



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 05:06 pm BST

PDB ID : 3WVG
Title : Time-Resolved Crystal Structure of HindIII with 0sec soaking
Authors : Kawamura, T.; Kobayashi, T.; Watanabe, N.
Deposited on : 2014-05-21
Resolution : 2.25 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

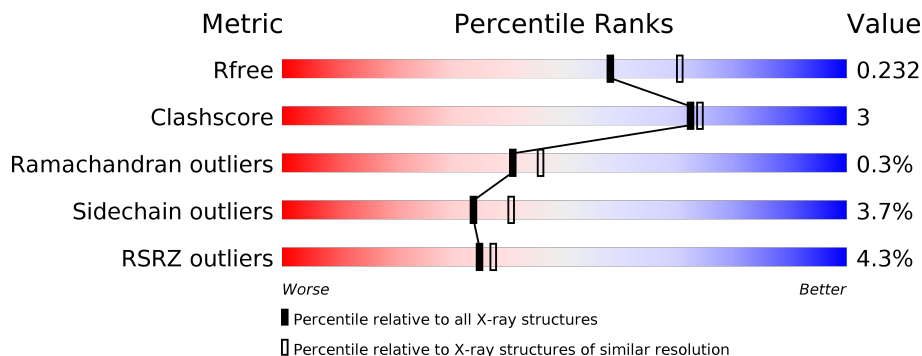
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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.






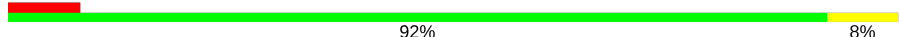


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	300	
1	B	300	
1	C	300	
1	D	300	
2	E	12	
2	F	12	

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Mol	Chain	Length	Quality of chain
2	G	12	 75% 25%
2	H	12	 75% 17% 8%
2	I	12	 17% 50% 50%
2	J	12	 8% 92% 8%
2	K	12	 92% 8%
2	L	12	 83% 17%

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
4	GOL	B	303	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 12207 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 Type-2 restriction enzyme HindIII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	298	Total 2452	C 1580	N 405	O 464	S 3	0	0	0
1	B	298	Total 2452	C 1580	N 405	O 464	S 3	0	0	0
1	C	298	Total 2452	C 1580	N 405	O 464	S 3	0	0	0
1	D	298	Total 2452	C 1580	N 405	O 464	S 3	0	0	0

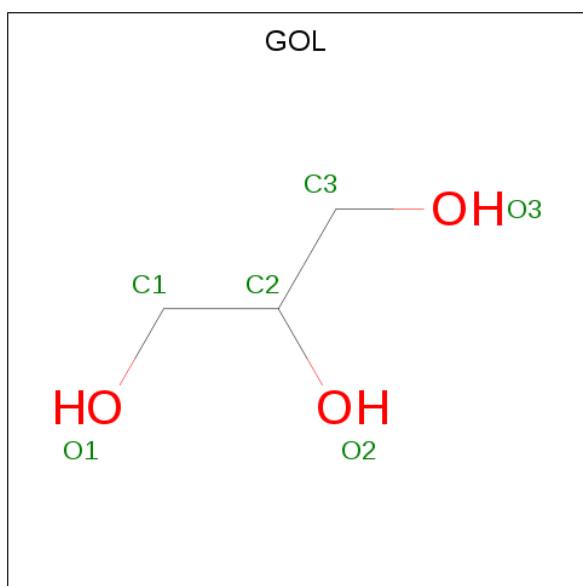
- Molecule 2 is a DNA chain called DNA (5'-D(*GP*CP*CP*AP*AP*GP*CP*TP*TP*GP*GP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	G	12	Total 243	C 116	N 46	O 70	P 11	0	0	0
2	H	12	Total 243	C 116	N 46	O 70	P 11	0	0	0
2	K	12	Total 243	C 116	N 46	O 70	P 11	0	0	0
2	L	12	Total 243	C 116	N 46	O 70	P 11	0	0	0
2	E	12	Total 243	C 116	N 46	O 70	P 11	0	0	0
2	F	12	Total 243	C 116	N 46	O 70	P 11	0	0	0
2	I	12	Total 243	C 116	N 46	O 70	P 11	0	0	0
2	J	12	Total 243	C 116	N 46	O 70	P 11	0	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total Na 1 1	0	0
3	D	2	Total Na 2 2	0	0
3	E	1	Total Na 1 1	0	0
3	B	1	Total Na 1 1	0	0
3	C	1	Total Na 1 1	0	0
3	A	1	Total Na 1 1	0	0
3	F	1	Total Na 1 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

