



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 08:01 pm BST

PDB ID : 4KTR
Title : Crystal structure of 2-O-alpha-glucosylglycerol phosphorylase in complex with isofagomine and glycerol
Authors : Touhara, K.K.; Nihira, T.; Kitaoka, M.; Nakai, H.; Fushinobu, S.
Deposited on : 2013-05-21
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
buster-report : 1.1.7 (2018)
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

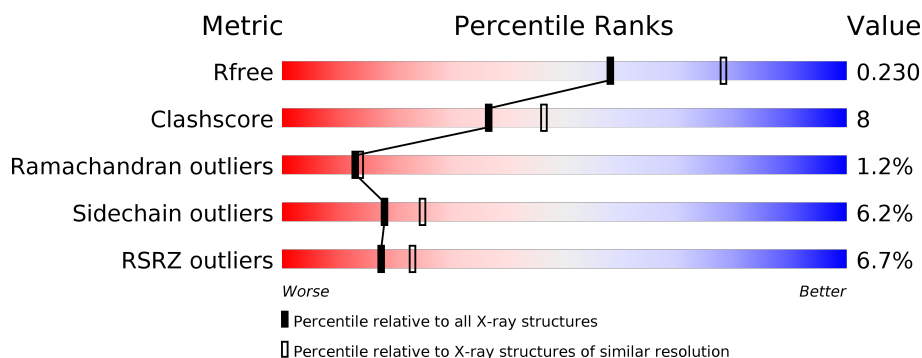
1 Overall quality at a glance

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	769	<div> <div>2%</div> <div>82% 14% ...</div> </div>
1	B	769	<div> <div>4%</div> <div>81% 16% ...</div> </div>
1	C	769	<div> <div>4%</div> <div>80% 16% ...</div> </div>
1	D	769	<div> <div>4%</div> <div>80% 17% ..</div> </div>
1	E	769	<div> <div>14%</div> <div>75% 20% ..</div> </div>
1	F	769	<div> <div>7%</div> <div>79% 17% ..</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	769	
1	H	769	

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
4	GOL	B	804	-	X	X	-
4	GOL	D	809	-	-	X	-
4	GOL	H	807	-	-	X	-
6	PGE	A	812	-	-	X	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 51264 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 Glycoside hydrolase family 65 central catalytic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	762	Total	C	N	O	S	0	0	0
			6093	3850	1036	1185	22			
1	B	761	Total	C	N	O	S	0	0	0
			6085	3844	1035	1184	22			
1	C	761	Total	C	N	O	S	0	0	0
			6085	3844	1035	1184	22			
1	D	761	Total	C	N	O	S	0	0	0
			6085	3844	1035	1184	22			
1	E	761	Total	C	N	O	S	0	0	0
			6085	3844	1035	1184	22			
1	F	761	Total	C	N	O	S	0	0	0
			6085	3844	1035	1184	22			
1	G	762	Total	C	N	O	S	0	0	0
			6093	3850	1036	1185	22			
1	H	761	Total	C	N	O	S	0	0	0
			6085	3844	1035	1184	22			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	475	GLN	GLU	ENGINEERED MUTATION	UNP D6XZ22
A	762	LEU	-	EXPRESSION TAG	UNP D6XZ22
A	763	GLU	-	EXPRESSION TAG	UNP D6XZ22
A	764	HIS	-	EXPRESSION TAG	UNP D6XZ22
A	765	HIS	-	EXPRESSION TAG	UNP D6XZ22
A	766	HIS	-	EXPRESSION TAG	UNP D6XZ22
A	767	HIS	-	EXPRESSION TAG	UNP D6XZ22
A	768	HIS	-	EXPRESSION TAG	UNP D6XZ22
A	769	HIS	-	EXPRESSION TAG	UNP D6XZ22
B	475	GLN	GLU	ENGINEERED MUTATION	UNP D6XZ22
B	762	LEU	-	EXPRESSION TAG	UNP D6XZ22
B	763	GLU	-	EXPRESSION TAG	UNP D6XZ22
B	764	HIS	-	EXPRESSION TAG	UNP D6XZ22

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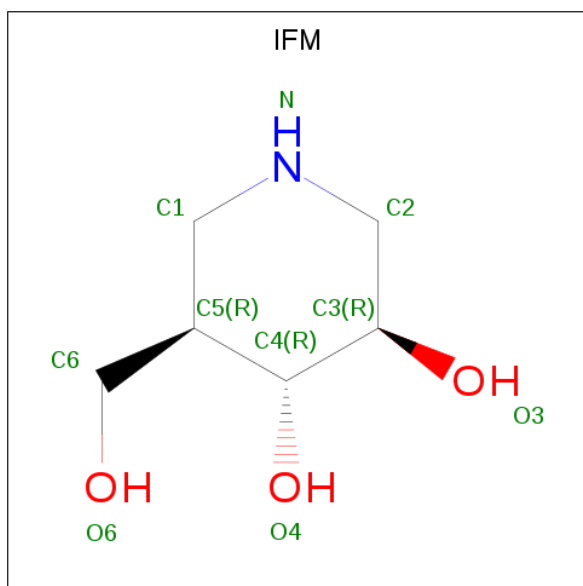
Chain	Residue	Modelled	Actual	Comment	Reference
B	765	HIS	-	EXPRESSION TAG	UNP D6XZ22
B	766	HIS	-	EXPRESSION TAG	UNP D6XZ22
B	767	HIS	-	EXPRESSION TAG	UNP D6XZ22
B	768	HIS	-	EXPRESSION TAG	UNP D6XZ22
B	769	HIS	-	EXPRESSION TAG	UNP D6XZ22
C	475	GLN	GLU	ENGINEERED MUTATION	UNP D6XZ22
C	762	LEU	-	EXPRESSION TAG	UNP D6XZ22
C	763	GLU	-	EXPRESSION TAG	UNP D6XZ22
C	764	HIS	-	EXPRESSION TAG	UNP D6XZ22
C	765	HIS	-	EXPRESSION TAG	UNP D6XZ22
C	766	HIS	-	EXPRESSION TAG	UNP D6XZ22
C	767	HIS	-	EXPRESSION TAG	UNP D6XZ22
C	768	HIS	-	EXPRESSION TAG	UNP D6XZ22
C	769	HIS	-	EXPRESSION TAG	UNP D6XZ22
D	475	GLN	GLU	ENGINEERED MUTATION	UNP D6XZ22
D	762	LEU	-	EXPRESSION TAG	UNP D6XZ22
D	763	GLU	-	EXPRESSION TAG	UNP D6XZ22
D	764	HIS	-	EXPRESSION TAG	UNP D6XZ22
D	765	HIS	-	EXPRESSION TAG	UNP D6XZ22
D	766	HIS	-	EXPRESSION TAG	UNP D6XZ22
D	767	HIS	-	EXPRESSION TAG	UNP D6XZ22
D	768	HIS	-	EXPRESSION TAG	UNP D6XZ22
D	769	HIS	-	EXPRESSION TAG	UNP D6XZ22
E	475	GLN	GLU	ENGINEERED MUTATION	UNP D6XZ22
E	762	LEU	-	EXPRESSION TAG	UNP D6XZ22
E	763	GLU	-	EXPRESSION TAG	UNP D6XZ22
E	764	HIS	-	EXPRESSION TAG	UNP D6XZ22
E	765	HIS	-	EXPRESSION TAG	UNP D6XZ22
E	766	HIS	-	EXPRESSION TAG	UNP D6XZ22
E	767	HIS	-	EXPRESSION TAG	UNP D6XZ22
E	768	HIS	-	EXPRESSION TAG	UNP D6XZ22
E	769	HIS	-	EXPRESSION TAG	UNP D6XZ22
F	475	GLN	GLU	ENGINEERED MUTATION	UNP D6XZ22
F	762	LEU	-	EXPRESSION TAG	UNP D6XZ22
F	763	GLU	-	EXPRESSION TAG	UNP D6XZ22
F	764	HIS	-	EXPRESSION TAG	UNP D6XZ22
F	765	HIS	-	EXPRESSION TAG	UNP D6XZ22
F	766	HIS	-	EXPRESSION TAG	UNP D6XZ22
F	767	HIS	-	EXPRESSION TAG	UNP D6XZ22
F	768	HIS	-	EXPRESSION TAG	UNP D6XZ22
F	769	HIS	-	EXPRESSION TAG	UNP D6XZ22
G	475	GLN	GLU	ENGINEERED MUTATION	UNP D6XZ22

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Chain	Residue	Modelled	Actual	Comment	Reference
G	762	LEU	-	EXPRESSION TAG	UNP D6XZ22
G	763	GLU	-	EXPRESSION TAG	UNP D6XZ22
G	764	HIS	-	EXPRESSION TAG	UNP D6XZ22
G	765	HIS	-	EXPRESSION TAG	UNP D6XZ22
G	766	HIS	-	EXPRESSION TAG	UNP D6XZ22
G	767	HIS	-	EXPRESSION TAG	UNP D6XZ22
G	768	HIS	-	EXPRESSION TAG	UNP D6XZ22
G	769	HIS	-	EXPRESSION TAG	UNP D6XZ22
H	475	GLN	GLU	ENGINEERED MUTATION	UNP D6XZ22
H	762	LEU	-	EXPRESSION TAG	UNP D6XZ22
H	763	GLU	-	EXPRESSION TAG	UNP D6XZ22
H	764	HIS	-	EXPRESSION TAG	UNP D6XZ22
H	765	HIS	-	EXPRESSION TAG	UNP D6XZ22
H	766	HIS	-	EXPRESSION TAG	UNP D6XZ22
H	767	HIS	-	EXPRESSION TAG	UNP D6XZ22
H	768	HIS	-	EXPRESSION TAG	UNP D6XZ22
H	769	HIS	-	EXPRESSION TAG	UNP D6XZ22

- Molecule 2 is 5-HYDROXYMETHYL-3,4-DIHYDROXYPIPERIDINE (three-letter code: IFM) (formula: $C_6H_{13}NO_3$).



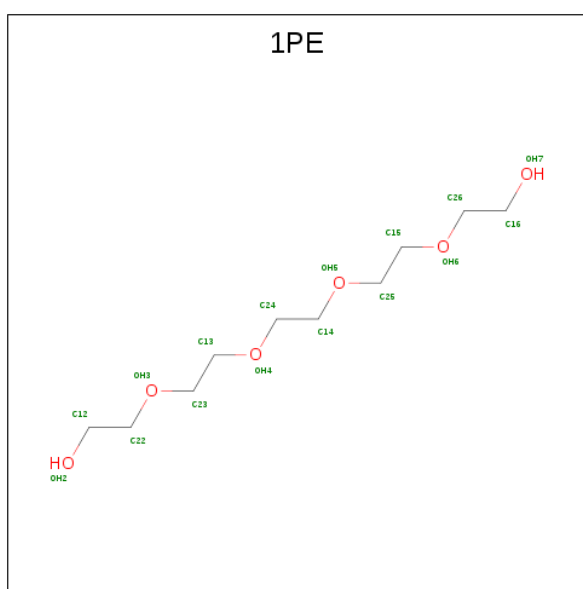
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	6	1	3		
2	D	1	Total	C	N	O	0	0
			10	6	1	3		

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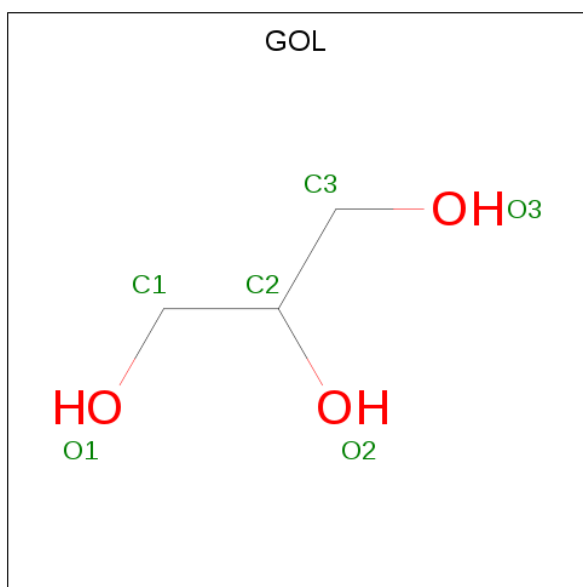
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	E	1	Total	C	N	O	0	0
			10	6	1	3		
2	F	1	Total	C	N	O	0	0
			10	6	1	3		
2	G	1	Total	C	N	O	0	0
			10	6	1	3		
2	H	1	Total	C	N	O	0	0
			10	6	1	3		

- Molecule 3 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			16	10	6		
3	C	1	Total	C	O	0	0
			16	10	6		
3	E	1	Total	C	O	0	0
			16	10	6		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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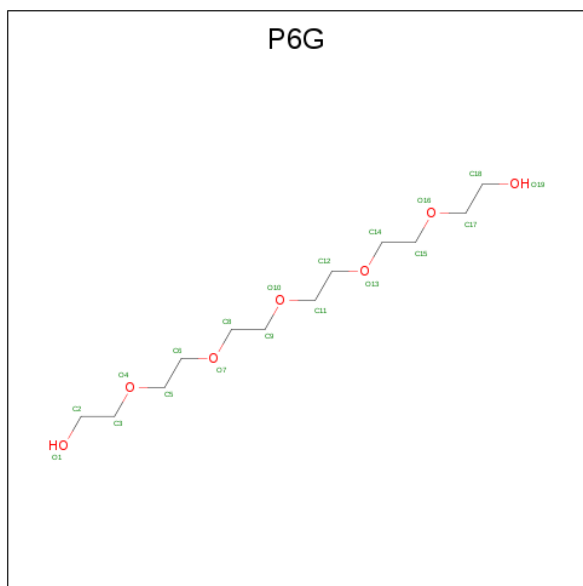
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		

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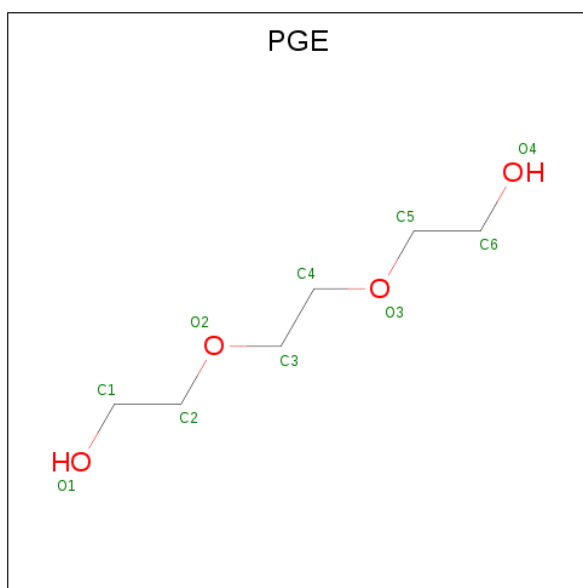
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	F	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: C₁₂H₂₆O₇).



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

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

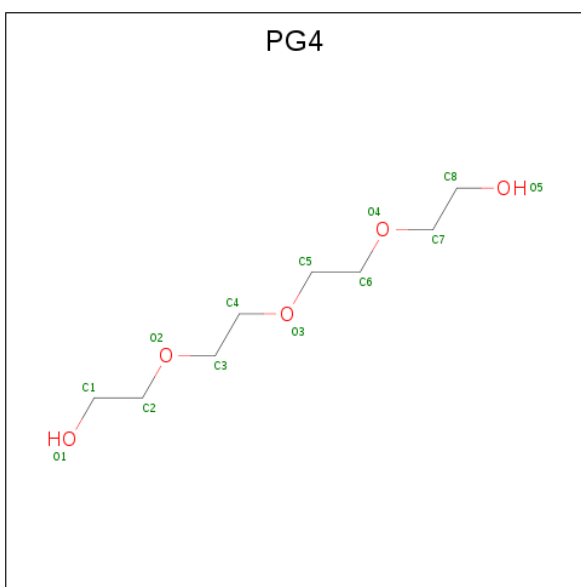


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			10	6	4		
6	C	1	Total	C	O	0	0
			10	6	4		
6	F	1	Total	C	O	0	0
			10	6	4		
6	G	1	Total	C	O	0	0
			10	6	4		

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

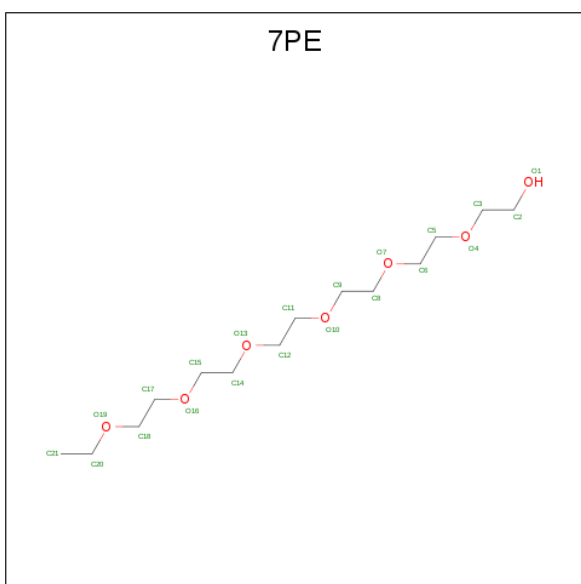
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	G	1	Total	Ca	0	0
			1	1		
7	D	2	Total	Ca	0	0
			2	2		
7	E	1	Total	Ca	0	0
			1	1		
7	B	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		
7	A	1	Total	Ca	0	0
			1	1		

- Molecule 8 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



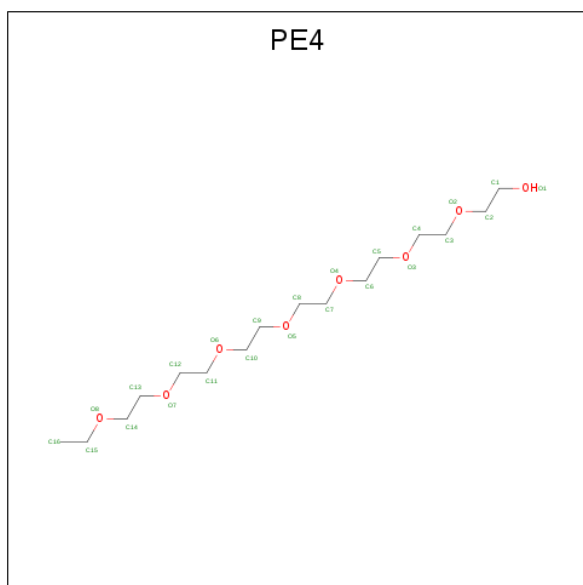
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			13	8	5		
8	D	1	Total	C	O	0	0
			13	8	5		
8	F	1	Total	C	O	0	0
			13	8	5		
8	H	1	Total	C	O	0	0
			13	8	5		

- Molecule 9 is 2-(2-(2-(2-(2-(2-ETHOXYETHOXY)ETHOXY)ETHOXY)ETHOXY)ETHOXY)ETHANOL (three-letter code: 7PE) (formula: C₁₄H₃₀O₇).



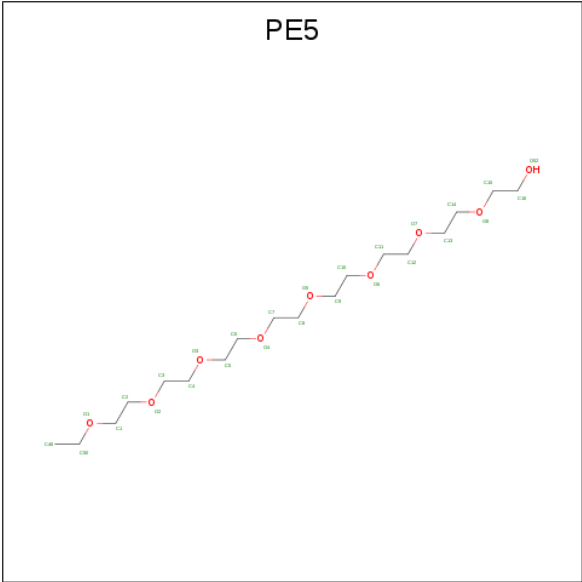
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			21	14	7		
9	D	1	Total	C	O	0	0
			21	14	7		

- Molecule 10 is 2-{2-[2-(2-{2-[2-(2-ETHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHOXY)-ETHOXY]-ETHOXY}-ETHANOL (three-letter code: PE4) (formula: C₁₆H₃₄O₈).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	C	1	Total	C	O	0	0
			24	16	8		

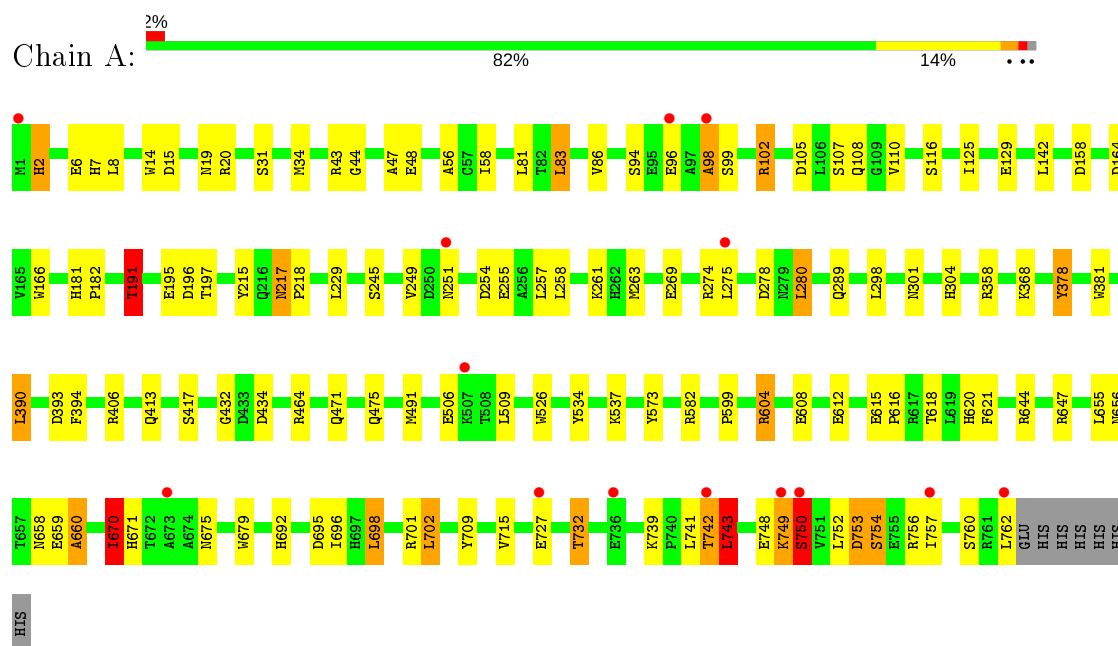
- Molecule 11 is 3,6,9,12,15,18,21,24-OCTAOXAHEXACOSAN-1-OL (three-letter code: PE5) (formula: C₁₈H₃₈O₉).



