



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:46 PM UTC

PDB ID : 4KTR / pdb_00004ktr
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

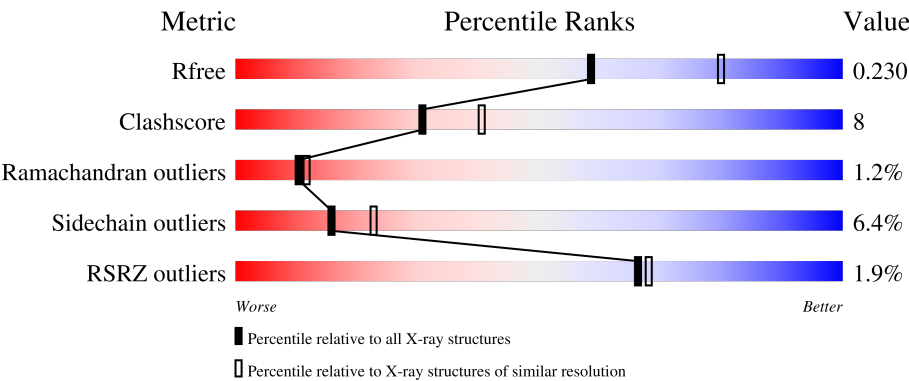
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



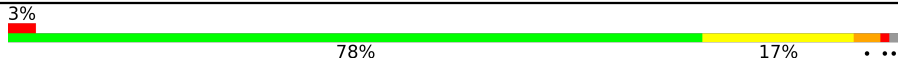
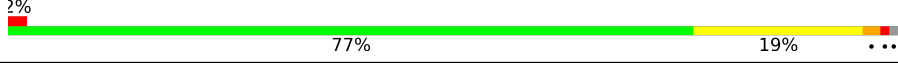
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	769	% 81%15% . . .
1	B	769	% 81%15% . . .
1	C	769	% 78%19% . . .
1	D	769	% 78%18% . .
1	E	769	5% 74%22% . . .

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Mol	Chain	Length	Quality of chain
1	F	769	 3% 78% 17% . .
1	G	769	 2% 76% 20% . .
1	H	769	 2% 77% 19% . . .

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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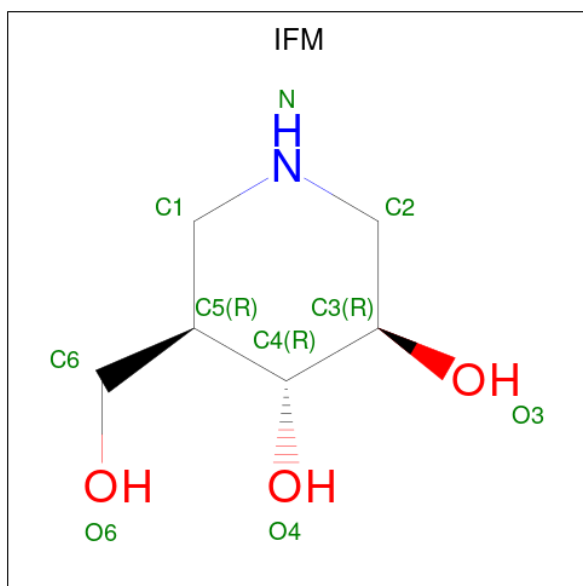
Chain	Residue	Modelled	Actual	Comment	Reference
B	765	HIS	-	expression tag	UNP D6XZ22
B	766	HIS	-	expression tag	UNP D6XZ22
B	767	HIS	-	expression tag	UNP D6XZ22
B	768	HIS	-	expression tag	UNP D6XZ22
B	769	HIS	-	expression tag	UNP D6XZ22
C	475	GLN	GLU	engineered mutation	UNP D6XZ22
C	762	LEU	-	expression 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 (CCD ID: IFM) (formula: $C_6H_{13}NO_3$).



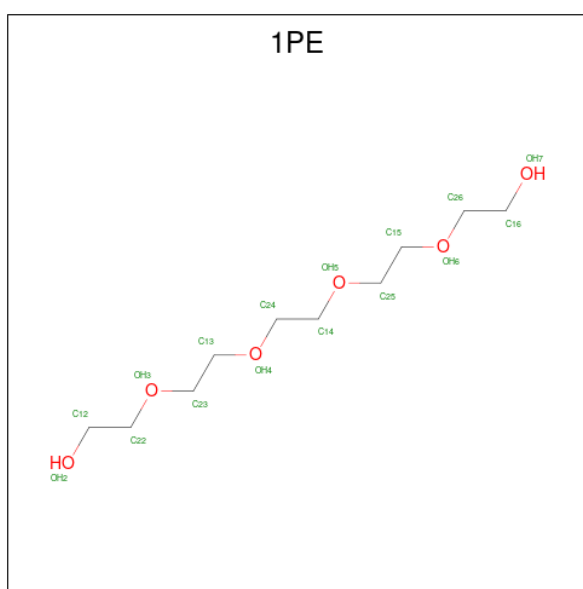
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	6	1	3		
2	D	1	Total	C	N	O	0	0
			10	6	1	3		

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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 (CCD ID: 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 (CCD ID: 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	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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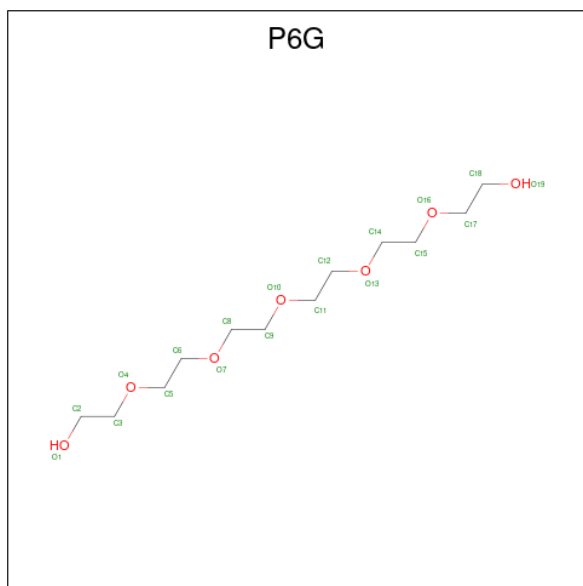
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	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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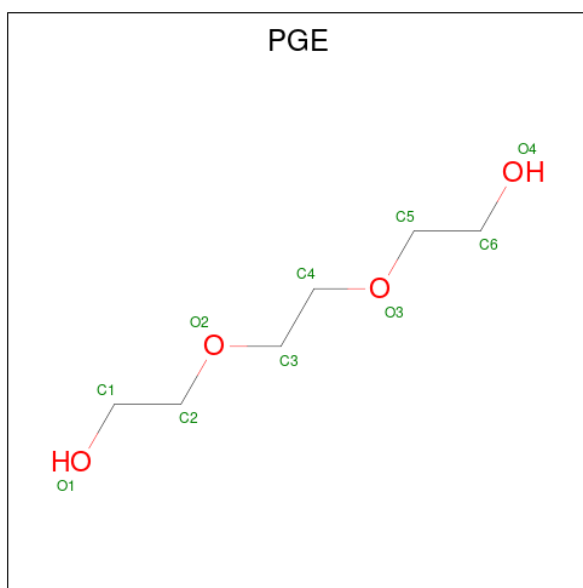
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	F	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is HEXAETHYLENE GLYCOL (CCD ID: P6G) (formula: $C_{12}H_{26}O_7$).



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 (CCD ID: PGE) (formula: $C_6H_{14}O_4$).

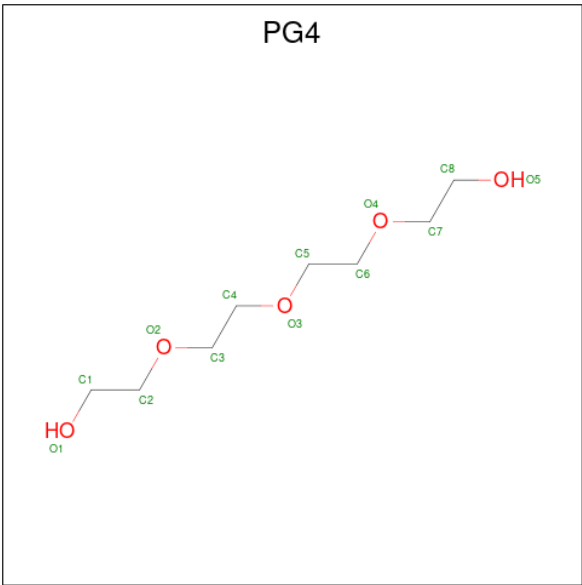


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			10	6	4		
6	C	1	Total	C	O	0	0
			10	6	4		
6	F	1	Total	C	O	0	0
			10	6	4		
6	G	1	Total	C	O	0	0
			10	6	4		

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

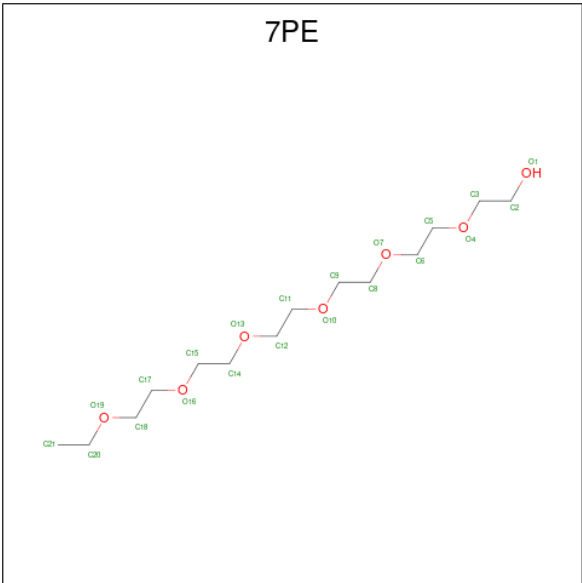
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	B	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		
7	D	2	Total	Ca	0	0
			2	2		
7	E	1	Total	Ca	0	0
			1	1		
7	G	1	Total	Ca	0	0
			1	1		

- Molecule 8 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



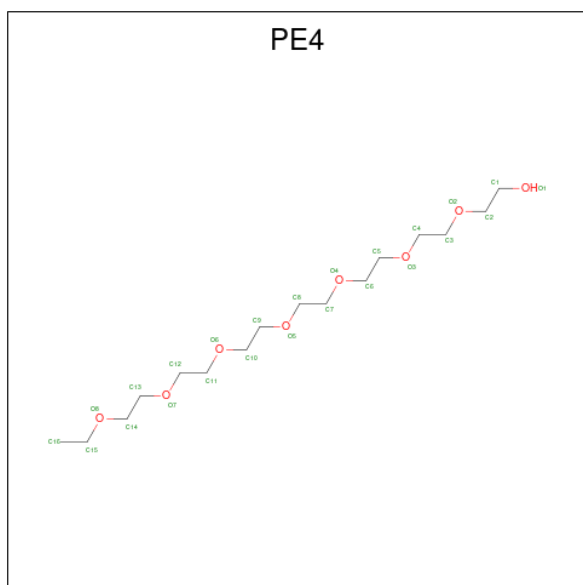
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			13	8	5		
8	D	1	Total	C	O	0	0
			13	8	5		
8	F	1	Total	C	O	0	0
			13	8	5		
8	H	1	Total	C	O	0	0
			13	8	5		

- Molecule 9 is 2-(2-(2-(2-(2-ETHOXYETHOXY)ETHOXY)ETHOXY)ETHOXY)ETHOXY)ETHANOL (CCD ID: 7PE) (formula: C₁₄H₃₀O₇).



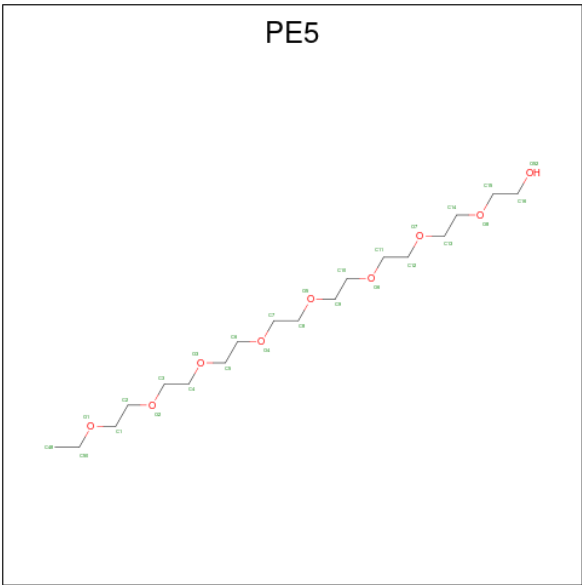
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			21	14	7		
9	D	1	Total	C	O	0	0
			21	14	7		

- Molecule 10 is 2-{2-[2-(2-{2-[2-(2-ETHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHOXY)-ETHOXY]-ETHOXY}-ETHANOL (CCD ID: 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 (CCD ID: PE5) (formula: C₁₈H₃₈O₉).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	H	1	Total	C	O	0	0
			27	18	9		

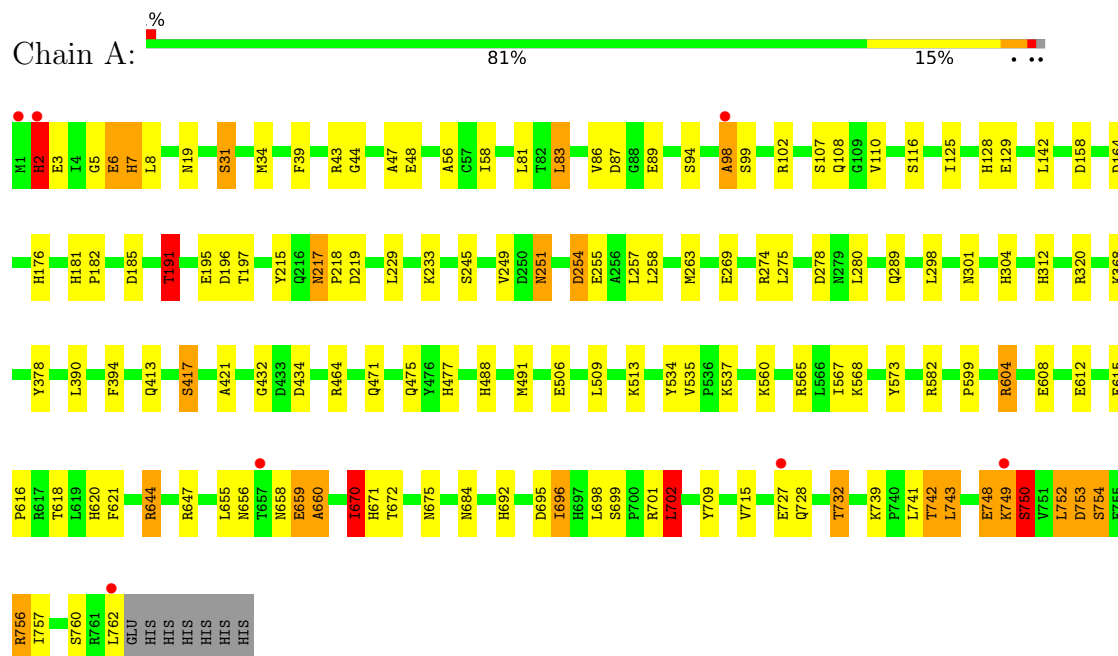
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	182	Total	O	0	0
			182	182		
12	B	303	Total	O	0	0
			303	303		
12	C	286	Total	O	0	0
			286	286		
12	D	348	Total	O	0	0
			348	348		
12	E	185	Total	O	0	0
			185	185		
12	F	247	Total	O	0	0
			247	247		
12	G	197	Total	O	0	0
			197	197		
12	H	218	Total	O	0	0
			218	218		

