



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 30, 2026 – 01:20 PM UTC

PDB ID : 8HSN / pdb_00008hsn
Title : Crystal structure of DFA I-forming Inulin Lyase from *Streptomyces peucetius* subsp. *caesius* ATCC 27952
Authors : Cheng, M.; Rao, Y.J.; Mu, W.M.
Deposited on : 2022-12-20
Resolution : 1.69 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

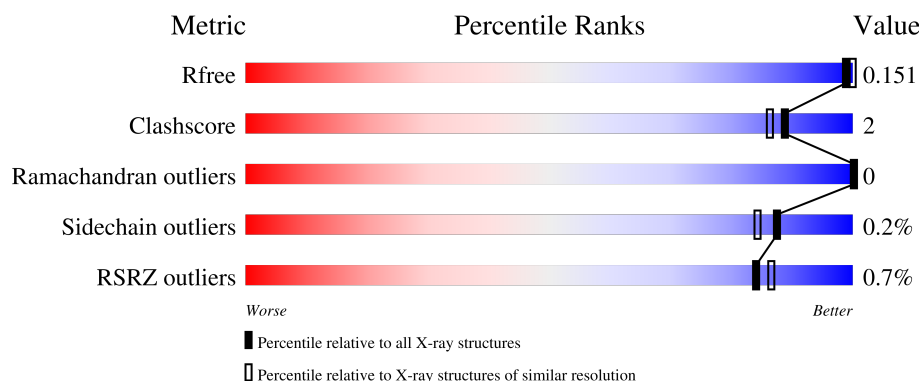
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.69 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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

Mol	Chain	Length	Quality of chain
1	A	400	% 95% 5% •
1	B	400	93% 5% •
1	C	400	% 93% 5% •

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 18817 atoms, of which 9067 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 Fructotransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	395	Total	C	H	N	O	S	0	7	0
			5862	1857	2892	523	584	6			
1	B	394	Total	C	H	N	O	S	0	5	0
			5866	1856	2899	521	584	6			
1	C	395	Total	C	H	N	O	S	0	6	0
			5888	1870	2903	525	584	6			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	395	HIS	-	expression tag	UNP A0A2D3U3Z1
A	396	HIS	-	expression tag	UNP A0A2D3U3Z1
A	397	HIS	-	expression tag	UNP A0A2D3U3Z1
A	398	HIS	-	expression tag	UNP A0A2D3U3Z1
A	399	HIS	-	expression tag	UNP A0A2D3U3Z1
A	400	HIS	-	expression tag	UNP A0A2D3U3Z1
B	395	HIS	-	expression tag	UNP A0A2D3U3Z1
B	396	HIS	-	expression tag	UNP A0A2D3U3Z1
B	397	HIS	-	expression tag	UNP A0A2D3U3Z1
B	398	HIS	-	expression tag	UNP A0A2D3U3Z1
B	399	HIS	-	expression tag	UNP A0A2D3U3Z1
B	400	HIS	-	expression tag	UNP A0A2D3U3Z1
C	395	HIS	-	expression tag	UNP A0A2D3U3Z1
C	396	HIS	-	expression tag	UNP A0A2D3U3Z1
C	397	HIS	-	expression tag	UNP A0A2D3U3Z1
C	398	HIS	-	expression tag	UNP A0A2D3U3Z1
C	399	HIS	-	expression tag	UNP A0A2D3U3Z1
C	400	HIS	-	expression tag	UNP A0A2D3U3Z1

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	B	1	Total	C	H	O	0	0
			14	3	8	3		
2	B	1	Total	C	H	O	0	0
			14	3	8	3		
2	B	1	Total	C	H	O	0	0
			14	3	8	3		
2	B	1	Total	C	H	O	0	0
			14	3	8	3		
2	C	1	Total	C	H	O	0	0
			14	3	8	3		
2	C	1	Total	C	H	O	0	0
			14	3	8	3		
2	C	1	Total	C	H	O	0	0
			14	3	8	3		
2	C	1	Total	C	H	O	0	0
			14	3	8	3		

Continued on next page...