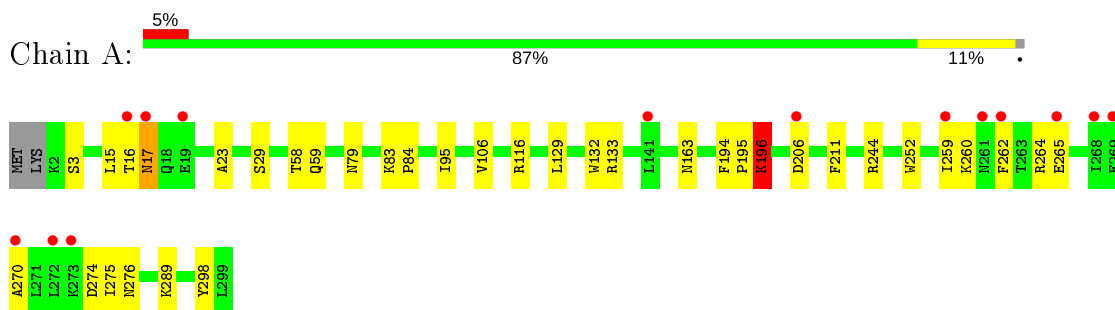
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	81	Total O 81 81	0	0
5	B	108	Total O 108 108	0	0
5	C	78	Total O 78 78	0	0
5	D	79	Total O 79 79	0	0
5	G	21	Total O 21 21	0	0
5	H	20	Total O 20 20	0	0
5	K	1	Total O 1 1	0	0
5	E	18	Total O 18 18	0	0
5	F	21	Total O 21 21	0	0
5	I	1	Total O 1 1	0	0
5	J	1	Total O 1 1	0	0

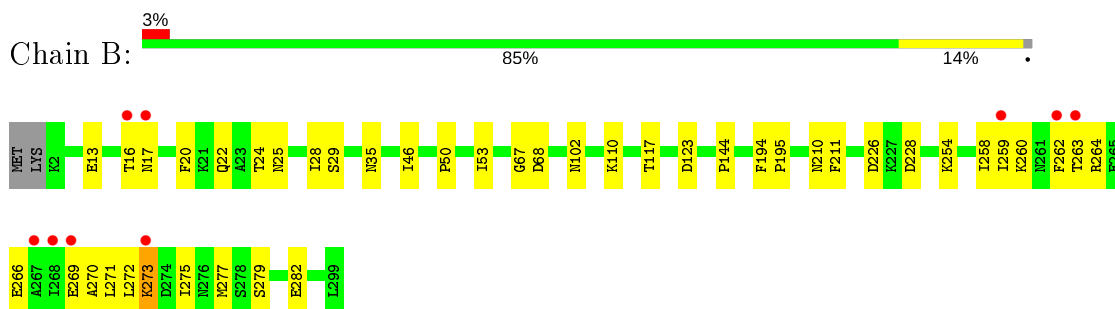
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

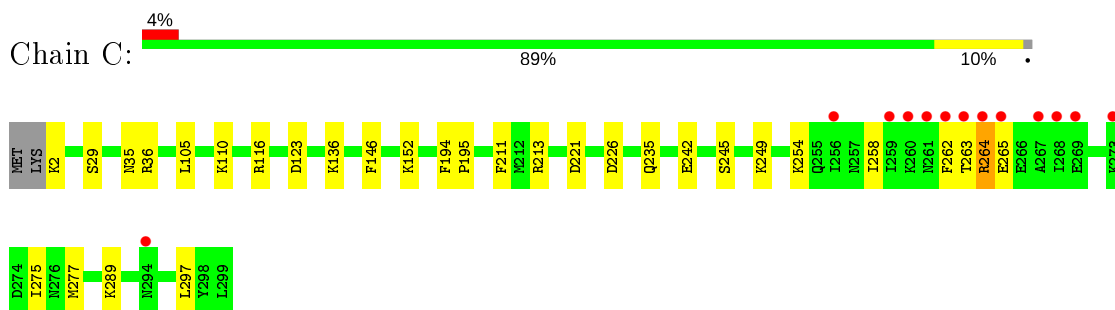
- Molecule 1: Type-2 restriction enzyme HindIII



