



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:46 PM UTC

PDB ID : 6JAU / pdb_00006jau
Title : The complex structure of Pseudomonas aeruginosa MucA/MucB.
Authors : Li, T.; He, L.H.; Li, C.C.; Liu, L.; Peng, C.T.; Shen, Y.L.; Qin, X.F.; Xiao, Q.J.; Zhu, Y.B.; Song, Y.J.; Zhao, N.I.; Zhao, C.; Yang, J.; Mu, X.Y.; Huang, Q.; Bao, R.
Deposited on : 2019-01-25
Resolution : 1.91 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

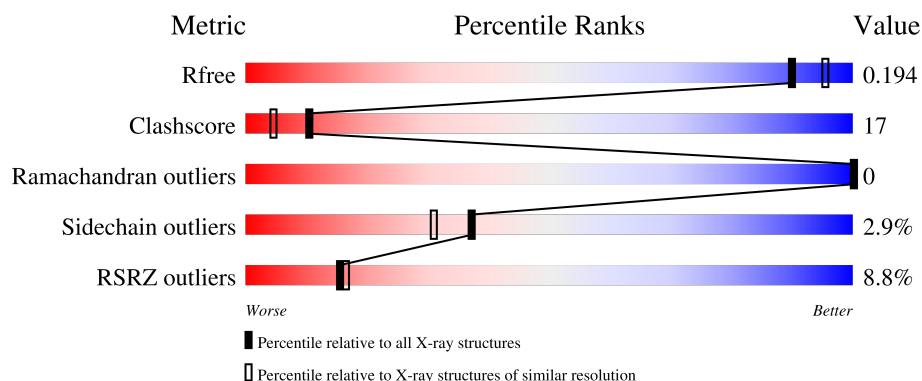
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.91 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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	303	
2	B	97	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 2782 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 Sigma factor AlgU regulatory protein MucB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	283	Total	C	N	O	S	0	0	0
			2201	1376	404	415	6			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	317	LEU	-	expression tag	UNP P38108
A	318	GLU	-	expression tag	UNP P38108
A	319	HIS	-	expression tag	UNP P38108
A	320	HIS	-	expression tag	UNP P38108
A	321	HIS	-	expression tag	UNP P38108
A	322	HIS	-	expression tag	UNP P38108
A	323	HIS	-	expression tag	UNP P38108
A	324	HIS	-	expression tag	UNP P38108

- Molecule 2 is a protein called Sigma factor AlgU negative regulatory protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	47	Total	C	N	O	0	0	0
			369	227	70	72			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	195	LEU	-	expression tag	UNP P38107
B	196	GLU	-	expression tag	UNP P38107
B	197	HIS	-	expression tag	UNP P38107
B	198	HIS	-	expression tag	UNP P38107
B	199	HIS	-	expression tag	UNP P38107
B	200	HIS	-	expression tag	UNP P38107
B	201	HIS	-	expression tag	UNP P38107
B	202	HIS	-	expression tag	UNP P38107

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

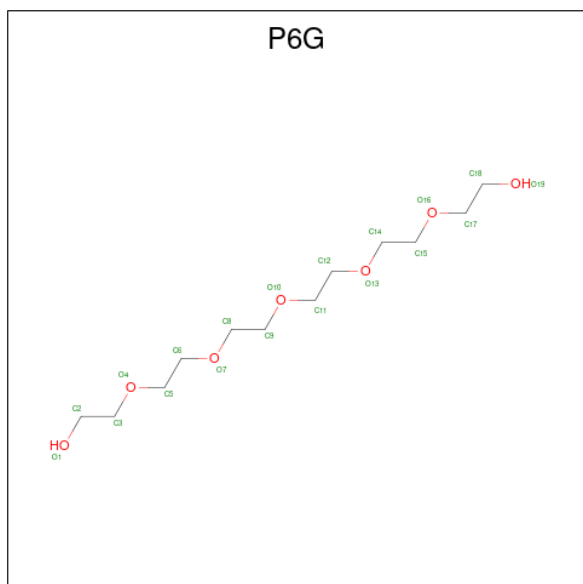
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 5 is HEXAETHYLENE GLYCOL (CCD ID: P6G) (formula: C₁₂H₂₆O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			19	12	7		

