Full wwPDB X-ray Structure Validation Report (i)

Sep 25, 2023 – 01:40 PM EDT

PDB ID	:	5WGM
Title	:	Crystal structure of Danio rerio histone deacetylase 6 catalytic domain 2 in complex with ACY-1083
Authors	:	Porter, N.J.; Christianson, D.W.
Deposited on	:	2017-07-14
Resolution	:	1.75 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:

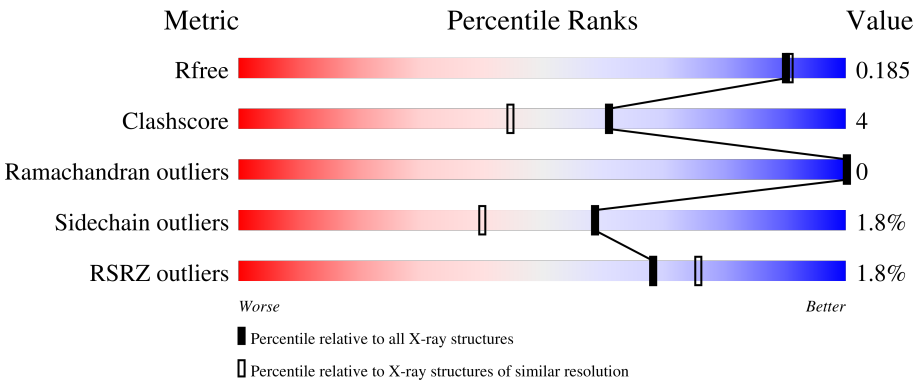
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 1.75 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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	A	364	2% 95% 5%
1	B	364	2% 93% 7%
1	C	364	% 91% 9%

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
5	EDO	B	807	-	-	X	-
6	PGE	A	816	-	-	X	-
6	PGE	C	816	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 9882 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 Hdac6 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	364	2904	1816	522	547	19	0	12	0
1	B	363	2859	1793	510	537	19	0	8	0
1	C	361	2867	1796	515	537	19	0	11	0

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	435	SER	-	expression tag	UNP A7YT55
A	436	ASN	-	expression tag	UNP A7YT55
A	437	ALA	-	expression tag	UNP A7YT55
A	438	GLY	-	expression tag	UNP A7YT55
A	439	GLY	-	expression tag	UNP A7YT55
B	435	SER	-	expression tag	UNP A7YT55
B	436	ASN	-	expression tag	UNP A7YT55
B	437	ALA	-	expression tag	UNP A7YT55
B	438	GLY	-	expression tag	UNP A7YT55
B	439	GLY	-	expression tag	UNP A7YT55
C	435	SER	-	expression tag	UNP A7YT55
C	436	ASN	-	expression tag	UNP A7YT55
C	437	ALA	-	expression tag	UNP A7YT55
C	438	GLY	-	expression tag	UNP A7YT55
C	439	GLY	-	expression tag	UNP A7YT55

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	A	1	1	1	0	0

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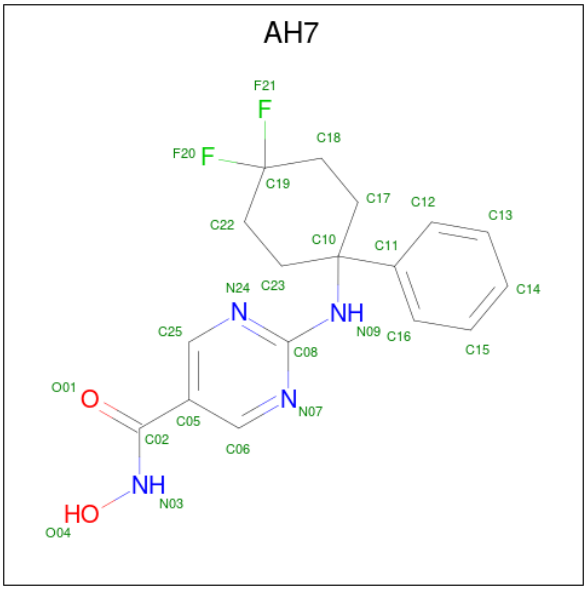
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	B	1	1	1	0	0
2	C	1	1	1	0	0

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

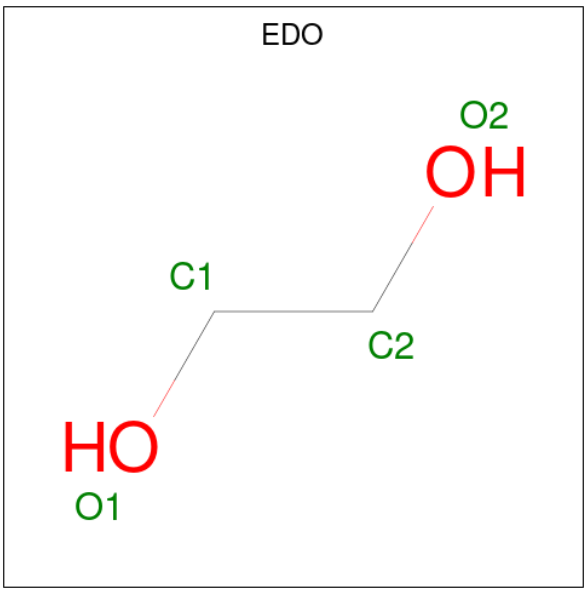
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	K		
3	A	2	2	2	0	0
3	B	2	2	2	0	0
3	C	2	2	2	0	0