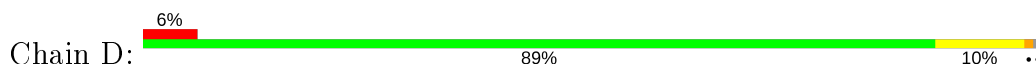
- Molecule 1: Type-2 restriction enzyme HindIII

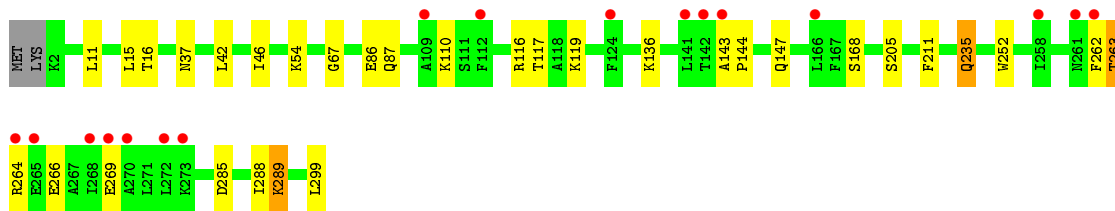


- Molecule 1: Type-2 restriction enzyme HindIII



- Molecule 1: Type-2 restriction enzyme HindIII





- Molecule 2: DNA (5'-D(*GP*CP*CP*AP*AP*GP*CP*TP*TP*GP*GP*C)-3')



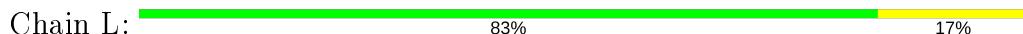
- Molecule 2: DNA (5'-D(*GP*CP*CP*AP*AP*GP*CP*TP*TP*GP*GP*C)-3')



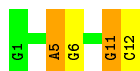
- Molecule 2: DNA (5'-D(*GP*CP*CP*AP*AP*GP*CP*TP*TP*GP*GP*C)-3')



- Molecule 2: DNA (5'-D(*GP*CP*CP*AP*AP*GP*CP*TP*TP*GP*GP*C)-3')



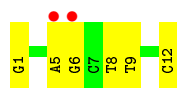
- Molecule 2: DNA (5'-D(*GP*CP*CP*AP*AP*GP*CP*TP*TP*GP*GP*C)-3')



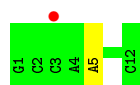
- Molecule 2: DNA (5'-D(*GP*CP*CP*AP*AP*GP*CP*TP*TP*GP*GP*C)-3')



- Molecule 2: DNA (5'-D(*GP*CP*CP*AP*AP*GP*CP*TP*TP*GP*GP*C)-3')



- Molecule 2: DNA (5'-D(*GP*CP*CP*AP*AP*GP*CP*TP*TP*GP*GP*C)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.66Å 140.58Å 96.29Å 90.00° 112.10° 90.00°	Depositor
Resolution (Å)	39.70 – 2.25 39.70 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.6 (39.70-2.25) 99.6 (39.70-2.25)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.13 (at 2.24Å)	Xtrriage
Refinement program	REFMAC 5.8.0069	Depositor
R, R_{free}	0.177 , 0.226 0.186 , 0.232	Depositor DCC
R_{free} test set	4714 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	31.5	Xtrriage
Anisotropy	0.093	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.048 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12207	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% 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, NA

