



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 13, 2024 – 12:30 AM EDT

PDB ID : 3WVP
Title : Time-Resolved Crystal Structure of HindIII with 60sec soaking
Authors : Kawamura, T.; Kobayashi, T.; Watanabe, N.
Deposited on : 2014-06-02
Resolution : 2.30 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 : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.20.1
EDS : 2.36.2
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) : 2.36.2

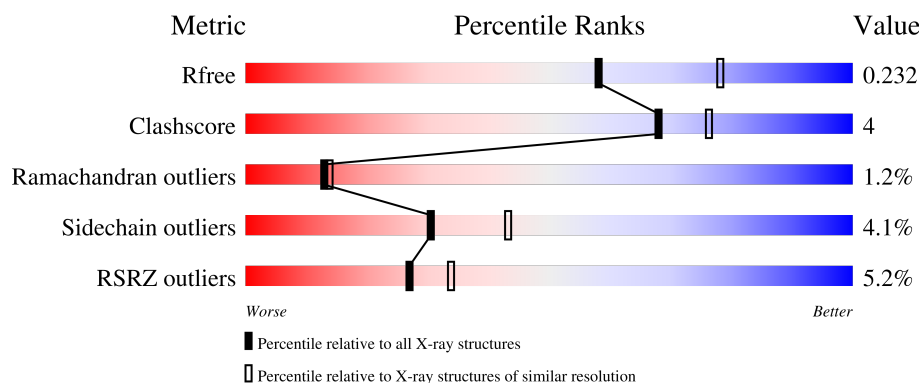
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	300	<div> <div>6%</div> <div> <div></div> <div>90%</div> <div>8%</div> <div>..</div> </div> </div>
1	B	300	<div> <div>3%</div> <div> <div></div> <div>85%</div> <div>14%</div> <div>.</div> </div> </div>
1	C	300	<div> <div>5%</div> <div> <div></div> <div>87%</div> <div>11%</div> <div>..</div> </div> </div>
1	D	300	<div> <div>9%</div> <div> <div></div> <div>88%</div> <div>10%</div> <div>..</div> </div> </div>
2	E	12	<div> <div></div> <div> <div></div> <div>83%</div> <div>17%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	F	12	 75%25%
2	G	12	 58%42%
2	H	12	 67%33%
2	I	12	 8%50%50%
2	J	12	 100%
2	K	12	 83%17%
2	L	12	 92%8%
3	M	8	 62%25%12%
3	N	8	 75%12%12%
3	Q	8	 75%12%12%
3	R	8	 62%25%12%
4	O	4	 100%
4	P	4	 100%
4	S	4	 100%
4	T	4	 75%25%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13226 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
1	C	298	Total	C	N	O	S	0	4	0
			2484	1597	414	470	3			
1	D	298	Total	C	N	O	S	0	4	0
			2484	1597	414	470	3			
1	A	298	Total	C	N	O	S	0	4	0
			2484	1597	414	470	3			
1	B	298	Total	C	N	O	S	0	4	0
			2484	1597	414	470	3			

- 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
2	K	12	Total	C	N	O	P	0	0	0
			243	116	46	70	11			
2	L	12	Total	C	N	O	P	0	0	0
			243	116	46	70	11			
2	I	12	Total	C	N	O	P	0	0	0
			243	116	46	70	11			
2	J	12	Total	C	N	O	P	0	0	0
			243	116	46	70	11			
2	E	12	Total	C	N	O	P	0	12	0
			243	116	46	70	11			
2	F	12	Total	C	N	O	P	0	12	0
			243	116	46	70	11			
2	G	12	Total	C	N	O	P	0	12	0
			243	116	46	70	11			
2	H	12	Total	C	N	O	P	0	12	0
			243	116	46	70	11			

