Full wwPDB X-ray Structure Validation Report ⓘ

Aug 25, 2020 – 02:19 PM BST

PDB ID	:	5T9J
Title	:	Crystal Structure of human GEN1 in complex with Holliday junction DNA in the upper interface
Authors	:	Lee, S.-H.; Biertumpfel, C.
Deposited on	:	2016-09-09
Resolution	:	3.00 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 ①) were used in the production of this report:

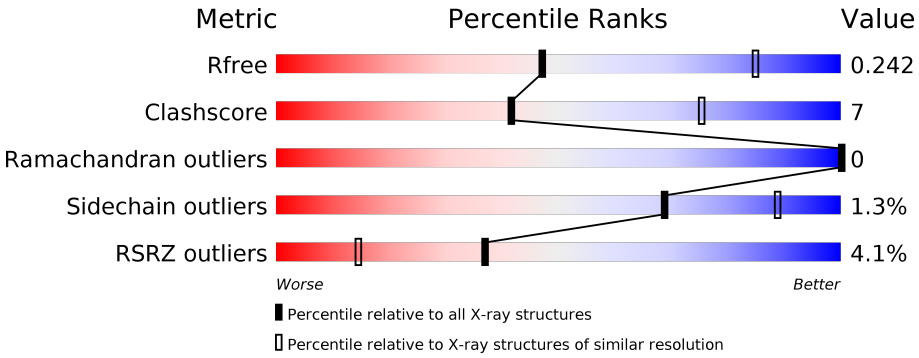
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13

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 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 <=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	506	3% 62% 15% 23%
1	B	506	4% 68% 9% 23%
2	C	20	65% 35%
3	D	20	50% 50%
4	E	20	70% 25% 5%
5	F	20	65% 30% 5%

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
6	GOL	A	601	-	-	-	X
6	GOL	A	604	-	-	-	X
6	GOL	A	607	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8002 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 Flap endonuclease GEN homolog 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	390	Total	C	N	O	S	0	0	0
			3144	2013	547	560	24			
1	B	391	Total	C	N	O	S	0	0	0
			3154	2020	549	561	24			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	ASN	ASP	engineered mutation	UNP Q17RS7
A	92	THR	SER	variant	UNP Q17RS7
A	310	ASN	SER	variant	UNP Q17RS7
A	506	LEU	-	expression tag	UNP Q17RS7
B	30	ASN	ASP	engineered mutation	UNP Q17RS7
B	92	THR	SER	variant	UNP Q17RS7
B	310	ASN	SER	variant	UNP Q17RS7
B	506	LEU	-	expression tag	UNP Q17RS7

- Molecule 2 is a DNA chain called DNA (5'-D(*DGP*DAP*DAP*DTP*DTP*DCP*DCP*DGP*DGP*DAP*DTP*DTP*DAP*DGP*DGP*DGP*DAP*DTP*DGP*DC)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	20	Total	C	N	O	P	0	0	0
			407	194	76	118	19			

- Molecule 3 is a DNA chain called DNA (5'-D(*DGP*DCP*DAP*DTP*DCP*DCP*DCP*DTP*DAP*DAP*DGP*DCP*DTP*DCP*DCP*DAP*DTP*DCP*DGP*DT)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	20	Total	C	N	O	P	0	0	0
			409	194	79	117	19			

- Molecule 4 is a DNA chain called DNA (5'-D(*DAP*DCP*DGP*DAP*DTP*DGP*DGP*

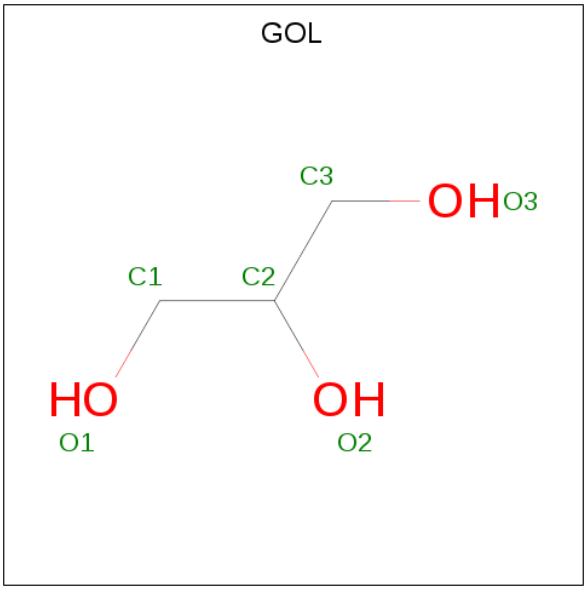
DAP*DGP*DCP*DCP*DGP*DCP*DTP*DAP*DGP*DGP*DCP*DTP*DC)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	19	Total	C	N	O	P	0	0	0
			379	182	67	112	18			

