



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:34 PM GMT

PDB ID : 4IML
Title : CrossFab binding to human Angiopoietin 2
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Deposited on : 2013-01-03
Resolution : 2.93 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

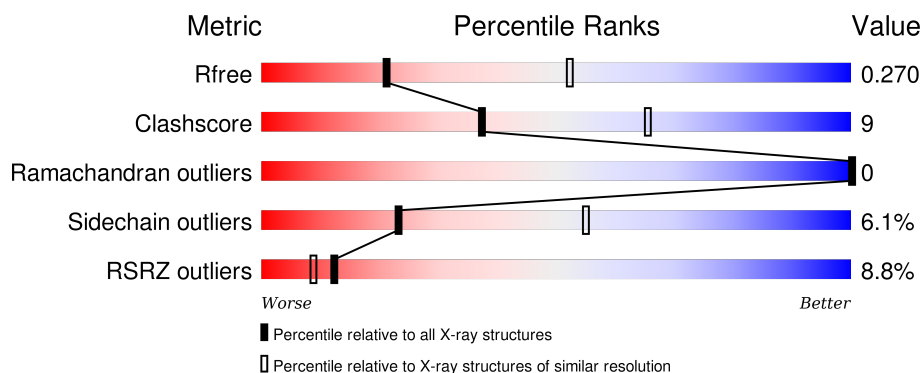
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.93 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}	91344	2057 (2.98-2.90)
Clashscore	102246	2308 (2.98-2.90)
Ramachandran outliers	100387	2245 (2.98-2.90)
Sidechain outliers	100360	2247 (2.98-2.90)
RSRZ outliers	91569	2065 (2.98-2.90)

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	A	245	<div> <div>11%</div> <div>75%</div> <div>20%</div> <div>.</div> </div>
1	H	245	<div> <div>3%</div> <div>70%</div> <div>24%</div> <div>..</div> </div>
2	B	213	<div> <div>13%</div> <div>82%</div> <div>16%</div> <div>.</div> </div>
2	L	213	<div> <div>8%</div> <div>80%</div> <div>17%</div> <div>..</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
3	GOL	B	301	-	-	-	X

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6743 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 Crossed heavy chain (VH-Ckappa).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	234	Total	C	N	O	S	81	0	0
			1816	1142	305	360	9			
1	A	234	Total	C	N	O	S	95	0	0
			1816	1142	305	360	9			

- Molecule 2 is a protein called Crossed light chain (VL-CH1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	210	Total	C	N	O	S	18	0	0
			1540	961	260	315	4			
2	B	212	Total	C	N	O	S	16	0	0
			1552	968	262	317	5			

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



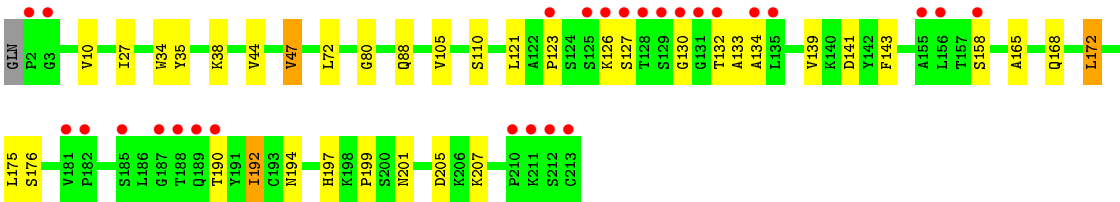
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	H	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	2	Total	O	0	0
			2	2		
4	L	2	Total	O	0	0
			2	2		
4	A	2	Total	O	0	0
			2	2		
4	B	1	Total	O	0	0
			1	1		

- Molecule 1: Crossed heavy chain (VH-Ckappa)





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	75.75Å 80.55Å 158.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.13 – 2.93 44.13 – 2.93	Depositor EDS
% Data completeness (in resolution range)	98.6 (44.13-2.93) 98.7 (44.13-2.93)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 2.96Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.237 , 0.269 0.237 , 0.270	Depositor DCC
R_{free} test set	1059 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	59.0	Xtriage
Anisotropy	0.421	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 63.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	2 of 21186 reflections (0.009%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6743	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.94 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 9.2315e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 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	0.24	0/1863	0.47	0/2532
1	H	0.23	0/1863	0.46	1/2532 (0.0%)
2	B	0.23	0/1591	0.46	0/2176
2	L	0.23	0/1579	0.45	0/2162
All	All	0.23	0/6896	0.46	1/9402 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	223	LEU	CA-CB-CG	5.80	128.63	115.30

