



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:10 AM UTC

PDB ID : 7FI3 / pdb_00007fi3
Title : Archaeal oligopeptide permease A (OppA) from *Thermococcus kodakaraensis*
in complex with an endogenous pentapeptide
Authors : Yokoyama, H.; Kamei, N.; Konishi, K.; Hara, K.; Hashimoto, H.
Deposited on : 2021-07-30
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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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

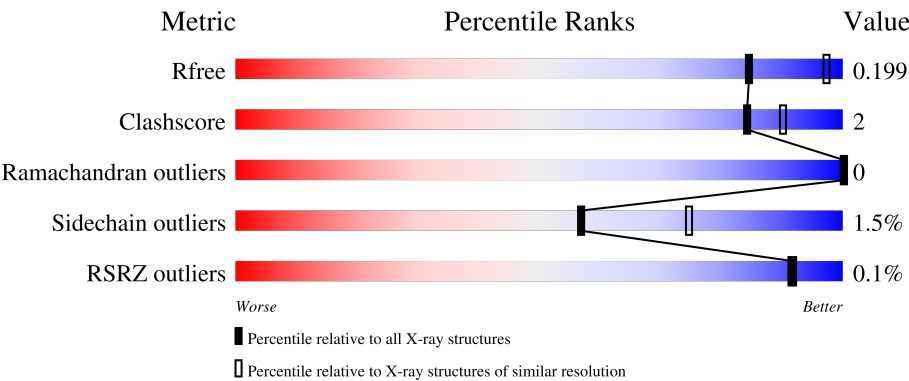
1 Overall quality at a glance i

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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	732	92%6% ..
1	B	732	93%5% .
1	C	732	91%8% .
1	D	732	91%7% ..
2	E	5	100%

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Mol	Chain	Length	Quality of chain
2	F	5	 100%
2	G	5	 100%
2	H	5	 100%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 24940 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 ABC-type dipeptide/oligopeptide transport system.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	724	Total	C	N	O	S	Se	0	0	0
			5862	3773	937	1135	2	15			
1	B	724	Total	C	N	O	S	Se	0	0	0
			5862	3773	937	1135	2	15			
1	C	724	Total	C	N	O	S	Se	0	0	0
			5862	3773	937	1135	2	15			
1	D	724	Total	C	N	O	S	Se	0	0	0
			5862	3773	937	1135	2	15			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	302	MSE	ILE	engineered mutation	UNP Q5JJ92
A	446	MSE	LEU	engineered mutation	UNP Q5JJ92
A	557	MSE	LEU	engineered mutation	UNP Q5JJ92
A	636	MSE	LEU	engineered mutation	UNP Q5JJ92
A	754	VAL	-	expression tag	UNP Q5JJ92
A	755	GLU	-	expression tag	UNP Q5JJ92
A	756	HIS	-	expression tag	UNP Q5JJ92
A	757	HIS	-	expression tag	UNP Q5JJ92
A	758	HIS	-	expression tag	UNP Q5JJ92
A	759	HIS	-	expression tag	UNP Q5JJ92
A	760	HIS	-	expression tag	UNP Q5JJ92
A	761	HIS	-	expression tag	UNP Q5JJ92
B	302	MSE	ILE	engineered mutation	UNP Q5JJ92
B	446	MSE	LEU	engineered mutation	UNP Q5JJ92
B	557	MSE	LEU	engineered mutation	UNP Q5JJ92
B	636	MSE	LEU	engineered mutation	UNP Q5JJ92
B	754	VAL	-	expression tag	UNP Q5JJ92
B	755	GLU	-	expression tag	UNP Q5JJ92
B	756	HIS	-	expression tag	UNP Q5JJ92
B	757	HIS	-	expression tag	UNP Q5JJ92
B	758	HIS	-	expression tag	UNP Q5JJ92

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Chain	Residue	Modelled	Actual	Comment	Reference
B	759	HIS	-	expression tag	UNP Q5JJ92
B	760	HIS	-	expression tag	UNP Q5JJ92
B	761	HIS	-	expression tag	UNP Q5JJ92
C	302	MSE	ILE	engineered mutation	UNP Q5JJ92
C	446	MSE	LEU	engineered mutation	UNP Q5JJ92
C	557	MSE	LEU	engineered mutation	UNP Q5JJ92
C	636	MSE	LEU	engineered mutation	UNP Q5JJ92
C	754	VAL	-	expression tag	UNP Q5JJ92
C	755	GLU	-	expression tag	UNP Q5JJ92
C	756	HIS	-	expression tag	UNP Q5JJ92
C	757	HIS	-	expression tag	UNP Q5JJ92
C	758	HIS	-	expression tag	UNP Q5JJ92
C	759	HIS	-	expression tag	UNP Q5JJ92
C	760	HIS	-	expression tag	UNP Q5JJ92
C	761	HIS	-	expression tag	UNP Q5JJ92
D	302	MSE	ILE	engineered mutation	UNP Q5JJ92
D	446	MSE	LEU	engineered mutation	UNP Q5JJ92
D	557	MSE	LEU	engineered mutation	UNP Q5JJ92
D	636	MSE	LEU	engineered mutation	UNP Q5JJ92
D	754	VAL	-	expression tag	UNP Q5JJ92
D	755	GLU	-	expression tag	UNP Q5JJ92
D	756	HIS	-	expression tag	UNP Q5JJ92
D	757	HIS	-	expression tag	UNP Q5JJ92
D	758	HIS	-	expression tag	UNP Q5JJ92
D	759	HIS	-	expression tag	UNP Q5JJ92
D	760	HIS	-	expression tag	UNP Q5JJ92
D	761	HIS	-	expression tag	UNP Q5JJ92