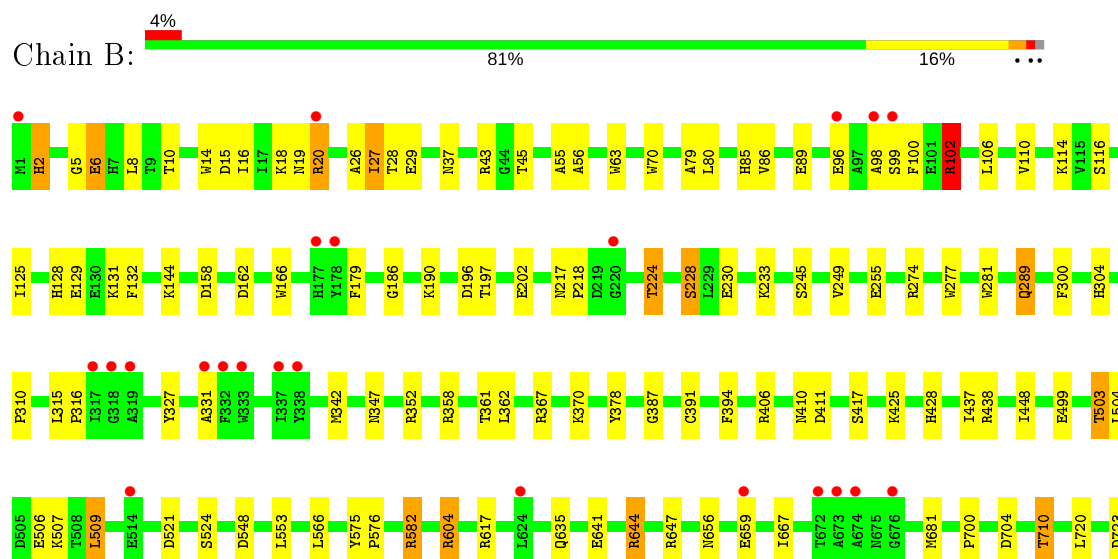
3 Residue-property plots [i](#)

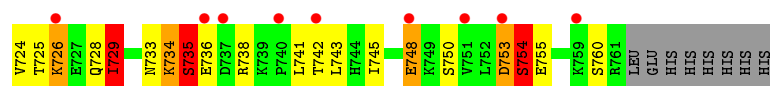
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Glycoside hydrolase family 65 central catalytic



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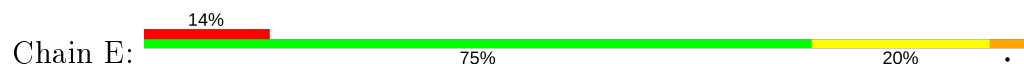
- Molecule 1: Glycoside hydrolase family 65 central catalytic



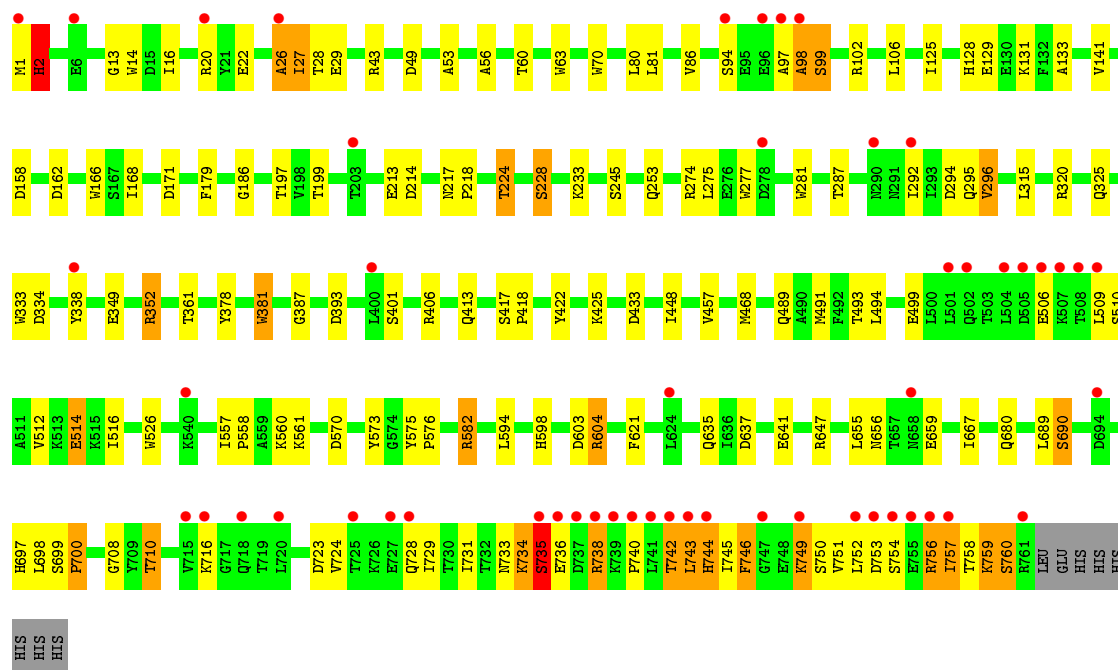
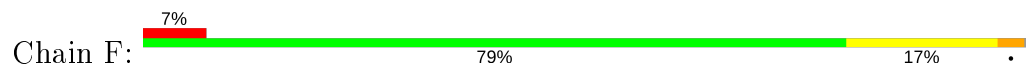
- Molecule 1: Glycoside hydrolase family 65 central catalytic



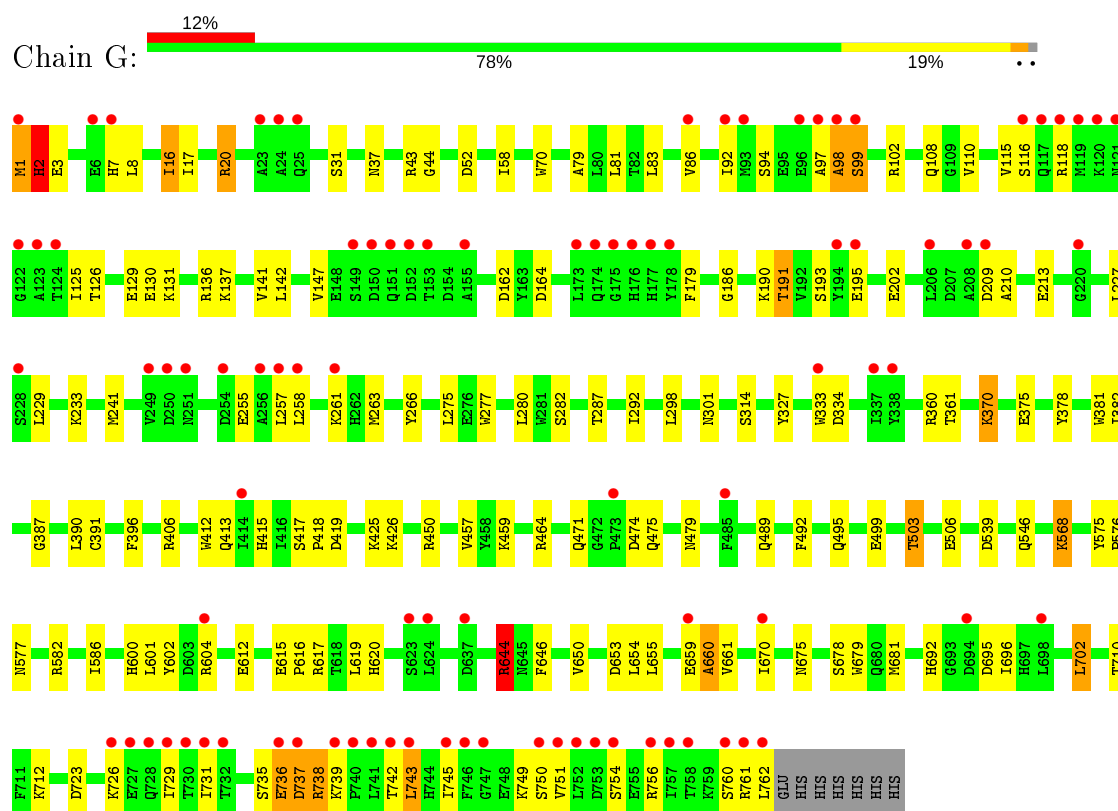
- Molecule 1: Glycoside hydrolase family 65 central catalytic



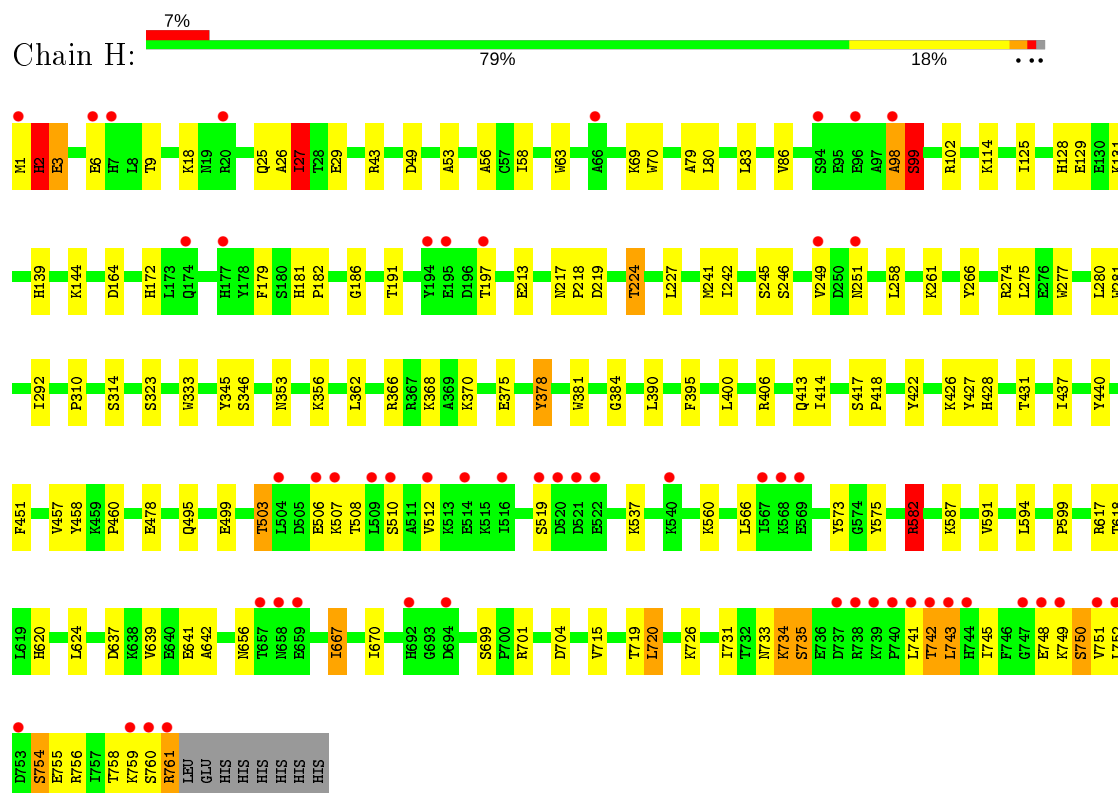
- Molecule 1: Glycoside hydrolase family 65 central catalytic



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• Molecule 1: Glycoside hydrolase family 65 central catalytic



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	109.00Å 263.21Å 138.79Å 90.00° 105.45° 90.00°	Depositor
Resolution (Å)	48.99 – 2.30 48.99 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.99-2.30) 99.8 (48.99-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.167 , 0.228 0.168 , 0.230	Depositor DCC
R_{free} test set	16702 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	37.3	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 65.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	51264	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.17% 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, PGE, PE4, PE5, CA, 1PE, PG4, P6G, IFM, 7PE

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	0.99	6/6236 (0.1%)	0.98	14/8456 (0.2%)
1	B	0.97	8/6228 (0.1%)	0.99	26/8445 (0.3%)
1	C	0.99	3/6228 (0.0%)	0.99	20/8445 (0.2%)
1	D	1.01	5/6228 (0.1%)	1.00	21/8445 (0.2%)
1	E	0.85	6/6228 (0.1%)	0.90	15/8445 (0.2%)
1	F	0.87	9/6228 (0.1%)	0.91	4/8445 (0.0%)
1	G	0.83	4/6236 (0.1%)	0.88	8/8456 (0.1%)
1	H	0.84	3/6228 (0.0%)	0.87	4/8445 (0.0%)
All	All	0.92	44/49840 (0.1%)	0.94	112/67582 (0.2%)

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	A	0	2
1	C	0	2
1	F	0	1
1	G	0	1
All	All	0	6

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	63	TRP	CD2-CE2	7.43	1.50	1.41
1	B	754	SER	CB-OG	6.83	1.51	1.42
1	E	70	TRP	CD2-CE2	6.81	1.49	1.41
1	F	333	TRP	CD2-CE2	6.40	1.49	1.41
1	F	63	TRP	CD2-CE2	6.39	1.49	1.41
1	C	333	TRP	CD2-CE2	6.38	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	333	TRP	CD2-CE2	6.30	1.49	1.41
1	F	166	TRP	CD2-CE2	6.25	1.48	1.41
1	F	281	TRP	CD2-CE2	6.19	1.48	1.41
1	E	412	TRP	CD2-CE2	6.19	1.48	1.41
1	G	333	TRP	CD2-CE2	6.05	1.48	1.41
1	B	70	TRP	CD2-CE2	6.01	1.48	1.41
1	H	281	TRP	CD2-CE2	5.96	1.48	1.41
1	A	14	TRP	CD2-CE2	5.94	1.48	1.41
1	B	14	TRP	CD2-CE2	5.85	1.48	1.41
1	B	166	TRP	CD2-CE2	5.84	1.48	1.41
1	G	70	TRP	CD2-CE2	5.82	1.48	1.41
1	H	63	TRP	CD2-CE2	5.80	1.48	1.41
1	F	70	TRP	CD2-CE2	5.80	1.48	1.41
1	B	304	HIS	CG-CD2	5.78	1.45	1.35
1	D	277	TRP	CD2-CE2	5.76	1.48	1.41
1	B	281	TRP	CD2-CE2	5.75	1.48	1.41
1	E	679	TRP	CD2-CE2	5.74	1.48	1.41
1	A	381	TRP	CD2-CE2	5.73	1.48	1.41
1	E	63	TRP	CD2-CE2	5.66	1.48	1.41
1	A	679	TRP	CD2-CE2	5.51	1.48	1.41
1	B	277	TRP	CD2-CE2	5.50	1.48	1.41
1	D	526	TRP	CD2-CE2	5.49	1.48	1.41
1	F	14	TRP	CD2-CE2	5.41	1.47	1.41
1	G	277	TRP	CD2-CE2	5.40	1.47	1.41
1	G	679	TRP	CD2-CE2	5.38	1.47	1.41
1	D	281	TRP	CD2-CE2	5.35	1.47	1.41
1	D	678	SER	CB-OG	5.30	1.49	1.42
1	F	526	TRP	CD2-CE2	5.25	1.47	1.41
1	F	381	TRP	CD2-CE2	5.22	1.47	1.41
1	C	63	TRP	CD2-CE2	5.19	1.47	1.41
1	E	381	TRP	CD2-CE2	5.17	1.47	1.41
1	B	63	TRP	CD2-CE2	5.17	1.47	1.41
1	C	381	TRP	CD2-CE2	5.17	1.47	1.41
1	F	277	TRP	CD2-CE2	5.15	1.47	1.41
1	A	166	TRP	CD2-CE2	5.11	1.47	1.41
1	E	333	TRP	CD2-CE2	5.09	1.47	1.41
1	A	191	THR	CB-CG2	-5.05	1.35	1.52
1	A	526	TRP	CD2-CE2	5.03	1.47	1.41

All (112) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	102	ARG	NE-CZ-NH2	12.77	126.69	120.30
1	D	102	ARG	NE-CZ-NH1	-11.92	114.34	120.30
1	A	670	ILE	CG1-CB-CG2	-11.80	85.43	111.40
1	E	438	ARG	NE-CZ-NH1	-9.91	115.35	120.30
1	B	644	ARG	NE-CZ-NH1	9.13	124.86	120.30
1	E	438	ARG	NE-CZ-NH2	8.85	124.72	120.30
1	C	406	ARG	NE-CZ-NH1	8.59	124.60	120.30
1	C	352	ARG	NE-CZ-NH1	8.40	124.50	120.30
1	C	406	ARG	NE-CZ-NH2	-8.14	116.23	120.30
1	A	406	ARG	NE-CZ-NH1	8.08	124.34	120.30
1	E	406	ARG	NE-CZ-NH1	7.95	124.28	120.30
1	B	644	ARG	NE-CZ-NH2	-7.84	116.38	120.30
1	D	16	ILE	CG1-CB-CG2	-7.81	94.23	111.40
1	A	15	ASP	CB-CG-OD1	7.70	125.23	118.30
1	A	406	ARG	NE-CZ-NH2	-7.56	116.52	120.30
1	E	406	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	D	43	ARG	NE-CZ-NH1	-7.44	116.58	120.30
1	B	102	ARG	NE-CZ-NH1	-7.34	116.63	120.30
1	B	102	ARG	NE-CZ-NH2	7.24	123.92	120.30
1	C	411	ASP	CB-CG-OD2	7.12	124.71	118.30
1	D	43	ARG	NE-CZ-NH2	7.05	123.82	120.30
1	B	729	ILE	CB-CA-C	-6.97	97.66	111.60
1	D	539	ASP	CB-CG-OD1	6.93	124.53	118.30
1	C	670	ILE	CG1-CB-CG2	-6.90	96.21	111.40
1	H	582	ARG	NE-CZ-NH2	6.82	123.71	120.30
1	D	15	ASP	CB-CG-OD1	6.80	124.42	118.30
1	B	367	ARG	NE-CZ-NH1	6.65	123.62	120.30
1	A	390	LEU	CB-CG-CD1	6.64	122.28	111.00
1	C	698	LEU	CA-CB-CG	6.59	130.45	115.30
1	B	358	ARG	NE-CZ-NH2	-6.55	117.02	120.30
1	D	223	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	B	617	ARG	NE-CZ-NH1	-6.53	117.03	120.30
1	B	15	ASP	CB-CG-OD1	6.50	124.15	118.30
1	B	521	ASP	CB-CG-OD1	6.44	124.10	118.30
1	C	644	ARG	NE-CZ-NH2	6.41	123.50	120.30
1	F	393	ASP	CB-CG-OD1	6.37	124.03	118.30
1	C	565	ARG	NE-CZ-NH2	-6.33	117.13	120.30
1	A	698	LEU	CA-CB-CG	6.33	129.85	115.30
1	G	464	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	G	644	ARG	NE-CZ-NH2	6.19	123.39	120.30
1	F	433	ASP	CB-CG-OD1	6.17	123.85	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	320	ARG	NE-CZ-NH1	6.17	123.38	120.30
1	G	702	LEU	CA-CB-CG	6.14	129.42	115.30
1	D	158	ASP	CB-CG-OD1	6.13	123.81	118.30
1	E	105	ASP	CB-CG-OD2	-6.08	112.83	118.30
1	D	8	LEU	CA-CB-CG	6.06	129.23	115.30
1	E	390	LEU	CB-CG-CD1	6.00	121.20	111.00
1	B	548	ASP	CB-CG-OD1	5.99	123.69	118.30
1	D	644	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	A	358	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	B	158	ASP	CB-CG-OD1	5.89	123.60	118.30
1	D	433	ASP	CB-CG-OD1	5.89	123.60	118.30
1	D	411	ASP	CB-CG-OD2	5.83	123.55	118.30
1	B	753	ASP	N-CA-C	-5.76	95.44	111.00
1	D	358	ARG	NE-CZ-NH2	-5.75	117.42	120.30
1	A	743	LEU	CA-CB-CG	5.74	128.49	115.30
1	H	406	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	B	274	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	D	105	ASP	CB-CG-OD1	5.71	123.44	118.30
1	B	362	LEU	CA-CB-CG	5.67	128.34	115.30
1	H	617	ARG	NE-CZ-NH1	-5.63	117.48	120.30
1	C	644	ARG	NE-CZ-NH1	-5.55	117.53	120.30
1	B	162	ASP	CB-CG-OD1	5.54	123.28	118.30
1	G	450	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	B	667	ILE	CG1-CB-CG2	5.50	123.49	111.40
1	A	280	LEU	CA-CB-CG	5.48	127.91	115.30
1	C	257	LEU	CA-CB-CG	5.47	127.89	115.30
1	C	362	LEU	CA-CB-CG	5.47	127.88	115.30
1	D	102	ARG	CD-NE-CZ	5.46	131.24	123.60
1	C	403	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	B	566	LEU	CB-CG-CD1	-5.44	101.75	111.00
1	B	358	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	B	406	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	D	433	ASP	CB-CG-OD2	-5.38	113.46	118.30
1	E	320	ARG	NE-CZ-NH1	-5.37	117.61	120.30
1	B	8	LEU	CA-CB-CG	5.37	127.65	115.30
1	E	670	ILE	CG1-CB-CG2	-5.37	99.59	111.40
1	D	371	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	G	539	ASP	CB-CG-OD1	5.35	123.12	118.30
1	G	43	ARG	NE-CZ-NH1	-5.33	117.63	120.30
1	B	438	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	C	191	THR	N-CA-CB	-5.31	100.21	110.30
1	C	548	ASP	CB-CG-OD1	5.29	123.06	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	227	LEU	CA-CB-CG	5.29	127.46	115.30
1	C	411	ASP	CB-CG-OD1	-5.27	113.56	118.30
1	A	102	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	G	406	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	E	698	LEU	CA-CB-CG	5.25	127.39	115.30
1	A	393	ASP	CB-CG-OD1	5.25	123.03	118.30
1	B	411	ASP	CB-CG-OD2	5.25	123.02	118.30
1	B	274	ARG	NE-CZ-NH2	-5.25	117.68	120.30
1	H	227	LEU	CA-CB-CG	5.24	127.36	115.30
1	E	299	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	D	644	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	A	105	ASP	CB-CG-OD1	5.18	122.97	118.30
1	F	406	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	D	743	LEU	CA-CB-CG	5.12	127.06	115.30
1	B	162	ASP	CB-CG-OD2	-5.10	113.71	118.30
1	C	469	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	E	464	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	C	15	ASP	CB-CG-OD1	5.07	122.86	118.30
1	E	355	LEU	CB-CG-CD1	-5.07	102.39	111.00
1	A	8	LEU	CB-CG-CD1	-5.06	102.40	111.00
1	C	298	LEU	CB-CG-CD2	5.06	119.60	111.00
1	E	702	LEU	CA-CB-CG	5.05	126.92	115.30
1	E	299	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	D	227	LEU	CB-CA-C	-5.03	100.64	110.20
1	G	164	ASP	CB-CG-OD2	-5.03	113.78	118.30
1	A	698	LEU	CB-CG-CD1	5.02	119.54	111.00
1	E	411	ASP	CB-CG-OD2	5.02	122.82	118.30
1	B	647	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	C	641	GLU	OE1-CD-OE2	5.01	129.32	123.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2	HIS	Peptide
1	A	748	GLU	Peptide
1	C	1	MET	Peptide
1	C	694	ASP	Peptide
1	F	26	ALA	Peptide
1	G	1	MET	Peptide

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	6093	0	5855	81	0
1	B	6085	0	5844	94	0
1	C	6085	0	5844	88	0
1	D	6085	0	5844	76	0
1	E	6085	0	5844	108	0
1	F	6085	0	5844	113	0
1	G	6093	0	5855	96	0
1	H	6085	0	5844	104	0
2	A	10	0	13	4	0
2	D	10	0	12	3	0
2	E	10	0	13	0	0
2	F	10	0	13	2	0
2	G	10	0	13	3	0
2	H	10	0	13	1	0
3	A	16	0	22	0	0
3	C	16	0	22	1	0
3	E	16	0	22	2	0
4	A	48	0	64	12	0
4	B	36	0	47	9	0
4	C	36	0	48	2	0
4	D	54	0	72	14	0
4	E	24	0	32	1	0
4	F	18	0	24	2	0
4	G	18	0	24	4	0
4	H	30	0	40	10	0
5	A	19	0	26	3	0
5	E	19	0	26	5	0
6	A	10	0	14	7	0
6	C	10	0	14	0	0
6	F	10	0	14	2	0
6	G	10	0	14	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	2	0	0	0	0
7	E	1	0	0	0	0
7	G	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	13	0	18	1	0
8	D	13	0	18	1	0
8	F	13	0	18	0	0
8	H	13	0	18	1	0
9	B	21	0	30	5	0
9	D	21	0	30	3	0
10	C	24	0	34	6	0
11	H	27	0	38	12	0
12	A	182	0	0	8	0
12	B	303	0	0	8	0
12	C	286	0	0	10	0
12	D	348	0	0	11	0
12	E	185	0	0	8	0
12	F	247	0	0	13	0
12	G	197	0	0	3	0
12	H	218	0	0	7	0
All	All	51264	0	47580	765	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 8.

