



Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 10:18 am BST

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

<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

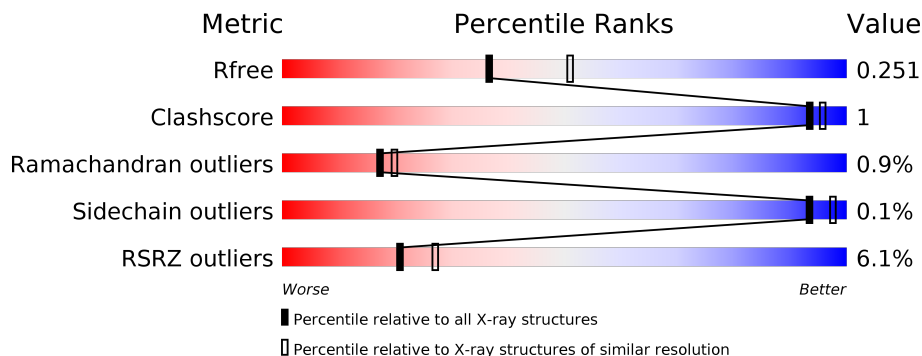
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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.



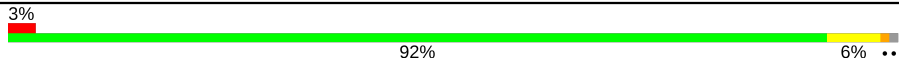
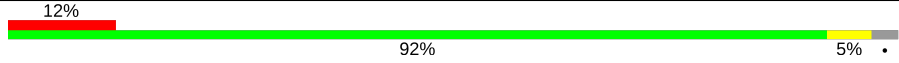
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 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	221	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 95%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">2% 95% 5% ..</p>
1	B	221	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 97%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">3% 97% ..</p>
1	C	221	<div style="display: flex; align-items: center;"> <div style="width: 10%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 92%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">10% 92% 5% ..</p>
1	D	221	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 96%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">4% 96% ..</p>
1	E	221	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 93%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">5% 93% 5% .</p>
1	F	221	<div style="display: flex; align-items: center;"> <div style="width: 10%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 96%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">10% 96% ..</p>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	221	 <p>3% 92% 6% ••</p>
1	H	221	 <p>12% 92% 5% •</p>

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

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

Continued on next page...

Continued from previous page...

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		

Continued on next page...

Continued from previous page...

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		

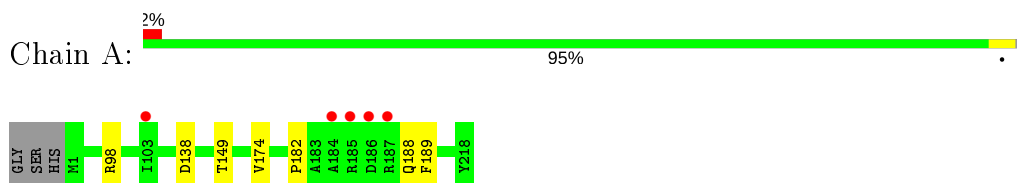
- Molecule 4 is water.

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		

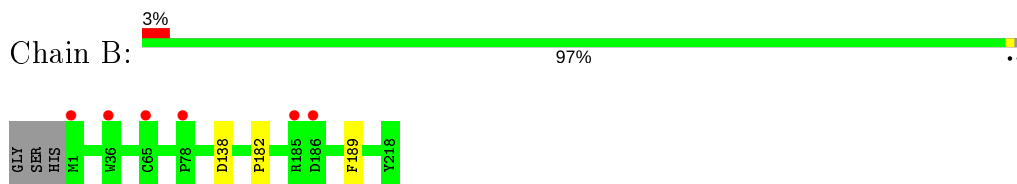
3 Residue-property plots [i](#)