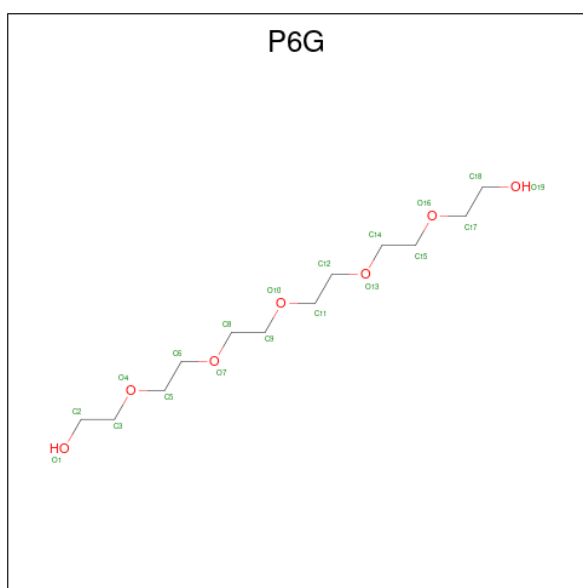
- Molecule 2 is a protein called endogenous pentapeptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	5	Total	C	N	O	0	0	0
			25	15	5	5			
2	F	5	Total	C	N	O	0	0	0
			25	15	5	5			
2	G	5	Total	C	N	O	0	0	0
			25	15	5	5			
2	H	5	Total	C	N	O	0	0	0
			25	15	5	5			

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Na	0	0
			2	2		
3	B	2	Total	Na	0	0
			2	2		
3	C	2	Total	Na	0	0
			2	2		
3	D	2	Total	Na	0	0
			2	2		

- Molecule 4 is HEXAETHYLENE GLYCOL (CCD ID: P6G) (formula: $C_{12}H_{26}O_7$).



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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

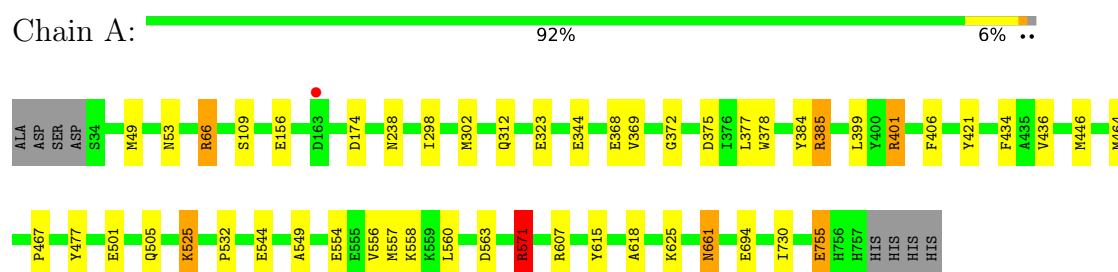
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	372	Total	O	0	0
			372	372		
6	B	265	Total	O	0	0
			265	265		
6	C	344	Total	O	0	0
			344	344		
6	D	323	Total	O	0	0
			323	323		

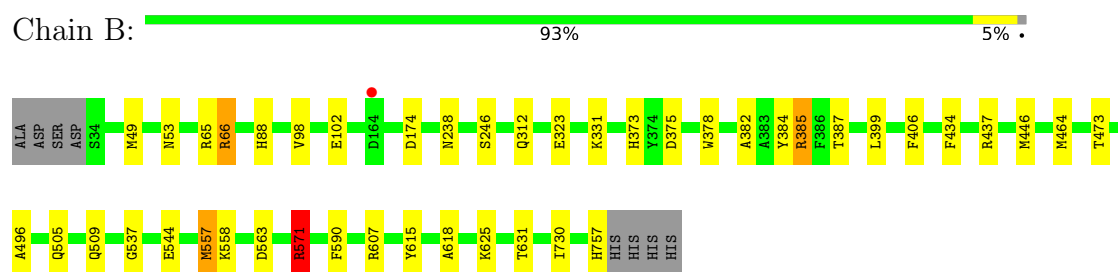
3 Residue-property plots [i](#)

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.

