Full wwPDB X-ray Structure Validation Report (i)

Aug 4, 2026 – 05:07 AM EDT

PDB ID	:	5BV2 / pdb_00005bv2
Title	:	Crystal structure of E. coli HPII catalase variant
Authors	:	Wang, J.; Lomkalin, I.V.
Deposited on	:	2015-06-04
Resolution	:	1.53 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 (i) 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 (i)) were used in the production of this report:

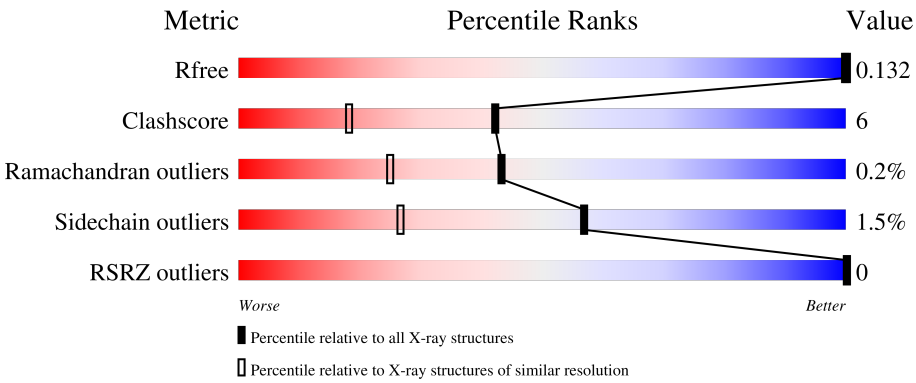
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.53 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	1003 (1.54-1.54)
Clashscore	190562	1025 (1.54-1.54)
Ramachandran outliers	187476	1007 (1.54-1.54)
Sidechain outliers	187428	1007 (1.54-1.54)
RSRZ outliers	180081	1002 (1.54-1.54)

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

Mol	Chain	Length	Quality of chain
1	P	753	91% 8% •
1	Q	753	91% 8% •
1	R	753	91% 8% •
1	S	753	91% 7% ••

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
2	HDD	P	801	X	-	-	-
2	HDD	Q	801	X	-	-	-
2	HDD	R	801	X	-	-	-
2	HDD	S	801	X	-	-	-
3	GOL	P	802	-	-	X	-
3	GOL	R	802	-	-	X	-
3	GOL	S	802	-	-	X	-
5	PGE	R	807	-	-	X	-
6	PEG	P	814	-	-	X	-
6	PEG	P	817	-	-	X	-

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 53930 atoms, of which 24516 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 Catalase HPII.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	P	747	11980	3836	5945	1059	1125	15	103	23	0
1	Q	746	12077	3864	6005	1065	1128	15	106	29	0
1	R	747	11933	3824	5920	1050	1124	15	106	23	0
1	S	747	12118	3875	6028	1069	1131	15	107	32	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	99	ASP	SER	conflict	UNP P21179
P	283	SER	GLU	conflict	UNP P21179
P	372	ASN	LYS	conflict	UNP P21179
P	565	SER	GLU	conflict	UNP P21179
P	710	VAL	ILE	conflict	UNP P21179
P	750	SER	LYS	conflict	UNP P21179
Q	99	ASP	SER	conflict	UNP P21179
Q	283	SER	GLU	conflict	UNP P21179
Q	372	ASN	LYS	conflict	UNP P21179
Q	565	SER	GLU	conflict	UNP P21179
Q	710	VAL	ILE	conflict	UNP P21179
Q	750	SER	LYS	conflict	UNP P21179
R	99	ASP	SER	conflict	UNP P21179
R	283	SER	GLU	conflict	UNP P21179
R	372	ASN	LYS	conflict	UNP P21179
R	565	SER	GLU	conflict	UNP P21179
R	710	VAL	ILE	conflict	UNP P21179
R	750	SER	LYS	conflict	UNP P21179
S	99	ASP	SER	conflict	UNP P21179
S	283	SER	GLU	conflict	UNP P21179
S	372	ASN	LYS	conflict	UNP P21179

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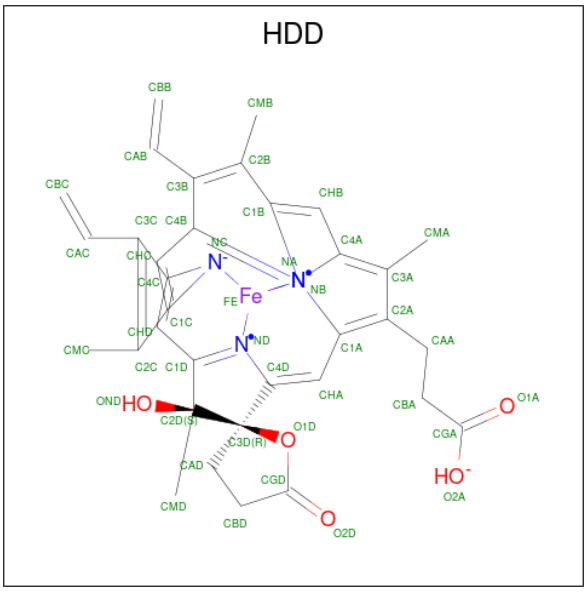
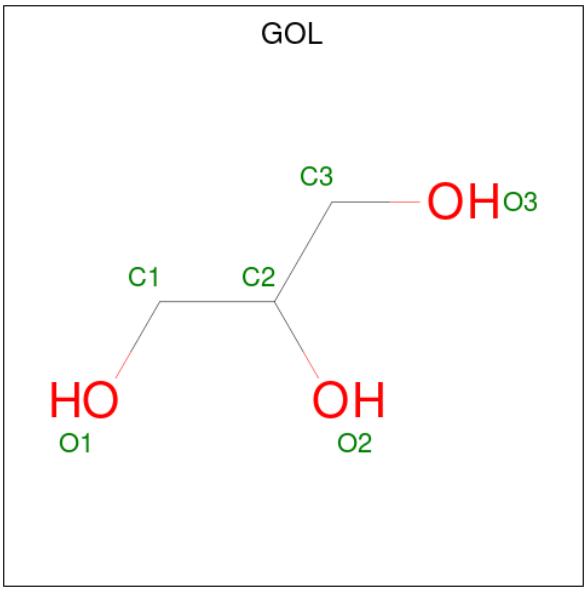
Chain	Residue	Modelled	Actual	Comment	Reference
S	565	SER	GLU	conflict	UNP P21179
S	710	VAL	ILE	conflict	UNP P21179
S	750	SER	LYS	conflict	UNP P21179

- Molecule 2 is CIS-HEME D HYDROXYCHLORIN GAMMA-SPIROLACTONE (CCD ID: HDD) (formula: $C_{34}H_{32}FeN_4O_5$).



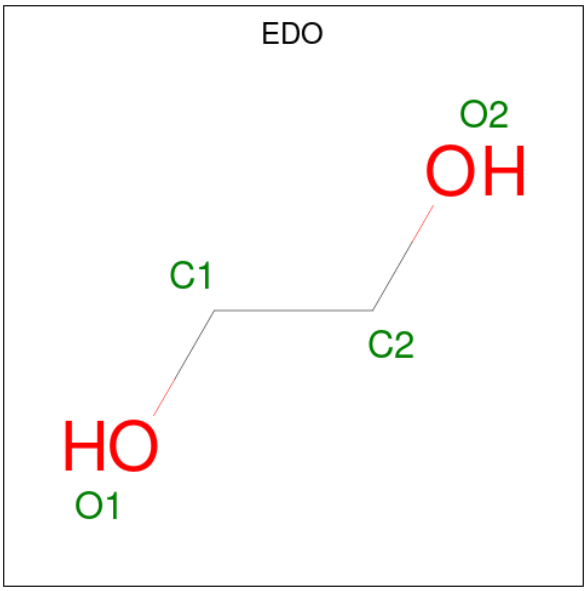
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Fe	H	N	O		
2	P	1	75	34	1	31	4	5	1	0
			Total	C	Fe	H	N	O		
2	Q	1	75	34	1	31	4	5	1	0
			Total	C	Fe	H	N	O		
2	R	1	75	34	1	31	4	5	1	0
			Total	C	Fe	H	N	O		
2	S	1	75	34	1	31	4	5	1	0

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
3	P	1	14	3	8	3	0	0
3	P	1	14	3	8	3	2	0
3	Q	1	14	3	8	3	0	0
3	Q	1	14	3	8	3	2	0
3	Q	1	14	3	8	3	2	0
3	R	1	14	3	8	3	0	0
3	R	1	14	3	8	3	2	0
3	R	1	14	3	8	3	2	0
3	S	1	14	3	8	3	0	0
3	S	1	14	3	8	3	2	0
3	S	1	14	3	8	3	2	0

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
4	P	1	10	2	6	2	1	0
4	P	1	10	2	6	2	1	0
4	P	1	10	2	6	2	1	0
4	P	1	10	2	6	2	1	0
4	P	1	10	2	6	2	1	0
4	P	1	10	2	6	2	1	0
4	P	1	10	2	6	2	1	0
4	P	1	10	2	6	2	1	0
4	P	1	10	2	6	2	0	0
4	Q	1	10	2	6	2	1	0
4	Q	1	10	2	6	2	1	0
4	Q	1	10	2	6	2	1	0
4	Q	1	10	2	6	2	1	0
4	Q	1	10	2	6	2	1	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
4	Q	1	10	2	6	2	1	0
			Total	C	H	O		
4	Q	1	10	2	6	2	1	0
			Total	C	H	O		
4	Q	1	10	2	6	2	1	0
			Total	C	H	O		
4	Q	1	10	2	6	2	1	0
			Total	C	H	O		
4	Q	1	10	2	6	2	1	0
			Total	C	H	O		
4	Q	1	10	2	6	2	1	0
			Total	C	H	O		
4	Q	1	10	2	6	2	1	0
			Total	C	H	O		
4	Q	1	10	2	6	2	1	0
			Total	C	H	O		
4	Q	1	10	2	6	2	1	0
			Total	C	H	O		
4	Q	1	10	2	6	2	1	0
			Total	C	H	O		
4	Q	1	10	2	6	2	1	0
			Total	C	H	O		
4	Q	1	10	2	6	2	1	0
			Total	C	H	O		
4	R	1	10	2	6	2	1	0
			Total	C	H	O		
4	R	1	10	2	6	2	1	0
			Total	C	H	O		
4	R	1	10	2	6	2	1	0
			Total	C	H	O		
4	R	1	10	2	6	2	1	0
			Total	C	H	O		
4	S	1	10	2	6	2	1	0
			Total	C	H	O		
4	S	1	10	2	6	2	1	0
			Total	C	H	O		
4	S	1	10	2	6	2	1	0
			Total	C	H	O		
4	S	1	10	2	6	2	1	0
			Total	C	H	O		
4	S	1	10	2	6	2	1	0

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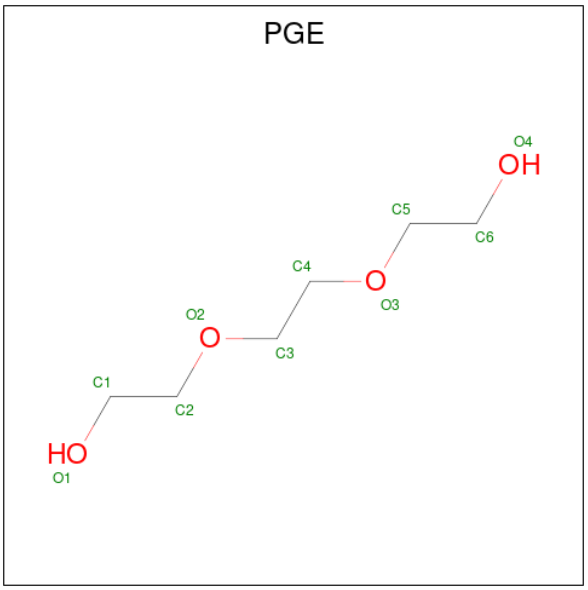
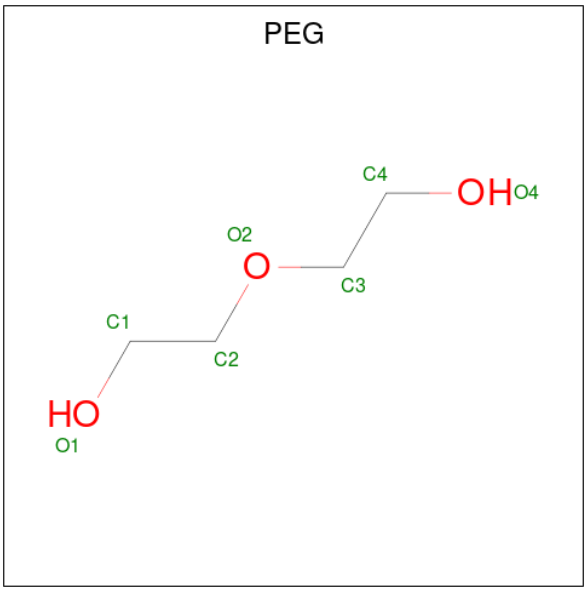
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
4	S	1	10	2	6	2	1	0
			Total	C	H	O		
4	S	1	10	2	6	2	1	0
			Total	C	H	O		
4	S	1	10	2	6	2	1	0
			Total	C	H	O		
4	S	1	10	2	6	2	1	0

- Molecule 5 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



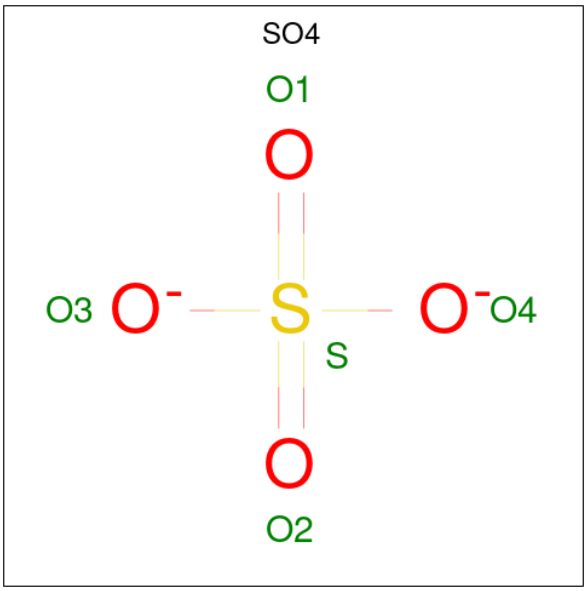
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
5	P	1	24	6	14	4	1	0
			Total	C	H	O		
5	R	1	24	6	14	4	1	0
			Total	C	H	O		
5	R	1	24	6	14	4	1	0

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
6	P	1	17	4	10	3	1	0
			Total	C	H	O		
6	P	1	17	4	10	3	1	0
			Total	C	H	O		
6	P	1	17	4	10	3	1	0
			Total	C	H	O		
6	P	1	17	4	10	3	1	0
			Total	C	H	O		
6	Q	1	17	4	10	3	1	0
			Total	C	H	O		
6	Q	1	17	4	10	3	1	0
			Total	C	H	O		
6	Q	1	17	4	10	3	1	0
			Total	C	H	O		
6	Q	1	17	4	10	3	1	0
			Total	C	H	O		
6	S	1	17	4	10	3	1	0
			Total	C	H	O		
6	S	1	17	4	10	3	1	0

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O_4S).