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	0.87	0/2494	0.89	4/3351 (0.1%)
1	B	0.87	1/2494 (0.0%)	0.89	1/3351 (0.0%)
1	C	0.87	0/2494	0.92	5/3351 (0.1%)
1	D	0.84	0/2494	0.85	1/3351 (0.0%)
2	E	0.79	0/272	1.06	2/418 (0.5%)
2	F	0.69	0/272	1.22	2/418 (0.5%)
2	G	0.87	1/272 (0.4%)	1.07	2/418 (0.5%)
2	H	0.90	0/272	1.05	1/418 (0.2%)
2	I	0.63	0/272	1.01	1/418 (0.2%)
2	J	0.60	0/272	0.99	0/418
2	K	0.62	0/272	1.12	1/418 (0.2%)
2	L	0.67	0/272	1.05	2/418 (0.5%)
All	All	0.84	2/12152 (0.0%)	0.93	22/16748 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	68	ASP	CB-CG	5.55	1.63	1.51
2	G	10	DG	O3'-P	-5.09	1.55	1.61

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	11	DG	O5'-P-OP2	-11.84	95.05	105.70
2	K	12	DC	O4'-C4'-C3'	-7.54	101.47	106.00
1	A	196	LYS	CD-CE-NZ	7.03	127.86	111.70
2	F	10	DG	O5'-P-OP2	-6.87	99.52	105.70
1	D	116	ARG	NE-CZ-NH1	6.80	123.70	120.30
2	E	11	DG	O5'-P-OP2	-6.70	99.67	105.70
1	C	123	ASP	CB-CG-OD1	6.66	124.30	118.30
2	I	12	DC	O4'-C4'-C3'	-6.54	101.89	104.50
2	L	12	DC	O4'-C4'-C3'	-5.94	102.12	104.50
1	A	244	ARG	NE-CZ-NH1	5.93	123.26	120.30
1	C	123	ASP	CB-CG-OD2	-5.84	113.04	118.30
1	C	36	ARG	NE-CZ-NH2	-5.83	117.39	120.30
2	G	7	DC	O4'-C4'-C3'	-5.72	102.21	104.50
1	C	116	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	A	206	ASP	CB-CG-OD1	5.28	123.05	118.30
1	A	116	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	B	123	ASP	CB-CG-OD1	5.26	123.03	118.30
1	C	116	ARG	NE-CZ-NH1	5.16	122.88	120.30
2	L	10	DG	O5'-P-OP1	-5.16	101.06	105.70
2	H	6	DG	O5'-P-OP1	5.15	116.88	110.70
2	E	5	DA	O5'-P-OP2	-5.05	101.15	105.70
2	G	5	DA	O4'-C4'-C3'	-5.00	102.50	104.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	17	ASN	Peptide