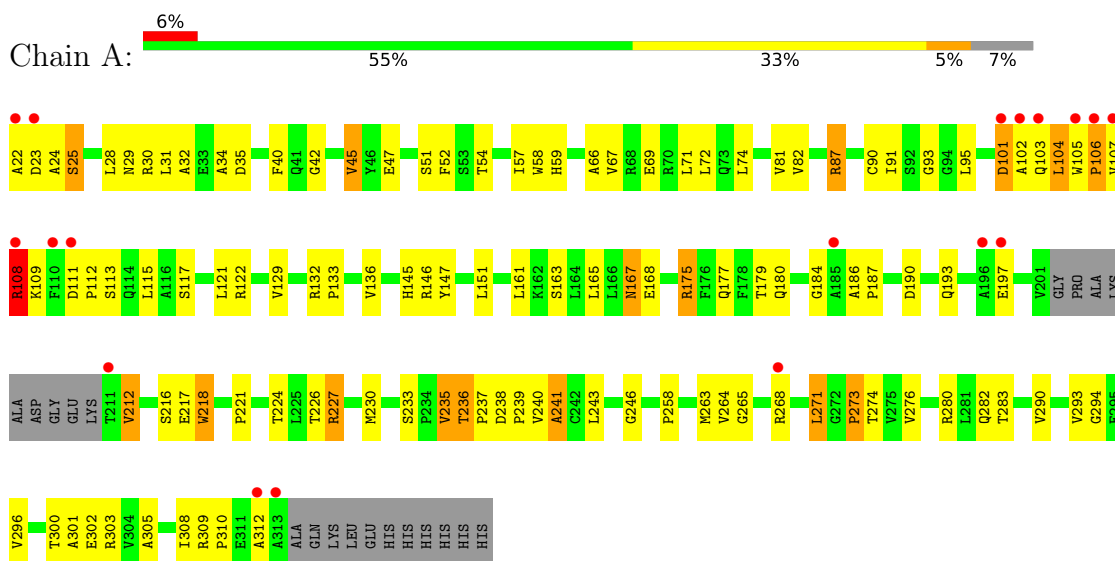
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	172	Total	O	0	0
			172	172		
6	B	14	Total	O	0	0
			14	14		

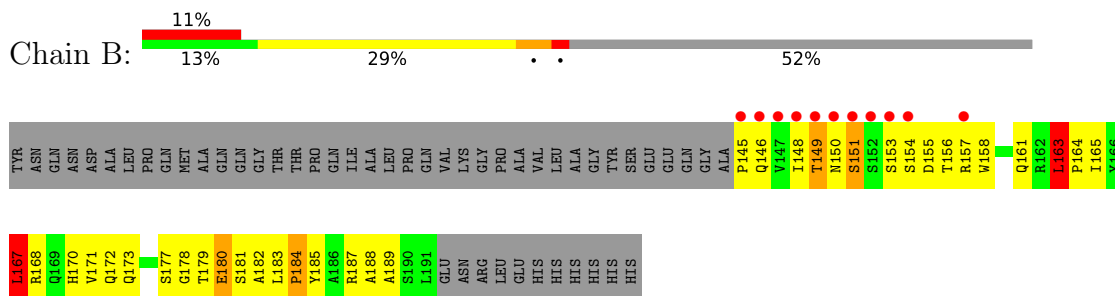
3 Residue-property plots

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: Sigma factor AlgU regulatory protein MucB



- Molecule 2: Sigma factor AlgU negative regulatory protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	71.91Å 186.43Å 50.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.95 – 1.91 35.95 – 1.91	Depositor EDS
% Data completeness (in resolution range)	98.9 (35.95-1.91) 98.9 (35.95-1.91)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	137.93 (at 1.91Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.173 , 0.193 0.174 , 0.194	Depositor DCC
R_{free} test set	2000 reflections (7.37%)	wwPDB-VP
Wilson B-factor (Å ²)	16.9	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 57.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2782	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.99% 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, P6G, CA

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	2.08	77/2246 (3.4%)	1.15	7/3052 (0.2%)
2	B	2.08	17/377 (4.5%)	1.47	6/513 (1.2%)
All	All	2.08	94/2623 (3.6%)	1.20	13/3565 (0.4%)