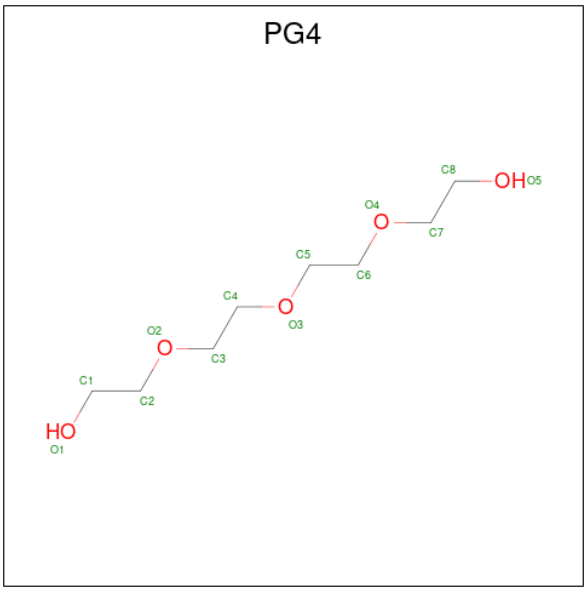


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	P	1	Total O S 5 4 1	0	0
7	S	1	Total O S 5 4 1	0	0

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	R	1	Total Mg 1 1	0	0
8	S	1	Total Mg 1 1	0	0

- Molecule 9 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
9	R	1	31	8	18	5	1	0

- Molecule 10 is water.

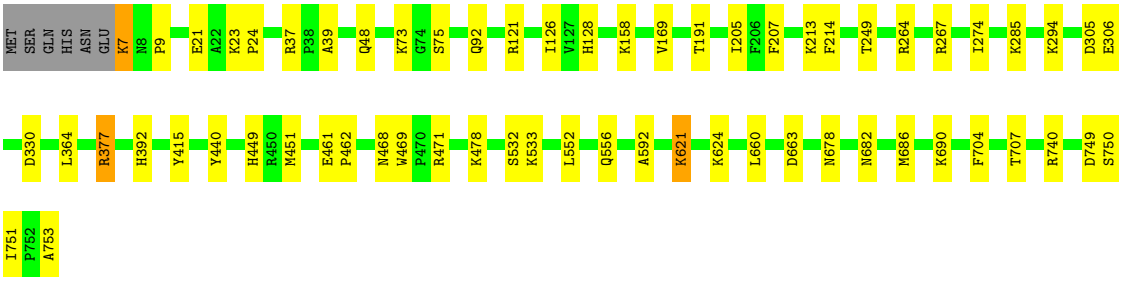
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O			
10	P	1171	1171	1171		0	0
			Total	O			
10	Q	1196	1196	1196		0	0
			Total	H	O		
10	R	1087	1093	6	1087	5	0
			Total	H	O		
10	S	1227	1233	6	1227	5	0

3 Residue-property plots (i)

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

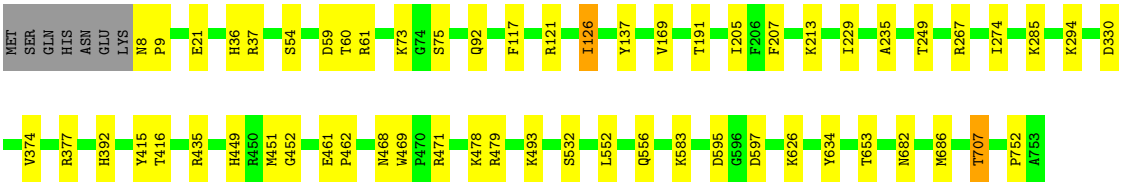
• Molecule 1: Catalase HPII

Chain P:



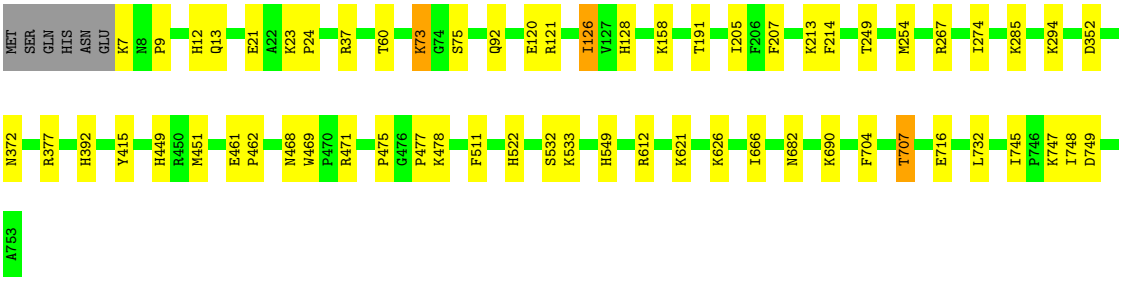
• Molecule 1: Catalase HPII

Chain Q:



• Molecule 1: Catalase HPII

Chain R:



• Molecule 1: Catalase HPII

Chain S:

MET
SER
GLN
HIS
ASN
GLU
K7
N8
P9
E21
D27
R37
T60
K73
G74
S75
Q92
F117
R121
I126
V127
H128
K142
F152
T168
V169
T191
I205
F206
F207
K213
F214
I229
T249
L250
H251
R267
I274
K285
K294
V303
R313
E335
R369
R377
H392
Y415
T416
H449
R450
M451
E461
P462
N468
W469
P470
R471
G476
P477
K478
R479
S532
H549
L552
Q556
L571
D597
K621
K631
Y634
T653
N682
M686
T707
D725
G726
S727
F728
A753

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	161.79Å 171.33Å 122.48Å 90.00° 121.55° 90.00°	Depositor
Resolution (Å)	50.00 – 1.53 50.00 – 1.53	Depositor EDS
% Data completeness (in resolution range)	71.8 (50.00-1.53) 71.8 (50.00-1.53)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.17 (at 1.53Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.082 , 0.132 0.082 , 0.132	Depositor DCC
R_{free} test set	15186 reflections (3.57%)	wwPDB-VP
Wilson B-factor (Å^2)	13.3	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 58.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.99	EDS
Total number of atoms	53930	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.81% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PG4, PEG, MG, SO4, HDD, PGE, GOL, EDO

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	P	0.56	0/6270	0.71	0/8523
1	Q	0.56	0/6331	0.72	1/8607 (0.0%)
1	R	0.55	0/6245	0.71	0/8485
1	S	0.55	0/6349	0.74	5/8622 (0.1%)
All	All	0.55	0/25195	0.72	6/34237 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	S	726[A]	GLY	CA-C-N	7.72	135.60	121.70
1	S	726[A]	GLY	C-N-CA	7.72	135.60	121.70
1	S	726[B]	GLY	CA-C-N	7.72	135.60	121.70
1	S	726[B]	GLY	C-N-CA	7.72	135.60	121.70
1	S	631	LYS	CB-CA-C	-5.96	100.27	110.16
1	Q	330	ASP	CB-CA-C	-5.30	104.16	112.12

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	P	6035	5945	5939	85	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Q	6072	6005	6007	74	0
1	R	6013	5920	5914	79	1
1	S	6090	6028	6030	82	0
2	P	44	31	31	4	0
2	Q	44	31	31	3	0
2	R	44	31	31	4	0
2	S	44	31	31	5	0
3	P	12	16	16	6	0
3	Q	18	24	24	1	0
3	R	18	24	23	13	0
3	S	18	24	24	4	0
4	P	36	54	54	6	0
4	Q	68	102	102	5	2
4	R	16	24	24	1	0
4	S	36	54	54	4	0
5	P	10	14	14	0	0
5	R	20	28	28	7	0
6	P	28	40	40	20	0
6	Q	28	40	40	3	0
6	S	14	20	20	3	0
7	P	5	0	0	0	0
7	S	5	0	0	0	0
8	R	1	0	0	0	0
8	S	1	0	0	0	0
9	R	13	18	18	0	0
10	P	1171	0	0	28	0
10	Q	1196	0	0	21	0
10	R	1087	6	0	27	1
10	S	1227	6	0	38	0
All	All	29414	24516	24495	312	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (312) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:449[B]:HIS:CD2	1:Q:451[B]:MET:CE	1.77	1.61
1:Q:392:HIS:ND1	1:Q:415:TYR:CB	1.86	1.38
1:S:392:HIS:ND1	1:S:415:TYR:CB	1.86	1.36
1:R:392:HIS:ND1	1:R:415:TYR:CB	1.87	1.35