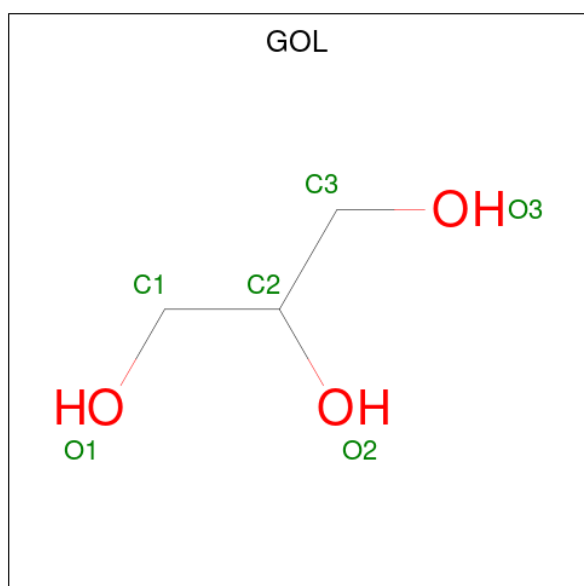
- Molecule 3 is a DNA chain called DNA (5'-D(P*AP*GP*CP*TP*TP*GP*GP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	8	Total	C	N	O	P	0	8	0
			166	78	30	50	8			
3	N	8	Total	C	N	O	P	0	8	0
			166	78	30	50	8			
3	Q	8	Total	C	N	O	P	0	8	0
			166	78	30	50	8			
3	R	8	Total	C	N	O	P	0	8	0
			166	78	30	50	8			

- Molecule 4 is a DNA chain called DNA (5'-D(*GP*CP*CP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	O	4	Total	C	N	O	P	0	4	0
			78	38	16	21	3			
4	P	4	Total	C	N	O	P	0	4	0
			78	38	16	21	3			
4	S	4	Total	C	N	O	P	0	4	0
			78	38	16	21	3			
4	T	4	Total	C	N	O	P	0	4	0
			78	38	16	21	3			

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



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

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

- Molecule 6 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	2	Total	Mn	0	0
			2	2		
6	D	2	Total	Mn	0	0
			2	2		
6	A	2	Total	Mn	0	0
			2	2		
6	B	2	Total	Mn	0	0
			2	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	72	Total	O	0	2
			72	72		
7	D	78	Total	O	0	3
			78	78		
7	K	1	Total	O	0	0
			1	1		
7	A	58	Total	O	0	2
			58	58		
7	B	70	Total	O	0	2
			70	70		
7	I	1	Total	O	0	0
			1	1		
7	J	1	Total	O	0	0
			1	1		
7	E	7	Total	O	0	0
			7	7		
7	F	6	Total	O	0	1
			6	6		
7	G	8	Total	O	0	1
			8	8		
7	H	7	Total	O	0	1
			7	7		

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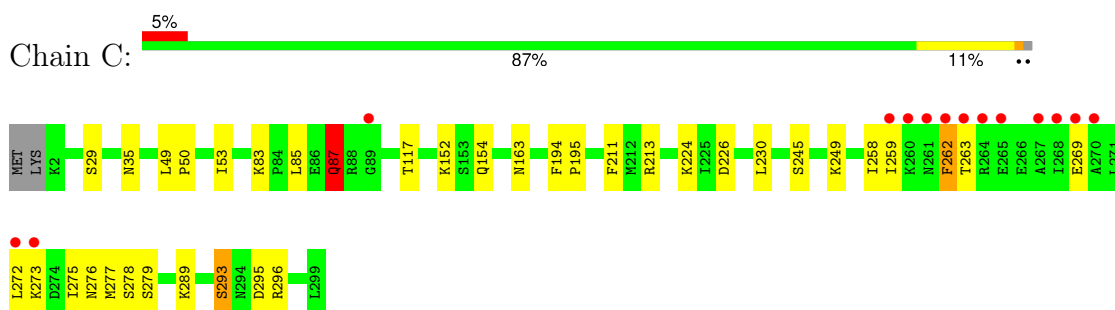
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	M	6	Total 6	O 6	0	0
7	N	3	Total 3	O 3	0	0
7	O	4	Total 4	O 4	0	0
7	P	2	Total 2	O 2	0	0
7	Q	5	Total 5	O 5	0	0
7	R	2	Total 2	O 2	0	0
7	S	3	Total 3	O 3	0	0
7	T	4	Total 4	O 4	0	0

