



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 2, 2017 – 08:10 PM EST

PDB ID : 5JX3
Title : Wild type D4 in orthorhombic space group
Authors : Schormann, N.; Chattopadhyay, D.
Deposited on : 2016-05-12
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

<http://wwpdb.org/validation/2016/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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20028442
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028442

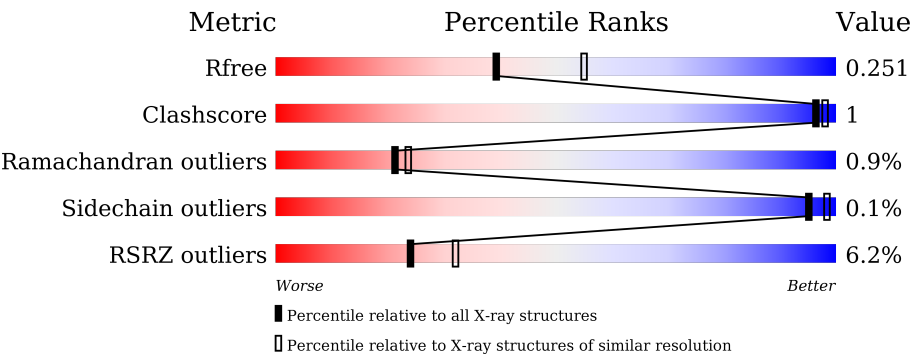
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	221	<div><div>2%</div><div>95%</div><div>5%</div><div>..</div></div>
1	B	221	<div><div>3%</div><div>97%</div><div>5%</div><div>..</div></div>
1	C	221	<div><div>10%</div><div>92%</div><div>5%</div><div>..</div></div>
1	D	221	<div><div>4%</div><div>96%</div><div>5%</div><div>..</div></div>
1	E	221	<div><div>5%</div><div>93%</div><div>5%</div><div>..</div></div>
1	F	221	<div><div>10%</div><div>96%</div><div>5%</div><div>..</div></div>

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Mol	Chain	Length	Quality of chain
1	G	221	
1	H	221	

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
2	GOL	B	302	-	-	-	X
2	GOL	D	301	-	-	-	X
2	GOL	D	303	-	-	-	X
2	GOL	E	301	-	-	-	X
2	GOL	F	301	-	-	-	X
2	GOL	G	301	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15051 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 Uracil-DNA glycosylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	218	Total	C	N	O	S	0	0	0
			1770	1147	294	323	6			
1	B	218	Total	C	N	O	S	0	1	0
			1776	1150	295	325	6			
1	C	217	Total	C	N	O	S	0	2	0
			1762	1141	292	323	6			
1	D	219	Total	C	N	O	S	0	2	0
			1795	1161	300	328	6			
1	E	218	Total	C	N	O	S	0	1	0
			1779	1152	296	325	6			
1	F	218	Total	C	N	O	S	0	0	0
			1770	1147	294	323	6			
1	G	218	Total	C	N	O	S	0	2	0
			1785	1155	297	327	6			
1	H	215	Total	C	N	O	S	0	0	0
			1720	1118	281	315	6			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P04303
A	-1	SER	-	expression tag	UNP P04303
A	0	HIS	-	expression tag	UNP P04303
A	17	ASN	ASP	see remark 999	UNP P04303
A	163	PHE	TYR	see remark 999	UNP P04303
B	-2	GLY	-	expression tag	UNP P04303
B	-1	SER	-	expression tag	UNP P04303
B	0	HIS	-	expression tag	UNP P04303
B	17	ASN	ASP	see remark 999	UNP P04303
B	163	PHE	TYR	see remark 999	UNP P04303
C	-2	GLY	-	expression tag	UNP P04303
C	-1	SER	-	expression tag	UNP P04303
C	0	HIS	-	expression tag	UNP P04303