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:392:HIS:ND1	1:P:415:TYR:CB	1.88	1.35
1:P:392:HIS:ND1	1:P:415:TYR:HB2	0.94	1.26
1:Q:449[B]:HIS:NE2	1:Q:451[B]:MET:HE1	1.50	1.26
1:Q:392:HIS:ND1	1:Q:415:TYR:HB2	0.92	1.25
1:R:392:HIS:ND1	1:R:415:TYR:HB2	0.94	1.24
1:Q:449[B]:HIS:CD2	1:Q:451[B]:MET:HE3	1.51	1.23
1:S:392:HIS:ND1	1:S:415:TYR:HB2	0.93	1.23
1:Q:449[B]:HIS:NE2	1:Q:451[B]:MET:CE	2.01	1.20
1:P:449[A]:HIS:CE1	10:P:902:HOH:O	1.95	1.18
6:P:814:PEG:H21	10:S:1356:HOH:O	1.42	1.17
1:R:449[A]:HIS:CE1	10:R:902:HOH:O	1.97	1.14
1:S:377[B]:ARG:HH11	1:S:377[B]:ARG:HG2	1.05	1.14
1:P:663:ASP:OD1	6:P:817:PEG:H31	1.48	1.12
1:Q:392:HIS:CE1	1:Q:415:TYR:HB2	1.87	1.10
1:Q:451[A]:MET:HE2	1:S:451[A]:MET:HE2	1.30	1.10
1:S:392:HIS:CE1	1:S:415:TYR:HB2	1.85	1.09
1:S:449[A]:HIS:CE1	10:S:905:HOH:O	2.03	1.09
1:R:392:HIS:CE1	1:R:415:TYR:HB2	1.87	1.09
1:P:392:HIS:CE1	1:P:415:TYR:HB2	1.88	1.09
1:Q:449[B]:HIS:CE1	10:Q:908:HOH:O	2.04	1.09
1:R:377[B]:ARG:HG2	1:R:377[B]:ARG:HH11	1.06	1.08
1:Q:449[B]:HIS:CD2	1:Q:451[B]:MET:HE2	1.72	1.07
1:P:451[A]:MET:HE2	1:R:451[A]:MET:HE2	1.31	1.06
1:P:740:ARG:HE	6:P:817:PEG:H41	1.23	1.02
1:Q:449[B]:HIS:HE2	1:Q:451[B]:MET:HE1	1.27	0.97
1:Q:377[B]:ARG:HH21	1:Q:377[B]:ARG:HG2	1.31	0.95
1:P:740:ARG:HE	6:P:817:PEG:C4	1.81	0.93
1:S:377[B]:ARG:HG2	1:S:377[B]:ARG:NH1	1.77	0.92
1:Q:449[B]:HIS:HD2	1:Q:451[B]:MET:CE	1.44	0.90
1:P:377[A]:ARG:HG2	1:P:377[A]:ARG:HH21	1.36	0.89
1:S:191[B]:THR:HG21	10:S:1520:HOH:O	1.71	0.89
1:P:682:ASN:OD1	1:P:707[B]:THR:HG21	1.73	0.88
1:P:478:LYS:NZ	10:P:901:HOH:O	1.93	0.88
1:S:377[B]:ARG:NE	10:S:901:HOH:O	1.95	0.88
1:Q:682:ASN:OD1	1:Q:707[A]:THR:HG21	1.75	0.87
1:R:267:ARG:CZ	10:R:937:HOH:O	2.22	0.87
1:P:663:ASP:OD1	6:P:817:PEG:C3	2.23	0.87
1:S:682:ASN:OD1	1:S:707[A]:THR:HG21	1.74	0.87
1:R:377[B]:ARG:HG2	1:R:377[B]:ARG:NH1	1.84	0.86
1:P:267[C]:ARG:NH1	10:P:903:HOH:O	2.09	0.86
1:S:37[A]:ARG:NH1	10:S:903:HOH:O	2.10	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:152:PHE:HB3	1:S:191[B]:THR:HG23	1.60	0.82
1:Q:435[B]:ARG:NH2	10:Q:906:HOH:O	2.15	0.79
1:R:449[A]:HIS:NE2	10:R:902:HOH:O	2.08	0.79
1:P:449[A]:HIS:NE2	10:P:902:HOH:O	2.05	0.79
1:R:745:ILE:HG12	5:R:807:PGE:H2	1.67	0.76
1:S:267[B]:ARG:NH2	10:S:906:HOH:O	2.17	0.76
1:S:377[B]:ARG:HH11	1:S:377[B]:ARG:CG	1.89	0.76
1:S:552:LEU:HD11	1:S:571:LEU:HD23	1.67	0.76
1:S:191[B]:THR:HG22	10:S:1063:HOH:O	1.86	0.75
1:P:740:ARG:NE	6:P:817:PEG:H41	2.01	0.75
1:S:37[A]:ARG:NE	10:S:903:HOH:O	2.19	0.75
4:S:805:EDO:H22	10:S:910:HOH:O	1.88	0.74
1:R:294:LYS:HG2	10:R:1602:HOH:O	1.87	0.73
1:P:753:ALA:O	6:P:814:PEG:H22	1.89	0.72
1:S:37[A]:ARG:CZ	10:S:903:HOH:O	2.38	0.72
1:Q:435[B]:ARG:CZ	10:Q:906:HOH:O	2.38	0.72
1:S:229:ILE:HG22	6:S:816:PEG:H21	1.71	0.71
1:S:532[A]:SER:OG	10:S:902:HOH:O	2.04	0.71
1:Q:294[C]:LYS:HG2	10:Q:1640:HOH:O	1.91	0.70
1:R:377[B]:ARG:HH11	1:R:377[B]:ARG:CG	1.96	0.69
1:Q:532[A]:SER:OG	10:Q:902:HOH:O	2.06	0.69
1:Q:449[B]:HIS:HD2	1:Q:451[B]:MET:HE3	1.07	0.69
1:Q:59:ASP:OD1	10:Q:903:HOH:O	2.11	0.68
1:Q:449[B]:HIS:CD2	1:Q:451[B]:MET:HE1	1.91	0.68
1:R:532[A]:SER:OG	10:R:903:HOH:O	2.10	0.68
1:S:449[A]:HIS:NE2	10:S:905:HOH:O	2.15	0.67
1:S:294:LYS:HG2	10:S:1653:HOH:O	1.96	0.66
10:Q:916:HOH:O	1:S:73[A]:LYS:HE3	1.95	0.66
2:S:801:HDD:C1B	3:S:802:GOL:H31	2.25	0.66
1:S:27[B]:ASP:OD2	10:S:904:HOH:O	2.12	0.66
1:Q:137:TYR:CE1	1:Q:374[B]:VAL:CG1	2.78	0.65
1:P:532[A]:SER:OG	10:P:904:HOH:O	2.11	0.65
1:P:294[A]:LYS:HG2	10:P:1627:HOH:O	1.96	0.65
1:S:152:PHE:HB3	1:S:191[B]:THR:CG2	2.28	0.64
1:P:624:LYS:HD3	10:P:1916:HOH:O	1.97	0.64
1:P:294[B]:LYS:HG2	10:P:1627:HOH:O	1.97	0.64
1:S:726[A]:GLY:HA3	1:S:728:PHE:H	1.59	0.64
1:P:449[B]:HIS:CG	1:R:449[B]:HIS:CG	2.47	0.63
1:R:748:ILE:HD11	5:R:807:PGE:H22	1.80	0.63
1:P:469:TRP:CE3	1:P:471:ARG:HG3	2.34	0.63
1:P:23:LYS:HA	10:P:972:HOH:O	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:749:ASP:OD1	4:R:803:EDO:H22	1.98	0.63
1:Q:449[B]:HIS:HE2	1:Q:451[B]:MET:CE	1.90	0.62
1:S:725[A]:ASP:O	1:S:726[A]:GLY:O	2.16	0.62
1:R:37:ARG:NH1	10:R:907:HOH:O	2.32	0.62
1:Q:449[B]:HIS:NE2	10:Q:908:HOH:O	2.17	0.62
1:P:740:ARG:HH21	6:P:817:PEG:C3	2.12	0.61
1:P:468:ASN:O	1:P:471:ARG:HG2	2.00	0.61
1:Q:73[A]:LYS:CD	10:S:1579:HOH:O	2.49	0.61
1:P:440:TYR:O	1:R:73[A]:LYS:HE2	2.01	0.61
1:Q:449[B]:HIS:HD2	1:Q:451[B]:MET:HE2	1.32	0.61
1:Q:435[B]:ARG:NE	10:Q:906:HOH:O	2.34	0.61
4:S:805:EDO:C2	10:S:910:HOH:O	2.47	0.60
1:R:24:PRO:HD3	10:R:932:HOH:O	2.02	0.60
1:P:37[A]:ARG:NH1	10:P:911:HOH:O	2.33	0.60
1:Q:267[B]:ARG:NH1	10:Q:912:HOH:O	2.34	0.60
1:S:335[B]:GLU:OE1	1:S:369[B]:ARG:NH1	2.34	0.60
1:S:335[B]:GLU:OE1	1:S:369[B]:ARG:CZ	2.49	0.60
1:R:468:ASN:O	1:R:471:ARG:HG2	2.03	0.59
1:P:305:ASP:OD2	6:P:814:PEG:H11	2.03	0.59
1:P:678:ASN:HD22	4:P:807:EDO:H11	1.68	0.59
1:R:666:ILE:HD11	1:R:732:LEU:HD22	1.85	0.59
1:S:469:TRP:CE3	1:S:471:ARG:HG3	2.38	0.59
1:R:128:HIS:NE2	3:R:802:GOL:H2	2.18	0.58
1:P:121:ARG:CZ	1:S:126[A]:ILE:HD12	2.32	0.58
1:S:468:ASN:O	1:S:471:ARG:HG2	2.02	0.58
1:Q:468:ASN:O	1:Q:471:ARG:HG2	2.03	0.58
1:R:254[B]:MET:HG2	1:R:511:PHE:HD2	1.69	0.58
1:Q:73[A]:LYS:HD3	10:S:1579:HOH:O	2.04	0.58
1:R:126[A]:ILE:CG2	2:R:801:HDD:HMD3	2.34	0.58
1:P:740:ARG:NE	6:P:817:PEG:C4	2.61	0.57
1:P:128:HIS:NE2	3:P:802:GOL:H2	2.19	0.57
1:P:126[B]:ILE:HD12	1:S:121:ARG:CZ	2.34	0.57
1:P:158:LYS:NZ	10:P:901:HOH:O	2.36	0.57
1:Q:121:ARG:CZ	1:R:126[A]:ILE:HD12	2.35	0.57
1:R:716:GLU:HG2	10:R:951:HOH:O	2.05	0.57
1:Q:126[A]:ILE:HD12	1:R:121:ARG:CZ	2.35	0.57
1:P:660:LEU:O	6:P:817:PEG:H12	2.05	0.57
1:P:740:ARG:HH21	6:P:817:PEG:C4	2.18	0.56
1:S:126[A]:ILE:CG2	2:S:801:HDD:HMD3	2.35	0.56
1:Q:169:VAL:HG13	3:Q:802:GOL:H11	1.85	0.56
1:S:478[B]:LYS:NZ	10:S:916:HOH:O	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:469:TRP:CE3	1:Q:471:ARG:HG3	2.39	0.56
1:P:678:ASN:HD22	4:P:807:EDO:C1	2.18	0.56
1:R:352:ASP:HA	3:R:809:GOL:H32	1.86	0.56
1:Q:126[A]:ILE:CG2	2:Q:801:HDD:HMD3	2.36	0.56
1:R:23:LYS:HA	10:R:932:HOH:O	2.04	0.56
1:R:214:PHE:CE1	3:R:802:GOL:H31	2.41	0.56
1:P:214:PHE:CE1	3:P:802:GOL:H31	2.41	0.55
1:P:121:ARG:NH2	1:S:126[A]:ILE:HD12	2.20	0.55
1:R:469:TRP:CE3	1:R:471:ARG:HG3	2.41	0.55
1:Q:377[B]:ARG:HG2	1:Q:377[B]:ARG:NH2	2.06	0.55
1:S:303:VAL:HG21	4:S:804:EDO:C1	2.37	0.55
1:P:126[B]:ILE:CG2	2:P:801:HDD:HMD3	2.37	0.55
1:P:305:ASP:OD2	6:P:814:PEG:C1	2.55	0.54
1:Q:449[B]:HIS:NE2	1:Q:451[B]:MET:HE3	1.90	0.54
1:R:747[A]:LYS:HE3	10:R:905:HOH:O	2.06	0.54
1:R:214:PHE:HZ	3:R:802:GOL:H32	1.72	0.54
10:Q:1348:HOH:O	1:S:73[A]:LYS:HE2	2.06	0.54
1:R:254[B]:MET:HG2	1:R:511:PHE:CD2	2.42	0.54
1:S:303:VAL:HG21	4:S:804:EDO:H12	1.89	0.53
1:Q:126[A]:ILE:HD12	1:R:121:ARG:NH2	2.23	0.53
1:P:267[C]:ARG:NE	10:P:908:HOH:O	2.42	0.53
1:S:377[B]:ARG:NH2	10:S:901:HOH:O	2.41	0.53
1:P:533:LYS:NZ	10:P:920:HOH:O	2.42	0.53
1:R:158:LYS:HB3	10:R:962:HOH:O	2.09	0.53
1:Q:121:ARG:NH2	1:R:126[A]:ILE:HD12	2.23	0.52
5:R:807:PGE:H1	10:R:919:HOH:O	2.09	0.52
1:P:126[B]:ILE:HD12	1:S:121:ARG:NH2	2.24	0.52
1:P:267[C]:ARG:CD	10:P:908:HOH:O	2.57	0.52
1:P:751:ILE:HB	10:P:1579:HOH:O	2.08	0.52
1:P:267[C]:ARG:HD3	10:P:908:HOH:O	2.09	0.52
1:P:377[A]:ARG:HG2	1:P:377[A]:ARG:NH2	2.10	0.52
1:S:205[B]:ILE:HD13	1:S:251:HIS:CG	2.45	0.52
1:P:24:PRO:HD3	10:P:972:HOH:O	2.09	0.52
1:S:377[B]:ARG:CZ	10:S:901:HOH:O	2.47	0.52
3:R:809:GOL:H32	10:R:1067:HOH:O	2.10	0.52
2:R:801:HDD:C1B	3:R:802:GOL:H12	2.40	0.52
1:S:274:ILE:HD12	2:S:801:HDD:HMB3	1.92	0.51
1:R:274:ILE:HD12	2:R:801:HDD:HMB3	1.92	0.51
1:P:556:GLN:NE2	10:P:922:HOH:O	2.43	0.51
1:R:214:PHE:CZ	3:R:802:GOL:H32	2.44	0.51
1:R:128:HIS:CD2	3:R:802:GOL:H2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:306:GLU:OE2	6:P:817:PEG:H22	2.11	0.51
1:R:690[A]:LYS:HE2	5:R:807:PGE:H62	1.93	0.50
1:S:205[B]:ILE:HD13	1:S:251:HIS:ND1	2.26	0.50
1:Q:452:GLY:HA3	1:S:73[A]:LYS:HE3	1.93	0.50
1:Q:556:GLN:HG2	10:Q:1179:HOH:O	2.11	0.50
1:P:274:ILE:HD12	2:P:801:HDD:HMB3	1.92	0.50
1:Q:8:ASN:HB2	1:Q:9:PRO:CD	2.42	0.50
1:S:169:VAL:HG13	3:S:802:GOL:H11	1.94	0.50
1:Q:60:THR:C	1:Q:61:ARG:HG2	2.36	0.50
1:Q:274:ILE:HD12	2:Q:801:HDD:HMB3	1.94	0.50
2:P:801:HDD:C1B	3:P:802:GOL:H12	2.41	0.50
1:R:690[A]:LYS:HE2	5:R:807:PGE:C6	2.41	0.50
1:P:73[A]:LYS:HE2	10:P:1184:HOH:O	2.12	0.49
10:Q:1581:HOH:O	1:S:416[B]:THR:HG21	2.13	0.49
1:P:690:LYS:HG3	10:P:1579:HOH:O	2.11	0.49
1:Q:294[C]:LYS:NZ	10:Q:926:HOH:O	2.45	0.49
1:R:60:THR:HB	1:R:377[B]:ARG:HD2	1.95	0.48
1:R:214:PHE:HE1	3:R:802:GOL:H31	1.78	0.48
6:P:814:PEG:C3	10:S:934:HOH:O	2.61	0.48
1:Q:137:TYR:CE1	1:Q:374[B]:VAL:HG13	2.47	0.48
2:S:801:HDD:NB	3:S:802:GOL:H31	2.27	0.48
1:P:440:TYR:O	1:R:73[A]:LYS:CE	2.61	0.48
1:S:369[A]:ARG:NH1	10:S:918:HOH:O	2.41	0.48
1:R:214:PHE:CZ	3:R:802:GOL:C3	2.96	0.48
4:Q:807:EDO:C2	1:R:12:HIS:HD2	2.26	0.48
1:P:364:LEU:HB3	6:P:815:PEG:H12	1.96	0.48
1:P:749[B]:ASP:OD1	1:P:750:SER:N	2.47	0.48
1:R:549:HIS:HD2	10:R:1812:HOH:O	1.97	0.48
1:P:621:LYS:HD3	10:P:1895:HOH:O	2.13	0.47
1:R:126[A]:ILE:CG2	2:R:801:HDD:CMD	2.92	0.47
1:S:267[B]:ARG:NH2	10:S:925:HOH:O	2.47	0.47
6:P:814:PEG:H12	1:S:313:ARG:HH22	1.78	0.47
1:Q:73[A]:LYS:HD2	10:S:1579:HOH:O	2.14	0.47
1:R:666:ILE:HD11	1:R:732:LEU:CD2	2.44	0.47
1:S:392:HIS:ND1	1:S:415:TYR:CG	2.77	0.47
1:P:749[B]:ASP:OD1	10:P:906:HOH:O	2.20	0.47
1:Q:229:ILE:HG22	6:Q:822:PEG:H21	1.96	0.47
1:P:37[A]:ARG:HD2	10:P:911:HOH:O	2.15	0.47
3:R:809:GOL:C3	10:R:1067:HOH:O	2.63	0.47
1:R:461:GLU:HA	1:R:462:PRO:C	2.40	0.46
1:P:461:GLU:HA	1:P:462:PRO:C	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:8:ASN:HB2	1:Q:9:PRO:HD2	1.97	0.46
1:R:267:ARG:NH1	10:R:916:HOH:O	2.42	0.46
1:Q:461:GLU:HA	1:Q:462:PRO:C	2.40	0.46
1:S:461:GLU:HA	1:S:462:PRO:C	2.40	0.46
1:P:7:LYS:HB3	1:P:9:PRO:HD2	1.97	0.46
1:Q:137:TYR:CZ	1:Q:374[B]:VAL:CG1	2.97	0.46
1:S:60:THR:HB	1:S:377[B]:ARG:HD3	1.98	0.46
1:P:704:PHE:O	1:P:707[A]:THR:HG22	2.16	0.46
1:S:7:LYS:HB3	1:S:9:PRO:HD2	1.98	0.46
1:Q:595[B]:ASP:OD2	10:Q:909:HOH:O	2.20	0.46
1:S:7:LYS:HD2	10:S:1703:HOH:O	2.16	0.46
1:R:682:ASN:HB3	1:R:707[A]:THR:HG21	1.97	0.46
1:P:592:ALA:HA	4:P:804:EDO:H22	1.97	0.45
1:P:128:HIS:CD2	3:P:802:GOL:H2	2.51	0.45
1:R:214:PHE:HZ	3:R:802:GOL:C3	2.29	0.45
1:R:13:GLN:NE2	10:R:930:HOH:O	2.50	0.45
1:R:372[B]:ASN:ND2	10:R:904:HOH:O	2.23	0.45
1:P:128:HIS:NE2	3:P:802:GOL:C2	2.80	0.45
1:P:214:PHE:HE1	3:P:802:GOL:H31	1.80	0.45
1:S:267[B]:ARG:HG3	10:S:1405:HOH:O	2.16	0.45
1:S:476:GLY:C	6:S:817:PEG:H42	2.42	0.45
1:Q:213:LYS:HD3	1:R:92:GLN:HA	1.99	0.44
1:Q:626:LYS:HE2	4:Q:819:EDO:C2	2.47	0.44
1:S:126[A]:ILE:CG2	2:S:801:HDD:CMD	2.95	0.44
1:P:264:ARG:HD3	6:P:817:PEG:H32	1.99	0.44
1:P:621:LYS:CD	10:P:1895:HOH:O	2.65	0.44
1:R:267:ARG:NE	10:R:912:HOH:O	2.50	0.44
1:R:267:ARG:HG3	10:R:1108:HOH:O	2.18	0.44
1:S:142:LYS:HE2	10:S:1604:HOH:O	2.17	0.44
6:S:817:PEG:H31	10:S:1768:HOH:O	2.16	0.44
1:Q:126[A]:ILE:CG2	2:Q:801:HDD:CMD	2.95	0.44
6:Q:822:PEG:O1	10:Q:904:HOH:O	2.11	0.44
1:P:92:GLN:HA	1:S:213:LYS:HD3	2.00	0.43
1:S:214:PHE:CZ	3:S:802:GOL:H2	2.53	0.43
1:P:740:ARG:HE	6:P:817:PEG:H42	1.76	0.43
1:R:626:LYS:HE2	10:R:1862:HOH:O	2.18	0.43
1:R:704:PHE:O	1:R:707[B]:THR:HG22	2.18	0.43
1:P:126[B]:ILE:CG2	2:P:801:HDD:CMD	2.97	0.43
1:Q:235:ALA:O	6:Q:822:PEG:H31	2.18	0.43
1:R:392:HIS:ND1	1:R:415:TYR:CG	2.78	0.43
1:R:533:LYS:NZ	10:R:931:HOH:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:725[B]:ASP:OD1	1:S:725[B]:ASP:C	2.62	0.43
1:P:73[B]:LYS:NZ	10:P:931:HOH:O	2.51	0.42
1:S:73[B]:LYS:NZ	10:S:932:HOH:O	2.49	0.42
1:P:740:ARG:HH21	6:P:817:PEG:H32	1.82	0.42
1:Q:137:TYR:CZ	1:Q:374[B]:VAL:HG11	2.54	0.42
1:S:207:PHE:O	1:S:249:THR:HA	2.20	0.42
1:P:213:LYS:HD3	1:S:92:GLN:HA	2.01	0.42
1:Q:61:ARG:HD2	10:Q:1537:HOH:O	2.19	0.42
1:R:128:HIS:NE2	3:R:802:GOL:C2	2.83	0.42
1:P:592:ALA:HA	4:P:804:EDO:H12	2.00	0.42
1:Q:36:HIS:CD2	1:Q:37[D]:ARG:HG2	2.55	0.42
1:R:207:PHE:O	1:R:249:THR:HA	2.18	0.42
1:R:475:PRO:HB2	5:R:808:PGE:H3	2.00	0.42
1:P:126[B]:ILE:HG12	1:S:117:PHE:CZ	2.55	0.42
1:Q:54[B]:SER:OG	1:Q:377[B]:ARG:NH1	2.52	0.42
1:S:556[A]:GLN:NE2	10:S:941:HOH:O	2.52	0.42
1:S:707[A]:THR:CG2	10:S:1639:HOH:O	2.67	0.42
1:S:549:HIS:HD2	10:S:1920:HOH:O	2.02	0.42
1:P:39:ALA:N	1:P:48[B]:GLN:OE1	2.53	0.42
1:P:158:LYS:HA	4:P:808:EDO:H21	2.01	0.42
1:Q:634:TYR:O	1:Q:653:THR:HA	2.20	0.42
1:S:478[B]:LYS:HG2	1:S:479:ARG:HG2	2.02	0.42
1:P:207:PHE:O	1:P:249:THR:HA	2.20	0.41
1:R:7:LYS:HB3	1:R:9:PRO:HD2	2.02	0.41
1:P:128:HIS:CE1	1:P:169:VAL:HG22	2.55	0.41
4:Q:807:EDO:H21	1:R:12:HIS:HD2	1.84	0.41
1:Q:126[A]:ILE:HD13	1:R:120:GLU:HB2	2.03	0.41
1:Q:478[A]:LYS:HG2	10:Q:987:HOH:O	2.20	0.41
1:Q:493:LYS:NZ	10:Q:941:HOH:O	2.53	0.41
1:Q:626:LYS:HE2	4:Q:819:EDO:H21	2.02	0.41
1:Q:117:PHE:CZ	1:R:126[A]:ILE:HG12	2.56	0.41
1:Q:479:ARG:NE	10:Q:924:HOH:O	2.52	0.41
1:Q:686[B]:MET:HE1	1:Q:752:PRO:HD2	2.01	0.41
1:R:254[B]:MET:CG	1:R:511:PHE:CD2	3.04	0.41
1:Q:452:GLY:HA3	1:S:73[A]:LYS:CE	2.50	0.41
1:R:612:ARG:NH1	10:R:921:HOH:O	2.45	0.41
1:P:678:ASN:ND2	4:P:807:EDO:H11	2.32	0.41
1:Q:207:PHE:O	1:Q:249:THR:HA	2.20	0.41
1:Q:416[B]:THR:HG21	10:S:1600:HOH:O	2.21	0.41
1:S:634:TYR:O	1:S:653:THR:HA	2.21	0.41
1:P:556:GLN:HG2	10:P:1742:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:92:GLN:HA	1:R:213:LYS:HD3	2.02	0.41
4:Q:803:EDO:C2	10:R:1589:HOH:O	2.69	0.41
1:R:23:LYS:CA	10:R:932:HOH:O	2.66	0.41
1:R:477:PRO:O	1:R:478[B]:LYS:HG3	2.21	0.41
1:S:267[B]:ARG:CZ	10:S:925:HOH:O	2.69	0.41
1:S:556[A]:GLN:NE2	10:S:946:HOH:O	2.53	0.41
1:S:707[A]:THR:HG22	10:S:1639:HOH:O	2.21	0.41
1:R:24:PRO:CD	10:R:932:HOH:O	2.65	0.41
1:S:128:HIS:HA	1:S:168:THR:O	2.21	0.41
1:S:478[A]:LYS:HG2	10:S:1686:HOH:O	2.19	0.41
1:P:294[B]:LYS:NZ	10:P:942:HOH:O	2.54	0.40
1:R:377[B]:ARG:NH2	10:R:901:HOH:O	2.54	0.40
1:S:726[B]:GLY:HA3	1:S:727:SER:HB3	2.02	0.40
10:P:1122:HOH:O	1:R:449[B]:HIS:HE1	2.02	0.40
1:Q:416[B]:THR:HG23	10:Q:1173:HOH:O	2.21	0.40
1:R:522:HIS:NE2	5:R:807:PGE:O2	2.51	0.40
1:S:37[A]:ARG:NH2	10:S:919:HOH:O	2.54	0.40
1:S:392:HIS:CG	1:S:415:TYR:CB	2.90	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:805:EDO:O1	4:Q:805:EDO:O1[2_656]	0.98	1.22
4:Q:805:EDO:O1	4:Q:805:EDO:HO1[2_656]	1.41	0.19
1:R:621:LYS:HZ3	10:R:1773:HOH:O[2_556]	1.51	0.09

