



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 12:16 PM UTC

PDB ID : 6KXK / pdb_00006kxk
Title : BON1
Authors : Wang, Q.C.; Jiang, M.Q.; Isupov, M.N.; Sun, L.F.; Wu, Y.K.
Deposited on : 2019-09-12
Resolution : 2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

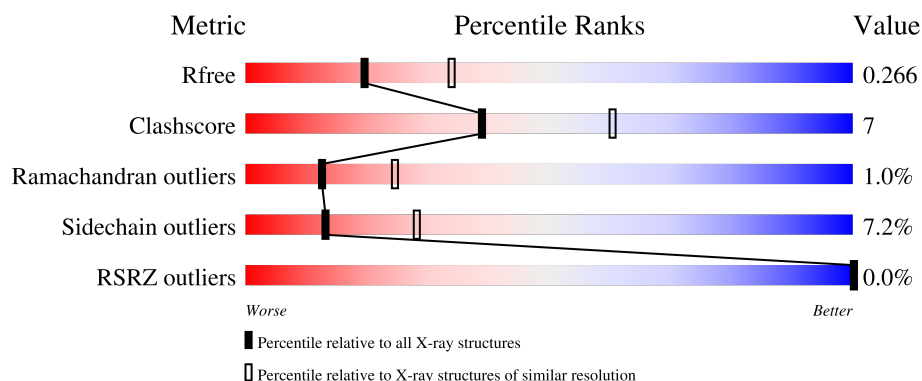
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	553	 82% 15% .
1	C	553	 83% 15% .
1	D	553	 82% 15% ..
1	F	553	 82% 16% .
2	B	528	 79% 16% ..

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Mol	Chain	Length	Quality of chain
3	E	550	79% 17% ...
4	G	527	80% 15% . .
5	H	553	81% 14% . .

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
6	PEG	D	611	-	-	X	-
6	PEG	D	614	-	-	X	-
7	EDO	A	804	-	-	X	-
7	EDO	A	805	-	-	X	-
7	EDO	A	817	-	-	X	-
7	EDO	B	608	-	-	X	-
7	EDO	B	609	-	-	X	-
7	EDO	D	612	-	-	X	-
7	EDO	F	1705	-	-	X	-
7	EDO	F	1719	-	-	X	-

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 35097 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 Protein BONZAI 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	553	Total	C	N	O	S	0	0	0
			4299	2735	719	832	13			
1	C	553	Total	C	N	O	S	0	0	0
			4299	2735	719	832	13			
1	D	553	Total	C	N	O	S	0	0	0
			4299	2735	719	832	13			
1	F	553	Total	C	N	O	S	0	0	0
			4299	2735	719	832	13			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	GLY	-	expression tag	UNP Q941L3
A	-8	THR	-	expression tag	UNP Q941L3
A	-7	SER	-	expression tag	UNP Q941L3
A	-6	SER	-	expression tag	UNP Q941L3
A	-5	MET	-	expression tag	UNP Q941L3
A	-4	ALA	-	expression tag	UNP Q941L3
A	-3	ASP	-	expression tag	UNP Q941L3
A	-2	ILE	-	expression tag	UNP Q941L3
A	-1	GLY	-	expression tag	UNP Q941L3
A	0	SER	-	expression tag	UNP Q941L3
C	-9	GLY	-	expression tag	UNP Q941L3
C	-8	THR	-	expression tag	UNP Q941L3
C	-7	SER	-	expression tag	UNP Q941L3
C	-6	SER	-	expression tag	UNP Q941L3
C	-5	MET	-	expression tag	UNP Q941L3
C	-4	ALA	-	expression tag	UNP Q941L3
C	-3	ASP	-	expression tag	UNP Q941L3
C	-2	ILE	-	expression tag	UNP Q941L3
C	-1	GLY	-	expression tag	UNP Q941L3
C	0	SER	-	expression tag	UNP Q941L3
D	-9	GLY	-	expression tag	UNP Q941L3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-8	THR	-	expression tag	UNP Q941L3
D	-7	SER	-	expression tag	UNP Q941L3
D	-6	SER	-	expression tag	UNP Q941L3
D	-5	MET	-	expression tag	UNP Q941L3
D	-4	ALA	-	expression tag	UNP Q941L3
D	-3	ASP	-	expression tag	UNP Q941L3
D	-2	ILE	-	expression tag	UNP Q941L3
D	-1	GLY	-	expression tag	UNP Q941L3
D	0	SER	-	expression tag	UNP Q941L3
F	-9	GLY	-	expression tag	UNP Q941L3
F	-8	THR	-	expression tag	UNP Q941L3
F	-7	SER	-	expression tag	UNP Q941L3
F	-6	SER	-	expression tag	UNP Q941L3
F	-5	MET	-	expression tag	UNP Q941L3
F	-4	ALA	-	expression tag	UNP Q941L3
F	-3	ASP	-	expression tag	UNP Q941L3
F	-2	ILE	-	expression tag	UNP Q941L3
F	-1	GLY	-	expression tag	UNP Q941L3
F	0	SER	-	expression tag	UNP Q941L3

- Molecule 2 is a protein called Protein BONZAI 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	528	Total	C	N	O	S	0	0	0
			4114	2621	690	791	12			

- Molecule 3 is a protein called Protein BONZAI 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	547	Total	C	N	O	S	0	0	0
			4259	2711	712	823	13			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-6	SER	-	expression tag	UNP Q941L3
E	-5	MET	-	expression tag	UNP Q941L3
E	-4	ALA	-	expression tag	UNP Q941L3
E	-3	ASP	-	expression tag	UNP Q941L3
E	-2	ILE	-	expression tag	UNP Q941L3
E	-1	GLY	-	expression tag	UNP Q941L3
E	0	SER	-	expression tag	UNP Q941L3

- Molecule 4 is a protein called Protein BONZAI 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	508	Total	C	N	O	S	0	0	0
			3963	2524	667	760	12			

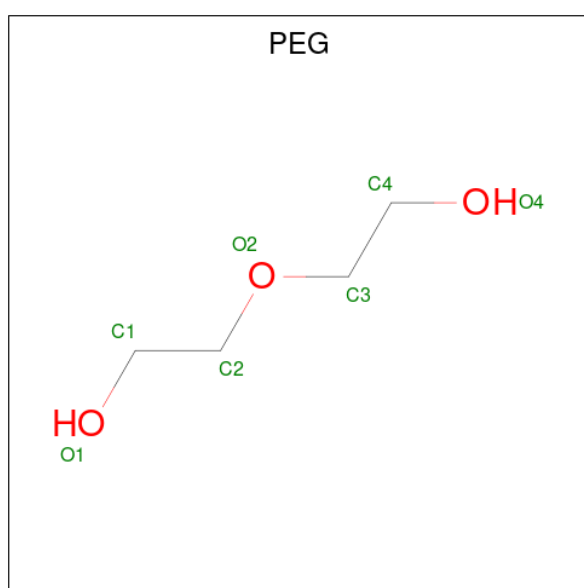
- Molecule 5 is a protein called Protein BONZAI 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	H	550	Total	C	N	O	S	0	0	0
			4277	2721	715	828	13			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	-9	GLY	-	expression tag	UNP Q941L3
H	-8	THR	-	expression tag	UNP Q941L3
H	-7	SER	-	expression tag	UNP Q941L3
H	-6	SER	-	expression tag	UNP Q941L3
H	-5	MET	-	expression tag	UNP Q941L3
H	-4	ALA	-	expression tag	UNP Q941L3
H	-3	ASP	-	expression tag	UNP Q941L3
H	-2	ILE	-	expression tag	UNP Q941L3
H	-1	GLY	-	expression tag	UNP Q941L3
H	0	THR	-	expression tag	UNP Q941L3