Continued from previous page...

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

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



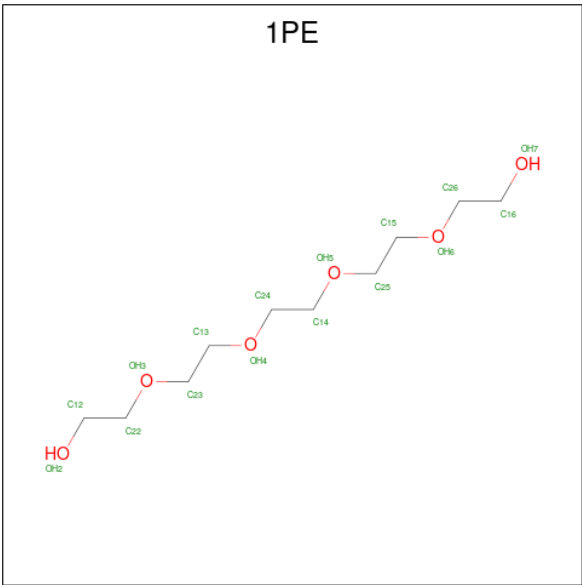
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	B	1	Total	C	H	O	0	0
			10	2	6	2		

Continued on next page...

Continued from previous page...

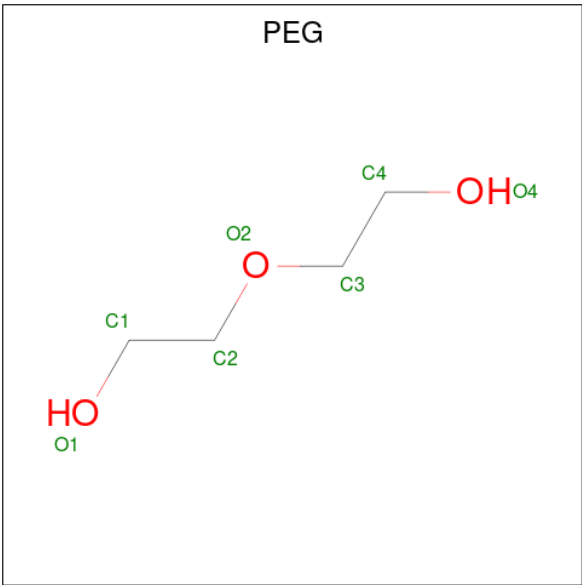
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	H	O	0	0
			10	2	6	2		
3	B	1	Total	C	H	O	0	0
			10	2	6	2		
3	B	1	Total	C	H	O	0	0
			10	2	6	2		
3	B	1	Total	C	H	O	0	0
			10	2	6	2		
3	B	1	Total	C	H	O	0	0
			10	2	6	2		
3	C	1	Total	C	H	O	0	0
			10	2	6	2		
3	C	1	Total	C	H	O	0	0
			10	2	6	2		
3	C	1	Total	C	H	O	0	0
			10	2	6	2		
3	C	1	Total	C	H	O	0	0
			10	2	6	2		
3	C	1	Total	C	H	O	0	0
			10	2	6	2		
3	C	1	Total	C	H	O	0	0
			10	2	6	2		
3	C	1	Total	C	H	O	0	0
			10	2	6	2		
3	C	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 4 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			38	10	22	6		
4	B	1	Total	C	H	O	0	0
			38	10	22	6		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



