



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 04:07 pm BST

PDB ID : 4K4T
Title : Poliovirus polymerase elongation complex (r4_form)
Authors : Gong, P.; Peersen, O.B.
Deposited on : 2013-04-12
Resolution : 2.75 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 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 : 2.11
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) : 2.11

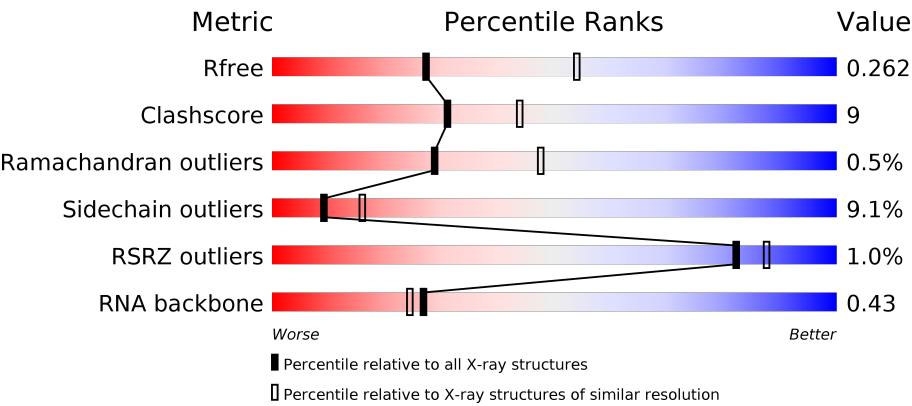
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)
RNA backbone	3102	1060 (3.02-2.50)

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 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	471	<div><div></div><div>71%24%..</div></div>
1	E	471	<div>%<div>73%21%..</div></div>
2	B	22	<div><div>36%32%9%23%</div></div>
2	F	22	<div><div>32%32%14%23%</div></div>

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Mol	Chain	Length	Quality of chain
3	C	12	<div><div></div><div>8%</div><div>25%</div><div>67%</div><div>8%</div></div>
3	G	12	<div><div></div><div>8%</div><div>58%</div><div>25%</div><div>17%</div></div>
4	D	9	<div><div></div><div>22%</div><div>22%</div><div>56%</div></div>
4	H	9	<div><div></div><div>11%</div><div>22%</div><div>22%</div><div>56%</div></div>

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 8944 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 RNA-directed RNA polymerase 3D-POL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	462	Total	C	N	O	S	0	0	0
			3701	2372	611	696	22			
1	E	462	Total	C	N	O	S	0	0	0
			3701	2372	611	696	22			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	446	ASP	LEU	ENGINEERED MUTATION	UNP P03300
A	462	GLY	-	EXPRESSION TAG	UNP P03300
A	463	SER	-	EXPRESSION TAG	UNP P03300
A	464	SER	-	EXPRESSION TAG	UNP P03300
A	465	SER	-	EXPRESSION TAG	UNP P03300
A	466	HIS	-	EXPRESSION TAG	UNP P03300
A	467	HIS	-	EXPRESSION TAG	UNP P03300
A	468	HIS	-	EXPRESSION TAG	UNP P03300
A	469	HIS	-	EXPRESSION TAG	UNP P03300
A	470	HIS	-	EXPRESSION TAG	UNP P03300
A	471	HIS	-	EXPRESSION TAG	UNP P03300
E	446	ASP	LEU	ENGINEERED MUTATION	UNP P03300
E	462	GLY	-	EXPRESSION TAG	UNP P03300
E	463	SER	-	EXPRESSION TAG	UNP P03300
E	464	SER	-	EXPRESSION TAG	UNP P03300
E	465	SER	-	EXPRESSION TAG	UNP P03300
E	466	HIS	-	EXPRESSION TAG	UNP P03300
E	467	HIS	-	EXPRESSION TAG	UNP P03300
E	468	HIS	-	EXPRESSION TAG	UNP P03300
E	469	HIS	-	EXPRESSION TAG	UNP P03300
E	470	HIS	-	EXPRESSION TAG	UNP P03300
E	471	HIS	-	EXPRESSION TAG	UNP P03300