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 7 4 3	0	0
6	A	1	Total C O 7 4 3	0	0
6	A	1	Total C O 7 4 3	0	0
6	A	1	Total C O 7 4 3	0	0
6	A	1	Total C O 7 4 3	0	0
6	B	1	Total C O 7 4 3	0	0
6	C	1	Total C O 7 4 3	0	0
6	C	1	Total C O 7 4 3	0	0
6	C	1	Total C O 7 4 3	0	0
6	D	1	Total C O 7 4 3	0	0
6	D	1	Total C O 7 4 3	0	0
6	D	1	Total C O 7 4 3	0	0
6	D	1	Total C O 7 4 3	0	0
6	D	1	Total C O 7 4 3	0	0
6	E	1	Total C O 7 4 3	0	0
6	E	1	Total C O 7 4 3	0	0
6	F	1	Total C O 7 4 3	0	0

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	D	1	Total 4	C 2	O 2	0	0
7	D	1	Total 4	C 2	O 2	0	0
7	D	1	Total 4	C 2	O 2	0	0
7	D	1	Total 4	C 2	O 2	0	0
7	D	1	Total 4	C 2	O 2	0	0
7	D	1	Total 4	C 2	O 2	0	0
7	D	1	Total 4	C 2	O 2	0	0
7	D	1	Total 4	C 2	O 2	0	0
7	D	1	Total 4	C 2	O 2	0	0
7	D	1	Total 4	C 2	O 2	0	0
7	D	1	Total 4	C 2	O 2	0	0
7	D	1	Total 4	C 2	O 2	0	0
7	D	1	Total 4	C 2	O 2	0	0
7	D	1	Total 4	C 2	O 2	0	0
7	E	1	Total 4	C 2	O 2	0	0
7	E	1	Total 4	C 2	O 2	0	0
7	E	1	Total 4	C 2	O 2	0	0
7	E	1	Total 4	C 2	O 2	0	0
7	E	1	Total 4	C 2	O 2	0	0
7	F	1	Total 4	C 2	O 2	0	0
7	F	1	Total 4	C 2	O 2	0	0

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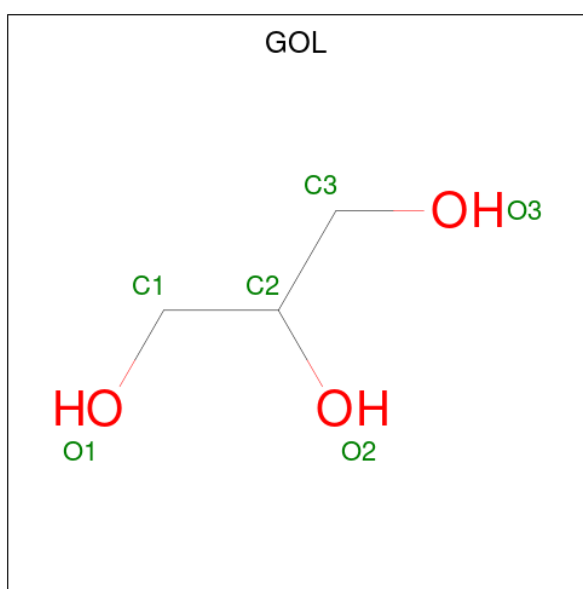
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	F	1	Total 4	C 2	O 2	0	0
7	F	1	Total 4	C 2	O 2	0	0
7	F	1	Total 4	C 2	O 2	0	0
7	F	1	Total 4	C 2	O 2	0	0
7	F	1	Total 4	C 2	O 2	0	0
7	F	1	Total 4	C 2	O 2	0	0
7	F	1	Total 4	C 2	O 2	0	0
7	F	1	Total 4	C 2	O 2	0	0
7	F	1	Total 4	C 2	O 2	0	0
7	F	1	Total 4	C 2	O 2	0	0
7	F	1	Total 4	C 2	O 2	0	0
7	F	1	Total 4	C 2	O 2	0	0
7	F	1	Total 4	C 2	O 2	0	0
7	F	1	Total 4	C 2	O 2	0	0
7	F	1	Total 4	C 2	O 2	0	0
7	F	1	Total 4	C 2	O 2	0	0
7	G	1	Total 4	C 2	O 2	0	0
7	G	1	Total 4	C 2	O 2	0	0
7	G	1	Total 4	C 2	O 2	0	0
7	G	1	Total 4	C 2	O 2	0	0
7	H	1	Total 4	C 2	O 2	0	0
7	H	1	Total 4	C 2	O 2	0	0

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

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



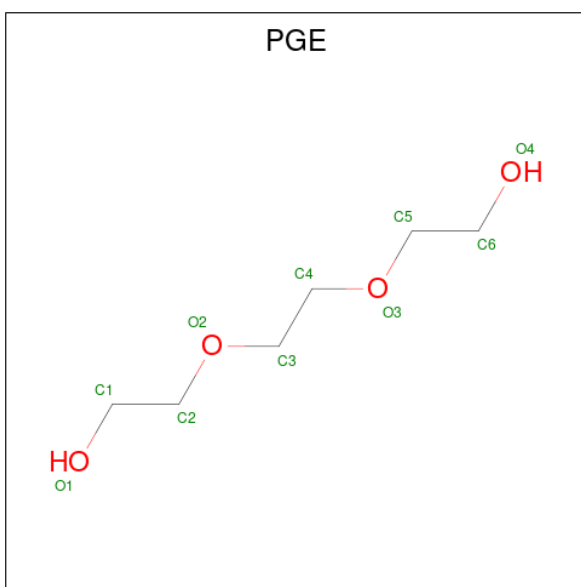
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		

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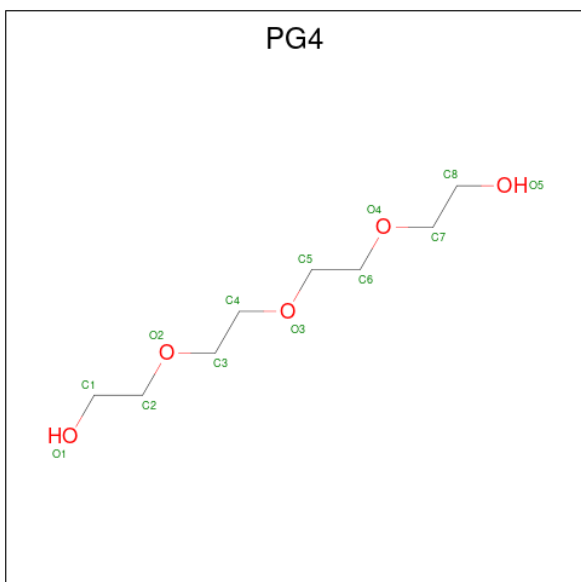
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	C	O	0	0
			6	3	3		
8	C	1	Total	C	O	0	0
			6	3	3		
8	C	1	Total	C	O	0	0
			6	3	3		
8	C	1	Total	C	O	0	0
			6	3	3		
8	D	1	Total	C	O	0	0
			6	3	3		
8	D	1	Total	C	O	0	0
			6	3	3		
8	D	1	Total	C	O	0	0
			6	3	3		
8	D	1	Total	C	O	0	0
			6	3	3		
8	E	1	Total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

- Molecule 9 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



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

- Molecule 10 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



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

- Molecule 11 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	C	1	Total	Cl	0	0
			1	1		
11	D	1	Total	Cl	0	0
			1	1		

- Molecule 12 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	D	1	Total	Ca	0	0
			1	1		
12	F	1	Total	Ca	0	0
			1	1		

- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	126	Total	O	0	0
			126	126		
13	B	89	Total	O	0	0
			89	89		
13	C	76	Total	O	0	0
			76	76		
13	D	95	Total	O	0	0
			95	95		
13	E	46	Total	O	0	0
			46	46		
13	F	86	Total	O	0	0
			86	86		
13	G	38	Total	O	0	0
			38	38		
13	H	47	Total	O	0	0
			47	47		