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	1816	0	1729	41	0
1	H	1816	0	1729	36	0
2	B	1552	0	1505	27	0
2	L	1540	0	1492	21	0
3	B	6	0	8	0	0
3	H	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	2	0	0	0	0
4	B	1	0	0	0	0
4	H	2	0	0	0	0
4	L	2	0	0	0	0
All	All	6743	0	6471	118	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 9.

All (118) 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:173:ASP:H	1:A:213:VAL:CG2	1.51	1.23
1:A:173:ASP:H	1:A:213:VAL:HG23	1.21	1.05
1:A:173:ASP:N	1:A:213:VAL:CG2	2.21	1.04
2:B:127:SER:HB2	2:B:133:ALA:HB2	1.41	1.01
1:A:173:ASP:HA	1:A:213:VAL:HG21	1.58	0.85
1:A:173:ASP:CA	1:A:213:VAL:HG21	2.11	0.80
1:A:173:ASP:N	1:A:213:VAL:HG23	1.93	0.79
1:H:14:PRO:HG2	1:H:129:SER:HB2	1.64	0.79
1:A:213:VAL:O	1:A:214:TYR:CG	2.36	0.79
1:A:213:VAL:O	1:A:214:TYR:CD1	2.38	0.77
1:H:186:THR:HG22	2:L:164:PRO:HD3	1.73	0.70
1:A:173:ASP:HA	1:A:213:VAL:CG2	2.20	0.70
1:A:173:ASP:CA	1:A:213:VAL:CG2	2.68	0.69
2:B:34:TRP:HB2	2:B:47:VAL:HG13	1.75	0.69
1:H:37:VAL:HG22	1:H:47:TRP:HA	1.74	0.68
2:L:46:VAL:HG12	2:L:47:VAL:HG23	1.74	0.67
1:H:212:LYS:O	1:H:232:ASN:ND2	2.26	0.67
1:A:37:VAL:HG22	1:A:47:TRP:HA	1.77	0.65
1:H:181:SER:HB3	1:H:201:LEU:HD23	1.79	0.64
1:A:158:LEU:HD12	1:A:197:LEU:HD22	1.80	0.63
1:A:173:ASP:H	1:A:213:VAL:HG22	1.55	0.63
1:H:2:VAL:HG11	1:H:98:ARG:HH21	1.63	0.63
1:H:12:LYS:NZ	1:H:17:SER:O	2.31	0.63
1:A:173:ASP:N	1:A:213:VAL:HG21	2.09	0.62
1:A:205:LYS:O	1:A:209:GLU:HG2	2.00	0.61
1:A:138:PHE:CD1	2:B:126:LYS:HB2	2.35	0.60
2:L:30:LYS:NZ	2:L:90:TRP:O	2.29	0.60
1:A:138:PHE:HD1	2:B:126:LYS:HB2	1.67	0.59
2:B:123:PRO:HA	2:B:126:LYS:NZ	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:130:GLY:C	2:B:132:THR:H	2.05	0.58
2:B:38:LYS:NZ	2:B:80:GLY:O	2.36	0.57
1:H:91:THR:HG23	1:H:126:THR:HA	1.86	0.56
2:L:124:SER:OG	2:L:125:SER:N	2.38	0.56
1:H:97:ALA:HB1	1:H:116:PHE:HB3	1.85	0.56
1:H:167:LYS:HB2	1:H:219:THR:HG23	1.87	0.56
1:H:159:ASN:OD1	1:H:160:ASN:ND2	2.35	0.55
1:H:39:GLN:HB3	1:H:45:LEU:HD23	1.88	0.55