- Molecule 2 is a RNA chain called RNA (5'-R(*AP*AP*GP*UP*CP*UP*CP*CP*AP*GP*GP*UP*CP*UP*CP*UP*CP*GP*GP*AP*AP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	17	Total	C	N	O	P	0	0	0
			360	161	63	119	17			
2	F	17	Total	C	N	O	P	0	0	0
			360	161	63	119	17			

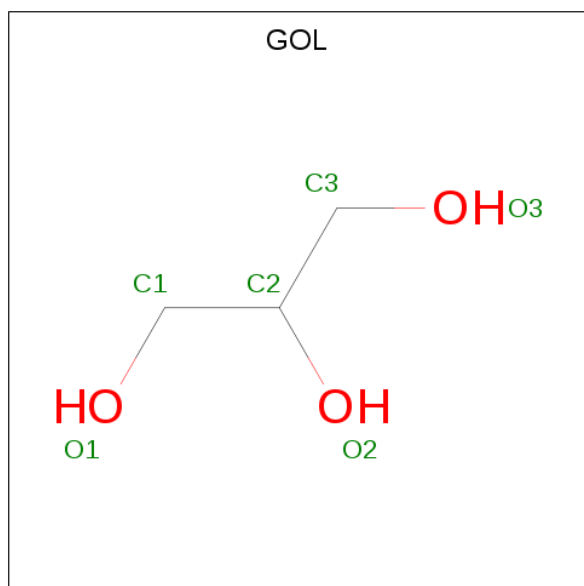
- Molecule 3 is a RNA chain called RNA (5'-R(P*UP*GP*UP*UP*CP*CP*GP*AP*GP*AP*GP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	12	Total	C	N	O	P	0	0	0
			258	115	47	84	12			
3	G	12	Total	C	N	O	P	0	0	0
			258	115	47	84	12			

- Molecule 4 is a RNA chain called RNA (5'-R(*GP*GP*GP*AP*GP*AP*UP*GP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	4	Total	C	N	O	P	0	0	0
			91	40	20	27	4			
4	H	4	Total	C	N	O	P	0	0	0
			91	40	20	27	4			

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

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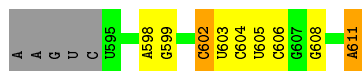
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	3	3		
5	E	1	Total	C	O	0	0
			6	3	3		
5	E	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Zn	0	0
			1	1		
6	E	1	Total	Zn	0	0
			1	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	35	Total	O	0	0
			35	35		
7	B	7	Total	O	0	0
			7	7		
7	C	6	Total	O	0	0
			6	6		
7	D	1	Total	O	0	0
			1	1		
7	E	35	Total	O	0	0
			35	35		
7	F	6	Total	O	0	0
			6	6		
7	G	6	Total	O	0	0
			6	6		
7	H	2	Total	O	0	0
			2	2		



- Molecule 2: RNA (5'-R(*AP*AP*GP*UP*CP*UP*CP*CP*AP*GP*GP*UP*CP*UP*CP*UP*CP*GP*GP*AP*AP*A)-3')



- Molecule 3: RNA (5'-R(P*UP*GP*UP*UP*CP*CP*GP*AP*GP*AP*GP*A)-3')



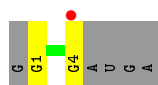
- Molecule 3: RNA (5'-R(P*UP*GP*UP*UP*CP*CP*GP*AP*GP*AP*GP*A)-3')



- Molecule 4: RNA (5'-R(*GP*GP*GP*AP*GP*AP*UP*GP*A)-3')



- Molecule 4: RNA (5'-R(*GP*GP*GP*AP*GP*AP*UP*GP*A)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	59.40Å 59.25Å 97.45Å 78.11° 78.09° 78.85°	Depositor
Resolution (Å)	46.96 – 2.75 46.96 – 2.75	Depositor EDS
% Data completeness (in resolution range)	96.0 (46.96-2.75) 95.4 (46.96-2.75)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.8.2 _1309	Depositor
R, R_{free}	0.202 , 0.262 0.202 , 0.262	Depositor DCC
R_{free} test set	1603 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	70.9	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.38$	Xtriage
Estimated twinning fraction	0.430 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8944	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.04% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN

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	0.47	0/3791	0.63	0/5127
1	E	0.47	0/3791	0.63	0/5127
2	B	0.61	0/401	1.02	0/622
2	F	0.61	0/401	1.06	1/622 (0.2%)
3	C	0.71	0/288	1.12	1/447 (0.2%)
3	G	0.62	0/288	1.15	1/447 (0.2%)
4	D	0.39	0/102	0.75	0/158
4	H	0.42	0/102	0.78	0/158
All	All	0.50	0/9164	0.73	3/12708 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	696	G	C4-C5-N7	-5.54	108.58	110.80
2	F	603	U	C5-C4-O4	-5.04	122.88	125.90
3	G	699	A	C2-N3-C4	5.01	113.10	110.60

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	3701	0	3661	73	0
1	E	3701	0	3661	63	0
2	B	360	0	184	11	0
2	F	360	0	184	11	0
3	C	258	0	130	5	0
3	G	258	0	130	3	0
4	D	91	0	45	1	0
4	H	91	0	45	2	0
5	A	6	0	8	1	0
5	B	6	0	8	0	0
5	E	12	0	16	1	0
6	A	1	0	0	0	0
6	E	1	0	0	0	0
7	A	35	0	0	3	0
7	B	7	0	0	1	0
7	C	6	0	0	0	0
7	D	1	0	0	0	0
7	E	35	0	0	1	0
7	F	6	0	0	1	0
7	G	6	0	0	0	0
7	H	2	0	0	0	0
All	All	8944	0	8072	154	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 (154) 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:599:G:N7	7:B:805:HOH:O	2.16	0.78
1:E:84:GLN:OE1	1:E:306:ARG:NH2	2.18	0.77
1:E:92:THR:O	1:E:261:ARG:NH2	2.21	0.74
1:A:18:ASN:ND2	4:D:1:G:O5'	2.24	0.70
1:A:84:GLN:OE1	1:A:306:ARG:NH2	2.20	0.70
1:A:92:THR:O	1:A:261:ARG:NH2	2.25	0.69
1:E:407:PRO:O	1:E:410:THR:OG1	2.10	0.69
1:A:24:LYS:NZ	2:B:599:G:O6	2.25	0.69
1:A:225:MET:O	7:A:621:HOH:O	2.12	0.67
1:E:345:GLN:HA	1:E:348:LYS:HE3	1.77	0.65
1:E:18:ASN:ND2	4:H:1:G:O5'	2.30	0.64
1:E:17:ILE:HD11	1:E:274:LEU:HD13	1.79	0.64
1:A:238:ASP:OD1	1:A:238:ASP:N	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:20:PRO:HG3	2:F:598:A:C5	2.33	0.63
1:A:358:ASP:OD2	1:A:372:THR:OG1	2.15	0.63
1:E:24:LYS:NZ	2:F:599:G:O6	2.32	0.62
1:A:406:ASP:OD1	1:A:408:ARG:HG2	2.01	0.61
1:A:407:PRO:O	1:A:410:THR:OG1	2.17	0.61
2:F:611:A:H2	3:G:691:G:H1	1.49	0.61
1:A:97:LEU:HD23	1:A:138:THR:HB	1.82	0.60
1:A:52:THR:OG1	1:A:53:ASP:N	2.35	0.60
2:B:611:A:H2	3:C:691:G:H1	1.52	0.58
1:E:108:GLU:O	1:E:188:ARG:NH2	2.25	0.58
2:F:604:C:H1'	7:F:703:HOH:O	2.04	0.58
1:E:406:ASP:OD1	1:E:408:ARG:HG2	2.04	0.57
1:A:260:ASP:OD1	1:A:261:ARG:NH1	2.37	0.57
1:E:238:ASP:OD1	1:E:238:ASP:N	2.35	0.57
1:E:236:GLY:O	1:E:240:SER:HB3	2.04	0.57
1:E:367:THR:O	1:E:369:GLU:N	2.38	0.57
1:A:411:GLN:HA	1:A:445:LEU:HD22	1.86	0.56
1:A:345:GLN:HA	1:A:348:LYS:HE3	1.86	0.56
1:E:260:ASP:OD1	1:E:260:ASP:N	2.38	0.56
1:A:367:THR:O	1:A:369:GLU:N	2.38	0.56
1:E:24:LYS:O	1:E:405:LYS:HA	2.06	0.56
1:E:97:LEU:HD23	1:E:138:THR:HB	1.86	0.56
2:B:602:C:H2'	2:B:603:U:C6	2.40	0.55
2:F:602:C:H2'	2:F:603:U:C6	2.41	0.55