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Chain	Residue	Modelled	Actual	Comment	Reference
C	17	ASN	ASP	see remark 999	UNP P04303
C	163	PHE	TYR	see remark 999	UNP P04303
D	-2	GLY	-	expression tag	UNP P04303
D	-1	SER	-	expression tag	UNP P04303
D	0	HIS	-	expression tag	UNP P04303
D	17	ASN	ASP	see remark 999	UNP P04303
D	163	PHE	TYR	see remark 999	UNP P04303
E	-2	GLY	-	expression tag	UNP P04303
E	-1	SER	-	expression tag	UNP P04303
E	0	HIS	-	expression tag	UNP P04303
E	17	ASN	ASP	see remark 999	UNP P04303
E	163	PHE	TYR	see remark 999	UNP P04303
F	-2	GLY	-	expression tag	UNP P04303
F	-1	SER	-	expression tag	UNP P04303
F	0	HIS	-	expression tag	UNP P04303
F	17	ASN	ASP	see remark 999	UNP P04303
F	163	PHE	TYR	see remark 999	UNP P04303
G	-2	GLY	-	expression tag	UNP P04303
G	-1	SER	-	expression tag	UNP P04303
G	0	HIS	-	expression tag	UNP P04303
G	17	ASN	ASP	see remark 999	UNP P04303
G	163	PHE	TYR	see remark 999	UNP P04303
H	-2	GLY	-	expression tag	UNP P04303
H	-1	SER	-	expression tag	UNP P04303
H	0	HIS	-	expression tag	UNP P04303
H	17	ASN	ASP	see remark 999	UNP P04303
H	163	PHE	TYR	see remark 999	UNP P04303

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		
2	G	1	Total	C	O	0	0
			6	3	3		

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

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	1	Total	Cl	0	0
			1	1		
3	G	1	Total	Cl	0	0
			1	1		
3	D	1	Total	Cl	0	0
			1	1		
3	F	1	Total	Cl	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	168	Total	O	0	0
			168	168		
4	B	107	Total	O	0	0
			107	107		
4	C	60	Total	O	0	0
			60	60		
4	D	127	Total	O	0	0
			127	127		
4	E	130	Total	O	0	0
			130	130		
4	F	60	Total	O	0	0
			60	60		
4	G	120	Total	O	0	0
			120	120		
4	H	28	Total	O	0	0
			28	28		

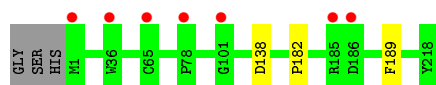
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

