Full wwPDB X-ray Structure Validation Report ⓘ

Jan 7, 2024 – 07:41 pm GMT

PDB ID	:	5MR3
Title	:	Crystal structure of red abalone egg VERL repeat 2 with linker in complex with sperm lysin at 1.8 A resolution
Authors	:	Nishimura, K.; Raj, I.; Sadat Al-Hosseini, H.; De Sanctis, D.; Jovine, L.
Deposited on	:	2016-12-21
Resolution	:	1.80 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:

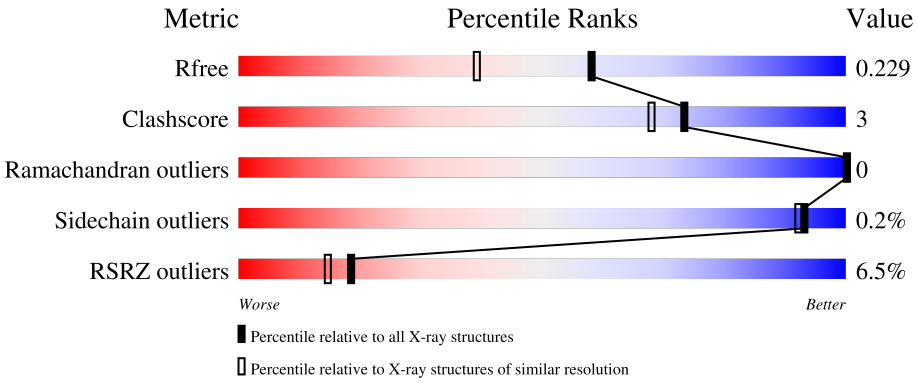
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 <=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	136	5% 85% 7% 8%
1	C	136	4% 89% 7%
1	E	136	3% 96%
1	G	136	3% 87% 8% 5%
2	B	134	7% 78% 10% 13%

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Mol	Chain	Length	Quality of chain
2	D	134	3% 72% 10% 18%
2	F	134	9% 71% 9% 20%
2	H	134	12% 75% 8% 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
3	GOL	D	902	-	-	-	X
3	GOL	H	902	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 16585 atoms, of which 8042 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 Egg-lysin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	125	Total	C	H	N	O	S	0	0	0
			2129	687	1079	185	171	7			
1	C	127	Total	C	H	N	O	S	0	0	0
			2166	698	1100	188	173	7			
1	E	133	Total	C	H	N	O	S	0	1	0
			2293	743	1158	201	184	7			
1	G	129	Total	C	H	N	O	S	0	0	0
			2196	708	1114	190	177	7			

- Molecule 2 is a protein called Vitelline envelope sperm lysin receptor.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	117	Total	C	H	N	O	S	0	0	0
			1810	588	893	149	170	10			
2	D	110	Total	C	H	N	O	S	0	0	0
			1698	552	835	140	161	10			
2	F	107	Total	C	H	N	O	S	0	0	0
			1670	543	824	138	155	10			
2	H	111	Total	C	H	N	O	S	0	0	0
			1733	561	859	143	160	10			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	173	GLU	-	expression tag	UNP Q8WR62
B	174	THR	-	expression tag	UNP Q8WR62
B	175	GLY	-	expression tag	UNP Q8WR62
B	293	ALA	SER	engineered mutation	UNP Q8WR62
B	296	ALA	SER	engineered mutation	UNP Q8WR62
B	297	ALA	SER	engineered mutation	UNP Q8WR62
B	299	LEU	-	expression tag	UNP Q8WR62
B	300	GLU	-	expression tag	UNP Q8WR62