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

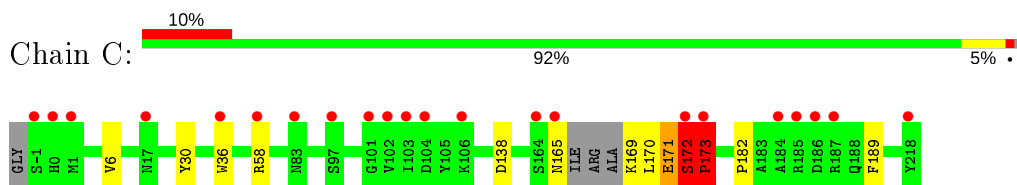
- Molecule 1: Uracil-DNA glycosylase



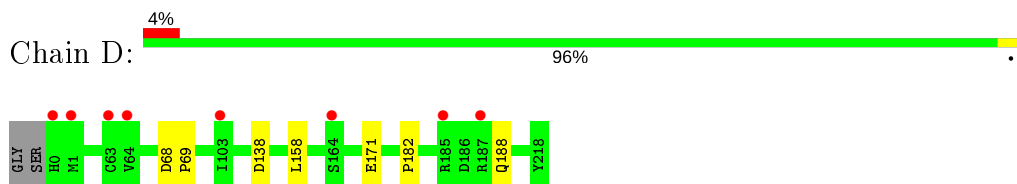
- Molecule 1: Uracil-DNA glycosylase



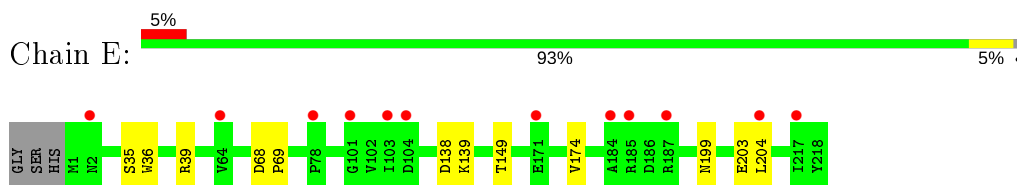
- Molecule 1: Uracil-DNA glycosylase



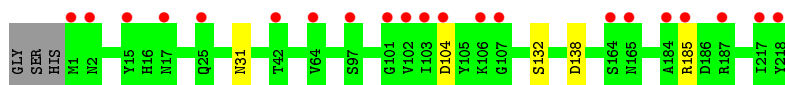
- Molecule 1: Uracil-DNA glycosylase



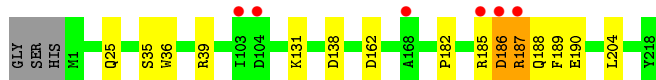
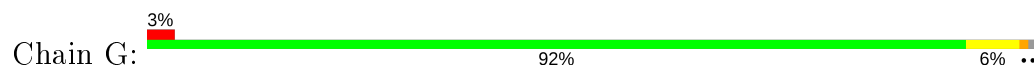
- Molecule 1: Uracil-DNA glycosylase



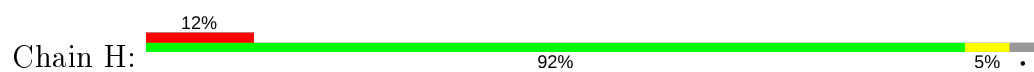
- Molecule 1: Uracil-DNA glycosylase



- 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)	Xtrriage
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 (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	28.6	Xtrriage
Anisotropy	0.032	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.011 for -h,l,k	Xtrriage
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

Xtrriage'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

Continued on next page...

Continued from previous page...

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 [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	216/221 (98%)	212 (98%)	3 (1%)	1 (0%)	29	35
1	B	217/221 (98%)	212 (98%)	4 (2%)	1 (0%)	29	35
1	C	215/221 (97%)	205 (95%)	6 (3%)	4 (2%)	8	7
1	D	219/221 (99%)	215 (98%)	3 (1%)	1 (0%)	29	35
1	E	217/221 (98%)	212 (98%)	4 (2%)	1 (0%)	29	35
1	F	216/221 (98%)	208 (96%)	5 (2%)	3 (1%)	11	11
1	G	218/221 (99%)	212 (97%)	4 (2%)	2 (1%)	17	20
1	H	211/221 (96%)	205 (97%)	3 (1%)	3 (1%)	11	11
All	All	1729/1768 (98%)	1681 (97%)	32 (2%)	16 (1%)	17	20

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%)	88	95
All	All	1590/1608 (99%)	1589 (100%)	1 (0%)	93	97