All (94) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	296	VAL	C-O	-9.04	1.17	1.24
1	A	212	VAL	C-O	-8.36	1.14	1.24
1	A	161	LEU	C-O	-7.97	1.14	1.24
1	A	32	ALA	C-O	-7.70	1.14	1.24
2	B	183	LEU	C-O	-7.48	1.17	1.24
1	A	309	ARG	C-O	-7.33	1.16	1.24
1	A	81	VAL	C-O	-7.19	1.16	1.24
1	A	310	PRO	C-O	-7.18	1.15	1.23
1	A	147	TYR	C-O	-7.00	1.15	1.23
2	B	188	ALA	C-O	-7.00	1.16	1.24
1	A	57	ILE	C-O	-6.96	1.16	1.24
1	A	308	ILE	C-O	-6.93	1.16	1.24
2	B	158	TRP	C-O	-6.74	1.16	1.24
1	A	133	PRO	C-O	-6.70	1.16	1.23
1	A	45	VAL	C-O	-6.68	1.16	1.24
1	A	47	GLU	C-O	-6.61	1.15	1.23
1	A	42	GLY	C-O	-6.55	1.17	1.23
1	A	31	LEU	C-O	-6.46	1.16	1.24
1	A	24	ALA	C-O	-6.41	1.16	1.24
1	A	235	VAL	C-O	-6.37	1.17	1.24
1	A	177	GLN	C-O	-6.29	1.16	1.23
1	A	218	TRP	C-O	-6.24	1.16	1.23
1	A	276	VAL	C-O	-6.22	1.17	1.24
1	A	122	ARG	C-O	-6.18	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	179	THR	C-O	-6.18	1.15	1.24
1	A	300	THR	C-O	-6.17	1.17	1.24
1	A	221	PRO	C-O	-6.16	1.16	1.23
2	B	181	SER	C-O	-6.13	1.16	1.23
1	A	52	PHE	C-O	-6.12	1.17	1.24
1	A	305	ALA	C-O	-6.11	1.17	1.24
1	A	115	LEU	C-O	-6.09	1.16	1.24
1	A	23	ASP	C-O	-6.08	1.16	1.24
1	A	236	THR	C-O	-6.04	1.19	1.24
1	A	82	VAL	C-O	-6.02	1.17	1.24
1	A	190	ASP	C-O	-5.94	1.17	1.24
1	A	66	ALA	C-O	-5.91	1.16	1.23
1	A	117	SER	C-O	-5.91	1.16	1.24
1	A	302	GLU	C-O	-5.87	1.17	1.24
1	A	301	ALA	C-O	-5.86	1.17	1.24
1	A	71	LEU	C-O	-5.85	1.17	1.24
1	A	175	ARG	C-O	-5.83	1.17	1.24
1	A	72	LEU	C-O	-5.82	1.17	1.23
2	B	167	LEU	C-O	-5.79	1.17	1.24
1	A	293	VAL	C-O	-5.79	1.18	1.24
1	A	91	ILE	C-O	-5.76	1.17	1.23
1	A	294	GLY	C-O	-5.76	1.17	1.24
2	B	187	ARG	C-O	-5.73	1.17	1.24
2	B	173	GLN	C-O	-5.71	1.17	1.24
1	A	40	PHE	C-O	-5.64	1.17	1.23
1	A	136	VAL	C-O	-5.63	1.18	1.24
1	A	67	VAL	C-O	-5.61	1.17	1.24
1	A	193	GLN	C-O	-5.61	1.17	1.23
1	A	180	GLN	C-O	-5.60	1.17	1.23
1	A	246	GLY	C-O	-5.59	1.17	1.24
1	A	93	GLY	C-O	-5.59	1.17	1.23
1	A	145	HIS	C-O	-5.59	1.16	1.24
1	A	167	ASN	C-O	-5.58	1.17	1.23
1	A	227	ARG	C-O	-5.56	1.17	1.23
2	B	170	HIS	C-O	-5.52	1.17	1.24
1	A	129	VAL	C-O	-5.50	1.18	1.24
1	A	273	PRO	C-O	-5.48	1.17	1.24
2	B	165	ILE	C-O	-5.47	1.18	1.24
1	A	274	THR	C-O	-5.46	1.17	1.24
1	A	216	SER	C-O	-5.43	1.17	1.23
1	A	151	LEU	C-O	-5.41	1.17	1.24
1	A	59	HIS	C-O	-5.38	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	185	TYR	C-O	-5.36	1.18	1.24
1	A	290	VAL	C-O	-5.34	1.18	1.24
1	A	243	LEU	C-O	-5.30	1.17	1.23
1	A	34	ALA	C-O	-5.29	1.18	1.24
1	A	283	THR	C-O	-5.27	1.17	1.23
1	A	241	ALA	C-O	-5.26	1.17	1.23
1	A	69	GLU	C-O	-5.25	1.17	1.23
1	A	58	TRP	C-O	-5.21	1.17	1.24
1	A	217	GLU	C-O	-5.21	1.17	1.24
1	A	258	PRO	C-O	-5.20	1.17	1.23
2	B	168	ARG	C-O	-5.20	1.18	1.24
1	A	51	SER	C-O	-5.19	1.18	1.23
2	B	172	GLN	C-O	-5.18	1.18	1.24
1	A	163	SER	C-O	-5.17	1.18	1.23
1	A	132	ARG	C-O	-5.16	1.17	1.24
2	B	180	GLU	C-O	-5.14	1.17	1.24
2	B	171	VAL	C-O	-5.14	1.18	1.24
1	A	95	LEU	C-O	-5.13	1.17	1.24
2	B	189	ALA	C-O	-5.12	1.17	1.24
2	B	184	PRO	C-O	-5.11	1.17	1.24
1	A	240	VAL	C-O	-5.09	1.18	1.24
1	A	146	ARG	C-O	-5.08	1.17	1.23
1	A	90	CYS	C-O	-5.05	1.17	1.23
2	B	163	LEU	C-O	-5.05	1.19	1.24
1	A	233	SER	C-O	-5.04	1.17	1.23
1	A	29	ASN	C-O	-5.04	1.18	1.24
1	A	224	THR	C-O	-5.03	1.17	1.23
1	A	25	SER	C-O	-5.00	1.18	1.24