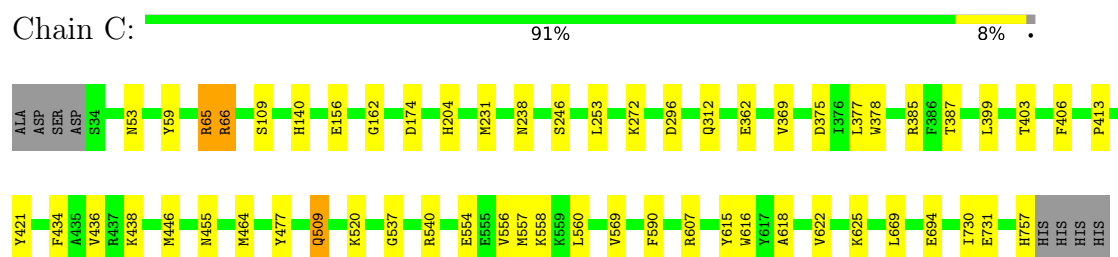
- Molecule 1: ABC-type dipeptide/oligopeptide transport system



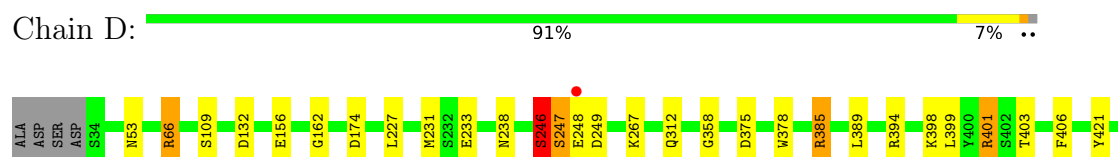
- Molecule 1: ABC-type dipeptide/oligopeptide transport system

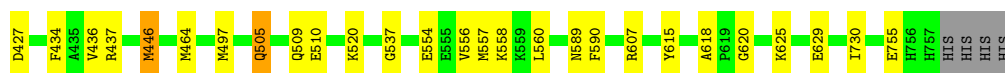


- Molecule 1: ABC-type dipeptide/oligopeptide transport system



- Molecule 1: ABC-type dipeptide/oligopeptide transport system





- Molecule 2: endogenous pentapeptide

Chain E:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: endogenous pentapeptide

Chain F:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: endogenous pentapeptide

Chain G:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: endogenous pentapeptide

Chain H:  100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	122.66Å 118.64Å 112.72Å 90.00° 105.32° 90.00°	Depositor
Resolution (Å)	19.98 – 2.30 19.98 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.98-2.30) 99.8 (19.98-2.30)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.49 (at 2.30Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.159 , 0.192 0.171 , 0.199	Depositor DCC
R_{free} test set	13814 reflections (10.02%)	wwPDB-VP
Wilson B-factor (Å ²)	26.0	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 35.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	24940	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, P6G, NA

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	1.14	4/6027 (0.1%)	1.28	9/8194 (0.1%)
1	B	1.09	3/6027 (0.0%)	1.26	12/8194 (0.1%)
1	C	1.11	4/6027 (0.1%)	1.27	8/8194 (0.1%)
1	D	1.11	2/6027 (0.0%)	1.27	11/8194 (0.1%)
All	All	1.11	13/24108 (0.1%)	1.27	40/32776 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	372	GLY	C-O	-6.66	1.15	1.24
1	C	140	HIS	CE1-NE2	6.31	1.38	1.32
1	B	382	ALA	C-O	6.15	1.31	1.23
1	B	88	HIS	CE1-NE2	6.10	1.38	1.32
1	A	467	PRO	C-O	-5.76	1.16	1.24
1	C	731	GLU	CD-OE2	5.63	1.36	1.25
1	D	358	GLY	C-O	-5.59	1.19	1.24
1	A	532	PRO	C-O	-5.51	1.17	1.23
1	B	373	HIS	CE1-NE2	5.40	1.38	1.32
1	D	620	GLY	N-CA	5.35	1.48	1.44
1	C	204	HIS	CE1-NE2	5.13	1.37	1.32
1	A	694	GLU	C-O	5.09	1.30	1.24
1	C	622	VAL	C-O	5.07	1.29	1.24