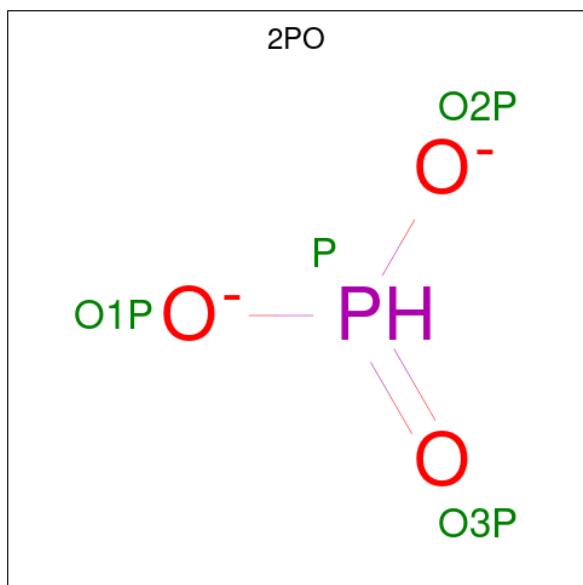
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			17	4	10	3		
5	B	1	Total	C	H	O	0	0
			17	4	10	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	H	O	0	0
			17	4	10	3		
5	B	1	Total	C	H	O	0	0
			17	4	10	3		
5	C	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 6 is PHOSPHONATE (CCD ID: 2PO) (formula: HO_3P).



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

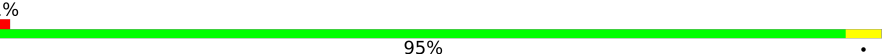
- Molecule 7 is water.

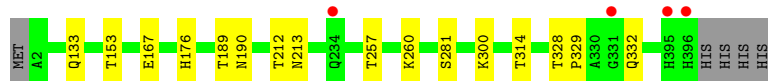
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	171	Total	O	0	0
			171	171		
7	B	189	Total	O	0	0
			189	189		
7	C	193	Total	O	0	0
			193	193		

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: Fructotransferase

Chain A:  95%

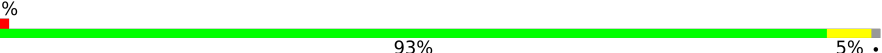


- Molecule 1: Fructotransferase

Chain B:  93% 5%



- Molecule 1: Fructotransferase

Chain C:  93% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	97.68Å 102.51Å 132.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.81 – 1.69 47.81 – 1.69	Depositor EDS
% Data completeness (in resolution range)	99.0 (47.81-1.69) 99.0 (47.81-1.69)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.65 (at 1.69Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.137 , 0.151 0.137 , 0.151	Depositor DCC
R_{free} test set	1994 reflections (1.34%)	wwPDB-VP
Wilson B-factor (Å ²)	11.9	Xtriage
Anisotropy	0.233	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.45 , 35.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.005 for k,h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	18817	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 2PO, EDO, GOL, 1PE, 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	0.37	0/3045	0.61	0/4154
1	B	0.39	1/3033 (0.0%)	0.63	1/4138 (0.0%)
1	C	0.37	0/3071	0.60	0/4193
All	All	0.37	1/9149 (0.0%)	0.61	1/12485 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	169	MET	C-O	-5.06	1.17	1.23

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	196	CYS	N-CA-C	-5.05	101.69	109.52