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	156	THR	N-CA-C	-9.80	100.43	111.71
2	B	151	SER	N-CA-C	9.56	124.44	111.24
2	B	150	ASN	N-CA-C	8.24	121.92	108.99
2	B	181	SER	N-CA-C	7.78	120.93	110.35
1	A	108	ARG	N-CA-C	7.75	119.44	108.74
2	B	148	ILE	N-CA-C	6.88	118.03	108.12
1	A	106	PRO	N-CA-C	-6.56	98.96	112.47
1	A	238	ASP	N-CA-C	6.14	117.63	109.83
1	A	23	ASP	N-CA-C	-6.09	104.70	111.71
1	A	235	VAL	N-CA-C	5.68	119.10	113.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	312	ALA	N-CA-C	5.25	118.30	109.95
1	A	74	LEU	N-CA-C	5.11	119.59	112.90
2	B	149	THR	CB-CA-C	-5.01	100.46	110.42

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	2201	0	2156	69	6
2	B	369	0	359	33	6
3	A	1	0	0	0	0
4	A	6	0	8	0	0
5	B	19	0	26	5	0
6	A	172	0	0	11	1
6	B	14	0	0	6	0
All	All	2782	0	2549	87	7

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 17.

All (87) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:GLY:H	2:B:154:SER:CB	1.12	1.58
1:A:265:GLY:N	2:B:154:SER:CB	1.98	1.24
1:A:265:GLY:N	2:B:154:SER:HB3	1.54	1.18
1:A:265:GLY:H	2:B:154:SER:HB2	1.04	1.15
1:A:102:ALA:O	1:A:105:TRP:CE3	2.10	1.04
1:A:265:GLY:H	2:B:154:SER:HB3	0.88	1.01
1:A:108:ARG:HH21	1:A:108:ARG:HG2	1.27	0.99
1:A:35:ASP:OD2	2:B:180:GLU:HG2	1.63	0.98
1:A:265:GLY:N	2:B:154:SER:HB2	1.70	0.94
2:B:177:SER:OG	6:B:401:HOH:O	1.88	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:PRO:HB3	2:B:178:GLY:HA3	1.51	0.90
1:A:108:ARG:NH2	6:A:501:HOH:O	2.06	0.88
1:A:105:TRP:CZ2	1:A:227:ARG:HD3	2.10	0.87
1:A:105:TRP:CE2	1:A:227:ARG:HD3	2.11	0.86
1:A:280:ARG:HH12	1:A:282:GLN:HG2	1.41	0.84
1:A:105:TRP:NE1	1:A:227:ARG:HD3	1.93	0.83
1:A:280:ARG:NH1	1:A:282:GLN:HG2	1.96	0.78
2:B:182:ALA:H	5:B:301:P6G:H121	1.47	0.78
1:A:35:ASP:CG	2:B:180:GLU:HG2	2.11	0.74
1:A:212:VAL:HG11	1:A:241:ALA:HB1	1.67	0.74
1:A:106:PRO:HB3	2:B:178:GLY:CA	2.16	0.74
1:A:102:ALA:O	1:A:105:TRP:HE3	1.71	0.73
1:A:263:MET:O	2:B:153:SER:O	2.09	0.70
2:B:155:ASP:OD1	6:B:402:HOH:O	2.11	0.69
1:A:35:ASP:OD2	2:B:180:GLU:CG	2.38	0.68
1:A:108:ARG:HH21	1:A:108:ARG:CG	2.04	0.68
1:A:112:PRO:O	6:A:503:HOH:O	2.12	0.67
1:A:28:LEU:HD12	1:A:121:LEU:HD13	1.79	0.65
1:A:28:LEU:CD1	1:A:121:LEU:HD13	2.28	0.64
1:A:236:THR:HB	1:A:237:PRO:HD2	1.80	0.63
1:A:87:ARG:O	1:A:87:ARG:HG3	1.95	0.62
1:A:175:ARG:NH2	6:A:502:HOH:O	2.09	0.62