1:E:250:LYS:HG2	1:E:262:VAL:HB	1.89	0.55
1:E:308:LEU:O	1:E:312:THR:OG1	2.20	0.55
1:A:306:ARG:HH11	1:A:306:ARG:HG3	1.71	0.55
1:A:340:ALA:HA	1:A:343:LEU:HD12	1.89	0.55
1:A:20:PRO:HG3	2:B:598:A:C5	2.42	0.55
1:E:442:GLY:HA2	1:E:445:LEU:HD12	1.88	0.55
1:A:17:ILE:HD11	1:A:274:LEU:HD13	1.89	0.54
1:E:356:PRO:HG3	1:E:363:PHE:CD2	2.43	0.54
1:A:260:ASP:OD1	1:A:260:ASP:N	2.41	0.54
1:E:159:LYS:HG3	1:E:176:ILE:CD1	2.38	0.53
1:A:250:LYS:HG2	1:A:262:VAL:HB	1.91	0.53
1:A:384:TYR:HB3	1:A:386:PHE:CE1	2.45	0.52
1:E:306:ARG:HG3	1:E:306:ARG:HH11	1.74	0.52
1:A:111:ASP:O	1:A:127:LYS:HD2	2.10	0.52
1:E:340:ALA:HA	1:E:343:LEU:HD12	1.91	0.52
1:A:426:GLU:HG3	1:A:450:TYR:CG	2.45	0.52
1:A:229:LEU:HD23	1:A:333:SER:HB3	1.90	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:358:ASP:OD2	1:E:372:THR:OG1	2.26	0.51
1:A:356:PRO:HG3	1:A:363:PHE:CD2	2.46	0.50
1:E:47:ASP:HB3	1:E:50:LEU:HD12	1.93	0.50
1:E:375:LYS:NZ	3:G:700:G:OP1	2.28	0.50
1:A:27:PRO:HB3	1:A:31:HIS:CD2	2.46	0.50
2:F:602:C:O2'	2:F:603:U:H5'	2.12	0.49
1:E:254:GLU:HG3	1:E:262:VAL:HG11	1.93	0.49
2:B:602:C:O2'	2:B:603:U:H5'	2.12	0.49
1:E:374:LEU:O	1:E:376:ARG:HD2	2.12	0.49
1:E:47:ASP:OD1	1:E:49:ARG:HG3	2.12	0.49
1:A:24:LYS:O	1:A:405:LYS:HA	2.13	0.49
1:E:111:ASP:O	1:E:127:LYS:HD2	2.12	0.48
1:E:2:GLU:HA	1:E:62:TYR:HB3	1.95	0.48
1:A:344:ALA:O	7:A:608:HOH:O	2.20	0.48
1:E:411:GLN:HA	1:E:445:LEU:HD22	1.95	0.48
1:A:108:GLU:O	1:A:188:ARG:NH2	2.33	0.48
1:E:159:LYS:HG3	1:E:176:ILE:HD12	1.94	0.48
1:E:214:PRO:O	1:E:390:PRO:HG3	2.13	0.48
1:A:236:GLY:O	1:A:240:SER:HB3	2.14	0.47
1:A:339:ASP:OD2	1:A:342:LEU:HG	2.14	0.47
1:E:330:VAL:O	5:E:501:GOL:O1	2.32	0.47
1:A:250:LYS:HE3	1:A:262:VAL:HG23	1.96	0.47
1:E:361:ALA:O	1:E:362:THR:HG23	2.14	0.47
1:A:234:TYR:O	5:A:501:GOL:H12	2.15	0.47
1:E:226:GLU:HG3	1:E:335:PRO:HD3	1.97	0.47
2:F:602:C:H2'	2:F:603:U:H6	1.78	0.47
1:E:218:TRP:CD1	1:E:390:PRO:HA	2.50	0.46
1:A:17:ILE:CD1	1:A:274:LEU:HB3	2.46	0.46
1:E:426:GLU:HG3	1:E:450:TYR:CG	2.51	0.46
1:A:8:PRO:HD2	1:A:11:GLU:OE2	2.16	0.46
2:B:602:C:H2'	2:B:603:U:H6	1.81	0.46
1:A:254:GLU:HG3	1:A:262:VAL:HG11	1.98	0.45
1:E:384:TYR:HB3	1:E:386:PHE:CE1	2.51	0.45
1:E:72:GLU:HB2	7:E:603:HOH:O	2.14	0.45
1:A:118:TYR:HA	1:A:119:PRO:HA	1.76	0.45
3:C:698:G:H2'	3:C:699:A:C8	2.51	0.45
1:E:45:LYS:HB3	1:E:45:LYS:HE2	1.87	0.45
2:B:603:U:H2'	2:B:604:C:C6	2.52	0.45
3:G:698:G:H2'	3:G:699:A:C8	2.52	0.45
1:A:441:ILE:HG22	1:A:442:GLY:N	2.32	0.45
1:E:208:SER:HA	1:E:325:ALA:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:237:TYR:CD2	1:E:328:ASP:HB3	2.52	0.45
1:A:208:SER:HA	1:A:325:ALA:O	2.16	0.44