- Molecule 5 is a DNA chain called DNA (5'-D(*DGP*DAP*DGP*DCP*DCP*DTP*DAP*DGP*DCP*DGP*DTP*DCP*DCP*DGP*DGP*DAP*DAP*DTP*DTP*DC)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	19	Total	C	N	O	P	0	0	0
			394	187	74	114	19			

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total Mg 1 1	0	0
7	A	1	Total Mg 1 1	0	0

- Molecule 8 is water.

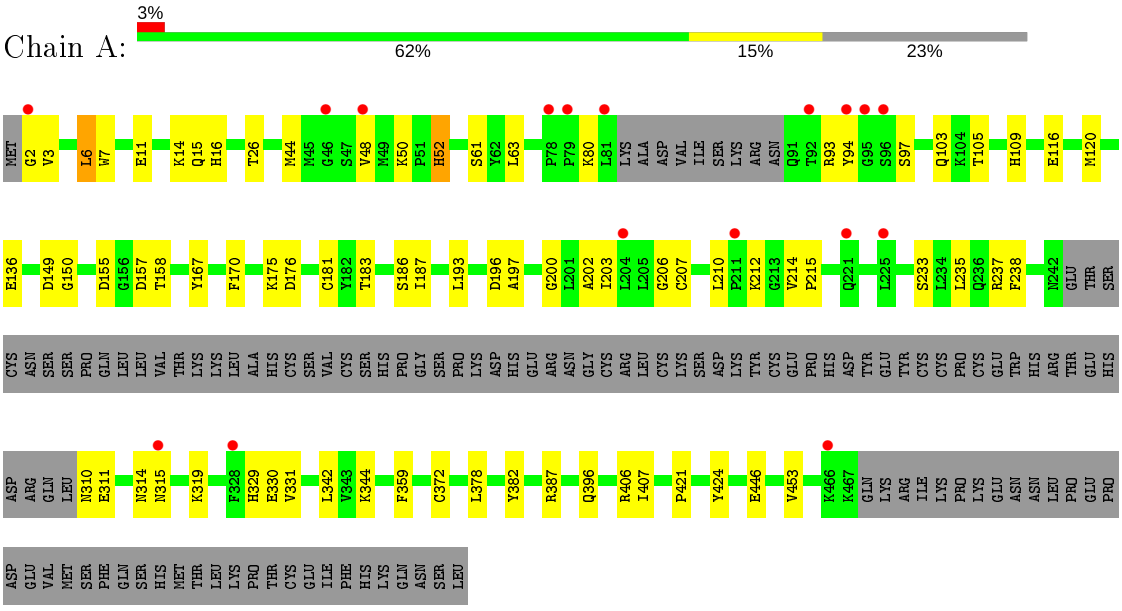
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	10	Total O 10 10	0	0
8	B	11	Total O 11 11	0	0
8	D	1	Total O 1 1	0	0
8	F	1	Total O 1 1	0	0

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.