3 Residue-property plots

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

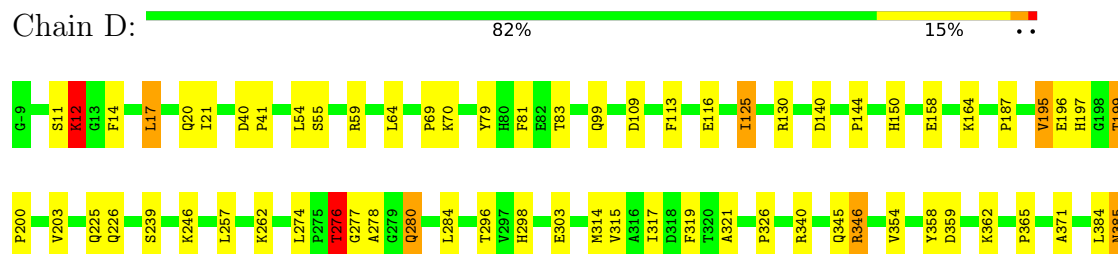
• Molecule 1: Protein BONZAI 1

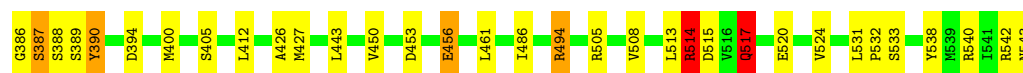


• Molecule 1: Protein BONZAI 1



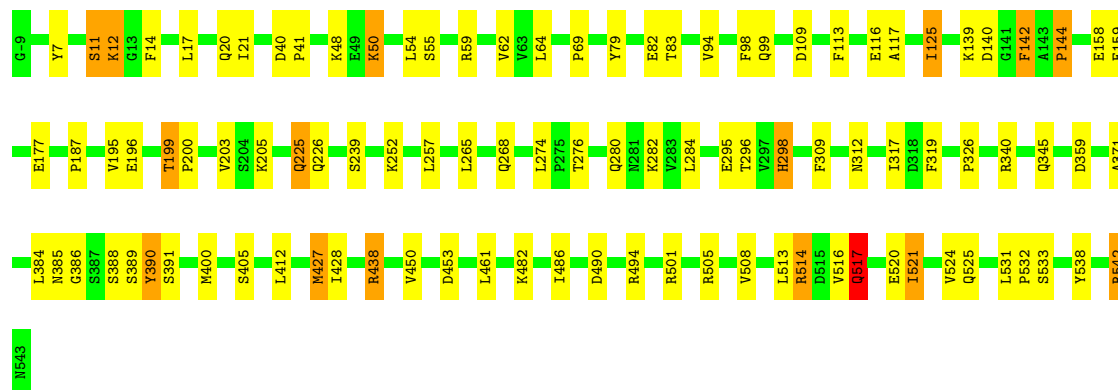
• Molecule 1: Protein BONZAI 1





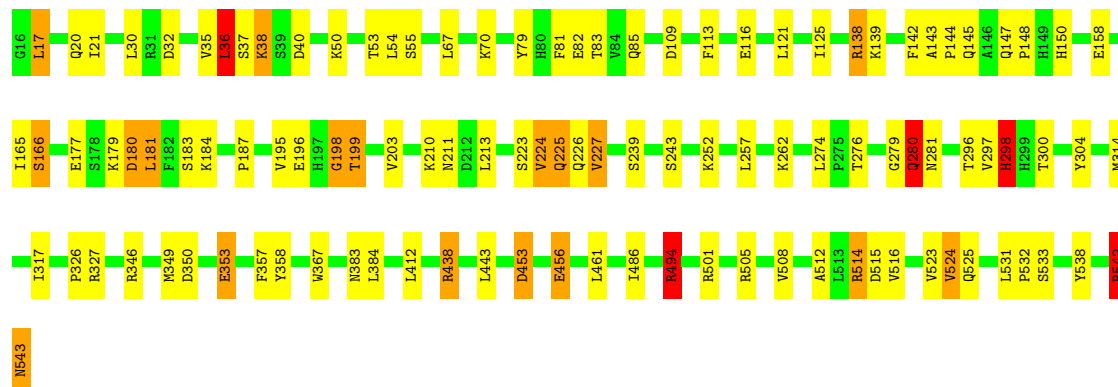
• Molecule 1: Protein BONZAI 1

Chain F: 82% 16%



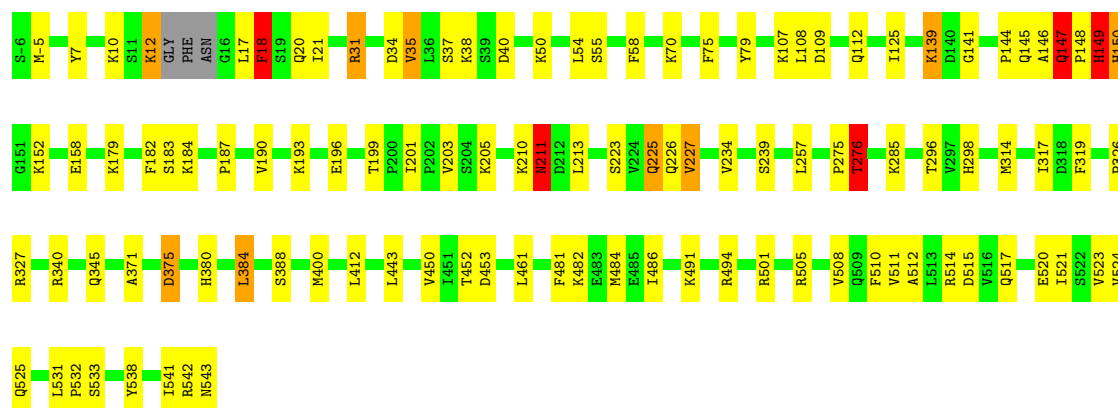
• Molecule 2: Protein BONZAI 1

Chain B: 79% 16%

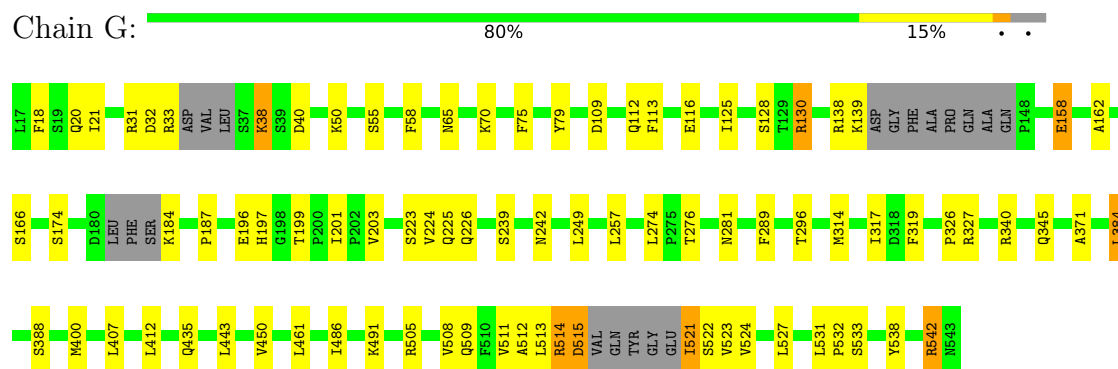


• Molecule 3: Protein BONZAI 1

Chain E: 79% 17%



• Molecule 4: Protein BONZAI 1



• Molecule 5: Protein BONZAI 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	122.28Å 118.72Å 222.25Å 90.00° 90.20° 90.00°	Depositor
Resolution (Å)	48.21 – 2.50 48.21 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.0 (48.21-2.50) 97.1 (48.21-2.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.227 , 0.266 0.227 , 0.266	Depositor DCC
R_{free} test set	10856 reflections (4.27%)	wwPDB-VP
Wilson B-factor (Å ²)	49.5	Xtriage
Anisotropy	0.428	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 56.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l 0.000 for -k,-h,-l 0.099 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	35097	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.11 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.1375e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, CL, PGE, CA, PG4, GOL, 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	0.60	0/4382	1.07	12/5929 (0.2%)
1	C	0.59	0/4382	1.06	15/5929 (0.3%)
1	D	0.61	0/4382	1.10	12/5929 (0.2%)
1	F	0.60	0/4382	1.05	5/5929 (0.1%)
2	B	0.63	0/4194	1.15	26/5676 (0.5%)
3	E	0.60	0/4340	1.07	14/5871 (0.2%)
4	G	0.58	0/4035	1.04	4/5452 (0.1%)
5	H	0.58	0/4358	1.04	8/5896 (0.1%)
All	All	0.60	0/34455	1.07	96/46611 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
1	F	0	1
2	B	0	2
All	All	0	4

There are no bond length outliers.

The worst 5 of 96 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	276	THR	CB-CA-C	-10.81	95.76	110.79
4	G	138	ARG	CB-CG-CD	-10.31	87.58	111.30
1	D	359	ASP	CA-CB-CG	9.61	122.21	112.60
1	A	540	ARG	CG-CD-NE	-9.52	91.06	112.00
2	B	515	ASP	N-CA-C	9.14	120.85	111.07

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	198	GLY	Peptide
2	B	514	ARG	Peptide
1	D	12	LYS	Peptide