1:E:145:LEU:HA	1:E:145:LEU:HD23	1.76	0.44
1:A:80:HIS:CD2	1:A:318:LEU:HB2	2.52	0.44
1:A:218:TRP:CD1	1:A:390:PRO:HA	2.53	0.44
1:E:177:GLU:O	1:E:289:GLY:HA3	2.17	0.44
2:F:603:U:H2'	2:F:604:C:C6	2.53	0.44
1:A:17:ILE:HD11	1:A:274:LEU:HB3	1.99	0.44
1:A:375:LYS:NZ	3:C:700:G:OP1	2.31	0.44
1:E:27:PRO:HB3	1:E:31:HIS:CD2	2.52	0.44
1:E:322:LYS:HB2	1:E:333:SER:OG	2.18	0.44
1:E:356:PRO:HG3	1:E:363:PHE:CE2	2.53	0.44
1:E:226:GLU:OE1	1:E:335:PRO:HG3	2.18	0.44
1:E:18:ASN:HB2	4:H:1:G:C1'	2.48	0.43
1:A:226:GLU:OE1	1:A:335:PRO:HG3	2.18	0.43
1:A:290:CYS:HB2	1:A:293:THR:CG2	2.49	0.43
1:A:63:VAL:HG23	1:A:64:GLY:N	2.33	0.43
3:C:693:U:H2'	3:C:694:C:C6	2.54	0.43
1:E:419:LEU:HA	1:E:419:LEU:HD22	1.75	0.43
1:A:250:LYS:HG3	1:A:265:ILE:HG21	2.01	0.43
2:B:605:U:H2'	2:B:606:C:C6	2.54	0.43
1:E:118:TYR:HA	1:E:119:PRO:HA	1.84	0.43
1:A:214:PRO:O	1:A:390:PRO:HG3	2.19	0.43
1:A:2:GLU:HA	1:A:62:TYR:HB3	2.01	0.42
1:A:63:VAL:HG23	1:A:64:GLY:H	1.84	0.42
1:E:63:VAL:HG23	1:E:64:GLY:N	2.34	0.42
1:A:152:LEU:HD12	1:A:180:SER:OG	2.20	0.42
1:A:47:ASP:HA	1:A:48:PRO:HD3	1.91	0.42
1:A:20:PRO:HG3	2:B:598:A:C4	2.53	0.42
1:A:310:LEU:HD11	1:A:318:LEU:HD11	2.01	0.42
3:C:697:A:H2'	3:C:698:G:C8	2.55	0.42
1:E:49:ARG:HH11	1:E:168:VAL:HG11	1.85	0.42
1:A:47:ASP:OD1	1:A:49:ARG:HG3	2.19	0.42
1:A:157:TYR:CD2	2:B:599:G:H4'	2.55	0.42
1:A:419:LEU:HD22	1:A:419:LEU:HA	1.80	0.42
1:A:81:TYR:CE1	1:A:302:ASN:HB3	2.55	0.42
1:E:142:GLN:NE2	1:E:142:GLN:O	2.50	0.42
1:A:237:TYR:CD2	1:A:328:ASP:HB3	2.55	0.41
1:A:177:GLU:O	1:A:289:GLY:HA3	2.20	0.41
1:A:200:LYS:HB2	1:A:200:LYS:HE3	1.84	0.41
1:E:63:VAL:HG23	1:E:64:GLY:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:112:LEU:HD23	1:E:112:LEU:HA	1.64	0.41
2:F:605:U:H2'	2:F:606:C:C6	2.56	0.41
1:A:392:MET:HA	1:A:393:PRO:HD3	1.88	0.41
1:A:356:PRO:HB2	1:A:360:SER:O	2.21	0.41
1:A:374:LEU:O	1:A:376:ARG:HD2	2.20	0.41
1:E:20:PRO:HG3	2:F:598:A:C4	2.56	0.41
1:A:386:PHE:HD1	1:A:386:PHE:H	1.69	0.41
1:E:277:ASN:OD1	1:E:278:LYS:HG2	2.21	0.41
1:A:286:MET:HE2	1:A:286:MET:HB2	1.95	0.40
1:A:294:SER:HB2	7:A:624:HOH:O	2.20	0.40
1:A:93:GLU:O	1:A:193:ASN:ND2	2.53	0.40
1:E:339:ASP:OD2	1:E:342:LEU:HG	2.21	0.40
1:A:306:ARG:NH1	1:A:306:ARG:HG3	2.36	0.40
1:A:76:GLU:HB3	1:A:310:LEU:HD13	2.03	0.40
1:A:356:PRO:HG3	1:A:363:PHE:CE2	2.56	0.40
1:E:176:ILE:HG12	2:F:600:G:C4	2.56	0.40
1:A:226:GLU:HB3	1:A:227:GLU:H	1.73	0.40
1:E:226:GLU:HB2	1:E:333:SER:HB2	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	460/471 (98%)	428 (93%)	29 (6%)	3 (1%)	22	39
1	E	460/471 (98%)	431 (94%)	27 (6%)	2 (0%)	34	53
All	All	920/942 (98%)	859 (93%)	56 (6%)	5 (0%)	29	47