- Molecule 4 is 2-[(4,4-difluoro-1-phenylcyclohexyl)amino]-N-hydroxypyrimidine-5-carboxamide (three-letter code: AH7) (formula: $C_{17}H_{18}F_2N_4O_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
4	A	1	25	17	2	4	2	0	0
4	B	1	25	17	2	4	2	0	0
4	C	1	25	17	2	4	2	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	4	2	2	0	0
5	A	1	4	2	2	0	0
5	A	1	4	2	2	0	0
5	A	1	4	2	2	0	0
5	A	1	4	2	2	0	0
5	A	1	4	2	2	0	0
5	A	1	4	2	2	0	0
5	A	1	4	2	2	0	0
5	A	1	4	2	2	0	0
5	A	1	4	2	2	0	0
5	A	1	4	2	2	0	0
5	A	1	4	2	2	0	0
5	B	1	4	2	2	0	0
5	B	1	4	2	2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	B	1	4	2	2	0	0
5	B	1	4	2	2	0	0
5	B	1	4	2	2	0	0
5	B	1	4	2	2	0	0
5	B	1	4	2	2	0	0
5	B	1	4	2	2	0	0
5	B	1	4	2	2	0	0
5	B	1	4	2	2	0	0
5	B	1	4	2	2	0	0
5	B	1	8	4	4	0	1
5	B	1	4	2	2	0	0
5	B	1	4	2	2	0	0
5	B	1	4	2	2	0	0
5	C	1	4	2	2	0	0
5	C	1	4	2	2	0	0
5	C	1	4	2	2	0	0
5	C	1	4	2	2	0	0
5	C	1	8	4	4	0	1
5	C	1	4	2	2	0	0
5	C	1	4	2	2	0	0
5	C	1	4	2	2	4	0

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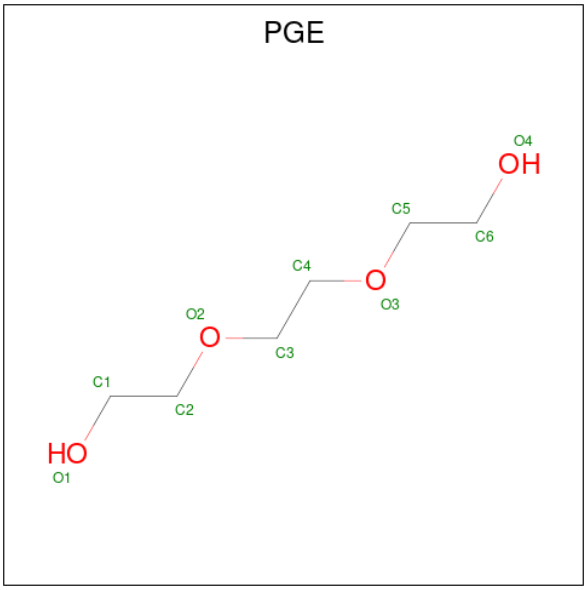
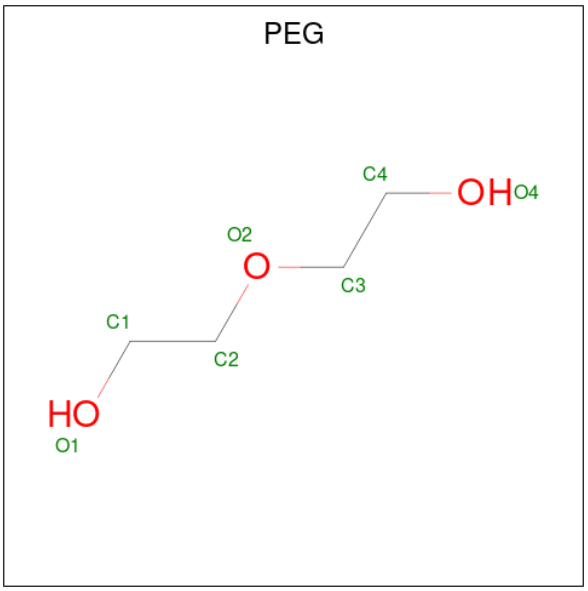
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	C	1	4	2	2	0	0
			Total	C	O		
5	C	1	4	2	2	0	0
			Total	C	O		
5	C	1	4	2	2	0	0

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



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

- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 7 4 3	0	0
7	C	1	Total C O 7 4 3	0	0

- Molecule 8 is water.

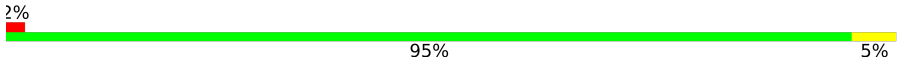
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	340	Total O 345 345	0	5
8	B	311	Total O 317 317	0	6
8	C	311	Total O 316 316	0	5

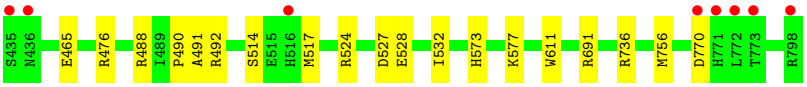
3 Residue-property plots (i)

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: Hdac6 protein

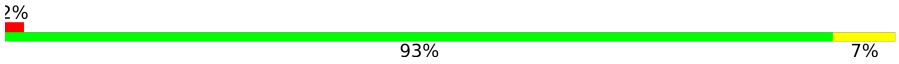
Chain A:

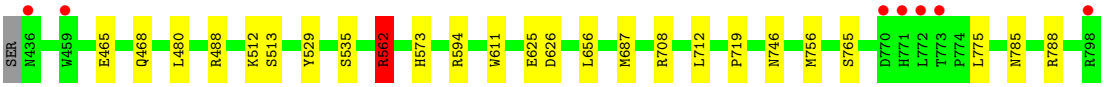




- Molecule 1: Hdac6 protein

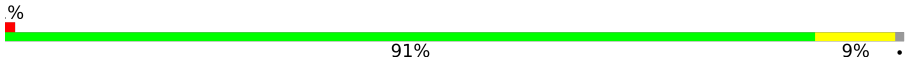
Chain B:

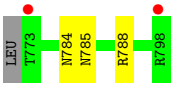




- Molecule 1: Hdac6 protein

Chain C:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	97.81Å 174.30Å 149.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.95 – 1.75 49.95 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.95-1.75) 99.9 (49.95-1.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.26 (at 1.75Å)	Xtriage
Refinement program	PHENIX (dev_2776: ???)	Depositor
R, R_{free}	0.159 , 0.185 0.159 , 0.185	Depositor DCC
R_{free} test set	6481 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	14.8	Xtriage
Anisotropy	0.396	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 44.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.026 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.028 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	9882	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% 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: K, ZN, EDO, AH7, PGE, PEG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.56	0/2981	0.65	0/4042
1	B	0.56	0/2930	0.68	1/3976 (0.0%)
1	C	0.53	0/2939	0.66	0/3986
All	All	0.55	0/8850	0.66	1/12004 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	562	ARG	NE-CZ-NH2	5.25	122.93	120.30

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	A	2904	0	2790	18	0
1	B	2859	0	2731	25	0
1	C	2867	0	2747	30	2
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	2	0	0	0	0
3	C	2	0	0	0	0
4	A	25	0	0	0	0
4	B	25	0	0	0	0
4	C	25	0	0	0	0
5	A	44	0	66	13	2
5	B	64	0	96	17	0
5	C	48	0	72	9	0
6	A	10	0	14	6	0
6	C	10	0	14	7	0
7	A	7	0	9	0	0
7	C	7	0	10	3	0
8	A	345	0	0	5	1
8	B	317	0	0	4	1
8	C	316	0	0	4	1
All	All	9882	0	8549	78	4

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 4.