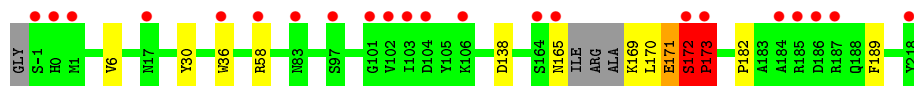
- Molecule 1: Uracil-DNA glycosylase



- Molecule 1: Uracil-DNA glycosylase



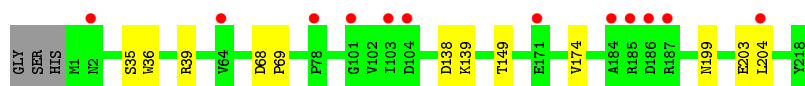
- Molecule 1: Uracil-DNA glycosylase



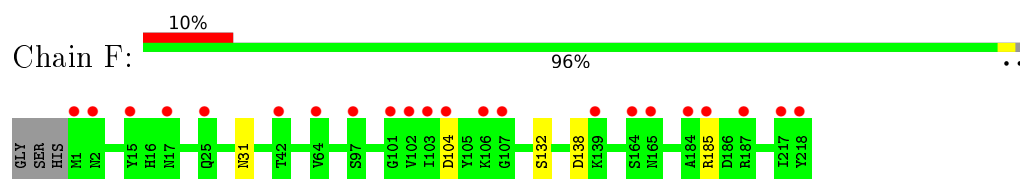
- Molecule 1: Uracil-DNA glycosylase



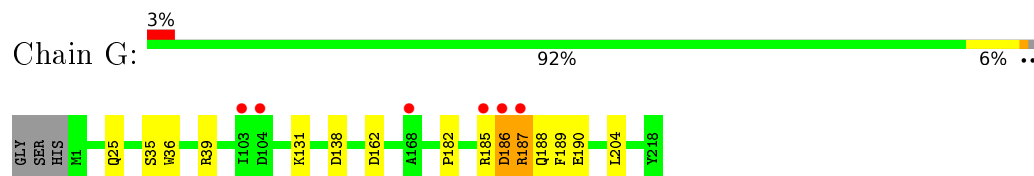
- Molecule 1: Uracil-DNA glycosylase



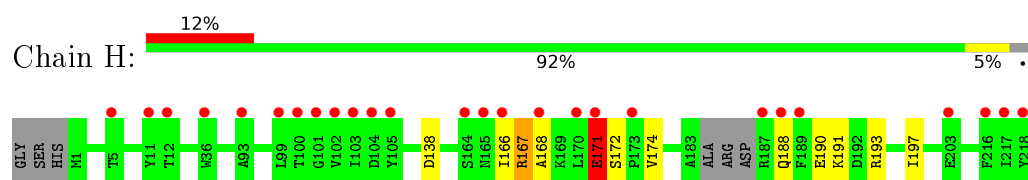
- Molecule 1: Uracil-DNA glycosylase



- Molecule 1: Uracil-DNA glycosylase



- Molecule 1: Uracil-DNA glycosylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	117.77Å 134.06Å 139.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.24 – 2.30 32.24 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (32.24-2.30) 100.0 (32.24-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.17 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, R_{free}	0.215 , 0.249 0.218 , 0.251	Depositor DCC
R_{free} test set	4905 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	28.6	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.011 for -h,l,k	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	15051	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.91% 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, CL

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	0.38	0/1819	0.60	0/2474
1	B	0.39	0/1825	0.59	0/2482
1	C	0.42	0/1811	0.68	4/2464 (0.2%)
1	D	0.39	0/1845	0.60	0/2509
1	E	0.39	0/1828	0.62	1/2486 (0.0%)
1	F	0.40	0/1819	0.59	0/2474
1	G	0.41	0/1834	0.62	1/2494 (0.0%)
1	H	0.41	0/1767	0.60	1/2406 (0.0%)
All	All	0.40	0/14548	0.61	7/19789 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	172	SER	C-N-CD	-8.93	100.95	120.60
1	C	170	LEU	N-CA-C	8.54	134.05	111.00
1	G	187	ARG	N-CA-C	-6.24	94.14	111.00
1	C	171	GLU	N-CA-C	5.71	126.41	111.00
1	H	190	GLU	N-CA-C	-5.35	96.55	111.00
1	E	204	LEU	CA-CB-CG	5.32	127.54	115.30
1	C	173	PRO	N-CA-C	-5.03	99.01	112.10

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	1770	0	1768	4	0
1	B	1776	0	1772	1	0
1	C	1762	0	1736	8	0
1	D	1795	0	1786	6	0
1	E	1779	0	1775	8	0
1	F	1770	0	1768	2	0
1	G	1785	0	1779	10	0
1	H	1720	0	1706	8	0
2	A	18	0	24	0	0
2	B	12	0	16	0	0
2	C	6	0	8	0	0
2	D	18	0	24	0	0
2	E	12	0	16	0	0
2	F	12	0	16	0	0
2	G	6	0	8	0	0
2	H	6	0	8	0	0
3	D	1	0	0	0	0
3	F	1	0	0	1	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	168	0	0	0	0
4	B	107	0	0	0	0
4	C	60	0	0	0	0
4	D	127	0	0	0	0
4	E	130	0	0	1	0
4	F	60	0	0	0	0
4	G	120	0	0	0	0
4	H	28	0	0	0	0
All	All	15051	0	14210	41	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 1.

