



Full wwPDB X-ray Structure Validation Report ⓘ

May 20, 2025 – 12:57 PM EDT

PDB ID : 9C2K / pdb_00009c2k
Title : The crystal structure of HIV-1 Rev Response Element Stem-Loop II in complex with a Fab
Authors : Ojha, M.; Koirala, D.
Deposited on : 2024-05-31
Resolution : 2.42 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 Phenix2.0rc1
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

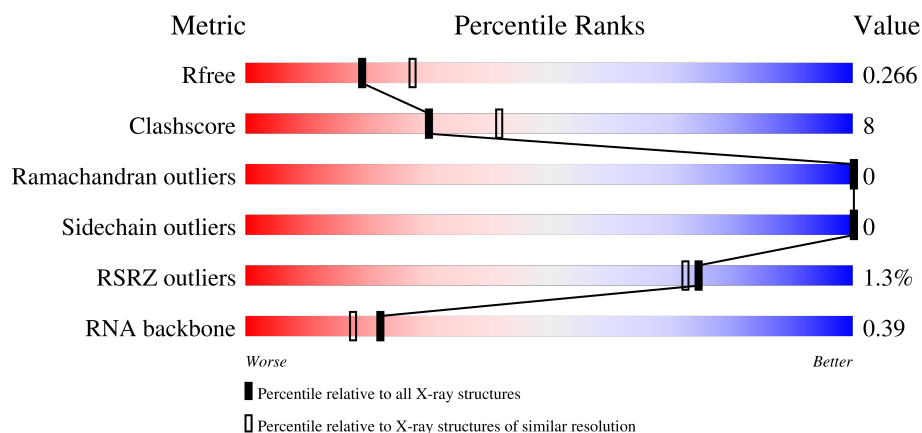
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.42 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}	164625	5670 (2.44-2.40)
Clashscore	180529	6299 (2.44-2.40)
Ramachandran outliers	177936	6232 (2.44-2.40)
Sidechain outliers	177891	6233 (2.44-2.40)
RSRZ outliers	164620	5670 (2.44-2.40)
RNA backbone	3690	1014 (2.72-2.12)

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	233	<div> <div></div> <div>86%</div> <div>11%</div> <div></div> </div>
1	H	233	<div> <div></div> <div>86%</div> <div>11%</div> <div></div> </div>
2	B	215	<div> <div></div> <div>83%</div> <div>17%</div> <div></div> </div>
2	L	215	<div> <div></div> <div>83%</div> <div>17%</div> <div></div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	C	72	<div><div></div><div>6%</div><div>31%</div><div>46%</div><div>24%</div></div>
3	R	72	<div><div></div><div>4%</div><div>44%</div><div>46%</div><div>10%</div></div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10271 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 BL3-6 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	226	Total	C	N	O	S	0	0	0
			1684	1058	288	332	6			
1	A	226	Total	C	N	O	S	0	0	0
			1684	1058	288	332	6			

- Molecule 2 is a protein called BL3-6 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	215	Total	C	N	O	S	0	0	0
			1643	1025	275	337	6			
2	B	215	Total	C	N	O	S	0	0	0
			1643	1025	275	337	6			

- Molecule 3 is a RNA chain called Rev Response Element.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	R	72	Total	C	N	O	P	0	0	0
			1543	689	285	497	72			
3	C	72	Total	C	N	O	P	0	0	0
			1543	689	285	497	72			

There are 16 discrepancies between the modelled and reference sequences:

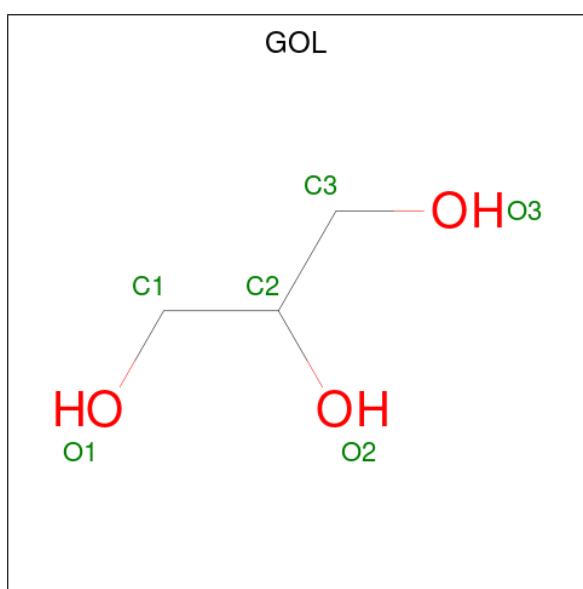
Chain	Residue	Modelled	Actual	Comment	Reference
R	1	G	-	insertion	GB 902798
R	49	G	U	conflict	GB 902798
R	50	A	U	conflict	GB 902798
R	52	A	-	insertion	GB 902798
R	53	C	-	insertion	GB 902798
R	54	A	-	insertion	GB 902798
R	55	C	-	insertion	GB 902798
R	72	C	-	insertion	GB 902798

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	G	-	insertion	GB 902798
C	49	G	U	conflict	GB 902798
C	50	A	U	conflict	GB 902798
C	52	A	-	insertion	GB 902798
C	53	C	-	insertion	GB 902798
C	54	A	-	insertion	GB 902798
C	55	C	-	insertion	GB 902798
C	72	C	-	insertion	GB 902798

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



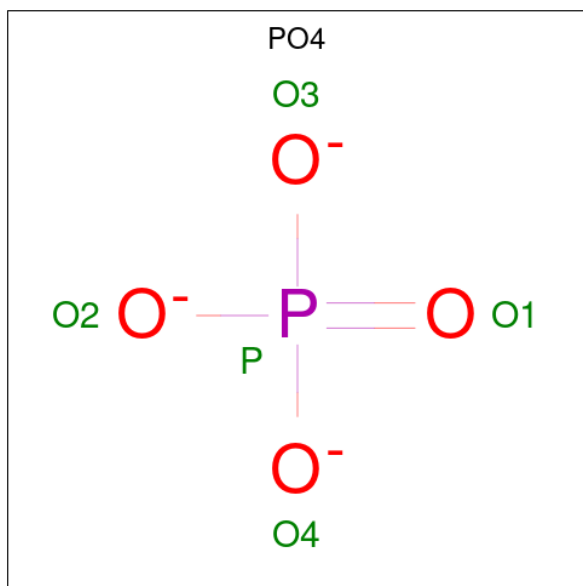
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	1	Total C O 6 3 3	0	0
4	H	1	Total C O 6 3 3	0	0
4	H	1	Total C O 6 3 3	0	0
4	H	1	Total C O 6 3 3	0	0
4	L	1	Total C O 6 3 3	0	0
4	L	1	Total C O 6 3 3	0	0
4	L	1	Total C O 6 3 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	L	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	R	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	P	0	0
			5	4	1		
5	R	1	Total	O	P	0	0
			5	4	1		
5	C	1	Total	O	P	0	0
			5	4	1		

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	R	1	Total	Mg	0	0
			1	1		


- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	H	102	Total	O	0	0
			102	102		
7	L	88	Total	O	0	0
			88	88		
7	A	83	Total	O	0	0
			83	83		
7	B	61	Total	O	0	0
			61	61		
7	R	46	Total	O	0	0
			46	46		
7	C	29	Total	O	0	0
			29	29		

3 Residue-property plots


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: BL3-6 Fab heavy chain

Chain H: 




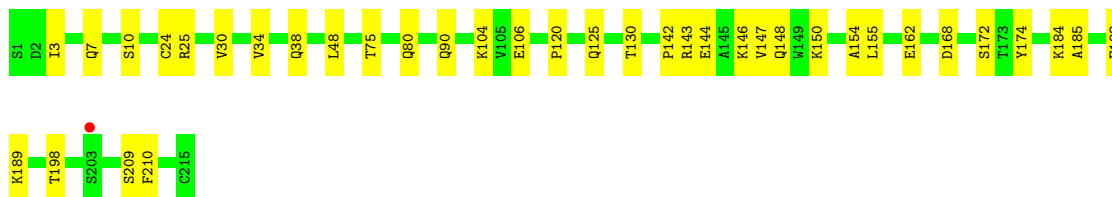
- Molecule 1: BL3-6 Fab heavy chain

Chain A: 