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	P	770/753 (102%)	751 (98%)	18 (2%)	1 (0%)	48 26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Q	778/753 (103%)	761 (98%)	16 (2%)	1 (0%)	48	26
1	R	769/753 (102%)	751 (98%)	17 (2%)	1 (0%)	48	26
1	S	780/753 (104%)	761 (98%)	17 (2%)	2 (0%)	36	19
All	All	3097/3012 (103%)	3024 (98%)	68 (2%)	5 (0%)	43	25

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	S	727	SER
1	P	75	SER
1	R	75	SER
1	S	75	SER
1	Q	75	SER

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	P	655/636 (103%)	644 (98%)	11 (2%)	53	23
1	Q	662/636 (104%)	651 (98%)	11 (2%)	53	23
1	R	654/636 (103%)	643 (98%)	11 (2%)	53	23
1	S	664/636 (104%)	643 (97%)	21 (3%)	34	7
All	All	2635/2544 (104%)	2581 (98%)	54 (2%)	57	18

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	7	LYS
1	P	21	GLU
1	P	191	THR
1	P	205	ILE
1	P	285	LYS
1	P	330[A]	ASP

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Mol	Chain	Res	Type
1	P	330[B]	ASP
1	P	377[A]	ARG
1	P	377[B]	ARG
1	P	552	LEU
1	P	621	LYS
1	Q	21	GLU
1	Q	126[A]	ILE
1	Q	126[B]	ILE
1	Q	191	THR
1	Q	205	ILE
1	Q	285	LYS
1	Q	552	LEU
1	Q	583	LYS
1	Q	597	ASP
1	Q	707[A]	THR
1	Q	707[B]	THR
1	R	21	GLU
1	R	73[A]	LYS
1	R	73[B]	LYS
1	R	73[C]	LYS
1	R	126[A]	ILE
1	R	126[B]	ILE
1	R	191	THR
1	R	205	ILE
1	R	285	LYS
1	R	707[A]	THR
1	R	707[B]	THR
1	S	7	LYS
1	S	21	GLU
1	S	37[A]	ARG
1	S	37[B]	ARG
1	S	37[C]	ARG
1	S	73[A]	LYS
1	S	73[B]	LYS
1	S	73[C]	LYS
1	S	126[A]	ILE
1	S	126[B]	ILE
1	S	191[A]	THR
1	S	191[B]	THR
1	S	205[A]	ILE
1	S	205[B]	ILE
1	S	285	LYS