1	F	11	SER	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4299	0	4300	65	0
1	C	4299	0	4300	50	0
1	D	4299	0	4300	61	0
1	F	4299	0	4300	68	0
2	B	4114	0	4125	60	0
3	E	4259	0	4266	57	0
4	G	3963	0	3986	46	0
5	H	4277	0	4283	53	0
6	A	35	0	50	6	0
6	B	7	0	10	0	0
6	C	21	0	30	4	0
6	D	35	0	50	10	0
6	E	14	0	20	3	0
6	F	7	0	10	2	0
7	A	48	0	72	21	0
7	B	52	0	78	16	0
7	C	40	0	60	4	0
7	D	56	0	84	7	0
7	E	20	0	30	2	0
7	F	68	0	102	18	0
7	G	16	0	24	0	0
7	H	24	0	36	3	0
8	A	36	0	48	0	0
8	B	6	0	8	0	0
8	C	24	0	32	3	0
8	D	24	0	32	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	E	30	0	40	2	0
8	F	24	0	32	2	0
8	G	6	0	8	1	0
8	H	12	0	16	1	0
9	A	20	0	28	2	0
9	B	10	0	14	2	0
9	C	10	0	14	1	0
9	F	10	0	14	5	0
10	B	13	0	18	3	0
10	D	13	0	18	3	0
11	C	1	0	0	0	0
11	D	1	0	0	0	0
12	D	1	0	0	0	0
12	F	1	0	0	0	0
13	A	126	0	0	8	0
13	B	89	0	0	3	0
13	C	76	0	0	2	0
13	D	95	0	0	7	0
13	E	46	0	0	2	0
13	F	86	0	0	6	0
13	G	38	0	0	1	0
13	H	47	0	0	0	0
All	All	35097	0	34838	472	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 7.

The worst 5 of 472 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)
4:G:249:LEU:HD12	4:G:249:LEU:O	1.52	1.10
3:E:10:LYS:HD3	3:E:541:ILE:HD11	1.35	1.06
2:B:85:GLN:H	7:B:609:EDO:H12	1.11	1.05
4:G:249:LEU:HD13	4:G:274:LEU:CD2	1.90	1.01
1:F:99:GLN:HA	7:F:1705:EDO:H12	1.39	1.01

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	551/553 (100%)	525 (95%)	22 (4%)	4 (1%)	18	34
1	C	551/553 (100%)	521 (95%)	24 (4%)	6 (1%)	11	22
1	D	551/553 (100%)	524 (95%)	21 (4%)	6 (1%)	11	22
1	F	551/553 (100%)	524 (95%)	21 (4%)	6 (1%)	11	22
2	B	526/528 (100%)	501 (95%)	20 (4%)	5 (1%)	12	24
3	E	543/550 (99%)	505 (93%)	31 (6%)	7 (1%)	9	18
4	G	498/527 (94%)	477 (96%)	19 (4%)	2 (0%)	30	49
5	H	546/553 (99%)	514 (94%)	25 (5%)	7 (1%)	9	18
All	All	4317/4370 (99%)	4091 (95%)	183 (4%)	43 (1%)	12	24

5 of 43 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	278	ALA
1	A	514	ARG
2	B	36	LEU
2	B	144	PRO
1	C	145	GLN

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	481/481 (100%)	446 (93%)	35 (7%)	13	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	481/481 (100%)	451 (94%)	30 (6%)	16	34
1	D	481/481 (100%)	451 (94%)	30 (6%)	16	34
1	F	481/481 (100%)	450 (94%)	31 (6%)	16	33
2	B	461/461 (100%)	427 (93%)	34 (7%)	13	27
3	E	477/479 (100%)	436 (91%)	41 (9%)	10	21
4	G	446/461 (97%)	416 (93%)	30 (7%)	15	31
5	H	479/481 (100%)	439 (92%)	40 (8%)	10	22
All	All	3787/3806 (100%)	3516 (93%)	271 (7%)	13	28