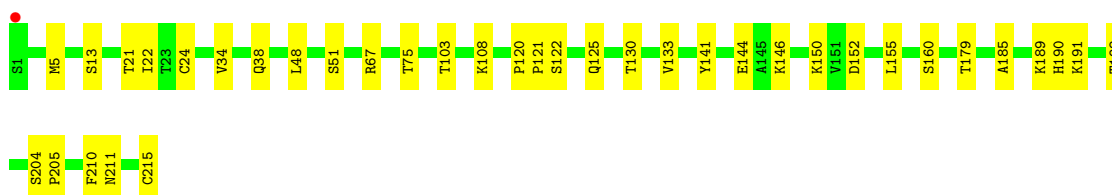
- Molecule 2: BL3-6 Fab light chain

Chain L: 

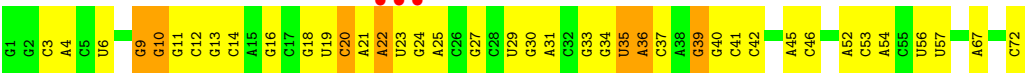


- Molecule 2: BL3-6 Fab light chain

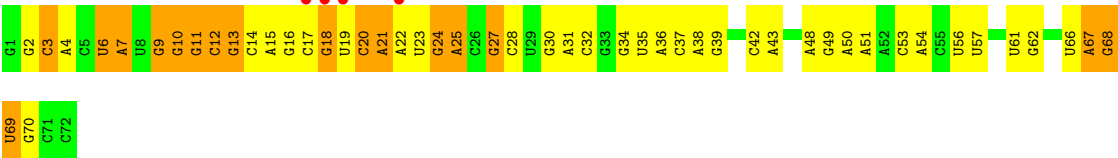
Chain B: 



- Molecule 3: Rev Response Element



● Molecule 3: Rev Response Element



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	72.36Å 76.24Å 82.60Å 116.56° 94.91° 102.75°	Depositor
Resolution (Å)	45.33 – 2.42 45.33 – 2.42	Depositor EDS
% Data completeness (in resolution range)	83.2 (45.33-2.42) 80.0 (45.33-2.42)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 2.42Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.205 , 0.265 0.208 , 0.266	Depositor DCC
R_{free} test set	55785 reflections (3.61%)	wwPDB-VP
Wilson B-factor (Å ²)	46.0	Xtriage
Anisotropy	0.275	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 60.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10271	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.55% 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, MG, PO4

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	0.51	0/1725	0.69	0/2347
1	H	0.54	0/1725	0.72	0/2347
2	B	0.46	0/1678	0.64	0/2277
2	L	0.47	0/1678	0.69	0/2277
3	C	0.31	0/1727	0.57	0/2691
3	R	0.32	0/1727	0.60	0/2691
All	All	0.45	0/10260	0.65	0/14630