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Chain	Residue	Modelled	Actual	Comment	Reference
B	301	HIS	-	expression tag	UNP Q8WR62
B	302	HIS	-	expression tag	UNP Q8WR62
B	303	HIS	-	expression tag	UNP Q8WR62
B	304	HIS	-	expression tag	UNP Q8WR62
B	305	HIS	-	expression tag	UNP Q8WR62
B	306	HIS	-	expression tag	UNP Q8WR62
D	173	GLU	-	expression tag	UNP Q8WR62
D	174	THR	-	expression tag	UNP Q8WR62
D	175	GLY	-	expression tag	UNP Q8WR62
D	293	ALA	SER	engineered mutation	UNP Q8WR62
D	296	ALA	SER	engineered mutation	UNP Q8WR62
D	297	ALA	SER	engineered mutation	UNP Q8WR62
D	299	LEU	-	expression tag	UNP Q8WR62
D	300	GLU	-	expression tag	UNP Q8WR62
D	301	HIS	-	expression tag	UNP Q8WR62
D	302	HIS	-	expression tag	UNP Q8WR62
D	303	HIS	-	expression tag	UNP Q8WR62
D	304	HIS	-	expression tag	UNP Q8WR62
D	305	HIS	-	expression tag	UNP Q8WR62
D	306	HIS	-	expression tag	UNP Q8WR62
F	173	GLU	-	expression tag	UNP Q8WR62
F	174	THR	-	expression tag	UNP Q8WR62
F	175	GLY	-	expression tag	UNP Q8WR62
F	293	ALA	SER	engineered mutation	UNP Q8WR62
F	296	ALA	SER	engineered mutation	UNP Q8WR62
F	297	ALA	SER	engineered mutation	UNP Q8WR62
F	299	LEU	-	expression tag	UNP Q8WR62
F	300	GLU	-	expression tag	UNP Q8WR62
F	301	HIS	-	expression tag	UNP Q8WR62
F	302	HIS	-	expression tag	UNP Q8WR62
F	303	HIS	-	expression tag	UNP Q8WR62
F	304	HIS	-	expression tag	UNP Q8WR62
F	305	HIS	-	expression tag	UNP Q8WR62
F	306	HIS	-	expression tag	UNP Q8WR62
H	173	GLU	-	expression tag	UNP Q8WR62
H	174	THR	-	expression tag	UNP Q8WR62
H	175	GLY	-	expression tag	UNP Q8WR62
H	293	ALA	SER	engineered mutation	UNP Q8WR62
H	296	ALA	SER	engineered mutation	UNP Q8WR62
H	297	ALA	SER	engineered mutation	UNP Q8WR62
H	299	LEU	-	expression tag	UNP Q8WR62
H	300	GLU	-	expression tag	UNP Q8WR62

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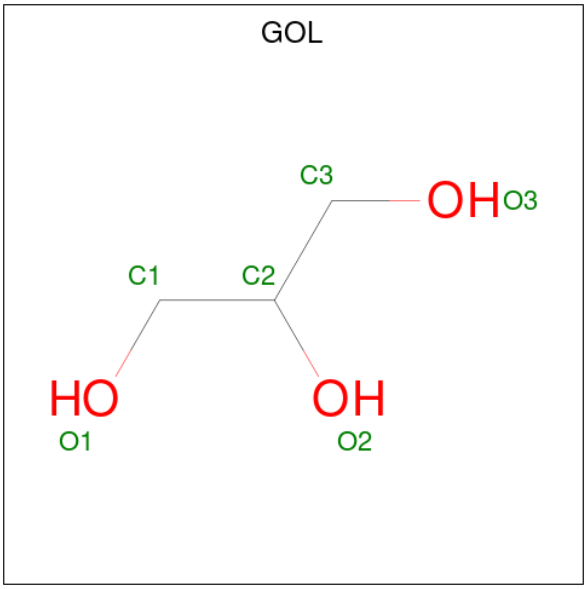
Chain	Residue	Modelled	Actual	Comment	Reference
H	301	HIS	-	expression tag	UNP Q8WR62
H	302	HIS	-	expression tag	UNP Q8WR62
H	303	HIS	-	expression tag	UNP Q8WR62
H	304	HIS	-	expression tag	UNP Q8WR62
H	305	HIS	-	expression tag	UNP Q8WR62
H	306	HIS	-	expression tag	UNP Q8WR62

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			14	3	8	3		
3	B	1	Total	C	H	O	0	0
			14	3	8	3		
3	B	1	Total	C	H	O	0	0
			14	3	8	3		
3	B	1	Total	C	H	O	0	0
			14	3	8	3		
3	C	1	Total	C	H	O	0	0
			14	3	8	3		
3	D	1	Total	C	H	O	0	0
			14	3	8	3		
3	D	1	Total	C	H	O	0	0
			14	3	8	3		
3	D	1	Total	C	H	O	0	0
			14	3	8	3		