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	2970	2892	2878	10	0
1	B	2967	2899	2894	13	0
1	C	2985	2903	2895	14	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	36	48	48	0	0
2	B	24	32	32	0	0
2	C	48	64	64	0	0
3	A	24	36	36	0	0
3	B	28	42	42	0	0
3	C	36	54	54	0	0
4	A	16	22	22	0	0
4	B	16	22	22	1	0
5	A	7	10	10	0	0
5	B	21	30	30	0	0
5	C	7	10	10	0	0
6	A	4	1	1	0	0
6	B	4	1	1	0	0
6	C	4	1	1	0	0
7	A	171	0	0	0	0
7	B	189	0	0	0	0
7	C	193	0	0	0	0
All	All	9750	9067	9040	35	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (35) 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:344:ASN:ND2	1:C:370:ARG:HH12	2.09	0.49
1:C:303:MET:HB2	1:C:336:ILE:O	2.14	0.47
1:B:106:ASN:OD1	1:B:106:ASN:C	2.58	0.47
1:B:281:SER:HA	1:B:314:THR:O	2.15	0.46
1:A:328:THR:HA	1:A:329:PRO:C	2.41	0.45
1:A:167:GLU:HA	1:A:189:THR:O	2.16	0.44
1:A:260:LYS:HB2	1:C:234:GLN:HG3	1.98	0.44
1:B:234:GLN:HE22	1:C:237:GLY:HA2	1.83	0.44
1:B:167:GLU:HA	1:B:189:THR:O	2.17	0.44
1:C:167:GLU:HA	1:C:189:THR:O	2.18	0.44
1:B:314:THR:HA	1:B:348:ALA:O	2.18	0.43
1:C:328:THR:HA	1:C:329:PRO:C	2.43	0.43
1:B:169:MET:HE3	1:B:169:MET:HB3	1.92	0.43
1:B:212:THR:HA	1:B:236:SER:O	2.19	0.43
1:A:153:THR:HA	1:A:176:HIS:O	2.18	0.43
1:A:281:SER:HA	1:A:314:THR:O	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:212:THR:HA	1:C:236:SER:O	2.19	0.43
1:C:5:VAL:HG22	1:C:47:VAL:CG1	2.49	0.42
1:C:257:THR:HA	1:C:281:SER:O	2.20	0.42
1:C:281:SER:HA	1:C:314:THR:O	2.20	0.42
1:B:133:GLN:HA	1:B:167:GLU:O	2.19	0.42
1:C:133:GLN:HA	1:C:167:GLU:O	2.20	0.42
1:B:257:THR:HA	1:B:281:SER:O	2.21	0.41
1:B:139:GLY:HA3	1:B:173:TYR:O	2.20	0.41
1:B:180:ILE:HG22	1:B:183:ALA:HB2	2.02	0.41
1:A:257:THR:HA	1:A:281:SER:O	2.20	0.41
1:C:335:THR:HG21	1:C:338:LEU:HB2	2.03	0.41
1:C:189:THR:HA	1:C:212:THR:O	2.20	0.41
1:B:184:ASP:CG	4:B:507:1PE:H251	2.45	0.41
1:A:133:GLN:HA	1:A:167:GLU:O	2.20	0.41
1:A:190:ASN:HA	1:A:213:ASN:O	2.21	0.41
1:A:300:LYS:HE2	1:A:332:GLN:HB3	2.02	0.41
1:B:328:THR:HA	1:B:329:PRO:C	2.46	0.41
1:A:189:THR:HA	1:A:212:THR:O	2.21	0.40
1:C:139:GLY:HA3	1:C:173:TYR:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	396/400 (99%)	380 (96%)	16 (4%)	0	100	100
1	B	395/400 (99%)	379 (96%)	16 (4%)	0	100	100
1	C	399/400 (100%)	385 (96%)	14 (4%)	0	100	100
All	All	1190/1200 (99%)	1144 (96%)	46 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	326/328 (99%)	326 (100%)	0	100	100
1	B	325/328 (99%)	324 (100%)	1 (0%)	86	83
1	C	327/328 (100%)	326 (100%)	1 (0%)	86	83
All	All	978/984 (99%)	976 (100%)	2 (0%)	87	84

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	233	LEU
1	C	370	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	GLN
1	A	207	GLN
1	A	229	ASN
1	A	332	GLN
1	B	109	HIS
1	B	158	GLN
1	B	207	GLN
1	B	234	GLN
1	B	326	ASN
1	B	332	GLN
1	C	69	GLN
1	C	87	GLN
1	C	158	GLN
1	C	207	GLN
1	C	234	GLN
1	C	344	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

50 ligands are modelled in this entry.