1:A:132:VAL:HG13	1:A:163:PRO:HD3	1.87	0.55
1:H:32:TYR:HD1	1:H:100:PRO:HA	1.72	0.55
1:A:172:VAL:O	1:A:175:ALA:N	2.39	0.54
2:B:165:ALA:HB2	2:B:175:LEU:HD23	1.89	0.54
2:L:139:VAL:HB	2:L:175:LEU:HB3	1.90	0.53
1:A:36:TRP:CE2	1:A:81:MET:HB2	2.43	0.53
1:A:180:ASN:ND2	1:A:202:THR:O	2.42	0.53
1:A:36:TRP:HB3	1:A:48:MET:HE3	1.91	0.52
2:B:123:PRO:HA	2:B:126:LYS:HZ1	1.73	0.52
2:B:126:LYS:HD2	2:B:134:ALA:H	1.74	0.52
1:A:207:ASP:HA	1:A:210:LYS:HD3	1.90	0.52
1:A:140:PHE:HB2	1:A:155:VAL:HB	1.90	0.52
2:B:194:ASN:ND2	2:B:205:ASP:OD1	2.43	0.51
1:H:32:TYR:OH	1:H:106:ASP:OD2	2.20	0.51
2:L:147:VAL:HG12	2:L:197:HIS:CD2	2.46	0.51
2:L:34:TRP:CD2	2:L:72:LEU:HB2	2.46	0.51
1:H:212:LYS:HA	1:H:233:ARG:NH1	2.27	0.50
1:H:169:GLN:HG2	1:H:217:GLU:HB3	1.93	0.50
1:A:213:VAL:C	1:A:214:TYR:CG	2.81	0.49
1:A:140:PHE:CD1	2:B:121:LEU:HB3	2.47	0.49
1:H:170:TRP:CE2	1:H:201:LEU:HB2	2.48	0.49
2:B:139:VAL:HB	2:B:175:LEU:HB3	1.93	0.49
2:B:141:ASP:OD1	2:B:168:GLN:NE2	2.46	0.49
1:A:167:LYS:HB2	1:A:219:THR:HG22	1.95	0.49
1:A:158:LEU:HB2	1:A:197:LEU:HB3	1.94	0.49
2:L:11:SER:HB3	2:L:108:LEU:HD21	1.94	0.48
1:H:136:SER:HB2	1:H:159:ASN:HB3	1.95	0.48
2:B:34:TRP:CD2	2:B:72:LEU:HB2	2.48	0.48
2:B:192:ILE:HG22	2:B:207:LYS:HA	1.96	0.47
2:B:143:PHE:HB2	2:B:172:LEU:HD12	1.97	0.47
2:B:126:LYS:O	2:B:130:GLY:N	2.47	0.47
1:A:39:GLN:HB3	1:A:45:LEU:HD23	1.96	0.47
1:H:138:PHE:HD1	2:L:126:LYS:HB2	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:143:SER:OG	2:L:120:PRO:O	2.33	0.46
1:H:138:PHE:CD1	2:L:126:LYS:HB2	2.50	0.46
1:A:172:VAL:HG21	1:A:211:HIS:CE1	2.50	0.46
2:B:35:TYR:HE1	2:B:88:GLN:HB3	1.79	0.46
2:L:197:HIS:CD2	2:L:199:PRO:HD2	2.50	0.46
2:B:127:SER:HB2	2:B:133:ALA:CB	2.29	0.46
1:A:29:PHE:CE2	1:A:53:PRO:HB3	2.51	0.45
1:H:208:TYR:HA	1:H:214:TYR:OH	2.17	0.45
1:H:154:VAL:HG23	1:H:201:LEU:HB3	1.99	0.45
2:L:10:VAL:O	2:L:105:VAL:HA	2.17	0.45
1:H:32:TYR:CD1	1:H:100:PRO:HA	2.51	0.44
1:A:208:TYR:O	1:A:214:TYR:OH	2.35	0.44
1:A:162:TYR:CG	1:A:163:PRO:HA	2.52	0.44
2:L:34:TRP:CE2	2:L:72:LEU:HB2	2.53	0.44