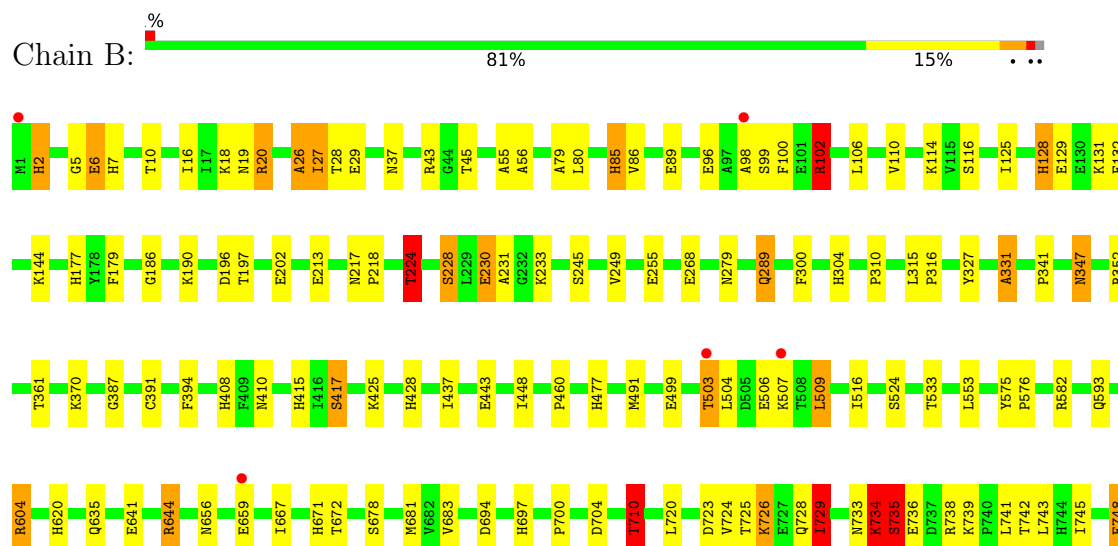
3 Residue-property plots

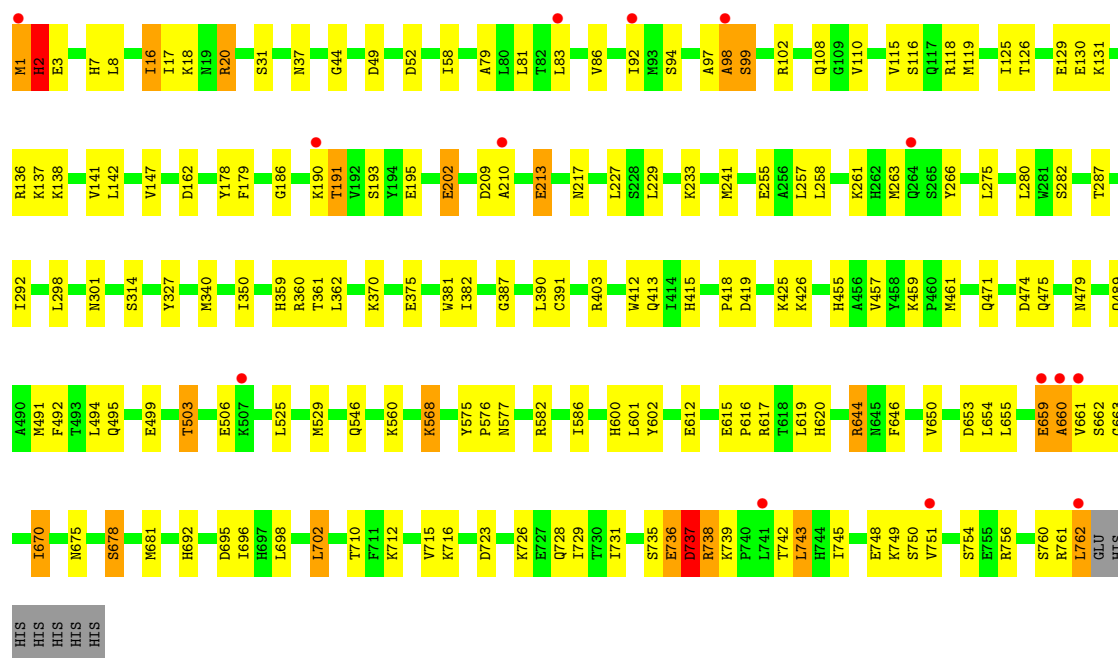
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Glycoside hydrolase family 65 central catalytic

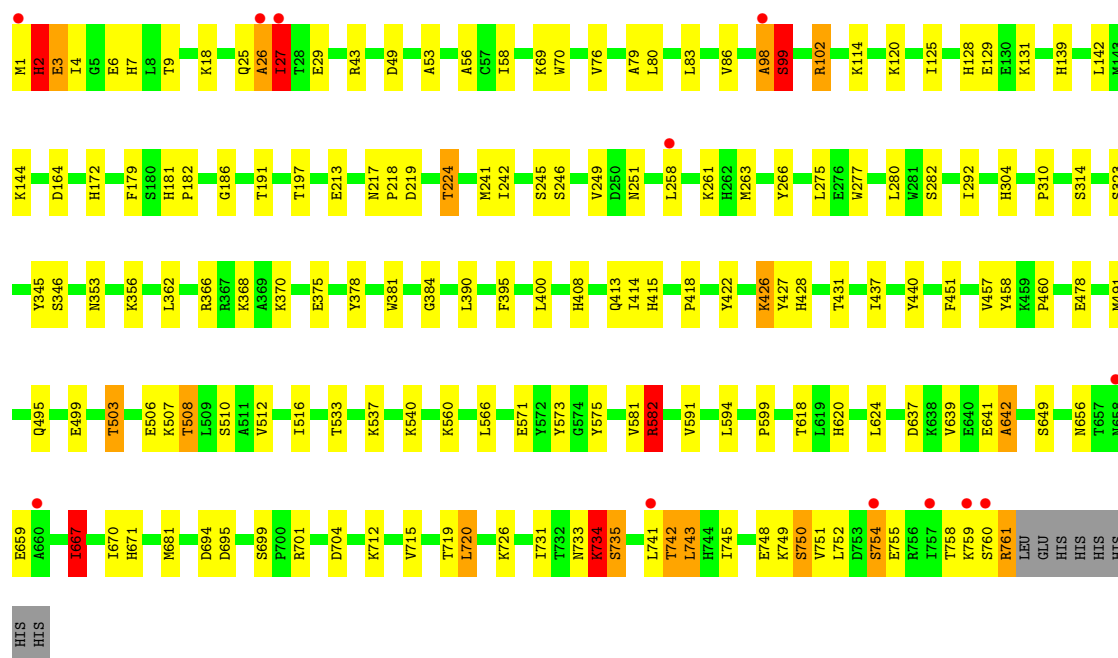
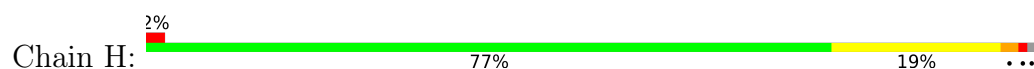


- Molecule 1: Glycoside hydrolase family 65 central catalytic





- 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 (5.03%)	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)	0.39 , 51.9	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: P6G, GOL, 7PE, PE4, 1PE, PG4, CA, PE5, PGE, IFM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.26	9/6236 (0.1%)	1.22	30/8456 (0.4%)
1	B	1.27	24/6228 (0.4%)	1.20	26/8445 (0.3%)
1	C	1.30	16/6228 (0.3%)	1.19	18/8445 (0.2%)
1	D	1.33	18/6228 (0.3%)	1.21	15/8445 (0.2%)
1	E	1.12	8/6228 (0.1%)	1.13	20/8445 (0.2%)
1	F	1.14	5/6228 (0.1%)	1.16	18/8445 (0.2%)
1	G	1.10	3/6236 (0.0%)	1.10	15/8456 (0.2%)
1	H	1.12	6/6228 (0.1%)	1.11	15/8445 (0.2%)
All	All	1.21	89/49840 (0.2%)	1.17	157/67582 (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 (89) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	304	HIS	CG-CD2	8.84	1.45	1.35
1	C	304	HIS	CG-CD2	7.36	1.44	1.35
1	A	417	SER	CA-C	7.32	1.60	1.52
1	D	598	HIS	CG-CD2	6.95	1.43	1.35
1	B	672	THR	C-O	-6.69	1.16	1.24
1	B	417	SER	C-O	-6.60	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	453	ALA	C-O	-6.50	1.16	1.24
1	H	671	HIS	CG-CD2	6.50	1.43	1.35
1	B	415	HIS	CE1-NE2	6.31	1.38	1.32
1	A	176	HIS	CG-CD2	6.30	1.42	1.35
1	C	754	SER	C-O	6.25	1.32	1.23
1	D	455	HIS	CD2-NE2	-6.25	1.30	1.37
1	B	304	HIS	CE1-NE2	6.19	1.38	1.32
1	B	304	HIS	ND1-CE1	6.16	1.38	1.32
1	B	620	HIS	CG-CD2	6.07	1.42	1.35
1	E	750	SER	N-CA	6.07	1.54	1.46
1	B	415	HIS	ND1-CE1	6.06	1.38	1.32
1	C	417	SER	C-O	-6.04	1.19	1.24
1	H	415	HIS	CG-CD2	6.03	1.42	1.35
1	B	279	ASN	CA-C	5.85	1.60	1.52
1	C	359	HIS	CG-CD2	5.82	1.42	1.35
1	B	408	HIS	CG-CD2	5.80	1.42	1.35
1	E	408	HIS	CG-CD2	5.79	1.42	1.35
1	C	671	HIS	CG-CD2	5.74	1.42	1.35
1	B	697	HIS	CG-CD2	5.67	1.42	1.35
1	D	359	HIS	CG-CD2	5.66	1.42	1.35
1	C	615	GLU	N-CA	5.65	1.51	1.46
1	C	304	HIS	ND1-CE1	5.64	1.38	1.32
1	B	443	GLU	CA-C	5.64	1.59	1.52
1	F	408	HIS	CG-CD2	5.61	1.42	1.35
1	E	312	HIS	CG-CD2	5.60	1.42	1.35
1	C	630	ALA	C-O	5.59	1.30	1.24
1	D	128	HIS	CG-CD2	5.58	1.42	1.35
1	F	177	HIS	CG-CD2	5.55	1.42	1.35
1	D	193	SER	CA-C	-5.55	1.46	1.52
1	F	408	HIS	CE1-NE2	5.54	1.38	1.32
1	C	455	HIS	CG-CD2	5.54	1.42	1.35
1	D	660	ALA	CA-C	5.53	1.60	1.52
1	H	7	HIS	CG-CD2	5.51	1.42	1.35
1	B	85	HIS	CG-CD2	5.51	1.42	1.35
1	D	600	HIS	CG-CD2	5.49	1.41	1.35
1	D	181	HIS	CG-CD2	5.48	1.41	1.35
1	D	598	HIS	CG-ND1	-5.46	1.32	1.38
1	D	415	HIS	CG-CD2	5.45	1.41	1.35
1	A	488	HIS	CG-CD2	5.41	1.41	1.35
1	A	128	HIS	CG-CD2	5.37	1.41	1.35
1	B	683	VAL	C-O	5.37	1.29	1.23
1	D	168	ILE	C-O	-5.36	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	312	HIS	CE1-NE2	5.36	1.38	1.32
1	D	598	HIS	CE1-NE2	5.36	1.38	1.32
1	B	415	HIS	CG-CD2	5.36	1.41	1.35
1	H	408	HIS	CG-CD2	5.35	1.41	1.35
1	C	455	HIS	CD2-NE2	-5.35	1.31	1.37
1	B	408	HIS	CE1-NE2	5.34	1.37	1.32
1	B	341	PRO	N-CA	5.34	1.54	1.47
1	G	359	HIS	CE1-NE2	5.33	1.37	1.32
1	C	408	HIS	CE1-NE2	5.32	1.37	1.32
1	E	751	VAL	N-CA	5.32	1.52	1.46
1	G	455	HIS	CD2-NE2	-5.31	1.32	1.37
1	C	312	HIS	CG-CD2	5.28	1.41	1.35
1	B	477	HIS	CE1-NE2	5.27	1.37	1.32
1	D	417	SER	CA-C	5.27	1.58	1.52
1	D	63	TRP	CD2-CE2	5.25	1.50	1.41
1	A	312	HIS	ND1-CE1	5.24	1.37	1.32
1	B	620	HIS	ND1-CE1	5.24	1.37	1.32
1	F	69	LYS	CA-C	5.23	1.57	1.52
1	H	304	HIS	ND1-CE1	5.23	1.37	1.32
1	B	671	HIS	CG-CD2	5.21	1.41	1.35
1	E	279	ASN	CA-C	5.17	1.59	1.52
1	H	415	HIS	CE1-NE2	5.17	1.37	1.32
1	E	104	LEU	CA-C	-5.14	1.46	1.52
1	B	754	SER	C-O	5.13	1.30	1.24
1	C	56	ALA	CA-C	-5.12	1.45	1.52
1	A	191	THR	CB-CG2	-5.11	1.35	1.52
1	C	467	PHE	C-O	5.11	1.29	1.24
1	A	31	SER	N-CA	5.10	1.52	1.46
1	B	331	ALA	C-O	5.09	1.30	1.24
1	E	304	HIS	CG-CD2	5.08	1.41	1.35
1	G	525	LEU	CA-C	5.08	1.59	1.52
1	A	8	LEU	N-CA	-5.07	1.40	1.46
1	D	697	HIS	CG-CD2	5.06	1.41	1.35
1	B	177	HIS	CG-CD2	5.05	1.41	1.35
1	D	541	HIS	CG-CD2	5.04	1.41	1.35
1	A	477	HIS	CG-CD2	5.03	1.41	1.35
1	B	128	HIS	CG-CD2	5.03	1.41	1.35
1	D	359	HIS	ND1-CE1	5.02	1.37	1.32
1	F	128	HIS	CG-CD2	5.01	1.41	1.35
1	E	176	HIS	CG-CD2	5.01	1.41	1.35
1	D	533	THR	CA-C	-5.00	1.46	1.52