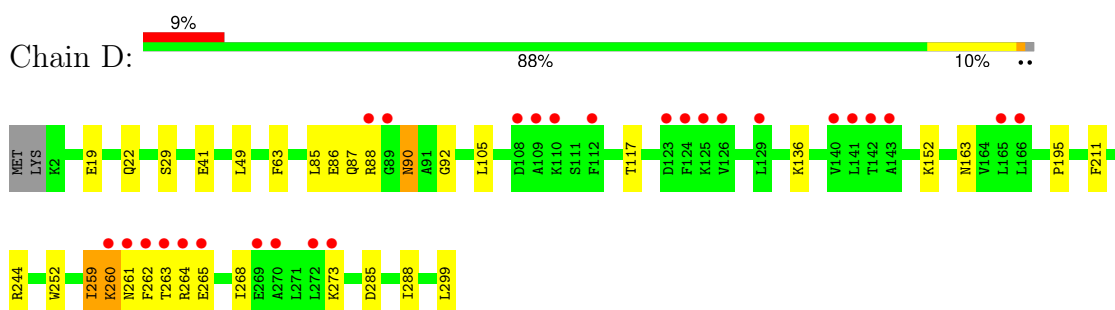
3 Residue-property plots [i](#)

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.

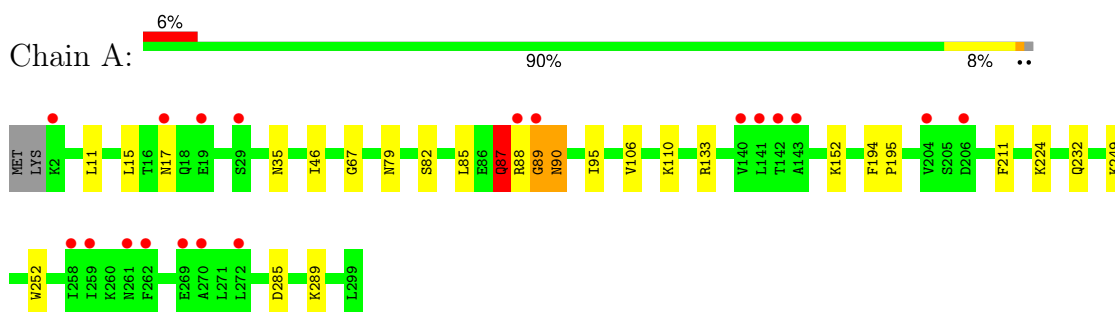
- Molecule 1: Type-2 restriction enzyme HindIII



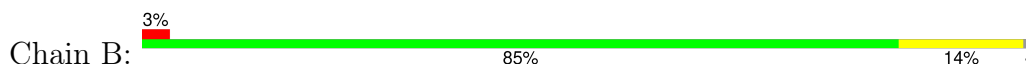
- Molecule 1: Type-2 restriction enzyme HindIII

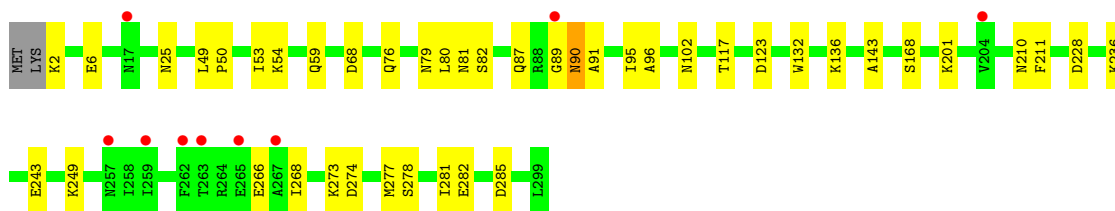


- Molecule 1: Type-2 restriction enzyme HindIII



- 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')

Chain K: 83% 17%



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

Chain L: 92% 8%



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

Chain I: 8% 50% 50%



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

Chain J: 100%

There are no outlier residues recorded for this chain.

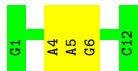
- Molecule 2: DNA (5'-D(*GP*CP*CP*AP*AP*GP*CP*TP*TP*GP*GP*C)-3')

Chain E: 83% 17%



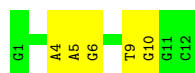
- Molecule 2: DNA (5'-D(*GP*CP*CP*AP*AP*GP*CP*TP*TP*GP*GP*C)-3')

Chain F: 75% 25%



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

Chain G:  58% 42%



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

Chain H:  67% 33%



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

Chain M:  62% 25% 12%



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

Chain N:  75% 12% 12%



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

Chain Q:  75% 12% 12%



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

Chain R:  62% 25% 12%



- Molecule 4: DNA (5'-D(*GP*CP*CP*A)-3')

Chain O:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: DNA (5'-D(*GP*CP*CP*A)-3')

Chain P:  100%


There are no outlier residues recorded for this chain.