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	SER
1	A	368	TRP
1	E	9	SER
1	E	368	TRP
1	A	361	ALA

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	403/412 (98%)	370 (92%)	33 (8%)	11	20
1	E	403/412 (98%)	363 (90%)	40 (10%)	8	13
All	All	806/824 (98%)	733 (91%)	73 (9%)	9	16

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	LYS
1	A	23	THR
1	A	26	GLU
1	A	35	GLU
1	A	42	VAL
1	A	45	LYS
1	A	49	ARG
1	A	52	THR
1	A	72	GLU
1	A	87	SER
1	A	93	GLU
1	A	163	ARG
1	A	164	SER
1	A	205	ILE
1	A	208	SER
1	A	215	ASP
1	A	218	TRP
1	A	238	ASP
1	A	240	SER

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Mol	Chain	Res	Type
1	A	242	SER
1	A	261	ARG
1	A	294	SER
1	A	319	ASP
1	A	337	GLU
1	A	338	VAL
1	A	362	THR
1	A	365	THR
1	A	372	THR
1	A	411	GLN
1	A	419	LEU
1	A	427	GLU
1	A	441	ILE
1	A	456	ARG
1	E	10	LYS
1	E	23	THR
1	E	24	LYS
1	E	26	GLU
1	E	35	GLU
1	E	42	VAL
1	E	45	LYS
1	E	49	ARG
1	E	68	THR
1	E	72	GLU
1	E	86	MET
1	E	93	GLU
1	E	163	ARG
1	E	164	SER
1	E	172	LYS
1	E	176	ILE
1	E	185	VAL
1	E	205	ILE
1	E	208	SER
1	E	215	ASP
1	E	218	TRP
1	E	238	ASP
1	E	240	SER
1	E	242	SER
1	E	261	ARG
1	E	294	SER
1	E	312	THR
1	E	319	ASP