All (78) 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:C:485:ARG:HH21	6:C:816:PGE:H42	1.31	0.95
1:C:762:LEU:HD23	6:C:816:PGE:H1	1.53	0.90
1:A:488:ARG:HH12	5:A:805:EDO:H21	1.40	0.85
1:C:485:ARG:HE	6:C:816:PGE:H5	1.43	0.84
6:A:816:PGE:H52	1:B:746:ASN:ND2	1.99	0.77
1:B:562:ARG:HG3	1:B:562:ARG:HH21	1.52	0.73
1:C:476:ARG:HH22	5:C:809[B]:EDO:H22	1.54	0.72
1:C:485:ARG:HH21	6:C:816:PGE:C4	2.03	0.71
1:C:785:ASN:OD1	1:C:788[B]:ARG:NH2	2.24	0.70
1:A:532:ILE:O	5:A:806:EDO:H12	1.91	0.70
5:B:816[B]:EDO:H21	1:C:672:LYS:HB2	1.74	0.69
1:A:492:ARG:HD2	5:A:811:EDO:H21	1.75	0.68
1:C:756[A]:MET:HG2	8:C:970:HOH:O	1.95	0.66
5:C:806:EDO:H11	8:C:1081:HOH:O	1.96	0.64
1:C:485:ARG:NH2	6:C:816:PGE:H42	2.08	0.64
1:B:513:SER:HB3	5:B:810:EDO:H21	1.79	0.63
1:A:488:ARG:NH1	5:A:805:EDO:H21	2.11	0.63
1:B:687:MET:HG3	5:B:818:EDO:H21	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:816:PGE:H52	1:B:746:ASN:HD21	1.64	0.60
6:A:816:PGE:H42	1:B:746:ASN:HD21	1.68	0.59
1:A:488:ARG:HH12	5:A:805:EDO:C2	2.14	0.58
6:A:816:PGE:H42	1:B:746:ASN:ND2	2.18	0.58
1:C:485:ARG:HE	6:C:816:PGE:C5	2.16	0.58
1:B:756[A]:MET:HG2	8:B:1019:HOH:O	2.04	0.57
5:A:810:EDO:H12	8:B:919:HOH:O	2.04	0.56
1:C:605:ARG:CD	7:C:817:PEG:H32	2.35	0.56
1:C:472:ARG:HG2	5:C:806:EDO:H21	1.87	0.56
1:A:756[B]:MET:HG2	8:A:936:HOH:O	2.04	0.56
1:A:527:ASP:OD1	5:A:806:EDO:H11	2.06	0.56
1:C:645:ASN:OD1	5:C:813:EDO:H21	2.06	0.56
1:B:480:LEU:HD22	5:B:812:EDO:H11	1.89	0.55
1:B:765:SER:OG	5:B:816[A]:EDO:H22	2.07	0.54
1:C:605:ARG:HD2	7:C:817:PEG:H32	1.90	0.54
1:A:490:PRO:HA	5:A:809:EDO:H22	1.92	0.51
1:B:488:ARG:HH12	5:B:807:EDO:H22	1.74	0.51
5:B:816[A]:EDO:H21	1:C:672:LYS:HB2	1.93	0.50
1:C:537:GLU:OE2	5:C:807:EDO:H21	2.11	0.50
1:A:476:ARG:NH1	6:A:816:PGE:H62	2.26	0.50
1:C:724:HIS:CE1	5:C:814:EDO:H21	2.47	0.49
1:B:785:ASN:OD1	1:B:788[A]:ARG:NH2	2.46	0.49
1:B:512[A]:LYS:HG2	5:B:810:EDO:H22	1.95	0.48
1:B:535:SER:HB2	5:B:809:EDO:H22	1.94	0.48
1:A:528:GLU:HB3	5:A:808:EDO:H22	1.96	0.48
1:C:711:PRO:HG2	1:C:712:LEU:HD13	1.95	0.47
1:B:594:ARG:NH1	1:B:626:ASP:OD2	2.46	0.47
5:B:816[B]:EDO:H21	1:C:672:LYS:HD2	1.97	0.47
1:C:565[A]:VAL:HG23	1:C:761:LEU:HD12	1.97	0.47
1:B:708:ARG:HD3	8:B:1006:HOH:O	2.14	0.47
1:C:746:ASN:HB3	1:C:749[A]:SER:HB2	1.97	0.47
1:A:476:ARG:HH12	6:A:816:PGE:H62	1.77	0.47
5:B:818:EDO:H11	8:B:953:HOH:O	2.15	0.46
5:C:806:EDO:H12	8:C:1116:HOH:O	2.15	0.46
1:C:456:HIS:CE1	5:C:807:EDO:H12	2.50	0.46
5:A:814:EDO:H11	8:A:916:HOH:O	2.16	0.45
1:B:488:ARG:HH22	5:B:807:EDO:H22	1.82	0.45
1:C:485:ARG:NE	6:C:816:PGE:H5	2.20	0.45
1:A:691:ARG:HD3	8:A:984:HOH:O	2.17	0.45
1:C:515:GLU:HG2	8:C:1043:HOH:O	2.16	0.45
1:B:488:ARG:HH22	5:B:807:EDO:C2	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:453:MET:O	5:C:810:EDO:H22	2.18	0.44
1:A:527:ASP:OD1	5:A:806:EDO:C1	2.65	0.44
1:C:565[B]:VAL:HG22	1:C:754:MET:CE	2.48	0.43
1:A:736[B]:ARG:CZ	8:A:1025:HOH:O	2.66	0.43
1:B:719:PRO:HB3	1:B:756[B]:MET:HG3	2.01	0.43
1:C:499:LEU:HD11	1:C:543:LEU:HD21	2.01	0.43
1:C:565[B]:VAL:HG22	1:C:754:MET:HE2	2.00	0.43
1:A:524[A]:ARG:HB2	5:A:815:EDO:H22	2.01	0.43
1:C:605:ARG:HD3	7:C:817:PEG:H32	1.99	0.43
1:B:512[A]:LYS:CG	5:B:810:EDO:H22	2.48	0.42
1:A:514:SER:HA	1:A:517:MET:HG3	2.01	0.42
1:B:529:TYR:CZ	5:B:813:EDO:H12	2.55	0.42
1:B:625:GLU:HG2	1:B:656:LEU:HB2	2.01	0.42
1:B:765:SER:CB	5:B:816[B]:EDO:H22	2.50	0.42
1:A:577:LYS:NZ	8:A:916:HOH:O	2.48	0.41
1:B:562:ARG:HH21	1:B:562:ARG:CG	2.28	0.41
1:B:488:ARG:NH1	5:B:807:EDO:H22	2.36	0.40
1:A:491:ALA:H	5:A:809:EDO:C1	2.35	0.40
1:C:784:ASN:O	1:C:788[B]:ARG:HG3	2.21	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:497:GLU:OE2	5:A:811:EDO:O1[5_545]	1.73	0.47
1:C:497:GLU:OE1	5:A:811:EDO:O1[5_545]	1.80	0.40
8:A:1208:HOH:O	8:B:1178:HOH:O[3_554]	2.14	0.06
8:C:997:HOH:O	8:C:997:HOH:O[4_555]	2.19	0.01