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	$\# Z > 2$
3	EDO	A	506	-	3,3,3	0.37	0	2,2,2	0.53	0
2	GOL	C	511	-	5,5,5	1.50	1 (20%)	5,5,5	1.10	0
3	EDO	C	505	-	3,3,3	0.40	0	2,2,2	0.37	0
2	GOL	C	510	-	5,5,5	1.24	1 (20%)	5,5,5	1.27	1 (20%)
3	EDO	C	506	-	3,3,3	0.49	0	2,2,2	0.52	0
3	EDO	A	514	-	3,3,3	0.46	0	2,2,2	0.44	0
2	GOL	B	510	-	5,5,5	0.90	0	5,5,5	0.73	0
2	GOL	C	514	-	5,5,5	1.11	0	5,5,5	1.01	0
3	EDO	A	504	-	3,3,3	0.68	0	2,2,2	0.16	0
3	EDO	B	506	-	3,3,3	0.43	0	2,2,2	0.37	0
3	EDO	C	516	-	3,3,3	0.43	0	2,2,2	1.17	0
3	EDO	C	504	-	3,3,3	0.41	0	2,2,2	0.87	0
2	GOL	A	502	-	5,5,5	0.85	0	5,5,5	0.78	0
3	EDO	B	516	-	3,3,3	0.46	0	2,2,2	0.57	0
2	GOL	B	511	-	5,5,5	1.27	0	5,5,5	1.06	1 (20%)
3	EDO	C	518	-	3,3,3	0.41	0	2,2,2	0.43	0
4	1PE	A	507	-	15,15,15	0.36	0	14,14,14	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	C	513	-	5,5,5	0.87	0	5,5,5	1.14	0
3	EDO	A	503	-	3,3,3	0.54	0	2,2,2	0.58	0
2	GOL	A	501	-	5,5,5	0.90	0	5,5,5	1.12	0
5	PEG	A	513	-	6,6,6	0.11	0	5,5,5	0.27	0
2	GOL	C	503	-	5,5,5	1.00	0	5,5,5	0.74	0
2	GOL	B	504	-	5,5,5	0.51	0	5,5,5	1.13	0
3	EDO	A	508	-	3,3,3	0.58	0	2,2,2	0.81	0
3	EDO	C	507	-	3,3,3	0.46	0	2,2,2	0.48	0
6	2PO	A	515	-	0,3,3	-	-	0,3,3	-	-
2	GOL	C	502	-	5,5,5	1.03	0	5,5,5	1.15	0
2	GOL	A	512	-	5,5,5	0.70	0	5,5,5	0.94	0
5	PEG	B	505	-	6,6,6	0.13	0	5,5,5	0.15	0
3	EDO	B	515	-	3,3,3	0.36	0	2,2,2	0.64	0
4	1PE	B	507	-	15,15,15	0.33	0	14,14,14	0.35	0
6	2PO	C	501	-	0,3,3	-	-	0,3,3	-	-
2	GOL	C	512	-	5,5,5	1.04	0	5,5,5	1.20	1 (20%)
3	EDO	B	503	-	3,3,3	0.42	0	2,2,2	0.62	0
3	EDO	C	508	-	3,3,3	0.32	0	2,2,2	0.89	0
3	EDO	C	519	-	3,3,3	0.40	0	2,2,2	0.56	0
3	EDO	C	517	-	3,3,3	0.41	0	2,2,2	0.65	0
2	GOL	A	511	-	5,5,5	1.20	0	5,5,5	0.89	0
5	PEG	C	515	-	6,6,6	0.28	0	5,5,5	0.09	0
6	2PO	B	502	-	0,3,3	-	-	0,3,3	-	-
3	EDO	B	501	-	3,3,3	0.52	0	2,2,2	0.12	0
5	PEG	B	508	-	6,6,6	0.12	0	5,5,5	0.11	0
2	GOL	C	509	-	5,5,5	0.80	0	5,5,5	0.96	0
3	EDO	A	505	-	3,3,3	0.66	0	2,2,2	0.28	0
2	GOL	B	509	-	5,5,5	0.69	0	5,5,5	1.30	1 (20%)
3	EDO	B	514	-	3,3,3	0.39	0	2,2,2	0.55	0