- Molecule 4: DNA (5'-D(*GP*CP*CP*A)-3')

Chain S:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: DNA (5'-D(*GP*CP*CP*A)-3')

Chain T:  75% 25%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.50Å 140.70Å 96.47Å 90.00° 112.07° 90.00°	Depositor
Resolution (Å)	39.71 – 2.30 39.71 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (39.71-2.30) 99.7 (39.71-2.30)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0069	Depositor
R, R_{free}	0.182 , 0.230 0.188 , 0.232	Depositor DCC
R_{free} test set	4430 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	36.2	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.047 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13226	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% 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, MN

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	0.81	0/2526	0.85	0/3393
1	B	0.79	0/2526	0.84	2/3393 (0.1%)
1	C	0.81	0/2526	0.83	0/3393
1	D	0.78	0/2526	0.82	1/3393 (0.0%)
2	E	0.53	0/272	0.83	0/418
2	F	0.52	0/272	0.84	0/418
2	G	0.48	0/272	0.78	0/418
2	H	0.49	0/272	0.75	0/418
2	I	0.54	0/272	0.93	0/418
2	J	0.56	0/272	0.92	0/418
2	K	0.57	0/272	1.07	2/418 (0.5%)
2	L	0.53	0/272	1.01	1/418 (0.2%)
3	M	0.89	1/185 (0.5%)	0.73	0/282
3	N	0.88	1/185 (0.5%)	0.83	0/282
3	Q	0.85	1/185 (0.5%)	0.81	0/282
3	R	0.92	1/185 (0.5%)	0.82	0/282
4	O	0.49	0/87	0.90	0/132
4	P	0.38	0/87	0.66	0/132
4	S	0.51	0/87	0.91	0/132
4	T	0.53	0/87	0.83	0/132
All	All	0.76	4/13368 (0.0%)	0.84	6/18572 (0.0%)

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	D	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	1[B]	DA	OP3-P	-10.29	1.48	1.61
3	R	1[B]	DA	OP3-P	-10.28	1.48	1.61
3	N	1[B]	DA	OP3-P	-9.95	1.49	1.61
3	Q	1[B]	DA	OP3-P	-9.70	1.49	1.61

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	4	DA	O5'-P-OP1	-8.35	98.19	105.70
1	B	68	ASP	CB-CG-OD1	7.79	125.31	118.30
1	B	123	ASP	CB-CG-OD1	6.78	124.40	118.30
2	L	12	DC	O4'-C4'-C3'	-6.16	102.04	104.50
1	D	244	ARG	NE-CZ-NH1	5.34	122.97	120.30
2	K	6	DG	C1'-O4'-C4'	-5.27	104.83	110.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	90[B]	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	2484	0	2531	17	0
1	B	2484	0	2531	21	0
1	C	2484	0	2531	23	0
1	D	2484	0	2531	23	0
2	E	243	0	134	1	0
2	F	243	0	134	4	0
2	G	243	0	134	3	0
2	H	243	0	134	3	0
2	I	243	0	136	5	0
2	J	243	0	136	0	0
2	K	243	0	136	0	0
2	L	243	0	136	0	0
3	M	166	0	90	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	N	166	0	90	1	0
3	Q	166	0	90	3	0
3	R	166	0	90	2	0
4	O	78	0	44	0	0
4	P	78	0	44	0	0
4	S	78	0	44	0	0
4	T	78	0	43	2	0
5	A	12	0	16	1	0
5	C	6	0	8	0	0
5	D	6	0	8	2	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
6	C	2	0	0	0	0
6	D	2	0	0	0	0
7	A	58	0	0	1	0
7	B	70	0	0	3	0
7	C	72	0	0	1	0
7	D	78	0	0	1	0
7	E	7	0	0	0	0
7	F	6	0	0	0	0
7	G	8	0	0	0	0
7	H	7	0	0	0	0
7	I	1	0	0	0	0
7	J	1	0	0	0	0
7	K	1	0	0	0	0
7	M	6	0	0	1	0
7	N	3	0	0	0	0
7	O	4	0	0	1	0
7	P	2	0	0	0	0
7	Q	5	0	0	0	0
7	R	2	0	0	0	0
7	S	3	0	0	0	0
7	T	4	0	0	0	0
All	All	13226	0	11771	92	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 4.