5 of 271 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	H	12	LYS
5	H	55	SER
5	H	450	VAL
1	C	533	SER
1	C	515	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 61 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	271	ASN
5	H	226	GLN
3	E	149	HIS
5	H	225	GLN
5	H	423	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 136 ligands modelled in this entry, 4 are monoatomic - leaving 132 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	$\# Z > 2$
6	PEG	D	617	-	6,6,6	0.20	0	5,5,5	0.09	0
7	EDO	H	608	-	3,3,3	0.09	0	2,2,2	0.02	0
7	EDO	D	624	-	3,3,3	0.09	0	2,2,2	0.13	0
7	EDO	B	615	-	3,3,3	0.02	0	2,2,2	0.24	0
9	PGE	B	612	-	9,9,9	0.29	0	8,8,8	0.29	0
6	PEG	B	611	-	6,6,6	0.36	0	5,5,5	0.24	0
7	EDO	B	603	-	3,3,3	0.19	0	2,2,2	0.64	0
6	PEG	C	603	-	6,6,6	0.33	0	5,5,5	0.26	0
7	EDO	C	611	-	3,3,3	0.07	0	2,2,2	0.06	0
6	PEG	F	1712	-	6,6,6	0.17	0	5,5,5	0.14	0
8	GOL	D	609	-	5,5,5	0.11	0	5,5,5	0.51	0
7	EDO	A	805	-	3,3,3	0.57	0	2,2,2	0.29	0
6	PEG	E	2001	-	6,6,6	0.12	0	5,5,5	0.12	0
7	EDO	A	806	-	3,3,3	0.06	0	2,2,2	0.20	0
7	EDO	C	604	-	3,3,3	0.19	0	2,2,2	0.33	0
8	GOL	C	602	-	5,5,5	0.16	0	5,5,5	0.49	0
7	EDO	B	608	-	3,3,3	0.11	0	2,2,2	0.81	0
7	EDO	B	605	-	3,3,3	0.10	0	2,2,2	0.13	0
7	EDO	F	1702	-	3,3,3	0.08	0	2,2,2	0.20	0
7	EDO	C	610	-	3,3,3	0.11	0	2,2,2	0.41	0
8	GOL	A	818	-	5,5,5	0.12	0	5,5,5	0.53	0
6	PEG	A	801	-	6,6,6	0.25	0	5,5,5	0.21	0
6	PEG	A	802	-	6,6,6	0.21	0	5,5,5	0.11	0
7	EDO	B	606	-	3,3,3	0.16	0	2,2,2	0.30	0
6	PEG	D	614	-	6,6,6	0.11	0	5,5,5	0.10	0
8	GOL	A	822	-	5,5,5	0.13	0	5,5,5	0.41	0
6	PEG	A	811	-	6,6,6	0.16	0	5,5,5	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	GOL	C	612	-	5,5,5	0.15	0	5,5,5	0.47	0
8	GOL	H	606	-	5,5,5	0.18	0	5,5,5	0.55	0
8	GOL	E	2008	-	5,5,5	0.10	0	5,5,5	0.35	0
7	EDO	A	819	-	3,3,3	0.08	0	2,2,2	0.33	0
7	EDO	H	605	-	3,3,3	0.21	0	2,2,2	0.71	0
7	EDO	C	616	-	3,3,3	0.12	0	2,2,2	0.18	0
7	EDO	C	601	-	3,3,3	0.19	0	2,2,2	0.40	0
7	EDO	D	623	-	3,3,3	0.07	0	2,2,2	0.04	0
7	EDO	E	2011	-	3,3,3	0.15	0	2,2,2	0.26	0
8	GOL	D	602	-	5,5,5	0.13	0	5,5,5	0.43	0
7	EDO	A	812	-	3,3,3	0.17	0	2,2,2	0.47	0
9	PGE	C	617	-	9,9,9	0.20	0	8,8,8	0.19	0
7	EDO	E	2010	-	3,3,3	0.08	0	2,2,2	0.18	0
7	EDO	A	817	-	3,3,3	0.24	0	2,2,2	0.23	0
7	EDO	A	809	-	3,3,3	0.06	0	2,2,2	0.19	0
7	EDO	H	604	-	3,3,3	0.10	0	2,2,2	0.26	0
7	EDO	A	804	-	3,3,3	0.11	0	2,2,2	0.40	0
6	PEG	E	2007	-	6,6,6	0.18	0	5,5,5	0.13	0
7	EDO	D	621	-	3,3,3	0.20	0	2,2,2	0.35	0
7	EDO	F	1713	-	3,3,3	0.14	0	2,2,2	0.42	0
7	EDO	F	1723	-	3,3,3	0.10	0	2,2,2	0.23	0
7	EDO	H	602	-	3,3,3	0.06	0	2,2,2	0.18	0
7	EDO	B	614	-	3,3,3	0.14	0	2,2,2	0.41	0
7	EDO	E	2002	-	3,3,3	0.07	0	2,2,2	0.20	0
7	EDO	D	622	-	3,3,3	0.15	0	2,2,2	0.05	0
7	EDO	B	613	-	3,3,3	0.13	0	2,2,2	0.43	0
7	EDO	B	617	-	3,3,3	0.10	0	2,2,2	0.15	0
8	GOL	G	605	-	5,5,5	0.11	0	5,5,5	0.40	0
7	EDO	E	2009	-	3,3,3	0.13	0	2,2,2	0.12	0
8	GOL	F	1708	-	5,5,5	0.08	0	5,5,5	0.34	0
7	EDO	E	2003	-	3,3,3	0.09	0	2,2,2	0.04	0
8	GOL	A	821	-	5,5,5	0.09	0	5,5,5	0.40	0
7	EDO	B	604	-	3,3,3	0.09	0	2,2,2	0.28	0
6	PEG	C	605	-	6,6,6	0.18	0	5,5,5	0.12	0
7	EDO	F	1705	-	3,3,3	0.11	0	2,2,2	0.69	0
8	GOL	A	820	-	5,5,5	0.17	0	5,5,5	0.56	0
8	GOL	E	2004	-	5,5,5	0.17	0	5,5,5	0.48	0
7	EDO	B	616	-	3,3,3	0.12	0	2,2,2	0.20	0
9	PGE	A	824	-	9,9,9	0.22	0	8,8,8	0.13	0
7	EDO	G	602	-	3,3,3	0.15	0	2,2,2	0.15	0
6	PEG	D	601	-	6,6,6	0.11	0	5,5,5	0.19	0
7	EDO	F	1721	-	3,3,3	0.08	0	2,2,2	0.09	0
7	EDO	F	1717	-	3,3,3	0.10	0	2,2,2	0.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	EDO	D	606	-	3,3,3	0.15	0	2,2,2	0.35	0
10	PG4	D	613	-	12,12,12	0.24	0	11,11,11	0.21	0
7	EDO	D	607	-	3,3,3	0.12	0	2,2,2	0.24	0
7	EDO	D	616	-	3,3,3	0.07	0	2,2,2	0.06	0
7	EDO	F	1709	-	3,3,3	0.09	0	2,2,2	0.30	0
7	EDO	F	1701	-	3,3,3	0.10	0	2,2,2	0.48	0
6	PEG	A	825	-	6,6,6	0.16	0	5,5,5	0.08	0
6	PEG	C	606	-	6,6,6	0.17	0	5,5,5	0.11	0
7	EDO	F	1707	-	3,3,3	0.32	0	2,2,2	0.89	0
7	EDO	D	619	-	3,3,3	0.12	0	2,2,2	0.54	0
8	GOL	B	607	-	5,5,5	0.17	0	5,5,5	0.48	0
6	PEG	A	807	-	6,6,6	0.16	0	5,5,5	0.09	0
7	EDO	D	618	-	3,3,3	0.09	0	2,2,2	0.09	0
7	EDO	H	607	-	3,3,3	0.11	0	2,2,2	0.53	0
7	EDO	A	816	-	3,3,3	0.12	0	2,2,2	0.20	0
7	EDO	F	1703	-	3,3,3	0.13	0	2,2,2	0.25	0
7	EDO	G	601	-	3,3,3	0.28	0	2,2,2	0.49	0
7	EDO	A	823	-	3,3,3	0.15	0	2,2,2	0.20	0
7	EDO	D	612	-	3,3,3	0.29	0	2,2,2	0.99	0
9	PGE	A	814	-	9,9,9	0.25	0	8,8,8	0.11	0
7	EDO	D	615	-	3,3,3	0.12	0	2,2,2	0.27	0
7	EDO	G	603	-	3,3,3	0.10	0	2,2,2	0.17	0
7	EDO	D	603	-	3,3,3	0.07	0	2,2,2	0.12	0
7	EDO	C	608	-	3,3,3	0.17	0	2,2,2	0.21	0
8	GOL	F	1722	-	5,5,5	0.09	0	5,5,5	0.35	0
7	EDO	F	1719	-	3,3,3	0.18	0	2,2,2	0.27	0
7	EDO	B	601	-	3,3,3	0.25	0	2,2,2	0.85	0
8	GOL	F	1716	-	5,5,5	0.07	0	5,5,5	0.40	0
7	EDO	F	1715	-	3,3,3	0.08	0	2,2,2	0.28	0
7	EDO	G	604	-	3,3,3	0.14	0	2,2,2	0.11	0
8	GOL	E	2006	-	5,5,5	0.14	0	5,5,5	0.41	0
8	GOL	A	815	-	5,5,5	0.18	0	5,5,5	0.29	0
8	GOL	F	1714	-	5,5,5	0.14	0	5,5,5	0.67	0
8	GOL	C	607	-	5,5,5	0.13	0	5,5,5	0.77	0
7	EDO	B	609	-	3,3,3	0.28	0	2,2,2	0.11	0
8	GOL	E	2012	-	5,5,5	0.10	0	5,5,5	0.35	0