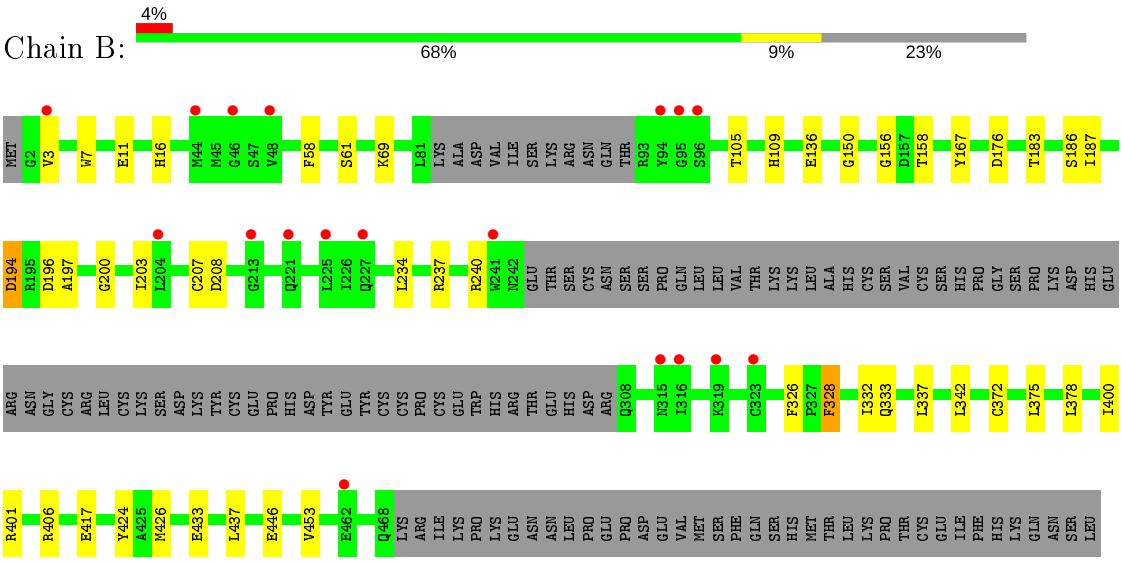
- Molecule 1: Flap endonuclease GEN homolog 1

Chain A:



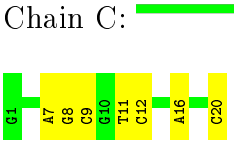
- Molecule 1: Flap endonuclease GEN homolog 1

Chain B:



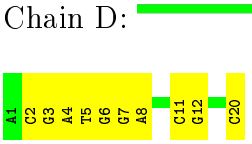
• Molecule 2: DNA (5'-D(*DGP*DAP*DAP*DTP*DTP*DCP*DCP*DGP*DGP*DAP*DTP*DTP*DAP*DGP*DGP*DGP*DAP*DTP*DGP*DC)-3')

Chain C:



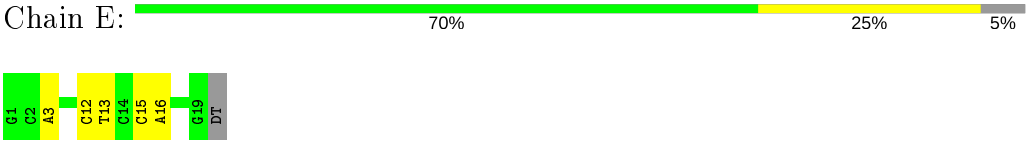
• Molecule 3: DNA (5'-D(*DGP*DCP*DAP*DTP*DCP*DCP*DCP*DTP*DAP*DAP*DGP*DCP*DTP*DCP*DCP*DAP*DTP*DCP*DGP*DT)-3')

Chain D:



• Molecule 4: DNA (5'-D(*DAP*DCP*DGP*DAP*DTP*DGP*DGP*DAP*DGP*DCP*DCP*DGP*DCP*DTP*DAP*DGP*DGP*DCP*DTP*DC)-3')

Chain E:



• Molecule 5: DNA (5'-D(*DGP*DAP*DGP*DCP*DCP*DTP*DAP*DGP*DCP*DGP*DTP*DCP*DCP*DGP*DGP*DAP*DAP*DTP*DTP*DC)-3')

Chain F:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	86.94Å 86.94Å 200.72Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	75.29 – 3.00 75.29 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (75.29-3.00) 100.0 (75.29-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	1.59 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.199 , 0.241 0.200 , 0.242	Depositor DCC
R_{free} test set	1720 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	93.2	Xtriage
Anisotropy	0.009	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 80.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.038 for -h,-k,l 0.478 for h,-h-k,-l 0.037 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8002	wwPDB-VP
Average B, all atoms (Å^2)	128.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.26	0/3210	0.44	0/4323
1	B	0.26	0/3220	0.42	0/4336
2	C	0.53	0/456	0.90	0/702
3	D	0.56	0/459	0.95	0/707
4	E	0.52	0/423	0.90	0/649
5	F	0.58	0/442	0.92	0/681
All	All	0.34	0/8210	0.59	0/11398

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	3144	0	3188	49	0
1	B	3154	0	3199	34	0
2	C	407	0	226	9	0
3	D	409	0	225	12	0
4	E	379	0	215	5	0
5	F	394	0	215	8	0
6	A	42	0	56	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	30	0	39	1	0
6	C	18	0	24	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	A	10	0	0	3	0
8	B	11	0	0	1	0
8	D	1	0	0	0	0
8	F	1	0	0	0	0
All	All	8002	0	7387	106	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 7.