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	1684	0	1643	18	0
1	H	1684	0	1643	15	0
2	B	1643	0	1595	23	0
2	L	1643	0	1595	27	0
3	C	1543	0	780	35	0
3	R	1543	0	780	24	0
4	A	12	0	16	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	30	0	40	1	0
4	H	24	0	32	0	0
4	L	24	0	31	3	0
4	R	6	0	8	0	0
5	B	10	0	0	1	0
5	C	5	0	0	0	0
5	L	5	0	0	0	0
5	R	5	0	0	0	0
6	R	1	0	0	0	0
7	A	83	0	0	2	0
7	B	61	0	0	0	0
7	C	29	0	0	0	0
7	H	102	0	0	1	0
7	L	88	0	0	2	0
7	R	46	0	0	0	0
All	All	10271	0	8163	136	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 (136) 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:B:191:LYS:HE3	2:B:211:ASN:HB3	1.76	0.68
3:C:49:G:H2'	3:C:51:A:H62	1.60	0.67
2:L:184:LYS:HE2	2:L:188:GLU:OE2	1.96	0.66
3:C:66:U:H2'	3:C:67:A:C8	2.31	0.65
3:C:9:G:H4'	3:C:10:G:OP2	1.97	0.63
3:C:9:G:OP1	3:C:9:G:H2'	1.99	0.62
3:C:4:A:N6	3:C:69:U:O4	2.33	0.62
2:L:143:ARG:HD3	4:L:305:GOL:H2	1.81	0.62
2:L:144:GLU:OE1	2:L:144:GLU:N	2.20	0.61
3:C:24:G:H3'	3:C:25:A:H8	1.64	0.61
1:H:101:ARG:NH2	1:H:113:ASP:OD2	2.30	0.60
3:C:43:A:H61	3:C:61:U:H3	1.46	0.60
1:H:88:SER:HB2	1:H:90:ARG:HH12	1.66	0.60
3:R:29:U:H2'	3:R:30:G:C8	2.37	0.60
3:C:24:G:H4'	3:C:24:G:OP1	2.04	0.58
2:L:104:LYS:HE2	2:L:106:GLU:OE2	2.04	0.57
3:R:29:U:H2'	3:R:30:G:H8	1.69	0.57
1:H:15:VAL:O	1:H:123:VAL:HA	2.05	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:106:GLU:OE1	2:L:174:TYR:OH	2.21	0.57
2:L:144:GLU:H	2:L:144:GLU:CD	2.12	0.57
1:H:46:LYS:HB3	7:H:465:HOH:O	2.06	0.56
2:B:120:PRO:HB3	2:B:210:PHE:CZ	2.41	0.56
1:A:41:ARG:NE	1:A:49:GLU:OE1	2.28	0.56
3:C:66:U:H2'	3:C:67:A:N7	2.21	0.55
2:L:3:ILE:HD13	2:L:30:VAL:HG12	1.89	0.55
1:A:92:GLU:H	1:A:92:GLU:CD	2.15	0.55
3:R:24:G:H2'	3:R:25:A:O4'	2.07	0.54
3:C:56:U:H2'	3:C:57:U:C6	2.43	0.54
3:R:10:G:O2'	3:R:11:G:H3'	2.07	0.54
2:B:38:GLN:HB2	2:B:48:LEU:HD11	1.88	0.54
2:B:152:ASP:OD2	2:B:190:HIS:HB3	2.07	0.53
3:R:6:U:H3	3:R:67:A:H61	1.55	0.53
2:B:150:LYS:HG2	2:B:155:LEU:HD23	1.89	0.53
1:H:15:VAL:HG13	1:H:123:VAL:HG22	1.91	0.53
1:A:190:LEU:HA	4:A:302:GOL:H32	1.91	0.53
1:H:110:ARG:NH2	3:R:52:A:O4'	2.42	0.53
1:A:212:HIS:HB3	1:A:217:THR:OG1	2.09	0.52
3:C:11:G:H8	3:C:62:G:H2'	1.74	0.52
2:B:185:ALA:O	2:B:189:LYS:HG3	2.09	0.52
3:C:24:G:H3'	3:C:25:A:C8	2.44	0.52
3:R:20:C:H3'	3:R:22:A:H61	1.75	0.52
