	59	VAL
2	B	161	VAL
2	B	182	LEU
2	B	213	CYS
1	C	98	LEU
1	C	141	VAL
2	D	59	VAL
2	D	161	VAL
2	D	182	LEU
2	D	213	CYS
1	E	98	LEU
1	E	141	VAL
1	E	156	VAL
2	F	59	VAL
2	F	94	TYR
2	F	161	VAL
2	F	182	LEU
2	F	213	CYS

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

Mol	Chain	Res	Type
1	H	73	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L	70	ASN
1	A	120	HIS
2	B	70	ASN
1	C	73	ASN
2	D	70	ASN
2	D	171	ASN
1	E	39	GLN
1	E	120	HIS
2	F	39	GLN
2	F	110	GLN

5.3.3 RNA [i](#)

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 oligosaccharides 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	GOL	B	301	-	5,5,5	0.96	0	5,5,5	1.06	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
3	GOL	B	301	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	301	GOL	C1-C2-C3-O3
3	B	301	GOL	O2-C2-C3-O3

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, 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	A	229/243 (94%)	0.14	3 (1%) 75 71	48, 89, 141, 187	0
1	C	227/243 (93%)	0.20	8 (3%) 47 41	46, 81, 131, 171	0
1	E	228/243 (93%)	0.30	5 (2%) 62 57	60, 93, 148, 161	0
1	H	232/243 (95%)	-0.02	3 (1%) 75 71	46, 72, 138, 174	0
2	B	211/214 (98%)	0.18	3 (1%) 73 70	63, 98, 143, 159	0
2	D	211/214 (98%)	0.18	6 (2%) 55 50	58, 88, 129, 153	0
2	F	211/214 (98%)	0.21	3 (1%) 73 70	65, 101, 134, 149	0
2	L	211/214 (98%)	0.17	4 (1%) 66 62	50, 86, 125, 141	0
All	All	1760/1828 (96%)	0.17	35 (1%) 65 60	46, 89, 138, 187	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	155	THR	5.3
1	C	153	SER	3.6
1	C	31	ASP	3.5
1	E	24	VAL	3.5
1	A	205	PRO	3.3
2	L	148	VAL	3.3
2	B	94	TYR	3.2
2	D	108	MET	3.1
1	C	32	HIS	3.1
1	E	153	SER	3.1
1	C	116	HIS	3.0
1	A	211	THR	2.9
1	E	105	GLY	2.9
1	C	114	LEU	2.7
2	F	56	PRO	2.6
2	D	12	GLY	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	53	SER	2.4
2	L	197	VAL	2.4
2	B	52	GLU	2.4
1	H	152	SER	2.3
2	F	3	VAL	2.3
1	A	119	PHE	2.3
1	C	152	SER	2.2
2	D	107	VAL	2.2
1	C	56	ASP	2.2
1	H	210	GLY	2.2
2	D	9	SER	2.2
2	L	150	TRP	2.1
2	L	108	MET	2.1
1	C	139	PRO	2.1
2	D	3	VAL	2.1
1	E	129	VAL	2.0
1	E	115	GLN	2.0
2	F	96	ILE	2.0
2	D	34	VAL	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 oligosaccharides 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, 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	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	B	301	6/6	0.80	0.11	107,108,109,109	0

6.5 Other polymers [i](#)

There are no such residues in this entry.