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	2452	0	2502	23	0
1	B	2452	0	2502	26	0
1	C	2452	0	2502	16	0
1	D	2452	0	2502	20	0
2	E	243	0	136	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	243	0	136	2	0
2	G	243	0	136	0	0
2	H	243	0	136	2	0
2	I	243	0	136	5	0
2	J	243	0	136	1	0
2	K	243	0	136	0	0
2	L	243	0	136	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	2	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
4	B	12	0	16	4	0
4	C	6	0	8	1	0
5	A	81	0	0	1	0
5	B	108	0	0	2	0
5	C	78	0	0	1	0
5	D	79	0	0	1	0
5	E	18	0	0	0	0
5	F	21	0	0	0	0
5	G	21	0	0	0	0
5	H	20	0	0	1	0
5	I	1	0	0	0	0
5	J	1	0	0	0	0
5	K	1	0	0	0	0
All	All	12207	0	11120	77	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (77) 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:262:PHE:O	1:B:264:ARG:NH1	1.96	0.98
1:A:264:ARG:NH1	1:B:262:PHE:O	2.07	0.87
1:B:102:ASN:HB2	5:B:419:HOH:O	1.79	0.83
1:C:264:ARG:HB3	1:D:264:ARG:HA	1.60	0.83
1:C:249:LYS:HE2	1:D:285:ASP:OD1	1.80	0.81
2:I:8:DT:O4	2:J:5:DA:N6	2.17	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:297:LEU:HD11	1:D:235:GLN:HE22	1.56	0.70
1:A:259:ILE:HD11	1:B:272:LEU:HD21	1.74	0.69
2:I:8:DT:H4'	2:I:9:DT:OP1	1.94	0.68
1:A:298:TYR:CE2	4:B:303:GOL:H31	2.31	0.66
1:A:16:THR:HG21	1:A:59:GLN:HE21	1.66	0.61
2:I:8:DT:C4'	2:I:9:DT:OP1	2.50	0.59
1:A:259:ILE:HD11	1:B:272:LEU:CD2	2.33	0.58
1:A:298:TYR:HE2	4:B:303:GOL:C3	2.18	0.56
1:C:249:LYS:CE	1:D:285:ASP:OD1	2.54	0.55
1:A:298:TYR:CE2	4:B:303:GOL:C3	2.90	0.55
1:C:277:MET:HG2	1:D:252:TRP:CE3	2.42	0.54
1:A:17:ASN:OD1	1:A:17:ASN:N	2.40	0.54
1:D:37:ASN:ND2	5:D:437:HOH:O	2.32	0.53
1:C:264:ARG:HB3	1:D:264:ARG:CA	2.36	0.52
1:C:275:ILE:HG22	1:C:277:MET:HG3	1.92	0.52
1:B:50:PRO:HG2	1:B:53:ILE:HD12	1.93	0.51
1:B:263:THR:OG1	1:B:266:GLU:HG2	2.12	0.49
1:A:298:TYR:HE2	4:B:303:GOL:H32	1.77	0.49
1:A:264:ARG:HB2	1:B:264:ARG:HB2	1.94	0.49
2:E:12:DC:OP2	2:I:1:DG:O5'	2.31	0.48
1:C:105:LEU:C	1:C:105:LEU:HD12	2.34	0.48
2:E:5:DA:H2'	2:E:6:DG:O4'	2.13	0.48
1:B:259:ILE:HD12	1:B:262:PHE:CE2	2.50	0.47
1:D:143:ALA:O	1:D:168:SER:HA	2.15	0.47
1:C:242:GLU:O	1:C:245:SER:OG	2.27	0.47
1:A:106:VAL:HG21	1:A:133:ARG:HA	1.96	0.47
1:D:11:LEU:O	1:D:15:LEU:HG	2.15	0.47
1:B:16:THR:HA	5:B:410:HOH:O	2.14	0.46
1:B:110:LYS:O	1:B:144:PRO:HD3	2.15	0.46
1:B:46:ILE:HG12	1:B:67:GLY:HA2	1.98	0.46
1:C:254:LYS:O	1:C:258:ILE:HD13	2.16	0.46
1:A:15:LEU:HD22	1:A:23:ALA:HA	1.96	0.46
1:A:270:ALA:HB3	1:B:271:LEU:HD11	1.98	0.46
1:B:275:ILE:HG22	1:B:277:MET:HG3	1.98	0.46
1:A:59:GLN:HG3	5:A:441:HOH:O	2.15	0.45
1:D:110:LYS:HG3	5:H:113:HOH:O	2.16	0.45
1:B:271:LEU:HD23	1:B:271:LEU:HA	1.87	0.45
1:D:264:ARG:CZ	1:D:264:ARG:HB3	2.46	0.45
1:A:252:TRP:CE3	1:B:277:MET:HG2	2.52	0.44
1:C:213:ARG:NH1	1:D:299:LEU:O	2.50	0.44
2:H:5:DA:H2'	2:H:6:DG:O4'	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:270:ALA:HA	1:B:273:LYS:HD3	2.00	0.43
1:A:58:THR:OG1	2:F:11:DG:OP1	2.22	0.43
2:F:5:DA:H2'	2:F:6:DG:O4'	2.18	0.43
1:B:279:SER:HA	1:B:282:GLU:OE1	2.18	0.43
1:D:143:ALA:HB1	1:D:144:PRO:CD	2.48	0.43
1:D:46:ILE:HG12	1:D:67:GLY:HA2	2.01	0.43
2:I:5:DA:H2''	2:I:6:DG:OP2	2.19	0.43
1:A:163:ASN:HB2	1:A:196:LYS:HE2	2.01	0.43
1:A:83:LYS:HG2	1:A:84:PRO:O	2.19	0.43
1:A:275:ILE:O	1:A:276:ASN:C	2.56	0.43
1:D:263:THR:HG1	1:D:266:GLU:H	1.66	0.43
1:B:13:GLU:O	1:B:16:THR:HG23	2.19	0.42
1:A:260:LYS:O	1:B:264:ARG:NH2	2.53	0.42
1:B:20:PHE:CD2	2:E:11:DG:H5''	2.54	0.42
1:C:297:LEU:HD11	1:D:235:GLN:NE2	2.27	0.42
1:A:129:LEU:HA	1:A:132:TRP:CE3	2.54	0.42
1:D:16:THR:HG22	1:D:16:THR:O	2.20	0.42
1:B:254:LYS:O	1:B:258:ILE:HD12	2.20	0.42
1:C:146:PHE:HA	4:C:302:GOL:H12	2.02	0.42
1:B:210:ASN:OD1	1:B:210:ASN:C	2.59	0.41
1:D:288:ILE:O	1:D:289:LYS:C	2.59	0.41
1:D:42:LEU:HA	1:D:42:LEU:HD23	1.83	0.41
1:C:110:LYS:HE2	5:C:476:HOH:O	2.20	0.41
1:C:194:PHE:N	1:C:195:PRO:CD	2.84	0.41
1:C:152:LYS:O	2:H:2:DC:H5''	2.20	0.41
1:A:194:PHE:HB3	1:A:195:PRO:HD3	2.03	0.41
1:B:35:ASN:C	1:B:35:ASN:OD1	2.60	0.41
1:D:119:LYS:HE3	1:D:147:GLN:OE1	2.21	0.41
1:B:194:PHE:HB3	1:B:195:PRO:HD3	2.03	0.40
1:B:24:THR:O	1:B:28:ILE:HG13	2.21	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	296/300 (99%)	285 (96%)	10 (3%)	1 (0%)	41	46
1	B	296/300 (99%)	286 (97%)	9 (3%)	1 (0%)	41	46
1	C	296/300 (99%)	291 (98%)	5 (2%)	0	100	100
1	D	296/300 (99%)	286 (97%)	8 (3%)	2 (1%)	22	21
All	All	1184/1200 (99%)	1148 (97%)	32 (3%)	4 (0%)	41	46