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Mol	Chain	Res	Type
1	S	369[A]	ARG
1	S	369[B]	ARG
1	S	597	ASP
1	S	621	LYS
1	S	707[A]	THR
1	S	707[B]	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	P	77	ASN
1	Q	11	GLN
1	Q	77	ASN
1	Q	549	HIS
1	R	549	HIS
1	S	492	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 72 ligands modelled in this entry, 2 are monoatomic - leaving 70 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	EDO	R	806	-	3,3,3	0.42	0	2,2,2	0.27	0
2	HDD	P	801	3,1	49,52,52	2.26	19 (38%)	62,89,89	2.49	22 (35%)
4	EDO	S	810	-	3,3,3	0.52	0	2,2,2	0.24	0
4	EDO	Q	812	-	3,3,3	0.48	0	2,2,2	0.24	0
3	GOL	Q	802	2	5,5,5	0.57	0	5,5,5	0.51	0
4	EDO	P	806	-	3,3,3	0.35	0	2,2,2	0.55	0
7	SO4	P	818	-	4,4,4	0.40	0	6,6,6	0.10	0
4	EDO	Q	816	-	3,3,3	0.40	0	2,2,2	0.54	0
3	GOL	P	802	2	5,5,5	0.72	0	5,5,5	1.29	1 (20%)
5	PGE	P	812	-	9,9,9	0.56	0	8,8,8	0.60	0
4	EDO	S	811	-	3,3,3	0.48	0	2,2,2	0.29	0
4	EDO	P	807	-	3,3,3	0.41	0	2,2,2	0.10	0
4	EDO	Q	808	-	3,3,3	0.39	0	2,2,2	0.55	0
4	EDO	Q	819	-	3,3,3	0.71	0	2,2,2	0.12	0
6	PEG	P	816	-	6,6,6	0.47	0	5,5,5	0.32	0
6	PEG	Q	822	-	6,6,6	0.43	0	5,5,5	0.30	0
6	PEG	Q	824	-	6,6,6	0.51	0	5,5,5	0.41	0
9	PG4	R	812	-	12,12,12	0.52	0	11,11,11	0.29	0
6	PEG	Q	823	-	6,6,6	0.69	0	5,5,5	0.59	0
4	EDO	P	804	-	3,3,3	0.52	0	2,2,2	0.09	0
4	EDO	P	811	-	3,3,3	0.34	0	2,2,2	0.41	0
3	GOL	S	813	-	5,5,5	0.34	0	5,5,5	0.79	0
4	EDO	Q	804	-	3,3,3	0.31	0	2,2,2	0.47	0
4	EDO	S	808	-	3,3,3	0.52	0	2,2,2	0.27	0
3	GOL	P	813	-	5,5,5	0.53	0	5,5,5	0.47	0
3	GOL	S	802	2	5,5,5	0.74	0	5,5,5	0.42	0
4	EDO	P	808	-	3,3,3	0.51	0	2,2,2	0.14	0
4	EDO	S	809	-	3,3,3	0.41	0	2,2,2	0.43	0
4	EDO	S	807	-	3,3,3	0.46	0	2,2,2	0.17	0
3	GOL	Q	820	-	5,5,5	0.49	0	5,5,5	0.32	0
2	HDD	R	801	3,1	49,52,52	2.28	19 (38%)	62,89,89	2.57	20 (32%)
4	EDO	Q	813	-	3,3,3	0.40	0	2,2,2	0.36	0
4	EDO	Q	803	-	3,3,3	0.48	0	2,2,2	0.26	0
4	EDO	Q	806	-	3,3,3	0.52	0	2,2,2	0.15	0
3	GOL	S	812	-	5,5,5	0.58	0	5,5,5	0.72	0
4	EDO	R	803	-	3,3,3	0.63	0	2,2,2	0.13	0
4	EDO	S	805	-	3,3,3	0.40	0	2,2,2	0.23	0
3	GOL	Q	821	-	5,5,5	0.39	0	5,5,5	0.23	0
4	EDO	P	803	-	3,3,3	0.32	0	2,2,2	0.25	0
6	PEG	P	817	-	6,6,6	0.56	0	5,5,5	1.27	0
4	EDO	R	805	-	3,3,3	0.58	0	2,2,2	0.54	0
4	EDO	Q	809	-	3,3,3	0.45	0	2,2,2	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
4	EDO	Q	807	-	3,3,3	0.60	0	2,2,2	0.36	0
4	EDO	Q	810	-	3,3,3	0.41	0	2,2,2	0.53	0
6	PEG	S	816	-	6,6,6	0.50	0	5,5,5	0.63	0
2	HDD	Q	801	3,1	49,52,52	2.32	20 (40%)	62,89,89	2.68	17 (27%)
3	GOL	R	810	-	5,5,5	0.45	0	5,5,5	0.83	0
4	EDO	Q	814	-	3,3,3	0.35	0	2,2,2	0.86	0
4	EDO	Q	818	-	3,3,3	0.42	0	2,2,2	0.42	0
4	EDO	Q	811	-	3,3,3	0.52	0	2,2,2	0.01	0
7	SO4	S	814	-	4,4,4	0.53	0	6,6,6	0.25	0
4	EDO	S	804	-	3,3,3	0.32	0	2,2,2	0.32	0
5	PGE	R	807	-	9,9,9	0.39	0	8,8,8	0.53	0
4	EDO	Q	805	-	3,3,3	0.66	0	2,2,2	0.12	0
4	EDO	R	804	-	3,3,3	0.53	0	2,2,2	0.28	0
6	PEG	P	815	-	6,6,6	0.39	0	5,5,5	0.38	0
4	EDO	P	809	-	3,3,3	0.58	0	2,2,2	0.43	0
6	PEG	Q	825	-	6,6,6	0.54	0	5,5,5	0.44	0
2	HDD	S	801	3,1	49,52,52	2.29	20 (40%)	62,89,89	2.49	22 (35%)
4	EDO	P	810	-	3,3,3	0.48	0	2,2,2	0.32	0
4	EDO	S	803	-	3,3,3	0.41	0	2,2,2	0.42	0
6	PEG	S	817	-	6,6,6	0.71	0	5,5,5	0.71	0
6	PEG	P	814	-	6,6,6	0.72	0	5,5,5	0.79	0
4	EDO	P	805	-	3,3,3	0.46	0	2,2,2	0.21	0
4	EDO	Q	817	-	3,3,3	0.46	0	2,2,2	0.29	0
3	GOL	R	809	-	5,5,5	0.45	0	5,5,5	0.73	0
5	PGE	R	808	-	9,9,9	0.61	0	8,8,8	0.39	0
4	EDO	S	806	-	3,3,3	0.52	0	2,2,2	0.22	0
4	EDO	Q	815	-	3,3,3	0.52	0	2,2,2	0.12	0
3	GOL	R	802	2	5,5,5	0.49	0	5,5,5	1.21	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	EDO	R	806	-	-	1/1/1/1	-
2	HDD	P	801	3,1	1/1/14/14	2/9/89/89	0/1/9/9
4	EDO	S	810	-	-	0/1/1/1	-
4	EDO	Q	812	-	-	1/1/1/1	-
3	GOL	Q	802	2	-	2/4/4/4	-
4	EDO	P	806	-	-	0/1/1/1	-
4	EDO	Q	816	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	P	802	2	-	2/4/4/4	-
5	PGE	P	812	-	-	6/7/7/7	-
4	EDO	S	811	-	-	0/1/1/1	-
4	EDO	P	807	-	-	1/1/1/1	-
4	EDO	Q	808	-	-	1/1/1/1	-
4	EDO	Q	819	-	-	1/1/1/1	-
6	PEG	P	816	-	-	4/4/4/4	-
6	PEG	Q	822	-	-	3/4/4/4	-
6	PEG	Q	824	-	-	3/4/4/4	-
9	PG4	R	812	-	-	5/10/10/10	-
6	PEG	Q	823	-	-	3/4/4/4	-
4	EDO	P	804	-	-	1/1/1/1	-
4	EDO	P	811	-	-	0/1/1/1	-
3	GOL	S	813	-	-	2/4/4/4	-
4	EDO	Q	804	-	-	0/1/1/1	-
4	EDO	S	808	-	-	1/1/1/1	-
3	GOL	P	813	-	-	1/4/4/4	-
3	GOL	S	802	2	-	2/4/4/4	-
4	EDO	P	808	-	-	1/1/1/1	-
4	EDO	S	809	-	-	0/1/1/1	-
4	EDO	S	807	-	-	1/1/1/1	-
3	GOL	Q	820	-	-	3/4/4/4	-
2	HDD	R	801	3,1	1/1/14/14	2/9/89/89	0/1/9/9
4	EDO	Q	813	-	-	1/1/1/1	-
4	EDO	Q	803	-	-	1/1/1/1	-
4	EDO	Q	806	-	-	1/1/1/1	-
3	GOL	S	812	-	-	4/4/4/4	-
4	EDO	R	803	-	-	0/1/1/1	-
4	EDO	S	805	-	-	1/1/1/1	-
3	GOL	Q	821	-	-	0/4/4/4	-
4	EDO	P	803	-	-	1/1/1/1	-
6	PEG	P	817	-	-	4/4/4/4	-
4	EDO	R	805	-	-	1/1/1/1	-
4	EDO	Q	809	-	-	0/1/1/1	-
4	EDO	Q	807	-	-	0/1/1/1	-
4	EDO	Q	810	-	-	0/1/1/1	-
6	PEG	S	816	-	-	2/4/4/4	-
2	HDD	Q	801	3,1	1/1/14/14	2/9/89/89	0/1/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	R	810	-	-	2/4/4/4	-
4	EDO	Q	814	-	-	1/1/1/1	-
4	EDO	Q	818	-	-	1/1/1/1	-
4	EDO	Q	811	-	-	1/1/1/1	-
4	EDO	S	804	-	-	1/1/1/1	-
5	PGE	R	807	-	-	6/7/7/7	-
4	EDO	Q	805	-	-	1/1/1/1	-
4	EDO	R	804	-	-	1/1/1/1	-
6	PEG	P	815	-	-	2/4/4/4	-
4	EDO	P	809	-	-	0/1/1/1	-
6	PEG	Q	825	-	-	3/4/4/4	-
2	HDD	S	801	3,1	1/1/14/14	2/9/89/89	0/1/9/9
4	EDO	P	810	-	-	1/1/1/1	-
4	EDO	S	803	-	-	0/1/1/1	-
6	PEG	S	817	-	-	2/4/4/4	-
6	PEG	P	814	-	-	3/4/4/4	-
4	EDO	P	805	-	-	1/1/1/1	-
4	EDO	Q	817	-	-	1/1/1/1	-
3	GOL	R	809	-	-	2/4/4/4	-
5	PGE	R	808	-	-	5/7/7/7	-
4	EDO	S	806	-	-	1/1/1/1	-
4	EDO	Q	815	-	-	1/1/1/1	-
3	GOL	R	802	2	-	0/4/4/4	-

All (78) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	801	HDD	O1D-CGD	6.18	1.45	1.35
2	Q	801	HDD	O1D-CGD	5.38	1.44	1.35
2	R	801	HDD	O1D-CGD	4.98	1.43	1.35
2	S	801	HDD	CHD-C4C	4.62	1.47	1.38
2	P	801	HDD	O1D-CGD	4.60	1.42	1.35
2	Q	801	HDD	CHD-C4C	4.45	1.47	1.38
2	R	801	HDD	CHD-C4C	4.31	1.46	1.38
2	R	801	HDD	C3B-C2B	4.29	1.45	1.37
2	Q	801	HDD	C3B-C2B	4.28	1.45	1.37
2	R	801	HDD	FE-NB	4.22	2.07	1.94
2	R	801	HDD	C3C-C2C	4.22	1.45	1.37
2	S	801	HDD	C3B-C2B	4.16	1.45	1.37
2	P	801	HDD	C3B-C2B	4.15	1.45	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	801	HDD	C3C-C2C	4.12	1.45	1.37
2	P	801	HDD	CHC-C1C	4.08	1.46	1.38
2	Q	801	HDD	FE-NB	4.07	2.07	1.94
2	P	801	HDD	FE-NB	4.01	2.07	1.94
2	P	801	HDD	CHD-C4C	3.96	1.46	1.38
2	Q	801	HDD	C3C-C2C	3.95	1.45	1.37
2	Q	801	HDD	FE-NC	3.90	2.08	1.95
2	S	801	HDD	FE-NB	3.85	2.06	1.94
2	S	801	HDD	C3C-C2C	3.77	1.44	1.37
2	R	801	HDD	FE-NC	3.67	2.07	1.95
2	P	801	HDD	FE-NC	3.64	2.07	1.95
2	S	801	HDD	CHC-C1C	3.61	1.45	1.38
2	R	801	HDD	CHC-C1C	3.59	1.45	1.38
2	S	801	HDD	CHA-C1A	3.57	1.47	1.39
2	Q	801	HDD	CHC-C1C	3.54	1.45	1.38
2	Q	801	HDD	CHA-C1A	3.49	1.47	1.39
2	Q	801	HDD	C1B-NB	-3.46	1.34	1.40
2	Q	801	HDD	C4C-NC	-3.45	1.33	1.39
2	R	801	HDD	C4C-NC	-3.37	1.33	1.39
2	P	801	HDD	C1D-ND	3.36	1.37	1.35
2	P	801	HDD	C1A-NA	-3.36	1.33	1.39
2	P	801	HDD	C4C-NC	-3.31	1.33	1.39
2	R	801	HDD	CHB-C4A	3.24	1.46	1.39
2	Q	801	HDD	CHC-C4B	3.23	1.46	1.39
2	S	801	HDD	FE-NC	3.21	2.05	1.95
2	Q	801	HDD	FE-NA	3.20	2.05	1.95
2	R	801	HDD	C1A-NA	-3.19	1.33	1.39
2	R	801	HDD	C1D-ND	3.16	1.37	1.35
2	R	801	HDD	CHA-C1A	3.15	1.46	1.39
2	R	801	HDD	CHB-C1B	3.14	1.44	1.38
2	P	801	HDD	FE-NA	3.11	2.05	1.95
2	R	801	HDD	C1B-NB	-3.10	1.34	1.40
2	S	801	HDD	C1B-NB	-3.09	1.34	1.40
2	S	801	HDD	FE-NA	3.08	2.05	1.95
2	P	801	HDD	CHB-C1B	3.08	1.44	1.38
2	S	801	HDD	CHB-C4A	3.05	1.46	1.39
2	Q	801	HDD	CHB-C1B	3.03	1.44	1.38
2	S	801	HDD	C4A-NA	-2.98	1.34	1.39
2	P	801	HDD	CHB-C4A	2.96	1.46	1.39
2	R	801	HDD	FE-NA	2.91	2.04	1.95
2	P	801	HDD	CHA-C1A	2.90	1.45	1.39
2	R	801	HDD	CHC-C4B	2.87	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	801	HDD	CHB-C1B	2.87	1.44	1.38
2	Q	801	HDD	C1D-ND	2.82	1.37	1.35
2	P	801	HDD	CHC-C4B	2.81	1.45	1.39
2	Q	801	HDD	C4A-NA	-2.80	1.34	1.39
2	S	801	HDD	C4C-NC	-2.76	1.34	1.39
2	P	801	HDD	C2A-C3A	2.76	1.46	1.38
2	S	801	HDD	C2A-C3A	2.68	1.45	1.38
2	R	801	HDD	C2A-C3A	2.67	1.45	1.38
2	Q	801	HDD	CHB-C4A	2.66	1.45	1.39
2	S	801	HDD	C1C-NC	-2.63	1.34	1.39
2	S	801	HDD	C1A-NA	-2.60	1.34	1.39
2	S	801	HDD	CHC-C4B	2.53	1.45	1.39
2	Q	801	HDD	C2A-C3A	2.52	1.45	1.38
2	P	801	HDD	C4A-NA	-2.50	1.34	1.39
2	P	801	HDD	C1B-NB	-2.44	1.36	1.40
2	Q	801	HDD	C1A-NA	-2.40	1.35	1.39
2	Q	801	HDD	C1B-C2B	2.21	1.49	1.44
2	S	801	HDD	CHD-C1D	-2.15	1.35	1.41
2	P	801	HDD	CHD-C1D	-2.14	1.35	1.41
2	R	801	HDD	C4A-C3A	2.10	1.48	1.43
2	S	801	HDD	C4B-NB	-2.09	1.34	1.38
2	Q	801	HDD	CHD-C1D	-2.08	1.35	1.41
2	R	801	HDD	C4A-NA	-2.06	1.35	1.39