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	H	301	-	5,5,5	0.37	0	5,5,5	0.56	0
2	GOL	E	302	-	5,5,5	0.39	0	5,5,5	0.25	0
2	GOL	C	301	-	5,5,5	0.31	0	5,5,5	0.18	0
2	GOL	B	301	-	5,5,5	0.30	0	5,5,5	0.41	0
2	GOL	G	301	-	5,5,5	0.44	0	5,5,5	0.42	0
2	GOL	E	301	-	5,5,5	0.37	0	5,5,5	0.55	0
2	GOL	A	401	-	5,5,5	0.30	0	5,5,5	0.57	0
2	GOL	F	301	-	5,5,5	0.34	0	5,5,5	0.26	0
2	GOL	B	302	-	5,5,5	0.41	0	5,5,5	0.50	0
2	GOL	D	302	-	5,5,5	0.32	0	5,5,5	0.40	0
2	GOL	A	402	-	5,5,5	0.29	0	5,5,5	0.43	0
2	GOL	F	302	-	5,5,5	0.28	0	5,5,5	0.30	0
2	GOL	D	301	-	5,5,5	0.29	0	5,5,5	0.22	0
2	GOL	D	303	-	5,5,5	0.36	0	5,5,5	0.39	0
2	GOL	A	403	-	5,5,5	0.51	0	5,5,5	0.61	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	H	301	-	-	2/4/4/4	-
2	GOL	E	302	-	-	2/4/4/4	-
2	GOL	C	301	-	-	0/4/4/4	-
2	GOL	B	301	-	-	4/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	G	301	-	-	0/4/4/4	-
2	GOL	E	301	-	-	2/4/4/4	-
2	GOL	A	401	-	-	3/4/4/4	-
2	GOL	F	301	-	-	4/4/4/4	-
2	GOL	B	302	-	-	0/4/4/4	-
2	GOL	D	302	-	-	2/4/4/4	-
2	GOL	A	402	-	-	2/4/4/4	-
2	GOL	F	302	-	-	2/4/4/4	-
2	GOL	D	301	-	-	0/4/4/4	-
2	GOL	D	303	-	-	2/4/4/4	-
2	GOL	A	403	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	301	GOL	O1-C1-C2-C3
2	E	302	GOL	O1-C1-C2-O2
2	E	302	GOL	O1-C1-C2-C3
2	A	401	GOL	C1-C2-C3-O3
2	F	301	GOL	C1-C2-C3-O3
2	F	301	GOL	O2-C2-C3-O3
2	D	302	GOL	O1-C1-C2-C3
2	F	302	GOL	O1-C1-C2-C3
2	D	303	GOL	C1-C2-C3-O3
2	D	303	GOL	O2-C2-C3-O3
2	B	301	GOL	O1-C1-C2-C3
2	B	301	GOL	C1-C2-C3-O3
2	E	301	GOL	O1-C1-C2-C3
2	F	301	GOL	O1-C1-C2-C3
2	A	402	GOL	C1-C2-C3-O3
2	H	301	GOL	O1-C1-C2-O2
2	B	301	GOL	O1-C1-C2-O2
2	D	302	GOL	O1-C1-C2-O2
2	F	302	GOL	O1-C1-C2-O2
2	E	301	GOL	O1-C1-C2-O2
2	A	401	GOL	O2-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	301	GOL	O2-C2-C3-O3
2	A	403	GOL	O1-C1-C2-O2
2	A	402	GOL	O2-C2-C3-O3
2	A	401	GOL	O1-C1-C2-C3
2	F	301	GOL	O1-C1-C2-O2
2	A	403	GOL	O1-C1-C2-C3