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	263	THR
1	A	79	ASN
1	B	117	THR
1	D	117	THR

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	274/276 (99%)	265 (97%)	9 (3%)	38	46
1	B	274/276 (99%)	265 (97%)	9 (3%)	38	46
1	C	274/276 (99%)	261 (95%)	13 (5%)	26	29
1	D	274/276 (99%)	264 (96%)	10 (4%)	35	42
All	All	1096/1104 (99%)	1055 (96%)	41 (4%)	34	40

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	17	ASN
1	A	29	SER
1	A	95	ILE

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Mol	Chain	Res	Type
1	A	196	LYS
1	A	211	PHE
1	A	265	GLU
1	A	274	ASP
1	A	289	LYS
1	B	22	GLN
1	B	25	ASN
1	B	29	SER
1	B	211	PHE
1	B	226	ASP
1	B	228	ASP
1	B	260	LYS
1	B	269	GLU
1	B	273	LYS
1	C	2	LYS
1	C	29	SER
1	C	35	ASN
1	C	136	LYS
1	C	211	PHE
1	C	221	ASP
1	C	226	ASP
1	C	235	GLN
1	C	262	PHE
1	C	263	THR
1	C	264	ARG
1	C	265	GLU
1	C	289	LYS
1	D	54	LYS
1	D	86	GLU
1	D	87	GLN
1	D	136	LYS
1	D	205	SER
1	D	211	PHE
1	D	235	GLN
1	D	262	PHE
1	D	269	GLU
1	D	289	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	GLN

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Mol	Chain	Res	Type
1	A	102	ASN
1	B	18	GLN
1	B	232	GLN
1	C	37	ASN
1	C	87	GLN
1	D	235	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](#)

Of 11 ligands modelled in this entry, 8 are monoatomic - leaving 3 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	B	303	-	5,5,5	0.39	0	5,5,5	0.61	0
4	GOL	C	302	-	5,5,5	0.64	0	5,5,5	0.84	0
4	GOL	B	302	-	5,5,5	0.39	0	5,5,5	0.70	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	303	-	-	0/4/4/4	-
4	GOL	C	302	-	-	2/4/4/4	-
4	GOL	B	302	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	302	GOL	O1-C1-C2-O2
4	C	302	GOL	O1-C1-C2-C3
4	B	302	GOL	O1-C1-C2-C3