2	GOL	A	509	-	5,5,5	1.12	0	5,5,5	1.97	2 (40%)
2	GOL	A	510	-	5,5,5	1.03	0	5,5,5	1.18	1 (20%)
3	EDO	B	513	-	3,3,3	0.55	0	2,2,2	0.30	0
5	PEG	B	512	-	6,6,6	0.19	0	5,5,5	0.14	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
3	EDO	A	506	-	-	1/1/1/1	-
2	GOL	C	511	-	-	2/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	C	505	-	-	1/1/1/1	-
2	GOL	C	510	-	-	0/4/4/4	-
3	EDO	C	506	-	-	0/1/1/1	-
3	EDO	A	514	-	-	1/1/1/1	-
2	GOL	B	510	-	-	2/4/4/4	-
2	GOL	C	514	-	-	2/4/4/4	-
3	EDO	A	504	-	-	1/1/1/1	-
3	EDO	B	506	-	-	1/1/1/1	-
3	EDO	C	516	-	-	1/1/1/1	-
3	EDO	C	504	-	-	0/1/1/1	-
2	GOL	A	502	-	-	0/4/4/4	-
3	EDO	B	516	-	-	1/1/1/1	-
2	GOL	B	511	-	-	2/4/4/4	-
3	EDO	C	518	-	-	1/1/1/1	-
4	1PE	A	507	-	-	7/13/13/13	-
2	GOL	C	513	-	-	2/4/4/4	-
3	EDO	A	503	-	-	1/1/1/1	-
2	GOL	A	501	-	-	0/4/4/4	-
5	PEG	A	513	-	-	2/4/4/4	-
2	GOL	C	503	-	-	0/4/4/4	-
2	GOL	B	504	-	-	0/4/4/4	-
3	EDO	A	508	-	-	1/1/1/1	-
3	EDO	C	507	-	-	1/1/1/1	-
2	GOL	C	502	-	-	0/4/4/4	-
2	GOL	A	512	-	-	0/4/4/4	-
5	PEG	B	505	-	-	1/4/4/4	-
3	EDO	B	515	-	-	1/1/1/1	-
4	1PE	B	507	-	-	9/13/13/13	-
2	GOL	C	512	-	-	1/4/4/4	-
3	EDO	B	503	-	-	1/1/1/1	-
3	EDO	C	508	-	-	1/1/1/1	-
3	EDO	C	519	-	-	1/1/1/1	-
3	EDO	C	517	-	-	1/1/1/1	-
2	GOL	A	511	-	-	2/4/4/4	-
5	PEG	C	515	-	-	3/4/4/4	-
3	EDO	B	501	-	-	1/1/1/1	-
5	PEG	B	508	-	-	2/4/4/4	-
2	GOL	C	509	-	-	2/4/4/4	-
3	EDO	A	505	-	-	0/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	B	509	-	-	2/4/4/4	-
3	EDO	B	514	-	-	1/1/1/1	-
2	GOL	A	509	-	-	2/4/4/4	-
2	GOL	A	510	-	-	0/4/4/4	-
3	EDO	B	513	-	-	0/1/1/1	-
5	PEG	B	512	-	-	4/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	511	GOL	C3-C2	2.17	1.60	1.51
2	C	510	GOL	C3-C2	2.05	1.59	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	509	GOL	C3-C2-C1	-3.46	99.09	111.80
2	B	509	GOL	C3-C2-C1	-2.52	102.55	111.80
2	C	510	GOL	C3-C2-C1	-2.42	102.92	111.80
2	A	509	GOL	O2-C2-C1	2.31	118.75	109.18
2	C	512	GOL	C3-C2-C1	-2.26	103.50	111.80
2	A	510	GOL	C3-C2-C1	-2.07	104.21	111.80
2	B	511	GOL	C3-C2-C1	-2.04	104.33	111.80