1:A:271:LEU:HG	2:B:145:PRO:HG3	1.80	0.62
1:A:197:GLU:HB2	6:A:515:HOH:O	2.01	0.61
2:B:177:SER:C	6:B:401:HOH:O	2.43	0.60
1:A:168:GLU:OE1	1:A:168:GLU:N	2.25	0.60
1:A:105:TRP:HE1	1:A:227:ARG:HD3	1.61	0.59
1:A:30:ARG:NH1	6:A:510:HOH:O	2.34	0.59
2:B:180:GLU:CG	6:B:403:HOH:O	2.48	0.59
2:B:182:ALA:H	5:B:301:P6G:C12	2.16	0.58
1:A:105:TRP:HE1	1:A:227:ARG:CD	2.08	0.57
2:B:146:GLN:O	2:B:146:GLN:HG3	2.06	0.56
1:A:212:VAL:CG1	1:A:241:ALA:HB1	2.37	0.55
1:A:102:ALA:O	1:A:105:TRP:CZ3	2.58	0.55
2:B:149:THR:O	2:B:149:THR:HG23	2.07	0.55
1:A:264:VAL:HA	2:B:154:SER:HA	1.88	0.54
1:A:105:TRP:NE1	1:A:227:ARG:CD	2.66	0.54
1:A:108:ARG:HG2	1:A:108:ARG:NH2	2.08	0.53
1:A:101:ASP:HA	1:A:104:LEU:HD23	1.90	0.53
2:B:167:LEU:C	2:B:167:LEU:HD13	2.34	0.53
1:A:22:ALA:HB3	1:A:25:SER:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:589:HOH:O	5:B:301:P6G:H82	2.09	0.52
2:B:179:THR:HG22	6:B:401:HOH:O	2.09	0.52
2:B:178:GLY:N	6:B:401:HOH:O	2.44	0.51
1:A:175:ARG:NE	6:A:502:HOH:O	2.40	0.51
1:A:105:TRP:CD1	1:A:105:TRP:O	2.65	0.49
1:A:230:MET:HE2	1:A:239:PRO:HB2	1.95	0.49
2:B:182:ALA:N	5:B:301:P6G:H121	2.24	0.49
1:A:268:ARG:NH1	1:A:268:ARG:HG2	2.28	0.48
1:A:167:ASN:HB2	1:A:168:GLU:OE1	2.13	0.48
1:A:264:VAL:HA	2:B:154:SER:CB	2.44	0.48
1:A:108:ARG:HG2	6:A:501:HOH:O	2.13	0.48
1:A:265:GLY:CA	2:B:154:SER:CB	2.86	0.48
1:A:175:ARG:CZ	6:A:502:HOH:O	2.56	0.47
1:A:107:VAL:HG11	1:A:226:THR:HB	1.97	0.47
1:A:111:ASP:OD1	1:A:113:SER:OG	2.28	0.47
1:A:264:VAL:HA	2:B:154:SER:CA	2.45	0.46
2:B:179:THR:HG21	2:B:184:PRO:HG2	1.99	0.45
1:A:105:TRP:HZ2	1:A:227:ARG:HD3	1.74	0.44
1:A:184:GLY:HA2	6:A:629:HOH:O	2.16	0.44
1:A:236:THR:HB	1:A:237:PRO:CD	2.47	0.44
2:B:146:GLN:H	2:B:146:GLN:HG2	1.54	0.44
1:A:104:LEU:HD13	1:A:104:LEU:HA	1.53	0.43
1:A:218:TRP:CE3	1:A:303:ARG:HG2	2.55	0.42
1:A:268:ARG:CG	1:A:268:ARG:HH11	2.33	0.42
1:A:109:LYS:O	6:A:501:HOH:O	2.21	0.41
5:B:301:P6G:H182	5:B:301:P6G:H151	1.43	0.41
1:A:103:GLN:HA	1:A:105:TRP:CH2	2.56	0.41
1:A:103:GLN:HA	1:A:105:TRP:CZ3	2.55	0.41
1:A:197:GLU:OE1	1:A:197:GLU:N	2.47	0.41
1:A:45:VAL:HG22	1:A:54:THR:HG22	2.02	0.41
1:A:101:ASP:O	1:A:104:LEU:HB2	2.20	0.41
1:A:165:LEU:HD23	1:A:273:PRO:HB3	2.02	0.41
1:A:186:ALA:HA	1:A:187:PRO:HD3	1.76	0.41
1:A:22:ALA:HB3	1:A:25:SER:CB	2.50	0.40
2:B:157:ARG:O	2:B:161:GLN:HG3	2.22	0.40
2:B:163:LEU:N	2:B:164:PRO:CD	2.84	0.40