All (41) 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:H:168:ALA:HA	1:H:171:GLU:OE2	1.64	0.97
1:C:172:SER:CB	1:C:173:PRO:HA	2.05	0.86
1:C:172:SER:CB	1:C:173:PRO:CA	2.70	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:188:GLN:O	1:H:191:LYS:NZ	2.20	0.67
1:E:199:ASN:O	1:E:203:GLU:HG2	1.95	0.66
1:G:185:ARG:O	1:G:186:ASP:HB2	1.96	0.66
1:E:199:ASN:O	1:E:203:GLU:CG	2.43	0.66
1:H:188:GLN:O	1:H:191:LYS:HG3	1.98	0.64
1:E:36:TRP:O	1:E:39:ARG:HD3	2.05	0.57
1:D:158:LEU:HD23	1:D:182:PRO:CG	2.35	0.55
1:H:166:ILE:O	1:H:167:ARG:CB	2.55	0.55
1:H:168:ALA:CA	1:H:171:GLU:OE2	2.50	0.53
1:G:187:ARG:O	1:G:188:GLN:HB2	2.08	0.53
1:D:158:LEU:HD23	1:D:182:PRO:CD	2.39	0.51
1:E:35:SER:HB2	1:G:35:SER:HB2	1.93	0.50
1:G:36:TRP:O	1:G:39:ARG:HD3	2.11	0.49
1:D:158:LEU:HD23	1:D:182:PRO:HD3	1.95	0.48
1:B:182:PRO:HA	1:B:189:PHE:CG	2.50	0.47
1:E:199:ASN:O	1:E:203:GLU:HG3	2.14	0.47
1:C:6:VAL:HG21	1:C:30:TYR:HD2	1.80	0.47
1:A:188:GLN:NE2	1:D:188:GLN:OE1	2.47	0.46
1:G:188:GLN:OE1	1:G:188:GLN:HA	2.15	0.45
1:G:187:ARG:HD2	1:G:190:GLU:OE1	2.16	0.45
1:G:182:PRO:HA	1:G:189:PHE:CG	2.52	0.44
1:A:149:THR:O	1:A:174:VAL:HG21	2.18	0.43
1:A:98:ARG:HD2	1:C:58:ARG:NE	2.32	0.43
1:G:204:LEU:HD11	1:H:197:ILE:HG21	2.01	0.43
1:G:131:LYS:NZ	1:G:162:ASP:OD1	2.50	0.42
1:H:172:SER:OG	1:H:174:VAL:HG12	2.19	0.42
1:E:149:THR:O	1:E:174:VAL:HG21	2.20	0.42
1:D:68:ASP:HB2	1:D:69:PRO:CD	2.50	0.42
1:G:25[A]:GLN:HA	1:G:25[A]:GLN:OE1	2.19	0.42
1:C:165:ASN:CB	1:C:169:LYS:CB	2.98	0.42
1:C:36:TRP:HZ2	1:F:132:SER:O	2.02	0.42
1:C:182:PRO:HA	1:C:189:PHE:CG	2.55	0.41
1:E:68:ASP:HB2	1:E:69:PRO:CD	2.50	0.41
1:A:182:PRO:HA	1:A:189:PHE:CG	2.55	0.41
1:H:193:ARG:HG3	1:H:197:ILE:HD11	2.02	0.41
1:F:31:ASN:HA	3:F:303:CL:CL	2.58	0.41
1:E:139:LYS:NZ	4:E:405:HOH:O	2.54	0.41
1:C:169:LYS:N	1:D:171:GLU:HA	2.35	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	216/221 (98%)	212 (98%)	3 (1%)	1 (0%)	34	41
1	B	217/221 (98%)	212 (98%)	4 (2%)	1 (0%)	34	41
1	C	215/221 (97%)	205 (95%)	6 (3%)	4 (2%)	10	8
1	D	219/221 (99%)	215 (98%)	3 (1%)	1 (0%)	34	41
1	E	217/221 (98%)	212 (98%)	4 (2%)	1 (0%)	34	41
1	F	216/221 (98%)	208 (96%)	5 (2%)	3 (1%)	14	13
1	G	218/221 (99%)	212 (97%)	4 (2%)	2 (1%)	21	24
1	H	211/221 (96%)	205 (97%)	3 (1%)	3 (1%)	14	13
All	All	1729/1768 (98%)	1681 (97%)	32 (2%)	16 (1%)	21	24

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	138	ASP
1	C	171	GLU
1	C	172	SER
1	E	138	ASP
1	G	138	ASP
1	H	167	ARG
1	H	171	GLU
1	B	138	ASP
1	F	138	ASP
1	D	138	ASP
1	H	138	ASP
1	C	138	ASP
1	C	173	PRO
1	F	185	ARG
1	G	186	ASP
1	F	104	ASP

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	199/201 (99%)	199 (100%)	0	100	100
1	B	200/201 (100%)	200 (100%)	0	100	100
1	C	197/201 (98%)	197 (100%)	0	100	100
1	D	202/201 (100%)	202 (100%)	0	100	100
1	E	200/201 (100%)	200 (100%)	0	100	100
1	F	199/201 (99%)	199 (100%)	0	100	100
1	G	201/201 (100%)	201 (100%)	0	100	100
1	H	192/201 (96%)	191 (100%)	1 (0%)	92	97
All	All	1590/1608 (99%)	1589 (100%)	1 (0%)	95	98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	171	GLU