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Q	801	HDD	O1D-CGD-O2D	9.71	128.99	120.81
2	Q	801	HDD	C3B-C2B-C1B	-8.68	99.90	106.41
2	R	801	HDD	O1D-CGD-O2D	8.17	127.69	120.81
2	S	801	HDD	O1D-CGD-O2D	8.12	127.65	120.81
2	P	801	HDD	O1D-CGD-O2D	7.83	127.41	120.81
2	S	801	HDD	C3B-C2B-C1B	-7.77	100.58	106.41
2	R	801	HDD	C3C-C2C-C1C	-7.74	99.72	107.05
2	Q	801	HDD	C3C-C2C-C1C	-7.70	99.76	107.05
2	P	801	HDD	C3C-C2C-C1C	-7.20	100.23	107.05
2	P	801	HDD	C3B-C2B-C1B	-7.04	101.13	106.41
2	R	801	HDD	C3B-C2B-C1B	-6.98	101.17	106.41
2	Q	801	HDD	C2B-C1B-NB	6.01	116.75	109.84
2	S	801	HDD	C3C-C2C-C1C	-5.74	101.61	107.05
2	R	801	HDD	C3B-C4B-NB	5.56	113.46	109.47
2	R	801	HDD	C2B-C1B-NB	5.41	116.06	109.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	S	801	HDD	C3B-C4B-NB	5.30	113.27	109.47
2	S	801	HDD	C2B-C1B-NB	5.23	115.85	109.84
2	Q	801	HDD	C3B-C4B-NB	5.21	113.21	109.47
2	P	801	HDD	C3B-C4B-NB	5.00	113.06	109.47
2	P	801	HDD	C2B-C1B-NB	4.90	115.47	109.84
2	P	801	HDD	O1D-CGD-CBD	-4.27	106.28	110.17
2	S	801	HDD	O1D-CGD-CBD	-4.21	106.34	110.17
2	S	801	HDD	OND-C2D-CMD	-4.12	101.48	109.45
2	P	801	HDD	C4A-C3A-C2A	-3.98	102.26	106.82
2	S	801	HDD	C4A-C3A-C2A	-3.88	102.38	106.82
2	Q	801	HDD	O1D-CGD-CBD	-3.81	106.70	110.17
2	R	801	HDD	O1D-CGD-CBD	-3.79	106.72	110.17
2	R	801	HDD	C4A-C3A-C2A	-3.62	102.67	106.82
2	R	801	HDD	OND-C2D-CMD	-3.62	102.46	109.45
2	R	801	HDD	C2C-C1C-NC	3.57	116.23	109.64
2	Q	801	HDD	CMC-C2C-C1C	3.56	131.00	124.73
2	P	801	HDD	OND-C2D-CMD	-3.55	102.58	109.45
2	Q	801	HDD	C2C-C1C-NC	3.52	116.16	109.64
2	P	801	HDD	C3D-O1D-CGD	3.51	114.41	111.14
2	R	801	HDD	CAA-CBA-CGA	-3.40	104.64	113.67
2	Q	801	HDD	C4A-C3A-C2A	-3.38	102.95	106.82
2	Q	801	HDD	OND-C2D-CMD	-3.25	103.16	109.45
2	Q	801	HDD	CAA-CBA-CGA	-3.20	105.17	113.67
2	S	801	HDD	CAA-CBA-CGA	-3.20	105.18	113.67
2	R	801	HDD	C3D-O1D-CGD	3.17	114.09	111.14
2	P	801	HDD	C2C-C1C-NC	3.15	115.45	109.64
2	R	801	HDD	C2A-C1A-NA	3.10	113.59	110.15
2	S	801	HDD	C2C-C1C-NC	3.10	115.36	109.64
2	R	801	HDD	CBD-CAD-C3D	3.08	108.37	103.98
2	P	801	HDD	C2D-C1D-CHD	-3.01	118.55	123.28
2	R	801	HDD	C2D-C1D-CHD	-2.90	118.71	123.28
2	P	801	HDD	CMC-C2C-C1C	2.89	129.82	124.73
2	Q	801	HDD	C2A-C1A-NA	2.85	113.32	110.15
2	R	801	HDD	CMC-C2C-C1C	2.85	129.75	124.73
2	S	801	HDD	C3D-O1D-CGD	2.85	113.80	111.14
2	R	801	HDD	CHC-C1C-C2C	-2.79	119.68	125.49
2	S	801	HDD	C3A-C4A-NA	2.75	114.55	110.14
2	P	801	HDD	CAA-CBA-CGA	-2.74	106.40	113.67
2	P	801	HDD	C3A-C4A-NA	2.70	114.47	110.14
2	Q	801	HDD	C2D-C1D-CHD	-2.65	119.11	123.28
2	P	801	HDD	CBD-CAD-C3D	2.59	107.68	103.98
2	S	801	HDD	CMB-C2B-C1B	2.57	129.05	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	P	801	HDD	CAA-C2A-C1A	2.54	129.89	124.94
2	S	801	HDD	CBD-CAD-C3D	2.53	107.58	103.98
2	S	801	HDD	CMC-C2C-C1C	2.50	129.13	124.73
2	P	801	HDD	C2A-C1A-NA	2.50	112.93	110.15
2	Q	801	HDD	C3A-C4A-NA	2.49	114.13	110.14
2	S	801	HDD	C2A-C1A-NA	2.40	112.82	110.15
2	S	801	HDD	CHC-C1C-C2C	-2.37	120.55	125.49
2	Q	801	HDD	CHB-C1B-C2B	-2.34	120.28	126.95
3	P	802	GOL	O2-C2-C3	2.34	118.87	109.18
2	S	801	HDD	CHB-C4A-C3A	-2.33	120.67	127.43
2	P	801	HDD	CHB-C4A-C3A	-2.32	120.70	127.43
2	R	801	HDD	CMA-C3A-C4A	2.31	128.94	125.42
2	R	801	HDD	C4B-C3B-C2B	-2.29	105.17	107.28
2	S	801	HDD	CHB-C1B-C2B	-2.29	120.44	126.95
2	S	801	HDD	CMA-C3A-C2A	2.29	130.47	125.62
2	S	801	HDD	C2D-C1D-CHD	-2.25	119.73	123.28
2	Q	801	HDD	CHC-C1C-C2C	-2.24	120.83	125.49
2	R	801	HDD	C3A-C4A-NA	2.15	113.59	110.14
2	P	801	HDD	CHB-C1B-C2B	-2.11	120.94	126.95
2	R	801	HDD	CHB-C1B-C2B	-2.10	120.97	126.95
2	S	801	HDD	C4C-C3C-C2C	-2.08	105.01	106.81
2	Q	801	HDD	CHB-C4A-C3A	-2.06	121.45	127.43
2	P	801	HDD	CMB-C2B-C1B	2.06	128.25	125.03
2	P	801	HDD	CMA-C3A-C4A	2.05	128.54	125.42
2	P	801	HDD	CHC-C1C-C2C	-2.03	121.27	125.49

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	P	801	HDD	NC
2	Q	801	HDD	NC
2	R	801	HDD	NC
2	S	801	HDD	NC

All (105) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	Q	802	GOL	C1-C2-C3-O3
3	Q	820	GOL	O1-C1-C2-C3
3	R	809	GOL	C1-C2-C3-O3
3	S	802	GOL	C1-C2-C3-O3
3	S	812	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	S	812	GOL	C1-C2-C3-O3
3	S	812	GOL	O2-C2-C3-O3
3	S	813	GOL	C1-C2-C3-O3
5	R	807	PGE	C3-C4-O3-C5
5	P	812	PGE	O2-C3-C4-O3
5	R	807	PGE	O3-C5-C6-O4
6	Q	824	PEG	O2-C3-C4-O4
3	Q	820	GOL	O1-C1-C2-O2
3	R	809	GOL	O2-C2-C3-O3
3	S	802	GOL	O2-C2-C3-O3
6	S	817	PEG	C1-C2-O2-C3
5	P	812	PGE	C6-C5-O3-C4
6	P	817	PEG	O2-C3-C4-O4
9	R	812	PG4	O2-C3-C4-O3
6	P	815	PEG	O2-C3-C4-O4
6	P	816	PEG	O2-C3-C4-O4
6	Q	823	PEG	O2-C3-C4-O4
6	Q	825	PEG	O1-C1-C2-O2
5	R	807	PGE	O2-C3-C4-O3
3	P	802	GOL	O1-C1-C2-C3
5	R	807	PGE	O1-C1-C2-O2
6	P	814	PEG	O2-C3-C4-O4
6	P	817	PEG	O1-C1-C2-O2
3	Q	802	GOL	O2-C2-C3-O3
3	S	813	GOL	O2-C2-C3-O3
5	P	812	PGE	O3-C5-C6-O4
5	R	808	PGE	O1-C1-C2-O2
6	Q	822	PEG	O1-C1-C2-O2
6	Q	824	PEG	O1-C1-C2-O2
4	P	805	EDO	O1-C1-C2-O2
4	S	805	EDO	O1-C1-C2-O2
5	R	808	PGE	O3-C5-C6-O4
5	P	812	PGE	O1-C1-C2-O2
3	S	812	GOL	O1-C1-C2-O2
6	P	815	PEG	O1-C1-C2-O2
9	R	812	PG4	O4-C7-C8-O5
4	P	808	EDO	O1-C1-C2-O2
4	Q	808	EDO	O1-C1-C2-O2
4	Q	817	EDO	O1-C1-C2-O2
4	Q	819	EDO	O1-C1-C2-O2
4	R	806	EDO	O1-C1-C2-O2
4	S	804	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	S	808	EDO	O1-C1-C2-O2
9	R	812	PG4	O3-C5-C6-O4
3	P	802	GOL	O1-C1-C2-O2
4	Q	805	EDO	O1-C1-C2-O2
4	Q	806	EDO	O1-C1-C2-O2
4	Q	818	EDO	O1-C1-C2-O2
4	R	804	EDO	O1-C1-C2-O2
6	S	817	PEG	O1-C1-C2-O2
5	R	808	PGE	C3-C4-O3-C5
6	Q	822	PEG	O2-C3-C4-O4
4	S	806	EDO	O1-C1-C2-O2
6	P	814	PEG	C4-C3-O2-C2
6	P	816	PEG	O1-C1-C2-O2
9	R	812	PG4	C1-C2-O2-C3
6	Q	823	PEG	C4-C3-O2-C2
6	S	816	PEG	O1-C1-C2-O2
6	P	817	PEG	C4-C3-O2-C2
6	P	816	PEG	C1-C2-O2-C3
6	Q	825	PEG	C4-C3-O2-C2
3	R	810	GOL	O1-C1-C2-C3
4	P	804	EDO	O1-C1-C2-O2
6	Q	825	PEG	C1-C2-O2-C3
5	R	808	PGE	C4-C3-O2-C2
6	P	816	PEG	C4-C3-O2-C2
2	P	801	HDD	CAA-CBA-CGA-O2A
2	S	801	HDD	CAA-CBA-CGA-O2A
2	P	801	HDD	CAA-CBA-CGA-O1A
2	Q	801	HDD	CAA-CBA-CGA-O1A
2	R	801	HDD	CAA-CBA-CGA-O1A
5	R	808	PGE	O2-C3-C4-O3
2	Q	801	HDD	CAA-CBA-CGA-O2A
2	R	801	HDD	CAA-CBA-CGA-O2A
4	Q	813	EDO	O1-C1-C2-O2
4	S	807	EDO	O1-C1-C2-O2
6	S	816	PEG	C4-C3-O2-C2
2	S	801	HDD	CAA-CBA-CGA-O1A
6	P	817	PEG	C1-C2-O2-C3
5	R	807	PGE	C1-C2-O2-C3
6	P	814	PEG	O1-C1-C2-O2
3	P	813	GOL	O2-C2-C3-O3
3	R	810	GOL	O1-C1-C2-O2
4	Q	803	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	Q	814	EDO	O1-C1-C2-O2
6	Q	823	PEG	C1-C2-O2-C3
6	Q	822	PEG	C1-C2-O2-C3
5	P	812	PGE	C3-C4-O3-C5
5	R	807	PGE	C6-C5-O3-C4
3	Q	820	GOL	O2-C2-C3-O3
4	P	803	EDO	O1-C1-C2-O2
4	Q	811	EDO	O1-C1-C2-O2
4	Q	812	EDO	O1-C1-C2-O2
4	Q	815	EDO	O1-C1-C2-O2
4	P	807	EDO	O1-C1-C2-O2
4	P	810	EDO	O1-C1-C2-O2
4	R	805	EDO	O1-C1-C2-O2
6	Q	824	PEG	C1-C2-O2-C3
9	R	812	PG4	C8-C7-O4-C6
5	P	812	PGE	C1-C2-O2-C3

There are no ring outliers.