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	374/364 (103%)	366 (98%)	8 (2%)	0	100	100
1	B	369/364 (101%)	362 (98%)	7 (2%)	0	100	100
1	C	368/364 (101%)	361 (98%)	7 (2%)	0	100	100
All	All	1111/1092 (102%)	1089 (98%)	22 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	313/305 (103%)	309 (99%)	4 (1%)	69	54
1	B	304/305 (100%)	297 (98%)	7 (2%)	50	28
1	C	306/305 (100%)	301 (98%)	5 (2%)	62	45
All	All	923/915 (101%)	907 (98%)	16 (2%)	59	42

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	465	GLU
1	A	573	HIS
1	A	611	TRP
1	A	770	ASP
1	B	465	GLU
1	B	468	GLN
1	B	562	ARG
1	B	573	HIS
1	B	611	TRP
1	B	712	LEU
1	B	775	LEU
1	C	441	SER
1	C	465	GLU
1	C	530	ASN
1	C	573	HIS

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Mol	Chain	Res	Type
1	C	611	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 55 ligands modelled in this entry, 9 are monoatomic - leaving 46 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	EDO	C	805	-	3,3,3	0.46	0	2,2,2	0.46	0
5	EDO	B	817	-	3,3,3	0.48	0	2,2,2	0.26	0
5	EDO	C	813	-	3,3,3	0.46	0	2,2,2	0.19	0
5	EDO	C	812	-	3,3,3	0.40	0	2,2,2	0.23	0
5	EDO	B	813	-	3,3,3	0.38	0	2,2,2	0.44	0
7	PEG	A	817	-	6,6,6	0.96	0	5,5,5	0.87	0
5	EDO	A	812	-	3,3,3	0.39	0	2,2,2	0.48	0
5	EDO	A	805	-	3,3,3	0.45	0	2,2,2	0.34	0
5	EDO	A	815	-	3,3,3	0.70	0	2,2,2	0.08	0
5	EDO	A	813	-	3,3,3	0.58	0	2,2,2	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	EDO	C	806	-	3,3,3	0.36	0	2,2,2	0.71	0
5	EDO	B	809	-	3,3,3	0.43	0	2,2,2	0.37	0
5	EDO	B	805	-	3,3,3	0.60	0	2,2,2	0.34	0
5	EDO	B	815	-	3,3,3	0.43	0	2,2,2	0.50	0
6	PGE	C	816	-	9,9,9	0.37	0	8,8,8	0.55	0
5	EDO	C	814	-	3,3,3	0.49	0	2,2,2	0.40	0
5	EDO	B	816[B]	-	3,3,3	0.58	0	2,2,2	0.47	0
5	EDO	C	807	-	3,3,3	0.41	0	2,2,2	0.66	0
6	PGE	A	816	-	9,9,9	0.35	0	8,8,8	0.61	0
5	EDO	B	807	-	3,3,3	0.45	0	2,2,2	0.19	0
5	EDO	C	808	-	3,3,3	0.47	0	2,2,2	0.21	0
4	AH7	C	804	2	25,27,27	2.15	7 (28%)	33,39,39	1.79	7 (21%)
5	EDO	A	808	-	3,3,3	0.42	0	2,2,2	0.38	0
5	EDO	C	811	-	3,3,3	0.53	0	2,2,2	0.29	0
7	PEG	C	817	-	6,6,6	0.74	0	5,5,5	0.59	0
5	EDO	C	810	-	3,3,3	0.72	0	2,2,2	0.62	0
5	EDO	B	808	-	3,3,3	0.47	0	2,2,2	0.28	0
4	AH7	B	804	2	25,27,27	2.46	10 (40%)	33,39,39	2.18	7 (21%)
5	EDO	A	811	1	3,3,3	0.61	0	2,2,2	0.52	0
5	EDO	C	809[A]	-	3,3,3	0.52	0	2,2,2	0.15	0
5	EDO	B	814	-	3,3,3	0.47	0	2,2,2	0.08	0
5	EDO	A	806	-	3,3,3	0.56	0	2,2,2	0.56	0
5	EDO	B	812	-	3,3,3	0.57	0	2,2,2	0.04	0
5	EDO	C	815	-	3,3,3	0.48	0	2,2,2	0.32	0
5	EDO	B	806	-	3,3,3	0.24	0	2,2,2	0.79	0
5	EDO	A	809	-	3,3,3	0.17	0	2,2,2	0.94	0
5	EDO	A	807	-	3,3,3	0.57	0	2,2,2	0.25	0