There are no chirality outliers.

All (65) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	509	GOL	C1-C2-C3-O3
2	A	511	GOL	O1-C1-C2-C3
2	B	509	GOL	O1-C1-C2-C3
2	B	510	GOL	O1-C1-C2-C3
2	C	511	GOL	C1-C2-C3-O3
4	B	507	1PE	OH6-C15-C25-OH5
4	A	507	1PE	OH5-C14-C24-OH4
2	B	510	GOL	O1-C1-C2-O2
2	C	513	GOL	O2-C2-C3-O3
5	B	508	PEG	O1-C1-C2-O2
5	B	512	PEG	O1-C1-C2-O2
5	C	515	PEG	O2-C3-C4-O4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	511	GOL	C1-C2-C3-O3
2	C	509	GOL	C1-C2-C3-O3
2	C	513	GOL	C1-C2-C3-O3
2	C	514	GOL	O1-C1-C2-C3
5	B	512	PEG	O2-C3-C4-O4
2	A	509	GOL	O2-C2-C3-O3
2	B	509	GOL	O1-C1-C2-O2
2	B	511	GOL	O2-C2-C3-O3
2	C	511	GOL	O2-C2-C3-O3
5	C	515	PEG	O1-C1-C2-O2
3	A	514	EDO	O1-C1-C2-O2
3	B	514	EDO	O1-C1-C2-O2
4	A	507	1PE	OH6-C15-C25-OH5
2	A	511	GOL	O1-C1-C2-O2
4	B	507	1PE	OH2-C12-C22-OH3
3	A	504	EDO	O1-C1-C2-O2
3	B	503	EDO	O1-C1-C2-O2
3	B	515	EDO	O1-C1-C2-O2
3	C	507	EDO	O1-C1-C2-O2
5	A	513	PEG	O2-C3-C4-O4
2	C	512	GOL	O2-C2-C3-O3
2	C	514	GOL	O1-C1-C2-O2
3	B	516	EDO	O1-C1-C2-O2
3	C	508	EDO	O1-C1-C2-O2
4	B	507	1PE	C13-C23-OH3-C22
4	B	507	1PE	C24-C14-OH5-C25
3	A	506	EDO	O1-C1-C2-O2
4	B	507	1PE	C25-C15-OH6-C26
4	B	507	1PE	OH7-C16-C26-OH6
5	C	515	PEG	C1-C2-O2-C3
5	B	512	PEG	C4-C3-O2-C2
3	C	505	EDO	O1-C1-C2-O2
4	B	507	1PE	OH5-C14-C24-OH4
5	B	508	PEG	C1-C2-O2-C3
4	A	507	1PE	OH2-C12-C22-OH3
5	A	513	PEG	O1-C1-C2-O2
2	C	509	GOL	O2-C2-C3-O3
5	B	505	PEG	C4-C3-O2-C2
4	B	507	1PE	C16-C26-OH6-C15
4	A	507	1PE	OH4-C13-C23-OH3
3	C	518	EDO	O1-C1-C2-O2
5	B	512	PEG	C1-C2-O2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	507	1PE	C14-C24-OH4-C13
3	A	503	EDO	O1-C1-C2-O2
3	B	506	EDO	O1-C1-C2-O2
3	C	516	EDO	O1-C1-C2-O2
4	A	507	1PE	C13-C23-OH3-C22
3	A	508	EDO	O1-C1-C2-O2
3	C	517	EDO	O1-C1-C2-O2
3	C	519	EDO	O1-C1-C2-O2
4	A	507	1PE	C12-C22-OH3-C23
4	B	507	1PE	C15-C25-OH5-C14
3	B	501	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	507	1PE	1	0

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	395/400 (98%)	-0.87	4 (1%) 79 82	5, 12, 24, 46	1 (0%)
1	B	394/400 (98%)	-0.85	1 (0%) 90 91	5, 13, 22, 35	2 (0%)
1	C	395/400 (98%)	-0.87	3 (0%) 82 85	6, 12, 24, 45	2 (0%)
All	All	1184/1200 (98%)	-0.86	8 (0%) 84 86	5, 12, 23, 46	5 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	396	HIS	4.1
1	C	395	HIS	3.8
1	A	395	HIS	3.7
1	C	396	HIS	3.6
1	C	331	GLY	3.0
1	A	234	GLN	2.9
1	B	395	HIS	2.6
1	A	331	GLY	2.3