All (157) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	251	ASN	CA-C-N	-10.88	108.57	119.56
1	A	251	ASN	C-N-CA	-10.88	108.57	119.56
1	B	753	ASP	N-CA-C	-9.49	95.44	110.14
1	A	233	LYS	CA-C-N	-9.29	110.53	120.66
1	A	233	LYS	C-N-CA	-9.29	110.53	120.66
1	F	702	LEU	CA-C-N	-8.79	111.82	120.52
1	F	702	LEU	C-N-CA	-8.79	111.82	120.52
1	F	4	ILE	N-CA-C	-8.51	105.01	111.90
1	A	89	GLU	CA-C-N	-8.45	111.31	119.85
1	A	89	GLU	C-N-CA	-8.45	111.31	119.85
1	A	670	ILE	CG1-CB-CG2	-8.42	85.43	110.70
1	B	729	ILE	CB-CA-C	-8.34	97.66	110.50
1	D	102	ARG	NE-CZ-NH2	8.32	126.69	119.20
1	E	735	SER	N-CA-C	8.00	119.69	110.97
1	B	26	ALA	N-CA-C	-7.83	98.88	110.23
1	E	749	LYS	N-CA-C	7.80	118.56	108.34
1	A	659	GLU	N-CA-C	7.68	122.72	113.12
1	E	354	ILE	N-CA-C	-7.48	103.50	110.53
1	H	4	ILE	N-CA-C	-7.41	105.44	111.81
1	D	102	ARG	NE-CZ-NH1	-7.16	114.34	121.50
1	A	7	HIS	N-CA-C	-7.00	102.15	110.41
1	C	191	THR	N-CA-CB	-6.92	100.21	110.17
1	A	699	SER	CA-C-N	-6.82	110.43	120.46
1	A	699	SER	C-N-CA	-6.82	110.43	120.46
1	C	440	TYR	CA-C-N	6.78	127.33	119.94
1	C	440	TYR	C-N-CA	6.78	127.33	119.94
1	B	213	GLU	N-CA-C	6.76	120.53	109.24
1	G	702	LEU	CA-C-N	-6.76	113.69	120.31
1	G	702	LEU	C-N-CA	-6.76	113.69	120.31
1	G	659	GLU	N-CA-C	6.75	121.56	113.12
1	E	112	SER	N-CA-C	6.72	119.16	109.14
1	A	3	GLU	N-CA-C	6.66	119.00	108.67
1	B	7	HIS	N-CA-C	-6.64	102.47	110.44
1	C	309	THR	CA-C-N	-6.64	112.93	119.90
1	C	309	THR	C-N-CA	-6.64	112.93	119.90
1	C	659	GLU	N-CA-C	6.60	120.55	112.23
1	A	535	VAL	CA-C-N	-6.59	113.17	119.76
1	A	535	VAL	C-N-CA	-6.59	113.17	119.76
1	E	153	THR	N-CA-C	6.38	119.00	108.99
1	A	567	ILE	N-CA-C	-6.38	106.33	111.81
1	C	486	THR	N-CA-C	-6.37	104.34	111.28
1	F	694	ASP	N-CA-C	-6.34	105.53	113.20
1	D	667	ILE	N-CA-C	-6.32	107.14	113.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	751	VAL	N-CA-C	6.30	122.45	109.34
1	B	347	ASN	CA-C-N	-6.26	113.17	119.56
1	B	347	ASN	C-N-CA	-6.26	113.17	119.56
1	D	737	ASP	N-CA-C	6.25	118.49	107.61
1	B	735	SER	N-CA-C	-6.24	97.51	110.80
1	E	339	ASN	N-CA-C	6.20	120.04	112.23
1	D	170	GLY	N-CA-C	-6.17	105.74	112.04
1	C	368	LYS	N-CA-C	-6.16	104.64	111.36
1	E	438	ARG	NE-CZ-NH1	-6.15	115.35	121.50
1	E	438	ARG	NE-CZ-NH2	6.14	124.72	119.20
1	F	728	GLN	N-CA-C	6.08	116.58	108.38
1	H	2	HIS	N-CA-C	-6.07	97.87	110.80
1	E	581	VAL	N-CA-C	6.07	117.54	110.62
1	G	748	GLU	N-CA-C	6.06	119.39	109.76
1	A	185	ASP	CA-C-N	6.05	129.25	121.27
1	A	185	ASP	C-N-CA	6.05	129.25	121.27
1	F	283	HIS	N-CA-C	6.04	118.83	111.82
1	B	734	LYS	N-CA-C	-6.02	97.97	110.80
1	A	728	GLN	N-CA-C	6.00	118.09	109.14
1	C	484	ALA	N-CA-C	5.99	118.58	111.33
1	A	191	THR	N-CA-CB	-5.97	101.57	110.17
1	B	224	THR	CB-CA-C	5.96	120.03	109.72
1	F	224	THR	CB-CA-C	5.92	119.97	109.72
1	A	39	PHE	N-CA-C	-5.92	105.72	113.12
1	B	268	GLU	N-CA-C	-5.90	104.93	111.36
1	B	516	ILE	N-CA-C	-5.88	107.39	113.10
1	A	2	HIS	N-CA-C	5.83	123.22	110.80
1	A	320	ARG	N-CA-C	-5.82	104.38	112.30
1	G	217	ASN	CA-C-N	-5.82	113.98	120.45
1	G	217	ASN	C-N-CA	-5.82	113.98	120.45
1	H	695	ASP	N-CA-C	5.82	119.12	109.46
1	H	694	ASP	N-CA-C	-5.82	105.44	112.54
1	F	224	THR	N-CA-CB	-5.81	101.45	110.57
1	H	26	ALA	N-CA-C	-5.80	98.45	110.80
1	E	750	SER	N-CA-C	5.78	123.11	110.80
1	F	93	MET	CB-CA-C	-5.77	102.71	109.80
1	D	395	PHE	N-CA-C	-5.75	105.94	113.12
1	B	710	THR	CB-CA-C	5.74	119.56	109.80
1	D	581	VAL	N-CA-C	5.72	117.15	110.62
1	F	648	LYS	N-CA-C	-5.72	105.12	111.36
1	F	749	LYS	N-CA-C	5.70	118.71	108.17
1	C	352	ARG	N-CA-C	-5.66	105.11	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	678	SER	N-CA-C	-5.63	105.04	111.07
1	F	224	THR	N-CA-C	-5.62	100.02	109.07
1	E	669	GLY	N-CA-C	-5.61	104.17	111.52
1	H	734	LYS	N-CA-C	-5.58	101.77	110.42
1	D	192	VAL	N-CA-C	5.53	115.73	110.53
1	G	213	GLU	N-CA-C	-5.53	101.56	110.14
1	A	748	GLU	N-CA-C	5.52	118.09	108.76
1	D	16	ILE	CG1-CB-CG2	-5.49	94.23	110.70
1	D	510	SER	CB-CA-C	-5.49	102.27	110.88
1	C	395	PHE	N-CA-C	-5.47	104.84	112.45
1	G	728	GLN	N-CA-C	5.47	116.58	108.86
1	G	49	ASP	N-CA-C	5.46	118.37	110.28
1	F	600	HIS	N-CA-C	5.46	118.73	112.57
1	E	714	ILE	CB-CA-C	-5.45	104.15	110.91
1	C	365	ALA	N-CA-C	5.44	117.21	111.28
1	C	191	THR	OG1-CB-CG2	5.42	120.15	109.30
1	A	219	ASP	N-CA-C	5.42	119.88	113.16
1	C	353	ASN	N-CA-C	5.42	117.19	111.28
1	E	62	THR	N-CA-C	-5.42	104.45	111.71
1	A	672	THR	N-CA-C	5.40	116.85	111.07
1	D	400	LEU	N-CA-C	-5.40	105.43	112.23
1	G	340	MET	CA-C-N	-5.38	113.19	119.32
1	G	340	MET	C-N-CA	-5.38	113.19	119.32
1	B	739	LYS	N-CA-C	-5.35	102.37	110.50
1	H	642	ALA	N-CA-C	-5.35	105.35	111.07
1	F	423	ALA	N-CA-C	-5.33	105.64	111.82
1	F	567	ILE	N-CA-C	-5.33	106.98	111.56
1	H	516	ILE	N-CA-C	5.31	118.09	112.83
1	E	205	SER	N-CA-C	5.31	122.10	110.80
1	E	347	ASN	CA-C-N	5.30	125.62	119.47
1	E	347	ASN	C-N-CA	5.30	125.62	119.47
1	D	27	ILE	CA-C-N	5.30	127.33	120.44
1	D	27	ILE	C-N-CA	5.30	127.33	120.44
1	B	2	HIS	N-CA-C	5.29	122.07	110.80
1	A	421	ALA	N-CA-C	-5.28	105.60	111.36
1	H	581	VAL	N-CA-CB	5.28	116.37	110.51
1	B	694	ASP	N-CA-C	-5.28	106.70	112.72
1	B	593	GLN	CA-C-N	5.25	127.26	120.44
1	B	593	GLN	C-N-CA	5.25	127.26	120.44
1	B	102	ARG	NE-CZ-NH2	5.24	123.92	119.20
1	B	460	PRO	CA-C-N	-5.24	111.97	120.72
1	B	460	PRO	C-N-CA	-5.24	111.97	120.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	550	TYR	N-CA-C	-5.23	105.58	111.28
1	B	644	ARG	N-CA-C	-5.22	105.77	111.82
1	G	737	ASP	CA-C-N	5.22	131.09	121.70
1	G	737	ASP	C-N-CA	5.22	131.09	121.70
1	H	282	SER	N-CA-C	-5.22	106.42	112.89
1	E	364	GLY	N-CA-C	-5.21	106.45	112.50
1	A	565	ARG	N-CA-C	-5.21	106.61	113.17
1	H	659	GLU	N-CA-C	5.19	116.80	110.41
1	E	739	LYS	N-CA-C	5.19	117.67	110.20
1	H	667	ILE	N-CA-CB	-5.17	105.64	112.36
1	A	644	ARG	N-CA-C	5.17	116.60	111.07
1	H	102	ARG	N-CA-C	-5.17	100.61	109.24
1	D	43	ARG	NE-CZ-NH2	5.14	123.82	119.20
1	B	736	GLU	CA-C-N	-5.12	115.55	122.77
1	B	736	GLU	C-N-CA	-5.12	115.55	122.77
1	E	27	ILE	N-CA-C	5.11	115.55	110.23
1	C	401	SER	N-CA-C	5.11	118.67	112.23
1	H	76	VAL	N-CA-C	5.11	113.51	107.84
1	D	667	ILE	N-CA-CB	-5.08	104.89	112.67
1	F	357	TYR	N-CA-C	-5.08	105.82	111.36
1	B	739	LYS	CA-C-N	-5.07	114.76	120.14
1	B	739	LYS	C-N-CA	-5.07	114.76	120.14
1	F	667	ILE	CB-CA-C	5.06	119.58	111.29
1	C	320	ARG	N-CA-C	-5.05	105.44	112.30
1	A	702	LEU	CA-C-N	-5.04	115.37	120.31
1	A	702	LEU	C-N-CA	-5.04	115.37	120.31
1	G	350	ILE	N-CA-C	-5.02	105.65	110.72
1	F	667	ILE	CA-CB-CG2	5.02	119.03	110.50
1	C	181	HIS	N-CA-C	-5.01	102.38	108.14
1	H	582	ARG	NE-CZ-NH2	5.01	123.71	119.20

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	85	0
1	B	6085	0	5844	95	0
1	C	6085	0	5844	93	0
1	D	6085	0	5844	83	0
1	E	6085	0	5844	114	0
1	F	6085	0	5844	120	0
1	G	6093	0	5855	102	0
1	H	6085	0	5844	107	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	3	0
4	D	54	0	72	15	0
4	E	24	0	32	1	0
4	F	18	0	24	2	0
4	G	18	0	24	3	0
4	H	30	0	40	10	0
5	A	19	0	26	4	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	7	0
12	C	286	0	0	11	0
12	D	348	0	0	12	0
12	E	185	0	0	12	0
12	F	247	0	0	15	0
12	G	197	0	0	3	0
12	H	218	0	0	6	0
All	All	51264	0	47580	803	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 (803) 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:HH11	1:F:756:ARG:HG3	1.09	1.12
4:D:806:GOL:H2	12:D:1202:HOH:O	1.51	1.09
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:HH11	1:F:604:ARG:HB3	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
1:D:637:ASP:HB3	12:D:1053:HOH:O	1.63	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:457:VAL:HG11	1:F:468:MET:HE2	1.51	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:G:735:SER:C	1:G:737:ASP:H	1.84	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