3:C:11:G:C8	3:C:62:G:H2'	2.44	0.52
2:B:144:GLU:OE1	2:B:144:GLU:N	2.24	0.51
3:R:41:C:H2'	3:R:42:C:O4'	2.10	0.51
3:C:20:C:N4	3:C:21:A:N7	2.59	0.51
3:C:13:G:N1	3:C:32:C:O2	2.43	0.51
3:C:30:G:H2'	3:C:31:A:C8	2.45	0.50
3:C:24:G:H5'	3:C:25:A:C8	2.46	0.50
1:H:9:GLU:CD	1:H:118:GLY:H	2.20	0.50
3:R:39:G:H3'	3:R:40:G:H8	1.77	0.49
3:C:35:U:H2'	3:C:36:A:C8	2.47	0.49
3:C:10:G:O2'	3:C:12:C:H3'	2.12	0.49
2:L:75:THR:HG23	7:L:418:HOH:O	2.11	0.49
2:L:150:LYS:HG2	2:L:155:LEU:HD23	1.93	0.49
1:A:68:LYS:HE3	7:A:450:HOH:O	2.12	0.49
1:A:190:LEU:C	1:A:190:LEU:HD12	2.37	0.49
2:L:125:GLN:HG2	2:L:130:THR:O	2.12	0.49
1:H:14:LEU:HD23	1:H:122:THR:HB	1.93	0.49
2:B:67:ARG:NH1	5:B:301:PO4:O2	2.37	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:38:A:H2'	3:C:39:G:H8	1.79	0.48
2:B:5:MET:HE3	2:B:24:CYS:SG	2.54	0.48
2:L:106:GLU:OE2	4:L:305:GOL:H31	2.13	0.48
1:A:228:CYS:C	2:B:215:CYS:HB3	2.38	0.48
1:A:130:GLY:HA3	1:A:217:THR:HG21	1.96	0.47
2:L:80:GLN:HG3	7:L:441:HOH:O	2.13	0.47
2:L:185:ALA:O	2:L:189:LYS:HG3	2.13	0.47
3:R:30:G:H2'	3:R:31:A:C8	2.49	0.47
1:H:164:VAL:HG22	1:H:210:VAL:HG22	1.97	0.47
2:L:147:VAL:HB	2:L:162:GLU:OE2	2.14	0.47
3:C:2:G:H2'	3:C:3:C:O4'	2.14	0.47
1:H:166:TRP:CH2	1:H:208:CYS:HB3	2.50	0.47
2:B:125:GLN:HG2	2:B:130:THR:O	2.15	0.47
3:R:3:C:H2'	3:R:4:A:C8	2.50	0.47
1:A:15:VAL:O	1:A:123:VAL:HA	2.15	0.46
3:C:6:U:O2'	3:C:7:A:OP1	2.22	0.46
2:B:160:SER:HA	2:B:179:THR:O	2.14	0.46
1:A:221:LYS:NZ	3:R:3:C:OP1	2.49	0.46
3:R:30:G:C6	3:R:31:A:C6	3.04	0.46
3:R:56:U:H2'	3:R:57:U:C6	2.50	0.46
3:R:53:C:H2'	3:R:54:A:H8	1.81	0.46
3:C:38:A:H2'	3:C:39:G:C8	2.50	0.46
2:L:38:GLN:HB2	2:L:48:LEU:HD11	1.98	0.45
3:R:35:U:H5'	3:R:36:A:OP2	2.16	0.45
3:C:17:C:H42	3:C:27:G:H1	1.64	0.45
1:H:41:ARG:NE	1:H:49:GLU:OE1	2.36	0.45
2:L:25:ARG:HG3	1:A:125:SER:OG	2.17	0.45
2:B:34:VAL:O	2:B:51:SER:O	2.35	0.45
3:R:11:G:N2	3:R:42:C:H1'	2.32	0.45
2:B:34:VAL:N	2:B:51:SER:O	2.37	0.45
3:R:9:G:N2	3:R:33:G:H1'	2.32	0.45
2:L:10:SER:N	4:L:302:GOL:O2	2.43	0.45
1:A:143:THR:O	1:A:147:THR:O	2.35	0.45
2:L:34:VAL:HA	2:L:90:GLN:O	2.18	0.44
2:B:21:THR:HG22	2:B:75:THR:HG22	1.98	0.44
3:C:9:G:HO2'	3:C:13:G:H8	1.64	0.44
3:C:66:U:H3	3:C:67:A:H62	1.65	0.44
2:B:22:ILE:HG12	2:B:103:THR:HG21	1.99	0.44
3:C:6:U:C2	3:C:68:G:N1	2.86	0.44
3:C:17:C:H2'	3:C:18:G:O4'	2.18	0.44