All (106) 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:C:16:DA:H2	5:F:5:DT:H3	1.12	0.93
1:A:200:GLY:HA2	1:A:203:ILE:HD12	1.66	0.77
2:C:16:DA:C2	5:F:5:DT:N3	2.51	0.75
2:C:16:DA:N1	5:F:5:DT:O4	2.26	0.69
1:A:15:GLN:HG3	1:A:181:CYS:HB3	1.76	0.68
1:A:183:THR:HG1	1:A:186:SER:HG	1.39	0.68
1:A:50:LYS:NZ	1:A:116:GLU:OE1	2.27	0.66
1:A:2:GLY:N	1:A:157:ASP:OD1	2.30	0.65
2:C:16:DA:H2	5:F:5:DT:N3	1.90	0.64
1:A:136:GLU:OE2	1:A:158:THR:OG1	2.16	0.64
1:B:200:GLY:HA2	1:B:203:ILE:HD12	1.79	0.63
1:A:6:LEU:HD13	1:A:7:TRP:H	1.66	0.61
1:B:16:HIS:NE2	1:B:176:ASP:OD1	2.25	0.61
3:D:7:DG:H2"	3:D:8:DA:C8	2.37	0.60
1:A:387:ARG:NH1	1:A:396:GLN:OE1	2.35	0.59
2:C:11:DT:H2'	2:C:12:DC:C6	2.38	0.58
1:B:234:LEU:HA	1:B:237:ARG:HD2	1.85	0.58
1:B:3:VAL:HA	1:B:207:CYS:HA	1.85	0.57
1:A:212:LYS:NZ	8:A:702:HOH:O	2.28	0.57
1:B:401:ARG:HH12	6:B:605:GOL:H32	1.68	0.57
1:A:3:VAL:HB	1:A:6:LEU:HB3	1.85	0.57
2:C:16:DA:N1	5:F:5:DT:C4	2.73	0.56
1:A:175:LYS:HE2	2:C:20:DC:H2"	1.87	0.56
1:B:400:ILE:HG22	1:B:401:ARG:HG2	1.87	0.56
1:B:208:ASP:N	1:B:208:ASP:OD1	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:ILE:HB	3:D:12:DG:H5"	1.89	0.55
3:D:3:DG:H2"	3:D:4:DA:C8	2.41	0.54
1:A:210:LEU:HD11	1:A:331:VAL:HG21	1.88	0.54
1:A:97:SER:O	8:A:701:HOH:O	2.18	0.54
4:E:15:DC:H2"	4:E:16:DA:H8	1.71	0.54
5:F:14:DG:H2'	5:F:15:DG:C8	2.43	0.54
1:A:382:TYR:HD1	6:A:605:GOL:H31	1.73	0.52
1:A:80:LYS:NZ	1:A:330:GLU:OE1	2.42	0.52
1:B:105:THR:O	1:B:109:HIS:ND1	2.42	0.52
3:D:3:DG:H4'	3:D:4:DA:OP1	2.10	0.51
1:A:105:THR:O	1:A:109:HIS:ND1	2.43	0.51
1:A:3:VAL:O	1:A:6:LEU:HD12	2.11	0.51
1:B:183:THR:OG1	1:B:186:SER:OG	2.28	0.51
1:B:406:ARG:NH1	5:F:12:DT:OP2	2.43	0.51
1:B:372:CYS:HB3	1:B:424:TYR:CE2	2.46	0.51
1:B:7:TRP:HZ2	1:B:156:GLY:H	1.58	0.50
3:D:5:DT:H2'	3:D:6:DG:C8	2.47	0.50
1:B:136:GLU:OE1	1:B:158:THR:OG1	2.27	0.50
1:A:16:HIS:NE2	1:A:176:ASP:OD1	2.32	0.50
1:A:372:CYS:HB3	1:A:424:TYR:CE2	2.47	0.50
1:A:446:GLU:HA	1:A:453:VAL:HG21	1.94	0.49
3:D:5:DT:H2'	3:D:6:DG:H8	1.77	0.49
1:A:6:LEU:HD13	1:A:7:TRP:N	2.27	0.49
1:B:7:TRP:O	1:B:11:GLU:HG2	2.13	0.49
1:A:7:TRP:NE1	1:A:155:ASP:OD2	2.41	0.48
1:B:240:ARG:HB2	1:B:326:PHE:HZ	1.78	0.48
1:A:311:GLU:HA	1:A:314:ASN:HD21	1.79	0.48
1:A:421:PRO:HG2	1:A:424:TYR:HB2	1.96	0.47
1:B:446:GLU:HA	1:B:453:VAL:HG21	1.95	0.47
1:A:315:ASN:O	1:A:319:LYS:HG3	2.13	0.47
4:E:15:DC:H2"	4:E:16:DA:C8	2.50	0.47
1:A:406:ARG:NH1	3:D:12:DG:OP2	2.45	0.47