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	757	HIS	CA-C-O	-10.80	102.43	120.80
1	D	247	SER	N-CA-C	-8.76	99.02	110.33
1	A	571	ARG	CB-CA-C	-8.58	96.60	110.84
1	B	757	HIS	CA-C-O	-8.47	106.41	120.80
1	D	427	ASP	CA-CB-CG	8.24	120.84	112.60
1	A	571	ARG	CG-CD-NE	-7.34	95.86	112.00
1	A	401	ARG	CG-CD-NE	-7.09	96.41	112.00
1	C	162	GLY	CA-C-O	-6.71	116.64	121.88
1	D	162	GLY	CA-C-O	-6.27	116.99	121.88
1	C	65	ARG	CG-CD-NE	6.23	125.70	112.00
1	D	401	ARG	CG-CD-NE	-6.08	98.63	112.00
1	D	401	ARG	CB-CA-C	-6.01	99.38	109.65
1	B	65	ARG	CG-CD-NE	-5.98	98.85	112.00
1	B	571	ARG	CB-CA-C	-5.89	98.69	110.42
1	B	557	MSE	CG-SE-CE	5.88	111.86	98.92
1	D	446	MSE	CG-SE-CE	-5.88	85.98	98.92
1	A	53	ASN	CB-CA-C	5.87	118.77	109.55
1	C	53	ASN	CB-CA-C	5.83	118.70	109.55
1	C	238	ASN	CB-CA-C	5.83	118.29	110.13
1	B	563	ASP	CA-CB-CG	5.82	118.42	112.60
1	B	571	ARG	CG-CD-NE	-5.81	99.22	112.00
1	C	509	GLN	CB-CA-C	5.77	121.25	110.70
1	D	53	ASN	CB-CA-C	5.75	118.58	109.55
1	D	629	GLU	CB-CG-CD	5.72	122.32	112.60
1	B	53	ASN	CB-CA-C	5.68	118.47	109.55
1	D	238	ASN	CB-CA-C	5.56	117.91	110.13
1	A	238	ASN	CB-CA-C	5.48	117.80	110.13
1	B	102	GLU	CA-CB-CG	-5.46	103.19	114.10
1	B	473	THR	CA-CB-OG1	-5.46	101.41	109.60
1	A	563	ASP	CA-CB-CG	5.44	118.04	112.60
1	A	401	ARG	CB-CA-C	-5.40	99.96	109.62
1	D	132	ASP	CA-CB-CG	5.39	117.99	112.60
1	B	238	ASN	CB-CA-C	5.38	117.66	110.13
1	C	387	THR	CA-CB-OG1	-5.38	101.53	109.60
1	D	589	ASN	CA-CB-CG	-5.28	107.32	112.60
1	A	549	ALA	N-CA-C	-5.21	105.61	111.28
1	B	323	GLU	CB-CG-CD	5.20	121.44	112.60
1	B	387	THR	CA-CB-OG1	-5.14	101.88	109.60
1	C	616	TRP	CA-C-O	-5.02	116.12	119.68
1	A	323	GLU	CB-CG-CD	5.01	121.12	112.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	246	SER	Mainchain

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	5862	0	5503	31	0
1	B	5862	0	5503	17	0
1	C	5862	0	5503	29	0
1	D	5862	0	5503	30	0
2	E	25	0	7	0	0
2	F	25	0	7	0	0
2	G	25	0	7	0	0
2	H	25	0	7	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	19	0	26	0	0
4	B	19	0	26	0	0
5	A	12	0	16	2	0
5	B	6	0	8	0	0
5	C	12	0	16	2	0
5	D	12	0	16	0	0
6	A	372	0	0	1	0
6	B	265	0	0	1	0
6	C	344	0	0	2	0
6	D	323	0	0	4	0
All	All	24940	0	22148	105	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 2.