7	EDO	D	608	-	3,3,3	0.11	0	2,2,2	0.05	0
7	EDO	F	1706	-	3,3,3	0.14	0	2,2,2	0.28	0
7	EDO	A	808	-	3,3,3	0.05	0	2,2,2	0.17	0
8	GOL	E	2005	-	5,5,5	0.16	0	5,5,5	0.47	0
7	EDO	F	1710	-	3,3,3	0.10	0	2,2,2	1.00	0
9	PGE	F	1718	-	9,9,9	0.27	0	8,8,8	0.13	0
10	PG4	B	610	-	12,12,12	0.35	0	11,11,11	0.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	PEG	D	611	-	6,6,6	0.15	0	5,5,5	0.10	0
7	EDO	A	803	-	3,3,3	0.61	0	2,2,2	1.87	1 (50%)
8	GOL	C	618	-	5,5,5	0.10	0	5,5,5	0.42	0
7	EDO	C	609	-	3,3,3	0.15	0	2,2,2	0.39	0
7	EDO	F	1704	-	3,3,3	0.04	0	2,2,2	0.10	0
7	EDO	F	1711	-	3,3,3	0.14	0	2,2,2	0.27	0
8	GOL	D	610	-	5,5,5	0.07	0	5,5,5	0.29	0
7	EDO	B	602	-	3,3,3	0.06	0	2,2,2	0.11	0
6	PEG	D	620	-	6,6,6	0.20	0	5,5,5	0.24	0
7	EDO	F	1720	-	3,3,3	0.14	0	2,2,2	0.15	0
8	GOL	A	810	-	5,5,5	0.10	0	5,5,5	0.37	0
7	EDO	H	603	-	3,3,3	0.05	0	2,2,2	0.35	0
7	EDO	C	614	-	3,3,3	0.08	0	2,2,2	0.26	0
7	EDO	D	605	-	3,3,3	0.14	0	2,2,2	0.32	0
7	EDO	A	813	-	3,3,3	0.07	0	2,2,2	0.09	0
8	GOL	H	601	-	5,5,5	0.09	0	5,5,5	0.25	0
8	GOL	D	604	-	5,5,5	0.11	0	5,5,5	0.39	0
7	EDO	C	613	-	3,3,3	0.14	0	2,2,2	0.10	0
7	EDO	C	615	-	3,3,3	0.13	0	2,2,2	0.17	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
6	PEG	D	617	-	-	3/4/4/4	-
7	EDO	H	608	-	-	1/1/1/1	-
7	EDO	D	624	-	-	1/1/1/1	-
7	EDO	B	615	-	-	0/1/1/1	-
9	PGE	B	612	-	-	4/7/7/7	-
6	PEG	B	611	-	-	4/4/4/4	-
7	EDO	B	603	-	-	0/1/1/1	-
6	PEG	C	603	-	-	2/4/4/4	-
7	EDO	C	611	-	-	1/1/1/1	-
6	PEG	F	1712	-	-	2/4/4/4	-
8	GOL	D	609	-	-	4/4/4/4	-
7	EDO	A	805	-	-	0/1/1/1	-
6	PEG	E	2001	-	-	1/4/4/4	-
7	EDO	A	806	-	-	0/1/1/1	-
7	EDO	C	604	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	GOL	C	602	-	-	2/4/4/4	-
7	EDO	B	608	-	-	1/1/1/1	-
7	EDO	B	605	-	-	1/1/1/1	-
7	EDO	F	1702	-	-	0/1/1/1	-
7	EDO	C	610	-	-	0/1/1/1	-
8	GOL	A	818	-	-	2/4/4/4	-
6	PEG	A	801	-	-	4/4/4/4	-
6	PEG	A	802	-	-	2/4/4/4	-
7	EDO	B	606	-	-	0/1/1/1	-
6	PEG	D	614	-	-	2/4/4/4	-
8	GOL	A	822	-	-	2/4/4/4	-
6	PEG	A	811	-	-	2/4/4/4	-
8	GOL	C	612	-	-	0/4/4/4	-
8	GOL	H	606	-	-	4/4/4/4	-
8	GOL	E	2008	-	-	4/4/4/4	-
7	EDO	A	819	-	-	1/1/1/1	-
7	EDO	H	605	-	-	0/1/1/1	-
7	EDO	C	616	-	-	1/1/1/1	-
7	EDO	C	601	-	-	1/1/1/1	-
7	EDO	D	623	-	-	0/1/1/1	-
7	EDO	E	2011	-	-	1/1/1/1	-
8	GOL	D	602	-	-	2/4/4/4	-
7	EDO	A	812	-	-	0/1/1/1	-
9	PGE	C	617	-	-	4/7/7/7	-
7	EDO	E	2010	-	-	1/1/1/1	-
7	EDO	A	817	-	-	0/1/1/1	-
7	EDO	A	809	-	-	0/1/1/1	-
7	EDO	H	604	-	-	0/1/1/1	-
7	EDO	A	804	-	-	1/1/1/1	-
6	PEG	E	2007	-	-	2/4/4/4	-
7	EDO	D	621	-	-	1/1/1/1	-
7	EDO	F	1713	-	-	1/1/1/1	-
7	EDO	F	1723	-	-	0/1/1/1	-
7	EDO	H	602	-	-	0/1/1/1	-
7	EDO	B	614	-	-	1/1/1/1	-
7	EDO	E	2002	-	-	0/1/1/1	-
7	EDO	D	622	-	-	0/1/1/1	-
7	EDO	B	613	-	-	1/1/1/1	-
7	EDO	B	617	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	GOL	G	605	-	-	2/4/4/4	-
7	EDO	E	2009	-	-	1/1/1/1	-
8	GOL	F	1708	-	-	2/4/4/4	-
7	EDO	E	2003	-	-	1/1/1/1	-
8	GOL	A	821	-	-	4/4/4/4	-
7	EDO	B	604	-	-	0/1/1/1	-
6	PEG	C	605	-	-	2/4/4/4	-
7	EDO	F	1705	-	-	1/1/1/1	-
8	GOL	A	820	-	-	0/4/4/4	-
8	GOL	E	2004	-	-	2/4/4/4	-
7	EDO	B	616	-	-	1/1/1/1	-
9	PGE	A	824	-	-	7/7/7/7	-
7	EDO	G	602	-	-	1/1/1/1	-
6	PEG	D	601	-	-	2/4/4/4	-
7	EDO	F	1721	-	-	1/1/1/1	-
7	EDO	F	1717	-	-	1/1/1/1	-
7	EDO	D	606	-	-	1/1/1/1	-
10	PG4	D	613	-	-	4/10/10/10	-
7	EDO	D	607	-	-	0/1/1/1	-
7	EDO	D	616	-	-	0/1/1/1	-
7	EDO	F	1709	-	-	1/1/1/1	-
7	EDO	F	1701	-	-	1/1/1/1	-
6	PEG	A	825	-	-	3/4/4/4	-
6	PEG	C	606	-	-	3/4/4/4	-
7	EDO	F	1707	-	-	0/1/1/1	-
7	EDO	D	619	-	-	0/1/1/1	-
8	GOL	B	607	-	-	0/4/4/4	-
6	PEG	A	807	-	-	2/4/4/4	-
7	EDO	D	618	-	-	0/1/1/1	-
7	EDO	H	607	-	-	1/1/1/1	-
7	EDO	A	816	-	-	1/1/1/1	-
7	EDO	F	1703	-	-	1/1/1/1	-
7	EDO	G	601	-	-	1/1/1/1	-
7	EDO	A	823	-	-	1/1/1/1	-
7	EDO	D	612	-	-	0/1/1/1	-
9	PGE	A	814	-	-	5/7/7/7	-
7	EDO	D	615	-	-	1/1/1/1	-
7	EDO	G	603	-	-	0/1/1/1	-
7	EDO	D	603	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	C	608	-	-	0/1/1/1	-
8	GOL	F	1722	-	-	2/4/4/4	-
7	EDO	F	1719	-	-	0/1/1/1	-
7	EDO	B	601	-	-	1/1/1/1	-
8	GOL	F	1716	-	-	2/4/4/4	-
7	EDO	F	1715	-	-	1/1/1/1	-
7	EDO	G	604	-	-	1/1/1/1	-
8	GOL	E	2006	-	-	1/4/4/4	-
8	GOL	A	815	-	-	2/4/4/4	-
8	GOL	F	1714	-	-	4/4/4/4	-
8	GOL	C	607	-	-	1/4/4/4	-
7	EDO	B	609	-	-	0/1/1/1	-
8	GOL	E	2012	-	-	2/4/4/4	-
7	EDO	D	608	-	-	1/1/1/1	-
7	EDO	F	1706	-	-	0/1/1/1	-
7	EDO	A	808	-	-	0/1/1/1	-
8	GOL	E	2005	-	-	2/4/4/4	-
7	EDO	F	1710	-	-	1/1/1/1	-
9	PGE	F	1718	-	-	4/7/7/7	-
10	PG4	B	610	-	-	6/10/10/10	-
6	PEG	D	611	-	-	2/4/4/4	-
7	EDO	A	803	-	-	1/1/1/1	-
8	GOL	C	618	-	-	2/4/4/4	-
7	EDO	C	609	-	-	1/1/1/1	-
7	EDO	F	1704	-	-	1/1/1/1	-
7	EDO	F	1711	-	-	0/1/1/1	-
8	GOL	D	610	-	-	2/4/4/4	-
7	EDO	B	602	-	-	0/1/1/1	-
6	PEG	D	620	-	-	2/4/4/4	-
7	EDO	F	1720	-	-	1/1/1/1	-
8	GOL	A	810	-	-	0/4/4/4	-
7	EDO	H	603	-	-	1/1/1/1	-
7	EDO	C	614	-	-	0/1/1/1	-
7	EDO	D	605	-	-	0/1/1/1	-
7	EDO	A	813	-	-	0/1/1/1	-
8	GOL	H	601	-	-	4/4/4/4	-
8	GOL	D	604	-	-	4/4/4/4	-
7	EDO	C	613	-	-	0/1/1/1	-
7	EDO	C	615	-	-	1/1/1/1	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	803	EDO	O2-C2-C1	-2.46	93.62	112.39