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	17	ASN

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

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 19 ligands modelled in this entry, 4 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	$\# Z > 2$
2	GOL	A	401	-	5,5,5	0.26	0	5,5,5	0.57	0
2	GOL	A	402	-	5,5,5	0.27	0	5,5,5	0.40	0
2	GOL	A	403	-	5,5,5	0.46	0	5,5,5	0.61	0
2	GOL	B	301	-	5,5,5	0.26	0	5,5,5	0.42	0
2	GOL	B	302	-	5,5,5	0.36	0	5,5,5	0.51	0
2	GOL	C	301	-	5,5,5	0.27	0	5,5,5	0.22	0
2	GOL	D	301	-	5,5,5	0.25	0	5,5,5	0.21	0
2	GOL	D	302	-	5,5,5	0.28	0	5,5,5	0.38	0
2	GOL	D	303	-	5,5,5	0.30	0	5,5,5	0.40	0
2	GOL	E	301	-	5,5,5	0.32	0	5,5,5	0.53	0
2	GOL	E	302	-	5,5,5	0.34	0	5,5,5	0.27	0
2	GOL	F	301	-	5,5,5	0.30	0	5,5,5	0.28	0
2	GOL	F	302	-	5,5,5	0.24	0	5,5,5	0.28	0
2	GOL	G	301	-	5,5,5	0.40	0	5,5,5	0.42	0
2	GOL	H	301	-	5,5,5	0.32	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
2	GOL	A	401	-	-	0/4/4/4	0/0/0/0
2	GOL	A	402	-	-	0/4/4/4	0/0/0/0
2	GOL	A	403	-	-	0/4/4/4	0/0/0/0
2	GOL	B	301	-	-	0/4/4/4	0/0/0/0
2	GOL	B	302	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	C	301	-	-	0/4/4/4	0/0/0/0
2	GOL	D	301	-	-	0/4/4/4	0/0/0/0
2	GOL	D	302	-	-	0/4/4/4	0/0/0/0
2	GOL	D	303	-	-	0/4/4/4	0/0/0/0
2	GOL	E	301	-	-	0/4/4/4	0/0/0/0
2	GOL	E	302	-	-	0/4/4/4	0/0/0/0
2	GOL	F	301	-	-	0/4/4/4	0/0/0/0
2	GOL	F	302	-	-	0/4/4/4	0/0/0/0
2	GOL	G	301	-	-	0/4/4/4	0/0/0/0
2	GOL	H	301	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	218/221 (98%)	-0.06	5 (2%) 64 72	13, 23, 41, 61	0
1	B	218/221 (98%)	0.16	7 (3%) 51 60	18, 31, 48, 68	0
1	C	217/221 (98%)	0.71	22 (10%) 9 13	24, 38, 63, 82	0
1	D	219/221 (99%)	0.16	8 (3%) 45 54	15, 26, 48, 71	0
1	E	218/221 (98%)	0.11	12 (5%) 29 37	15, 25, 51, 75	0
1	F	218/221 (98%)	0.65	22 (10%) 9 13	24, 40, 60, 84	0
1	G	218/221 (98%)	0.11	6 (2%) 56 66	15, 26, 53, 69	0
1	H	215/221 (97%)	0.84	26 (12%) 6 9	28, 47, 69, 80	0
All	All	1741/1768 (98%)	0.34	108 (6%) 24 32	13, 32, 59, 84	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	103	ILE	7.6
1	C	-1	SER	6.7
1	C	101	GLY	6.3
1	E	103	ILE	6.1
1	C	0	HIS	5.7
1	H	104	ASP	5.6
1	H	103	ILE	5.5
1	C	1	MET	5.1
1	C	102	VAL	5.0
1	C	172	SER	4.9
1	C	185	ARG	4.8
1	A	187	ARG	4.7
1	H	218	TYR	4.7
1	D	103	ILE	4.6
1	D	185	ARG	4.5
1	F	185	ARG	4.4