All (7) 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)
1:A:268:ARG:NE	2:B:151:SER:CB[4_556]	1.74	0.46
1:A:268:ARG:CD	2:B:151:SER:O[4_556]	1.76	0.44
1:A:268:ARG:CG	2:B:151:SER:O[4_556]	1.84	0.36
1:A:268:ARG:CB	2:B:151:SER:O[4_556]	1.84	0.36
6:A:671:HOH:O	6:A:672:HOH:O[6_655]	2.05	0.15
1:A:268:ARG:CD	2:B:151:SER:C[4_556]	2.09	0.11
1:A:268:ARG:CD	2:B:151:SER:CB[4_556]	2.11	0.09

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	279/303 (92%)	275 (99%)	4 (1%)	0	100	100
2	B	45/97 (46%)	42 (93%)	3 (7%)	0	100	100
All	All	324/400 (81%)	317 (98%)	7 (2%)	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	232/247 (94%)	226 (97%)	6 (3%)	40	35
2	B	41/81 (51%)	39 (95%)	2 (5%)	22	14
All	All	273/328 (83%)	265 (97%)	8 (3%)	37	31

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	87	ARG
1	A	101	ASP
1	A	104	LEU
1	A	108	ARG
1	A	235	VAL
1	A	271	LEU
2	B	163	LEU
2	B	167	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	89	GLN
1	A	145	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	A	402	-	5,5,5	0.25	0	5,5,5	0.46	0
5	P6G	B	301	-	18,18,18	0.53	0	17,17,17	0.51	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	402	-	-	4/4/4/4	-
5	P6G	B	301	-	-	7/16/16/16	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	402	GOL	C1-C2-C3-O3
4	A	402	GOL	O2-C2-C3-O3
5	B	301	P6G	C18-C17-O16-C15
5	B	301	P6G	O10-C11-C12-O13
4	A	402	GOL	O1-C1-C2-C3
5	B	301	P6G	O1-C2-C3-O4
5	B	301	P6G	O7-C8-C9-O10
5	B	301	P6G	O16-C17-C18-O19
4	A	402	GOL	O1-C1-C2-O2
5	B	301	P6G	C12-C11-O10-C9
5	B	301	P6G	C15-C14-O13-C12