All (92) 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:B:278:SER:O	1:B:282:GLU:HG3	1.74	0.86
1:D:88[B]:ARG:HB2	3:R:8[B]:DC:O3'	1.76	0.85
1:A:88[B]:ARG:O	1:A:89[B]:GLY:O	1.98	0.82
1:D:88[B]:ARG:O	1:D:88[B]:ARG:HD3	1.80	0.81
1:D:88[B]:ARG:O	1:D:88[B]:ARG:CG	2.31	0.78
1:D:88[B]:ARG:O	1:D:88[B]:ARG:HG2	1.87	0.75
1:A:11:LEU:O	1:A:15:LEU:HB2	1.89	0.73
1:D:88[B]:ARG:O	1:D:88[B]:ARG:CD	2.36	0.72
1:C:272:LEU:HD21	1:D:259:ILE:HG21	1.80	0.64
1:C:230:LEU:HD23	1:D:299:LEU:HD21	1.80	0.63
2:F:4[A]:DA:H2'	2:F:5[A]:DA:C8	2.35	0.62
1:C:275:ILE:HG22	1:C:277:MET:HG3	1.82	0.61
1:B:102:ASN:HB2	7:B:416:HOH:O	1.99	0.61
1:A:110:LYS:HE2	7:M:106:HOH:O	2.01	0.59
1:A:249:LYS:HD3	1:B:285:ASP:OD1	2.03	0.58
2:E:5[A]:DA:H2'	2:E:6[A]:DG:O4'	2.03	0.58
1:C:277:MET:HG2	1:D:252:TRP:CE3	2.39	0.57
2:H:4[A]:DA:H2'	2:H:5[A]:DA:C8	2.39	0.57
1:A:252:TRP:CE3	1:B:277:MET:HG2	2.41	0.55
3:R:1[B]:DA:H2'	3:R:2[B]:DG:O4'	2.07	0.55
3:Q:1[B]:DA:H2'	3:Q:2[B]:DG:O4'	2.07	0.54
1:C:249:LYS:NZ	1:D:285:ASP:OD1	2.34	0.53
2:F:5[A]:DA:H2'	2:F:6[A]:DG:O4'	2.08	0.53
1:B:59:GLN:NE2	7:B:443:HOH:O	2.41	0.53
1:C:296:ARG:HE	5:D:301:GOL:H32	1.74	0.53
1:D:90[B]:ASN:ND2	7:D:457:HOH:O	2.41	0.53
1:A:88[A]:ARG:HD3	7:A:455:HOH:O	2.08	0.53
1:A:252:TRP:HB2	1:B:281:ILE:HD11	1.91	0.52
3:M:1[B]:DA:H2'	3:M:2[B]:DG:O4'	2.09	0.52
1:C:258:ILE:HG22	1:C:258:ILE:O	2.08	0.52
2:G:5[A]:DA:H2'	2:G:6[A]:DG:O4'	2.10	0.52
1:D:265:GLU:O	1:D:268:ILE:HG13	2.09	0.52
1:B:89[A]:GLY:HA3	7:O:102:HOH:O	2.08	0.51
3:N:1[B]:DA:H2'	3:N:2[B]:DG:O4'	2.10	0.51
5:A:302:GOL:O1	1:B:210:ASN:ND2	2.40	0.50
1:C:245:SER:HB3	1:D:288:ILE:HD11	1.95	0.49
2:I:5:DA:H2''	2:I:6:DG:OP2	2.11	0.49
2:H:5[A]:DA:H2'	2:H:6[A]:DG:O4'	2.13	0.49
1:C:259:ILE:O	1:C:262:PHE:HB2	2.13	0.48
1:B:50:PRO:HG2	1:B:53:ILE:HD12	1.94	0.48
2:I:4:DA:H1'	2:I:5:DA:C8	2.48	0.48
2:G:9[A]:DT:H2''	2:G:10[A]:DG:C8	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:1[B]:DA:O5'	4:T:4[B]:DA:H2''	2.13	0.48
1:A:106:VAL:HG21	1:A:133:ARG:HA	1.97	0.47
1:A:89[B]:GLY:O	1:A:90[B]:ASN:C	2.53	0.47
2:I:1:DG:O5'	2:H:12[A]:DC:OP2	2.29	0.47
1:C:213:ARG:NH1	1:D:299:LEU:O	2.47	0.47
2:I:1:DG:O5'	3:M:8[B]:DC:OP2	2.29	0.47