5	EDO	B	810	-	3,3,3	0.40	0	2,2,2	0.53	0
5	EDO	A	814	-	3,3,3	0.42	0	2,2,2	0.37	0
5	EDO	B	819	-	3,3,3	0.56	0	2,2,2	0.24	0
5	EDO	A	810	-	3,3,3	0.22	0	2,2,2	1.44	1 (50%)
5	EDO	B	816[A]	-	3,3,3	0.47	0	2,2,2	0.40	0
5	EDO	C	809[B]	-	3,3,3	0.58	0	2,2,2	0.27	0
5	EDO	B	811	-	3,3,3	0.55	0	2,2,2	0.30	0
4	AH7	A	804	2	25,27,27	1.60	5 (20%)	33,39,39	2.29	10 (30%)
5	EDO	B	818	-	3,3,3	0.45	0	2,2,2	0.49	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	C	805	-	-	0/1/1/1	-
5	EDO	B	817	-	-	1/1/1/1	-
5	EDO	C	813	-	-	1/1/1/1	-
5	EDO	C	812	-	-	1/1/1/1	-
5	EDO	B	813	-	-	0/1/1/1	-
7	PEG	A	817	-	-	4/4/4/4	-
5	EDO	A	812	-	-	0/1/1/1	-
5	EDO	A	805	-	-	1/1/1/1	-
5	EDO	A	815	-	-	1/1/1/1	-
5	EDO	A	813	-	-	1/1/1/1	-
5	EDO	C	806	-	-	0/1/1/1	-
5	EDO	B	809	-	-	0/1/1/1	-
5	EDO	B	805	-	-	0/1/1/1	-
5	EDO	B	815	-	-	1/1/1/1	-
6	PGE	C	816	-	-	4/7/7/7	-
5	EDO	C	814	-	-	0/1/1/1	-
5	EDO	B	816[B]	-	-	1/1/1/1	-
5	EDO	C	807	-	-	0/1/1/1	-
6	PGE	A	816	-	-	6/7/7/7	-
5	EDO	B	807	-	-	1/1/1/1	-
5	EDO	C	808	-	-	1/1/1/1	-
4	AH7	C	804	2	-	2/17/31/31	0/3/3/3
5	EDO	A	808	-	-	1/1/1/1	-
5	EDO	C	811	-	-	0/1/1/1	-
7	PEG	C	817	-	-	2/4/4/4	-
5	EDO	C	810	-	-	1/1/1/1	-
5	EDO	B	808	-	-	1/1/1/1	-
4	AH7	B	804	2	-	2/17/31/31	0/3/3/3
5	EDO	A	811	1	-	0/1/1/1	-
5	EDO	C	809[A]	-	-	1/1/1/1	-
5	EDO	B	814	-	-	0/1/1/1	-
5	EDO	A	806	-	-	1/1/1/1	-
5	EDO	B	812	-	-	1/1/1/1	-
5	EDO	C	815	-	-	0/1/1/1	-
5	EDO	B	806	-	-	1/1/1/1	-
5	EDO	A	809	-	-	1/1/1/1	-
5	EDO	A	807	-	-	1/1/1/1	-
5	EDO	B	810	-	-	0/1/1/1	-
5	EDO	A	814	-	-	0/1/1/1	-
5	EDO	B	819	-	-	0/1/1/1	-
5	EDO	A	810	-	-	0/1/1/1	-
5	EDO	B	816[A]	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	C	809[B]	-	-	0/1/1/1	-
5	EDO	B	811	-	-	1/1/1/1	-
4	AH7	A	804	2	-	2/17/31/31	0/3/3/3
5	EDO	B	818	-	-	1/1/1/1	-

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	804	AH7	C23-C10	5.45	1.61	1.54
4	B	804	AH7	C18-C19	4.91	1.55	1.50
4	C	804	AH7	C23-C10	4.68	1.60	1.54
4	B	804	AH7	C08-N09	4.68	1.41	1.34
4	C	804	AH7	C18-C19	3.99	1.54	1.50
4	C	804	AH7	C08-N09	3.86	1.40	1.34
4	A	804	AH7	C08-N09	3.30	1.39	1.34
4	B	804	AH7	C08-N07	3.22	1.39	1.34
4	C	804	AH7	C08-N24	3.19	1.39	1.34
4	B	804	AH7	C25-C05	3.07	1.44	1.39
4	B	804	AH7	C22-C19	3.06	1.53	1.50
4	C	804	AH7	C05-C02	-2.80	1.44	1.50
4	A	804	AH7	C17-C10	2.71	1.57	1.54
4	B	804	AH7	C08-N24	2.45	1.38	1.34
4	A	804	AH7	C06-C05	2.44	1.43	1.39
4	C	804	AH7	C02-N03	2.35	1.35	1.32
4	A	804	AH7	C05-C02	-2.27	1.45	1.50
4	C	804	AH7	C15-C14	2.16	1.43	1.38
4	B	804	AH7	F20-C19	2.14	1.42	1.38
4	B	804	AH7	F21-C19	2.12	1.42	1.38
4	A	804	AH7	C23-C22	-2.04	1.46	1.53
4	B	804	AH7	C05-C02	-2.03	1.46	1.50