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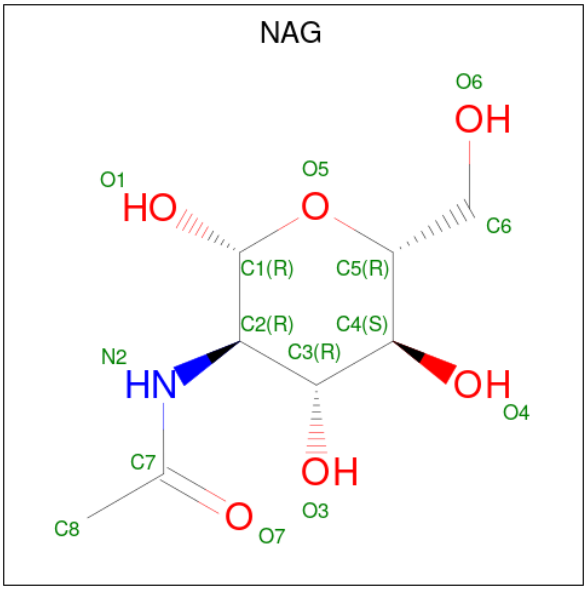
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	1	Total C H O 14 3 8 3	0	0
3	E	1	Total C H O 14 3 8 3	0	0
3	H	1	Total C H O 14 3 8 3	0	0
3	H	1	Total C H O 14 3 8 3	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Cl 1 1	0	0
4	F	1	Total Cl 1 1	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C H N O 28 8 14 1 5	0	0
5	D	1	Total C H N O 28 8 14 1 5	0	0
5	F	1	Total C H N O 28 8 14 1 5	0	0

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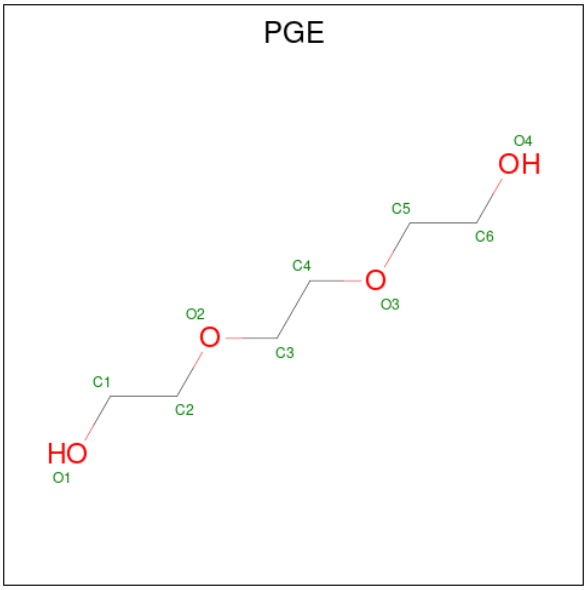
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	H	1	Total	C	H	N	O	0	0
			28	8	14	1	5		

- Molecule 6 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	G	1	Total	C	H	O		0	0
			24	6	14	4			
6	G	1	Total	C	H	O		0	0
			24	6	14	4			

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	70	Total	O	0	0
			70	70		
7	B	79	Total	O	0	0
			79	79		
7	C	57	Total	O	0	0
			57	57		
7	D	61	Total	O	0	0
			61	61		
7	E	94	Total	O	0	1
			95	95		
7	F	69	Total	O	0	0
			69	69		

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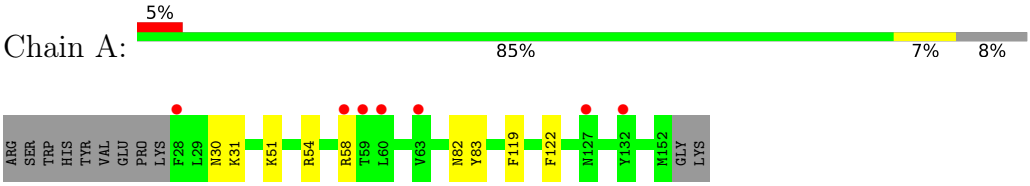
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	G	76	Total O 76 76	0	0
7	H	53	Total O 53 53	0	0

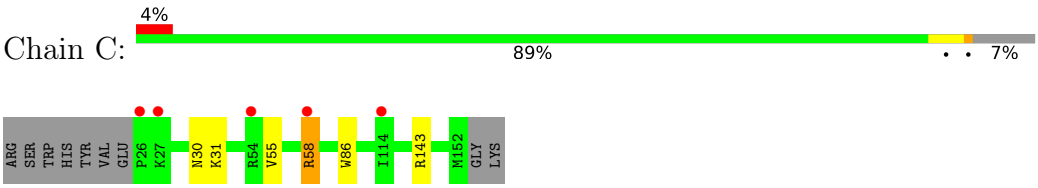
3 Residue-property plots (i)

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.