1:B:196:ASP:OD1	1:B:197:ALA:N	2.48	0.47
3:D:11:DC:H2"	3:D:12:DG:C8	2.50	0.46
1:B:61:SER:HA	1:B:378:LEU:HD21	1.97	0.46
1:A:26:THR:O	1:A:149:ASP:N	2.47	0.46
1:B:3:VAL:HG22	1:B:207:CYS:HB3	1.97	0.46
4:E:12:DC:H2"	4:E:13:DT:H5'	1.98	0.46
1:A:150:GLY:HA3	1:A:167:TYR:HE2	1.81	0.45
3:D:5:DT:H2"	3:D:6:DG:O4'	2.17	0.45
1:A:50:LYS:HB3	1:A:52:HIS:ND1	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:333:GLN:O	1:B:337:LEU:HB2	2.16	0.45
3:D:2:DC:H2'	3:D:3:DG:C8	2.52	0.45
1:B:426:MET:SD	1:B:433:GLU:HG2	2.57	0.44
4:E:15:DC:H4'	4:E:16:DA:OP1	2.16	0.44
1:A:187:ILE:HG22	1:A:193:LEU:HB2	1.99	0.44
1:A:63:LEU:HD21	1:A:170:PHE:HE2	1.82	0.44
1:A:214:VAL:HB	1:A:215:PRO:HA	1.98	0.44
1:A:3:VAL:HA	1:A:206:GLY:O	2.18	0.44
1:A:183:THR:OG1	1:A:186:SER:OG	2.19	0.44
1:A:103:GLN:HG3	8:A:701:HOH:O	2.18	0.43
1:A:7:TRP:O	1:A:11:GLU:HG3	2.18	0.43
1:B:194:ASP:N	1:B:194:ASP:OD1	2.29	0.43
1:B:326:PHE:CD1	1:B:326:PHE:O	2.72	0.43
1:A:196:ASP:OD1	1:A:197:ALA:N	2.52	0.43
1:A:235:LEU:HA	1:A:238:PHE:CD2	2.54	0.43
1:A:61:SER:HA	1:A:378:LEU:HD21	2.00	0.43
1:B:375:LEU:HD12	1:B:378:LEU:HD12	1.99	0.43
1:B:58:PHE:CG	4:E:3:DA:H5"	2.54	0.43
1:A:310:ASN:O	1:A:314:ASN:ND2	2.52	0.43
1:B:203:ILE:HD11	1:B:332:ILE:HG12	2.01	0.42
2:C:7:DA:H2'	2:C:8:DG:C8	2.54	0.42
1:A:233:SER:O	1:A:237:ARG:HG3	2.19	0.42
1:B:240:ARG:HB2	1:B:326:PHE:CZ	2.53	0.42
5:F:7:DC:H2"	5:F:8:DG:C8	2.54	0.42
1:A:202:ALA:HB1	1:A:207:CYS:SG	2.60	0.41
1:A:344:LYS:HB3	1:A:344:LYS:HE2	1.84	0.41
1:A:120:MET:HB2	1:A:359:PHE:CE1	2.55	0.41
1:B:150:GLY:HA3	1:B:167:TYR:HE2	1.85	0.41
1:B:417:GLU:HA	1:B:437:LEU:HD23	2.01	0.41
1:A:14:LYS:HA	1:A:181:CYS:O	2.20	0.41
1:A:342:LEU:HA	1:A:342:LEU:HD23	1.88	0.41
1:B:342:LEU:HD23	1:B:342:LEU:HA	1.82	0.41
1:A:149:ASP:OD1	6:A:606:GOL:O3	2.39	0.41
1:B:183:THR:O	1:B:187:ILE:HG13	2.21	0.41
2:C:9:DC:H42	3:D:12:DG:H1	1.68	0.41
1:B:326:PHE:CD1	1:B:328:PHE:CE2	3.09	0.40
1:A:183:THR:O	1:A:187:ILE:HG13	2.20	0.40
3:D:20:DC:H6	3:D:20:DC:H5'	1.87	0.40
1:B:337:LEU:HD23	1:B:337:LEU:HA	1.82	0.40
1:B:69:LYS:NZ	8:B:701:HOH:O	2.38	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	384/506 (76%)	375 (98%)	9 (2%)	0	100	100
1	B	385/506 (76%)	378 (98%)	7 (2%)	0	100	100
All	All	769/1012 (76%)	753 (98%)	16 (2%)	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	344/456 (75%)	337 (98%)	7 (2%)	55	83
1	B	345/456 (76%)	343 (99%)	2 (1%)	86	95
All	All	689/912 (76%)	680 (99%)	9 (1%)	69	89