2:B:126:LYS:HD2	2:B:134:ALA:O	2.18	0.44
2:L:38:LYS:HG2	2:L:83:ALA:HB2	2.00	0.44
1:H:106:ASP:OD1	1:H:107:SER:N	2.47	0.43
2:L:116:PRO:HB3	2:L:142:TYR:HB3	2.00	0.43
1:H:163:PRO:HB2	1:H:165:GLU:OE1	2.19	0.43
1:A:220:HIS:CD2	1:A:221:GLN:H	2.36	0.43
1:H:29:PHE:CE1	1:H:53:PRO:HB3	2.54	0.43
2:L:27:ILE:HD13	2:L:27:ILE:HA	1.90	0.42
1:A:161:PHE:HB2	1:A:220:HIS:HE1	1.85	0.42
2:B:10:VAL:O	2:B:105:VAL:HA	2.19	0.42
1:H:173:ASP:N	1:H:173:ASP:OD2	2.53	0.42
1:A:162:TYR:CD1	1:A:163:PRO:HA	2.55	0.42
2:B:197:HIS:CD2	2:B:199:PRO:HD2	2.55	0.42
1:H:64:PHE:O	1:H:68:VAL:HG12	2.19	0.42
1:A:137:VAL:HG13	1:A:158:LEU:HD23	2.02	0.42
2:L:209:GLU:HB2	2:L:210:PRO:HD2	2.01	0.42
1:H:156:CYS:HB2	1:H:170:TRP:CH2	2.54	0.41
2:L:143:PHE:HA	2:L:144:PRO:HA	1.84	0.41
1:H:47:TRP:CZ2	1:H:49:GLY:HA2	2.56	0.41
1:H:67:ARG:NH1	1:H:90:ASP:OD2	2.47	0.41
2:B:126:LYS:O	2:B:130:GLY:HA3	2.20	0.41
2:L:35:TYR:HE1	2:L:88:GLN:HB3	1.85	0.41
2:B:34:TRP:CE2	2:B:72:LEU:HB2	2.56	0.41
1:H:212:LYS:HA	1:H:233:ARG:HH12	1.85	0.41
1:A:140:PHE:HA	1:A:141:PRO:HD2	1.94	0.41
1:H:135:PRO:HA	1:H:161:PHE:HB3	2.01	0.41
1:H:32:TYR:CG	1:H:98:ARG:HD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:126:LYS:CD	2:B:134:ALA:H	2.32	0.41
1:A:50:TRP:CE2	1:A:59:ASN:HB3	2.56	0.41
1:H:207:ASP:O	1:H:211:HIS:ND1	2.46	0.41
2:B:130:GLY:C	2:B:132:THR:N	2.73	0.40
1:A:156:CYS:HB2	1:A:170:TRP:CH2	2.56	0.40
2:L:22:CYS:HB3	2:L:70:ALA:HB3	2.02	0.40
1:A:207:ASP:HA	1:A:210:LYS:HG2	2.03	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	232/245 (95%)	223 (96%)	9 (4%)	0	100	100
1	H	232/245 (95%)	225 (97%)	7 (3%)	0	100	100
2	B	210/213 (99%)	203 (97%)	7 (3%)	0	100	100
2	L	208/213 (98%)	198 (95%)	10 (5%)	0	100	100
All	All	882/916 (96%)	849 (96%)	33 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	199/208 (96%)	188 (94%)	11 (6%)	27	60
1	H	199/208 (96%)	185 (93%)	14 (7%)	19	47
2	B	180/181 (99%)	170 (94%)	10 (6%)	26	59
2	L	178/181 (98%)	167 (94%)	11 (6%)	23	54
All	All	756/778 (97%)	710 (94%)	46 (6%)	23	55