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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:HG2	1:H:582:ARG:HH21	1.50	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:F:491:MET:HE2	1:F:491:MET:HA	1.69	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: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:HH11	1:F:756:ARG:CG	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:659:GLU:O	1:A:660:ALA:HB3	1.88	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:142:LEU:HD21	1:G:263:MET:HE1	1.71	0.72
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:B:734:LYS:HD2	1:B:734:LYS:H	1.54	0.71
1:E:735:SER:O	1:E:736:GLU:HB3	1.90	0.71
1:A:158:ASP:CG	6:A:812:PGE:H6	2.15	0.71
1:G:1:MET:HG3	1:G:2:HIS:HB2	1.73	0.70
1:H:129:GLU:OE2	1:H:131:LYS:NZ	2.24	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:HD2	1:B:734:LYS:N	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:G:735:SER:C	1:G:737:ASP:N	2.50	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:83:LEU:HD12	6:A:812:PGE:O4	1.93	0.68
1:A:612:GLU:OE2	4:A:805:GOL:H11	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:A:756:ARG:HG2	1:A:756:ARG:HH11	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:H42	11:H:808:PE5:C7	2.21	0.67
1:D:499:GLU:O	1:D:503:THR:HB	1.94	0.66
1:E:468:MET:CE	12:E:974:HOH:O	2.44	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:E:466:GLU:OE1	1:E:468:MET:HE3	1.95	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: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:C:491:MET:HE2	1:C:491:MET:HA	1.79	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:F:26:ALA:C	1:F:27:ILE:HG22	2.23	0.63
1:E:8:LEU:HD22	1:E:16:ILE:HD12	1.81	0.63
1:H:582:ARG:HG2	1:H:582:ARG:NH2	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:A:491:MET:HE2	1:A:491:MET:HA	1.82	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:656:ASN:CG	1:H:656:ASN:O	2.42	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:B:656:ASN:O	1:B:656:ASN:CG	2.42	0.60
1:E:31:SER:HB3	1:E:670:ILE:HG12	1.83	0.60
1:F:97:ALA:C	1:F:99:SER:H	2.08	0.60
1:A:659:GLU:O	1:A:660:ALA:CB	2.49	0.60
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: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:58:ILE:N	1:G:58:ILE:HD12	2.18	0.59
1:G:79:ALA:HB1	1:G:202:GLU:HB2	1.84	0.59
1:E:751:VAL:O	1:E:752:LEU:HB2	2.02	0.59
1:B:27:ILE:HG22	1:B:28:THR:H	1.68	0.59
1:B:726:LYS:CD	1:B:726:LYS:H	2.16	0.59
1:C:99:SER:HB3	1:C:116:SER:HB2	1.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:658:ASN:HB3	4:A:803:GOL:H31	1.86	0.58
1:E:693:GLY:C	1:E:695:ASP:H	2.11	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:B:43:ARG:HD3	1:B:56:ALA:HB3	1.85	0.57
1:B:79:ALA:HB1	1:B:202:GLU:HB2	1.86	0.57
1:C:142:LEU:HD21	1:C:263:MET:CE	2.34	0.57
1:D:97:ALA:O	1:D:99:SER:N	2.38	0.57
1:E:738:ARG:O	1:E:738:ARG:CG	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:B:428:HIS:CD2	1:B:437:ILE:HG13	2.39	0.56
1:C:97:ALA:O	1:C:99:SER:N	2.39	0.56
1:E:370:LYS:NZ	12:E:1083:HOH:O	2.38	0.56
1:F:656:ASN:HA	12:F:1054:HOH:O	2.03	0.56
1:F:745:ILE:O	1:F:745:ILE:HG22	2.04	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:D:18:LYS:NZ	1:D:29:GLU:OE1	2.35	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:G:653:ASP:CG	1:G:670:ILE:HD13	2.31	0.56
1:D:418:PRO:HB2	1:D:489:GLN:HB3	1.88	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:E:468:MET:HE2	12:E:974:HOH:O	2.02	0.55
1:H:759:LYS:HG3	1:H:760:SER:H	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:491:MET:HE3	1:B:533:THR:HG21	1.88	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:F:507:LYS:NZ	12:F:977:HOH:O	2.33	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
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:E:737:ASP:CA	1:E:738:ARG:CB	2.70	0.54
1:D:504:LEU:HB2	1:D:509:LEU:HD22	1.88	0.54
1:H:25:GLN:C	1:H:26:ALA:O	2.47	0.54
1:B:114:LYS:NZ	12:B:1091:HOH:O	2.39	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:B:5:GLY:O	1:B:6:GLU:C	2.51	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:HD13	1:E:714:ILE:N	2.23	0.54
1:B:2:HIS:HB3	1:B:10:THR:O	2.08	0.54
1:E:5:GLY:O	1:E:6:GLU:C	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:HD12	1:C:293:ILE:H	1.74	0.53
1:E:468:MET:HE1	12:E:974:HOH:O	2.06	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
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:H:649:SER:HB3	1:H:681:MET:HE1	1.91	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:F:425:LYS:NZ	1:F:499:GLU:OE1	2.32	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:1:MET:SD	1:D:1:MET:N	2.83	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:O6	10:C:805:PE4:C13	2.57	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:58:ILE:N	1:H:58:ILE:HD12	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: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:G:494:LEU:HD11	1:G:529:MET:HE2	1.91	0.51
1:A:573:TYR:HE2	1:A:621:PHE:HE1	1.59	0.51
1:E:714:ILE:N	1:E:714:ILE:CD1	2.74	0.51
1:H:1:MET:HA	1:H:292:ILE:CG2	2.39	0.51
1:E:86:VAL:HB	1:E:119:MET:HE2	1.93	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:77:PRO:HD3	1:E:173:LEU:HD12	1.92	0.50
1:E:749:LYS:O	1:E:750:SER:HB2	2.11	0.50
1:H:172:HIS:O	1:H:191:THR:HA	2.11	0.50
11:H:808:PE5:H72	11:H:808:PE5:C4	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:F:656:ASN:CG	1:F:656:ASN:O	2.55	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:E:727:GLU:CD	1:E:727:GLU:H	2.19	0.50
1:F:224:THR:HG23	12:F:984:HOH:O	2.12	0.50
1:F:655:LEU:O	1:F:656:ASN:C	2.55	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: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:B:678:SER:HA	1:B:681:MET:HE2	1.93	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:164:ASP:CG	4:H:807:GOL:H2	2.35	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:A:656:ASN:CG	1:A:656:ASN:O	2.51	0.49
1:D:649:SER:HB3	1:D:681:MET:HE1	1.93	0.49
1:E:693:GLY:C	1:E:695:ASP:N	2.71	0.49
1:H:591:VAL:O	1:H:594:LEU:HB3	2.12	0.49
1:D:79:ALA:HB1	1:D:202:GLU:HB2	1.94	0.49
1:D:130:GLU:HG3	1:D:266:TYR:OH	2.12	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
1:C:635:GLN:HB2	10:C:805:PE4:H22	1.93	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:H:491:MET:HE3	1:H:533:THR:HG21	1.95	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:O	1:D:560:LYS:HG3	2.13	0.48
1:B:754:SER:OG	1:B:755:GLU:N	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:142:LEU:HD21	1:G:263:MET:CE	2.42	0.48
1:H:26:ALA:O	1:H:27:ILE:HG22	2.13	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:E:468:MET:HB2	1:F:468:MET:HE1	1.95	0.48
1:G:413:GLN:NE2	1:G:475:GLN:NE2	2.56	0.48
1:C:154:ASP:CG	1:G:644:ARG:NH1	2.72	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
1:F:557:ILE:HA	1:F:558:PRO:C	2.39	0.47
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:D:733:ASN:OD1	1:D:733:ASN:C	2.57	0.47
1:E:71:GLU:O	1:E:328:GLN:HG2	2.14	0.47
1:G:16:ILE:CD1	1:G:654:LEU:HD22	2.44	0.47
1:G:44:GLY:O	1:G:102:ARG:NH2	2.38	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:C:86:VAL:HG21	1:C:125:ILE:HG13	1.97	0.47
1:C:113:ARG:NH2	1:C:129:GLU:OE1	2.45	0.47
1:C:302:ILE:O	1:C:306:ILE:HG13	2.14	0.47
1:C:752:LEU:HD13	1:C:757:ILE:HG12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:712:LYS:NZ	12:G:1058:HOH:O	2.32	0.47
1:H:98:ALA:O	1:H:99:SER:CB	2.63	0.47
1:B:729:ILE:CD1	1:B:745:ILE:HG21	2.45	0.47
1:B:738:ARG:CZ	1:B:755:GLU:HG3	2.45	0.47
1:B:745:ILE:O	1:B:748:GLU:HG2	2.14	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:HD12	1:E:624:LEU:N	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:98:ALA:HB2	12:F:1136:HOH:O	2.15	0.46
1:F:422:TYR:HE2	6:F:806:PGE:H42	1.79	0.46
1:B:100:PHE:CZ	1:B:102:ARG:HB2	2.50	0.46
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:96:GLU:HG3	1:E:96:GLU:O	2.15	0.46
1:E:670:ILE:HD12	1:E:670:ILE:HG23	1.68	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: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:E:637:ASP:CG	1:E:637:ASP:O	2.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:731:ILE:HB	1:D:757:ILE:CG2	2.45	0.45
1:A:98:ALA:O	1:A:99:SER:HB3	2.15	0.45
1:A:671:HIS:HB3	12:A:957:HOH:O	2.16	0.45
1:C:315:LEU:O	4:C:809:GOL:H32	2.16	0.45
1:E:6:GLU:HB3	1:E:7:HIS:H	1.49	0.45
1:E:545:GLU:HG2	1:E:547:PHE:O	2.16	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: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:684:ASN:HB3	9:D:808:7PE:H112	1.97	0.45
1:D:696:ILE:HG12	1:D:715:VAL:HG11	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:G:97:ALA:O	1:G:98:ALA:C	2.58	0.45
1:H:427:TYR:CE1	1:H:431:THR:HG21	2.51	0.45
1:C:142:LEU:HD21	1:C:263:MET:HE1	1.99	0.45
1:E:230:GLU:CD	1:E:233:LYS:HE3	2.42	0.45
1:G:115:VAL:O	1:G:126:THR:HA	2.17	0.45
1:B:733:ASN:C	1:B:734:LYS:O	2.58	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:D:741:LEU:C	1:D:742:THR:HG23	2.42	0.45
1:E:47:ALA:HB1	1:E:82:THR:HB	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:119:MET:HG2	1:E:123:ALA:O	2.16	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:1:MET:O	1:H:1:MET:HG3	2.17	0.45
1:H:381:TRP:CH2	1:H:413:GLN:CD	2.95	0.45
1:C:587:LYS:HE2	1:C:622:SER:HB2	1.99	0.45
1:D:244:TYR:OH	1:D:259:GLU:OE2	2.31	0.45
1:D:327:TYR:OH	4:D:802:GOL:C3	2.65	0.45
1:H:754:SER:O	1:H:755:GLU:C	2.59	0.45
1:A:394:PHE:HZ	1:B:582:ARG:HG2	1.82	0.45
1:F:27:ILE:HG23	1:F:28:THR:H	1.82	0.45
1:F:611:TYR:CD1	1:F:611:TYR:C	2.94	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:C:51:LYS:HE2	1:C:164:ASP:CG	2.42	0.44
1:C:561:LYS:NZ	4:C:803:GOL:O2	2.50	0.44
1:D:129:GLU:OE2	1:D:131:LYS:NZ	2.45	0.44
1:D:756:ARG:CG	1:D:757:ILE:N	2.81	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:18:LYS:NZ	1:C:29:GLU:OE1	2.50	0.44
1:C:229:LEU:N	1:C:229:LEU:HD12	2.33	0.44
1:C:718:GLN:CD	1:C:733:ASN:HD21	2.24	0.44
1:B:129:GLU:OE2	1:B:131:LYS:NZ	2.47	0.44
1:D:98:ALA:O	1:D:99:SER:CB	2.64	0.44
1:D:501:LEU:HD23	1:D:509:LEU:HD11	2.00	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:G:263:MET:HB3	1:G:263:MET:HE3	1.63	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:422:TYR:CE2	6:F:806:PGE:H42	2.53	0.44
1:F:457:VAL:CG1	1:F:468:MET:HE2	2.36	0.44
1:G:715:VAL:O	1:G:716:LYS:C	2.61	0.44
1:A:142:LEU:HD21	1:A:263:MET:HE2	1.98	0.44
1:A:215:TYR:HE1	6:A:812:PGE:H22	1.83	0.44
1:A:301:ASN:O	1:A:675:ASN:HB3	2.18	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: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
4:A:811:GOL:C3	1:F:158:ASP:OD1	2.66	0.43
1:C:501:LEU:HD23	1:C:509:LEU:HD11	2.00	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:D:515:LYS:NZ	12:D:1132:HOH:O	2.50	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
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:A:5:GLY:O	1:A:6:GLU:C	2.60	0.43
1:G:178:TYR:CD2	1:G:178:TYR:C	2.97	0.43
1:G:381:TRP:CH2	1:G:413:GLN:CD	2.96	0.43
1:H:277:TRP:HA	1:H:280:LEU:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:ARG:HD3	1:A:56:ALA:HB3	2.01	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:H	1:E:95:GLU:HG2	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:G:662:SER:O	1:G:663:GLY:C	2.62	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:A:753:ASP:O	1:A:754:SER:CB	2.66	0.43
1:D:727:GLU:O	1:D:761:ARG:N	2.45	0.43
1:E:138:LYS:NZ	12:E:1025:HOH:O	2.52	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
12:A:1080:HOH:O	1:C:644:ARG:HD2	2.19	0.42
1:B:249:VAL:HG11	1:B:255:GLU:HG2	2.01	0.42
1:E:287:THR:HB	1:E:710:THR:HG23	2.01	0.42
1:F:747:GLY:C	1:F:748:GLU:HG2	2.44	0.42
1:D:756:ARG:CG	1:D:757:ILE:H	2.32	0.42
1:H:49:ASP:HB3	1:H:53:ALA:HB3	2.01	0.42
1:H:667:ILE:HD12	1:H:667:ILE:HA	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
1:H:731:ILE:HD13	1:H:743:LEU:HD23	2.01	0.42
1:H:761:ARG:HB3	1:H:761:ARG:HH21	1.84	0.42
1:B:18:LYS:HG2	1:B:29:GLU:OE1	2.19	0.42
1:D:340:MET:HE3	1:D:351:ALA:HB1	2.01	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:468:MET:SD	1:F:468:MET:CE	3.08	0.42
1:E:491:MET:HG3	1:E:535:VAL:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:97:ALA:C	1:F:99:SER:N	2.72	0.42
1:F:338:TYR:HA	1:F:680:GLN:HE22	1.84	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:C:356:LYS:NZ	12:C:1039:HOH:O	2.43	0.42
1:D:374:TYR:HH	4:D:809:GOL:H12	1.81	0.42
1:F:512:VAL:O	1:F:516:ILE:HG12	2.20	0.42
1:A:684:ASN:CG	5:A:806:P6G:H82	2.44	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:H:142:LEU:HD21	1:H:263:MET:HE2	2.01	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:C:91:PHE:CD1	1:C:91:PHE:C	2.98	0.42
1:D:686:PHE:CE1	1:D:703:PRO:HG3	2.55	0.42
1:F:697:HIS:C	1:F:698:LEU:HG	2.45	0.42
1:D:336:GLU:O	9:D:808:7PE:H32	2.20	0.41
1:D:459:LYS:HB3	1:D:459:LYS:HE3	1.84	0.41
1:D:709:TYR:C	1:D:710:THR:HG22	2.45	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:F:26:ALA:C	1:F:27:ILE:CG2	2.93	0.41
1:F:513:LYS:NZ	12:F:1123:HOH:O	2.52	0.41
1:G:644:ARG:HD3	12:G:1020:HOH:O	2.19	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:G:461:MET:HE2	1:G:461:MET:HB3	1.90	0.41
1:A:368:LYS:HD3	1:A:378:TYR:O	2.20	0.41
1:A:582:ARG:HD2	1:B:394:PHE:HZ	1.84	0.41
1:A:618:THR:HG22	1:A:620:HIS:H	1.85	0.41
5:A:806:P6G:H22	5:A:806:P6G:H52	1.90	0.41
1:D:6:GLU:O	1:D:7:HIS:HB2	2.19	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:F:734:LYS:H	1:F:734:LYS:HG2	1.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:551:TYR:CZ	4:D:807:GOL:H11	2.55	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
12:A:1080:HOH:O	1:C:644:ARG:CD	2.68	0.41
1:B:20:ARG:HD2	1:B:20:ARG:HA	1.76	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:85:HIS:HA	1:B:89:GLU:O	2.20	0.41
1:B:315:LEU:H	4:B:803:GOL:H12	1.86	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:58:ILE:HD12	1:G:58:ILE:H	1.84	0.41
1:G:179:PHE:CZ	1:G:186:GLY:HA3	2.55	0.41
1:G:403:ARG:HH22	1:H:571:GLU:CD	2.27	0.41
1:G:646:PHE:O	1:G:650:VAL:HG22	2.21	0.41
1:H:79:ALA:HB3	1:H:241:MET:HB2	2.01	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: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:A:752:LEU:O	1:A:753:ASP:C	2.63	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:N	1:C:696:ILE:CD1	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:OD1	1:F:570:ASP:N	2.51	0.41
1:G:31:SER:HB3	1:G:670:ILE:HG12	2.02	0.41
1:G:415:HIS:ND1	1:G:419:ASP:OD2	2.44	0.41
1:H:69:LYS:HA	8:H:803:PG4:H72	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:A:432:GLY:O	1:A:434:ASP:N	2.54	0.41
1:A:644:ARG:NH1	1:F:228:SER:HB3	2.33	0.41
1:C:16:ILE:CG1	1:C:104:LEU:HB3	2.50	0.41
10:C:805:PE4:H142	10:C:805:PE4:C8	2.50	0.41
1:D:45:THR:HG21	1:D:55:ALA:HA	2.01	0.41
1:D:573:TYR:HE2	1:D:621:PHE:HE1	1.68	0.41
1:D:605:LYS:HD3	1:D:605:LYS:HA	1.92	0.41
8:D:803:PG4:H11	8:D:803:PG4:H32	1.76	0.41
1:E:28:THR:HG21	1:E:656:ASN:HB2	2.02	0.41
1:F:49:ASP:HB3	1:F:53:ALA:HB3	2.02	0.41
1:F:573:TYR:CE2	1:F:621:PHE:HE1	2.38	0.41
1:F:635:GLN:NE2	1:F:635:GLN:HA	2.24	0.41
1:F:751:VAL:HG12	1:F:752:LEU:N	2.35	0.41
1:G:86:VAL:HB	1:G:119:MET:HE2	2.03	0.41
1:G:491:MET:HA	1:G:491:MET:HE2	2.01	0.41
1:H:356:LYS:HE3	1:H:440:TYR:CZ	2.56	0.41
1:A:86:VAL:O	1:A:87:ASP:C	2.60	0.41
1:E:653:ASP:CG	1:E:670:ILE:HD13	2.46	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:F:529:MET:HB3	1:F:529:MET:HE2	1.85	0.40
1:A:58:ILE:HD12	1:A:58:ILE:N	2.36	0.40
1:E:15:ASP:OD2	1:E:17:ILE:HD11	2.22	0.40
1:F:415:HIS:O	1:F:416:ILE:C	2.64	0.40
1:G:619:LEU:O	1:G:620:HIS:HB2	2.21	0.40
1:A:31:SER:HB3	1:A:670:ILE:HG12	2.02	0.40
1:B:230:GLU:O	1:B:231:ALA:C	2.64	0.40
1:B:726:LYS:HD2	1:B:726:LYS:N	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: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:E:29:GLU:HG2	1:E:102:ARG:NH1	2.37	0.40
1:F:594:LEU:HD12	1:F:598:HIS:HD2	1.86	0.40
1:B:604:ARG:HE	1:B:604:ARG:HB3	1.47	0.40
1:D:79:ALA:HB3	1:D:241:MET:HB2	2.04	0.40
1:D:201:VAL:HG11	1:D:260:ALA:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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