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	303	GOL	4	0
4	C	302	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 i

6.1 Protein, DNA and RNA chains i

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	298/300 (99%)	0.17	14 (4%) 31 34	16, 36, 68, 89	0
1	B	298/300 (99%)	-0.05	9 (3%) 50 53	16, 35, 63, 80	0
1	C	298/300 (99%)	-0.08	13 (4%) 34 37	18, 34, 73, 100	0
1	D	298/300 (99%)	0.18	17 (5%) 23 25	19, 35, 71, 105	0
2	E	12/12 (100%)	-0.26	0 100 100	23, 25, 30, 34	0
2	F	12/12 (100%)	-0.46	0 100 100	19, 24, 34, 37	0
2	G	12/12 (100%)	-0.51	0 100 100	19, 21, 27, 29	0
2	H	12/12 (100%)	-0.34	0 100 100	19, 23, 26, 26	0
2	I	12/12 (100%)	1.01	2 (16%) 1 1	33, 55, 68, 74	0
2	J	12/12 (100%)	1.00	1 (8%) 11 12	29, 54, 70, 74	0
2	K	12/12 (100%)	0.28	0 100 100	27, 49, 53, 54	0
2	L	12/12 (100%)	0.33	0 100 100	27, 45, 57, 60	0
All	All	1288/1296 (99%)	0.06	56 (4%) 35 37	16, 35, 68, 105	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	263	THR	5.2
1	D	265	GLU	4.7
1	D	261	ASN	4.3
1	A	16	THR	4.2
1	A	272	LEU	4.1
1	D	264	ARG	3.8
1	A	17	ASN	3.5
1	C	262	PHE	3.4
1	D	262	PHE	3.4
1	C	265	GLU	3.3
1	C	264	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	256	ILE	3.1
1	A	269	GLU	3.1
1	D	141	LEU	3.1
1	A	259	ILE	3.1
1	B	259	ILE	3.0
1	D	273	LYS	2.9
1	B	17	ASN	2.9
1	C	261	ASN	2.9
1	D	272	LEU	2.8
1	A	261	ASN	2.8
1	B	263	THR	2.7
1	C	260	LYS	2.7
2	I	6	DG	2.7
1	C	273	LYS	2.7
1	A	270	ALA	2.6
1	B	16	THR	2.6
1	C	269	GLU	2.6
1	D	269	GLU	2.5
1	A	19	GLU	2.5
1	B	269	GLU	2.5
1	B	273	LYS	2.4
1	C	268	ILE	2.4
1	B	267	ALA	2.3
1	D	124	PHE	2.3
1	A	262	PHE	2.3
1	D	258	ILE	2.3
1	A	268	ILE	2.3
1	B	268	ILE	2.3
1	A	265	GLU	2.3
1	A	206	ASP	2.2
1	D	112	PHE	2.2
2	J	3	DC	2.2
1	D	270	ALA	2.2
1	A	273	LYS	2.2
1	B	262	PHE	2.1
1	C	267	ALA	2.1
1	D	268	ILE	2.1
1	D	143	ALA	2.1
1	D	166	LEU	2.1
2	I	5	DA	2.1
1	C	294	ASN	2.1
1	D	109	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	141	LEU	2.0
1	D	142	THR	2.0
1	C	259	ILE	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. 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
4	GOL	C	302	6/6	0.92	0.15	35,41,43,44	0
3	NA	G	101	1/1	0.93	0.09	38,38,38,38	0
3	NA	E	101	1/1	0.94	0.14	37,37,37,37	0
3	NA	D	301	1/1	0.95	0.16	40,40,40,40	0
4	GOL	B	302	6/6	0.96	0.17	35,37,39,41	0
3	NA	A	301	1/1	0.96	0.10	35,35,35,35	0
4	GOL	B	303	6/6	0.96	0.13	32,40,45,49	0
3	NA	B	301	1/1	0.98	0.09	40,40,40,40	0
3	NA	C	301	1/1	0.99	0.04	28,28,28,28	0
3	NA	D	302	1/1	0.99	0.11	37,37,37,37	0
3	NA	F	101	1/1	0.99	0.07	29,29,29,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.