All (765) 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:801:IFM:H2C2	12:D:1243:HOH:O	1.38	1.23
2:A:801:IFM:H2C2	12:A:917:HOH:O	1.35	1.21
1:B:352:ARG:HD3	12:B:1019:HOH:O	1.45	1.17
1:A:278:ASP:HB3	12:A:1031:HOH:O	1.45	1.14
1:F:756:ARG:HG3	1:F:756:ARG:HH11	1.09	1.12
4:D:806:GOL:H2	12:D:1202:HOH:O	1.51	1.09
1:E:468:MET:HE1	12:E:974:HOH:O	1.51	1.08
1:E:737:ASP:HA	1:E:738:ARG:CB	1.85	1.06
1:H:599:PRO:HB3	11:H:808:PE5:H142	1.38	1.06
1:D:310:PRO:O	4:D:812:GOL:H11	1.59	1.03
1:H:213:GLU:HB3	1:H:224:THR:HG22	1.40	1.02
1:G:737:ASP:HA	1:G:738:ARG:HB2	1.40	1.00
1:F:604:ARG:HB3	1:F:604:ARG:HH11	1.27	1.00
1:E:737:ASP:HA	1:E:738:ARG:HB3	1.41	0.99
1:E:6:GLU:HG2	12:E:1030:HOH:O	1.59	0.99
11:H:808:PE5:H42	11:H:808:PE5:H72	1.45	0.97
1:B:734:LYS:O	1:B:735:SER:HB2	1.66	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:637:ASP:HB3	12:D:1053:HOH:O	1.63	0.96
1:A:608:GLU:OE2	4:A:805:GOL:H12	1.66	0.96
1:F:98:ALA:O	1:F:99:SER:HB2	1.62	0.95
1:F:604:ARG:HB3	1:F:604:ARG:NH1	1.82	0.94
1:A:604:ARG:HD2	12:A:1059:HOH:O	1.67	0.94
1:E:226:SER:HB3	1:H:704:ASP:OD2	1.69	0.93
1:H:499:GLU:O	1:H:503:THR:HB	1.69	0.93
1:G:710:THR:HG22	1:G:723:ASP:OD2	1.69	0.93
1:B:26:ALA:O	1:B:27:ILE:CB	2.18	0.91
1:C:1:MET:HG3	1:C:2:HIS:HB2	1.51	0.91
1:C:499:GLU:O	1:C:503:THR:HB	1.71	0.91
1:B:327:TYR:H	4:B:804:GOL:H32	1.37	0.90
1:F:753:ASP:HB2	12:F:979:HOH:O	1.70	0.90
1:B:644:ARG:HD3	12:D:1128:HOH:O	1.69	0.89
1:B:26:ALA:O	1:B:27:ILE:HB	1.71	0.88
1:H:164:ASP:OD1	4:H:807:GOL:H2	1.75	0.87
1:A:217:ASN:HB2	1:A:218:PRO:HD2	1.57	0.86
1:F:510:SER:O	1:F:514:GLU:HG2	1.75	0.86
4:H:804:GOL:H12	12:H:986:HOH:O	1.74	0.86
1:G:108:GLN:HG3	1:G:110:VAL:HG23	1.56	0.85
1:C:18:LYS:HE3	1:C:29:GLU:OE1	1.76	0.85
1:C:352:ARG:HD2	12:C:1073:HOH:O	1.77	0.84
1:B:604:ARG:HG2	9:B:802:7PE:H211	1.59	0.84
1:G:413:GLN:HE22	1:G:475:GLN:HE22	1.24	0.83
1:B:228:SER:HB3	1:E:644:ARG:HH22	1.41	0.83
1:C:18:LYS:CE	1:C:29:GLU:OE1	2.27	0.82
1:E:732:THR:HG23	12:E:1064:HOH:O	1.78	0.82
1:E:684:ASN:HB3	5:E:803:P6G:H91	1.60	0.82
1:F:560:LYS:HG3	12:F:1068:HOH:O	1.79	0.81
1:F:756:ARG:O	1:F:757:ILE:HB	1.78	0.81
1:G:737:ASP:HA	1:G:738:ARG:CB	2.11	0.81
1:C:191:THR:HG23	12:C:954:HOH:O	1.79	0.80
1:A:83:LEU:HD12	6:A:812:PGE:H62	1.64	0.80
1:F:731:ILE:O	1:F:757:ILE:HG22	1.80	0.80
1:F:749:LYS:HE2	12:F:1073:HOH:O	1.81	0.80
1:H:224:THR:HG23	12:H:995:HOH:O	1.82	0.80
1:E:352:ARG:HD3	12:E:956:HOH:O	1.82	0.80
1:B:734:LYS:O	1:B:735:SER:CB	2.29	0.80
1:G:731:ILE:HD13	1:G:743:LEU:HD23	1.62	0.80
1:H:219:ASP:OD1	4:H:807:GOL:H11	1.82	0.79
1:G:735:SER:C	1:G:737:ASP:H	1.84	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:499:GLU:O	1:E:503:THR:HB	1.83	0.78
1:E:738:ARG:O	1:E:738:ARG:HG3	1.83	0.78
1:H:217:ASN:HB2	1:H:218:PRO:HD2	1.64	0.78
1:C:128:HIS:HB3	12:C:1164:HOH:O	1.84	0.78
1:E:210:ALA:HB1	1:E:226:SER:O	1.83	0.78
1:G:413:GLN:HE22	1:G:475:GLN:NE2	1.81	0.78
1:C:459:LYS:HZ3	4:D:809:GOL:H32	1.49	0.77
1:E:230:GLU:HB2	1:E:233:LYS:HD2	1.67	0.77
1:A:83:LEU:HD12	6:A:812:PGE:C6	2.14	0.77
1:C:22:GLU:OE1	1:C:25:GLN:HG3	1.83	0.77
1:B:499:GLU:O	1:B:503:THR:HB	1.84	0.77
8:B:801:PG4:H21	12:B:976:HOH:O	1.85	0.77
1:A:107:SER:HB2	4:A:808:GOL:H11	1.67	0.77
10:C:805:PE4:H131	10:C:805:PE4:O6	1.84	0.76
1:C:459:LYS:NZ	4:D:809:GOL:H32	1.99	0.76
1:A:158:ASP:OD2	6:A:812:PGE:H6	1.85	0.75
3:E:802:1PE:H222	12:E:1006:HOH:O	1.85	0.75
1:E:737:ASP:HA	1:E:738:ARG:HB2	1.68	0.75
2:F:801:IFM:H2C1	4:F:802:GOL:O3	1.87	0.75
1:F:756:ARG:HG3	1:F:756:ARG:NH1	1.88	0.75
1:D:374:TYR:OH	4:D:809:GOL:H12	1.86	0.75
1:F:352:ARG:HD3	12:F:1034:HOH:O	1.87	0.75
1:H:213:GLU:HB3	1:H:224:THR:CG2	2.16	0.75
1:D:742:THR:HG22	1:D:751:VAL:HG13	1.69	0.75
1:H:582:ARG:HH21	1:H:582:ARG:HG2	1.50	0.74
1:G:142:LEU:HD21	1:G:263:MET:HE1	1.68	0.74
1:A:742:THR:O	1:A:743:LEU:HB2	1.86	0.74
1:B:644:ARG:HH12	1:D:228:SER:HB3	1.51	0.74
1:H:114:LYS:HG3	1:H:128:HIS:CD2	2.23	0.74
1:E:190:LYS:HE2	12:E:1044:HOH:O	1.87	0.73
1:A:659:GLU:O	1:A:660:ALA:HB3	1.88	0.73
1:D:136:ARG:HD3	12:D:1041:HOH:O	1.88	0.73
1:H:1:MET:HA	1:H:292:ILE:HG21	1.70	0.73
1:F:756:ARG:CG	1:F:756:ARG:HH11	1.95	0.73
1:H:2:HIS:O	1:H:3:GLU:HB3	1.87	0.73
1:H:656:ASN:HA	12:H:1075:HOH:O	1.88	0.73
1:H:733:ASN:HD22	1:H:741:LEU:HD11	1.51	0.72
1:A:83:LEU:CD1	6:A:812:PGE:O4	2.37	0.72
1:F:745:ILE:O	1:F:746:PHE:HB2	1.88	0.72
1:G:94:SER:O	1:G:97:ALA:HB2	1.90	0.72
1:F:98:ALA:O	1:F:99:SER:CB	2.37	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:425:LYS:HD3	1:G:492:PHE:CZ	2.25	0.72
1:F:97:ALA:O	1:F:99:SER:N	2.23	0.72
1:H:345:TYR:OH	11:H:808:PE5:H22	1.90	0.71
1:E:735:SER:O	1:E:736:GLU:CB	2.39	0.71
1:E:735:SER:O	1:E:736:GLU:HB3	1.90	0.71
1:B:734:LYS:H	1:B:734:LYS:HD2	1.54	0.71
1:G:1:MET:HG3	1:G:2:HIS:HB2	1.73	0.70
1:B:289:GLN:OE1	1:B:710:THR:HG22	1.92	0.70
1:D:635:GLN:HG3	9:D:808:7PE:H152	1.74	0.70
1:H:70:TRP:CZ3	4:H:804:GOL:H32	2.26	0.70
1:H:353:ASN:HB3	4:H:805:GOL:H11	1.72	0.70
1:F:759:LYS:O	1:F:760:SER:HB3	1.92	0.69
1:B:327:TYR:N	4:B:804:GOL:H32	2.06	0.69
1:G:413:GLN:NE2	1:G:475:GLN:HE22	1.90	0.69
1:D:334:ASP:OD1	2:D:801:IFM:O4	2.09	0.69
1:B:734:LYS:N	1:B:734:LYS:HD2	2.08	0.69
1:E:741:LEU:O	1:E:751:VAL:CG2	2.41	0.69
1:H:426:LYS:HE2	11:H:808:PE5:H482	1.73	0.69
1:B:27:ILE:CG2	1:B:28:THR:N	2.56	0.69
1:F:699:SER:N	1:F:700:PRO:HD3	2.07	0.69
1:B:26:ALA:O	1:B:27:ILE:CG2	2.40	0.69
1:E:370:LYS:HE3	1:E:375:GLU:OE2	1.93	0.69
1:H:2:HIS:O	1:H:3:GLU:CB	2.39	0.69
1:B:26:ALA:O	1:B:27:ILE:HG22	1.93	0.68
1:B:553:LEU:HD21	4:B:807:GOL:H11	1.76	0.68
1:A:612:GLU:OE2	4:A:805:GOL:H11	1.93	0.68
1:A:83:LEU:HD12	6:A:812:PGE:O4	1.93	0.68
1:B:733:ASN:OD1	1:B:734:LYS:O	2.11	0.68
1:C:190:LYS:HE3	4:C:806:GOL:H31	1.76	0.68
1:H:129:GLU:OE2	1:H:131:LYS:NZ	2.24	0.68
1:A:756:ARG:HH11	1:A:756:ARG:HG2	1.59	0.68
1:B:224:THR:HG23	12:B:1171:HOH:O	1.92	0.68
1:A:644:ARG:HH12	1:F:228:SER:HB3	1.58	0.67
1:A:608:GLU:OE2	4:A:805:GOL:C1	2.41	0.67
1:F:28:THR:HG21	1:F:656:ASN:HB2	1.77	0.67
11:H:808:PE5:C7	11:H:808:PE5:H42	2.21	0.67
1:D:499:GLU:O	1:D:503:THR:HB	1.94	0.66
1:A:158:ASP:CG	6:A:812:PGE:H6	2.15	0.66
3:E:802:1PE:C22	12:E:1006:HOH:O	2.41	0.66
1:G:499:GLU:O	1:G:503:THR:HB	1.93	0.66
1:A:48:GLU:HB2	1:A:83:LEU:HD23	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:599:PRO:HG3	10:C:805:PE4:H52	1.77	0.66
1:G:287:THR:HB	1:G:710:THR:OG1	1.95	0.66
2:A:801:IFM:C2	12:A:917:HOH:O	2.12	0.66
1:F:217:ASN:HB2	1:F:218:PRO:CD	2.25	0.66
1:E:44:GLY:O	1:E:102:ARG:NH2	2.29	0.66
1:G:710:THR:CG2	1:G:723:ASP:OD2	2.43	0.65
1:A:599:PRO:HB3	5:A:806:P6G:H141	1.78	0.65
1:F:604:ARG:NH2	12:F:1091:HOH:O	2.30	0.65
1:G:735:SER:O	1:G:737:ASP:N	2.25	0.65
1:H:128:HIS:HB3	12:H:997:HOH:O	1.95	0.65
1:G:742:THR:HG22	1:G:751:VAL:HG22	1.77	0.65
1:H:742:THR:HG22	1:H:751:VAL:HG22	1.79	0.65
1:B:27:ILE:HG23	1:B:28:THR:N	2.12	0.65
1:E:204:CYS:O	1:E:205:SER:HB2	1.95	0.65
1:B:27:ILE:CG2	1:B:28:THR:H	2.08	0.64
1:G:735:SER:C	1:G:737:ASP:N	2.50	0.64
1:F:1:MET:HA	1:F:292:ILE:HG21	1.79	0.64
1:H:582:ARG:HH21	1:H:582:ARG:CG	2.10	0.64
1:F:734:LYS:O	1:F:735:SER:HB2	1.96	0.64
1:E:680:GLN:OE1	5:E:803:P6G:H141	1.98	0.64
1:A:108:GLN:HG3	1:A:110:VAL:HG23	1.79	0.63
1:E:8:LEU:HD22	1:E:16:ILE:HD12	1.81	0.63
1:H:582:ARG:NH2	1:H:582:ARG:HG2	2.11	0.63
1:C:213:GLU:OE2	1:G:617:ARG:NH2	2.26	0.63
1:G:108:GLN:HG3	1:G:110:VAL:CG2	2.29	0.63
1:H:599:PRO:HB3	11:H:808:PE5:C14	2.24	0.63
1:A:217:ASN:HB2	1:A:218:PRO:CD	2.24	0.63
1:H:428:HIS:HB2	1:H:437:ILE:HD11	1.81	0.62
1:G:116:SER:HA	1:G:125:ILE:O	2.00	0.62
1:H:734:LYS:O	1:H:735:SER:CB	2.47	0.62
1:F:558:PRO:HD2	1:F:561:LYS:HE2	1.82	0.61
1:B:110:VAL:HG22	1:B:132:PHE:HB3	1.81	0.61
1:D:217:ASN:HB2	1:D:218:PRO:CD	2.31	0.61
1:F:742:THR:HA	1:F:751:VAL:HA	1.82	0.61
1:H:506:GLU:O	1:H:510:SER:HB2	2.00	0.61
1:D:352:ARG:HD3	12:D:1010:HOH:O	2.00	0.61
1:F:743:LEU:O	1:F:744:HIS:HB2	2.00	0.61
1:C:700:PRO:HD2	1:C:746:PHE:CZ	2.35	0.61
1:B:635:GLN:HG3	9:B:802:7PE:H152	1.83	0.61
1:E:31:SER:HB3	1:E:670:ILE:HG12	1.83	0.60
1:A:659:GLU:O	1:A:660:ALA:CB	2.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:26:ALA:O	1:F:27:ILE:HG22	2.02	0.60
1:B:347:ASN:HD21	4:B:805:GOL:H2	1.67	0.60
1:C:700:PRO:HG3	1:C:729:ILE:HD12	1.84	0.60
4:A:811:GOL:H32	1:F:158:ASP:OD1	2.00	0.60
1:E:577:ASN:OD1	1:E:582:ARG:NH2	2.33	0.60
1:H:219:ASP:OD1	4:H:807:GOL:C1	2.49	0.60
1:C:659:GLU:O	1:C:660:ALA:HB3	2.01	0.60
1:E:748:GLU:O	1:E:749:LYS:HD2	2.02	0.60
1:F:217:ASN:HB2	1:F:218:PRO:HD2	1.83	0.60
1:F:740:PRO:HA	1:F:752:LEU:O	2.02	0.60
1:E:751:VAL:O	1:E:752:LEU:HB2	2.02	0.59
1:F:457:VAL:HG11	1:F:468:MET:HE2	1.84	0.59
1:C:31:SER:HB3	1:C:670:ILE:HG12	1.84	0.59
1:E:116:SER:HA	1:E:125:ILE:O	2.02	0.59
1:G:79:ALA:HB1	1:G:202:GLU:HB2	1.84	0.59
1:G:58:ILE:HD12	1:G:58:ILE:N	2.18	0.59
1:B:27:ILE:HG22	1:B:28:THR:H	1.68	0.59
1:B:726:LYS:H	1:B:726:LYS:CD	2.16	0.59
1:C:99:SER:HB3	1:C:116:SER:HB2	1.84	0.59
1:F:26:ALA:C	1:F:27:ILE:HG22	2.23	0.59
1:B:753:ASP:O	1:B:754:SER:HB3	2.03	0.58
2:H:801:IFM:H2C1	4:H:802:GOL:O1	2.02	0.58
1:E:84:LEU:HD23	1:E:91:PHE:HB2	1.85	0.58
1:F:129:GLU:OE2	1:F:131:LYS:NZ	2.32	0.58
1:C:209:ASP:OD1	4:G:803:GOL:H32	2.02	0.58
1:C:752:LEU:HD13	1:C:757:ILE:CG1	2.33	0.58
1:E:696:ILE:HG12	1:E:743:LEU:HD12	1.84	0.58
1:F:352:ARG:CD	12:F:1034:HOH:O	2.50	0.58
1:C:696:ILE:N	1:C:696:ILE:HD12	2.18	0.58
1:D:450:ARG:NH1	4:D:804:GOL:H11	2.18	0.58
1:E:659:GLU:O	1:E:660:ALA:HB3	2.03	0.58
1:E:635:GLN:HG3	5:E:803:P6G:H61	1.86	0.58
1:E:641:GLU:HG3	12:E:965:HOH:O	2.03	0.58
1:F:1:MET:O	1:F:2:HIS:ND1	2.36	0.58
1:A:658:ASN:HB3	4:A:803:GOL:H31	1.86	0.58
1:E:58:ILE:N	1:E:58:ILE:HD12	2.19	0.58
1:C:573:TYR:HE2	1:C:621:PHE:HE1	1.50	0.57
1:G:396:PHE:HZ	4:G:802:GOL:HO3	1.51	0.57
1:B:79:ALA:HB1	1:B:202:GLU:HB2	1.86	0.57
1:B:43:ARG:HD3	1:B:56:ALA:HB3	1.85	0.57
1:C:142:LEU:HD21	1:C:263:MET:CE	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:97:ALA:O	1:D:99:SER:N	2.38	0.57
1:E:738:ARG:CG	1:E:738:ARG:O	2.51	0.57
1:B:417:SER:HB3	1:B:448:ILE:HG23	1.86	0.57
1:H:735:SER:HA	12:H:984:HOH:O	2.04	0.57
1:B:217:ASN:HB2	1:B:218:PRO:CD	2.34	0.57
1:C:728:GLN:HG2	1:C:729:ILE:N	2.18	0.57
1:G:600:HIS:CD2	1:G:692:HIS:HB2	2.39	0.57
1:H:742:THR:HA	1:H:751:VAL:HA	1.85	0.57
1:D:742:THR:HA	1:D:750:SER:O	2.04	0.57
1:E:64:ASP:OD1	1:E:191:THR:HG23	2.04	0.57
1:G:601:LEU:HD23	1:G:602:TYR:CE2	2.40	0.57
1:B:16:ILE:HD12	1:B:106:LEU:HD11	1.86	0.57
1:F:213:GLU:HB3	1:F:224:THR:HG22	1.86	0.57
1:H:217:ASN:HB2	1:H:218:PRO:CD	2.35	0.57
1:C:97:ALA:O	1:C:99:SER:N	2.39	0.56
1:F:656:ASN:HA	12:F:1054:HOH:O	2.03	0.56
1:B:428:HIS:CD2	1:B:437:ILE:HG13	2.39	0.56
1:F:491:MET:HE1	1:F:494:LEU:HD12	1.88	0.56
1:F:745:ILE:HG22	1:F:745:ILE:O	2.04	0.56
1:H:656:ASN:O	1:H:656:ASN:CG	2.42	0.56
1:C:591:VAL:O	1:C:594:LEU:HB3	2.06	0.56
1:H:251:ASN:HB3	12:H:969:HOH:O	2.06	0.56
1:F:656:ASN:ND2	12:F:1054:HOH:O	2.36	0.56
1:B:228:SER:HB3	1:E:644:ARG:NH2	2.16	0.56
1:H:310:PRO:O	4:H:805:GOL:H2	2.06	0.56
1:B:85:HIS:ND1	12:B:1055:HOH:O	2.33	0.56
1:D:418:PRO:HB2	1:D:489:GLN:HB3	1.88	0.56
1:F:97:ALA:C	1:F:99:SER:H	2.08	0.56
1:B:656:ASN:CG	1:B:656:ASN:O	2.42	0.56
1:C:491:MET:HG3	1:C:535:VAL:HG21	1.87	0.56
1:H:395:PHE:CE1	4:H:802:GOL:H31	2.41	0.56
1:C:264:GLN:HB3	1:C:268:GLU:HB2	1.88	0.55
1:D:217:ASN:HB2	1:D:218:PRO:HD2	1.88	0.55
1:H:759:LYS:HG3	1:H:760:SER:H	1.72	0.55
1:A:749:LYS:O	1:A:750:SER:O	2.23	0.55
1:B:604:ARG:CG	9:B:802:7PE:H211	2.34	0.55
1:A:191:THR:HG22	1:A:196:ASP:H	1.70	0.55
1:E:737:ASP:CA	1:E:738:ARG:HB3	2.27	0.55
1:F:168:ILE:HD12	1:F:325:GLN:HB2	1.89	0.55
1:B:644:ARG:CD	12:D:1128:HOH:O	2.38	0.55
1:A:742:THR:O	1:A:743:LEU:CB	2.52	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2:HIS:O	1:E:9:THR:HA	2.07	0.55
1:G:731:ILE:HD13	1:G:743:LEU:CD2	2.35	0.55
1:E:394:PHE:CZ	1:F:582:ARG:HG2	2.42	0.55
1:G:413:GLN:HG3	1:G:471:GLN:O	2.07	0.55
1:G:731:ILE:HG21	1:G:743:LEU:HD21	1.89	0.55
1:B:114:LYS:NZ	12:B:1091:HOH:O	2.39	0.54
1:E:693:GLY:C	1:E:695:ASP:H	2.11	0.54
1:E:737:ASP:CA	1:E:738:ARG:CB	2.70	0.54
1:H:587:LYS:NZ	12:H:1094:HOH:O	2.40	0.54
1:D:504:LEU:HB2	1:D:509:LEU:HD22	1.88	0.54
1:B:86:VAL:HG21	1:B:125:ILE:HG13	1.90	0.54
1:C:110:VAL:HG22	1:C:132:PHE:HB3	1.89	0.54
1:F:287:THR:OG1	1:F:710:THR:HG23	2.07	0.54
1:H:426:LYS:HG2	11:H:808:PE5:H41	1.89	0.54
1:E:714:ILE:N	1:E:714:ILE:HD13	2.23	0.54
1:B:2:HIS:HB3	1:B:10:THR:O	2.08	0.54
1:F:199:THR:HG21	1:F:253:GLN:HA	1.89	0.54
1:H:733:ASN:ND2	1:H:741:LEU:HD11	2.22	0.54
1:H:758:THR:HG22	1:H:759:LYS:N	2.23	0.54
1:C:537:LYS:HG2	12:C:1072:HOH:O	2.07	0.54
4:D:812:GOL:H12	12:D:1114:HOH:O	2.08	0.54
1:F:742:THR:HG22	1:F:751:VAL:HG13	1.89	0.54
1:D:464:ARG:HD2	1:D:534:TYR:HB2	1.90	0.53
1:G:86:VAL:HG21	1:G:125:ILE:HG13	1.89	0.53
1:A:671:HIS:CD2	4:A:803:GOL:H12	2.43	0.53
1:B:2:HIS:CB	1:B:10:THR:O	2.57	0.53
1:A:658:ASN:HB3	4:A:803:GOL:C3	2.38	0.53
1:G:475:GLN:HG3	2:G:801:IFM:H2C1	1.90	0.53
1:E:394:PHE:HZ	1:F:582:ARG:HG2	1.73	0.53
1:D:448:ILE:HG22	1:D:493:THR:HG21	1.90	0.53
1:E:741:LEU:O	1:E:751:VAL:HG22	2.08	0.53
1:F:81:LEU:HD22	1:F:162:ASP:HB2	1.91	0.53
1:F:697:HIS:O	1:F:698:LEU:HG	2.09	0.53
1:B:754:SER:OG	1:B:755:GLU:N	2.36	0.53
1:E:341:PRO:HG3	5:E:803:P6G:H172	1.91	0.53
1:E:86:VAL:HG21	1:E:125:ILE:HD11	1.90	0.53
1:B:45:THR:HG21	1:B:55:ALA:HA	1.90	0.53
1:C:293:ILE:H	1:C:293:ILE:HD12	1.74	0.53
1:G:191:THR:HG22	1:G:195:GLU:H	1.73	0.53
1:D:43:ARG:HD3	1:D:56:ALA:HB3	1.91	0.52
1:F:16:ILE:CD1	1:F:106:LEU:HD11	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:ASN:HB3	1:A:254:ASP:OD2	2.08	0.52
1:F:179:PHE:CZ	1:F:186:GLY:HA3	2.44	0.52
1:F:294:ASP:OD1	1:F:647:ARG:NH1	2.33	0.52
1:H:745:ILE:O	1:H:748:GLU:HG2	2.08	0.52
1:G:425:LYS:HD3	1:G:492:PHE:HZ	1.75	0.52
1:H:426:LYS:HD3	11:H:808:PE5:H12	1.90	0.52
1:C:718:GLN:CG	1:C:733:ASN:HD21	2.22	0.52
1:D:710:THR:HB	1:D:723:ASP:HA	1.91	0.52
1:A:696:ILE:HD13	1:A:696:ILE:N	2.25	0.52
1:B:27:ILE:HA	1:B:43:ARG:NH1	2.24	0.52
1:D:152:ASP:OD2	4:D:805:GOL:H12	2.09	0.52
1:B:504:LEU:HB2	1:B:509:LEU:HD22	1.91	0.52
1:C:191:THR:HG22	1:C:196:ASP:H	1.74	0.52
1:G:16:ILE:HD13	1:G:654:LEU:CD2	2.39	0.52
1:A:217:ASN:CB	1:A:218:PRO:HD2	2.36	0.52
1:H:734:LYS:O	1:H:735:SER:HB3	2.10	0.52
1:D:81:LEU:HD22	1:D:162:ASP:HB2	1.92	0.52
1:F:334:ASP:OD1	2:F:801:IFM:O4	2.14	0.52
1:F:418:PRO:HB2	1:F:489:GLN:HB3	1.92	0.52
1:A:142:LEU:HD21	1:A:263:MET:CE	2.40	0.52
1:A:413:GLN:HG3	1:A:471:GLN:O	2.10	0.52
1:C:573:TYR:HE2	1:C:621:PHE:CE1	2.28	0.51
1:B:327:TYR:HA	4:B:804:GOL:H32	1.91	0.51
1:D:450:ARG:HH11	4:D:804:GOL:H11	1.73	0.51
1:E:230:GLU:CB	1:E:233:LYS:HE3	2.39	0.51
1:E:744:HIS:HA	1:E:748:GLU:O	2.10	0.51
1:F:733:ASN:HD22	1:F:752:LEU:HD21	1.75	0.51
10:C:805:PE4:C13	10:C:805:PE4:O6	2.57	0.51
1:H:58:ILE:HD12	1:H:58:ILE:N	2.25	0.51
1:A:197:THR:O	1:A:245:SER:HA	2.11	0.51
2:D:801:IFM:C2	12:D:1243:HOH:O	2.17	0.51
1:E:110:VAL:HG22	1:E:132:PHE:HB3	1.91	0.51
1:G:653:ASP:CG	1:G:670:ILE:HD13	2.31	0.51
1:A:164:ASP:OD1	4:A:809:GOL:O1	2.10	0.51
1:C:28:THR:HG21	1:C:656:ASN:HB2	1.92	0.51
1:F:575:TYR:CG	1:F:576:PRO:HA	2.46	0.51
1:H:181:HIS:HB2	1:H:182:PRO:CD	2.40	0.51
1:H:741:LEU:HD13	1:H:752:LEU:HD23	1.90	0.51
1:A:191:THR:HG22	1:A:195:GLU:N	2.26	0.51
1:D:382:ILE:HG13	1:D:391:CYS:HB2	1.92	0.51
1:A:573:TYR:HE2	1:A:621:PHE:HE1	1.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:714:ILE:CD1	1:E:714:ILE:N	2.74	0.51
1:H:1:MET:HA	1:H:292:ILE:CG2	2.39	0.51
1:E:560:LYS:HE3	1:E:563:THR:HG21	1.92	0.51
1:G:475:GLN:CG	2:G:801:IFM:H2C1	2.41	0.51
1:E:400:LEU:HD13	1:F:401:SER:HB2	1.93	0.51
1:E:749:LYS:O	1:E:750:SER:HB2	2.11	0.50
1:E:77:PRO:HD3	1:E:173:LEU:HD12	1.92	0.50
1:F:635:GLN:HA	1:F:635:GLN:NE2	2.24	0.50
1:H:172:HIS:O	1:H:191:THR:HA	2.11	0.50
11:H:808:PE5:C4	11:H:808:PE5:H72	2.32	0.50
1:H:181:HIS:HB2	1:H:182:PRO:HD2	1.92	0.50
1:A:274:ARG:NH2	4:A:808:GOL:H2	2.25	0.50
1:B:710:THR:HB	1:B:723:ASP:HA	1.93	0.50
1:E:659:GLU:O	1:E:660:ALA:CB	2.60	0.50
1:G:361:THR:HB	1:G:387:GLY:HA3	1.93	0.50
1:G:731:ILE:CD1	1:G:745:ILE:HD11	2.41	0.50
1:F:224:THR:HG23	12:F:984:HOH:O	2.12	0.50
1:B:116:SER:HA	1:B:125:ILE:O	2.12	0.50
1:D:615:GLU:N	1:D:616:PRO:CD	2.75	0.50
1:H:25:GLN:C	1:H:26:ALA:O	2.47	0.50
1:E:135:TYR:O	1:E:138:LYS:HE3	2.12	0.50
1:F:699:SER:N	1:F:700:PRO:CD	2.73	0.50
1:F:745:ILE:O	1:F:746:PHE:CB	2.58	0.50
1:F:425:LYS:NZ	1:F:499:GLU:OE1	2.32	0.50
1:D:212:GLU:OE1	4:D:806:GOL:O2	2.30	0.49
1:H:1:MET:CA	1:H:292:ILE:HG21	2.39	0.49
1:A:217:ASN:CB	1:A:218:PRO:CD	2.89	0.49
1:B:28:THR:HG21	1:B:656:ASN:HB2	1.94	0.49
1:G:418:PRO:HB2	1:G:489:GLN:HB3	1.95	0.49
1:H:591:VAL:O	1:H:594:LEU:HB3	2.12	0.49
1:B:5:GLY:O	1:B:6:GLU:C	2.51	0.49
1:D:130:GLU:HG3	1:D:266:TYR:OH	2.12	0.49
1:D:79:ALA:HB1	1:D:202:GLU:HB2	1.94	0.49
1:G:1:MET:HG3	1:G:2:HIS:CB	2.39	0.49
1:A:696:ILE:CD1	1:A:715:VAL:HG11	2.43	0.49
1:C:114:LYS:HG2	1:C:128:HIS:HD2	1.78	0.49
1:C:333:TRP:HB3	1:C:416:ILE:HD13	1.93	0.49
1:F:689:LEU:HG	1:F:690:SER:N	2.25	0.49
1:B:641:GLU:HB2	12:B:1151:HOH:O	2.13	0.49
1:H:197:THR:O	1:H:245:SER:HA	2.13	0.49
1:A:249:VAL:HG11	1:A:255:GLU:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:635:GLN:HB2	10:C:805:PE4:H22	1.93	0.49