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%)	9	10
1	B	759/769 (99%)	720 (95%)	33 (4%)	6 (1%)	16	20
1	C	759/769 (99%)	728 (96%)	25 (3%)	6 (1%)	16	20
1	D	759/769 (99%)	723 (95%)	34 (4%)	2 (0%)	36	46
1	E	759/769 (99%)	696 (92%)	48 (6%)	15 (2%)	6	5
1	F	759/769 (99%)	701 (92%)	44 (6%)	14 (2%)	6	6
1	G	760/769 (99%)	718 (94%)	31 (4%)	11 (1%)	9	9
1	H	759/769 (99%)	715 (94%)	35 (5%)	9 (1%)	10	12
All	All	6074/6152 (99%)	5722 (94%)	279 (5%)	73 (1%)	10	12

All (73) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	742	THR
1	A	750	SER
1	A	754	SER

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Mol	Chain	Res	Type
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
1	C	660	ALA
1	D	99	SER

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Mol	Chain	Res	Type
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%)	614 (94%)	37 (6%)	18	27
1	B	650/658 (99%)	618 (95%)	32 (5%)	22	34
1	C	650/658 (99%)	607 (93%)	43 (7%)	15	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	650/658 (99%)	611 (94%)	39 (6%)	17	25
1	E	650/658 (99%)	595 (92%)	55 (8%)	10	13
1	F	650/658 (99%)	610 (94%)	40 (6%)	16	24
1	G	651/658 (99%)	597 (92%)	54 (8%)	10	14
1	H	650/658 (99%)	617 (95%)	33 (5%)	21	32
All	All	5202/5264 (99%)	4869 (94%)	333 (6%)	16	23

All (333) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	LEU
1	A	94	SER
1	A	129	GLU
1	A	191	THR
1	A	217	ASN
1	A	229	LEU
1	A	254	ASP
1	A	257	LEU
1	A	258	LEU
1	A	275	LEU
1	A	280	LEU
1	A	289	GLN
1	A	298	LEU
1	A	390	LEU
1	A	417	SER
1	A	506	GLU
1	A	509	LEU
1	A	513	LYS
1	A	537	LYS
1	A	560	LYS
1	A	568	LYS
1	A	604	ARG
1	A	647	ARG
1	A	655	LEU
1	A	670	ILE
1	A	696	ILE
1	A	698	LEU
1	A	701	ARG
1	A	702	LEU
1	A	727	GLU

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Mol	Chain	Res	Type
1	A	732	THR
1	A	739	LYS
1	A	741	LEU
1	A	750	SER
1	A	752	LEU
1	A	756	ARG
1	A	757	ILE
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	425	LYS
1	B	503	THR
1	B	506	GLU
1	B	507	LYS
1	B	509	LEU
1	B	524	SER
1	B	604	ARG
1	B	659	GLU
1	B	667	ILE
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	741	LEU
1	B	742	THR
1	B	743	LEU
1	B	748	GLU
1	B	750	SER
1	B	760	SER
1	C	2	HIS
1	C	6	GLU
1	C	18	LYS

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Mol	Chain	Res	Type
1	C	93	MET
1	C	94	SER
1	C	96	GLU
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	390	LEU
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	696	ILE
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
1	D	16	ILE

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Mol	Chain	Res	Type
1	D	27	ILE
1	D	80	LEU
1	D	94	SER
1	D	101	GLU
1	D	102	ARG
1	D	141	VAL
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	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	716	LYS
1	D	720	LEU
1	D	726	LYS
1	D	729	ILE
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	759	LYS
1	D	761	ARG
1	E	2	HIS
1	E	16	ILE
1	E	18	LYS
1	E	22	GLU
1	E	29	GLU

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Mol	Chain	Res	Type
1	E	89	GLU
1	E	96	GLU
1	E	99	SER
1	E	114	LYS
1	E	174	GLN
1	E	191	THR
1	E	193	SER
1	E	203	THR
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	349	GLU
1	E	390	LEU
1	E	495	GLN
1	E	503	THR
1	E	507	LYS
1	E	509	LEU
1	E	540	LYS
1	E	560	LYS
1	E	655	LEU
1	E	658	ASN
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	716	LYS
1	E	726	LYS
1	E	732	THR
1	E	734	LYS

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Mol	Chain	Res	Type
1	E	741	LEU
1	E	742	THR
1	E	743	LEU
1	E	749	LYS
1	E	751	VAL
1	E	753	ASP
1	E	755	GLU
1	E	757	ILE
1	F	2	HIS
1	F	16	ILE
1	F	20	ARG
1	F	22	GLU
1	F	27	ILE
1	F	80	LEU
1	F	96	GLU
1	F	102	ARG
1	F	171	ASP
1	F	224	THR
1	F	228	SER
1	F	233	LYS
1	F	275	LEU
1	F	296	VAL
1	F	349	GLU
1	F	416	ILE
1	F	417	SER
1	F	502	GLN
1	F	506	GLU
1	F	509	LEU
1	F	514	GLU
1	F	582	ARG
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	734	LYS
1	F	735	SER
1	F	736	GLU
1	F	738	ARG
1	F	739	LYS

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Mol	Chain	Res	Type
1	F	742	THR
1	F	743	LEU
1	F	749	LYS
1	F	750	SER
1	F	756	ARG
1	F	759	LYS
1	G	2	HIS
1	G	3	GLU
1	G	16	ILE
1	G	18	LYS
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	138	LYS
1	G	147	VAL
1	G	190	LYS
1	G	191	THR
1	G	193	SER
1	G	202	GLU
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	362	LEU
1	G	390	LEU
1	G	426	LYS
1	G	495	GLN
1	G	503	THR
1	G	506	GLU
1	G	560	LYS

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Mol	Chain	Res	Type
1	G	568	LYS
1	G	644	ARG
1	G	655	LEU
1	G	661	VAL
1	G	670	ILE
1	G	696	ILE
1	G	698	LEU
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	G	762	LEU
1	H	27	ILE
1	H	80	LEU
1	H	83	LEU
1	H	99	SER
1	H	102	ARG
1	H	120	LYS
1	H	224	THR
1	H	258	LEU
1	H	261	LYS
1	H	275	LEU
1	H	346	SER
1	H	370	LYS
1	H	400	LEU
1	H	426	LYS
1	H	495	GLN
1	H	503	THR
1	H	507	LYS
1	H	508	THR
1	H	537	LYS
1	H	540	LYS
1	H	560	LYS
1	H	582	ARG
1	H	641	GLU
1	H	667	ILE

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Mol	Chain	Res	Type
1	H	699	SER
1	H	712	LYS
1	H	720	LEU
1	H	726	LYS
1	H	734	LYS
1	H	742	THR
1	H	743	LEU
1	H	754	SER
1	H	761	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	290	ASN
1	A	339	ASN
1	A	495	GLN
1	A	684	ASN
1	B	85	HIS
1	B	262	HIS
1	B	290	ASN
1	B	328	GLN
1	B	347	ASN
1	B	684	ASN
1	C	128	HIS
1	C	217	ASN
1	C	247	ASN
1	C	253	GLN
1	C	413	GLN
1	C	429	GLN
1	C	475	GLN
1	C	680	GLN
1	C	684	ASN
1	C	697	HIS
1	D	169	ASN
1	D	253	GLN
1	D	262	HIS
1	D	413	GLN
1	D	429	GLN
1	D	475	GLN
1	D	675	ASN
1	D	684	ASN

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Mol	Chain	Res	Type
1	E	121	ASN
1	E	128	HIS
1	E	151	GLN
1	E	251	ASN
1	E	289	GLN
1	E	328	GLN
1	E	697	HIS
1	F	85	HIS
1	F	279	ASN
1	F	593	GLN
1	F	680	GLN
1	F	718	GLN
1	F	744	HIS
1	G	7	HIS
1	G	25	GLN
1	G	117	GLN
1	G	128	HIS
1	G	151	GLN
1	G	217	ASN
1	G	429	GLN
1	G	455	HIS
1	G	475	GLN
1	G	588	GLN
1	G	684	ASN
1	H	680	GLN
1	H	733	ASN