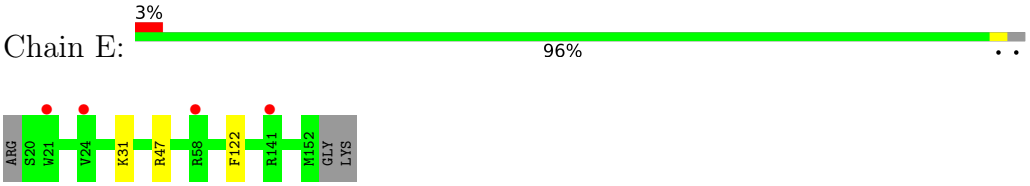
• Molecule 1: Egg-lysin



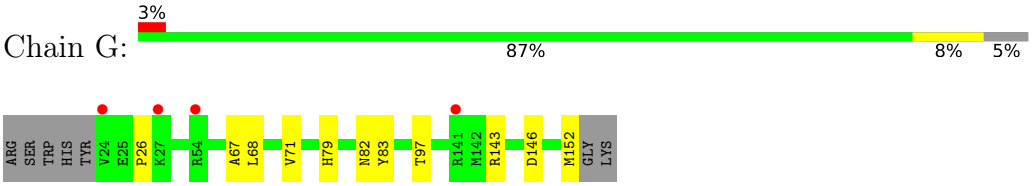
• Molecule 1: Egg-lysin



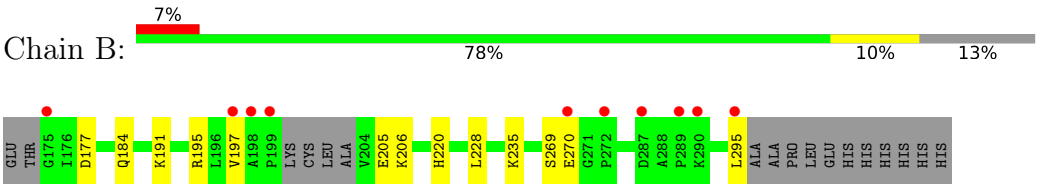
• Molecule 1: Egg-lysin



• Molecule 1: Egg-lysin

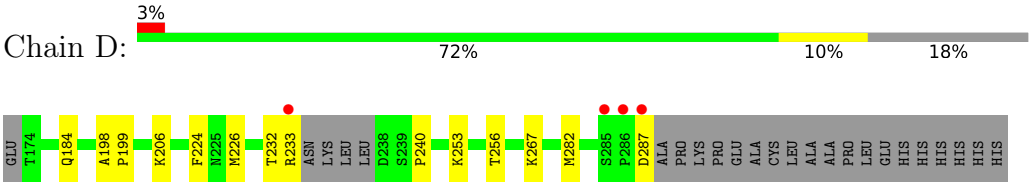


• Molecule 2: Vitelline envelope sperm lysin receptor



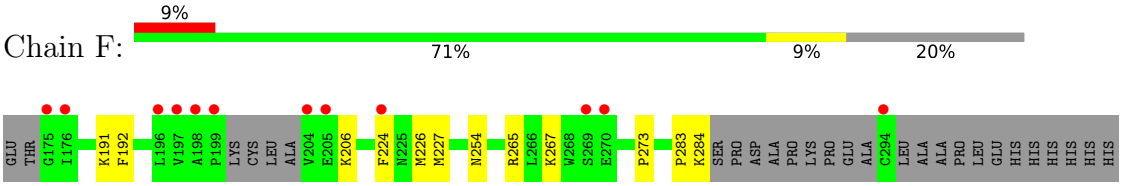
• Molecule 2: Vitelline envelope sperm lysin receptor

Chain D:



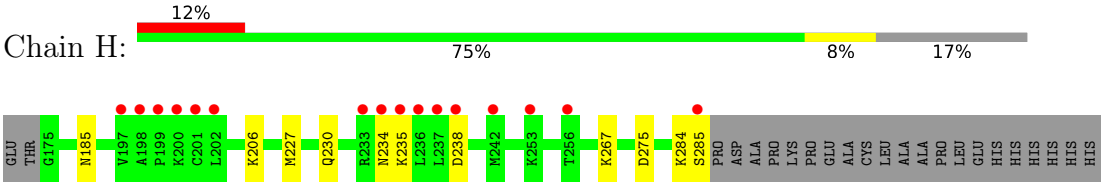
• Molecule 2: Vitelline envelope sperm lysin receptor