2:L:120:PRO:HB3	2:L:210:PHE:CE2	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:45:A:H2'	3:R:46:C:O4'	2.18	0.44
3:R:53:C:H2'	3:R:54:A:C8	2.52	0.44
2:B:121:PRO:HD3	2:B:133:VAL:HG22	1.99	0.44
3:C:37:C:H3'	3:C:38:A:H8	1.83	0.43
1:H:56:PRO:C	1:H:58:SER:H	2.26	0.43
1:A:86:MET:HB3	1:A:89:LEU:HD21	1.99	0.43
3:C:67:A:O2'	3:C:68:G:OP1	2.33	0.43
1:A:3:SER:OG	7:A:401:HOH:O	2.21	0.43
2:L:168:ASP:O	2:L:172:SER:HA	2.19	0.42
2:L:146:LYS:HB3	2:L:198:THR:HB	2.01	0.42
1:A:166:TRP:CH2	1:A:208:CYS:HB3	2.55	0.42
3:C:27:G:H2'	3:C:28:C:O4'	2.20	0.42
3:C:42:C:H42	3:C:62:G:H1	1.68	0.42
1:H:174:GLY:O	1:H:194:VAL:HA	2.19	0.42
2:L:155:LEU:HD23	2:L:155:LEU:HA	1.69	0.42
1:A:56:PRO:C	1:A:58:SER:H	2.29	0.41
3:C:53:C:H2'	3:C:54:A:H8	1.85	0.41
2:L:150:LYS:HA	2:L:154:ALA:O	2.20	0.41
2:B:108:LYS:HA	2:B:141:TYR:OH	2.20	0.41
2:B:204:SER:HB2	2:B:205:PRO:HD2	2.03	0.41
3:R:10:G:HO2'	3:R:11:G:H3'	1.84	0.41
3:R:10:G:C4	3:R:12:C:C4	3.08	0.41
3:R:30:G:C2	3:R:31:A:C4	3.08	0.41
1:H:141:LYS:HD2	2:L:209:SER:O	2.21	0.41
2:B:122:SER:HB2	4:B:307:GOL:H2	2.03	0.41
1:H:163:THR:OG1	1:H:211:ASN:HB3	2.21	0.41
2:L:148:GLN:CD	2:L:155:LEU:HD22	2.45	0.41
1:A:34:TYR:HB3	3:C:50:A:O2'	2.20	0.41
2:B:146:LYS:HB3	2:B:198:THR:HB	2.03	0.40
2:B:120:PRO:HB3	2:B:210:PHE:CE2	2.55	0.40
3:C:48:A:H2'	3:C:49:G:O4'	2.21	0.40
2:L:142:PRO:HB2	2:L:144:GLU:OE1	2.21	0.40
1:A:9:GLU:CD	1:A:118:GLY:H	2.30	0.40
2:B:13:SER:HB3	2:B:108:LYS:HD2	2.03	0.40
2:L:7:GLN:HG2	2:L:24:CYS:HB2	2.03	0.40
3:R:6:U:H3	3:R:67:A:N6	2.20	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	224/233 (96%)	215 (96%)	9 (4%)	0	100	100
1	H	224/233 (96%)	218 (97%)	6 (3%)	0	100	100
2	B	213/215 (99%)	208 (98%)	5 (2%)	0	100	100
2	L	213/215 (99%)	208 (98%)	5 (2%)	0	100	100
All	All	874/896 (98%)	849 (97%)	25 (3%)	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	187/194 (96%)	187 (100%)	0	100	100
1	H	187/194 (96%)	187 (100%)	0	100	100
2	B	190/190 (100%)	190 (100%)	0	100	100
2	L	190/190 (100%)	190 (100%)	0	100	100
All	All	754/768 (98%)	754 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	42	GLN
2	L	39	GLN
2	L	80	GLN
2	L	190	HIS
1	A	85	GLN
2	B	38	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	C	71/72 (98%)	24 (33%)	4 (5%)
3	R	71/72 (98%)	18 (25%)	0
All	All	142/144 (98%)	42 (29%)	4 (2%)