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 oligosaccharides 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$
4	GOL	C	803	-	5,5,5	0.23	0	5,5,5	1.34	1 (20%)
4	GOL	D	802	-	5,5,5	0.49	0	5,5,5	0.82	0
4	GOL	D	805	-	5,5,5	0.09	0	5,5,5	1.02	0
4	GOL	G	802	-	5,5,5	0.19	0	5,5,5	0.84	0
4	GOL	G	803	-	5,5,5	0.20	0	5,5,5	0.84	0
2	IFM	D	801	-	10,10,10	1.87	5 (50%)	9,13,13	3.51	6 (66%)
4	GOL	D	810	-	5,5,5	0.39	0	5,5,5	1.90	1 (20%)
4	GOL	A	804	-	5,5,5	0.82	0	5,5,5	2.24	3 (60%)
11	PE5	H	808	-	26,26,26	0.78	0	25,25,25	0.89	0
4	GOL	B	808	-	5,5,5	0.56	0	5,5,5	2.06	1 (20%)
4	GOL	D	812	-	5,5,5	1.34	0	5,5,5	2.08	3 (60%)
3	1PE	E	802	-	15,15,15	0.71	0	14,14,14	0.40	0
4	GOL	E	807	-	5,5,5	0.22	0	5,5,5	1.01	0
6	PGE	F	806	-	9,9,9	0.51	0	8,8,8	0.47	0
2	IFM	H	801	-	10,10,10	1.16	2 (20%)	9,13,13	3.64	4 (44%)
4	GOL	H	802	-	5,5,5	0.31	0	5,5,5	0.58	0
4	GOL	B	807	-	5,5,5	0.60	0	5,5,5	0.93	0
8	PG4	F	803	-	12,12,12	0.54	0	11,11,11	0.48	0
4	GOL	H	805	-	5,5,5	0.43	0	5,5,5	1.07	1 (20%)
6	PGE	C	807	-	9,9,9	0.46	0	8,8,8	0.84	0
4	GOL	D	804	-	5,5,5	0.35	0	5,5,5	0.48	0
4	GOL	A	811	-	5,5,5	0.46	0	5,5,5	1.30	0
3	1PE	C	801	-	15,15,15	0.66	0	14,14,14	0.95	0
4	GOL	D	811	-	5,5,5	0.35	0	5,5,5	0.33	0
2	IFM	A	801	-	10,10,10	1.27	1 (10%)	9,13,13	3.70	3 (33%)
4	GOL	F	804	-	5,5,5	0.56	0	5,5,5	0.55	0
5	P6G	E	803	-	18,18,18	0.66	0	17,17,17	0.78	0
9	7PE	D	808	-	20,20,20	0.73	0	19,19,19	1.42	3 (15%)
4	GOL	B	806	-	5,5,5	0.32	0	5,5,5	0.56	0
4	GOL	D	807	-	5,5,5	0.32	0	5,5,5	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	PG4	B	801	-	12,12,12	0.58	0	11,11,11	0.44	0
8	PG4	H	803	-	12,12,12	0.69	0	11,11,11	0.48	0
4	GOL	A	803	-	5,5,5	0.59	0	5,5,5	1.15	0
4	GOL	C	808	-	5,5,5	0.50	0	5,5,5	0.73	0
4	GOL	A	810	-	5,5,5	0.57	0	5,5,5	0.91	0
4	GOL	C	802	-	5,5,5	0.54	0	5,5,5	0.38	0
4	GOL	F	802	-	5,5,5	0.27	0	5,5,5	0.87	0
4	GOL	A	809	-	5,5,5	0.54	0	5,5,5	0.49	0
4	GOL	D	806	-	5,5,5	0.78	0	5,5,5	1.15	1 (20%)
9	7PE	B	802	-	20,20,20	0.61	0	19,19,19	0.99	1 (5%)
2	IFM	G	801	-	10,10,10	1.14	2 (20%)	9,13,13	3.03	5 (55%)
4	GOL	D	809	-	5,5,5	0.37	0	5,5,5	1.45	2 (40%)
4	GOL	C	809	-	5,5,5	0.62	0	5,5,5	2.45	1 (20%)
4	GOL	B	804	-	5,5,5	0.72	0	5,5,5	1.67	2 (40%)
8	PG4	D	803	-	12,12,12	0.60	0	11,11,11	0.61	0
2	IFM	E	801	-	10,10,10	1.33	2 (20%)	9,13,13	3.02	4 (44%)
4	GOL	H	807	-	5,5,5	0.46	0	5,5,5	0.67	0
2	IFM	F	801	-	10,10,10	1.19	2 (20%)	9,13,13	3.09	3 (33%)
4	GOL	E	806	-	5,5,5	0.53	0	5,5,5	0.85	0
4	GOL	E	805	-	5,5,5	0.43	0	5,5,5	0.22	0
4	GOL	F	805	-	5,5,5	0.66	0	5,5,5	0.69	0
4	GOL	C	806	-	5,5,5	0.66	0	5,5,5	0.79	0
4	GOL	G	804	-	5,5,5	0.34	0	5,5,5	0.60	0
4	GOL	H	804	-	5,5,5	0.37	0	5,5,5	0.65	0
5	P6G	A	806	-	18,18,18	0.59	0	17,17,17	0.83	0
10	PE4	C	805	-	23,23,23	0.92	0	22,22,22	1.32	2 (9%)
4	GOL	A	807	-	5,5,5	0.59	0	5,5,5	1.19	1 (20%)
4	GOL	B	805	-	5,5,5	0.55	0	5,5,5	0.95	0
4	GOL	A	808	-	5,5,5	0.44	0	5,5,5	0.76	0
3	1PE	A	802	-	15,15,15	0.73	0	14,14,14	0.70	0
4	GOL	E	804	-	5,5,5	0.21	0	5,5,5	0.72	0
4	GOL	B	803	-	5,5,5	0.59	0	5,5,5	1.83	2 (40%)
4	GOL	A	805	-	5,5,5	0.26	0	5,5,5	0.72	0
4	GOL	C	804	-	5,5,5	0.42	0	5,5,5	1.35	1 (20%)
4	GOL	H	806	-	5,5,5	0.51	0	5,5,5	1.10	0
6	PGE	G	805	-	9,9,9	0.71	0	8,8,8	0.59	0
6	PGE	A	812	-	9,9,9	0.56	0	8,8,8	0.44	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	C	803	-	-	0/4/4/4	-
4	GOL	D	802	-	-	2/4/4/4	-
4	GOL	D	805	-	-	1/4/4/4	-
4	GOL	G	802	-	-	2/4/4/4	-
4	GOL	G	803	-	-	3/4/4/4	-
2	IFM	D	801	-	-	0/2/16/16	0/1/1/1
4	GOL	D	810	-	-	3/4/4/4	-
4	GOL	A	804	-	-	2/4/4/4	-
11	PE5	H	808	-	-	21/24/24/24	-
4	GOL	B	808	-	-	3/4/4/4	-
4	GOL	D	812	-	-	0/4/4/4	-
3	1PE	E	802	-	-	9/13/13/13	-
4	GOL	E	807	-	-	2/4/4/4	-
6	PGE	F	806	-	-	4/7/7/7	-
2	IFM	H	801	-	-	0/2/16/16	1/1/1/1
4	GOL	H	802	-	-	0/4/4/4	-
4	GOL	B	807	-	-	0/4/4/4	-
8	PG4	F	803	-	-	8/10/10/10	-
4	GOL	H	805	-	-	2/4/4/4	-
6	PGE	C	807	-	-	3/7/7/7	-
4	GOL	D	804	-	-	4/4/4/4	-
4	GOL	A	811	-	-	4/4/4/4	-
3	1PE	C	801	-	-	5/13/13/13	-
4	GOL	D	811	-	-	4/4/4/4	-
2	IFM	A	801	-	-	1/2/16/16	0/1/1/1
4	GOL	F	804	-	-	2/4/4/4	-
5	P6G	E	803	-	-	10/16/16/16	-
9	7PE	D	808	-	-	4/18/18/18	-
4	GOL	B	806	-	-	2/4/4/4	-
4	GOL	D	807	-	-	1/4/4/4	-
8	PG4	B	801	-	-	3/10/10/10	-
8	PG4	H	803	-	-	6/10/10/10	-
4	GOL	A	803	-	-	4/4/4/4	-
4	GOL	C	808	-	-	0/4/4/4	-
4	GOL	A	810	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	C	802	-	-	0/4/4/4	-
4	GOL	F	802	-	-	2/4/4/4	-
4	GOL	A	809	-	-	2/4/4/4	-
4	GOL	D	806	-	-	4/4/4/4	-
9	7PE	B	802	-	-	8/18/18/18	-
2	IFM	G	801	-	-	0/2/16/16	0/1/1/1
4	GOL	D	809	-	-	3/4/4/4	-
4	GOL	C	809	-	-	2/4/4/4	-
4	GOL	B	804	-	-	4/4/4/4	-
8	PG4	D	803	-	-	5/10/10/10	-
2	IFM	E	801	-	-	0/2/16/16	0/1/1/1
4	GOL	H	807	-	-	4/4/4/4	-
2	IFM	F	801	-	-	0/2/16/16	1/1/1/1
4	GOL	E	806	-	-	1/4/4/4	-
4	GOL	E	805	-	-	2/4/4/4	-
4	GOL	F	805	-	-	2/4/4/4	-
4	GOL	C	806	-	-	0/4/4/4	-
4	GOL	G	804	-	-	0/4/4/4	-
4	GOL	H	804	-	-	4/4/4/4	-
5	P6G	A	806	-	-	10/16/16/16	-
10	PE4	C	805	-	-	9/21/21/21	-
4	GOL	A	807	-	-	4/4/4/4	-
4	GOL	B	805	-	-	3/4/4/4	-
4	GOL	A	808	-	-	4/4/4/4	-
3	1PE	A	802	-	-	9/13/13/13	-
4	GOL	E	804	-	-	2/4/4/4	-
4	GOL	B	803	-	-	2/4/4/4	-
4	GOL	A	805	-	-	4/4/4/4	-
4	GOL	C	804	-	-	2/4/4/4	-
4	GOL	H	806	-	-	0/4/4/4	-
6	PGE	G	805	-	-	4/7/7/7	-
6	PGE	A	812	-	-	4/7/7/7	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	801	IFM	O4-C4	-2.88	1.35	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	801	IFM	C3-C4	2.71	1.56	1.52
2	F	801	IFM	C3-C4	2.62	1.56	1.52
2	D	801	IFM	C3-C4	2.53	1.56	1.52
2	D	801	IFM	O3-C3	2.41	1.48	1.43
2	D	801	IFM	C2-N	-2.32	1.41	1.47
2	G	801	IFM	C3-C4	2.31	1.56	1.52
2	E	801	IFM	O3-C3	2.22	1.48	1.43
2	H	801	IFM	O3-C3	2.20	1.47	1.43
2	D	801	IFM	C2-C3	2.13	1.54	1.52
2	F	801	IFM	O3-C3	2.13	1.47	1.43
2	G	801	IFM	C2-C3	2.04	1.54	1.52
2	A	801	IFM	C3-C4	2.03	1.55	1.52
2	H	801	IFM	C3-C4	2.03	1.55	1.52

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	801	IFM	C1-N-C2	8.52	121.66	111.78
2	F	801	IFM	C1-N-C2	7.91	120.96	111.78
2	D	801	IFM	O4-C4-C5	-7.64	97.27	110.01
2	A	801	IFM	C1-N-C2	7.60	120.59	111.78
2	G	801	IFM	C1-N-C2	6.88	119.75	111.78
2	E	801	IFM	O4-C4-C5	-6.72	98.79	110.01
2	A	801	IFM	O4-C4-C5	-6.70	98.83	110.01
2	H	801	IFM	O4-C4-C5	-5.60	100.67	110.01
2	E	801	IFM	C1-N-C2	4.64	117.16	111.78
4	C	809	GOL	C3-C2-C1	-4.34	95.89	111.80
4	B	808	GOL	O3-C3-C2	-4.14	91.73	110.38
2	D	801	IFM	O3-C3-C4	3.92	118.27	110.15
4	D	810	GOL	O1-C1-C2	-3.90	92.80	110.38
2	D	801	IFM	C1-N-C2	3.79	116.18	111.78
10	C	805	PE4	C15-O8-C14	3.50	125.33	113.06
2	G	801	IFM	C1-C5-C4	3.37	115.43	108.72
4	A	804	GOL	O1-C1-C2	-3.28	95.63	110.38
2	F	801	IFM	O3-C3-C4	3.26	116.90	110.15
4	D	812	GOL	O2-C2-C3	3.22	122.50	109.18
2	G	801	IFM	O4-C4-C5	-3.13	104.80	110.01
9	D	808	7PE	O4-C5-C6	-3.11	96.18	110.35
2	D	801	IFM	O6-C6-C5	-3.07	104.27	111.26
2	H	801	IFM	O3-C3-C4	3.02	116.40	110.15
2	E	801	IFM	O3-C3-C4	3.01	116.39	110.15
9	D	808	7PE	O7-C8-C9	-2.78	97.67	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	804	GOL	C3-C2-C1	-2.75	101.69	111.80
4	A	804	GOL	O2-C2-C3	2.71	120.41	109.18
2	D	801	IFM	C1-C5-C4	-2.68	103.40	108.72
4	D	812	GOL	C3-C2-C1	-2.58	102.33	111.80
2	F	801	IFM	O4-C4-C5	-2.54	105.78	110.01
2	A	801	IFM	O4-C4-C3	2.53	115.22	110.05
4	C	804	GOL	O1-C1-C2	-2.52	99.01	110.38
4	C	803	GOL	O1-C1-C2	-2.32	99.92	110.38
4	B	803	GOL	O3-C3-C2	-2.32	99.95	110.38
4	B	804	GOL	O2-C2-C3	-2.28	99.74	109.18
10	C	805	PE4	O7-C13-C14	2.24	120.58	110.35
4	B	803	GOL	C3-C2-C1	-2.23	103.62	111.80
4	D	809	GOL	O2-C2-C1	-2.22	100.00	109.18
9	B	802	7PE	C20-O19-C18	2.21	120.83	113.06
2	E	801	IFM	O6-C6-C5	-2.21	106.22	111.26
2	G	801	IFM	O4-C4-C3	2.18	114.51	110.05
4	H	805	GOL	O1-C1-C2	-2.18	100.57	110.38
2	G	801	IFM	O3-C3-C4	2.13	114.57	110.15
9	D	808	7PE	C20-O19-C18	2.13	120.55	113.06
4	A	804	GOL	C3-C2-C1	-2.11	104.06	111.80
4	D	809	GOL	O1-C1-C2	-2.11	100.89	110.38
2	D	801	IFM	C2-C3-C4	-2.10	107.68	110.25
4	D	806	GOL	O2-C2-C3	2.05	117.67	109.18
2	H	801	IFM	C2-C3-C4	-2.04	107.75	110.25
4	D	812	GOL	O2-C2-C1	-2.03	100.75	109.18
4	A	807	GOL	O1-C1-C2	-2.02	101.30	110.38

There are no chirality outliers.

All (217) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	808	GOL	O1-C1-C2-C3
4	A	808	GOL	C1-C2-C3-O3
4	A	809	GOL	O1-C1-C2-O2
4	A	809	GOL	O1-C1-C2-C3
4	A	811	GOL	C1-C2-C3-O3
4	B	804	GOL	O1-C1-C2-C3
4	B	804	GOL	C1-C2-C3-O3
4	B	806	GOL	C1-C2-C3-O3
4	B	808	GOL	C1-C2-C3-O3
4	B	808	GOL	O2-C2-C3-O3
4	C	804	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	C	804	GOL	O1-C1-C2-C3
4	C	809	GOL	C1-C2-C3-O3
4	D	804	GOL	O1-C1-C2-C3
4	D	806	GOL	O1-C1-C2-C3
4	D	809	GOL	O1-C1-C2-C3
4	D	811	GOL	C1-C2-C3-O3
4	E	805	GOL	C1-C2-C3-O3
4	E	805	GOL	O2-C2-C3-O3
4	E	807	GOL	O1-C1-C2-O2
4	F	802	GOL	C1-C2-C3-O3
4	F	804	GOL	O1-C1-C2-C3
4	F	805	GOL	O1-C1-C2-C3
4	G	802	GOL	O1-C1-C2-C3
4	H	804	GOL	O1-C1-C2-O2
4	H	804	GOL	O1-C1-C2-C3
4	H	805	GOL	C1-C2-C3-O3
4	H	807	GOL	C1-C2-C3-O3
5	A	806	P6G	C2-C3-O4-C5
8	F	803	PG4	C1-C2-O2-C3
8	D	803	PG4	C1-C2-O2-C3
11	H	808	PE5	C2-C1-O1-C50
3	E	802	1PE	OH4-C13-C23-OH3
10	C	805	PE4	O2-C3-C4-O3
3	C	801	1PE	OH4-C13-C23-OH3
9	D	808	7PE	O10-C11-C12-O13
10	C	805	PE4	O4-C7-C8-O5
9	D	808	7PE	O4-C5-C6-O7
11	H	808	PE5	O7-C13-C14-O8
8	H	803	PG4	O3-C5-C6-O4
11	H	808	PE5	C6-C5-O3-C4
3	E	802	1PE	OH5-C14-C24-OH4
8	D	803	PG4	O2-C3-C4-O3
3	C	801	1PE	OH5-C14-C24-OH4
8	F	803	PG4	O3-C5-C6-O4
4	A	805	GOL	O1-C1-C2-O2
4	B	804	GOL	O2-C2-C3-O3
4	B	806	GOL	O2-C2-C3-O3
4	D	806	GOL	O1-C1-C2-O2
4	H	805	GOL	O2-C2-C3-O3
4	H	807	GOL	O2-C2-C3-O3
10	C	805	PE4	O3-C5-C6-O4
11	H	808	PE5	O6-C10-C9-O5