There are no chirality outliers.

5 of 176 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	815	GOL	C1-C2-C3-O3
8	A	815	GOL	O2-C2-C3-O3
8	A	818	GOL	C1-C2-C3-O3
8	A	821	GOL	O1-C1-C2-C3
8	A	821	GOL	C1-C2-C3-O3

There are no ring outliers.

49 monomers are involved in 122 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	612	PGE	2	0
6	C	603	PEG	3	0
7	C	611	EDO	1	0
6	F	1712	PEG	2	0
7	A	805	EDO	10	0
7	B	608	EDO	6	0
7	C	610	EDO	1	0
6	A	801	PEG	2	0
6	A	802	PEG	3	0
6	D	614	PEG	4	0
8	C	612	GOL	1	0
8	D	602	GOL	3	0
9	C	617	PGE	1	0
7	E	2010	EDO	2	0
7	A	817	EDO	4	0
7	A	809	EDO	2	0
7	A	804	EDO	5	0
6	E	2007	PEG	3	0
7	F	1723	EDO	2	0
7	D	622	EDO	1	0
8	G	605	GOL	1	0
7	B	604	EDO	2	0
6	C	605	PEG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	F	1705	EDO	7	0
9	A	824	PGE	1	0
6	D	601	PEG	1	0
7	F	1721	EDO	2	0
10	D	613	PG4	3	0
6	A	825	PEG	1	0
7	F	1707	EDO	2	0
7	A	816	EDO	1	0
7	D	612	EDO	5	0
9	A	814	PGE	1	0
7	F	1719	EDO	5	0
7	B	601	EDO	3	0
8	F	1714	GOL	2	0
8	C	607	GOL	2	0
7	B	609	EDO	7	0
8	E	2012	GOL	1	0
7	D	608	EDO	1	0
8	E	2005	GOL	1	0
9	F	1718	PGE	5	0
10	B	610	PG4	3	0
6	D	611	PEG	4	0
6	D	620	PEG	1	0
7	H	603	EDO	3	0
7	C	614	EDO	2	0
8	H	601	GOL	1	0
8	D	604	GOL	2	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	553/553 (100%)	-1.20	0 100 100	27, 53, 112, 173	0
1	C	553/553 (100%)	-1.16	1 (0%) 91 89	35, 56, 118, 183	0
1	D	553/553 (100%)	-1.13	0 100 100	25, 55, 123, 163	0
1	F	553/553 (100%)	-1.10	0 100 100	27, 58, 128, 200	0
2	B	528/528 (100%)	-1.15	0 100 100	27, 54, 130, 173	0
3	E	547/550 (99%)	-1.06	0 100 100	29, 60, 154, 199	0
4	G	508/527 (96%)	-1.05	0 100 100	35, 65, 144, 187	0
5	H	550/553 (99%)	-1.03	0 100 100	39, 66, 165, 204	0
All	All	4345/4370 (99%)	-1.11	1 (0%) 100 100	25, 58, 143, 204	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	144	PRO	2.2