Chain F:



• Molecule 2: Vitelline envelope sperm lysin receptor

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	75.87Å 87.86Å 92.55Å 90.00° 100.93° 90.00°	Depositor
Resolution (Å)	45.32 – 1.80 45.32 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.5 (45.32-1.80) 89.8 (45.32-1.80)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.78 (at 1.79Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.201 , 0.227 0.203 , 0.229	Depositor DCC
R_{free} test set	5504 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	30.1	Xtriage
Anisotropy	0.331	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 48.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	16585	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, PGE, CL, GOL

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	0.29	0/1077	0.45	0/1451
1	C	0.29	0/1094	0.47	0/1473
1	E	0.29	0/1167	0.45	0/1574
1	G	0.34	0/1110	0.47	0/1496
2	B	0.31	0/943	0.55	0/1286
2	D	0.33	0/887	0.55	0/1209
2	F	0.30	0/868	0.53	0/1180
2	H	0.31	0/898	0.55	0/1223
All	All	0.31	0/8044	0.50	0/10892

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1050	1079	1079	7	0
1	C	1066	1100	1100	3	1
1	E	1135	1158	1157	3	0
1	G	1082	1114	1114	9	1
2	B	917	893	893	10	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	863	835	835	10	1
2	F	846	824	823	7	0
2	H	874	859	859	12	1
3	A	6	8	8	0	0
3	B	18	24	24	0	0
3	C	6	8	8	0	0
3	D	18	24	24	1	0
3	E	12	16	16	0	0
3	H	12	16	16	1	0
4	B	1	0	0	0	0
4	F	1	0	0	0	0
5	B	14	14	13	0	0
5	D	14	14	13	0	0
5	F	14	14	13	1	0
5	H	14	14	13	0	0
6	G	20	28	28	0	0
7	A	70	0	0	0	0
7	B	79	0	0	2	0
7	C	57	0	0	0	0
7	D	61	0	0	2	0
7	E	95	0	0	2	0
7	F	69	0	0	0	0
7	G	76	0	0	1	0
7	H	53	0	0	5	0
All	All	8543	8042	8036	52	3