1:B:143:ALA:O	1:B:168:SER:HA	2.14	0.47
2:I:7:DC:H1'	2:I:8:DT:H5'	1.96	0.46
1:C:154:GLN:CD	1:D:90[B]:ASN:OD1	2.54	0.46
1:C:85:LEU:O	1:C:87[B]:GLN:HG3	2.16	0.46
1:B:81:ASN:O	1:B:96:ALA:HA	2.16	0.46
1:B:90[B]:ASN:HB3	1:B:132:TRP:NE1	2.31	0.46
1:A:46:ILE:HG12	1:A:67:GLY:HA2	1.97	0.45
1:A:285:ASP:OD1	1:B:249:LYS:NZ	2.42	0.45
1:C:275:ILE:CG2	1:C:277:MET:HG3	2.46	0.45
1:A:194:PHE:HB3	1:A:195:PRO:HD3	1.99	0.45
1:A:82:SER:HA	1:A:95:ILE:O	2.17	0.45
1:A:89[B]:GLY:O	1:A:90[B]:ASN:O	2.34	0.45
1:B:201:LYS:O	1:B:201:LYS:HG3	2.16	0.45
1:B:90[B]:ASN:O	1:B:91:ALA:HB2	2.17	0.45
1:B:201:LYS:O	1:B:201:LYS:CG	2.65	0.45
1:D:49:LEU:HD23	1:D:63:PHE:CD2	2.51	0.45
1:A:85:LEU:O	1:A:87[B]:GLN:HG3	2.18	0.44
1:B:82:SER:HA	1:B:95:ILE:O	2.17	0.44
1:D:163:ASN:HA	1:D:195:PRO:HB2	1.98	0.44
1:A:90[B]:ASN:OD1	1:A:90[B]:ASN:N	2.49	0.44
1:C:258:ILE:O	1:C:258:ILE:CG2	2.66	0.43
1:C:87[B]:GLN:NE2	7:C:467:HOH:O	2.48	0.43
1:B:59:GLN:HG3	7:B:433:HOH:O	2.19	0.43
1:A:35:ASN:OD1	1:A:35:ASN:C	2.57	0.43
1:B:266:GLU:C	1:B:268:ILE:H	2.22	0.43
1:D:85:LEU:O	1:D:87[B]:GLN:HG3	2.19	0.42
1:C:276:ASN:OD1	1:C:279:SER:HB2	2.20	0.42
1:C:296:ARG:HE	5:D:301:GOL:C3	2.32	0.42
1:D:105:LEU:C	1:D:105:LEU:HD12	2.39	0.42
1:C:194:PHE:N	1:C:195:PRO:CD	2.83	0.42
1:D:87[B]:GLN:OE1	1:D:92:GLY:O	2.38	0.42
2:F:4[A]:DA:H2'	2:F:5[A]:DA:H8	1.81	0.41
1:B:76:GLN:HA	1:B:80:LEU:O	2.21	0.41
1:C:163:ASN:HA	1:C:195:PRO:HB2	2.02	0.41
1:C:50:PRO:HD2	1:C:53:ILE:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:293:SER:OG	1:C:295:ASP:OD1	2.38	0.41
1:D:260:LYS:O	1:D:262:PHE:N	2.53	0.41
1:C:262:PHE:O	1:D:264:ARG:NH1	2.50	0.41
1:D:88[B]:ARG:HD3	1:D:88[B]:ARG:C	2.40	0.41
2:G:4[A]:DA:H2'	2:G:5[A]:DA:C8	2.56	0.41
3:Q:1[B]:DA:C6	4:T:4[B]:DA:C6	3.09	0.40
1:C:272:LEU:CD2	1:D:259:ILE:HG21	2.49	0.40
1:B:90[A]:ASN:HD22	1:B:132:TRP:HE1	1.69	0.40
2:F:4[A]:DA:H2''	2:F:5[A]:DA:H5'	2.03	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	300/300 (100%)	284 (95%)	9 (3%)	7 (2%)	6	5
1	B	300/300 (100%)	288 (96%)	8 (3%)	4 (1%)	12	12
1	C	300/300 (100%)	283 (94%)	12 (4%)	5 (2%)	9	8
1	D	300/300 (100%)	283 (94%)	14 (5%)	3 (1%)	15	17
All	All	1200/1200 (100%)	1138 (95%)	43 (4%)	19 (2%)	13	9