1:E:5:GLY:O	1:E:6:GLU:C	2.51	0.49
1:F:274:ARG:HD3	12:F:1062:HOH:O	2.12	0.49
1:A:475:GLN:CG	2:A:801:IFM:H2C1	2.42	0.49
1:B:19:ASN:O	1:B:20:ARG:HD3	2.13	0.49
1:C:160:GLY:HA2	1:C:202:GLU:OE2	2.13	0.49
1:F:86:VAL:HG21	1:F:125:ILE:HG13	1.95	0.49
1:F:179:PHE:CE1	1:F:186:GLY:HA3	2.48	0.49
1:C:142:LEU:HD21	1:C:263:MET:HE1	1.94	0.49
1:C:79:ALA:HB1	1:C:202:GLU:HB2	1.94	0.49
1:D:707:ASP:OD1	1:D:726:LYS:HE2	2.13	0.49
1:E:84:LEU:HD23	1:E:91:PHE:CD2	2.48	0.49
1:D:560:LYS:HG3	1:D:560:LYS:O	2.13	0.48
1:G:81:LEU:HD22	1:G:162:ASP:HB2	1.95	0.48
1:E:81:LEU:HD22	1:E:162:ASP:HB2	1.94	0.48
1:G:130:GLU:HG3	1:G:266:TYR:OH	2.14	0.48
1:D:608:GLU:HA	1:D:636:ILE:HD12	1.94	0.48
1:E:684:ASN:HB3	5:E:803:P6G:C9	2.39	0.48
1:H:43:ARG:HD3	1:H:56:ALA:HB3	1.94	0.48
1:A:86:VAL:HG21	1:A:125:ILE:HG13	1.95	0.48
1:G:370:LYS:HD3	12:G:1093:HOH:O	2.13	0.48
1:C:144:LYS:HG2	12:C:1167:HOH:O	2.13	0.48
1:C:371:ARG:NH1	3:C:801:1PE:H222	2.28	0.48
1:D:413:GLN:HG3	1:D:471:GLN:O	2.13	0.48
1:G:412:TRP:CZ3	1:G:479:ASN:HB2	2.49	0.48
1:C:684:ASN:O	1:C:688:GLY:HA2	2.13	0.48
1:E:141:VAL:HG13	1:E:241:MET:HB3	1.95	0.48
1:E:727:GLU:OE1	1:E:727:GLU:N	2.42	0.48
1:G:327:TYR:CE1	2:G:801:IFM:H6C1	2.49	0.48
1:G:457:VAL:HB	1:H:457:VAL:HB	1.94	0.48
1:C:604:ARG:NH1	1:C:637:ASP:OD1	2.46	0.48
1:F:604:ARG:CZ	12:F:1091:HOH:O	2.62	0.48
1:H:26:ALA:O	1:H:27:ILE:HG22	2.13	0.48
1:A:656:ASN:O	1:A:656:ASN:CG	2.51	0.48
1:B:114:LYS:HG2	1:B:128:HIS:CD2	2.49	0.48
1:B:310:PRO:O	4:B:803:GOL:H31	2.14	0.48
1:D:742:THR:HA	1:D:751:VAL:HA	1.94	0.48
1:G:413:GLN:NE2	1:G:475:GLN:NE2	2.56	0.48
1:F:708:GLY:HA2	1:F:724:VAL:O	2.14	0.48
1:D:600:HIS:CD2	1:D:692:HIS:HB2	2.49	0.47
1:E:191:THR:HB	1:E:196:ASP:H	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:368:LYS:HD3	1:H:378:TYR:O	2.13	0.47
1:G:459:LYS:HB3	1:G:459:LYS:HE3	1.70	0.47
1:G:615:GLU:HB3	1:G:616:PRO:HD3	1.95	0.47
1:G:678:SER:HA	1:G:681:MET:CE	2.44	0.47
1:A:263:MET:CE	1:A:269:GLU:HG3	2.45	0.47
1:D:575:TYR:HB2	12:D:1074:HOH:O	2.15	0.47
1:E:136:ARG:HG3	1:E:137:LYS:HG3	1.97	0.47
1:G:136:ARG:HG3	1:G:137:LYS:HG3	1.97	0.47
1:H:179:PHE:CZ	1:H:186:GLY:HA3	2.48	0.47
1:C:575:TYR:HB2	12:C:1035:HOH:O	2.14	0.47
1:E:71:GLU:O	1:E:328:GLN:HG2	2.14	0.47
1:G:44:GLY:O	1:G:102:ARG:NH2	2.38	0.47
1:G:16:ILE:CD1	1:G:654:LEU:HD22	2.44	0.47
1:A:34:MET:HG2	1:A:304:HIS:HE1	1.80	0.47
1:B:724:VAL:HG22	1:B:729:ILE:HG23	1.96	0.47
1:F:457:VAL:HG11	1:F:468:MET:CE	2.43	0.47
1:C:302:ILE:O	1:C:306:ILE:HG13	2.14	0.47
1:C:86:VAL:HG21	1:C:125:ILE:HG13	1.97	0.47
1:H:98:ALA:O	1:H:99:SER:CB	2.63	0.47
1:C:113:ARG:NH2	1:C:129:GLU:OE1	2.45	0.47
1:C:752:LEU:HD13	1:C:757:ILE:HG12	1.96	0.47
1:G:712:LYS:NZ	12:G:1058:HOH:O	2.32	0.47
1:B:729:ILE:CD1	1:B:745:ILE:HG21	2.45	0.47
1:B:745:ILE:O	1:B:748:GLU:HG2	2.14	0.47
1:B:738:ARG:CZ	1:B:755:GLU:HG3	2.45	0.47
1:C:448:ILE:HG22	1:C:493:THR:HG21	1.97	0.47
1:D:80:LEU:HD23	1:D:131:LYS:HD3	1.96	0.47
1:F:26:ALA:HA	1:F:29:GLU:HB2	1.97	0.47
1:G:191:THR:HG22	1:G:195:GLU:N	2.29	0.47
1:D:738:ARG:HE	1:D:755:GLU:HA	1.80	0.47
1:E:624:LEU:N	1:E:624:LEU:HD12	2.30	0.47
1:G:370:LYS:HE3	1:G:375:GLU:OE2	2.15	0.47
1:C:191:THR:CG2	12:C:954:HOH:O	2.53	0.47
1:F:731:ILE:HB	1:F:757:ILE:HG21	1.97	0.47
1:H:715:VAL:CG2	1:H:720:LEU:HD22	2.45	0.47
1:A:475:GLN:HG3	2:A:801:IFM:H2C1	1.95	0.46
1:D:741:LEU:O	1:D:742:THR:HG23	2.15	0.46
1:F:422:TYR:HE2	6:F:806:PGE:H42	1.79	0.46
1:F:98:ALA:HB2	12:F:1136:HOH:O	2.15	0.46
1:A:491:MET:HA	1:A:491:MET:HE2	1.97	0.46
1:B:100:PHE:CZ	1:B:102:ARG:HB2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:55:ALA:O	1:E:56:ALA:HB2	2.15	0.46
1:F:13:GLY:O	1:F:296:VAL:HG23	2.15	0.46
1:C:99:SER:O	1:C:115:VAL:HA	2.15	0.46
1:D:692:HIS:O	1:D:695:ASP:HB2	2.16	0.46
1:F:756:ARG:O	1:F:757:ILE:CB	2.59	0.46
1:E:670:ILE:HD12	1:E:670:ILE:HG23	1.68	0.46
1:E:96:GLU:O	1:E:96:GLU:HG3	2.15	0.46
1:F:743:LEU:O	1:F:744:HIS:CB	2.64	0.46
1:G:141:VAL:HG13	1:G:241:MET:HB3	1.96	0.46
1:G:287:THR:HB	1:G:710:THR:HG1	1.80	0.46
1:B:327:TYR:CA	4:B:804:GOL:H32	2.45	0.46
1:C:728:GLN:HG3	1:C:758:THR:HG23	1.98	0.46
1:E:359:HIS:HB2	1:E:444:MET:SD	2.56	0.46
1:F:733:ASN:HD22	1:F:752:LEU:CD2	2.28	0.46
1:A:692:HIS:O	1:A:695:ASP:HB2	2.15	0.46
1:B:575:TYR:CG	1:B:576:PRO:HA	2.50	0.46
1:B:726:LYS:H	1:B:726:LYS:HD2	1.80	0.46
1:G:301:ASN:O	1:G:675:ASN:HB3	2.16	0.46
1:E:230:GLU:HB3	1:E:233:LYS:HE3	1.97	0.46
1:E:332:PHE:CZ	1:E:382:ILE:HG12	2.50	0.46
1:G:729:ILE:HD11	1:G:761:ARG:HG3	1.98	0.46
1:H:618:THR:HG22	1:H:620:HIS:H	1.80	0.46
1:E:197:THR:O	1:E:245:SER:HA	2.16	0.46
1:C:718:GLN:OE1	1:C:738:ARG:HA	2.16	0.46
1:H:362:LEU:HD13	1:H:366:ARG:NH2	2.30	0.46
1:C:382:ILE:O	1:C:390:LEU:HB2	2.16	0.45
1:C:738:ARG:CZ	1:C:755:GLU:HG3	2.46	0.45
1:D:1:MET:N	1:D:1:MET:SD	2.83	0.45
1:D:731:ILE:HB	1:D:757:ILE:CG2	2.45	0.45
1:F:656:ASN:O	1:F:656:ASN:CG	2.55	0.45
1:A:671:HIS:HB3	12:A:957:HOH:O	2.16	0.45
1:A:98:ALA:O	1:A:99:SER:HB3	2.15	0.45
1:C:315:LEU:O	4:C:809:GOL:H32	2.16	0.45
1:E:545:GLU:HG2	1:E:547:PHE:O	2.16	0.45
1:E:6:GLU:HB3	1:E:7:HIS:H	1.49	0.45
1:A:615:GLU:HB3	1:A:616:PRO:HD3	1.99	0.45
1:B:504:LEU:HD12	1:B:509:LEU:HD13	1.98	0.45
1:B:700:PRO:HG3	1:B:729:ILE:HG12	1.97	0.45
1:C:575:TYR:CG	1:C:576:PRO:HA	2.51	0.45
1:D:584:GLN:O	1:D:586:ILE:HG23	2.16	0.45
1:F:655:LEU:O	1:F:656:ASN:C	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:214:ASP:OD1	4:F:805:GOL:O2	2.34	0.45
1:G:94:SER:O	1:G:97:ALA:CB	2.64	0.45
1:H:86:VAL:HG21	1:H:125:ILE:HG13	1.98	0.45
1:C:191:THR:HG22	1:C:195:GLU:N	2.31	0.45
1:C:375:GLU:O	1:C:451:PHE:HA	2.15	0.45
1:D:582:ARG:HD3	12:D:985:HOH:O	2.16	0.45
1:D:696:ILE:HG12	1:D:715:VAL:HG11	1.97	0.45
1:D:684:ASN:HB3	9:D:808:7PE:H112	1.97	0.45
1:E:84:LEU:HD13	1:E:147:VAL:HG21	1.96	0.45
1:F:224:THR:CG2	12:F:984:HOH:O	2.65	0.45
1:F:710:THR:HB	1:F:723:ASP:HA	1.98	0.45
1:G:8:LEU:HA	1:G:17:ILE:O	2.17	0.45
1:C:697:HIS:HD2	12:C:1087:HOH:O	1.98	0.45
1:F:197:THR:O	1:F:245:SER:HA	2.16	0.45
1:H:427:TYR:CE1	1:H:431:THR:HG21	2.51	0.45
1:G:115:VAL:O	1:G:126:THR:HA	2.17	0.45
1:H:1:MET:O	1:H:1:MET:HG3	2.17	0.45
1:C:172:HIS:HE1	12:C:923:HOH:O	1.99	0.45
1:C:599:PRO:HB3	10:C:805:PE4:H42	1.99	0.45
1:E:119:MET:HG2	1:E:123:ALA:O	2.16	0.45
1:E:47:ALA:HB1	1:E:82:THR:HB	1.99	0.45
1:G:382:ILE:HD12	1:G:391:CYS:HB2	1.99	0.45
1:G:761:ARG:O	1:G:762:LEU:HD13	2.16	0.45
1:H:164:ASP:CG	4:H:807:GOL:H2	2.35	0.45
1:C:587:LYS:HE2	1:C:622:SER:HB2	1.99	0.45
1:D:327:TYR:OH	4:D:802:GOL:C3	2.65	0.45
1:A:394:PHE:HZ	1:B:582:ARG:HG2	1.82	0.45
1:E:468:MET:SD	1:F:468:MET:HE3	2.57	0.45
1:F:27:ILE:HG23	1:F:28:THR:H	1.82	0.45
1:B:197:THR:O	1:B:245:SER:HA	2.17	0.45
1:D:508:THR:O	1:D:512:VAL:HG23	2.17	0.44
1:F:491:MET:CE	1:F:491:MET:HA	2.47	0.44
1:D:18:LYS:NZ	1:D:29:GLU:OE1	2.35	0.44
1:D:756:ARG:CG	1:D:757:ILE:N	2.81	0.44
1:E:727:GLU:H	1:E:727:GLU:CD	2.19	0.44
1:H:345:TYR:OH	11:H:808:PE5:H11	2.17	0.44
1:A:604:ARG:NH1	1:A:608:GLU:OE1	2.50	0.44
9:B:802:7PE:H201	12:B:1039:HOH:O	2.16	0.44
1:C:229:LEU:HD12	1:C:229:LEU:N	2.33	0.44
1:C:18:LYS:NZ	1:C:29:GLU:OE1	2.50	0.44
1:B:129:GLU:OE2	1:B:131:LYS:NZ	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:501:LEU:HD23	1:D:509:LEU:HD11	2.00	0.44
1:D:98:ALA:O	1:D:99:SER:CB	2.64	0.44
1:E:594:LEU:HD12	1:E:598:HIS:HD2	1.81	0.44
1:H:2:HIS:ND1	1:H:9:THR:HB	2.32	0.44
1:H:478:GLU:HB2	1:H:575:TYR:CD2	2.52	0.44
1:H:323:SER:HB3	1:H:670:ILE:HG22	2.00	0.44
1:A:181:HIS:HB2	1:A:182:PRO:CD	2.47	0.44
1:E:13:GLY:N	1:E:292:ILE:HD11	2.33	0.44
1:F:731:ILE:HB	1:F:757:ILE:CG2	2.47	0.44
1:H:566:LEU:HD11	1:H:573:TYR:OH	2.17	0.44
1:C:659:GLU:O	1:C:660:ALA:CB	2.65	0.44
1:E:577:ASN:N	4:E:805:GOL:O3	2.37	0.44
1:G:659:GLU:O	1:G:660:ALA:HB3	2.16	0.44
1:C:643:TYR:O	1:C:646:PHE:HB3	2.18	0.44
1:E:718:GLN:HA	1:E:735:SER:OG	2.18	0.44
1:F:422:TYR:CE2	6:F:806:PGE:H42	2.53	0.44
1:A:301:ASN:O	1:A:675:ASN:HB3	2.18	0.44
1:A:753:ASP:O	1:A:754:SER:CB	2.66	0.44
1:A:215:TYR:HE1	6:A:812:PGE:H22	1.83	0.44
1:B:327:TYR:CE2	4:B:808:GOL:H32	2.53	0.44
1:C:320:ARG:HA	1:C:670:ILE:O	2.18	0.44
1:C:754:SER:O	1:C:755:GLU:HB2	2.17	0.44
1:E:203:THR:O	1:E:239:LYS:HA	2.17	0.44
1:E:693:GLY:C	1:E:695:ASP:N	2.71	0.44
1:G:577:ASN:OD1	1:G:582:ARG:NH2	2.46	0.44
1:H:639:VAL:O	1:H:642:ALA:HB3	2.17	0.44
1:H:715:VAL:HG22	1:H:720:LEU:HD22	2.00	0.44
1:C:501:LEU:HD23	1:C:509:LEU:HD11	2.00	0.43
4:A:811:GOL:C3	1:F:158:ASP:OD1	2.66	0.43
1:H:508:THR:O	1:H:512:VAL:HG23	2.18	0.43
1:A:47:ALA:O	1:A:81:LEU:HD12	2.18	0.43
1:B:99:SER:HB3	1:B:116:SER:HB2	1.99	0.43
1:C:233:LYS:HA	1:C:234:PRO:HD3	1.82	0.43
1:E:693:GLY:O	1:E:694:ASP:HB2	2.18	0.43
1:A:108:GLN:HG3	1:A:110:VAL:CG2	2.46	0.43
1:C:459:LYS:HZ1	4:D:809:GOL:H32	1.83	0.43
1:G:179:PHE:CE1	1:G:186:GLY:HA3	2.53	0.43
1:H:749:LYS:O	1:H:750:SER:HB3	2.18	0.43
1:A:732:THR:HG23	12:A:980:HOH:O	2.17	0.43
1:B:391:CYS:HB3	1:B:410:ASN:HB3	1.99	0.43
1:G:731:ILE:HD12	1:G:745:ILE:HD11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:199:THR:HG21	1:E:253:GLN:HA	2.00	0.43
1:B:428:HIS:CG	1:B:437:ILE:HG13	2.53	0.43
1:C:573:TYR:CE2	1:C:621:PHE:CE1	3.07	0.43
1:E:630:ALA:HB2	1:E:645:ASN:HB3	2.01	0.43
1:G:7:HIS:CE1	1:G:20:ARG:HD3	2.54	0.43
1:G:382:ILE:HD12	1:G:391:CYS:CB	2.49	0.43
1:G:568:LYS:HB3	1:G:568:LYS:HE2	1.76	0.43
1:H:18:LYS:NZ	1:H:29:GLU:OE1	2.47	0.43
1:H:345:TYR:OH	11:H:808:PE5:C2	2.64	0.43
1:C:154:ASP:CG	1:G:644:ARG:NH1	2.72	0.43
1:H:277:TRP:HA	1:H:280:LEU:HD12	2.01	0.43
1:A:43:ARG:HD3	1:A:56:ALA:HB3	2.01	0.43
1:B:342:MET:HE2	12:B:970:HOH:O	2.17	0.43
1:B:725:THR:OG1	1:B:728:GLN:HG3	2.18	0.43
1:D:172:HIS:O	1:D:191:THR:HA	2.17	0.43
1:E:95:GLU:HG2	1:E:95:GLU:H	1.68	0.43
1:F:689:LEU:O	1:F:690:SER:HB3	2.18	0.43
1:F:731:ILE:O	1:F:757:ILE:CG2	2.59	0.43
1:H:144:LYS:HE3	1:H:266:TYR:CD2	2.53	0.43
1:A:191:THR:CG2	1:A:196:ASP:H	2.32	0.43
1:D:727:GLU:O	1:D:761:ARG:N	2.45	0.43
1:G:575:TYR:CG	1:G:576:PRO:HA	2.54	0.43
1:H:741:LEU:O	1:H:742:THR:HG23	2.18	0.43
1:H:758:THR:CG2	1:H:759:LYS:N	2.82	0.43
1:B:16:ILE:HD13	1:B:300:PHE:CD2	2.54	0.43
1:H:139:HIS:O	1:H:242:ILE:HA	2.19	0.43
1:B:249:VAL:HG11	1:B:255:GLU:HG2	2.01	0.42
12:A:1080:HOH:O	1:C:644:ARG:HD2	2.19	0.42
1:E:287:THR:HB	1:E:710:THR:HG23	2.01	0.42
1:D:733:ASN:OD1	1:D:733:ASN:C	2.57	0.42
1:D:756:ARG:CG	1:D:757:ILE:H	2.32	0.42
1:F:557:ILE:HA	1:F:558:PRO:C	2.39	0.42
1:H:49:ASP:HB3	1:H:53:ALA:HB3	2.01	0.42
1:H:667:ILE:HA	1:H:667:ILE:HD12	1.75	0.42
1:A:116:SER:HA	1:A:125:ILE:O	2.19	0.42
1:C:6:GLU:H	1:C:6:GLU:HG2	1.51	0.42
1:D:327:TYR:HD1	1:D:327:TYR:HA	1.71	0.42
1:E:319:ALA:HB2	1:E:332:PHE:CD1	2.55	0.42
1:G:97:ALA:O	1:G:99:SER:N	2.53	0.42
1:H:114:LYS:HG3	1:H:128:HIS:HD2	1.78	0.42
1:H:384:GLY:HA3	1:H:390:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:731:ILE:HD13	1:H:743:LEU:HD23	2.01	0.42
1:H:761:ARG:HH21	1:H:761:ARG:HB3	1.84	0.42
1:B:18:LYS:HG2	1:B:29:GLU:OE1	2.19	0.42
1:E:139:HIS:O	1:E:242:ILE:HA	2.18	0.42
1:F:729:ILE:HD12	1:F:760:SER:HA	2.01	0.42
1:A:702:LEU:HD23	1:A:709:TYR:CE2	2.55	0.42
1:C:229:LEU:N	1:C:229:LEU:CD1	2.82	0.42
1:E:491:MET:HG3	1:E:535:VAL:HG21	2.02	0.42
1:F:338:TYR:HA	1:F:680:GLN:HE22	1.84	0.42
1:E:468:MET:SD	1:F:468:MET:CE	3.08	0.42
1:F:514:GLU:HG2	1:F:514:GLU:H	1.73	0.42
1:A:760:SER:OG	1:A:762:LEU:HD12	2.19	0.42
1:C:116:SER:HA	1:C:125:ILE:O	2.20	0.42
1:F:512:VAL:O	1:F:516:ILE:HG12	2.20	0.42
1:G:142:LEU:HD21	1:G:263:MET:CE	2.42	0.42
1:B:681:MET:HE3	1:B:681:MET:HB2	1.91	0.42
1:D:615:GLU:HB3	1:D:616:PRO:HD3	2.02	0.42
1:E:287:THR:O	1:E:709:TYR:HA	2.20	0.42
1:G:17:ILE:HA	1:G:102:ARG:O	2.20	0.42
1:G:360:ARG:HH11	1:G:360:ARG:HG2	1.85	0.42
1:A:599:PRO:CB	5:A:806:P6G:H141	2.46	0.42
1:C:508:THR:O	1:C:512:VAL:HG23	2.19	0.42
1:H:637:ASP:OD2	1:H:701:ARG:NH1	2.53	0.42
1:A:464:ARG:HD2	1:A:534:TYR:HB2	2.02	0.42
1:B:361:THR:HB	1:B:387:GLY:HA3	2.02	0.42
1:D:686:PHE:CE1	1:D:703:PRO:HG3	2.55	0.42
1:D:459:LYS:HB3	1:D:459:LYS:HE3	1.84	0.41
1:D:336:GLU:O	9:D:808:7PE:H32	2.20	0.41
1:E:233:LYS:HA	1:E:234:PRO:HD3	1.90	0.41
1:E:412:TRP:CZ3	1:E:479:ASN:HB2	2.55	0.41
1:G:644:ARG:HD3	12:G:1020:HOH:O	2.19	0.41
1:A:263:MET:HE3	1:A:269:GLU:HG3	2.03	0.41
1:A:696:ILE:HD12	1:A:715:VAL:HG11	2.02	0.41
1:C:165:VAL:HB	12:C:1184:HOH:O	2.20	0.41
1:A:368:LYS:HD3	1:A:378:TYR:O	2.20	0.41
1:A:618:THR:HG22	1:A:620:HIS:H	1.85	0.41
5:A:806:P6G:H52	5:A:806:P6G:H22	1.90	0.41
1:A:582:ARG:HD2	1:B:394:PHE:HZ	1.84	0.41
1:D:178:TYR:OH	1:D:180:SER:HB3	2.20	0.41
1:D:181:HIS:HB2	1:D:182:PRO:CD	2.50	0.41
1:D:6:GLU:O	1:D:7:HIS:HB2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:734:LYS:H	1:F:734:LYS:HG2	1.76	0.41
1:G:678:SER:HA	1:G:681:MET:HE3	2.01	0.41
1:D:551:TYR:CZ	4:D:807:GOL:H11	2.55	0.41
1:E:637:ASP:O	1:E:637:ASP:CG	2.58	0.41
1:F:381:TRP:CH2	1:F:413:GLN:NE2	2.88	0.41
1:F:448:ILE:HG22	1:F:493:THR:HG21	2.03	0.41
1:H:375:GLU:O	1:H:451:PHE:HA	2.19	0.41
1:A:274:ARG:NE	4:A:808:GOL:O1	2.52	0.41
1:B:20:ARG:HD2	1:B:20:ARG:HA	1.76	0.41
12:A:1080:HOH:O	1:C:644:ARG:CD	2.68	0.41
1:D:361:THR:HB	1:D:387:GLY:HA3	2.03	0.41
1:G:327:TYR:OH	4:G:802:GOL:H31	2.20	0.41
1:B:315:LEU:H	4:B:803:GOL:H12	1.86	0.41
1:B:85:HIS:HA	1:B:89:GLU:O	2.20	0.41
1:C:293:ILE:HD12	1:C:293:ILE:N	2.35	0.41
1:D:131:LYS:HA	1:D:142:LEU:O	2.21	0.41
1:F:734:LYS:HB2	1:F:735:SER:H	1.70	0.41
1:G:179:PHE:CZ	1:G:186:GLY:HA3	2.55	0.41
1:G:58:ILE:H	1:G:58:ILE:HD12	1.84	0.41
1:G:646:PHE:O	1:G:650:VAL:HG22	2.21	0.41
1:H:356:LYS:HB3	1:H:356:LYS:HE2	1.90	0.41
1:H:414:ILE:O	1:H:418:PRO:HD2	2.21	0.41
1:H:79:ALA:HB3	1:H:241:MET:HB2	2.01	0.41
1:B:179:PHE:CE1	1:B:186:GLY:HA3	2.56	0.41
1:C:47:ALA:HB1	1:C:82:THR:HB	2.02	0.41
1:D:477:HIS:HE1	1:D:585:CYS:O	2.04	0.41
1:E:301:ASN:O	1:E:675:ASN:HB3	2.20	0.41
1:F:60:THR:HB	1:F:315:LEU:HD13	2.02	0.41
1:G:546:GLN:OE1	1:G:586:ILE:HG21	2.21	0.41
1:G:692:HIS:O	1:G:695:ASP:HB2	2.21	0.41
1:H:246:SER:HA	1:H:249:VAL:O	2.20	0.41
1:A:7:HIS:HB3	1:A:19:ASN:OD1	2.21	0.41
1:B:190:LYS:HA	1:B:196:ASP:O	2.21	0.41
1:B:704:ASP:OD2	4:D:805:GOL:O3	2.38	0.41
1:C:696:ILE:CD1	1:C:696:ILE:N	2.84	0.41
1:E:341:PRO:HG2	1:E:680:GLN:NE2	2.35	0.41
1:F:133:ALA:HA	1:F:141:VAL:HA	2.02	0.41
1:F:570:ASP:N	1:F:570:ASP:OD1	2.51	0.41
1:G:415:HIS:ND1	1:G:419:ASP:OD2	2.44	0.41
1:G:31:SER:HB3	1:G:670:ILE:HG12	2.02	0.41
1:H:458:TYR:CE2	1:H:460:PRO:HA	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:69:LYS:HA	8:H:803:PG4:H72	2.02	0.41
1:C:16:ILE:CG1	1:C:104:LEU:HB3	2.50	0.41
1:C:491:MET:HA	1:C:491:MET:CE	2.51	0.41
1:D:45:THR:HG21	1:D:55:ALA:HA	2.01	0.41
1:E:28:THR:HG21	1:E:656:ASN:HB2	2.02	0.41
1:F:573:TYR:CE2	1:F:621:PHE:HE1	2.38	0.41
1:F:751:VAL:HG12	1:F:752:LEU:N	2.35	0.41
1:G:737:ASP:CA	1:G:738:ARG:CB	2.92	0.41
1:A:432:GLY:O	1:A:434:ASP:N	2.54	0.41
10:C:805:PE4:C8	10:C:805:PE4:H142	2.50	0.41
1:D:573:TYR:HE2	1:D:621:PHE:HE1	1.68	0.41
1:D:605:LYS:HA	1:D:605:LYS:HD3	1.92	0.41
8:D:803:PG4:H11	8:D:803:PG4:H32	1.76	0.41
1:A:644:ARG:NH1	1:F:228:SER:HB3	2.33	0.41
1:F:49:ASP:HB3	1:F:53:ALA:HB3	2.02	0.41
1:H:356:LYS:HE3	1:H:440:TYR:CZ	2.56	0.41
1:G:129:GLU:OE2	1:G:131:LYS:NZ	2.38	0.41
1:H:422:TYR:HE2	11:H:808:PE5:H62	1.86	0.41
1:A:44:GLY:O	1:A:102:ARG:NH2	2.38	0.40
1:F:43:ARG:HD3	1:F:56:ALA:HB3	2.02	0.40
1:A:58:ILE:HD12	1:A:58:ILE:N	2.36	0.40
1:B:733:ASN:C	1:B:734:LYS:O	2.58	0.40
1:E:15:ASP:OD2	1:E:17:ILE:HD11	2.22	0.40
1:G:619:LEU:O	1:G:620:HIS:HB2	2.21	0.40
1:G:97:ALA:O	1:G:98:ALA:C	2.58	0.40
1:A:31:SER:HB3	1:A:670:ILE:HG12	2.02	0.40
1:B:726:LYS:N	1:B:726:LYS:HD2	2.37	0.40
1:B:729:ILE:HD11	1:B:745:ILE:HG21	2.02	0.40
1:D:612:GLU:OE2	1:D:638:LYS:NZ	2.54	0.40
1:E:230:GLU:CD	1:E:233:LYS:HE3	2.42	0.40
1:G:612:GLU:OE2	4:G:803:GOL:H31	2.21	0.40
1:A:573:TYR:CE2	1:A:621:PHE:HE1	2.39	0.40
1:B:316:PRO:CB	1:B:331:ALA:HB2	2.52	0.40
1:B:604:ARG:HG2	9:B:802:7PE:C21	2.42	0.40
1:D:741:LEU:C	1:D:742:THR:HG23	2.42	0.40
1:E:29:GLU:HG2	1:E:102:ARG:NH1	2.37	0.40
1:E:466:GLU:OE1	1:E:468:MET:CE	2.70	0.40
1:F:491:MET:HE1	1:F:491:MET:HA	2.01	0.40
1:F:594:LEU:HD12	1:F:598:HIS:HD2	1.86	0.40
1:H:381:TRP:CH2	1:H:413:GLN:CD	2.95	0.40
1:B:604:ARG:HB3	1:B:604:ARG:HE	1.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:201:VAL:HG11	1:D:260:ALA:HB2	2.03	0.40
1:D:79:ALA:HB3	1:D:241:MET:HB2	2.04	0.40
1:D:412:TRP:CZ3	1:D:479:ASN:HB2	2.57	0.40
1:E:117:GLN:O	1:E:124:THR:HA	2.21	0.40
1:F:361:THR:HB	1:F:387:GLY:HA3	2.04	0.40
1:G:381:TRP:CH2	1:G:413:GLN:NE2	2.90	0.40
1:G:615:GLU:HB3	1:G:616:PRO:CD	2.51	0.40
1:H:624:LEU:HD12	1:H:624:LEU:N	2.36	0.40
1:H:719:THR:H	1:H:735:SER:HB3	1.86	0.40
1:H:754:SER:O	1:H:755:GLU:C	2.59	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	760/769 (99%)	721 (95%)	29 (4%)	10 (1%)	12	12
1	B	759/769 (99%)	720 (95%)	33 (4%)	6 (1%)	19	23
1	C	759/769 (99%)	728 (96%)	25 (3%)	6 (1%)	19	23
1	D	759/769 (99%)	723 (95%)	34 (4%)	2 (0%)	41	50
1	E	759/769 (99%)	696 (92%)	48 (6%)	15 (2%)	7	6
1	F	759/769 (99%)	701 (92%)	44 (6%)	14 (2%)	8	7
1	G	760/769 (99%)	718 (94%)	31 (4%)	11 (1%)	11	11
1	H	759/769 (99%)	715 (94%)	35 (5%)	9 (1%)	13	14
All	All	6074/6152 (99%)	5722 (94%)	279 (5%)	73 (1%)	13	14