All (105) 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:446:MSE:HE3	1:A:560:LEU:HD21	1.58	0.85
1:D:446:MSE:HE3	1:D:560:LEU:HD21	1.59	0.83
1:C:446:MSE:HE3	1:C:560:LEU:HD21	1.59	0.82
1:A:385:ARG:HH21	1:A:385:ARG:HA	1.52	0.74
1:A:477:TYR:HE1	5:A:804:GOL:H12	1.52	0.72
1:A:174:ASP:HB3	1:A:615:TYR:O	2.01	0.60
1:D:174:ASP:HB3	1:D:615:TYR:O	2.01	0.60
1:D:401:ARG:HD2	6:D:1091:HOH:O	2.01	0.60
1:A:477:TYR:CE1	5:A:804:GOL:H12	2.34	0.60
1:B:174:ASP:HB3	1:B:615:TYR:O	2.01	0.60
1:C:477:TYR:CE1	5:C:803:GOL:H12	2.37	0.59
1:C:477:TYR:HE1	5:C:803:GOL:H12	1.67	0.59
1:C:174:ASP:HB3	1:C:615:TYR:O	2.02	0.59
1:D:406:PHE:HB2	1:D:464:MSE:HE1	1.83	0.59
1:B:49:MSE:HB2	1:B:571:ARG:HG2	1.85	0.58
1:A:49:MSE:HB2	1:A:571:ARG:HG2	1.86	0.58
1:D:505:GLN:OE1	1:D:509:GLN:NE2	2.36	0.58
1:A:406:PHE:HB2	1:A:464:MSE:HE1	1.86	0.58
1:A:385:ARG:HA	1:A:385:ARG:NH2	2.17	0.56
1:B:446:MSE:HG2	1:B:496:ALA:HB1	1.88	0.56
1:A:755:GLU:HG3	6:C:938:HOH:O	2.06	0.55
1:A:446:MSE:HG2	1:A:556:VAL:HG13	1.87	0.55
1:B:406:PHE:HB2	1:B:464:MSE:HE1	1.90	0.54
1:C:406:PHE:CD1	1:C:464:MSE:HE1	2.43	0.53
1:D:109:SER:HB3	1:D:156:GLU:HA	1.91	0.53
1:B:406:PHE:CD1	1:B:464:MSE:HE1	2.44	0.53
1:C:406:PHE:HB2	1:C:464:MSE:HE1	1.90	0.53
1:D:446:MSE:HG2	1:D:556:VAL:HG13	1.92	0.51
1:A:434:PHE:HZ	1:A:557:MSE:SE	2.44	0.51
1:C:109:SER:HB3	1:C:156:GLU:HA	1.94	0.50
1:C:434:PHE:HZ	1:C:557:MSE:SE	2.44	0.50
1:D:389:LEU:O	1:D:394:ARG:NH1	2.45	0.50
1:A:501:GLU:O	1:A:505:GLN:HG3	2.11	0.50
1:C:446:MSE:HG2	1:C:556:VAL:HG13	1.93	0.49
1:D:554:GLU:OE1	1:D:558:LYS:HE3	2.12	0.49
1:C:59:TYR:HB3	1:C:65:ARG:HD3	1.95	0.49
1:D:246:SER:C	1:D:247:SER:O	2.51	0.49
1:D:618:ALA:O	1:D:625:LYS:HA	2.13	0.48
1:C:446:MSE:CE	1:C:560:LEU:HD21	2.38	0.48
1:D:406:PHE:HB2	1:D:464:MSE:CE	2.44	0.48
1:B:434:PHE:HZ	1:B:557:MSE:SE	2.45	0.48
1:A:406:PHE:HB2	1:A:464:MSE:CE	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:MSE:CE	1:A:560:LEU:HD21	2.38	0.48
1:A:554:GLU:OE1	1:A:558:LYS:HE3	2.13	0.47
1:A:618:ALA:O	1:A:625:LYS:HA	2.14	0.47
1:A:109:SER:HB3	1:A:156:GLU:HA	1.95	0.47
1:D:406:PHE:CD1	1:D:464:MSE:HE1	2.49	0.47
1:B:384:TYR:OH	1:B:544:GLU:OE2	2.27	0.47
1:A:406:PHE:CD1	1:A:464:MSE:HE1	2.49	0.47
1:D:434:PHE:HZ	1:D:557:MSE:SE	2.48	0.47
1:A:401:ARG:HD2	6:A:947:HOH:O	2.14	0.46
1:C:66:ARG:HG2	1:C:378:TRP:CE2	2.51	0.46
1:C:375:ASP:HB3	1:C:730:ILE:CD1	2.46	0.46
1:C:554:GLU:OE1	1:C:558:LYS:HE3	2.16	0.46
1:C:618:ALA:O	1:C:625:LYS:HA	2.15	0.46
1:C:231:MSE:HE2	1:C:253:LEU:HD23	1.97	0.45
1:B:618:ALA:O	1:B:625:LYS:HA	2.15	0.45
1:C:607:ARG:HA	1:C:607:ARG:HD3	1.85	0.44
1:A:369:VAL:HG21	1:A:377:LEU:HB2	1.99	0.44