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Mol	Chain	Res	Type
1	E	326	TYR
1	E	337	GLU
1	E	355	THR
1	E	359	LYS
1	E	362	THR
1	E	372	THR
1	E	410	THR
1	E	419	LEU
1	E	427	GLU
1	E	428	GLU
1	E	441	ILE
1	E	456	ARG

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	398	HIS
1	E	409	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	16/22 (72%)	3 (18%)	0
2	F	16/22 (72%)	3 (18%)	0
3	C	11/12 (91%)	2 (18%)	0
3	G	11/12 (91%)	2 (18%)	0
4	D	3/9 (33%)	1 (33%)	0
4	H	3/9 (33%)	1 (33%)	0
All	All	60/86 (69%)	12 (20%)	0

All (12) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	602	C
2	B	608	G
2	B	611	A
3	C	691	G
3	C	692	U
4	D	4	G
2	F	602	C

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Mol	Chain	Res	Type
2	F	608	G
2	F	611	A
3	G	691	G
3	G	692	U
4	H	4	G

There are no RNA pucker outliers to report.

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](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	$\# Z > 2$
5	GOL	A	501	-	5,5,5	0.28	0	5,5,5	0.43	0
5	GOL	E	502	-	5,5,5	0.34	0	5,5,5	0.40	0
5	GOL	E	501	-	5,5,5	0.36	0	5,5,5	0.35	0
5	GOL	B	701	-	5,5,5	0.44	0	5,5,5	0.24	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
5	GOL	A	501	-	-	2/4/4/4	-
5	GOL	E	502	-	-	4/4/4/4	-
5	GOL	E	501	-	-	2/4/4/4	-
5	GOL	B	701	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	502	GOL	O1-C1-C2-C3
5	A	501	GOL	O1-C1-C2-O2
5	A	501	GOL	O1-C1-C2-C3
5	E	502	GOL	C1-C2-C3-O3
5	B	701	GOL	O1-C1-C2-C3
5	E	501	GOL	O1-C1-C2-C3
5	E	502	GOL	O1-C1-C2-O2
5	E	501	GOL	O1-C1-C2-O2
5	E	502	GOL	O2-C2-C3-O3
5	B	701	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	501	GOL	1	0
5	E	501	GOL	1	0

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	462/471 (98%)	0.05	1 (0%) 95 97	46, 63, 83, 103	0
1	E	462/471 (98%)	0.05	4 (0%) 84 89	45, 63, 81, 104	0
2	B	17/22 (77%)	-0.36	0 100 100	49, 62, 139, 141	0
2	F	17/22 (77%)	-0.45	0 100 100	46, 60, 137, 140	0
3	C	12/12 (100%)	-0.03	1 (8%) 11 13	51, 58, 143, 155	0
3	G	12/12 (100%)	0.02	1 (8%) 11 13	49, 57, 142, 155	0
4	D	4/9 (44%)	1.85	2 (50%) 0 0	128, 138, 148, 152	0
4	H	4/9 (44%)	0.99	1 (25%) 0 0	126, 137, 146, 149	0
All	All	990/1028 (96%)	0.05	10 (1%) 82 87	45, 63, 87, 155	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	4	G	3.1
1	A	334	TYR	3.0
1	E	21	SER	3.0
3	C	690	U	2.5
1	E	1	GLY	2.3
3	G	690	U	2.2
1	E	41	ALA	2.2
1	E	169	GLU	2.2
4	D	3	A	2.1
4	H	4	G	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 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. 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(\AA^2)	Q<0.9
5	GOL	A	501	6/6	0.85	0.23	62,71,75,76	0
5	GOL	E	502	6/6	0.92	0.17	63,68,71,73	0
5	GOL	B	701	6/6	0.95	0.18	53,56,60,64	0
5	GOL	E	501	6/6	0.97	0.11	63,67,69,71	0
6	ZN	A	502	1/1	0.99	0.19	43,43,43,43	0
6	ZN	E	503	1/1	0.99	0.18	40,40,40,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.