All (73) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	742	THR
1	A	750	SER
1	A	754	SER
1	B	6	GLU
1	B	27	ILE
1	B	735	SER
1	C	6	GLU
1	C	98	ALA
1	C	694	ASP
1	D	98	ALA
1	E	736	GLU
1	E	738	ARG
1	E	750	SER
1	E	751	VAL
1	F	27	ILE
1	F	98	ALA
1	F	99	SER
1	F	744	HIS
1	F	746	PHE
1	F	757	ILE
1	G	209	ASP
1	G	660	ALA
1	G	736	GLU
1	G	738	ARG
1	H	3	GLU
1	H	735	SER
1	A	6	GLU
1	A	98	ALA
1	A	743	LEU
1	A	749	LYS
1	A	753	ASP
1	E	660	ALA
1	F	738	ARG
1	F	754	SER
1	F	760	SER
1	G	2	HIS
1	G	98	ALA
1	H	2	HIS
1	H	6	GLU
1	H	98	ALA
1	H	99	SER
1	A	2	HIS
1	A	660	ALA

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Mol	Chain	Res	Type
1	C	660	ALA
1	D	99	SER
1	E	6	GLU
1	E	98	ALA
1	E	205	SER
1	E	209	ASP
1	F	2	HIS
1	F	690	SER
1	F	700	PRO
1	G	210	ALA
1	H	750	SER
1	B	37	ASN
1	B	98	ALA
1	B	754	SER
1	C	2	HIS
1	C	37	ASN
1	E	26	ALA
1	E	474	ASP
1	E	746	PHE
1	F	735	SER
1	F	758	THR
1	G	314	SER
1	G	737	ASP
1	H	314	SER
1	G	474	ASP
1	E	87	ASP
1	G	37	ASN
1	E	182	PRO
1	H	27	ILE
1	E	757	ILE

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	651/658 (99%)	616 (95%)	35 (5%)	22	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	650/658 (99%)	615 (95%)	35 (5%)	22	30
1	C	650/658 (99%)	609 (94%)	41 (6%)	18	24
1	D	650/658 (99%)	615 (95%)	35 (5%)	22	30
1	E	650/658 (99%)	598 (92%)	52 (8%)	12	15
1	F	650/658 (99%)	609 (94%)	41 (6%)	18	24
1	G	651/658 (99%)	600 (92%)	51 (8%)	12	16
1	H	650/658 (99%)	616 (95%)	34 (5%)	23	32
All	All	5202/5264 (99%)	4878 (94%)	324 (6%)	18	25

All (324) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	ARG
1	A	83	LEU
1	A	94	SER
1	A	96	GLU
1	A	129	GLU
1	A	191	THR
1	A	217	ASN
1	A	229	LEU
1	A	257	LEU
1	A	258	LEU
1	A	261	LYS
1	A	275	LEU
1	A	280	LEU
1	A	289	GLN
1	A	298	LEU
1	A	378	TYR
1	A	390	LEU
1	A	417	SER
1	A	506	GLU
1	A	509	LEU
1	A	537	LYS
1	A	604	ARG
1	A	647	ARG
1	A	655	LEU
1	A	670	ILE
1	A	698	LEU
1	A	701	ARG
1	A	702	LEU

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Mol	Chain	Res	Type
1	A	727	GLU
1	A	732	THR
1	A	739	LYS
1	A	741	LEU
1	A	750	SER
1	A	752	LEU
1	A	757	ILE
1	B	2	HIS
1	B	20	ARG
1	B	80	LEU
1	B	96	GLU
1	B	102	ARG
1	B	144	LYS
1	B	224	THR
1	B	228	SER
1	B	230	GLU
1	B	233	LYS
1	B	289	GLN
1	B	370	LYS
1	B	378	TYR
1	B	425	LYS
1	B	503	THR
1	B	506	GLU
1	B	507	LYS
1	B	509	LEU
1	B	524	SER
1	B	582	ARG
1	B	604	ARG
1	B	659	GLU
1	B	710	THR
1	B	720	LEU
1	B	726	LYS
1	B	729	ILE
1	B	734	LYS
1	B	735	SER
1	B	736	GLU
1	B	741	LEU
1	B	742	THR
1	B	743	LEU
1	B	748	GLU
1	B	750	SER
1	B	760	SER

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Mol	Chain	Res	Type
1	C	1	MET
1	C	2	HIS
1	C	6	GLU
1	C	18	LYS
1	C	94	SER
1	C	118	ARG
1	C	147	VAL
1	C	191	THR
1	C	227	LEU
1	C	228	SER
1	C	230	GLU
1	C	257	LEU
1	C	258	LEU
1	C	261	LYS
1	C	275	LEU
1	C	280	LEU
1	C	289	GLN
1	C	298	LEU
1	C	349	GLU
1	C	352	ARG
1	C	370	LYS
1	C	378	TYR
1	C	495	GLN
1	C	503	THR
1	C	509	LEU
1	C	510	SER
1	C	537	LYS
1	C	569	GLU
1	C	582	ARG
1	C	604	ARG
1	C	655	LEU
1	C	698	LEU
1	C	702	LEU
1	C	710	THR
1	C	718	GLN
1	C	728	GLN
1	C	735	SER
1	C	750	SER
1	C	754	SER
1	C	757	ILE
1	C	760	SER
1	D	1	MET

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Mol	Chain	Res	Type
1	D	27	ILE
1	D	80	LEU
1	D	94	SER
1	D	99	SER
1	D	101	GLU
1	D	102	ARG
1	D	147	VAL
1	D	205	SER
1	D	228	SER
1	D	233	LYS
1	D	275	LEU
1	D	289	GLN
1	D	349	GLU
1	D	370	LYS
1	D	378	TYR
1	D	397	LYS
1	D	417	SER
1	D	426	LYS
1	D	503	THR
1	D	509	LEU
1	D	524	SER
1	D	582	ARG
1	D	605	LYS
1	D	667	ILE
1	D	699	SER
1	D	710	THR
1	D	726	LYS
1	D	735	SER
1	D	736	GLU
1	D	741	LEU
1	D	742	THR
1	D	748	GLU
1	D	750	SER
1	D	761	ARG
1	E	2	HIS
1	E	16	ILE
1	E	22	GLU
1	E	29	GLU
1	E	89	GLU
1	E	96	GLU
1	E	99	SER
1	E	114	LYS