1:D:227:LEU:HG	1:D:231:MSE:HE2	2.00	0.44
1:D:385:ARG:NH1	6:D:920:HOH:O	2.50	0.44
1:D:233:GLU:HB3	1:D:267:LYS:HE3	2.00	0.44
1:C:406:PHE:HB2	1:C:464:MSE:CE	2.47	0.44
1:A:298:ILE:O	1:A:302:MSE:HG3	2.18	0.43
1:B:537:GLY:HA3	1:B:590:PHE:CZ	2.53	0.43
1:D:248:GLU:O	1:D:249:ASP:HB2	2.18	0.43
1:D:375:ASP:HB3	1:D:730:ILE:CD1	2.48	0.43
1:C:362:GLU:OE1	1:C:385:ARG:NH1	2.51	0.43
1:D:403:THR:HB	6:D:902:HOH:O	2.18	0.43
1:A:607:ARG:HD3	1:A:607:ARG:HA	1.87	0.43
1:C:403:THR:HB	6:C:903:HOH:O	2.18	0.43
1:D:421:TYR:CD1	1:D:436:VAL:HG22	2.54	0.42
1:D:537:GLY:HA3	1:D:590:PHE:CZ	2.54	0.42
1:B:66:ARG:HG2	1:B:378:TRP:CE2	2.54	0.42
1:C:537:GLY:HA3	1:C:590:PHE:CZ	2.54	0.42
1:D:505:GLN:HE21	1:D:505:GLN:HB3	1.68	0.42
1:A:421:TYR:CD1	1:A:436:VAL:HG22	2.54	0.42
1:B:385:ARG:HA	1:B:385:ARG:NH1	2.34	0.42
1:D:446:MSE:CE	1:D:560:LEU:HD21	2.40	0.42
1:C:455:ASN:OD1	1:D:385:ARG:NH2	2.53	0.42
1:B:505:GLN:HG2	1:B:509:GLN:NE2	2.33	0.42
1:A:344:GLU:OE2	1:C:694:GLU:OE2	2.38	0.42
1:B:385:ARG:HA	1:B:385:ARG:HH11	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:558:LYS:HE2	6:B:1136:HOH:O	2.19	0.42
1:C:554:GLU:CD	1:C:558:LYS:HE3	2.44	0.42
1:A:525:LYS:HB3	1:A:525:LYS:HE3	1.80	0.41
1:B:607:ARG:HA	1:B:607:ARG:HD3	1.82	0.41
1:A:375:ASP:HB3	1:A:730:ILE:CD1	2.50	0.41
1:D:446:MSE:HE2	1:D:446:MSE:HB2	1.90	0.41
1:C:421:TYR:CD1	1:C:436:VAL:HG22	2.56	0.41
1:D:607:ARG:HD3	1:D:607:ARG:HA	1.85	0.41
1:A:66:ARG:HG2	1:A:378:TRP:CE2	2.55	0.41
1:A:375:ASP:HB3	1:A:730:ILE:HD11	2.03	0.41
1:B:375:ASP:HB3	1:B:730:ILE:CD1	2.51	0.41
1:D:66:ARG:HG2	1:D:378:TRP:CE2	2.56	0.41
1:C:272:LYS:HE3	1:C:296:ASP:OD1	2.21	0.41
1:C:540:ARG:HA	1:C:569:VAL:O	2.21	0.41
1:D:446:MSE:HE1	1:D:497:MSE:SE	2.71	0.41
1:A:384:TYR:OH	1:A:544:GLU:OE2	2.34	0.40
1:A:434:PHE:CZ	1:A:557:MSE:SE	3.24	0.40
1:C:464:MSE:HE2	1:C:464:MSE:HB3	2.02	0.40
1:D:398:LYS:NZ	6:D:907:HOH:O	2.45	0.40
1:C:369:VAL:HG21	1:C:377:LEU:HB2	2.02	0.40
1:A:661:ASN:C	1:A:661:ASN:HD22	2.28	0.40
1:B:406:PHE:HB2	1:B:464:MSE:CE	2.50	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	722/732 (99%)	709 (98%)	13 (2%)	0	100	100
1	B	722/732 (99%)	707 (98%)	15 (2%)	0	100	100
1	C	722/732 (99%)	711 (98%)	11 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	722/732 (99%)	708 (98%)	14 (2%)	0	100	100
All	All	2888/2928 (99%)	2835 (98%)	53 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	620/612 (101%)	611 (98%)	9 (2%)	57	75
1	B	620/612 (101%)	610 (98%)	10 (2%)	55	73
1	C	620/612 (101%)	611 (98%)	9 (2%)	57	75
1	D	620/612 (101%)	610 (98%)	10 (2%)	55	73
All	All	2480/2448 (101%)	2442 (98%)	38 (2%)	57	75