All (42) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	R	9	G
3	R	10	G
3	R	13	G
3	R	14	C
3	R	16	G
3	R	18	G
3	R	19	U
3	R	20	C
3	R	21	A
3	R	22	A
3	R	23	U
3	R	27	G
3	R	34	G
3	R	35	U
3	R	36	A
3	R	37	C
3	R	39	G
3	R	72	C
3	C	3	C
3	C	6	U
3	C	7	A
3	C	9	G
3	C	10	G
3	C	11	G
3	C	12	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	13	G
3	C	14	C
3	C	15	A
3	C	16	G
3	C	18	G
3	C	19	U
3	C	20	C
3	C	21	A
3	C	22	A
3	C	23	U
3	C	24	G
3	C	25	A
3	C	27	G
3	C	34	G
3	C	67	A
3	C	68	G
3	C	70	G

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	C	6	U
3	C	9	G
3	C	67	A
3	C	69	U

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](#)

Of 22 ligands modelled in this entry, 1 is monoatomic - leaving 21 for Mogul analysis.

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	GOL	H	302	-	5,5,5	0.93	0	5,5,5	1.17	1 (20%)
4	GOL	B	307	-	5,5,5	0.77	0	5,5,5	1.23	0
4	GOL	A	302	-	5,5,5	1.20	0	5,5,5	1.06	0
4	GOL	L	304	-	5,5,5	1.41	1 (20%)	5,5,5	0.93	0
4	GOL	A	301	-	5,5,5	1.03	0	5,5,5	1.00	0
4	GOL	B	305	-	5,5,5	1.43	1 (20%)	5,5,5	0.91	0
5	PO4	C	101	-	4,4,4	0.86	0	6,6,6	0.51	0
4	GOL	L	305	-	5,5,5	1.08	0	5,5,5	1.00	0
4	GOL	L	302	-	5,5,5	0.96	0	5,5,5	1.12	0
5	PO4	L	301	-	4,4,4	0.67	0	6,6,6	0.93	0
5	PO4	R	101	-	4,4,4	0.87	0	6,6,6	0.49	0
4	GOL	R	103	-	5,5,5	0.97	0	5,5,5	1.28	0
4	GOL	L	303	-	5,5,5	0.99	0	5,5,5	1.11	0
4	GOL	B	304	-	5,5,5	1.00	0	5,5,5	1.02	0
4	GOL	B	306	-	5,5,5	1.15	0	5,5,5	1.44	1 (20%)
4	GOL	H	301	-	5,5,5	0.73	0	5,5,5	0.99	0
4	GOL	H	303	-	5,5,5	1.47	2 (40%)	5,5,5	1.05	0
5	PO4	B	302	-	4,4,4	0.76	0	6,6,6	0.50	0
4	GOL	H	304	-	5,5,5	1.18	0	5,5,5	0.89	0
5	PO4	B	301	-	4,4,4	1.09	0	6,6,6	0.29	0
4	GOL	B	303	-	5,5,5	1.06	0	5,5,5	1.16	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	GOL	B	306	-	-	2/4/4/4	-
4	GOL	H	302	-	-	2/4/4/4	-
4	GOL	H	303	-	-	2/4/4/4	-
4	GOL	H	301	-	-	2/4/4/4	-
4	GOL	A	302	-	-	4/4/4/4	-
4	GOL	H	304	-	-	2/4/4/4	-
4	GOL	B	307	-	-	4/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	L	302	-	-	2/4/4/4	-
4	GOL	L	304	-	-	2/4/4/4	-
4	GOL	A	301	-	-	2/4/4/4	-
4	GOL	R	103	-	-	4/4/4/4	-
4	GOL	L	303	-	-	1/4/4/4	-
4	GOL	B	303	-	-	2/4/4/4	-
4	GOL	B	305	-	-	2/4/4/4	-
4	GOL	L	305	-	-	1/4/4/4	-
4	GOL	B	304	-	-	2/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	304	GOL	O2-C2	-2.48	1.36	1.43
4	B	305	GOL	C1-C2	2.44	1.61	1.51
4	H	303	GOL	C3-C2	2.33	1.60	1.51
4	H	303	GOL	C1-C2	2.15	1.60	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	302	GOL	C3-C2-C1	-2.08	104.16	111.80
4	B	306	GOL	C3-C2-C1	-2.06	104.22	111.80