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Mol	Chain	Res	Type
1	E	171	ASP
1	E	174	GLN
1	E	193	SER
1	E	217	ASN
1	E	226	SER
1	E	228	SER
1	E	243	ILE
1	E	257	LEU
1	E	258	LEU
1	E	259	GLU
1	E	261	LYS
1	E	262	HIS
1	E	275	LEU
1	E	280	LEU
1	E	289	GLN
1	E	298	LEU
1	E	370	LYS
1	E	378	TYR
1	E	390	LEU
1	E	503	THR
1	E	506	GLU
1	E	509	LEU
1	E	540	LYS
1	E	560	LYS
1	E	604	ARG
1	E	655	LEU
1	E	659	GLU
1	E	661	VAL
1	E	696	ILE
1	E	698	LEU
1	E	702	LEU
1	E	710	THR
1	E	714	ILE
1	E	726	LYS
1	E	732	THR
1	E	734	LYS
1	E	741	LEU
1	E	742	THR
1	E	743	LEU
1	E	749	LYS
1	E	751	VAL
1	E	753	ASP

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Mol	Chain	Res	Type
1	E	755	GLU
1	E	757	ILE
1	F	2	HIS
1	F	20	ARG
1	F	22	GLU
1	F	80	LEU
1	F	94	SER
1	F	102	ARG
1	F	128	HIS
1	F	171	ASP
1	F	224	THR
1	F	228	SER
1	F	233	LYS
1	F	275	LEU
1	F	295	GLN
1	F	296	VAL
1	F	349	GLU
1	F	352	ARG
1	F	378	TYR
1	F	417	SER
1	F	506	GLU
1	F	509	LEU
1	F	514	GLU
1	F	582	ARG
1	F	603	ASP
1	F	604	ARG
1	F	637	ASP
1	F	641	GLU
1	F	659	GLU
1	F	667	ILE
1	F	710	THR
1	F	716	LYS
1	F	728	GLN
1	F	734	LYS
1	F	735	SER
1	F	736	GLU
1	F	738	ARG
1	F	742	THR
1	F	743	LEU
1	F	749	LYS
1	F	750	SER
1	F	756	ARG

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Mol	Chain	Res	Type
1	F	759	LYS
1	G	2	HIS
1	G	3	GLU
1	G	16	ILE
1	G	20	ARG
1	G	52	ASP
1	G	83	LEU
1	G	92	ILE
1	G	99	SER
1	G	118	ARG
1	G	147	VAL
1	G	190	LYS
1	G	191	THR
1	G	193	SER
1	G	213	GLU
1	G	227	LEU
1	G	229	LEU
1	G	233	LYS
1	G	255	GLU
1	G	257	LEU
1	G	258	LEU
1	G	261	LYS
1	G	275	LEU
1	G	280	LEU
1	G	282	SER
1	G	292	ILE
1	G	298	LEU
1	G	334	ASP
1	G	370	LYS
1	G	378	TYR
1	G	390	LEU
1	G	417	SER
1	G	426	LYS
1	G	495	GLN
1	G	503	THR
1	G	506	GLU
1	G	568	LYS
1	G	604	ARG
1	G	644	ARG
1	G	655	LEU
1	G	661	VAL
1	G	696	ILE

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Mol	Chain	Res	Type
1	G	702	LEU
1	G	726	LYS
1	G	736	GLU
1	G	739	LYS
1	G	743	LEU
1	G	749	LYS
1	G	750	SER
1	G	754	SER
1	G	756	ARG
1	G	760	SER
1	H	2	HIS
1	H	27	ILE
1	H	80	LEU
1	H	83	LEU
1	H	99	SER
1	H	102	ARG
1	H	224	THR
1	H	258	LEU
1	H	261	LYS
1	H	274	ARG
1	H	275	LEU
1	H	346	SER
1	H	370	LYS
1	H	378	TYR
1	H	400	LEU
1	H	417	SER
1	H	495	GLN
1	H	503	THR
1	H	507	LYS
1	H	519	SER
1	H	537	LYS
1	H	560	LYS
1	H	582	ARG
1	H	641	GLU
1	H	667	ILE
1	H	699	SER
1	H	720	LEU
1	H	726	LYS
1	H	734	LYS
1	H	742	THR
1	H	743	LEU
1	H	754	SER

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Mol	Chain	Res	Type
1	H	756	ARG
1	H	761	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	495	GLN
1	A	680	GLN
1	B	128	HIS
1	B	347	ASN
1	C	128	HIS
1	C	217	ASN
1	C	429	GLN
1	C	680	GLN
1	D	429	GLN
1	E	289	GLN
1	E	697	HIS
1	F	429	GLN
1	F	455	HIS
1	F	680	GLN
1	G	7	HIS
1	G	264	GLN
1	G	429	GLN
1	G	475	GLN
1	H	7	HIS
1	H	680	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 74 ligands modelled in this entry, 7 are monoatomic - leaving 67 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$
9	7PE	B	802	-	20,20,20	0.61	0	19,19,19	0.99	1 (5%)
11	PE5	H	808	-	26,26,26	0.77	0	25,25,25	0.90	0
4	GOL	C	809	-	5,5,5	0.60	0	5,5,5	2.29	1 (20%)
4	GOL	A	810	-	5,5,5	0.56	0	5,5,5	0.85	0
2	IFM	D	801	-	9,10,10	2.40	5 (55%)	9,13,13	3.56	6 (66%)
4	GOL	A	808	-	5,5,5	0.44	0	5,5,5	0.72	0
4	GOL	D	806	-	5,5,5	0.75	0	5,5,5	1.08	0
4	GOL	E	806	-	5,5,5	0.51	0	5,5,5	0.78	0
4	GOL	D	802	-	5,5,5	0.49	0	5,5,5	0.76	0
4	GOL	C	802	-	5,5,5	0.52	0	5,5,5	0.36	0
2	IFM	E	801	-	9,10,10	1.51	2 (22%)	9,13,13	3.09	4 (44%)
8	PG4	D	803	-	12,12,12	0.60	0	11,11,11	0.62	0
6	PGE	C	807	-	9,9,9	0.45	0	8,8,8	0.85	0
4	GOL	A	805	-	5,5,5	0.26	0	5,5,5	0.67	0
8	PG4	B	801	-	12,12,12	0.57	0	11,11,11	0.44	0
4	GOL	B	807	-	5,5,5	0.59	0	5,5,5	0.89	0
4	GOL	D	804	-	5,5,5	0.35	0	5,5,5	0.45	0
4	GOL	B	806	-	5,5,5	0.31	0	5,5,5	0.54	0
4	GOL	E	804	-	5,5,5	0.21	0	5,5,5	0.67	0
4	GOL	E	807	-	5,5,5	0.22	0	5,5,5	0.93	0
4	GOL	D	809	-	5,5,5	0.37	0	5,5,5	1.35	1 (20%)
6	PGE	G	805	-	9,9,9	0.71	0	8,8,8	0.60	0
4	GOL	F	805	-	5,5,5	0.65	0	5,5,5	0.66	0
4	GOL	H	806	-	5,5,5	0.49	0	5,5,5	1.03	0
4	GOL	D	805	-	5,5,5	0.08	0	5,5,5	0.94	0
4	GOL	D	812	-	5,5,5	1.29	0	5,5,5	1.95	2 (40%)
2	IFM	G	801	-	9,10,10	1.22	1 (11%)	9,13,13	3.17	5 (55%)
4	GOL	F	802	-	5,5,5	0.26	0	5,5,5	0.80	0
4	GOL	G	802	-	5,5,5	0.19	0	5,5,5	0.78	0
8	PG4	F	803	-	12,12,12	0.54	0	11,11,11	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	G	803	-	5,5,5	0.20	0	5,5,5	0.77	0
4	GOL	D	810	-	5,5,5	0.38	0	5,5,5	1.77	1 (20%)
6	PGE	F	806	-	9,9,9	0.50	0	8,8,8	0.48	0
4	GOL	A	809	-	5,5,5	0.53	0	5,5,5	0.45	0
4	GOL	B	804	-	5,5,5	0.72	0	5,5,5	1.56	2 (40%)
4	GOL	C	804	-	5,5,5	0.42	0	5,5,5	1.25	1 (20%)
4	GOL	A	803	-	5,5,5	0.58	0	5,5,5	1.10	0
4	GOL	A	804	-	5,5,5	0.80	0	5,5,5	2.09	2 (40%)
4	GOL	C	808	-	5,5,5	0.48	0	5,5,5	0.66	0
4	GOL	B	803	-	5,5,5	0.55	0	5,5,5	1.70	2 (40%)
4	GOL	E	805	-	5,5,5	0.42	0	5,5,5	0.21	0
8	PG4	H	803	-	12,12,12	0.68	0	11,11,11	0.48	0
4	GOL	H	802	-	5,5,5	0.31	0	5,5,5	0.53	0
5	P6G	E	803	-	18,18,18	0.66	0	17,17,17	0.79	0
4	GOL	D	811	-	5,5,5	0.35	0	5,5,5	0.29	0
4	GOL	H	805	-	5,5,5	0.43	0	5,5,5	1.00	1 (20%)
3	1PE	C	801	-	15,15,15	0.65	0	14,14,14	0.96	0
2	IFM	F	801	-	9,10,10	1.36	2 (22%)	9,13,13	3.26	3 (33%)
4	GOL	B	808	-	5,5,5	0.55	0	5,5,5	1.91	1 (20%)
4	GOL	C	806	-	5,5,5	0.64	0	5,5,5	0.75	0
4	GOL	D	807	-	5,5,5	0.32	0	5,5,5	0.53	0
2	IFM	H	801	-	9,10,10	1.27	2 (22%)	9,13,13	3.81	4 (44%)
4	GOL	H	804	-	5,5,5	0.36	0	5,5,5	0.61	0
3	1PE	E	802	-	15,15,15	0.70	0	14,14,14	0.40	0
4	GOL	F	804	-	5,5,5	0.55	0	5,5,5	0.52	0
4	GOL	G	804	-	5,5,5	0.33	0	5,5,5	0.55	0
9	7PE	D	808	-	20,20,20	0.73	0	19,19,19	1.43	3 (15%)
6	PGE	A	812	-	9,9,9	0.56	0	8,8,8	0.45	0
4	GOL	C	803	-	5,5,5	0.22	0	5,5,5	1.24	1 (20%)
4	GOL	A	807	-	5,5,5	0.57	0	5,5,5	1.10	0
3	1PE	A	802	-	15,15,15	0.72	0	14,14,14	0.71	0
4	GOL	B	805	-	5,5,5	0.53	0	5,5,5	0.88	0
2	IFM	A	801	-	9,10,10	1.75	3 (33%)	9,13,13	3.85	3 (33%)
4	GOL	A	811	-	5,5,5	0.45	0	5,5,5	1.21	0
5	P6G	A	806	-	18,18,18	0.59	0	17,17,17	0.83	0
4	GOL	H	807	-	5,5,5	0.44	0	5,5,5	0.64	0
10	PE4	C	805	-	23,23,23	0.91	0	22,22,22	1.33	2 (9%)

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
9	7PE	B	802	-	-	8/18/18/18	-
11	PE5	H	808	-	-	21/24/24/24	-
4	GOL	C	809	-	-	2/4/4/4	-
4	GOL	A	810	-	-	1/4/4/4	-
2	IFM	D	801	-	-	0/2/16/16	0/1/1/1
4	GOL	A	808	-	-	4/4/4/4	-
4	GOL	D	806	-	-	3/4/4/4	-
4	GOL	E	806	-	-	1/4/4/4	-
4	GOL	D	802	-	-	2/4/4/4	-
4	GOL	C	802	-	-	0/4/4/4	-
2	IFM	E	801	-	-	0/2/16/16	0/1/1/1
8	PG4	D	803	-	-	4/10/10/10	-
6	PGE	C	807	-	-	3/7/7/7	-
4	GOL	A	805	-	-	4/4/4/4	-
8	PG4	B	801	-	-	3/10/10/10	-
4	GOL	B	807	-	-	0/4/4/4	-
4	GOL	D	804	-	-	4/4/4/4	-
4	GOL	B	806	-	-	2/4/4/4	-
4	GOL	E	804	-	-	2/4/4/4	-
4	GOL	E	807	-	-	2/4/4/4	-
4	GOL	D	809	-	-	3/4/4/4	-
6	PGE	G	805	-	-	4/7/7/7	-
4	GOL	F	805	-	-	2/4/4/4	-
4	GOL	H	806	-	-	0/4/4/4	-
4	GOL	D	805	-	-	2/4/4/4	-
4	GOL	D	812	-	-	0/4/4/4	-
2	IFM	G	801	-	-	0/2/16/16	0/1/1/1
4	GOL	F	802	-	-	2/4/4/4	-
4	GOL	G	802	-	-	2/4/4/4	-
8	PG4	F	803	-	-	8/10/10/10	-
4	GOL	G	803	-	-	3/4/4/4	-
4	GOL	D	810	-	-	4/4/4/4	-
6	PGE	F	806	-	-	4/7/7/7	-
4	GOL	A	809	-	-	2/4/4/4	-
4	GOL	B	804	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	C	804	-	-	2/4/4/4	-
4	GOL	A	803	-	-	4/4/4/4	-
4	GOL	A	804	-	-	2/4/4/4	-
4	GOL	C	808	-	-	0/4/4/4	-
4	GOL	B	803	-	-	2/4/4/4	-
4	GOL	E	805	-	-	2/4/4/4	-
8	PG4	H	803	-	-	6/10/10/10	-
4	GOL	H	802	-	-	0/4/4/4	-
5	P6G	E	803	-	-	10/16/16/16	-
4	GOL	D	811	-	-	4/4/4/4	-
4	GOL	H	805	-	-	2/4/4/4	-
3	1PE	C	801	-	-	5/13/13/13	-
2	IFM	F	801	-	-	0/2/16/16	1/1/1/1
4	GOL	B	808	-	-	3/4/4/4	-
4	GOL	C	806	-	-	0/4/4/4	-
4	GOL	D	807	-	-	2/4/4/4	-
2	IFM	H	801	-	-	0/2/16/16	1/1/1/1
4	GOL	H	804	-	-	4/4/4/4	-
3	1PE	E	802	-	-	9/13/13/13	-
4	GOL	F	804	-	-	2/4/4/4	-
4	GOL	G	804	-	-	0/4/4/4	-
9	7PE	D	808	-	-	4/18/18/18	-
6	PGE	A	812	-	-	4/7/7/7	-
4	GOL	C	803	-	-	0/4/4/4	-
4	GOL	A	807	-	-	4/4/4/4	-
3	1PE	A	802	-	-	9/13/13/13	-
4	GOL	B	805	-	-	3/4/4/4	-
2	IFM	A	801	-	-	1/2/16/16	0/1/1/1
4	GOL	A	811	-	-	4/4/4/4	-
5	P6G	A	806	-	-	11/16/16/16	-
4	GOL	H	807	-	-	4/4/4/4	-
10	PE4	C	805	-	-	8/21/21/21	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	801	IFM	C2-N	-3.71	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	IFM	C5-C4	-3.20	1.49	1.53
2	D	801	IFM	C5-C4	-3.10	1.49	1.53
2	D	801	IFM	O4-C4	-3.04	1.35	1.43
2	E	801	IFM	C3-C4	2.80	1.56	1.52
2	F	801	IFM	C3-C4	2.70	1.56	1.52
2	D	801	IFM	C3-C4	2.62	1.56	1.52
2	G	801	IFM	C3-C4	2.38	1.56	1.52
2	D	801	IFM	O3-C3	2.38	1.48	1.43
2	A	801	IFM	C2-N	-2.36	1.43	1.46
2	E	801	IFM	O3-C3	2.19	1.48	1.43
2	H	801	IFM	O3-C3	2.17	1.47	1.43
2	F	801	IFM	O3-C3	2.10	1.47	1.43
2	A	801	IFM	C3-C4	2.09	1.55	1.52
2	H	801	IFM	C3-C4	2.09	1.55	1.52

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	801	IFM	C1-N-C2	9.07	121.66	111.70
2	F	801	IFM	C1-N-C2	8.43	120.96	111.70
2	A	801	IFM	C1-N-C2	8.10	120.59	111.70
2	D	801	IFM	O4-C4-C5	-7.59	97.27	110.08
2	G	801	IFM	C1-N-C2	7.34	119.75	111.70
2	E	801	IFM	O4-C4-C5	-6.68	98.79	110.08
2	A	801	IFM	O4-C4-C5	-6.66	98.83	110.08
2	H	801	IFM	O4-C4-C5	-5.57	100.67	110.08
2	E	801	IFM	C1-N-C2	4.97	117.16	111.70
2	D	801	IFM	C1-N-C2	4.08	116.18	111.70
4	C	809	GOL	C3-C2-C1	-4.07	95.89	111.70
2	D	801	IFM	O3-C3-C4	4.06	118.27	110.14
4	B	808	GOL	O3-C3-C2	-3.85	91.73	110.20
4	D	810	GOL	O1-C1-C2	-3.63	92.80	110.20
10	C	805	PE4	C15-O8-C14	3.47	125.33	112.90
2	F	801	IFM	O3-C3-C4	3.38	116.90	110.14
2	G	801	IFM	C1-C5-C4	3.37	115.43	108.72
9	D	808	7PE	O4-C5-C6	-3.15	96.18	110.39
2	G	801	IFM	O4-C4-C5	-3.13	104.80	110.08
2	H	801	IFM	O3-C3-C4	3.13	116.40	110.14
2	E	801	IFM	O3-C3-C4	3.12	116.39	110.14
2	D	801	IFM	O6-C6-C5	-3.09	104.27	111.36
4	A	804	GOL	O1-C1-C2	-3.04	95.63	110.20
4	D	812	GOL	O2-C2-C3	3.04	122.50	109.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	808	7PE	O7-C8-C9	-2.82	97.67	110.39
2	A	801	IFM	O4-C4-C3	2.73	115.22	109.99
2	D	801	IFM	C1-C5-C4	-2.68	103.40	108.72
4	B	804	GOL	C3-C2-C1	-2.57	101.69	111.70
4	A	804	GOL	O2-C2-C3	2.56	120.41	109.12
2	F	801	IFM	O4-C4-C5	-2.55	105.78	110.08
4	D	812	GOL	C3-C2-C1	-2.41	102.33	111.70
2	G	801	IFM	O4-C4-C3	2.36	114.51	109.99
4	C	804	GOL	O1-C1-C2	-2.33	99.01	110.20
10	C	805	PE4	O7-C13-C14	2.26	120.58	110.39
2	D	801	IFM	C2-C3-C4	-2.25	107.68	110.33
2	E	801	IFM	O6-C6-C5	-2.24	106.22	111.36
2	G	801	IFM	O3-C3-C4	2.21	114.57	110.14
9	B	802	7PE	C20-O19-C18	2.21	120.83	112.90
2	H	801	IFM	C2-C3-C4	-2.19	107.75	110.33
4	C	803	GOL	O1-C1-C2	-2.14	99.92	110.20
4	B	803	GOL	O3-C3-C2	-2.14	99.95	110.20
9	D	808	7PE	C20-O19-C18	2.14	120.55	112.90
4	B	804	GOL	O2-C2-C3	-2.13	99.74	109.12
4	B	803	GOL	C3-C2-C1	-2.08	103.62	111.70
4	D	809	GOL	O2-C2-C1	-2.07	100.00	109.12
4	H	805	GOL	O1-C1-C2	-2.01	100.57	110.20

There are no chirality outliers.

All (217) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	809	GOL	C1-C2-C3-O3
4	D	809	GOL	O1-C1-C2-C3
4	A	808	GOL	O1-C1-C2-C3
4	A	808	GOL	C1-C2-C3-O3
4	D	806	GOL	O1-C1-C2-C3
4	D	804	GOL	O1-C1-C2-C3
4	B	806	GOL	C1-C2-C3-O3
4	E	807	GOL	O1-C1-C2-O2
4	F	805	GOL	O1-C1-C2-C3
4	F	802	GOL	C1-C2-C3-O3
4	G	802	GOL	O1-C1-C2-C3
4	E	805	GOL	C1-C2-C3-O3
4	E	805	GOL	O2-C2-C3-O3
4	A	809	GOL	O1-C1-C2-O2
4	A	809	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
4	B	804	GOL	O1-C1-C2-C3
4	B	804	GOL	C1-C2-C3-O3
4	C	804	GOL	O1-C1-C2-O2
4	C	804	GOL	O1-C1-C2-C3
4	D	811	GOL	C1-C2-C3-O3
4	H	805	GOL	C1-C2-C3-O3
4	B	808	GOL	C1-C2-C3-O3
4	B	808	GOL	O2-C2-C3-O3
4	H	804	GOL	O1-C1-C2-O2
4	H	804	GOL	O1-C1-C2-C3
4	F	804	GOL	O1-C1-C2-C3
4	B	805	GOL	O1-C1-C2-C3
4	A	811	GOL	C1-C2-C3-O3
4	H	807	GOL	C1-C2-C3-O3
8	F	803	PG4	C1-C2-O2-C3
5	A	806	P6G	C2-C3-O4-C5
8	D	803	PG4	C1-C2-O2-C3
11	H	808	PE5	C2-C1-O1-C50
3	E	802	1PE	OH4-C13-C23-OH3
3	C	801	1PE	OH4-C13-C23-OH3
9	D	808	7PE	O10-C11-C12-O13
9	D	808	7PE	O4-C5-C6-O7
10	C	805	PE4	O2-C3-C4-O3
10	C	805	PE4	O4-C7-C8-O5
8	H	803	PG4	O3-C5-C6-O4
11	H	808	PE5	C6-C5-O3-C4
11	H	808	PE5	O7-C13-C14-O8
3	E	802	1PE	OH5-C14-C24-OH4
8	D	803	PG4	O2-C3-C4-O3
11	H	808	PE5	O8-C15-C16-O52
10	C	805	PE4	O1-C1-C2-O2
10	C	805	PE4	O3-C5-C6-O4
11	H	808	PE5	O6-C10-C9-O5
3	C	801	1PE	OH5-C14-C24-OH4
8	F	803	PG4	O3-C5-C6-O4
5	E	803	P6G	O13-C14-C15-O16
4	D	806	GOL	O1-C1-C2-O2
4	A	805	GOL	O1-C1-C2-O2
4	B	806	GOL	O2-C2-C3-O3
4	B	804	GOL	O2-C2-C3-O3
4	H	805	GOL	O2-C2-C3-O3
4	H	807	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
9	B	802	7PE	O13-C14-C15-O16
9	B	802	7PE	O4-C5-C6-O7
11	H	808	PE5	O1-C1-C2-O2
8	F	803	PG4	O4-C7-C8-O5
8	D	803	PG4	O1-C1-C2-O2
3	E	802	1PE	OH2-C12-C22-OH3
3	C	801	1PE	OH7-C16-C26-OH6
6	A	812	PGE	O1-C1-C2-O2
9	D	808	7PE	O13-C14-C15-O16
3	A	802	1PE	OH5-C14-C24-OH4
10	C	805	PE4	O6-C10-C9-O5
10	C	805	PE4	O7-C13-C14-O8
6	F	806	PGE	O2-C3-C4-O3
6	G	805	PGE	O2-C3-C4-O3
6	C	807	PGE	O1-C1-C2-O2
6	C	807	PGE	O3-C5-C6-O4
11	H	808	PE5	O4-C7-C8-O5
5	A	806	P6G	C11-C12-O13-C14
4	D	806	GOL	C1-C2-C3-O3
4	D	802	GOL	O1-C1-C2-C3
4	A	805	GOL	O1-C1-C2-C3
4	A	805	GOL	C1-C2-C3-O3
4	D	804	GOL	C1-C2-C3-O3
4	E	804	GOL	C1-C2-C3-O3
4	E	807	GOL	O1-C1-C2-C3
4	D	810	GOL	O1-C1-C2-C3
4	A	803	GOL	C1-C2-C3-O3
4	A	804	GOL	O1-C1-C2-C3
4	B	803	GOL	O1-C1-C2-C3
4	G	803	GOL	C1-C2-C3-O3
4	D	811	GOL	O1-C1-C2-C3
4	H	804	GOL	C1-C2-C3-O3
4	A	807	GOL	O1-C1-C2-C3
4	A	807	GOL	C1-C2-C3-O3
4	A	811	GOL	O1-C1-C2-C3
4	H	807	GOL	O1-C1-C2-C3
8	F	803	PG4	O1-C1-C2-O2
5	A	806	P6G	O1-C2-C3-O4
9	B	802	7PE	O10-C11-C12-O13
3	A	802	1PE	OH4-C13-C23-OH3
4	C	809	GOL	O2-C2-C3-O3
4	A	808	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	A	808	GOL	O2-C2-C3-O3
4	D	802	GOL	O1-C1-C2-O2
4	D	804	GOL	O1-C1-C2-O2
4	F	805	GOL	O1-C1-C2-O2
4	F	802	GOL	O2-C2-C3-O3
4	D	810	GOL	O1-C1-C2-O2
4	D	810	GOL	O2-C2-C3-O3
4	A	803	GOL	O2-C2-C3-O3
4	A	804	GOL	O1-C1-C2-O2
4	G	803	GOL	O2-C2-C3-O3
4	D	811	GOL	O1-C1-C2-O2
4	D	811	GOL	O2-C2-C3-O3
4	A	811	GOL	O2-C2-C3-O3
4	H	807	GOL	O1-C1-C2-O2
5	A	806	P6G	O7-C8-C9-O10
6	A	812	PGE	O2-C3-C4-O3
9	B	802	7PE	O1-C2-C3-O4
6	G	805	PGE	O1-C1-C2-O2
3	E	802	1PE	OH6-C15-C25-OH5
5	E	803	P6G	O7-C8-C9-O10
5	A	806	P6G	O16-C17-C18-O19
9	B	802	7PE	C6-C5-O4-C3
4	B	804	GOL	O1-C1-C2-O2
4	F	804	GOL	O1-C1-C2-O2
4	B	805	GOL	O1-C1-C2-O2
4	A	811	GOL	O1-C1-C2-O2
8	H	803	PG4	O1-C1-C2-O2
4	A	810	GOL	C1-C2-C3-O3
4	G	803	GOL	O1-C1-C2-C3
9	B	802	7PE	C5-C6-O7-C8
5	A	806	P6G	O4-C5-C6-O7
5	E	803	P6G	O16-C17-C18-O19
11	H	808	PE5	C48-C50-O1-C1
11	H	808	PE5	C11-C12-O7-C13
10	C	805	PE4	C4-C3-O2-C2
3	A	802	1PE	OH2-C12-C22-OH3
3	A	802	1PE	C23-C13-OH4-C24
11	H	808	PE5	O2-C3-C4-O3
3	A	802	1PE	C13-C23-OH3-C22
3	A	802	1PE	C24-C14-OH5-C25
11	H	808	PE5	C10-C9-O5-C8
11	H	808	PE5	C9-C10-O6-C11