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
3	EDO	B	503	4/4	0.71	0.20	25,32,43,51	0
3	EDO	B	515	4/4	0.73	0.22	35,42,49,53	0
6	2PO	C	501	4/4	0.73	0.18	26,28,72,86	0
4	1PE	B	507	16/16	0.75	0.27	21,45,57,59	0
3	EDO	A	506	4/4	0.77	0.19	27,39,47,51	0
5	PEG	A	513	7/7	0.79	0.18	29,36,46,53	0
4	1PE	A	507	16/16	0.80	0.21	13,38,53,53	0
3	EDO	C	506	4/4	0.80	0.15	31,38,43,50	0
5	PEG	C	515	7/7	0.81	0.21	30,49,63,63	0
5	PEG	B	512	7/7	0.81	0.19	29,37,61,61	0
3	EDO	B	516	4/4	0.82	0.17	30,37,44,50	0
2	GOL	C	503	6/6	0.82	0.15	26,34,44,49	0
3	EDO	C	516	4/4	0.82	0.17	30,36,40,49	0
3	EDO	A	504	4/4	0.83	0.17	25,35,51,51	0
3	EDO	C	519	4/4	0.84	0.15	23,37,44,48	0
3	EDO	C	504	4/4	0.85	0.14	28,34,44,44	0
3	EDO	A	514	4/4	0.85	0.19	24,41,56,56	0
2	GOL	A	511	6/6	0.86	0.17	28,40,48,57	0
2	GOL	C	514	6/6	0.86	0.17	18,42,55,66	0
3	EDO	B	514	4/4	0.86	0.16	24,40,46,56	0
2	GOL	A	512	6/6	0.87	0.18	16,47,57,66	0
2	GOL	C	513	6/6	0.87	0.13	27,44,55,55	0
2	GOL	C	512	6/6	0.88	0.14	23,37,45,54	0
3	EDO	C	517	4/4	0.88	0.14	34,41,48,48	0
2	GOL	B	509	6/6	0.88	0.12	25,36,48,52	0
2	GOL	B	511	6/6	0.89	0.12	20,33,42,47	0
2	GOL	B	510	6/6	0.90	0.13	21,26,32,35	0
3	EDO	A	505	4/4	0.90	0.12	17,32,36,39	0
6	2PO	B	502	4/4	0.90	0.20	26,26,66,80	0
5	PEG	B	508	7/7	0.90	0.16	19,34,59,59	0
3	EDO	B	513	4/4	0.91	0.15	14,28,49,49	0
2	GOL	A	509	6/6	0.91	0.14	15,31,42,45	0
3	EDO	B	501	4/4	0.91	0.15	16,36,51,54	0
6	2PO	A	515	4/4	0.91	0.12	19,43,62,75	0
2	GOL	C	511	6/6	0.91	0.13	17,35,49,50	0
5	PEG	B	505	7/7	0.91	0.14	13,35,58,58	0
3	EDO	A	508	4/4	0.92	0.11	16,26,38,38	0
3	EDO	C	507	4/4	0.92	0.14	16,43,51,61	0
3	EDO	C	505	4/4	0.92	0.15	26,35,48,58	0
3	EDO	C	518	4/4	0.93	0.14	24,39,50,50	0
2	GOL	C	509	6/6	0.93	0.10	20,28,40,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	C	508	4/4	0.93	0.12	20,28,47,47	0
3	EDO	A	503	4/4	0.94	0.10	17,22,41,49	0
2	GOL	C	510	6/6	0.95	0.10	15,28,34,34	0
2	GOL	A	502	6/6	0.95	0.09	18,23,30,31	0
3	EDO	B	506	4/4	0.96	0.11	17,29,35,35	0
2	GOL	A	510	6/6	0.96	0.09	15,22,42,51	0
2	GOL	C	502	6/6	0.97	0.06	12,17,20,23	0
2	GOL	B	504	6/6	0.97	0.06	12,16,21,21	0
2	GOL	A	501	6/6	0.98	0.05	11,14,18,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.