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	87[A]	GLN
1	C	87[B]	GLN
1	D	261	ASN
1	D	263	THR
1	A	89[A]	GLY
1	A	89[B]	GLY

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Mol	Chain	Res	Type
1	A	90[A]	ASN
1	A	90[B]	ASN
1	C	263	THR
1	A	87[A]	GLN
1	A	87[B]	GLN
1	B	87[A]	GLN
1	B	87[B]	GLN
1	C	269	GLU
1	A	79	ASN
1	B	117	THR
1	C	117	THR
1	D	117	THR
1	B	79	ASN

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	277/276 (100%)	269 (97%)	8 (3%)	42	58
1	B	277/276 (100%)	263 (95%)	14 (5%)	24	33
1	C	277/276 (100%)	262 (95%)	15 (5%)	22	30
1	D	277/276 (100%)	266 (96%)	11 (4%)	31	44
All	All	1108/1104 (100%)	1060 (96%)	48 (4%)	30	40

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	29	SER
1	C	35	ASN
1	C	49	LEU
1	C	83	LYS
1	C	87[A]	GLN
1	C	87[B]	GLN
1	C	152	LYS
1	C	211	PHE

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Mol	Chain	Res	Type
1	C	224	LYS
1	C	226	ASP
1	C	262	PHE
1	C	273	LYS
1	C	278	SER
1	C	289	LYS
1	C	293	SER
1	D	19	GLU
1	D	22	GLN
1	D	29	SER
1	D	41	GLU
1	D	86	GLU
1	D	136	LYS
1	D	152	LYS
1	D	211	PHE
1	D	259	ILE
1	D	260	LYS
1	D	273	LYS
1	A	17	ASN
1	A	87[A]	GLN
1	A	87[B]	GLN
1	A	152	LYS
1	A	211	PHE
1	A	224	LYS
1	A	232	GLN
1	A	289	LYS
1	B	2	LYS
1	B	6	GLU
1	B	25	ASN
1	B	49	LEU
1	B	54	LYS
1	B	90[A]	ASN
1	B	90[B]	ASN
1	B	136	LYS
1	B	211	PHE
1	B	228	ASP
1	B	236	LYS
1	B	243	GLU
1	B	273	LYS
1	B	274	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	154	GLN
1	D	22	GLN
1	B	154	GLN
1	B	232	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 8 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	C	301	-	5,5,5	0.73	0	5,5,5	0.63	0
5	GOL	D	301	-	5,5,5	0.20	0	5,5,5	0.66	0
5	GOL	A	302	-	5,5,5	0.38	0	5,5,5	0.65	0
5	GOL	A	301	-	5,5,5	0.35	0	5,5,5	0.57	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	C	301	-	-	0/4/4/4	-
5	GOL	D	301	-	-	2/4/4/4	-
5	GOL	A	302	-	-	2/4/4/4	-
5	GOL	A	301	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	301	GOL	C1-C2-C3-O3
5	A	301	GOL	O1-C1-C2-C3
5	A	301	GOL	C1-C2-C3-O3
5	A	302	GOL	O1-C1-C2-C3
5	D	301	GOL	O2-C2-C3-O3
5	A	301	GOL	O1-C1-C2-O2
5	A	301	GOL	O2-C2-C3-O3
5	A	302	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	301	GOL	2	0
5	A	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 ⓘ

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	298/300 (99%)	0.23	19 (6%) 19 25	20, 38, 73, 100	4 (1%)
1	B	298/300 (99%)	0.02	9 (3%) 50 57	21, 37, 68, 89	0
1	C	298/300 (99%)	0.01	14 (4%) 31 38	23, 37, 76, 108	0
1	D	298/300 (99%)	0.28	27 (9%) 9 12	22, 38, 73, 102	0
2	E	12/12 (100%)	-0.27	0 100 100	21, 26, 33, 34	12 (100%)
2	F	12/12 (100%)	-0.35	0 100 100	22, 28, 36, 39	12 (100%)
2	G	12/12 (100%)	-0.34	0 100 100	24, 30, 41, 45	12 (100%)
2	H	12/12 (100%)	-0.12	0 100 100	20, 30, 34, 35	12 (100%)
2	I	12/12 (100%)	0.75	1 (8%) 11 15	38, 62, 75, 82	0
2	J	12/12 (100%)	0.60	0 100 100	33, 59, 73, 77	0
2	K	12/12 (100%)	0.40	0 100 100	34, 55, 60, 61	0
2	L	12/12 (100%)	0.31	0 100 100	32, 50, 66, 67	0
3	M	8/8 (100%)	-0.05	0 100 100	26, 29, 31, 36	8 (100%)
3	N	8/8 (100%)	-0.17	0 100 100	22, 29, 37, 42	8 (100%)
3	Q	8/8 (100%)	-0.24	0 100 100	27, 29, 30, 33	8 (100%)
3	R	8/8 (100%)	-0.33	0 100 100	25, 28, 31, 37	8 (100%)
4	O	4/4 (100%)	-0.66	0 100 100	20, 21, 21, 28	4 (100%)
4	P	4/4 (100%)	-0.23	0 100 100	34, 37, 41, 43	4 (100%)
4	S	4/4 (100%)	-0.38	0 100 100	18, 19, 22, 25	4 (100%)
4	T	4/4 (100%)	-0.34	0 100 100	23, 27, 28, 32	4 (100%)
All	All	1336/1344 (99%)	0.12	70 (5%) 27 34	18, 37, 73, 108	100 (7%)