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 (52) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:282:MET:HG2	7:D:1002:HOH:O	1.79	0.81
2:B:206:LYS:HB2	7:B:1041:HOH:O	1.85	0.75
2:H:238:ASP:OD1	2:H:238:ASP:O	2.06	0.74
1:C:55:VAL:O	1:C:58:ARG:NH2	2.22	0.72
1:E:47:ARG:NH2	7:E:1001:HOH:O	2.23	0.72
1:G:97:THR:HG23	7:G:1038:HOH:O	1.88	0.71
2:H:285:SER:HB3	7:H:1036:HOH:O	1.93	0.68
1:G:82:ASN:OD1	1:G:83:TYR:N	2.28	0.66
1:G:68:LEU:O	1:G:71:VAL:HG22	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:234:ASN:OD1	2:H:235:LYS:N	2.31	0.64
3:D:902:GOL:O2	7:D:1001:HOH:O	2.16	0.59
2:B:177:ASP:OD1	2:D:253:LYS:NZ	2.36	0.59
1:E:31:LYS:NZ	7:E:1003:HOH:O	2.36	0.59
2:D:224:PHE:HE2	2:D:226:MET:HE2	1.71	0.55
2:B:269:SER:O	2:B:270:GLU:HG2	2.07	0.55
2:F:206:LYS:HE2	2:F:267:LYS:HD2	1.89	0.54
2:B:197:VAL:O	2:B:197:VAL:HG13	2.07	0.54
2:H:284:LYS:O	7:H:1002:HOH:O	2.17	0.54
2:D:256:THR:HG22	2:D:287:ASP:HB2	1.90	0.53
2:H:284:LYS:O	2:H:285:SER:CB	2.56	0.53
1:A:54:ARG:HE	1:G:26:PRO:HB3	1.75	0.52
1:A:51:LYS:HD2	1:G:152:MET:HE3	1.91	0.52
2:B:195:ARG:NH1	7:B:1005:HOH:O	2.46	0.49
1:A:58:ARG:H	1:A:58:ARG:HD3	1.78	0.49
1:A:122:PHE:CG	2:B:191:LYS:HD2	2.49	0.47
1:E:122:PHE:CG	2:F:191:LYS:HD2	2.49	0.47
1:G:67:ALA:O	1:G:71:VAL:HG13	2.14	0.47
1:A:82:ASN:OD1	1:A:83:TYR:N	2.48	0.46
1:G:79:HIS:HE1	2:H:227:MET:HB2	1.81	0.46
1:C:30:ASN:OD1	1:C:31:LYS:N	2.48	0.46
2:D:232:THR:HG22	2:D:233:ARG:N	2.31	0.46
3:H:902:GOL:O2	7:H:1001:HOH:O	2.17	0.45
1:A:30:ASN:OD1	1:A:31:LYS:N	2.49	0.45
2:D:224:PHE:HE2	2:D:226:MET:CE	2.29	0.44
2:F:192:PHE:HB3	2:F:227:MET:HG2	1.99	0.44
2:D:198:ALA:HB1	2:D:199:PRO:HD2	1.99	0.44
2:D:206:LYS:HE3	2:D:267:LYS:HD2	1.99	0.44
2:B:197:VAL:O	2:B:197:VAL:CG1	2.65	0.43
2:F:265:ARG:HD2	2:F:273:PRO:HB2	2.01	0.43
2:B:235:LYS:HE3	2:H:275:ASP:OD2	2.19	0.43
1:A:119:PHE:CE1	2:B:228:LEU:HG	2.54	0.43
2:H:285:SER:CB	7:H:1036:HOH:O	2.62	0.42
1:G:79:HIS:CE1	2:H:227:MET:HB2	2.54	0.42
2:F:224:PHE:CE2	2:F:226:MET:SD	3.13	0.42
2:H:284:LYS:O	2:H:285:SER:HB2	2.20	0.42
2:F:254:ASN:OD1	5:F:402:NAG:N2	2.52	0.41
1:G:143:ARG:HD3	1:G:146:ASP:OD2	2.20	0.41
2:B:295:LEU:HD11	2:D:199:PRO:HG3	2.02	0.41
2:H:230:GLN:NE2	7:H:1006:HOH:O	2.45	0.41
2:F:283:PRO:O	2:F:284:LYS:HB2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:86:TRP:CB	2:D:240:PRO:HB3	2.51	0.40
2:H:206:LYS:HE3	2:H:267:LYS:HD2	2.04	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:205:GLU:OE2	1:G:143:ARG:NH2[2_646]	1.97	0.23
2:B:184:GLN:OE1	1:C:143:ARG:HH21[2_555]	1.51	0.09
2:D:184:GLN:O	2:H:185:ASN:HD22[1_455]	1.58	0.02

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	123/136 (90%)	123 (100%)	0	0	100	100
1	C	125/136 (92%)	125 (100%)	0	0	100	100
1	E	132/136 (97%)	132 (100%)	0	0	100	100
1	G	127/136 (93%)	127 (100%)	0	0	100	100
2	B	113/134 (84%)	110 (97%)	3 (3%)	0	100	100
2	D	106/134 (79%)	105 (99%)	1 (1%)	0	100	100
2	F	102/134 (76%)	101 (99%)	1 (1%)	0	100	100
2	H	109/134 (81%)	108 (99%)	1 (1%)	0	100	100
All	All	937/1080 (87%)	931 (99%)	6 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	109/119 (92%)	109 (100%)	0	100 100
1	C	111/119 (93%)	110 (99%)	1 (1%)	78 75
1	E	118/119 (99%)	118 (100%)	0	100 100
1	G	113/119 (95%)	113 (100%)	0	100 100
2	B	106/120 (88%)	105 (99%)	1 (1%)	78 75
2	D	100/120 (83%)	100 (100%)	0	100 100
2	F	98/120 (82%)	98 (100%)	0	100 100
2	H	101/120 (84%)	101 (100%)	0	100 100
All	All	856/956 (90%)	854 (100%)	2 (0%)	93 92