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%) 60 67	13, 23, 41, 61	0
1	B	218/221 (98%)	0.16	6 (2%) 53 60	18, 31, 48, 68	0
1	C	217/221 (98%)	0.71	22 (10%) 7 9	24, 38, 63, 82	0
1	D	219/221 (99%)	0.15	8 (3%) 41 48	15, 26, 48, 71	0
1	E	218/221 (98%)	0.11	12 (5%) 25 31	15, 25, 51, 75	0
1	F	218/221 (98%)	0.64	21 (9%) 8 10	24, 40, 60, 84	0
1	G	218/221 (98%)	0.11	6 (2%) 53 60	15, 26, 53, 69	0
1	H	215/221 (97%)	0.84	26 (12%) 4 6	28, 47, 69, 80	0
All	All	1741/1768 (98%)	0.33	106 (6%) 21 27	13, 32, 59, 84	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	103	ILE	7.6
1	C	-1	SER	6.9
1	C	101	GLY	6.6
1	E	103	ILE	6.2
1	C	0	HIS	5.7
1	H	103	ILE	5.5
1	H	104	ASP	5.5
1	C	172	SER	5.1
1	C	102	VAL	5.1
1	C	1	MET	5.0
1	D	103	ILE	4.7
1	A	187	ARG	4.7
1	C	185	ARG	4.7
1	D	185	ARG	4.6
1	H	218	TYR	4.5
1	F	102	VAL	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	101	GLY	4.4
1	F	185	ARG	4.4
1	F	2	ASN	4.3
1	G	103	ILE	4.2
1	C	218	TYR	4.1
1	F	106	LYS	4.1
1	F	218	TYR	4.1
1	B	186	ASP	4.0
1	F	107	GLY	4.0
1	H	102	VAL	3.9
1	C	186	ASP	3.9
1	H	187	ARG	3.8
1	H	36	TRP	3.7
1	H	105	TYR	3.6
1	H	93	ALA	3.5
1	H	164	SER	3.4
1	E	101	GLY	3.3
1	H	166	ILE	3.3
1	H	101	GLY	3.2
1	G	104	ASP	3.2
1	H	168	ALA	3.2
1	C	104	ASP	3.2
1	B	185	ARG	3.1
1	C	36	TRP	3.1
1	H	165	ASN	3.1
1	D	1	MET	3.0
1	F	184	ALA	3.0
1	A	186	ASP	3.0
1	H	216	PHE	2.9
1	C	165	ASN	2.9
1	F	1	MET	2.9
1	C	184	ALA	2.8
1	G	168	ALA	2.8
1	E	187	ARG	2.8
1	H	100	THR	2.8
1	H	99	LEU	2.8
1	F	187	ARG	2.8
1	E	184	ALA	2.8
1	C	106	LYS	2.8
1	H	189	PHE	2.7
1	B	36	TRP	2.7
1	C	97	SER	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	185	ARG	2.7
1	E	204	LEU	2.7
1	C	164	SER	2.7
1	D	64	VAL	2.6
1	H	171	GLU	2.6
1	H	5	THR	2.6
1	E	185	ARG	2.5
1	F	97	SER	2.5
1	F	164	SER	2.5
1	C	83	ASN	2.5
1	F	64	VAL	2.5
1	F	217	ILE	2.5
1	B	1	MET	2.5
1	A	184	ALA	2.5
1	C	58	ARG	2.4
1	F	17	ASN	2.4
1	H	12	THR	2.4
1	D	0	HIS	2.4
1	E	104	ASP	2.4
1	E	171	GLU	2.4
1	H	188	GLN	2.4
1	C	173	PRO	2.4
1	F	15	TYR	2.4
1	B	78	PRO	2.4
1	G	186	ASP	2.3
1	B	65	CYS	2.3
1	F	104	ASP	2.3
1	H	11	TYR	2.3
1	D	187	ARG	2.3
1	G	187	ARG	2.3
1	A	103	ILE	2.2
1	H	170	LEU	2.2
1	F	25	GLN	2.2
1	C	187	ARG	2.2
1	D	164	SER	2.2
1	F	165	ASN	2.2
1	G	185	ARG	2.2
1	H	97	SER	2.1
1	E	64	VAL	2.1
1	E	78	PRO	2.1
1	F	103	ILE	2.1
1	F	42	THR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	173	PRO	2.1
1	H	203	GLU	2.0
1	D	63	CYS	2.0
1	E	2	ASN	2.0
1	C	17	ASN	2.0
1	E	217	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
2	GOL	B	302	6/6	0.67	0.20	47,48,50,50	0
2	GOL	F	302	6/6	0.73	0.16	59,61,61,62	0
2	GOL	F	301	6/6	0.74	0.30	55,57,57,58	0
2	GOL	D	303	6/6	0.74	0.28	39,41,41,41	0
2	GOL	E	301	6/6	0.78	0.27	25,28,29,30	0
2	GOL	E	302	6/6	0.80	0.16	69,70,70,71	0
2	GOL	A	403	6/6	0.80	0.17	27,28,29,29	0
2	GOL	D	301	6/6	0.82	0.20	30,33,34,35	0
2	GOL	H	301	6/6	0.83	0.21	41,44,45,46	0
2	GOL	G	301	6/6	0.84	0.25	29,32,33,35	0
2	GOL	B	301	6/6	0.88	0.19	39,40,41,41	0
2	GOL	A	402	6/6	0.90	0.21	23,24,25,26	0
2	GOL	D	302	6/6	0.91	0.22	24,27,28,29	0
3	CL	F	303	1/1	0.92	0.13	52,52,52,52	0
2	GOL	C	301	6/6	0.92	0.14	36,37,38,39	0
2	GOL	A	401	6/6	0.93	0.15	31,31,32,32	0
3	CL	D	304	1/1	0.97	0.17	50,50,50,50	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	CL	G	302	1/1	0.97	0.10	47,47,47,47	0
3	CL	H	302	1/1	0.98	0.07	44,44,44,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.