27 monomers are involved in 87 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	P	801	HDD	4	0
3	Q	802	GOL	1	0
3	P	802	GOL	6	0
4	P	807	EDO	3	0
4	Q	819	EDO	2	0
6	Q	822	PEG	3	0
4	P	804	EDO	2	0
3	S	802	GOL	4	0
4	P	808	EDO	1	0
2	R	801	HDD	4	0
4	Q	803	EDO	1	0
4	R	803	EDO	1	0
4	S	805	EDO	2	0
6	P	817	PEG	13	0
4	Q	807	EDO	2	0
6	S	816	PEG	1	0
2	Q	801	HDD	3	0
4	S	804	EDO	2	0
5	R	807	PGE	6	0
4	Q	805	EDO	0	2
6	P	815	PEG	1	0

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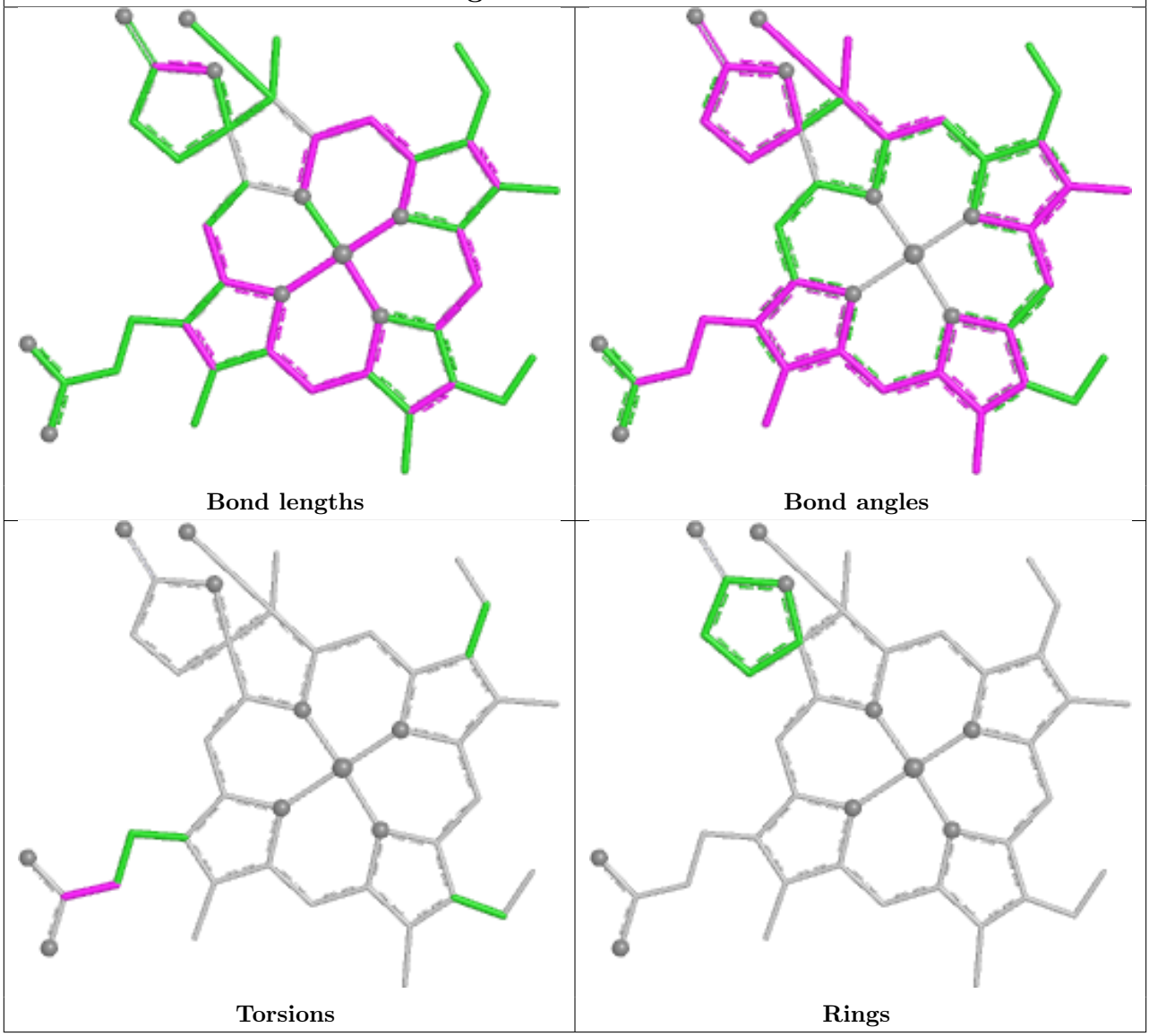
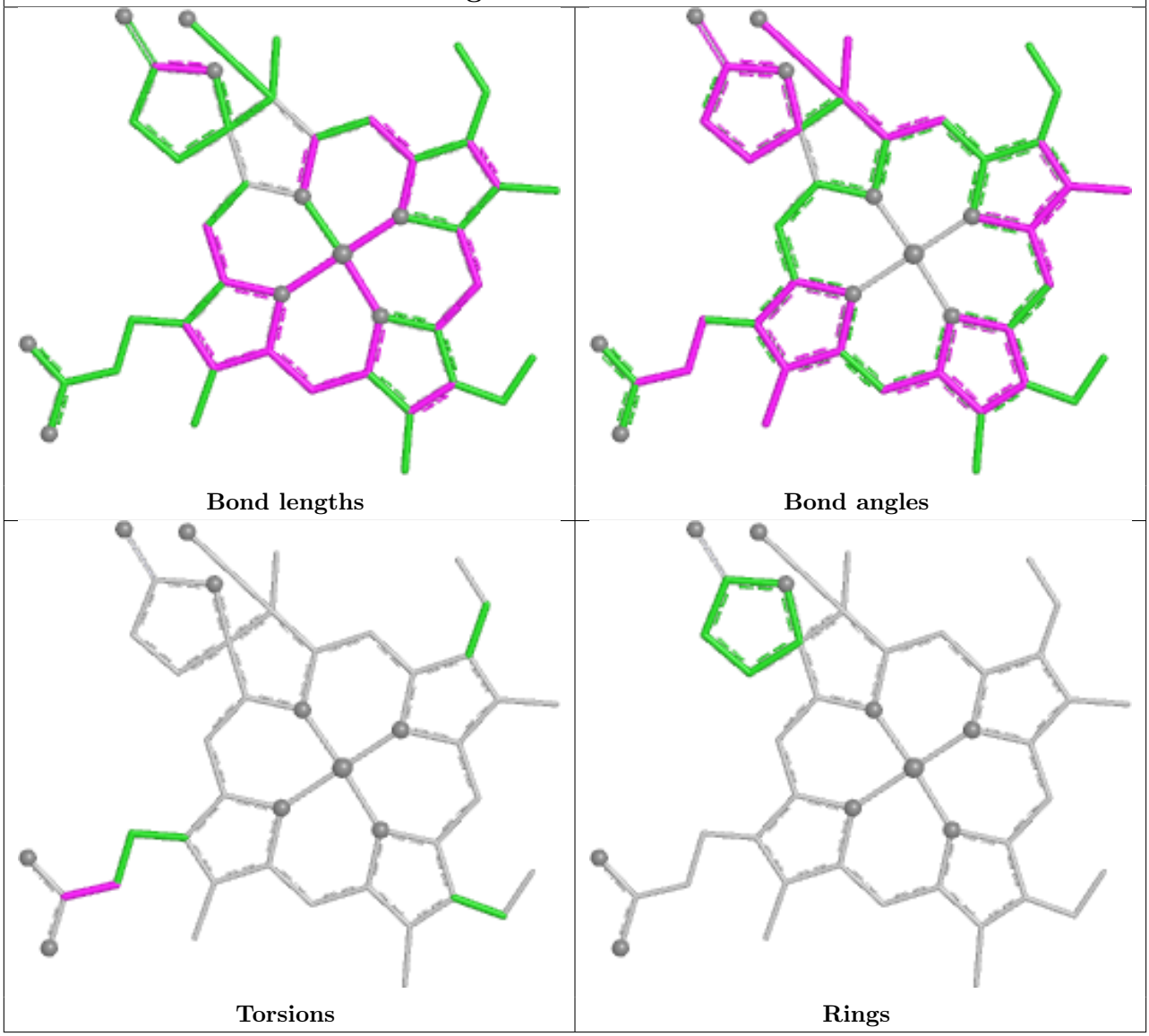
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	S	801	HDD	5	0
6	S	817	PEG	2	0
6	P	814	PEG	6	0
3	R	809	GOL	3	0
5	R	808	PGE	1	0
3	R	802	GOL	10	0

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 then 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.

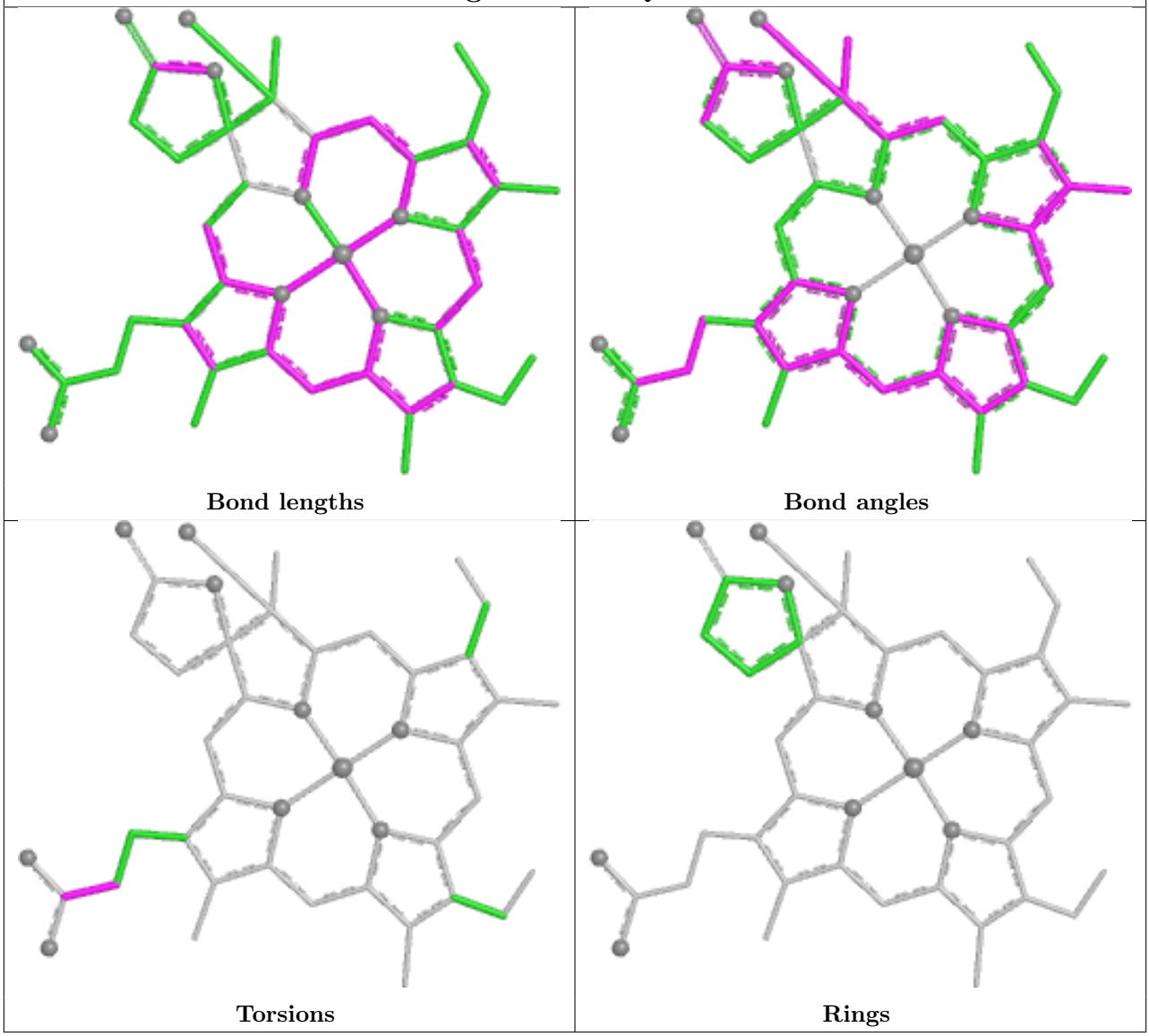
Ligand HDD P 801



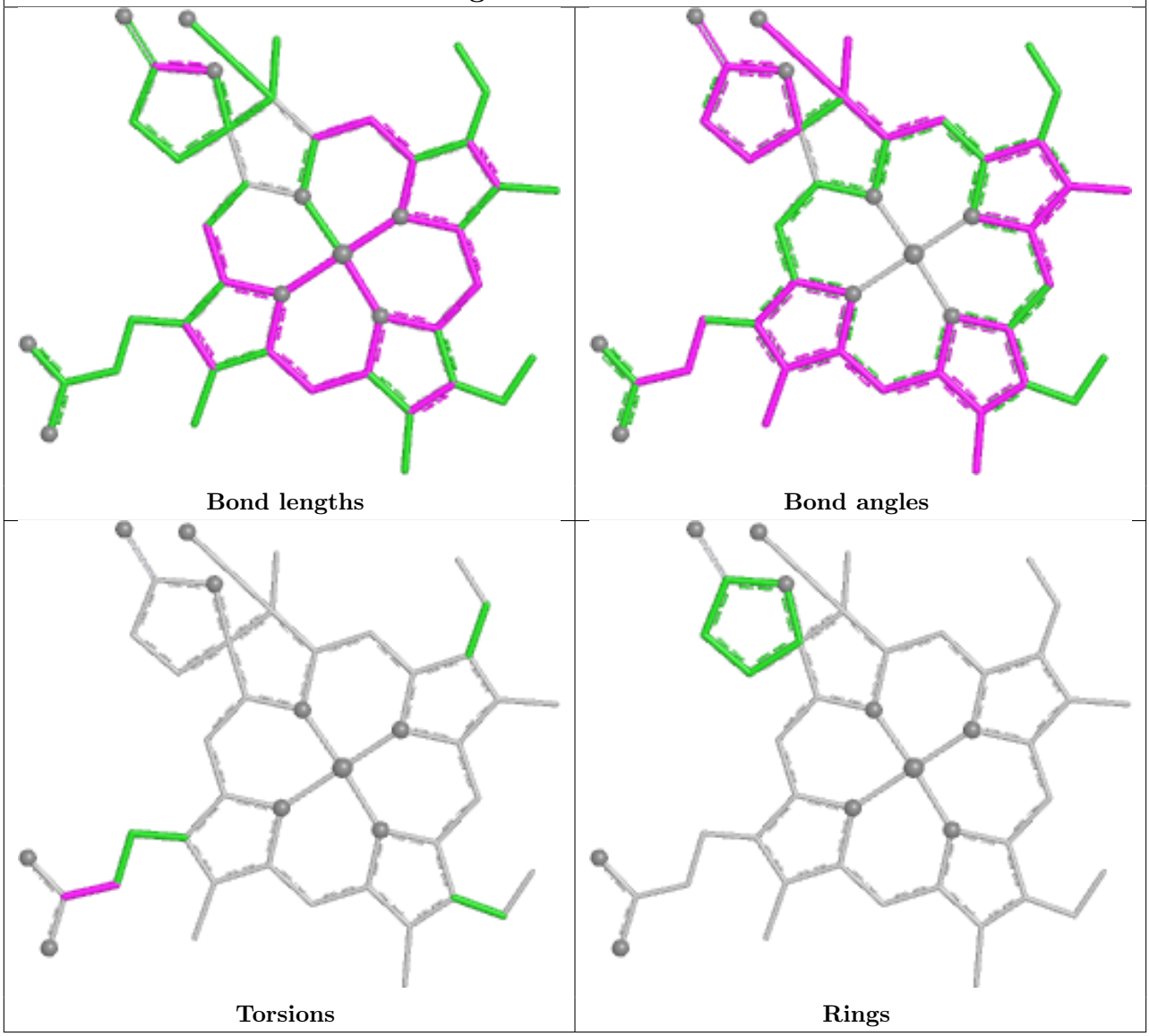
Ligand HDD R 801



Ligand HDD Q 801



Ligand HDD S 801



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	P	747/753 (99%)	-1.23	0	100	100	4, 12, 29, 105	23 (3%)
1	Q	746/753 (99%)	-1.23	0	100	100	4, 13, 28, 74	29 (3%)
1	R	747/753 (99%)	-1.18	0	100	100	4, 14, 33, 94	23 (3%)
1	S	747/753 (99%)	-1.24	0	100	100	4, 12, 28, 87	32 (4%)
All	All	2987/3012 (99%)	-1.22	0	100	100	4, 13, 30, 105	107 (3%)

There are no RSRZ outliers to report.