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	220	HIS
1	C	58	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 20 ligands modelled in this entry, 2 are monoatomic - leaving 18 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	NAG	H	903	2	14,14,15	0.24	0	17,19,21	0.38	0
3	GOL	B	901	-	5,5,5	0.41	0	5,5,5	0.16	0
3	GOL	H	902	-	5,5,5	0.36	0	5,5,5	0.41	0
3	GOL	D	903	-	5,5,5	0.36	0	5,5,5	0.39	0
3	GOL	C	900	-	5,5,5	0.42	0	5,5,5	0.09	0
3	GOL	E	900	-	5,5,5	0.35	0	5,5,5	0.24	0
3	GOL	B	904	-	5,5,5	0.33	0	5,5,5	0.38	0
3	GOL	D	902	-	5,5,5	0.38	0	5,5,5	0.12	0
3	GOL	A	201	-	5,5,5	0.35	0	5,5,5	0.39	0
3	GOL	D	901	-	5,5,5	0.33	0	5,5,5	0.58	0
3	GOL	E	901	-	5,5,5	0.37	0	5,5,5	0.27	0
5	NAG	B	905	2	14,14,15	0.34	0	17,19,21	0.47	0
6	PGE	G	900	-	9,9,9	0.32	0	8,8,8	0.29	0
3	GOL	B	902	-	5,5,5	0.40	0	5,5,5	0.23	0
6	PGE	G	901	-	9,9,9	0.30	0	8,8,8	0.34	0
5	NAG	F	402	2	14,14,15	0.27	0	17,19,21	0.58	0
5	NAG	D	904	2	14,14,15	0.18	0	17,19,21	0.48	0
3	GOL	H	901	-	5,5,5	0.46	0	5,5,5	0.39	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	NAG	H	903	2	-	1/6/23/26	0/1/1/1
3	GOL	B	901	-	-	0/4/4/4	-
3	GOL	H	902	-	-	2/4/4/4	-
3	GOL	D	903	-	-	2/4/4/4	-
3	GOL	C	900	-	-	2/4/4/4	-
3	GOL	E	900	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	904	-	-	2/4/4/4	-
3	GOL	D	902	-	-	0/4/4/4	-
3	GOL	A	201	-	-	2/4/4/4	-
3	GOL	D	901	-	-	2/4/4/4	-
3	GOL	E	901	-	-	0/4/4/4	-
5	NAG	B	905	2	-	2/6/23/26	0/1/1/1
6	PGE	G	900	-	-	3/7/7/7	-
3	GOL	B	902	-	-	2/4/4/4	-
6	PGE	G	901	-	-	1/7/7/7	-
5	NAG	F	402	2	-	1/6/23/26	0/1/1/1
5	NAG	D	904	2	-	0/6/23/26	0/1/1/1
3	GOL	H	901	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	904	GOL	O1-C1-C2-C3
3	C	900	GOL	O1-C1-C2-O2
3	C	900	GOL	O1-C1-C2-C3
3	D	901	GOL	C1-C2-C3-O3
3	D	903	GOL	O1-C1-C2-C3
3	H	902	GOL	O1-C1-C2-C3
5	B	905	NAG	O5-C5-C6-O6
5	B	905	NAG	C4-C5-C6-O6
6	G	900	PGE	O2-C3-C4-O3
6	G	900	PGE	O1-C1-C2-O2
3	B	902	GOL	O1-C1-C2-C3
3	E	900	GOL	C1-C2-C3-O3
3	B	904	GOL	O1-C1-C2-O2
3	D	903	GOL	O1-C1-C2-O2
3	H	902	GOL	O1-C1-C2-O2
5	H	903	NAG	O5-C5-C6-O6
6	G	900	PGE	C1-C2-O2-C3
3	A	201	GOL	O2-C2-C3-O3
3	D	901	GOL	O2-C2-C3-O3
3	H	901	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	H	901	GOL	O2-C2-C3-O3
6	G	901	PGE	C3-C4-O3-C5
3	B	902	GOL	O1-C1-C2-O2
3	E	900	GOL	O2-C2-C3-O3
3	A	201	GOL	C1-C2-C3-O3
5	F	402	NAG	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	902	GOL	1	0
3	D	902	GOL	1	0
5	F	402	NAG	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	125/136 (91%)	0.18	7 (5%) 24 19	30, 46, 74, 128	0
1	C	127/136 (93%)	0.03	5 (3%) 39 33	32, 49, 78, 111	0
1	E	133/136 (97%)	-0.08	4 (3%) 50 44	29, 42, 75, 107	0
1	G	129/136 (94%)	-0.09	4 (3%) 49 43	34, 46, 78, 101	0
2	B	117/134 (87%)	0.55	10 (8%) 10 8	28, 40, 101, 147	0
2	D	110/134 (82%)	0.33	4 (3%) 42 37	27, 42, 90, 131	0
2	F	107/134 (79%)	0.64	12 (11%) 5 4	28, 41, 104, 139	0
2	H	111/134 (82%)	0.65	16 (14%) 2 1	31, 43, 122, 139	0
All	All	959/1080 (88%)	0.26	62 (6%) 18 15	27, 45, 92, 147	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	237	LEU	10.9
2	H	201	CYS	8.7
2	B	197	VAL	8.0
2	F	198	ALA	7.8
2	H	235	LYS	6.6
2	F	197	VAL	6.2
1	A	28	PHE	6.0
2	F	199	PRO	6.0
2	F	196	LEU	5.4
2	F	175	GLY	5.3
2	B	289	PRO	5.2
2	B	270	GLU	5.1
2	B	199	PRO	5.1
2	H	236	LEU	5.1
1	A	59	THR	4.9
2	B	295	LEU	4.6