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Mol	Chain	Res	Type	RSRZ
1	F	101	GLY	4.3
1	F	102	VAL	4.3
1	G	103	ILE	4.3
1	C	218	TYR	4.3
1	F	2	ASN	4.1
1	F	218	TYR	4.1
1	F	107	GLY	4.1
1	B	186	ASP	4.0
1	F	106	LYS	4.0
1	C	186	ASP	3.8
1	H	102	VAL	3.7
1	H	187	ARG	3.7
1	H	36	TRP	3.5
1	H	105	TYR	3.5
1	H	93	ALA	3.4
1	H	164	SER	3.4
1	G	104	ASP	3.3
1	H	168	ALA	3.2
1	H	166	ILE	3.2
1	A	186	ASP	3.2
1	C	104	ASP	3.2
1	E	101	GLY	3.2
1	C	36	TRP	3.1
1	B	185	ARG	3.1
1	H	165	ASN	3.1
1	D	1	MET	3.1
1	F	184	ALA	3.0
1	H	101	GLY	3.0
1	H	216	PHE	2.9
1	E	187	ARG	2.9
1	A	185	ARG	2.9
1	C	165	ASN	2.9
1	F	1	MET	2.9
1	G	168	ALA	2.9
1	F	187	ARG	2.8
1	C	184	ALA	2.8
1	B	36	TRP	2.8
1	H	171	GLU	2.8
1	H	99	LEU	2.7
1	H	189	PHE	2.7
1	F	164	SER	2.7
1	E	184	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	204	LEU	2.7
1	H	100	THR	2.7
1	C	106	LYS	2.6
1	D	64	VAL	2.6
1	C	164	SER	2.6
1	F	217	ILE	2.6
1	D	0	HIS	2.5
1	C	97	SER	2.5
1	F	97	SER	2.5
1	E	185	ARG	2.5
1	A	184	ALA	2.5
1	F	64	VAL	2.4
1	C	83	ASN	2.4
1	H	5	THR	2.4
1	C	58	ARG	2.4
1	H	12	THR	2.4
1	E	171	GLU	2.4
1	B	1	MET	2.4
1	F	17	ASN	2.4
1	B	78	PRO	2.4
1	G	187	ARG	2.4
1	C	173	PRO	2.4
1	H	11	TYR	2.3
1	H	188	GLN	2.3
1	E	104	ASP	2.3
1	B	65	CYS	2.3
1	F	15	TYR	2.3
1	D	187	ARG	2.3
1	F	104	ASP	2.3
1	G	186	ASP	2.3
1	H	170	LEU	2.3
1	A	103	ILE	2.2
1	F	25	GLN	2.2
1	F	165	ASN	2.2
1	C	187	ARG	2.2
1	E	64	VAL	2.2
1	D	164	SER	2.2
1	E	78	PRO	2.1
1	G	185	ARG	2.1
1	E	2	ASN	2.1
1	H	173	PRO	2.1
1	E	186	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	203	GLU	2.1
1	B	101	GLY	2.1
1	C	17	ASN	2.0
1	F	42	THR	2.0
1	F	139	LYS	2.0
1	F	103	ILE	2.0
1	H	217	ILE	2.0
1	D	63	CYS	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	GOL	F	301	6/6	0.74	0.30	4.48	55,57,57,58	0
2	GOL	G	301	6/6	0.84	0.25	3.85	29,32,33,35	0
2	GOL	D	303	6/6	0.74	0.28	3.41	39,41,41,41	0
2	GOL	D	301	6/6	0.82	0.21	2.47	30,33,34,35	0
2	GOL	E	301	6/6	0.78	0.27	2.34	25,28,29,30	0
2	GOL	B	302	6/6	0.67	0.21	2.15	47,48,50,50	0
2	GOL	H	301	6/6	0.83	0.22	1.85	41,44,45,46	0
2	GOL	D	302	6/6	0.91	0.22	1.69	24,27,28,29	0
2	GOL	A	402	6/6	0.90	0.21	0.94	23,24,25,26	0
2	GOL	A	401	6/6	0.93	0.15	0.89	31,31,32,32	0
2	GOL	A	403	6/6	0.80	0.17	0.78	27,28,29,29	0
2	GOL	B	301	6/6	0.89	0.19	0.54	39,40,41,41	0
2	GOL	F	302	6/6	0.73	0.16	-0.35	59,61,61,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	GOL	C	301	6/6	0.92	0.15	-0.41	36,37,38,39	0
3	CL	G	302	1/1	0.97	0.09	-1.05	47,47,47,47	0
3	CL	F	303	1/1	0.91	0.13	-1.16	52,52,52,52	0
2	GOL	E	302	6/6	0.80	0.16	-	69,70,70,71	0
3	CL	H	302	1/1	0.98	0.07	-	44,44,44,44	0
3	CL	D	304	1/1	0.97	0.17	-	50,50,50,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.