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	268	ILE	4.9
1	D	261	ASN	4.6
1	D	262	PHE	4.5
1	A	89[A]	GLY	4.3
1	B	17	ASN	4.2
1	A	262	PHE	4.2
1	C	265	GLU	4.1
1	C	263	THR	4.1
1	D	141	LEU	3.9
1	D	89[A]	GLY	3.8
1	D	264	ARG	3.7
1	A	17	ASN	3.7
1	D	269	GLU	3.7
1	B	259	ILE	3.7
1	C	262	PHE	3.5
1	D	272	LEU	3.4
1	B	267	ALA	3.3
1	D	142	THR	3.3
1	B	262	PHE	3.2
1	D	88[A]	ARG	3.2
1	D	273	LYS	3.1
1	C	264	ARG	3.1
1	A	269	GLU	3.1
1	A	272	LEU	3.1
1	B	263	THR	3.1
1	D	124	PHE	3.1
1	A	141	LEU	3.0
1	A	258	ILE	2.8
1	C	261	ASN	2.8
1	C	273	LYS	2.8
1	D	263	THR	2.8
1	D	265	GLU	2.8
1	D	110	LYS	2.8
1	A	261	ASN	2.7
1	A	88[A]	ARG	2.6
1	D	166	LEU	2.6
1	C	89[A]	GLY	2.6
1	D	126	VAL	2.6
1	A	270	ALA	2.6
1	A	19	GLU	2.5
2	I	6	DG	2.5
1	D	143	ALA	2.4
1	B	265	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	112	PHE	2.4
1	D	123	ASP	2.4
1	C	269	GLU	2.4
1	B	204	VAL	2.3
1	D	108	ASP	2.3
1	C	260	LYS	2.3
1	D	125	LYS	2.3
1	A	142	THR	2.3
1	A	2	LYS	2.3
1	D	140	VAL	2.3
1	A	140	VAL	2.3
1	C	267	ALA	2.3
1	A	204	VAL	2.2
1	D	129	LEU	2.2
1	B	89[A]	GLY	2.2
1	C	259	ILE	2.2
1	D	165	LEU	2.2
1	D	109	ALA	2.2
1	D	270	ALA	2.2
1	A	206	ASP	2.2
1	C	272	LEU	2.1
1	B	257	ASN	2.1
1	A	143	ALA	2.1
1	A	259	ILE	2.0
1	A	29	SER	2.0
1	C	270	ALA	2.0
1	D	260	LYS	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, 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	GOL	A	302	6/6	0.93	0.15	40,47,53,54	0
5	GOL	D	301	6/6	0.94	0.18	38,44,55,55	0
5	GOL	C	301	6/6	0.95	0.12	36,38,39,40	0
5	GOL	A	301	6/6	0.96	0.17	42,46,50,50	0
6	MN	A	304	1/1	0.98	0.16	34,34,34,34	1
6	MN	C	303	1/1	0.99	0.09	33,33,33,33	1
6	MN	A	303	1/1	0.99	0.14	33,33,33,33	0
6	MN	C	302	1/1	0.99	0.13	28,28,28,28	0
6	MN	B	301	1/1	0.99	0.15	29,29,29,29	0
6	MN	B	302	1/1	0.99	0.09	37,37,37,37	1
6	MN	D	302	1/1	1.00	0.18	32,32,32,32	0
6	MN	D	303	1/1	1.00	0.15	40,40,40,40	1

6.5 Other polymers [i](#)

There are no such residues in this entry.