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	804	AH7	F20-C19-C22	8.04	114.60	109.37
4	B	804	AH7	C23-C22-C19	-6.67	106.98	110.93
4	B	804	AH7	F21-C19-C18	-5.91	105.52	109.37
4	C	804	AH7	C17-C18-C19	-5.88	107.44	110.93
4	A	804	AH7	N24-C08-N07	-4.69	121.49	126.43
4	B	804	AH7	N24-C08-N07	-4.56	121.63	126.43
4	C	804	AH7	N24-C08-N07	-4.43	121.77	126.43
4	A	804	AH7	F21-C19-C22	-4.18	106.64	109.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	804	AH7	C17-C18-C19	-3.87	108.64	110.93
4	A	804	AH7	F21-C19-C18	-3.25	107.25	109.37
4	B	804	AH7	C05-C02-N03	3.22	121.31	116.16
4	C	804	AH7	F20-C19-C18	2.87	111.23	109.37
4	A	804	AH7	C18-C17-C10	2.84	115.57	112.15
4	A	804	AH7	C17-C18-C19	-2.79	109.28	110.93
4	C	804	AH7	F20-C19-C22	2.79	111.18	109.37
4	C	804	AH7	C22-C23-C10	2.76	115.48	112.15
4	A	804	AH7	F20-C19-C18	2.75	111.15	109.37
4	B	804	AH7	F20-C19-C18	2.73	111.14	109.37
4	A	804	AH7	C06-N07-C08	2.73	120.00	115.88
4	A	804	AH7	C25-N24-C08	2.46	119.59	115.88
4	C	804	AH7	C23-C22-C19	-2.30	109.57	110.93
4	A	804	AH7	C05-C02-N03	2.17	119.64	116.16
4	B	804	AH7	C25-N24-C08	2.14	119.11	115.88
4	C	804	AH7	C06-N07-C08	2.06	118.99	115.88
5	A	810	EDO	O2-C2-C1	-2.03	97.28	111.91

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	816	PGE	O3-C5-C6-O4
6	A	816	PGE	O3-C5-C6-O4
7	A	817	PEG	O1-C1-C2-O2
7	A	817	PEG	O2-C3-C4-O4
6	A	816	PGE	O1-C1-C2-O2
5	A	806	EDO	O1-C1-C2-O2
5	A	813	EDO	O1-C1-C2-O2
5	B	807	EDO	O1-C1-C2-O2
5	B	811	EDO	O1-C1-C2-O2
5	B	816[B]	EDO	O1-C1-C2-O2
5	B	817	EDO	O1-C1-C2-O2
5	C	808	EDO	O1-C1-C2-O2
5	C	809[A]	EDO	O1-C1-C2-O2
5	A	815	EDO	O1-C1-C2-O2
5	C	810	EDO	O1-C1-C2-O2
5	C	812	EDO	O1-C1-C2-O2
4	A	804	AH7	C17-C10-N09-C08
4	B	804	AH7	C17-C10-N09-C08
4	C	804	AH7	C17-C10-N09-C08
5	A	805	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	A	808	EDO	O1-C1-C2-O2
5	B	815	EDO	O1-C1-C2-O2
6	C	816	PGE	C4-C3-O2-C2
7	C	817	PEG	C1-C2-O2-C3
7	A	817	PEG	C1-C2-O2-C3
6	A	816	PGE	C1-C2-O2-C3
6	C	816	PGE	C3-C4-O3-C5
7	A	817	PEG	C4-C3-O2-C2
4	A	804	AH7	C23-C10-C11-C16
4	B	804	AH7	C23-C10-C11-C16
4	C	804	AH7	C23-C10-C11-C16
6	A	816	PGE	C3-C4-O3-C5
5	B	806	EDO	O1-C1-C2-O2
5	B	808	EDO	O1-C1-C2-O2
7	C	817	PEG	C4-C3-O2-C2
5	B	818	EDO	O1-C1-C2-O2
5	A	807	EDO	O1-C1-C2-O2
5	A	809	EDO	O1-C1-C2-O2
5	C	813	EDO	O1-C1-C2-O2
6	A	816	PGE	C4-C3-O2-C2
6	A	816	PGE	O2-C3-C4-O3
5	B	812	EDO	O1-C1-C2-O2
6	C	816	PGE	C6-C5-O3-C4

There are no ring outliers.

25 monomers are involved in 57 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	813	EDO	1	0
5	B	813	EDO	1	0
5	A	805	EDO	3	0
5	A	815	EDO	1	0
5	C	806	EDO	3	0
5	B	809	EDO	1	0
6	C	816	PGE	7	0
5	C	814	EDO	1	0
5	B	816[B]	EDO	3	0
5	C	807	EDO	2	0
6	A	816	PGE	6	0
5	B	807	EDO	4	0
5	A	808	EDO	1	0
7	C	817	PEG	3	0