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	44	MET
1	A	48	VAL
1	A	52	HIS
1	A	93	ARG
1	A	94	TYR
1	A	329	HIS
1	B	194	ASP

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Mol	Chain	Res	Type
1	B	328	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	314	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 17 ligands modelled in this entry, 2 are monoatomic - leaving 15 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	$\#\|Z\| > 2$
6	GOL	A	606	-	5,5,5	0.36	0	5,5,5	0.29	0
6	GOL	B	604	-	5,5,5	0.37	0	5,5,5	0.28	0
6	GOL	B	603	-	5,5,5	0.34	0	5,5,5	0.26	0
6	GOL	A	603	-	5,5,5	0.38	0	5,5,5	0.23	0
6	GOL	C	103	-	5,5,5	0.38	0	5,5,5	0.23	0
6	GOL	A	607	-	5,5,5	0.39	0	5,5,5	0.17	0
6	GOL	B	602	-	5,5,5	0.37	0	5,5,5	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	GOL	A	604	-	5,5,5	0.37	0	5,5,5	0.21	0
6	GOL	C	102	-	5,5,5	0.37	0	5,5,5	0.18	0
6	GOL	B	601	-	5,5,5	0.37	0	5,5,5	0.26	0
6	GOL	B	605	-	5,5,5	0.37	0	5,5,5	0.26	0
6	GOL	A	601	-	5,5,5	0.38	0	5,5,5	0.24	0
6	GOL	C	101	-	5,5,5	0.37	0	5,5,5	0.21	0
6	GOL	A	602	-	5,5,5	0.38	0	5,5,5	0.19	0
6	GOL	A	605	-	5,5,5	0.37	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
6	GOL	A	606	-	-	2/4/4/4	-
6	GOL	B	604	-	-	2/4/4/4	-
6	GOL	B	603	-	-	0/4/4/4	-
6	GOL	A	603	-	-	2/4/4/4	-
6	GOL	C	103	-	-	2/4/4/4	-
6	GOL	A	607	-	-	2/4/4/4	-
6	GOL	B	602	-	-	2/4/4/4	-
6	GOL	A	604	-	-	2/4/4/4	-
6	GOL	C	102	-	-	2/4/4/4	-
6	GOL	B	601	-	-	2/4/4/4	-
6	GOL	B	605	-	-	2/4/4/4	-
6	GOL	A	601	-	-	2/4/4/4	-
6	GOL	C	101	-	-	2/4/4/4	-
6	GOL	A	602	-	-	2/4/4/4	-
6	GOL	A	605	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	606	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
6	A	603	GOL	O1-C1-C2-C3
6	C	103	GOL	O1-C1-C2-C3
6	A	607	GOL	O1-C1-C2-C3
6	B	602	GOL	O1-C1-C2-C3
6	A	604	GOL	O1-C1-C2-C3
6	C	102	GOL	O1-C1-C2-C3
6	B	601	GOL	O1-C1-C2-C3
6	B	605	GOL	O1-C1-C2-C3
6	C	101	GOL	O1-C1-C2-C3
6	A	602	GOL	O1-C1-C2-C3
6	A	605	GOL	O1-C1-C2-C3
6	B	604	GOL	O1-C1-C2-C3
6	B	602	GOL	O1-C1-C2-O2
6	C	101	GOL	O1-C1-C2-O2
6	A	602	GOL	O1-C1-C2-O2
6	A	605	GOL	O1-C1-C2-O2
6	A	606	GOL	O1-C1-C2-O2
6	B	604	GOL	O1-C1-C2-O2
6	C	103	GOL	O1-C1-C2-O2
6	C	102	GOL	O1-C1-C2-O2
6	B	601	GOL	O1-C1-C2-O2
6	B	605	GOL	O1-C1-C2-O2
6	A	603	GOL	O1-C1-C2-O2
6	A	604	GOL	O1-C1-C2-O2
6	A	607	GOL	O1-C1-C2-O2
6	A	601	GOL	O1-C1-C2-C3
6	A	601	GOL	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	606	GOL	1	0
6	B	605	GOL	1	0
6	A	605	GOL	1	0