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Mol	Chain	Res	Type	Atoms
6	F	806	PGE	C6-C5-O3-C4
5	A	806	P6G	C5-C6-O7-C8
3	A	802	1PE	C16-C26-OH6-C15
8	B	801	PG4	C3-C4-O3-C5
3	E	802	1PE	C23-C13-OH4-C24
3	A	802	1PE	C14-C24-OH4-C13
5	E	803	P6G	C12-C11-O10-C9
9	B	802	7PE	O7-C8-C9-O10
11	H	808	PE5	C12-C11-O6-C10
4	D	809	GOL	O1-C1-C2-O2
4	D	809	GOL	O2-C2-C3-O3
4	D	804	GOL	O2-C2-C3-O3
4	G	802	GOL	O1-C1-C2-O2
4	A	803	GOL	O1-C1-C2-O2
4	B	808	GOL	O1-C1-C2-O2
4	H	804	GOL	O2-C2-C3-O3
4	A	807	GOL	O1-C1-C2-O2
4	B	805	GOL	O2-C2-C3-O3
8	H	803	PG4	O4-C7-C8-O5
5	E	803	P6G	O1-C2-C3-O4
11	H	808	PE5	C4-C3-O2-C2
6	G	805	PGE	C1-C2-O2-C3
11	H	808	PE5	C5-C6-O4-C7
3	C	801	1PE	C25-C15-OH6-C26
3	E	802	1PE	C16-C26-OH6-C15
5	E	803	P6G	C6-C5-O4-C3
4	A	803	GOL	O1-C1-C2-C3
11	H	808	PE5	O6-C11-C12-O7
10	C	805	PE4	C13-C14-O8-C15
2	A	801	IFM	C1-C5-C6-O6
9	B	802	7PE	C2-C3-O4-C5
11	H	808	PE5	C13-C14-O8-C15
8	D	803	PG4	C8-C7-O4-C6
3	E	802	1PE	C14-C24-OH4-C13
5	A	806	P6G	C12-C11-O10-C9
3	E	802	1PE	C12-C22-OH3-C23
3	C	801	1PE	C12-C22-OH3-C23
5	A	806	P6G	C15-C14-O13-C12
3	A	802	1PE	OH6-C15-C25-OH5
11	H	808	PE5	C7-C8-O5-C9
8	H	803	PG4	O2-C3-C4-O3
6	F	806	PGE	C4-C3-O2-C2

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Mol	Chain	Res	Type	Atoms
5	E	803	P6G	C2-C3-O4-C5
6	A	812	PGE	C4-C3-O2-C2
5	E	803	P6G	O4-C5-C6-O7
9	D	808	7PE	C18-C17-O16-C15
11	H	808	PE5	O3-C5-C6-O4
6	F	806	PGE	C1-C2-O2-C3
4	B	803	GOL	O1-C1-C2-O2
11	H	808	PE5	C14-C13-O7-C12
6	A	812	PGE	O3-C5-C6-O4
8	F	803	PG4	C5-C6-O4-C7
11	H	808	PE5	C1-C2-O2-C3
8	H	803	PG4	C8-C7-O4-C6
5	E	803	P6G	C11-C12-O13-C14
6	C	807	PGE	C3-C4-O3-C5
8	B	801	PG4	C1-C2-O2-C3
3	E	802	1PE	C24-C14-OH5-C25
8	F	803	PG4	C3-C4-O3-C5
5	E	803	P6G	O10-C11-C12-O13
8	H	803	PG4	C1-C2-O2-C3
4	A	805	GOL	O2-C2-C3-O3
4	E	804	GOL	O2-C2-C3-O3
8	F	803	PG4	C4-C3-O2-C2
8	F	803	PG4	O2-C3-C4-O3
4	D	807	GOL	O2-C2-C3-O3
4	A	807	GOL	O2-C2-C3-O3
5	A	806	P6G	O13-C14-C15-O16
4	D	805	GOL	C1-C2-C3-O3
4	D	810	GOL	C1-C2-C3-O3
4	D	807	GOL	C1-C2-C3-O3
8	B	801	PG4	O3-C5-C6-O4
6	G	805	PGE	C4-C3-O2-C2
5	A	806	P6G	O10-C11-C12-O13
4	E	806	GOL	O1-C1-C2-O2
4	D	805	GOL	O2-C2-C3-O3

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	801	IFM	C1-C2-C3-C4-C5-N
2	H	801	IFM	C1-C2-C3-C4-C5-N

46 monomers are involved in 114 short contacts:

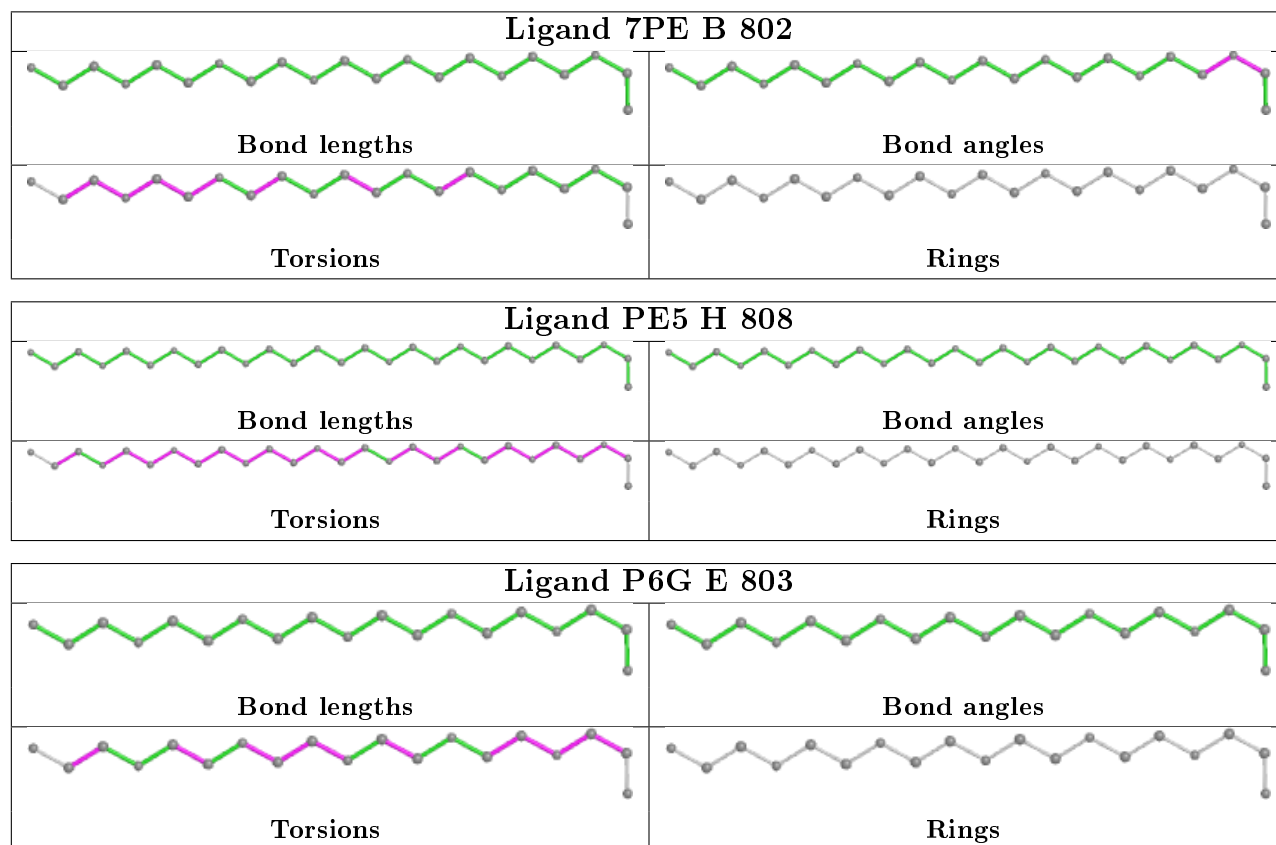
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	802	7PE	5	0
11	H	808	PE5	12	0
4	C	809	GOL	1	0
2	D	801	IFM	3	0
4	A	808	GOL	3	0
4	D	806	GOL	2	0
4	D	802	GOL	1	0
8	D	803	PG4	1	0
4	A	805	GOL	3	0
8	B	801	PG4	1	0
4	B	807	GOL	1	0
4	D	804	GOL	2	0
4	D	809	GOL	4	0
4	F	805	GOL	1	0
4	D	805	GOL	2	0
4	D	812	GOL	2	0
2	G	801	IFM	3	0
4	F	802	GOL	1	0
4	G	802	GOL	2	0
4	G	803	GOL	2	0
6	F	806	PGE	2	0
4	A	809	GOL	1	0
4	B	804	GOL	4	0
4	A	803	GOL	3	0
4	B	803	GOL	2	0
4	E	805	GOL	1	0
8	H	803	PG4	1	0
4	H	802	GOL	2	0
5	E	803	P6G	5	0
4	H	805	GOL	2	0
3	C	801	1PE	1	0
2	F	801	IFM	2	0
4	B	808	GOL	1	0
4	C	806	GOL	1	0
4	D	807	GOL	1	0
2	H	801	IFM	1	0
4	H	804	GOL	2	0
3	E	802	1PE	2	0
9	D	808	7PE	3	0
6	A	812	PGE	7	0
4	B	805	GOL	1	0
2	A	801	IFM	4	0
4	A	811	GOL	2	0

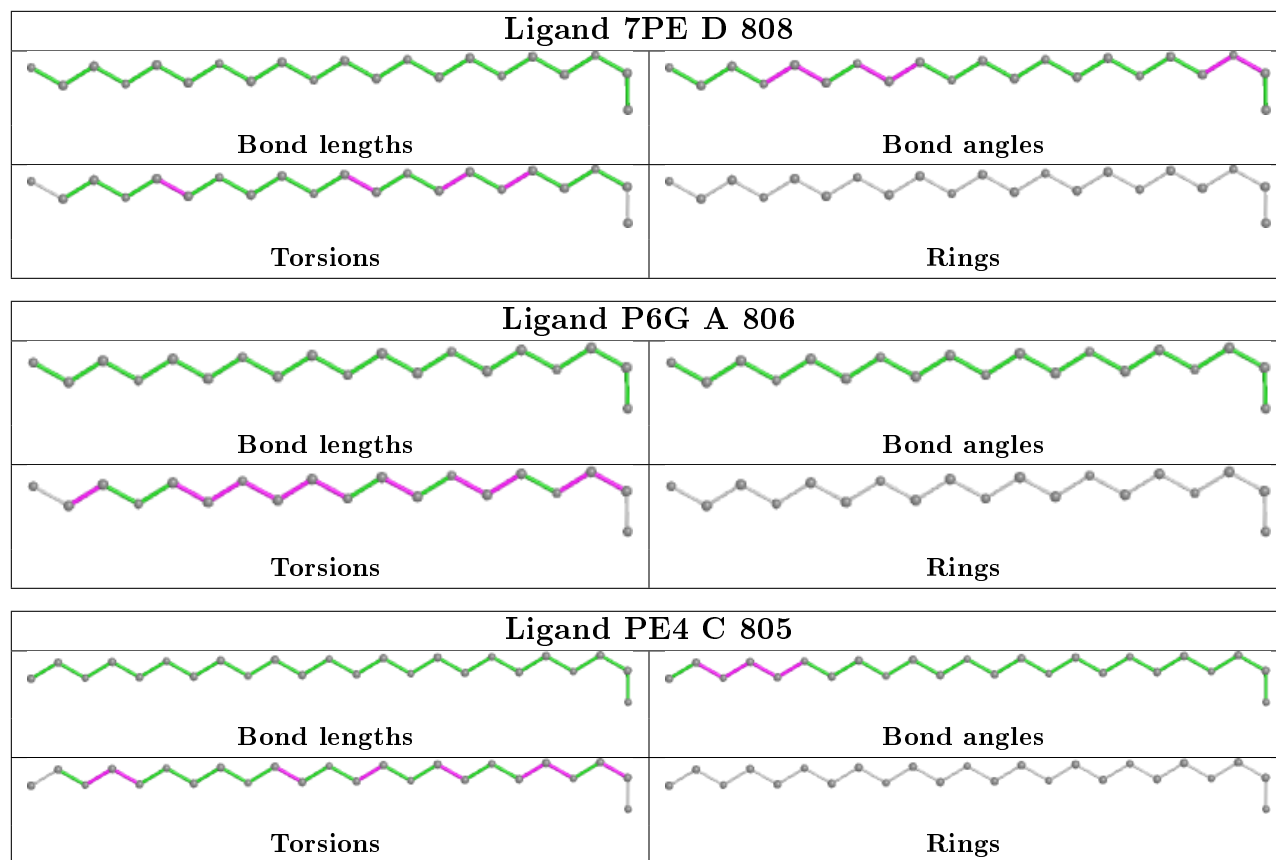
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	806	P6G	3	0
4	H	807	GOL	4	0
10	C	805	PE4	6	0

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	762/769 (99%)	0.04	14 (1%) 68 74	30, 40, 65, 98	0
1	B	761/769 (98%)	0.22	32 (4%) 36 43	28, 40, 64, 97	0
1	C	761/769 (98%)	0.18	28 (3%) 41 48	28, 40, 64, 99	0
1	D	761/769 (98%)	0.13	29 (3%) 40 47	28, 39, 68, 97	0
1	E	761/769 (98%)	0.68	108 (14%) 2 3	35, 53, 101, 142	0
1	F	761/769 (98%)	0.33	52 (6%) 17 22	32, 49, 86, 131	0
1	G	762/769 (99%)	0.56	91 (11%) 4 6	38, 52, 83, 110	0
1	H	761/769 (98%)	0.32	53 (6%) 16 21	37, 50, 85, 115	0
All	All	6090/6152 (98%)	0.31	407 (6%) 17 23	28, 46, 80, 142	0

All (407) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	98	ALA	12.3
1	G	98	ALA	9.7
1	H	751	VAL	8.4
1	E	753	ASP	7.9
1	F	754	SER	7.4
1	F	98	ALA	7.0
1	E	752	LEU	6.8
1	F	761	ARG	6.7
1	H	98	ALA	6.6
1	A	762	LEU	6.2
1	E	208	ALA	6.0
1	F	736	GLU	5.8
1	E	98	ALA	5.8
1	D	98	ALA	5.6
1	C	1	MET	5.6
1	E	125	ILE	5.5