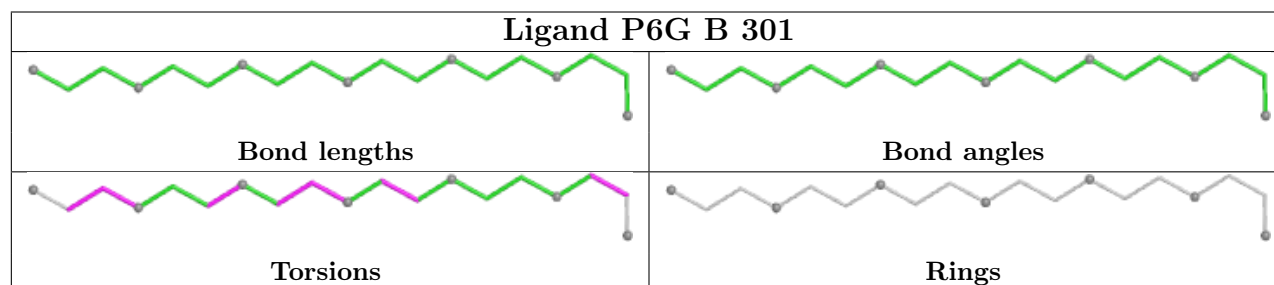
There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	301	P6G	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	283/303 (93%)	-0.01	18 (6%) 25 27	8, 18, 50, 82	4 (1%)
2	B	47/97 (48%)	0.73	11 (23%) 2 1	11, 20, 78, 87	3 (6%)
All	All	330/400 (82%)	0.10	29 (8%) 15 16	8, 18, 58, 87	7 (2%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	105	TRP	8.0
2	B	152	SER	6.6
1	A	185	ALA	4.8
2	B	149	THR	4.5
2	B	151	SER	4.2
1	A	106	PRO	3.7
1	A	22	ALA	3.6
2	B	145	PRO	3.5
1	A	107	VAL	3.4
1	A	110	PHE	3.4
1	A	313	ALA	3.2
2	B	146	GLN	2.9
2	B	148	ILE	2.9
1	A	108	ARG	2.8
1	A	197	GLU	2.8
1	A	101	ASP	2.7
2	B	153	SER	2.5
2	B	154	SER	2.5
1	A	196	ALA	2.5
1	A	23	ASP	2.5
1	A	111	ASP	2.5
2	B	150	ASN	2.4
1	A	102	ALA	2.3
2	B	147	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	157	ARG	2.2
1	A	211	THR	2.2
1	A	312	ALA	2.1
1	A	103	GLN	2.0
1	A	268	ARG	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

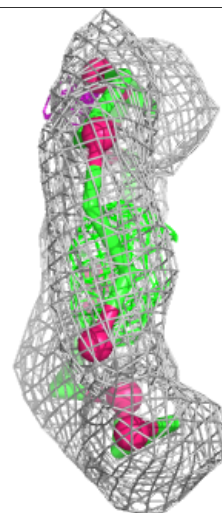
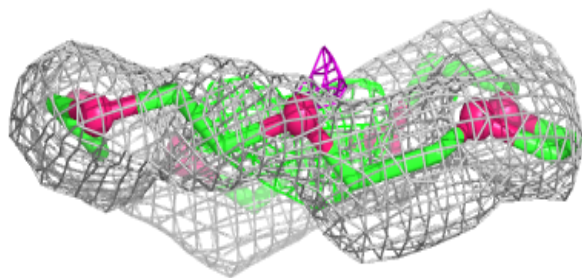
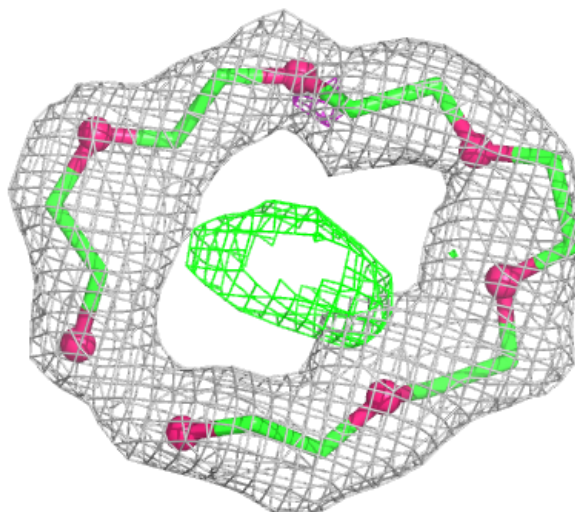
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	A	402	6/6	0.84	0.14	45,51,52,53	0
5	P6G	B	301	19/19	0.87	0.15	31,41,50,52	0
3	CA	A	401	1/1	0.98	0.13	37,37,37,37	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around P6G B 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.