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Mol	Chain	Res	Type	Atoms
3	E	802	1PE	OH2-C12-C22-OH3
6	A	812	PGE	O1-C1-C2-O2
8	D	803	PG4	O1-C1-C2-O2
8	F	803	PG4	O4-C7-C8-O5
10	C	805	PE4	O1-C1-C2-O2
11	H	808	PE5	O8-C15-C16-O52
5	E	803	P6G	O13-C14-C15-O16
9	B	802	7PE	O13-C14-C15-O16
9	B	802	7PE	O4-C5-C6-O7
11	H	808	PE5	O1-C1-C2-O2
9	D	808	7PE	O13-C14-C15-O16
10	C	805	PE4	O6-C10-C9-O5
3	A	802	1PE	OH5-C14-C24-OH4
6	F	806	PGE	O2-C3-C4-O3
10	C	805	PE4	O7-C13-C14-O8
3	C	801	1PE	OH7-C16-C26-OH6
6	C	807	PGE	O1-C1-C2-O2
11	H	808	PE5	O4-C7-C8-O5
4	A	803	GOL	C1-C2-C3-O3
4	A	804	GOL	O1-C1-C2-C3
4	A	805	GOL	O1-C1-C2-C3
4	A	805	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	B	803	GOL	O1-C1-C2-C3
4	B	805	GOL	O1-C1-C2-C3
4	D	802	GOL	O1-C1-C2-C3
4	D	804	GOL	C1-C2-C3-O3
4	D	806	GOL	C1-C2-C3-O3
4	D	810	GOL	O1-C1-C2-C3
4	D	811	GOL	O1-C1-C2-C3
4	E	804	GOL	C1-C2-C3-O3
4	E	807	GOL	O1-C1-C2-C3
4	G	803	GOL	C1-C2-C3-O3
4	H	804	GOL	C1-C2-C3-O3
4	H	807	GOL	O1-C1-C2-C3
6	C	807	PGE	O3-C5-C6-O4
6	G	805	PGE	O2-C3-C4-O3
4	A	803	GOL	O2-C2-C3-O3
4	A	804	GOL	O1-C1-C2-O2
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	A	811	GOL	O2-C2-C3-O3
4	C	809	GOL	O2-C2-C3-O3
4	D	802	GOL	O1-C1-C2-O2
4	D	804	GOL	O1-C1-C2-O2
4	D	810	GOL	O1-C1-C2-O2
4	D	810	GOL	O2-C2-C3-O3
4	D	811	GOL	O1-C1-C2-O2
4	D	811	GOL	O2-C2-C3-O3
4	F	802	GOL	O2-C2-C3-O3
4	F	805	GOL	O1-C1-C2-O2
4	G	803	GOL	O2-C2-C3-O3
4	H	807	GOL	O1-C1-C2-O2
5	A	806	P6G	C11-C12-O13-C14
9	B	802	7PE	O10-C11-C12-O13
5	A	806	P6G	O1-C2-C3-O4
6	G	805	PGE	O1-C1-C2-O2
9	B	802	7PE	O1-C2-C3-O4
6	A	812	PGE	O2-C3-C4-O3
3	A	802	1PE	OH4-C13-C23-OH3
8	F	803	PG4	O1-C1-C2-O2
5	A	806	P6G	O7-C8-C9-O10
3	E	802	1PE	OH6-C15-C25-OH5
5	A	806	P6G	O16-C17-C18-O19
4	A	811	GOL	O1-C1-C2-O2
4	B	804	GOL	O1-C1-C2-O2
4	B	805	GOL	O1-C1-C2-O2
4	F	804	GOL	O1-C1-C2-O2
5	E	803	P6G	O7-C8-C9-O10
4	G	803	GOL	O1-C1-C2-C3
9	B	802	7PE	C6-C5-O4-C3
8	H	803	PG4	O1-C1-C2-O2
11	H	808	PE5	C48-C50-O1-C1
5	A	806	P6G	O4-C5-C6-O7
5	E	803	P6G	O16-C17-C18-O19
9	B	802	7PE	C5-C6-O7-C8
4	A	803	GOL	O1-C1-C2-O2
4	A	807	GOL	O1-C1-C2-O2
4	B	805	GOL	O2-C2-C3-O3
4	B	808	GOL	O1-C1-C2-O2
4	D	804	GOL	O2-C2-C3-O3
4	D	809	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	D	809	GOL	O2-C2-C3-O3
4	G	802	GOL	O1-C1-C2-O2
4	H	804	GOL	O2-C2-C3-O3
3	A	802	1PE	C23-C13-OH4-C24
10	C	805	PE4	C4-C3-O2-C2
11	H	808	PE5	C9-C10-O6-C11
3	A	802	1PE	C13-C23-OH3-C22
3	A	802	1PE	C24-C14-OH5-C25
11	H	808	PE5	C10-C9-O5-C8
4	A	810	GOL	C1-C2-C3-O3
3	A	802	1PE	C16-C26-OH6-C15
6	F	806	PGE	C6-C5-O3-C4
8	B	801	PG4	C3-C4-O3-C5
5	A	806	P6G	C5-C6-O7-C8
3	A	802	1PE	OH2-C12-C22-OH3
3	E	802	1PE	C23-C13-OH4-C24
3	A	802	1PE	C14-C24-OH4-C13
5	E	803	P6G	C12-C11-O10-C9
11	H	808	PE5	C12-C11-O6-C10
6	G	805	PGE	C1-C2-O2-C3
11	H	808	PE5	C5-C6-O4-C7
9	B	802	7PE	O7-C8-C9-O10
11	H	808	PE5	C4-C3-O2-C2
11	H	808	PE5	C11-C12-O7-C13
5	E	803	P6G	O1-C2-C3-O4
8	H	803	PG4	O4-C7-C8-O5
11	H	808	PE5	O2-C3-C4-O3
3	C	801	1PE	C25-C15-OH6-C26
3	E	802	1PE	C16-C26-OH6-C15
5	E	803	P6G	C6-C5-O4-C3
2	A	801	IFM	C1-C5-C6-O6
10	C	805	PE4	C13-C14-O8-C15
3	C	801	1PE	C12-C22-OH3-C23
3	E	802	1PE	C12-C22-OH3-C23
9	B	802	7PE	C2-C3-O4-C5
11	H	808	PE5	C13-C14-O8-C15
8	D	803	PG4	C8-C7-O4-C6
11	H	808	PE5	O6-C11-C12-O7
3	E	802	1PE	C14-C24-OH4-C13
5	A	806	P6G	C12-C11-O10-C9
5	A	806	P6G	C15-C14-O13-C12
11	H	808	PE5	C7-C8-O5-C9

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Mol	Chain	Res	Type	Atoms
4	B	803	GOL	O1-C1-C2-O2
3	A	802	1PE	OH6-C15-C25-OH5
6	F	806	PGE	C4-C3-O2-C2
8	H	803	PG4	O2-C3-C4-O3
5	E	803	P6G	C2-C3-O4-C5
6	A	812	PGE	O3-C5-C6-O4
6	A	812	PGE	C4-C3-O2-C2
11	H	808	PE5	C14-C13-O7-C12
11	H	808	PE5	O3-C5-C6-O4
9	D	808	7PE	C18-C17-O16-C15
11	H	808	PE5	C1-C2-O2-C3
5	E	803	P6G	O4-C5-C6-O7
6	F	806	PGE	C1-C2-O2-C3
8	F	803	PG4	C5-C6-O4-C7
6	C	807	PGE	C3-C4-O3-C5
4	A	803	GOL	O1-C1-C2-C3
8	H	803	PG4	C8-C7-O4-C6
5	E	803	P6G	C11-C12-O13-C14
8	B	801	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	C3-C4-O3-C5
3	E	802	1PE	C24-C14-OH5-C25
4	A	807	GOL	O2-C2-C3-O3
5	E	803	P6G	O10-C11-C12-O13
8	H	803	PG4	C1-C2-O2-C3
8	F	803	PG4	C4-C3-O2-C2
4	D	807	GOL	O2-C2-C3-O3
4	E	806	GOL	O1-C1-C2-O2
8	F	803	PG4	O2-C3-C4-O3
4	D	805	GOL	O2-C2-C3-O3
8	B	801	PG4	O3-C5-C6-O4
5	A	806	P6G	O13-C14-C15-O16
4	A	810	GOL	O2-C2-C3-O3
4	D	806	GOL	O2-C2-C3-O3
6	G	805	PGE	C4-C3-O2-C2
8	D	803	PG4	C6-C5-O3-C4
10	C	805	PE4	C6-C5-O3-C4

All (2) ring outliers are listed below:

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Mol	Chain	Res	Type	Atoms
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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

47 monomers are involved in 116 short contacts:

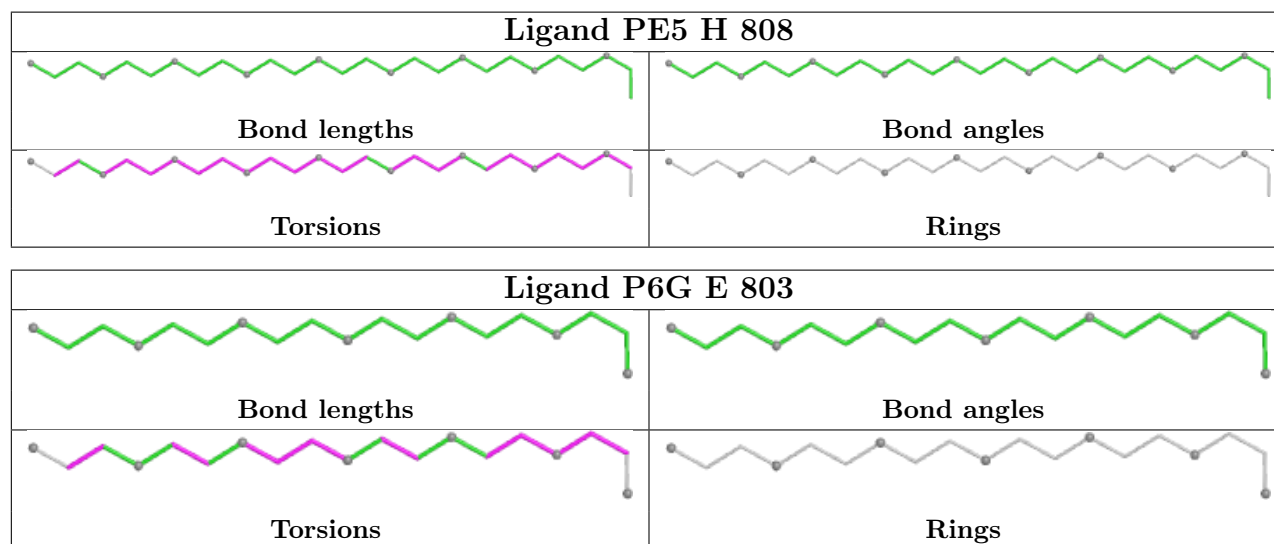
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	803	GOL	1	0
4	D	802	GOL	1	0
4	D	805	GOL	2	0
4	G	802	GOL	1	0
4	G	803	GOL	2	0
2	D	801	IFM	3	0
11	H	808	PE5	12	0
4	B	808	GOL	1	0
4	D	812	GOL	2	0
3	E	802	1PE	2	0
6	F	806	PGE	2	0
2	H	801	IFM	1	0
4	H	802	GOL	2	0
4	B	807	GOL	1	0
4	H	805	GOL	2	0
4	D	804	GOL	2	0
4	A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

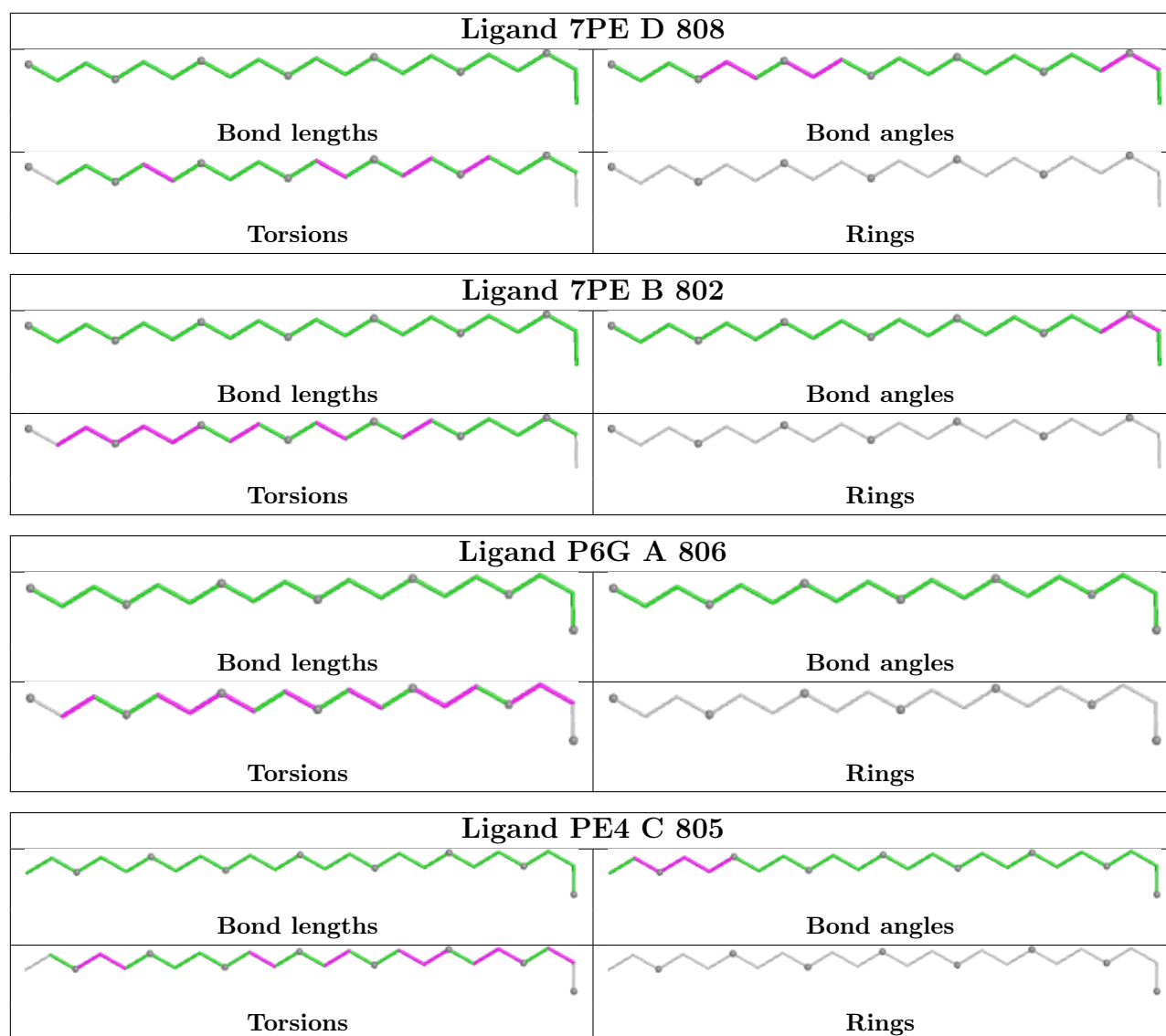
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	801	IFM	2	0
4	E	805	GOL	1	0
4	F	805	GOL	1	0
4	C	806	GOL	1	0
4	H	804	GOL	2	0
5	A	806	P6G	4	0
10	C	805	PE4	6	0
4	B	805	GOL	1	0
4	A	808	GOL	3	0
4	B	803	GOL	2	0
4	A	805	GOL	3	0
6	A	812	PGE	7	0