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Mol	Chain	Res	Type	RSRZ
1	B	98	ALA	5.5
1	G	118	ARG	5.4
1	G	741	LEU	5.3
1	C	97	ALA	5.1
1	E	231	ALA	5.1
1	F	741	LEU	5.1
1	A	98	ALA	5.1
1	E	228	SER	4.9
1	G	97	ALA	4.9
1	E	232	GLY	4.9
1	G	737	ASP	4.9
1	E	726	LYS	4.8
1	F	752	LEU	4.8
1	F	757	ILE	4.7
1	G	740	PRO	4.7
1	D	761	ARG	4.7
1	E	150	ASP	4.6
1	H	506	GLU	4.6
1	E	230	GLU	4.5
1	E	118	ARG	4.5
1	F	1	MET	4.5
1	F	739	LYS	4.5
1	E	229	LEU	4.5
1	E	729	ILE	4.4
1	E	124	THR	4.4
1	E	659	GLU	4.4
1	H	753	ASP	4.3
1	G	153	THR	4.3
1	G	752	LEU	4.3
1	G	6	GLU	4.3
1	B	737	ASP	4.3
1	G	746	PHE	4.3
1	E	233	LYS	4.3
1	G	751	VAL	4.1
1	E	742	THR	4.1
1	H	761	ARG	4.1
1	E	149	SER	4.1
1	E	757	ILE	4.0
1	E	1	MET	4.0
1	G	694	ASP	3.9
1	H	752	LEU	3.9
1	G	96	GLU	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	753	ASP	3.9
1	E	754	SER	3.9
1	C	96	GLU	3.8
1	H	96	GLU	3.8
1	E	227	LEU	3.8
1	G	249	VAL	3.8
1	E	117	GLN	3.8
1	E	151	GLN	3.8
1	G	758	THR	3.8
1	G	762	LEU	3.8
1	H	20	ARG	3.8
1	E	234	PRO	3.8
1	G	731	ILE	3.7
1	D	736	GLU	3.7
1	H	194	TYR	3.7
1	E	708	GLY	3.7
1	G	756	ARG	3.7
1	E	192	VAL	3.6
1	H	742	THR	3.6
1	G	258	LEU	3.6
1	H	504	LEU	3.6
1	G	760	SER	3.6
1	E	123	ALA	3.6
1	G	124	THR	3.6
1	E	728	GLN	3.6
1	E	152	ASP	3.6
1	F	725	THR	3.6
1	H	740	PRO	3.6
1	E	92	ILE	3.6
1	E	119	MET	3.6
1	E	756	ARG	3.6
1	D	727	GLU	3.5
1	E	147	VAL	3.5
1	G	151	GLN	3.5
1	G	209	ASP	3.5
1	H	759	LYS	3.5
1	E	177	HIS	3.4
1	H	567	ILE	3.4
1	A	96	GLU	3.4
1	D	751	VAL	3.4
1	E	178	TYR	3.4
1	G	753	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	E	727	GLU	3.4
1	F	756	ARG	3.4
1	E	94	SER	3.4
1	G	251	ASN	3.4
1	E	738	ARG	3.4
1	C	232	GLY	3.3
1	F	753	ASP	3.3
1	E	338	TYR	3.3
1	H	741	LEU	3.3
1	G	119	MET	3.3
1	B	736	GLU	3.3
1	E	86	VAL	3.3
1	B	337	ILE	3.2
1	G	730	THR	3.2
1	G	750	SER	3.2
1	F	743	LEU	3.2
1	E	658	ASN	3.2
1	B	333	TRP	3.2
1	E	235	VAL	3.2
1	E	623	SER	3.2
1	F	6	GLU	3.2
1	G	120	LYS	3.2
1	G	333	TRP	3.2
1	D	96	GLU	3.2
1	C	20	ARG	3.2
1	G	726	LYS	3.2
1	C	751	VAL	3.1
1	E	524	SER	3.1
1	E	218	PRO	3.1
1	B	1	MET	3.1
1	D	748	GLU	3.1
1	E	100	PHE	3.1
1	G	149	SER	3.1
1	F	738	ARG	3.1
1	E	673	ALA	3.1
1	G	122	GLY	3.1
1	E	96	GLU	3.1
1	D	317	ILE	3.1
1	F	728	GLN	3.1
1	H	509	LEU	3.1
1	E	674	ALA	3.1
1	C	676	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	F	747	GLY	3.0
1	G	177	HIS	3.0
1	E	724	VAL	3.0
1	G	194	TYR	3.0
1	C	209	ASP	3.0
1	E	730	THR	3.0
1	E	2	HIS	3.0
1	H	7	HIS	3.0
1	E	755	GLU	3.0
1	C	118	ARG	3.0
1	G	739	LYS	3.0
1	E	760	SER	3.0
1	H	748	GLU	3.0
1	H	747	GLY	3.0
1	E	672	THR	3.0
1	F	508	THR	2.9
1	C	21	TYR	2.9
1	E	206	LEU	2.9
1	G	99	SER	2.9
1	E	337	ILE	2.9
1	E	174	GLN	2.9
1	E	209	ASP	2.9
1	F	727	GLU	2.9
1	G	742	THR	2.9
1	G	250	ASP	2.9
1	H	520	ASP	2.9
1	H	749	LYS	2.9
1	G	659	GLU	2.9
1	E	624	LEU	2.9
1	H	568	LYS	2.9
1	E	333	TRP	2.9
1	B	331	ALA	2.9
1	G	121	ASN	2.9
1	E	597	LEU	2.9
1	G	206	LEU	2.9
1	F	505	ASP	2.9
1	D	744	HIS	2.9
1	H	659	GLU	2.8
1	H	1	MET	2.8
1	A	727	GLU	2.8
1	A	749	LYS	2.8
1	G	123	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	624	LEU	2.8
1	C	99	SER	2.8
1	F	94	SER	2.8
1	G	743	LEU	2.8
1	E	676	GLY	2.8
1	D	672	THR	2.8
1	D	742	THR	2.8
1	B	177	HIS	2.8
1	D	757	ILE	2.8
1	B	740	PRO	2.7
1	E	66	ALA	2.7
1	H	569	GLU	2.8
1	E	116	SER	2.7
1	D	624	LEU	2.7
1	H	743	LEU	2.7
1	C	317	ILE	2.7
1	E	120	LYS	2.7
1	F	502	GLN	2.7
1	H	760	SER	2.7
1	E	251	ASN	2.7
1	F	278	ASP	2.7
1	H	658	ASN	2.7
1	G	195	GLU	2.7
1	G	623	SER	2.7
1	C	231	ALA	2.7
1	B	99	SER	2.7
1	F	292	ILE	2.7
1	F	26	ALA	2.7
1	E	473	PRO	2.7
1	E	761	ARG	2.6
1	F	507	LYS	2.6
1	F	755	GLU	2.6
1	G	208	ALA	2.6
1	G	728	GLN	2.6
1	F	742	THR	2.6
1	E	171	ASP	2.6
1	G	729	ILE	2.6
1	B	659	GLU	2.6
1	B	751	VAL	2.6
1	G	228	SER	2.6
1	H	694	ASP	2.6
1	G	757	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	720	LEU	2.6
1	A	1	MET	2.6
1	F	506	GLU	2.6
1	G	736	GLU	2.6
1	H	507	LYS	2.6
1	F	658	ASN	2.6
1	F	735	SER	2.6
1	G	116	SER	2.6
1	B	332	PHE	2.6
1	E	759	LYS	2.6
1	C	23	ALA	2.6
1	C	677	ALA	2.6
1	D	637	ASP	2.6
1	E	751	VAL	2.6
1	G	175	GLY	2.6
1	E	93	MET	2.5
1	H	692	HIS	2.5
1	G	23	ALA	2.5
1	G	155	ALA	2.5
1	E	670	ILE	2.5
1	H	177	HIS	2.5
1	F	715	VAL	2.5
1	G	176	HIS	2.5
1	G	761	ARG	2.5
1	G	150	ASP	2.5
1	G	698	LEU	2.5
1	C	92	ILE	2.5
1	B	759	LYS	2.5
1	C	233	LYS	2.5
1	G	254	ASP	2.5
1	A	251	ASN	2.5
1	E	122	GLY	2.5
1	G	624	LEU	2.5
1	G	485	PHE	2.4
1	G	732	THR	2.4
1	H	739	LYS	2.4
1	F	504	LEU	2.4
1	H	6	GLU	2.4
1	G	261	LYS	2.4
1	E	189	ALA	2.4
1	F	718	GLN	2.4
1	B	178	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	317	ILE	2.4
1	G	173	LEU	2.4
1	C	672	THR	2.4
1	E	197	THR	2.4
1	H	657	THR	2.4
1	A	736	GLU	2.4
1	G	178	TYR	2.4
1	G	92	ILE	2.4
1	E	155	ALA	2.4
1	G	220	GLY	2.4
1	F	20	ARG	2.4
1	B	514	GLU	2.4
1	A	673	ALA	2.4
1	F	290	ASN	2.4
1	F	694	ASP	2.4
1	G	152	ASP	2.4
1	E	677	ALA	2.4
1	D	759	LYS	2.3
1	H	737	ASP	2.3
1	E	731	ILE	2.3
1	B	220	GLY	2.3
1	E	262	HIS	2.3
1	B	748	GLU	2.3
1	D	677	ALA	2.3
1	A	742	THR	2.3
1	E	121	ASN	2.3
1	E	266	TYR	2.3
1	G	473	PRO	2.3
1	G	24	ALA	2.3
1	D	737	ASP	2.3
1	B	96	GLU	2.3
1	G	670	ILE	2.3
1	E	207	ASP	2.3
1	A	507	LYS	2.3
1	D	746	PHE	2.3
1	E	176	HIS	2.3
1	F	744	HIS	2.3
1	G	174	GLN	2.3
1	B	673	ALA	2.3
1	C	673	ALA	2.3
1	B	338	TYR	2.3
1	E	750	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	510	SER	2.3
1	B	726	LYS	2.3
1	G	1	MET	2.3
1	E	740	PRO	2.3
1	B	319	ALA	2.3
1	D	673	ALA	2.3
1	B	672	THR	2.3
1	G	754	SER	2.3
1	E	736	GLU	2.3
1	G	637	ASP	2.3
1	A	750	SER	2.3
1	B	674	ALA	2.3
1	G	745	ILE	2.3
1	H	197	THR	2.2
1	C	748	GLU	2.2
1	G	727	GLU	2.2
1	D	333	TRP	2.2
1	D	382	ILE	2.2
1	G	256	ALA	2.2
1	G	604	ARG	2.2
1	H	251	ASN	2.2
1	G	86	VAL	2.2
1	B	20	ARG	2.2
1	D	319	ALA	2.2
1	E	260	ALA	2.2
1	E	319	ALA	2.2
1	G	337	ILE	2.2
1	F	501	LEU	2.2
1	G	25	GLN	2.2
1	F	740	PRO	2.2
1	E	91	PHE	2.2
1	E	308	ALA	2.2
1	H	521	ASP	2.2
1	A	275	LEU	2.2
1	H	738	ARG	2.2
1	G	338	TYR	2.2
1	C	235	VAL	2.2
1	E	267	GLU	2.2
1	E	334	ASP	2.2
1	F	338	TYR	2.2
1	F	737	ASP	2.2
1	F	540	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	744	HIS	2.2
1	C	95	GLU	2.2
1	H	519	SER	2.2
1	F	749	LYS	2.1
1	H	174	GLN	2.2
1	H	540	LYS	2.1
1	G	7	HIS	2.1
1	F	624	LEU	2.1
1	D	626	PRO	2.1
1	F	97	ALA	2.1
1	A	757	ILE	2.1
1	B	317	ILE	2.1
1	G	117	GLN	2.1
1	C	94	SER	2.1
1	D	738	ARG	2.1
1	H	195	GLU	2.1
1	B	742	THR	2.1
1	C	208	ALA	2.1
1	D	674	ALA	2.1
1	F	203	THR	2.1
1	H	66	ALA	2.1
1	B	318	GLY	2.1
1	C	341	PRO	2.1
1	F	96	GLU	2.1
1	G	414	ILE	2.1
1	G	747	GLY	2.1
1	E	732	THR	2.1
1	E	758	THR	2.1
1	D	337	ILE	2.1
1	E	173	LEU	2.1
1	F	400	LEU	2.1
1	E	254	ASP	2.1
1	E	156	VAL	2.1
1	C	149	SER	2.1
1	H	516	ILE	2.1
1	C	694	ASP	2.1
1	G	93	MET	2.1
1	H	249	VAL	2.1
1	E	195	GLU	2.0
1	F	509	LEU	2.0
1	B	676	GLY	2.0
1	D	676	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	740	PRO	2.0
1	E	261	LYS	2.0
1	E	675	ASN	2.0
1	H	514	GLU	2.0
1	E	725	THR	2.0
1	D	623	SER	2.0
1	H	512	VAL	2.0
1	E	21	TYR	2.0
1	G	257	LEU	2.0
1	H	522	GLU	2.0
1	E	723	ASP	2.0
1	F	716	LYS	2.0
1	H	94	SER	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates 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(Å ²)	Q<0.9
4	GOL	C	806	6/6	0.66	0.24	64,77,87,89	0
4	GOL	H	807	6/6	0.70	0.17	70,70,73,76	0
4	GOL	B	805	6/6	0.74	0.24	59,73,75,75	0
4	GOL	A	807	6/6	0.80	0.19	57,59,72,79	0
4	GOL	D	806	6/6	0.82	0.12	56,64,67,71	0
4	GOL	H	806	6/6	0.82	0.15	48,62,65,73	0
4	GOL	A	809	6/6	0.82	0.14	58,66,67,73	0
4	GOL	G	803	6/6	0.82	0.10	65,76,86,86	0
4	GOL	F	805	6/6	0.83	0.15	39,62,67,70	0
6	PGE	G	805	10/10	0.83	0.23	54,66,73,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	IFM	G	801	10/10	0.83	0.38	55,79,87,98	0
3	1PE	E	802	16/16	0.84	0.23	62,75,101,104	0
11	PE5	H	808	27/27	0.85	0.22	53,72,84,96	0
8	PG4	H	803	13/13	0.86	0.18	57,68,83,88	0
2	IFM	E	801	10/10	0.86	0.35	44,59,71,73	0
4	GOL	B	807	6/6	0.86	0.22	59,65,74,82	0
8	PG4	D	803	13/13	0.87	0.17	48,65,75,77	0
4	GOL	A	808	6/6	0.87	0.19	59,61,66,85	0
4	GOL	D	805	6/6	0.88	0.14	63,64,69,70	0
4	GOL	E	805	6/6	0.88	0.18	63,77,85,87	0
3	1PE	A	802	16/16	0.88	0.23	50,62,83,101	0
5	P6G	E	803	19/19	0.88	0.30	52,67,71,73	0
3	1PE	C	801	16/16	0.88	0.16	44,61,79,82	0
2	IFM	H	801	10/10	0.89	0.25	56,70,75,82	0
6	PGE	A	812	10/10	0.89	0.22	40,51,58,60	0
4	GOL	D	811	6/6	0.89	0.13	49,56,61,71	0
2	IFM	F	801	10/10	0.90	0.28	49,56,65,72	0
4	GOL	D	807	6/6	0.90	0.19	55,64,71,72	0
4	GOL	G	804	6/6	0.91	0.21	68,68,70,72	0
4	GOL	B	806	6/6	0.91	0.23	57,64,70,77	0
4	GOL	A	803	6/6	0.91	0.28	46,60,72,75	0
6	PGE	F	806	10/10	0.92	0.24	62,65,71,74	0
8	PG4	F	803	13/13	0.93	0.16	56,62,75,77	0
6	PGE	C	807	10/10	0.93	0.15	42,51,57,59	0
4	GOL	A	805	6/6	0.93	0.09	57,64,74,75	0
4	GOL	E	804	6/6	0.93	0.19	54,59,62,63	0
8	PG4	B	801	13/13	0.93	0.18	46,57,87,88	0
2	IFM	A	801	10/10	0.93	0.22	38,51,60,62	0
5	P6G	A	806	19/19	0.93	0.21	41,49,64,70	0
4	GOL	G	802	6/6	0.93	0.38	52,64,71,76	0
4	GOL	H	802	6/6	0.94	0.24	58,73,84,85	0
7	CA	G	806	1/1	0.94	0.11	55,55,55,55	0
4	GOL	F	802	6/6	0.94	0.25	52,58,61,65	0
9	7PE	B	802	21/21	0.94	0.22	36,45,52,55	0
9	7PE	D	808	21/21	0.94	0.17	41,48,54,59	0
4	GOL	D	812	6/6	0.94	0.23	32,38,40,45	0
10	PE4	C	805	24/24	0.94	0.27	39,48,59,68	0
4	GOL	D	804	6/6	0.95	0.18	47,54,57,62	0
4	GOL	D	809	6/6	0.95	0.16	45,54,57,60	0
4	GOL	H	805	6/6	0.95	0.20	51,52,59,60	0
4	GOL	B	804	6/6	0.95	0.20	33,35,40,47	0
4	GOL	E	806	6/6	0.95	0.17	46,47,50,54	0

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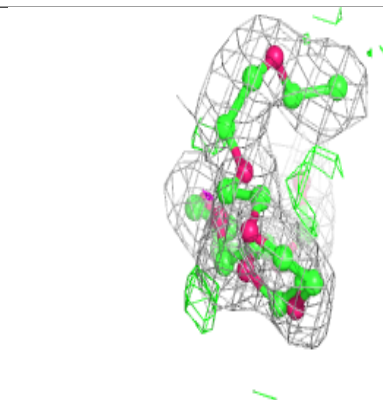
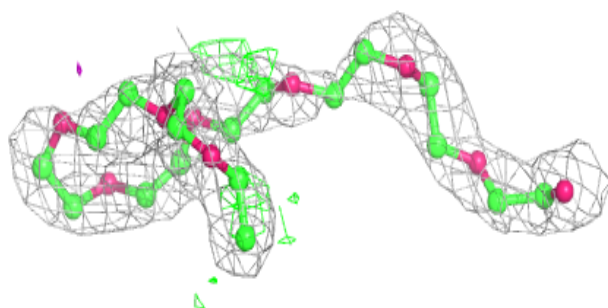
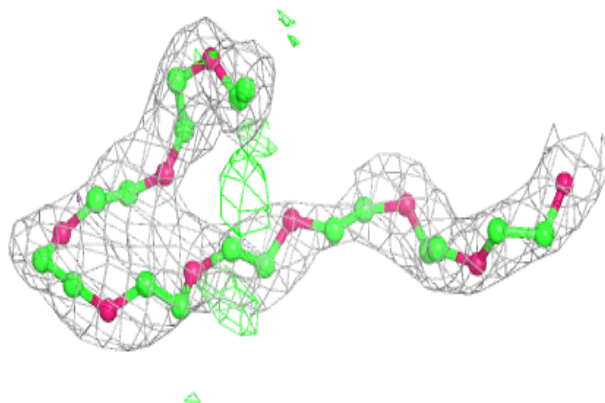
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GOL	A	804	6/6	0.95	0.18	42,43,46,52	0
2	IFM	D	801	10/10	0.95	0.21	35,44,50,63	0
4	GOL	C	809	6/6	0.95	0.21	37,42,49,52	0
4	GOL	H	804	6/6	0.95	0.17	46,52,57,61	0
4	GOL	F	804	6/6	0.95	0.20	47,48,50,53	0
4	GOL	D	802	6/6	0.96	0.33	50,58,60,62	0
4	GOL	E	807	6/6	0.96	0.20	43,53,60,60	0
4	GOL	B	808	6/6	0.96	0.28	36,43,46,48	0
4	GOL	C	804	6/6	0.96	0.24	43,46,53,57	0
4	GOL	C	802	6/6	0.96	0.16	43,57,62,73	0
7	CA	D	813	1/1	0.96	0.04	54,54,54,54	0
7	CA	D	814	1/1	0.97	0.16	45,45,45,45	0
4	GOL	B	803	6/6	0.97	0.16	35,41,44,46	0
4	GOL	A	811	6/6	0.97	0.14	45,50,51,51	0
7	CA	A	813	1/1	0.98	0.10	44,44,44,44	0
4	GOL	C	803	6/6	0.98	0.13	45,48,52,59	0
4	GOL	A	810	6/6	0.98	0.14	37,37,39,40	0
4	GOL	D	810	6/6	0.98	0.21	33,37,40,41	0
4	GOL	C	808	6/6	0.98	0.14	35,38,39,42	0
7	CA	C	810	1/1	0.99	0.13	36,36,36,36	0
7	CA	E	808	1/1	0.99	0.11	54,54,54,54	0
7	CA	B	809	1/1	1.00	0.12	43,43,43,43	0

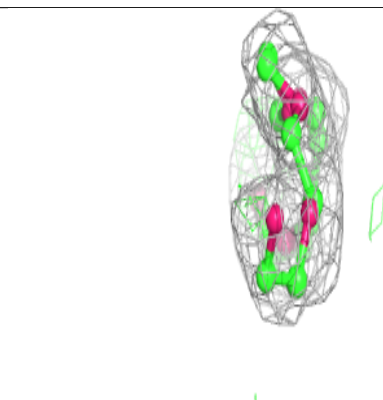
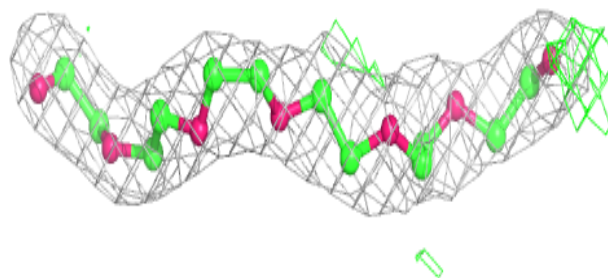
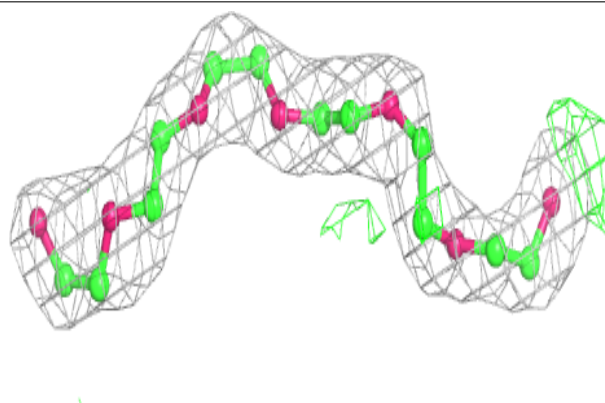
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PE5 H 808:

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

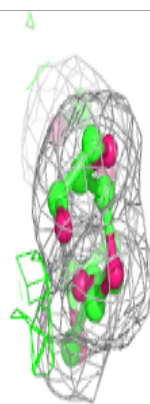
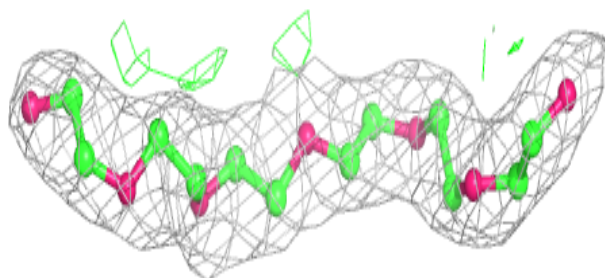
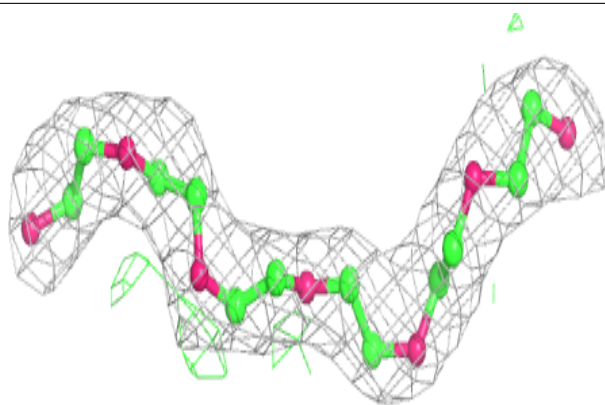
**Electron density around P6G E 803:**

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

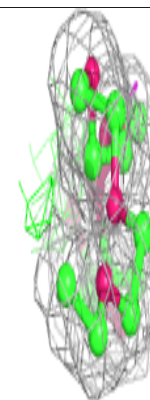
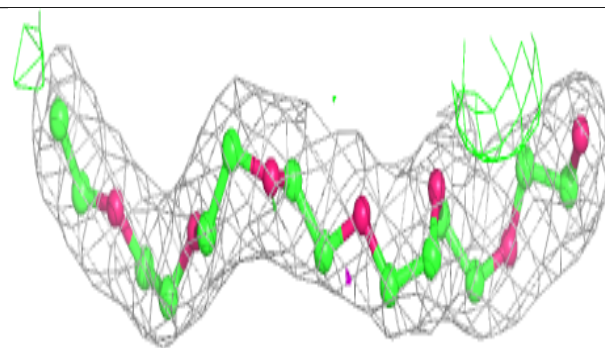
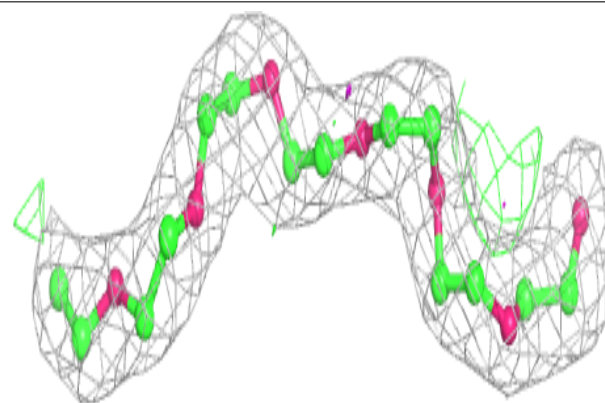


Electron density around P6G A 806:

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

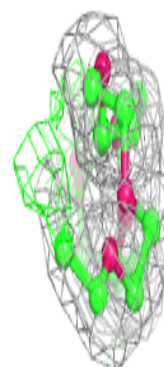
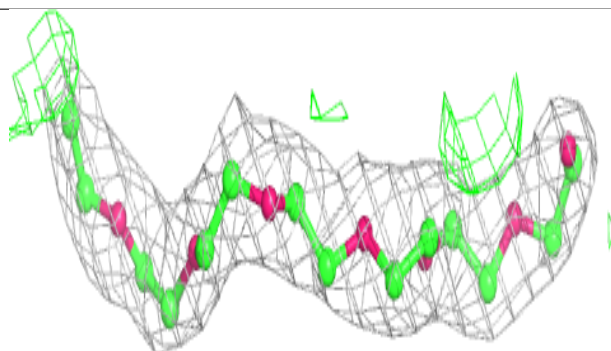
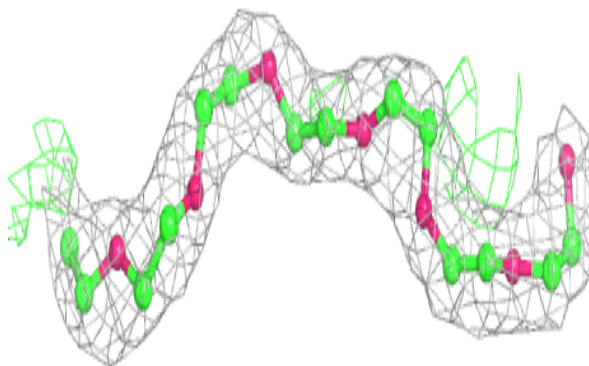
**Electron density around 7PE B 802:**

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

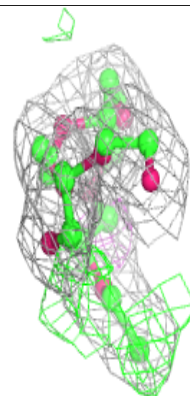
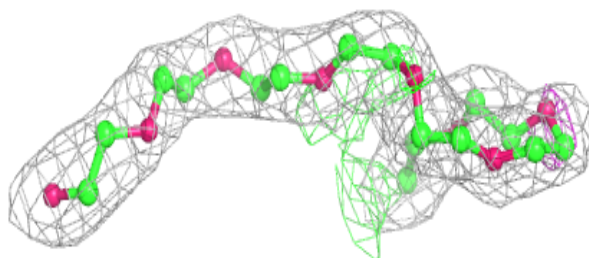
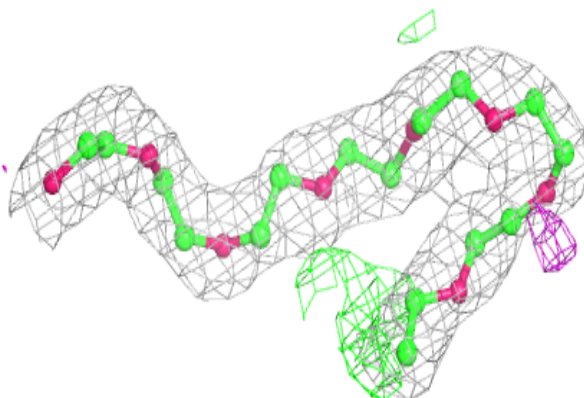


Electron density around 7PE D 808:

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

**Electron density around PE4 C 805:**

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



6.5 Other polymers

There are no such residues in this entry.