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	303	GOL	C1-C2-C3-O3
4	L	302	GOL	C1-C2-C3-O3
4	L	304	GOL	O1-C1-C2-C3
4	A	301	GOL	O1-C1-C2-C3
4	A	302	GOL	C1-C2-C3-O3
4	B	303	GOL	O1-C1-C2-C3
4	B	304	GOL	C1-C2-C3-O3
4	B	304	GOL	O2-C2-C3-O3
4	B	305	GOL	O1-C1-C2-C3
4	B	307	GOL	O1-C1-C2-O2
4	B	307	GOL	O1-C1-C2-C3
4	R	103	GOL	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	H	301	GOL	O1-C1-C2-C3
4	H	302	GOL	C1-C2-C3-O3
4	H	304	GOL	C1-C2-C3-O3
4	A	302	GOL	O1-C1-C2-C3
4	B	306	GOL	C1-C2-C3-O3
4	B	307	GOL	C1-C2-C3-O3
4	R	103	GOL	O1-C1-C2-C3
4	R	103	GOL	C1-C2-C3-O3
4	H	303	GOL	O2-C2-C3-O3
4	H	304	GOL	O2-C2-C3-O3
4	A	301	GOL	O1-C1-C2-O2
4	A	302	GOL	O2-C2-C3-O3
4	B	303	GOL	O1-C1-C2-O2
4	B	305	GOL	O1-C1-C2-O2
4	B	306	GOL	O2-C2-C3-O3
4	R	103	GOL	O2-C2-C3-O3
4	H	302	GOL	O2-C2-C3-O3
4	L	303	GOL	O1-C1-C2-O2
4	L	304	GOL	O1-C1-C2-O2
4	L	305	GOL	O2-C2-C3-O3
4	L	302	GOL	O2-C2-C3-O3
4	A	302	GOL	O1-C1-C2-O2
4	B	307	GOL	O2-C2-C3-O3
4	H	301	GOL	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	307	GOL	1	0
4	A	302	GOL	1	0
4	L	305	GOL	2	0
4	L	302	GOL	1	0
5	B	301	PO4	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

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	226/233 (96%)	-0.20	3 (1%) 74 72	35, 45, 68, 138	0
1	H	226/233 (96%)	-0.19	1 (0%) 89 87	32, 43, 67, 114	0
2	B	215/215 (100%)	0.03	1 (0%) 87 86	38, 57, 79, 118	0
2	L	215/215 (100%)	-0.13	1 (0%) 87 86	33, 50, 77, 133	0
3	C	72/72 (100%)	0.71	4 (5%) 31 29	48, 164, 285, 317	0
3	R	72/72 (100%)	0.41	3 (4%) 41 39	39, 113, 214, 274	0
All	All	1026/1040 (98%)	-0.03	13 (1%) 74 72	32, 50, 166, 317	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	145	GLY	3.4
2	L	203	SER	2.9
1	A	3	SER	2.7
2	B	1	SER	2.6
3	C	19	U	2.6
3	R	22	A	2.3
3	C	17	C	2.3
3	C	18	G	2.2
3	R	24	G	2.2
3	R	23	U	2.1
1	H	4	GLU	2.1
3	C	22	A	2.1
1	A	33	SER	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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, 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(Å ²)	Q<0.9
5	PO4	C	101	5/5	0.67	0.13	109,111,115,117	0
5	PO4	R	101	5/5	0.74	0.11	123,125,128,132	0
4	GOL	R	103	6/6	0.75	0.10	64,65,67,68	0
4	GOL	B	306	6/6	0.76	0.15	52,53,55,58	0
4	GOL	B	305	6/6	0.77	0.12	72,74,77,78	0
5	PO4	B	302	5/5	0.77	0.08	86,90,92,104	0
4	GOL	H	304	6/6	0.78	0.13	72,76,79,79	0
4	GOL	H	303	6/6	0.79	0.17	47,50,53,54	0
4	GOL	B	303	6/6	0.80	0.15	57,61,69,70	0
4	GOL	L	303	6/6	0.83	0.10	65,69,76,77	0
4	GOL	L	305	6/6	0.83	0.12	58,63,66,67	0
5	PO4	L	301	5/5	0.83	0.15	68,70,80,85	0
4	GOL	A	301	6/6	0.84	0.12	78,87,88,94	0
4	GOL	B	304	6/6	0.85	0.10	73,74,75,75	0
4	GOL	B	307	6/6	0.86	0.14	59,62,63,64	0
4	GOL	H	302	6/6	0.86	0.15	49,53,55,58	0
4	GOL	H	301	6/6	0.87	0.11	54,62,66,66	0
5	PO4	B	301	5/5	0.89	0.14	65,68,72,75	0
4	GOL	L	302	6/6	0.89	0.10	57,59,63,65	0
4	GOL	L	304	6/6	0.90	0.13	50,51,54,56	0
4	GOL	A	302	6/6	0.92	0.10	45,46,49,50	0
6	MG	R	102	1/1	0.96	0.18	67,67,67,67	0

6.5 Other polymers [i](#)

There are no such residues in this entry.