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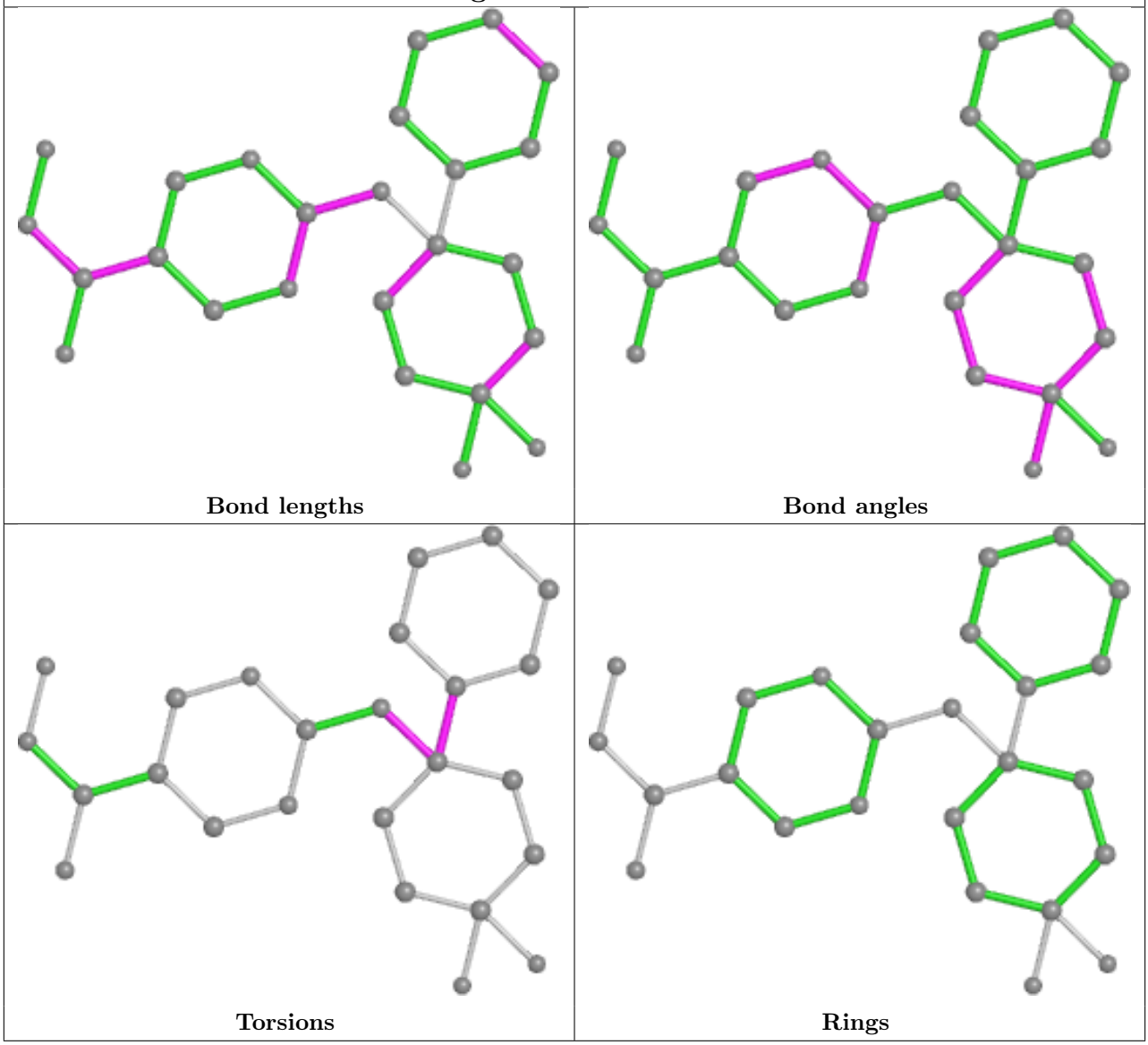
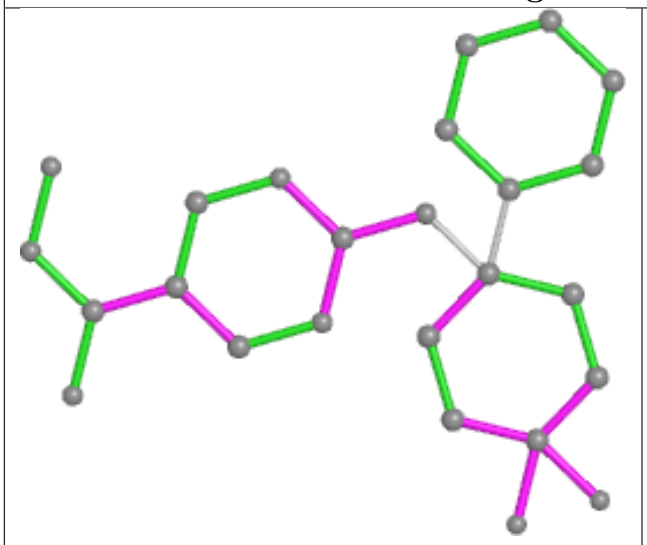
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	810	EDO	1	0
5	A	811	EDO	1	2
5	A	806	EDO	3	0
5	B	812	EDO	1	0
5	A	809	EDO	2	0
5	B	810	EDO	3	0
5	A	814	EDO	1	0
5	A	810	EDO	1	0
5	B	816[A]	EDO	2	0
5	C	809[B]	EDO	1	0
5	B	818	EDO	2	0