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%)	-0.35	7 (0%) 81 82	30, 40, 65, 98	0
1	B	761/769 (98%)	-0.35	6 (0%) 82 83	28, 40, 64, 97	0
1	C	761/769 (98%)	-0.31	7 (0%) 81 82	28, 40, 64, 99	0
1	D	761/769 (98%)	-0.38	6 (0%) 82 83	28, 39, 68, 97	0
1	E	761/769 (98%)	0.23	39 (5%) 33 35	35, 53, 101, 142	0
1	F	761/769 (98%)	0.10	26 (3%) 48 50	32, 49, 86, 131	0
1	G	762/769 (99%)	0.11	14 (1%) 67 69	38, 52, 83, 110	0
1	H	761/769 (98%)	-0.02	12 (1%) 70 72	37, 50, 85, 115	0
All	All	6090/6152 (98%)	-0.12	117 (1%) 66 68	28, 46, 80, 142	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	752	LEU	6.7
1	G	762	LEU	6.6
1	F	98	ALA	6.0
1	C	98	ALA	5.9
1	F	26	ALA	5.8
1	A	762	LEU	5.4
1	E	229	LEU	5.0
1	C	1	MET	4.5
1	G	1	MET	4.5
1	D	98	ALA	4.4
1	D	1	MET	4.2
1	E	125	ILE	4.1
1	H	98	ALA	4.0
1	E	92	ILE	4.0
1	F	754	SER	4.0
1	E	751	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
1	F	752	LEU	3.5
1	E	693	GLY	3.5
1	F	660	ALA	3.5
1	F	757	ILE	3.4
1	H	757	ILE	3.4
1	G	210	ALA	3.4
1	A	749	LYS	3.4
1	E	98	ALA	3.3
1	G	661	VAL	3.3
1	F	743	LEU	3.3
1	B	659	GLU	3.2
1	B	98	ALA	3.2
1	E	150	ASP	3.2
1	C	97	ALA	3.1
1	A	1	MET	3.1
1	E	1	MET	3.1
1	A	2	HIS	3.1
1	F	741	LEU	3.0
1	E	124	THR	3.0
1	E	753	ASP	3.0
1	H	1	MET	3.0
1	G	741	LEU	2.9
1	F	761	ARG	2.9
1	E	86	VAL	2.9
1	D	97	ALA	2.8
1	E	231	ALA	2.8
1	E	149	SER	2.8
1	D	759	LYS	2.7
1	A	98	ALA	2.6
1	E	83	LEU	2.6
1	F	705	ALA	2.6
1	H	26	ALA	2.6
1	E	659	GLU	2.6
1	F	755	GLU	2.6
1	E	147	VAL	2.6
1	F	1	MET	2.6
1	F	720	LEU	2.6
1	F	706	TRP	2.6
1	F	658	ASN	2.5
1	G	98	ALA	2.5
1	E	2	HIS	2.5
1	E	208	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	G	660	ALA	2.5
1	F	504	LEU	2.5
1	H	258	LEU	2.5
1	H	660	ALA	2.5
1	H	760	SER	2.4
1	F	751	VAL	2.4
1	B	503	THR	2.4
1	F	503	THR	2.4
1	G	751	VAL	2.4
1	G	659	GLU	2.4
1	E	708	GLY	2.3
1	E	153	THR	2.3
1	E	228	SER	2.3
1	B	1	MET	2.3
1	F	2	HIS	2.3
1	F	759	LYS	2.3
1	G	190	LYS	2.3
1	E	738	ARG	2.3
1	C	16	ILE	2.3
1	F	114	LYS	2.3
1	G	83	LEU	2.3
1	E	658	ASN	2.3
1	E	657	THR	2.3
1	E	227	LEU	2.2
1	E	154	ASP	2.2
1	E	747	GLY	2.2
1	E	524	SER	2.2
1	E	16	ILE	2.2
1	D	661	VAL	2.2
1	F	702	LEU	2.2
1	E	261	LYS	2.2
1	E	156	VAL	2.2
1	H	759	LYS	2.2
1	E	66	ALA	2.2
1	F	400	LEU	2.1
1	C	694	ASP	2.1
1	A	657	THR	2.1
1	B	754	SER	2.1
1	F	742	THR	2.1
1	H	754	SER	2.1
1	H	741	LEU	2.1
1	E	91	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	264	GLN	2.1
1	C	232	GLY	2.1
1	E	232	GLY	2.1
1	D	657	THR	2.1
1	E	750	SER	2.1
1	C	231	ALA	2.1
1	A	727	GLU	2.1
1	H	27	ILE	2.1
1	F	715	VAL	2.1
1	E	118	ARG	2.1
1	E	726	LYS	2.0
1	H	658	ASN	2.0
1	E	21	TYR	2.0
1	B	507	LYS	2.0
1	F	718	GLN	2.0
1	G	92	ILE	2.0
1	G	507	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	B	805	6/6	0.74	0.17	59,73,75,75	0
4	GOL	F	805	6/6	0.81	0.20	39,62,67,70	0
4	GOL	A	809	6/6	0.82	0.17	58,66,67,73	0
4	GOL	A	807	6/6	0.83	0.18	57,59,72,79	0
2	IFM	G	801	10/10	0.83	0.19	55,79,87,98	0
4	GOL	D	805	6/6	0.84	0.15	63,64,69,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	D	806	6/6	0.85	0.13	56,64,67,71	0
4	GOL	G	803	6/6	0.85	0.15	65,76,86,86	0
2	IFM	E	801	10/10	0.86	0.15	44,59,71,73	0
4	GOL	E	805	6/6	0.86	0.19	63,77,85,87	0
4	GOL	H	807	6/6	0.86	0.13	70,70,73,76	0
11	PE5	H	808	27/27	0.86	0.18	53,72,84,96	0
8	PG4	H	803	13/13	0.87	0.14	57,68,83,88	0
4	GOL	C	806	6/6	0.88	0.19	64,77,87,89	0
4	GOL	A	805	6/6	0.88	0.12	57,64,74,75	0
4	GOL	B	807	6/6	0.88	0.18	59,65,74,82	0
4	GOL	A	803	6/6	0.89	0.17	46,60,72,75	0
4	GOL	D	811	6/6	0.90	0.12	49,56,61,71	0
4	GOL	G	804	6/6	0.90	0.13	68,68,70,72	0
3	1PE	E	802	16/16	0.90	0.15	62,75,101,104	0
5	P6G	E	803	19/19	0.90	0.14	52,67,71,73	0
6	PGE	G	805	10/10	0.90	0.13	54,66,73,78	0
4	GOL	A	808	6/6	0.90	0.13	59,61,66,85	0
4	GOL	G	802	6/6	0.90	0.13	52,64,71,76	0
4	GOL	D	802	6/6	0.91	0.13	50,58,60,62	0
6	PGE	A	812	10/10	0.91	0.10	40,51,58,60	0
6	PGE	F	806	10/10	0.91	0.13	62,65,71,74	0
4	GOL	D	809	6/6	0.91	0.10	45,54,57,60	0
8	PG4	B	801	13/13	0.91	0.12	46,57,87,88	0
8	PG4	D	803	13/13	0.91	0.15	48,65,75,77	0
4	GOL	H	806	6/6	0.91	0.10	48,62,65,73	0
10	PE4	C	805	24/24	0.91	0.12	39,48,59,68	0
3	1PE	A	802	16/16	0.91	0.15	50,62,83,101	0
3	1PE	C	801	16/16	0.92	0.12	44,61,79,82	0
4	GOL	D	812	6/6	0.92	0.10	32,38,40,45	0
2	IFM	H	801	10/10	0.92	0.14	56,70,75,82	0
2	IFM	F	801	10/10	0.93	0.13	49,56,65,72	0
4	GOL	H	805	6/6	0.93	0.11	51,52,59,60	0
6	PGE	C	807	10/10	0.93	0.09	42,51,57,59	0
9	7PE	B	802	21/21	0.93	0.10	36,45,52,55	0
9	7PE	D	808	21/21	0.93	0.11	41,48,54,59	0
4	GOL	A	804	6/6	0.93	0.10	42,43,46,52	0
4	GOL	F	802	6/6	0.93	0.11	52,58,61,65	0
4	GOL	E	804	6/6	0.94	0.13	54,59,62,63	0
5	P6G	A	806	19/19	0.94	0.11	41,49,64,70	0
8	PG4	F	803	13/13	0.94	0.10	56,62,75,77	0
4	GOL	B	806	6/6	0.94	0.13	57,64,70,77	0
4	GOL	E	806	6/6	0.94	0.08	46,47,50,54	0

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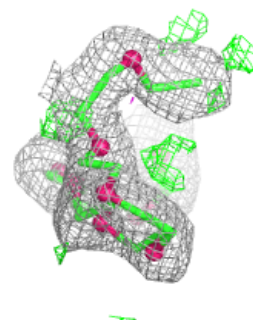
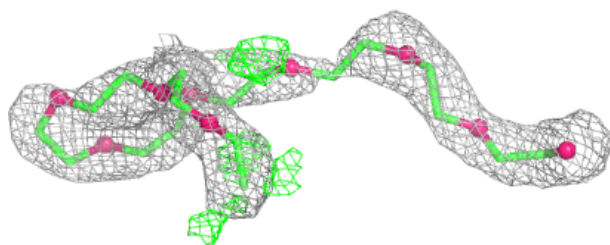
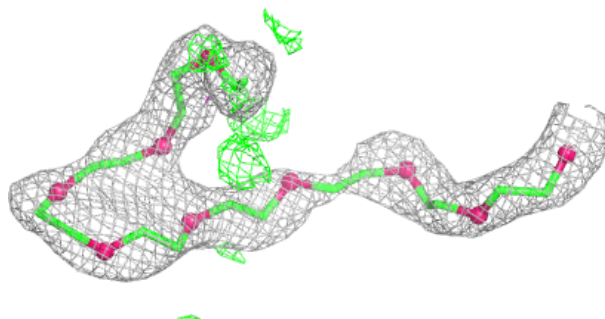
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	H	802	6/6	0.94	0.11	58,73,84,85	0
2	IFM	A	801	10/10	0.94	0.12	38,51,60,62	0
4	GOL	D	807	6/6	0.94	0.13	55,64,71,72	0
4	GOL	C	809	6/6	0.95	0.11	37,42,49,52	0
4	GOL	B	808	6/6	0.95	0.09	36,43,46,48	0
4	GOL	H	804	6/6	0.95	0.09	46,52,57,61	0
4	GOL	D	804	6/6	0.95	0.09	47,54,57,62	0
4	GOL	B	804	6/6	0.95	0.09	33,35,40,47	0
2	IFM	D	801	10/10	0.96	0.09	35,44,50,63	0
4	GOL	A	811	6/6	0.96	0.09	45,50,51,51	0
4	GOL	E	807	6/6	0.96	0.08	43,53,60,60	0
4	GOL	C	802	6/6	0.96	0.11	43,57,62,73	0
4	GOL	F	804	6/6	0.96	0.08	47,48,50,53	0
4	GOL	C	804	6/6	0.96	0.07	43,46,53,57	0
4	GOL	B	803	6/6	0.96	0.08	35,41,44,46	0
4	GOL	D	810	6/6	0.97	0.08	33,37,40,41	0
4	GOL	C	803	6/6	0.97	0.07	45,48,52,59	0
4	GOL	C	808	6/6	0.97	0.07	35,38,39,42	0
4	GOL	A	810	6/6	0.97	0.06	37,37,39,40	0
7	CA	D	813	1/1	0.98	0.04	54,54,54,54	0
7	CA	D	814	1/1	0.98	0.03	45,45,45,45	0
7	CA	E	808	1/1	0.99	0.02	54,54,54,54	0
7	CA	G	806	1/1	0.99	0.03	55,55,55,55	0
7	CA	C	810	1/1	0.99	0.02	36,36,36,36	0
7	CA	A	813	1/1	0.99	0.03	44,44,44,44	0
7	CA	B	809	1/1	0.99	0.03	43,43,43,43	0

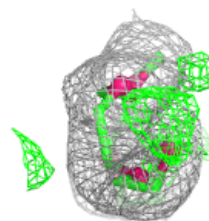
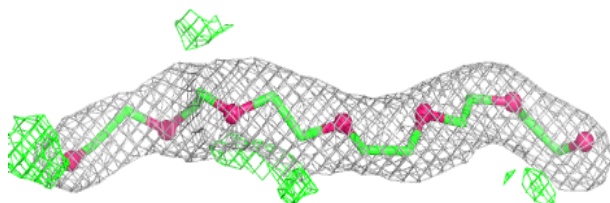
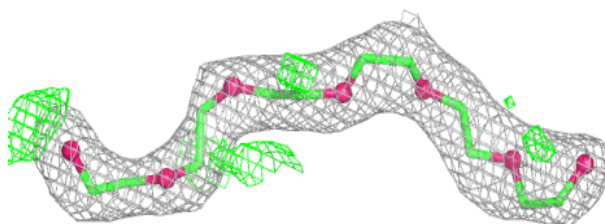
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

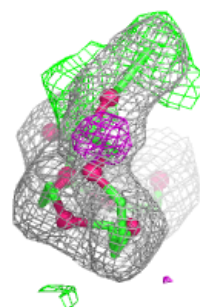
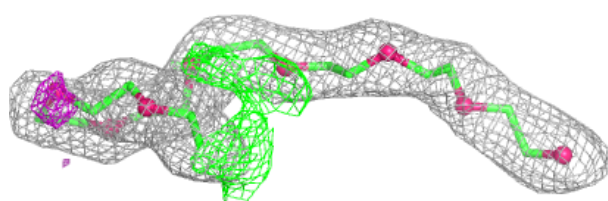
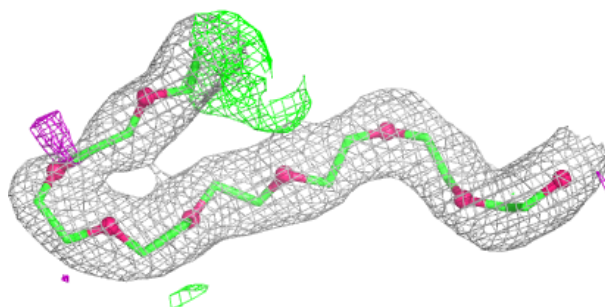
**Electron density around P6G E 803:**

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

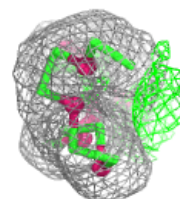
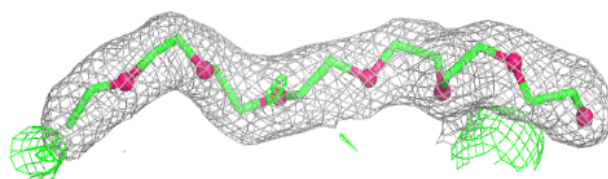
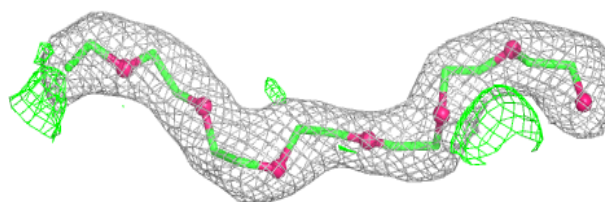


Electron density around PE4 C 805:

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

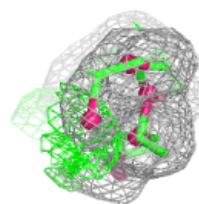
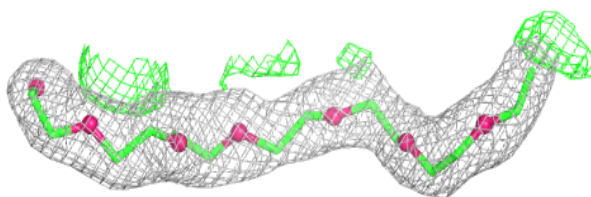
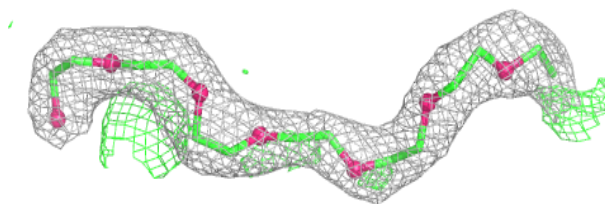
**Electron density around 7PE B 802:**

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

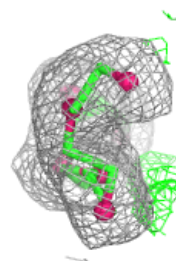
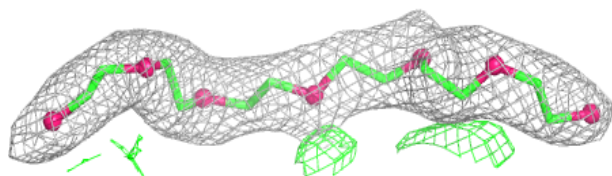
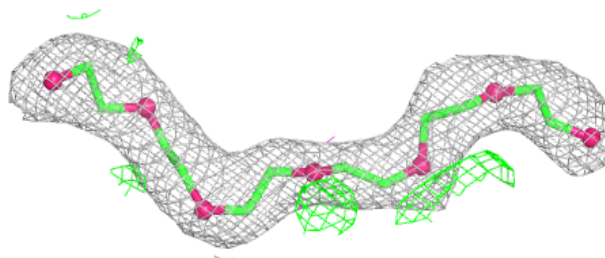


Electron density around 7PE D 808:

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

**Electron density around 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.