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	ARG
1	A	312	GLN
1	A	368	GLU
1	A	385	ARG
1	A	399	LEU
1	A	525	LYS
1	A	571	ARG
1	A	661	ASN
1	A	755	GLU
1	B	66	ARG
1	B	98	VAL
1	B	246	SER
1	B	312	GLN
1	B	331	LYS
1	B	385	ARG
1	B	399	LEU

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Mol	Chain	Res	Type
1	B	437	ARG
1	B	571	ARG
1	B	631	THR
1	C	66	ARG
1	C	246	SER
1	C	312	GLN
1	C	399	LEU
1	C	413	PRO
1	C	438	LYS
1	C	509	GLN
1	C	520	LYS
1	C	669	LEU
1	D	66	ARG
1	D	246	SER
1	D	312	GLN
1	D	385	ARG
1	D	399	LEU
1	D	437	ARG
1	D	505	GLN
1	D	510	GLU
1	D	520	LYS
1	D	755	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	587	GLN
1	A	661	ASN
1	A	701	ASN
1	B	509	GLN
1	B	529	ASN
1	B	645	ASN
1	C	645	ASN
1	D	262	GLN
1	D	505	GLN
1	D	509	GLN
1	D	701	ASN

5.3.3 RNA ⓘ

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 17 ligands modelled in this entry, 8 are monoatomic - leaving 9 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	GOL	A	805	-	5,5,5	0.24	0	5,5,5	0.74	0
4	P6G	A	803	-	18,18,18	0.50	0	17,17,17	0.51	0
5	GOL	C	804	-	5,5,5	0.10	0	5,5,5	0.36	0
5	GOL	B	804	-	5,5,5	0.18	0	5,5,5	0.49	0
5	GOL	D	803	-	5,5,5	0.15	0	5,5,5	0.32	0
5	GOL	A	804	-	5,5,5	0.11	0	5,5,5	0.55	0
4	P6G	B	803	-	18,18,18	0.45	0	17,17,17	0.67	0
5	GOL	D	804	-	5,5,5	0.16	0	5,5,5	0.46	0
5	GOL	C	803	-	5,5,5	0.22	0	5,5,5	0.52	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	805	-	-	4/4/4/4	-
4	P6G	A	803	-	-	5/16/16/16	-
5	GOL	C	804	-	-	3/4/4/4	-
5	GOL	B	804	-	-	0/4/4/4	-
5	GOL	D	803	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	804	-	-	2/4/4/4	-
4	P6G	B	803	-	-	4/16/16/16	-
5	GOL	D	804	-	-	4/4/4/4	-
5	GOL	C	803	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	804	GOL	O1-C1-C2-C3
5	A	805	GOL	O1-C1-C2-C3
5	C	804	GOL	C1-C2-C3-O3
4	B	803	P6G	O1-C2-C3-O4
4	A	803	P6G	O1-C2-C3-O4
4	B	803	P6G	O16-C17-C18-O19
5	A	805	GOL	C1-C2-C3-O3
5	D	804	GOL	O1-C1-C2-C3
5	D	804	GOL	C1-C2-C3-O3
5	A	804	GOL	O1-C1-C2-O2
5	A	805	GOL	O1-C1-C2-O2
5	D	804	GOL	O2-C2-C3-O3
5	C	804	GOL	O2-C2-C3-O3
5	D	804	GOL	O1-C1-C2-O2
5	C	804	GOL	O1-C1-C2-O2
4	B	803	P6G	C14-C15-O16-C17
4	A	803	P6G	C18-C17-O16-C15
4	A	803	P6G	O13-C14-C15-O16
4	B	803	P6G	O13-C14-C15-O16
4	A	803	P6G	C8-C9-O10-C11
5	A	805	GOL	O2-C2-C3-O3
5	D	803	GOL	C1-C2-C3-O3
4	A	803	P6G	O16-C17-C18-O19

There are no ring outliers.

2 monomers are involved in 4 short contacts:

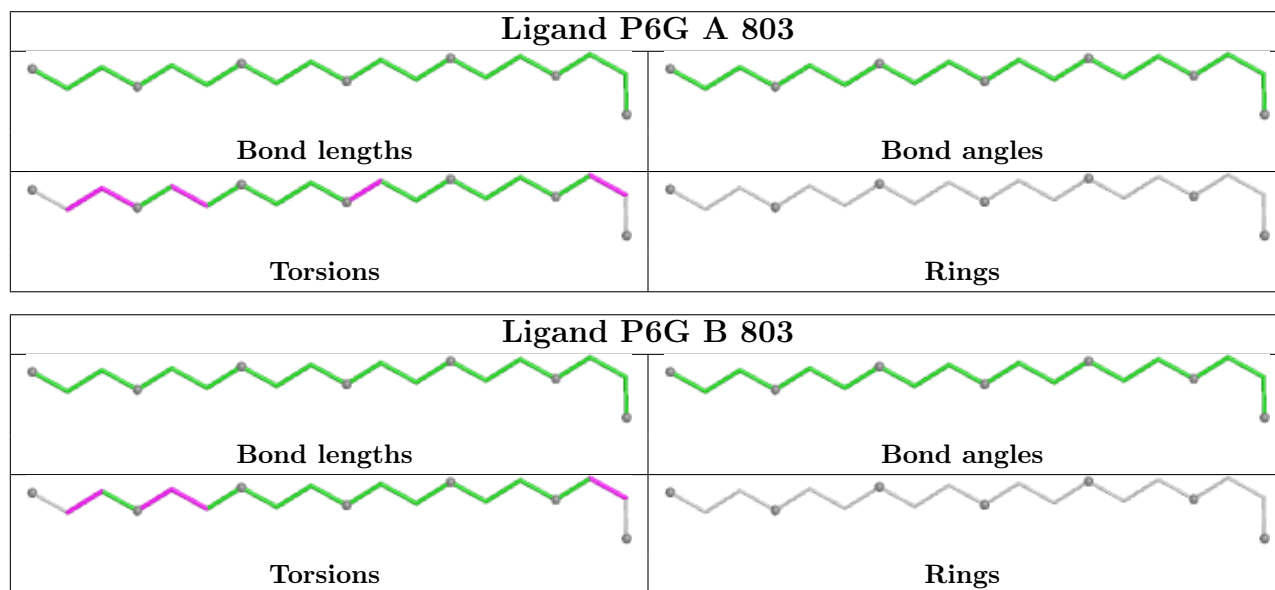
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	804	GOL	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	803	GOL	2	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	709/732 (96%)	-0.65	1 (0%) 92 91	15, 23, 39, 65	0
1	B	709/732 (96%)	-0.44	1 (0%) 92 91	18, 30, 52, 77	0
1	C	709/732 (96%)	-0.62	0 100 100	17, 24, 44, 68	0
1	D	709/732 (96%)	-0.56	1 (0%) 92 91	17, 27, 45, 90	0
2	E	0/5	-	-	-	-
2	F	0/5	-	-	-	-
2	G	0/5	-	-	-	-
2	H	0/5	-	-	-	-
All	All	2836/2948 (96%)	-0.57	3 (0%) 92 91	15, 26, 46, 90	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	164	ASP	2.7
1	A	163	ASP	2.3
1	D	248	GLU	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