5.7 Other polymers (i)

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, 95^{th} 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	390/506 (77%)	0.12	17 (4%) 34 13	60, 106, 226, 284	0
1	B	391/506 (77%)	0.13	18 (4%) 32 12	61, 107, 228, 321	0
2	C	20/20 (100%)	-0.38	0 100 100	85, 110, 273, 274	0
3	D	20/20 (100%)	-0.52	0 100 100	88, 113, 289, 303	0
4	E	19/20 (95%)	-0.48	0 100 100	81, 110, 266, 282	0
5	F	19/20 (95%)	-0.53	0 100 100	89, 113, 258, 278	0
All	All	859/1092 (78%)	0.07	35 (4%) 37 14	60, 107, 244, 321	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	95	GLY	6.6
1	A	211	PRO	6.0
1	B	95	GLY	4.6
1	A	81	LEU	4.6
1	B	96	SER	3.7
1	A	315	ASN	3.6
1	B	315	ASN	3.6
1	A	79	PRO	3.4
1	A	2	GLY	3.4
1	B	221	GLN	3.3
1	B	241	TRP	3.1
1	B	46	GLY	3.1
1	B	94	TYR	3.1
1	A	221	GLN	3.1
1	B	323	CYS	3.0
1	A	78	PRO	3.0
1	B	48	VAL	3.0
1	A	225	LEU	2.9
1	B	213	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	3	VAL	2.8
1	A	328	PHE	2.8
1	B	227	GLN	2.8
1	B	319	LYS	2.7
1	B	44	MET	2.6
1	B	316	ILE	2.6
1	A	94	TYR	2.6
1	A	92	THR	2.5
1	A	466	LYS	2.5
1	A	204	LEU	2.5
1	B	204	LEU	2.3
1	A	46	GLY	2.2
1	A	48	VAL	2.1
1	B	462	GLU	2.1
1	B	225	LEU	2.0
1	A	96	SER	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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
7	MG	A	608	1/1	0.56	0.14	122,122,122,122	0
6	GOL	A	603	6/6	0.57	0.28	135,140,151,154	0
6	GOL	B	603	6/6	0.63	0.17	122,137,145,146	0
6	GOL	A	604	6/6	0.69	0.54	94,125,138,145	0
6	GOL	A	607	6/6	0.72	0.57	99,122,141,155	0
7	MG	B	606	1/1	0.73	0.13	133,133,133,133	0
6	GOL	C	103	6/6	0.79	0.26	126,139,143,144	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	GOL	A	602	6/6	0.79	0.30	117,125,132,136	0
6	GOL	A	601	6/6	0.80	0.41	108,128,130,133	0
6	GOL	B	601	6/6	0.81	0.43	105,130,132,142	0
6	GOL	C	102	6/6	0.82	0.23	114,133,137,143	0
6	GOL	B	602	6/6	0.82	0.22	96,116,122,128	0
6	GOL	A	606	6/6	0.84	0.18	116,122,137,142	0
6	GOL	A	605	6/6	0.87	0.46	127,143,151,157	0
6	GOL	B	604	6/6	0.89	0.20	116,124,135,143	0
6	GOL	B	605	6/6	0.92	0.43	77,111,125,136	0
6	GOL	C	101	6/6	0.92	0.23	93,113,126,140	0

6.5 Other polymers (i)

There are no such residues in this entry.