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

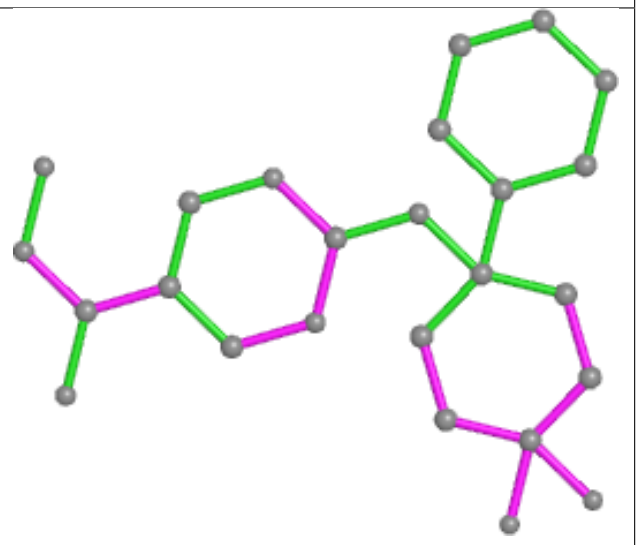
Ligand AH7 C 804



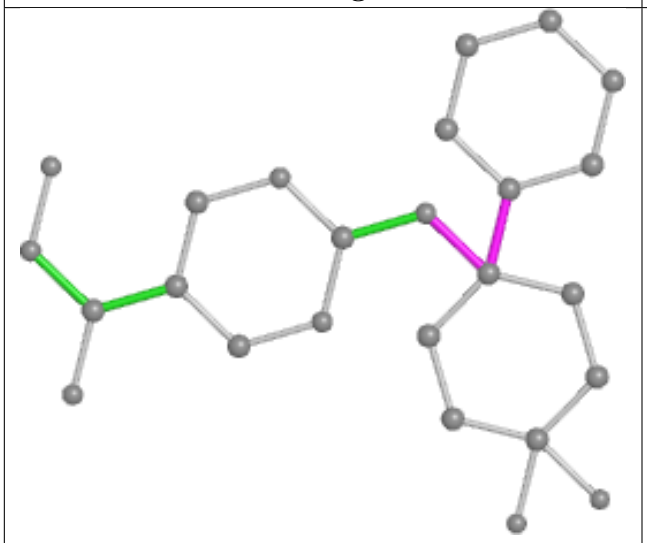
Ligand AH7 B 804



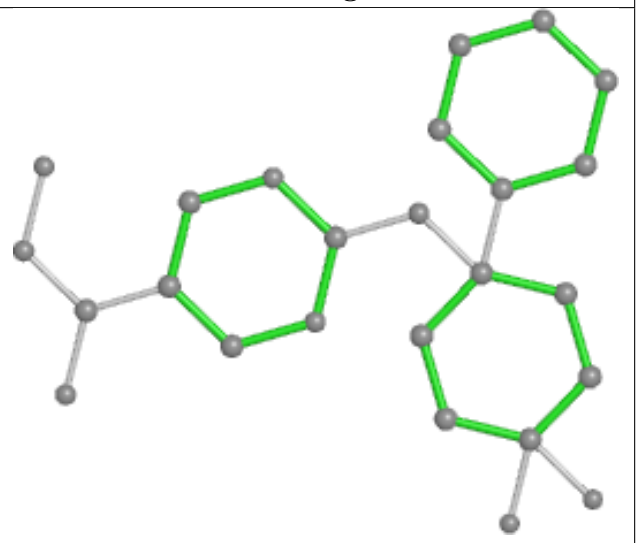
Bond lengths



Bond angles

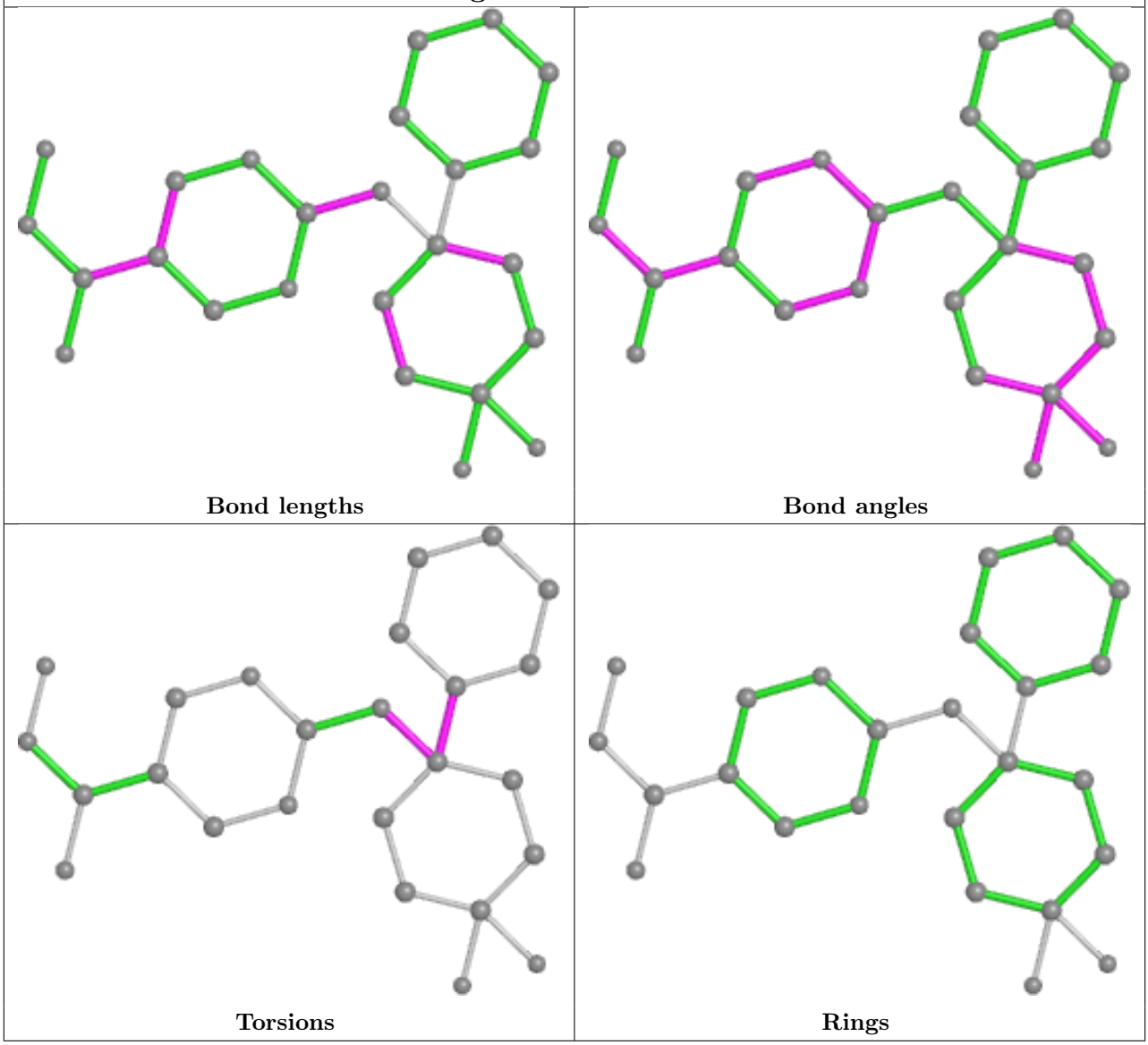


Torsions



Rings

Ligand AH7 A 804



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	364/364 (100%)	-0.18	8 (2%)	62	69	7, 14, 27, 51	1 (0%)
1	B	363/364 (99%)	-0.15	7 (1%)	66	74	7, 14, 28, 58	2 (0%)
1	C	361/364 (99%)	-0.21	5 (1%)	75	82	8, 15, 28, 52	1 (0%)
All	All	1088/1092 (99%)	-0.18	20 (1%)	68	76	7, 14, 28, 58	4 (0%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	773	THR	7.1
1	A	435	SER	5.7
1	B	772	LEU	5.3
1	B	436	ASN	3.8
1	A	771	HIS	3.5
1	A	773	THR	3.5
1	B	771	HIS	3.4
1	A	798	ARG	3.4
1	B	798	ARG	3.2
1	B	773	THR	3.0
1	C	516	HIS	2.9
1	A	772	LEU	2.8
1	A	770	ASP	2.5
1	A	516	HIS	2.4
1	A	436	ASN	2.3
1	C	435	SER	2.3
1	C	497	GLU	2.2
1	B	459	TRP	2.0
1	C	798	ARG	2.0
1	B	770	ASP	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 monosaccharides in this entry.

6.4 Ligands (i)

LIGAND-RSR INFOmissingINFO

6.5 Other polymers (i)

There are no such residues in this entry.