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	12	LYS
1	H	43	GLN
1	H	72	ARG
1	H	87	ARG
1	H	88	SER
1	H	172	VAL
1	H	173	ASP
1	H	189	ASP
1	H	203	LEU
1	H	209	GLU
1	H	213	VAL
1	H	218	VAL
1	H	219	THR
1	H	223	LEU
2	L	12	VAL
2	L	69	THR
2	L	89	VAL
2	L	105	VAL
2	L	106	THR
2	L	126	LYS
2	L	156	LEU
2	L	157	THR
2	L	175	LEU
2	L	201	ASN
2	L	209	GLU
1	A	1	GLN
1	A	72	ARG
1	A	89	ASP
1	A	125	VAL
1	A	148	LYS
1	A	173	ASP
1	A	186	THR
1	A	190	SER

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Mol	Chain	Res	Type
1	A	192	ASP
1	A	201	LEU
1	A	223	LEU
2	B	27	ILE
2	B	44	VAL
2	B	47	VAL
2	B	110	SER
2	B	158	SER
2	B	172	LEU
2	B	176	SER
2	B	190	THR
2	B	192	ILE
2	B	201	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	A	146	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

2 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	$\# Z > 2$
3	GOL	B	301	-	5,5,5	0.35	0	5,5,5	0.28	0
3	GOL	H	301	-	5,5,5	0.36	0	5,5,5	0.23	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	-	-	0/4/4/4	0/0/0/0
3	GOL	H	301	-	-	0/4/4/4	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.

No monomer is involved in short contacts.

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, 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	234/245 (95%)	0.67	26 (11%) 7 5	32, 70, 134, 161	24 (10%)
1	H	234/245 (95%)	0.45	7 (2%) 54 50	31, 74, 111, 127	21 (8%)
2	B	212/213 (99%)	0.63	27 (12%) 5 3	24, 57, 147, 253	4 (1%)
2	L	210/213 (98%)	0.47	18 (8%) 13 9	27, 56, 136, 180	5 (2%)
All	All	890/916 (97%)	0.56	78 (8%) 12 9	24, 64, 131, 253	54 (6%)

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	127	SER	11.9
2	B	128	THR	7.4
2	B	185	SER	6.5
2	B	135	LEU	5.2
1	A	154	VAL	5.1
2	L	127	SER	5.1
1	A	140	PHE	5.1
2	B	3	GLY	5.0
1	A	222	GLY	4.7
1	A	214	TYR	4.5
2	L	185	SER	4.3
2	B	129	SER	4.3
2	L	128	THR	4.2
2	L	184	SER	4.1
2	L	112	SER	4.0
1	A	230	SER	4.0
2	L	187	GLY	3.9
1	A	223	LEU	3.9
2	L	181	VAL	3.9
1	A	208	TYR	3.8
2	B	212	SER	3.7

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Mol	Chain	Res	Type	RSRZ
2	L	157	THR	3.6
2	B	188	THR	3.5
2	B	190	THR	3.5
2	B	213	CYS	3.5
2	B	130	GLY	3.4
1	A	224	SER	3.3
2	L	3	GLY	3.3
1	H	190	SER	3.2
2	B	125	SER	3.2
2	B	123	PRO	3.2
1	A	176	LEU	3.2
2	B	156	LEU	3.2
1	A	170	TRP	3.2
2	B	131	GLY	3.2
1	A	211	HIS	3.1
2	L	132	THR	3.0
1	A	227	VAL	3.0
2	B	134	ALA	3.0
1	H	192	ASP	2.9
2	B	210	PRO	2.9
1	A	228	THR	2.8
2	B	182	PRO	2.8
2	B	181	VAL	2.8
2	B	126	LYS	2.8
2	B	189	GLN	2.8
1	A	219	THR	2.7
2	L	191	TYR	2.7
1	A	207	ASP	2.6
1	A	138	PHE	2.6
1	A	157	LEU	2.6
1	A	168	VAL	2.6
1	H	189	ASP	2.5
1	A	197	LEU	2.5
2	B	187	GLY	2.5
2	B	155	ALA	2.5
1	A	195	TYR	2.4
1	A	171	LYS	2.4
1	A	136	SER	2.4
2	B	2	PRO	2.4
2	B	132	THR	2.4
1	A	158	LEU	2.3
1	A	160	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
2	L	208	VAL	2.3
1	H	158	LEU	2.3
1	H	206	ALA	2.3
2	L	210	PRO	2.3
2	B	211	LYS	2.3
1	H	154	VAL	2.3
2	B	158	SER	2.2
2	L	186	LEU	2.2
1	H	86	LEU	2.2
2	L	180	THR	2.2
2	L	182	PRO	2.2
1	A	196	SER	2.1
1	A	226	PRO	2.1
2	L	129	SER	2.1
2	L	2	PRO	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. 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(Å ²)	Q<0.9
3	GOL	B	301	6/6	0.92	0.25	3.29	47,49,51,54	0
3	GOL	H	301	6/6	0.95	0.16	-0.51	43,44,45,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.