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Mol	Chain	Res	Type	RSRZ
2	F	204	VAL	4.6
2	H	198	ALA	4.4
2	D	286	PRO	4.4
2	F	176	ILE	4.4
2	F	294	CYS	4.3
2	B	198	ALA	4.3
2	D	287	ASP	4.1
2	F	269	SER	4.1
2	F	205	GLU	3.9
2	H	200	LYS	3.9
1	A	60	LEU	3.8
2	H	238	ASP	3.7
2	H	234	ASN	3.5
1	A	63	VAL	3.5
1	A	58	ARG	3.4
2	B	175	GLY	3.3
1	E	21	TRP	3.2
2	F	270	GLU	3.2
1	E	24	VAL	3.2
2	H	233	ARG	3.0
2	H	197	VAL	2.9
2	H	202	LEU	2.9
2	D	233	ARG	2.8
1	G	24	VAL	2.7
1	C	114	ILE	2.6
1	G	141	ARG	2.5
1	C	26	PRO	2.5
1	G	54	ARG	2.5
2	H	253	LYS	2.4
2	H	256	THR	2.4
2	F	224	PHE	2.4
1	C	54	ARG	2.4
1	A	127	ASN	2.4
1	G	27	LYS	2.4
1	C	27	LYS	2.3
1	E	58	ARG	2.3
2	B	287	ASP	2.3
2	D	285	SER	2.2
1	C	58	ARG	2.2
2	H	285	SER	2.1
1	A	132	TYR	2.1
2	B	290	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	141	ARG	2.0
2	B	272	PRO	2.0
2	H	199	PRO	2.0
2	H	242	MET	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	E	900	6/6	0.44	0.38	134,161,167,168	0
3	GOL	E	901	6/6	0.54	0.38	121,146,147,147	0
6	PGE	G	901	10/10	0.54	0.22	126,152,183,183	0
3	GOL	C	900	6/6	0.55	0.17	119,143,145,147	0
5	NAG	F	402	14/15	0.58	0.30	98,104,123,125	0
3	GOL	H	902	6/6	0.68	0.52	117,141,148,151	0
3	GOL	B	904	6/6	0.72	0.22	75,91,95,95	0
3	GOL	D	902	6/6	0.76	0.47	91,110,116,116	0
6	PGE	G	900	10/10	0.78	0.19	70,84,96,97	0
5	NAG	B	905	14/15	0.79	0.23	76,91,103,103	0
3	GOL	D	903	6/6	0.82	0.41	148,178,182,185	0
5	NAG	H	903	14/15	0.83	0.17	63,76,93,93	0
3	GOL	A	201	6/6	0.84	0.55	109,130,134,137	0
3	GOL	D	901	6/6	0.86	0.15	45,54,56,57	0
5	NAG	D	904	14/15	0.86	0.13	75,87,100,105	0
3	GOL	B	901	6/6	0.86	0.20	110,132,144,148	0
3	GOL	B	902	6/6	0.91	0.18	83,100,104,108	0
3	GOL	H	901	6/6	0.94	0.11	43,53,63,64	0
4	CL	B	903	1/1	0.99	0.18	33,33,33,33	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CL	F	401	1/1	0.99	0.09	36,36,36,36	0

6.5 Other polymers (i)

There are no such residues in this entry.