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	EDO	R	803	4/4	0.81	0.14	42,53,63,72	1
5	PGE	R	808	10/10	0.82	0.14	36,62,103,104	1
6	PEG	Q	824	7/7	0.82	0.12	38,52,73,74	1
4	EDO	P	810	4/4	0.84	0.11	48,63,66,67	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	PGE	P	812	10/10	0.84	0.13	50,74,84,84	1
9	PG4	R	812	13/13	0.84	0.12	50,71,80,82	1
4	EDO	Q	815	4/4	0.85	0.13	45,70,82,83	1
3	GOL	S	812	6/6	0.86	0.10	32,58,64,67	2
4	EDO	Q	819	4/4	0.86	0.10	42,52,54,56	1
6	PEG	P	816	7/7	0.86	0.11	47,59,69,69	1
3	GOL	Q	821	6/6	0.86	0.10	59,77,85,106	2
4	EDO	R	806	4/4	0.86	0.11	58,76,90,95	1
6	PEG	S	817	7/7	0.87	0.11	25,47,63,64	1
4	EDO	Q	817	4/4	0.87	0.10	69,80,91,91	1
6	PEG	P	817	7/7	0.88	0.11	17,21,27,32	17
6	PEG	P	814	7/7	0.89	0.10	29,38,48,52	1
4	EDO	Q	818	4/4	0.89	0.10	52,55,67,68	1
4	EDO	S	811	4/4	0.89	0.11	51,73,76,78	1
3	GOL	Q	820	6/6	0.90	0.09	48,62,69,71	2
4	EDO	P	808	4/4	0.90	0.09	43,56,62,72	1
4	EDO	S	808	4/4	0.90	0.10	30,39,52,52	1
4	EDO	Q	816	4/4	0.90	0.09	34,41,54,57	1
4	EDO	R	804	4/4	0.91	0.09	32,49,53,57	1
6	PEG	Q	825	7/7	0.91	0.09	41,50,62,66	1
5	PGE	R	807	10/10	0.91	0.11	12,14,15,15	24
4	EDO	Q	806	4/4	0.91	0.11	49,69,73,79	4
3	GOL	R	809	6/6	0.92	0.09	31,40,49,60	2
4	EDO	S	807	4/4	0.92	0.07	46,53,56,58	1
4	EDO	Q	812	4/4	0.92	0.09	66,72,74,76	1
4	EDO	S	810	4/4	0.92	0.09	32,42,52,52	1
4	EDO	P	806	4/4	0.92	0.09	36,50,54,58	1
3	GOL	S	802	6/6	0.93	0.10	15,18,30,34	14
4	EDO	S	806	4/4	0.93	0.09	42,56,62,68	1
3	GOL	Q	802	6/6	0.93	0.09	16,22,35,38	0
4	EDO	Q	809	4/4	0.93	0.08	34,40,43,44	1
6	PEG	S	816	7/7	0.93	0.08	21,27,38,39	1
4	EDO	Q	811	4/4	0.93	0.09	38,43,50,51	1
6	PEG	P	815	7/7	0.93	0.08	35,42,51,52	1
3	GOL	S	813	6/6	0.94	0.09	19,25,34,45	2
4	EDO	S	803	4/4	0.94	0.07	33,40,46,48	1
6	PEG	Q	822	7/7	0.94	0.07	19,30,39,40	1
4	EDO	S	804	4/4	0.94	0.16	23,26,29,30	1
4	EDO	P	804	4/4	0.94	0.09	6,32,40,43	1
3	GOL	R	802	6/6	0.94	0.10	16,20,37,45	14
3	GOL	P	802	6/6	0.94	0.10	17,24,34,45	0
4	EDO	S	809	4/4	0.94	0.08	38,48,54,68	1

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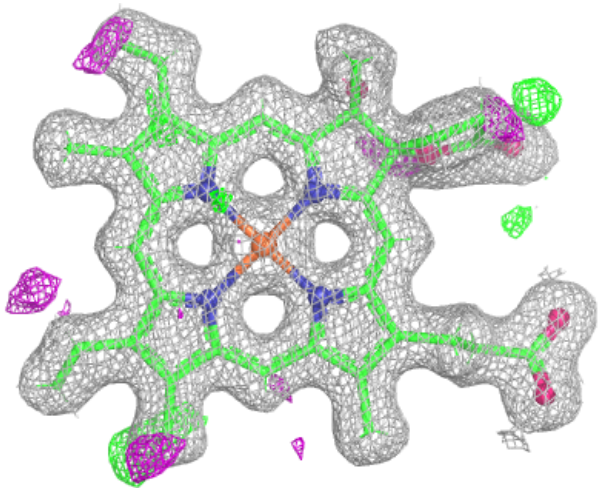
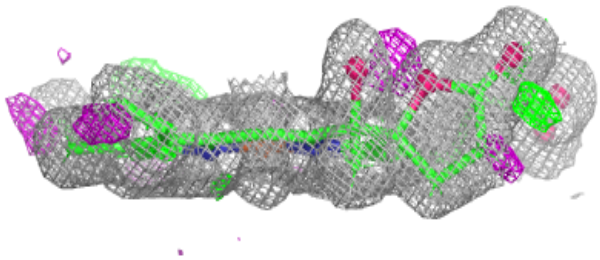
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	EDO	Q	808	4/4	0.95	0.09	22,26,29,32	1
3	GOL	R	810	6/6	0.95	0.10	22,27,39,55	2
4	EDO	P	809	4/4	0.95	0.07	21,24,34,35	1
4	EDO	P	805	4/4	0.95	0.06	28,40,50,58	1
4	EDO	R	805	4/4	0.95	0.09	23,26,38,38	1
4	EDO	Q	813	4/4	0.95	0.06	35,38,51,54	1
4	EDO	Q	803	4/4	0.95	0.08	30,38,43,44	1
3	GOL	P	813	6/6	0.95	0.08	16,24,43,50	2
8	MG	S	815	1/1	0.95	0.12	49,49,49,49	0
4	EDO	Q	807	4/4	0.95	0.08	29,35,40,43	1
4	EDO	Q	814	4/4	0.96	0.08	20,30,42,54	1
7	SO4	P	818	5/5	0.96	0.09	35,37,49,51	5
7	SO4	S	814	5/5	0.96	0.08	41,50,64,68	0
4	EDO	Q	810	4/4	0.96	0.06	30,35,42,44	1
6	PEG	Q	823	7/7	0.96	0.08	18,33,55,56	1
4	EDO	S	805	4/4	0.97	0.05	25,32,37,38	1
4	EDO	P	807	4/4	0.97	0.05	32,35,45,46	1
4	EDO	Q	804	4/4	0.97	0.07	23,26,31,32	1
8	MG	R	811	1/1	0.98	0.13	41,41,41,41	0
4	EDO	P	803	4/4	0.98	0.06	23,28,29,29	1
4	EDO	Q	805	4/4	0.98	0.09	23,33,69,69	1
2	HDD	R	801	44/44	0.99	0.03	8,10,15,19	1
4	EDO	P	811	4/4	0.99	0.03	25,30,38,40	0
2	HDD	S	801	44/44	0.99	0.03	7,9,15,17	1
2	HDD	P	801	44/44	0.99	0.03	7,9,15,20	1
2	HDD	Q	801	44/44	0.99	0.04	7,9,14,18	1

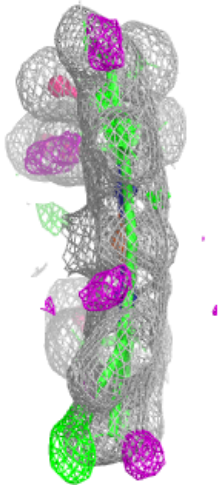
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HDD R 801:

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

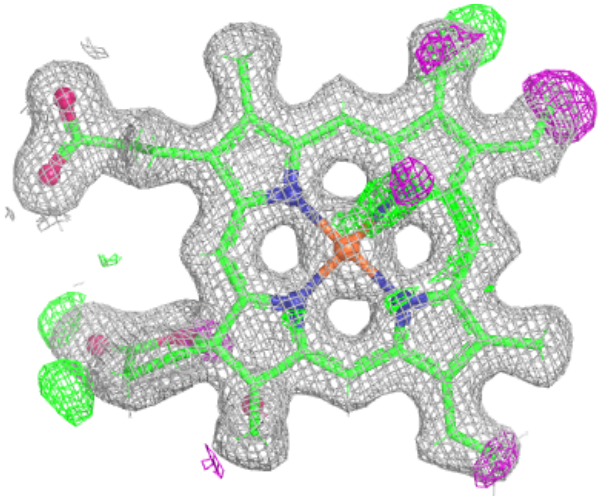


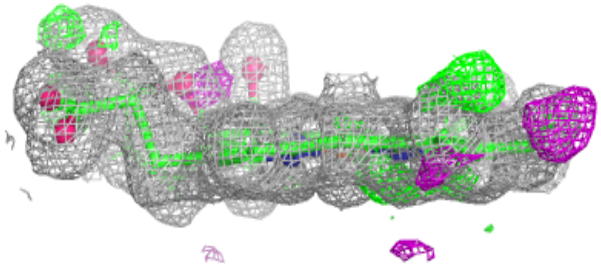


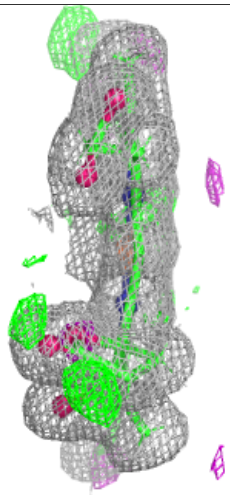


Electron density around HDD S 801:

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

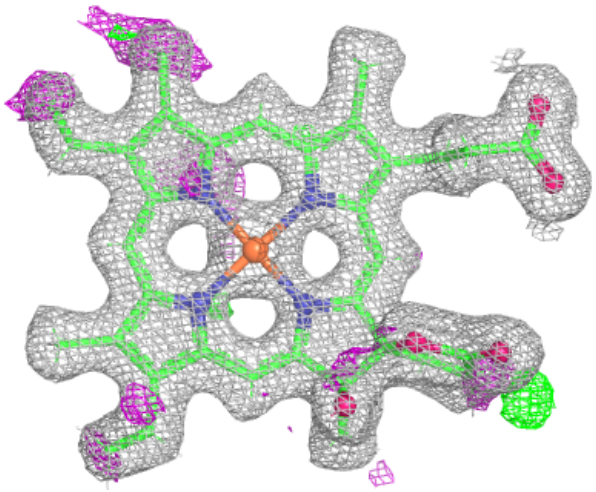


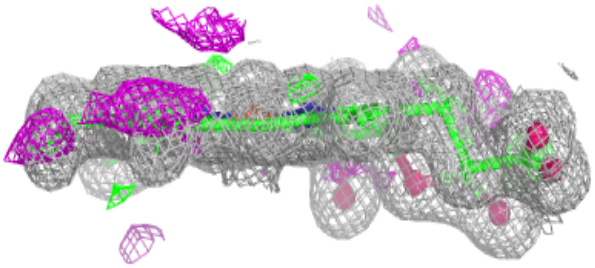


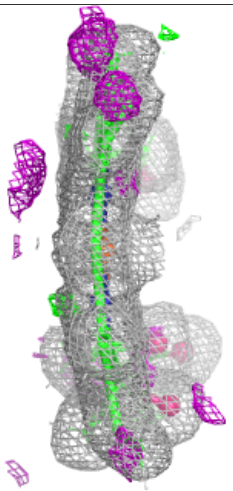


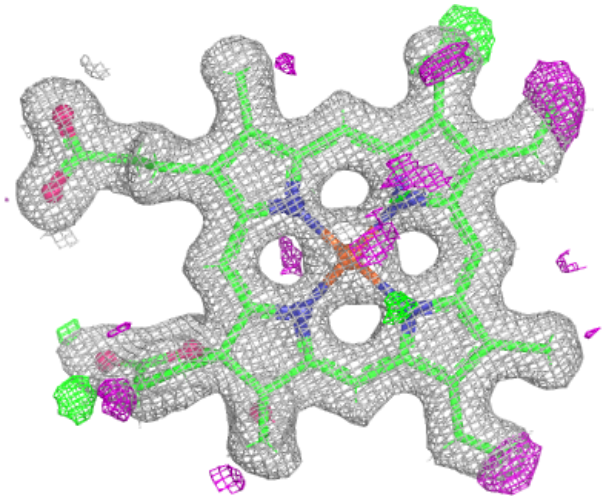
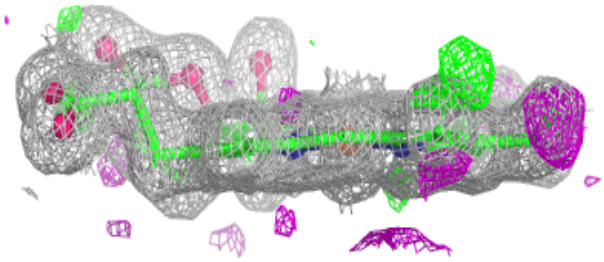
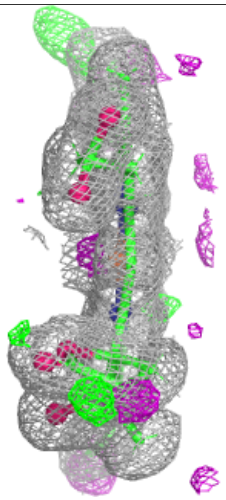
Electron density around HDD P 801:

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 HDD Q 801: 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.