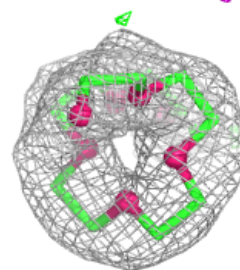
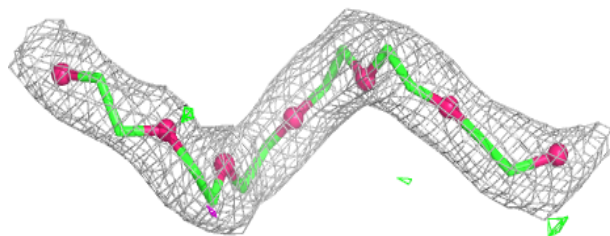
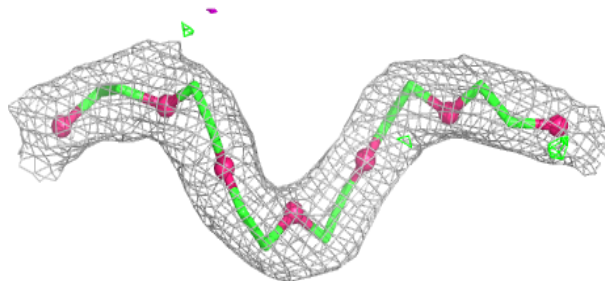
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	NA	C	802	1/1	0.72	0.11	47,47,47,47	0
5	GOL	A	805	6/6	0.81	0.12	41,44,48,52	0
5	GOL	C	804	6/6	0.81	0.11	43,45,48,51	0
3	NA	D	802	1/1	0.90	0.07	38,38,38,38	0
4	P6G	B	803	19/19	0.91	0.09	37,41,48,50	0
4	P6G	A	803	19/19	0.92	0.09	39,44,50,51	0
5	GOL	D	804	6/6	0.92	0.08	39,42,43,43	0
5	GOL	B	804	6/6	0.94	0.09	30,33,34,36	0
5	GOL	A	804	6/6	0.94	0.07	22,27,28,28	0
3	NA	B	802	1/1	0.94	0.04	36,36,36,36	0
5	GOL	D	803	6/6	0.95	0.06	25,27,28,30	0
5	GOL	C	803	6/6	0.95	0.07	24,26,27,30	0
3	NA	C	801	1/1	0.96	0.04	25,25,25,25	0
3	NA	B	801	1/1	0.98	0.03	29,29,29,29	0
3	NA	D	801	1/1	0.98	0.03	23,23,23,23	0
3	NA	A	801	1/1	0.98	0.03	21,21,21,21	0
3	NA	A	802	1/1	0.98	0.02	34,34,34,34	0

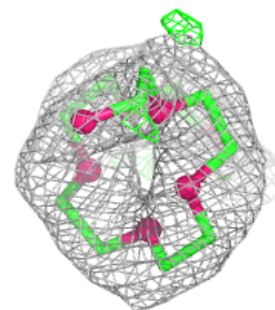
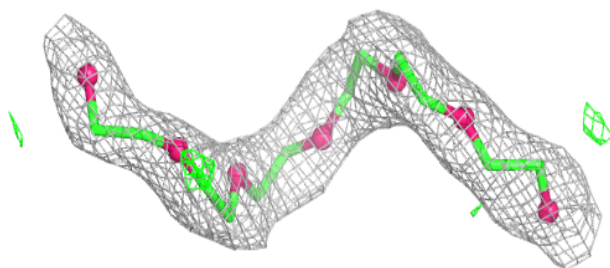
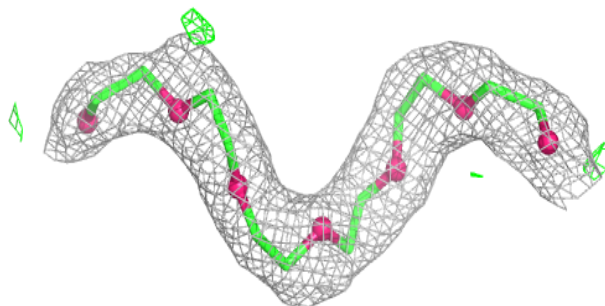
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around P6G B 803:

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

**Electron density around P6G A 803:**

$2mF_o-DF_c$ (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.