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($\text{\AA}^2$)	Q<0.9
7	EDO	E	2009	4/4	0.91	0.30	67,75,77,80	4
7	EDO	E	2010	4/4	0.92	0.13	67,68,71,71	4
7	EDO	H	608	4/4	0.93	0.21	77,79,80,81	4
7	EDO	E	2002	4/4	0.94	0.13	63,68,68,72	4
7	EDO	B	613	4/4	0.94	0.17	78,88,92,96	0
7	EDO	D	603	4/4	0.95	0.15	77,80,81,84	0
7	EDO	D	618	4/4	0.95	0.14	79,86,88,90	0
7	EDO	A	819	4/4	0.95	0.14	53,53,61,61	4
7	EDO	A	808	4/4	0.95	0.13	77,77,86,88	0
7	EDO	B	617	4/4	0.95	0.12	60,70,72,73	4
7	EDO	F	1703	4/4	0.95	0.09	88,90,90,91	0
7	EDO	F	1704	4/4	0.95	0.25	61,63,66,66	4
7	EDO	F	1711	4/4	0.95	0.08	67,71,72,75	0
7	EDO	F	1717	4/4	0.95	0.10	61,69,71,73	4
7	EDO	C	609	4/4	0.95	0.19	71,72,73,74	4
8	GOL	B	607	6/6	0.95	0.15	62,70,80,80	6
8	GOL	E	2012	6/6	0.95	0.09	66,69,73,76	0
7	EDO	D	624	4/4	0.96	0.14	66,78,79,82	4
6	PEG	D	620	7/7	0.96	0.07	60,66,69,69	7
7	EDO	E	2003	4/4	0.96	0.06	96,96,103,103	0
7	EDO	C	604	4/4	0.96	0.13	90,92,93,104	4
7	EDO	B	602	4/4	0.96	0.08	71,71,78,82	0
7	EDO	F	1702	4/4	0.96	0.12	78,88,92,94	0
7	EDO	C	610	4/4	0.96	0.08	72,73,78,80	0
7	EDO	C	615	4/4	0.96	0.21	76,79,79,80	4
7	EDO	F	1706	4/4	0.96	0.08	57,63,70,72	0
7	EDO	C	616	4/4	0.96	0.10	67,71,77,78	0
6	PEG	D	601	7/7	0.96	0.09	81,85,97,99	0
7	EDO	G	603	4/4	0.96	0.11	66,83,85,86	0
7	EDO	H	604	4/4	0.96	0.11	82,92,93,95	0
7	EDO	D	616	4/4	0.96	0.10	67,68,73,74	0
7	EDO	B	616	4/4	0.96	0.12	79,84,93,95	0
7	EDO	D	621	4/4	0.96	0.14	54,55,63,64	4
6	PEG	C	606	7/7	0.97	0.08	59,70,77,79	7
7	EDO	A	812	4/4	0.97	0.09	76,81,82,87	0
7	EDO	A	813	4/4	0.97	0.20	72,74,74,79	4
7	EDO	A	816	4/4	0.97	0.14	64,73,73,77	0
7	EDO	F	1701	4/4	0.97	0.12	94,97,104,109	0
7	EDO	C	613	4/4	0.97	0.12	64,73,74,78	4
7	EDO	C	614	4/4	0.97	0.09	76,82,83,88	0
6	PEG	A	811	7/7	0.97	0.12	59,71,82,83	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	PEG	D	611	7/7	0.97	0.08	72,77,85,89	7
7	EDO	B	603	4/4	0.97	0.11	59,69,72,75	0
7	EDO	F	1713	4/4	0.97	0.10	71,77,84,92	0
7	EDO	D	605	4/4	0.97	0.09	55,69,70,79	0
7	EDO	F	1719	4/4	0.97	0.09	80,81,81,83	4
7	EDO	G	602	4/4	0.97	0.07	71,73,73,75	0
7	EDO	B	604	4/4	0.97	0.16	91,92,94,102	0
7	EDO	G	604	4/4	0.97	0.09	64,65,75,75	0
7	EDO	H	602	4/4	0.97	0.08	63,68,73,75	0
6	PEG	D	617	7/7	0.97	0.13	82,84,93,94	0
7	EDO	H	605	4/4	0.97	0.07	56,61,65,66	0
7	EDO	B	614	4/4	0.97	0.09	76,91,91,96	0
7	EDO	D	623	4/4	0.97	0.12	64,65,66,67	4
8	GOL	C	612	6/6	0.97	0.07	53,61,62,66	6
8	GOL	D	602	6/6	0.97	0.08	78,85,87,92	0
6	PEG	C	605	7/7	0.97	0.07	56,64,71,71	7
9	PGE	A	824	10/10	0.97	0.07	85,88,93,95	0
10	PG4	B	610	13/13	0.97	0.10	73,84,88,90	13
10	PG4	D	613	13/13	0.97	0.11	57,85,95,100	13
7	EDO	A	804	4/4	0.98	0.08	64,74,76,76	0
7	EDO	A	805	4/4	0.98	0.13	40,41,44,47	0
7	EDO	C	601	4/4	0.98	0.10	62,62,63,64	0
7	EDO	E	2011	4/4	0.98	0.07	59,68,73,76	0
6	PEG	A	807	7/7	0.98	0.08	57,63,68,74	7
7	EDO	C	608	4/4	0.98	0.11	51,53,58,61	4
7	EDO	A	809	4/4	0.98	0.08	68,77,90,94	0
6	PEG	A	801	7/7	0.98	0.05	61,69,71,76	7
7	EDO	F	1705	4/4	0.98	0.24	52,59,59,64	0
7	EDO	C	611	4/4	0.98	0.08	74,85,91,95	0
7	EDO	F	1707	4/4	0.98	0.09	63,65,68,72	0
6	PEG	B	611	7/7	0.98	0.07	65,77,81,86	0
6	PEG	D	614	7/7	0.98	0.09	75,80,89,92	7
7	EDO	F	1715	4/4	0.98	0.05	73,78,81,82	0
6	PEG	C	603	7/7	0.98	0.07	66,79,88,90	0
7	EDO	A	823	4/4	0.98	0.09	64,65,69,69	0
7	EDO	F	1723	4/4	0.98	0.06	76,80,80,81	0
7	EDO	G	601	4/4	0.98	0.05	60,61,62,63	0
6	PEG	A	802	7/7	0.98	0.07	75,86,92,93	0
6	PEG	E	2001	7/7	0.98	0.09	74,85,93,93	0
7	EDO	D	606	4/4	0.98	0.12	67,75,76,85	0
7	EDO	D	607	4/4	0.98	0.05	70,71,72,74	0
7	EDO	D	608	4/4	0.98	0.08	53,64,65,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	EDO	D	615	4/4	0.98	0.09	68,72,80,82	0
7	EDO	H	607	4/4	0.98	0.14	79,81,84,87	0
6	PEG	E	2007	7/7	0.98	0.08	55,72,76,76	0
8	GOL	A	810	6/6	0.98	0.06	79,82,88,88	0
8	GOL	A	818	6/6	0.98	0.06	54,61,67,69	0
8	GOL	A	820	6/6	0.98	0.06	66,81,84,84	0
7	EDO	B	605	4/4	0.98	0.11	77,78,82,85	0
7	EDO	D	619	4/4	0.98	0.14	69,79,80,81	0
8	GOL	C	618	6/6	0.98	0.08	70,78,80,82	0
7	EDO	B	606	4/4	0.98	0.13	66,70,82,86	0
8	GOL	D	610	6/6	0.98	0.10	60,68,77,78	6
8	GOL	E	2004	6/6	0.98	0.07	75,85,91,93	0
8	GOL	E	2006	6/6	0.98	0.05	90,94,96,103	0
7	EDO	D	622	4/4	0.98	0.09	62,69,70,72	0
8	GOL	F	1708	6/6	0.98	0.06	74,80,81,86	0
8	GOL	F	1714	6/6	0.98	0.05	61,66,68,70	0
8	GOL	F	1716	6/6	0.98	0.07	72,82,84,86	0
8	GOL	F	1722	6/6	0.98	0.06	67,90,92,96	0
8	GOL	G	605	6/6	0.98	0.06	60,69,69,71	0
8	GOL	H	601	6/6	0.98	0.07	62,70,73,74	0
8	GOL	H	606	6/6	0.98	0.08	71,75,85,89	0
9	PGE	A	814	10/10	0.98	0.07	56,73,82,83	10
6	PEG	F	1712	7/7	0.98	0.07	58,77,83,87	7
9	PGE	C	617	10/10	0.98	0.07	56,68,74,78	10
9	PGE	F	1718	10/10	0.98	0.07	63,78,80,84	10
7	EDO	A	803	4/4	0.98	0.06	43,45,48,49	0
7	EDO	B	615	4/4	0.98	0.10	78,82,82,89	0
8	GOL	D	604	6/6	0.99	0.06	76,89,92,92	0
8	GOL	D	609	6/6	0.99	0.04	82,91,97,100	0
7	EDO	H	603	4/4	0.99	0.06	68,70,73,74	0
7	EDO	A	817	4/4	0.99	0.11	33,49,50,57	0
8	GOL	E	2005	6/6	0.99	0.07	61,71,75,77	0
7	EDO	B	608	4/4	0.99	0.11	66,67,69,71	0
8	GOL	E	2008	6/6	0.99	0.07	62,73,76,77	0
7	EDO	B	609	4/4	0.99	0.08	52,52,55,58	0
7	EDO	F	1720	4/4	0.99	0.08	72,76,83,87	0
7	EDO	F	1721	4/4	0.99	0.07	75,78,80,87	0
8	GOL	A	815	6/6	0.99	0.03	52,56,59,64	0
7	EDO	A	806	4/4	0.99	0.08	64,65,70,71	0
6	PEG	A	825	7/7	0.99	0.10	56,58,63,68	0
8	GOL	A	821	6/6	0.99	0.07	69,86,92,93	0
8	GOL	A	822	6/6	0.99	0.05	78,81,87,88	0

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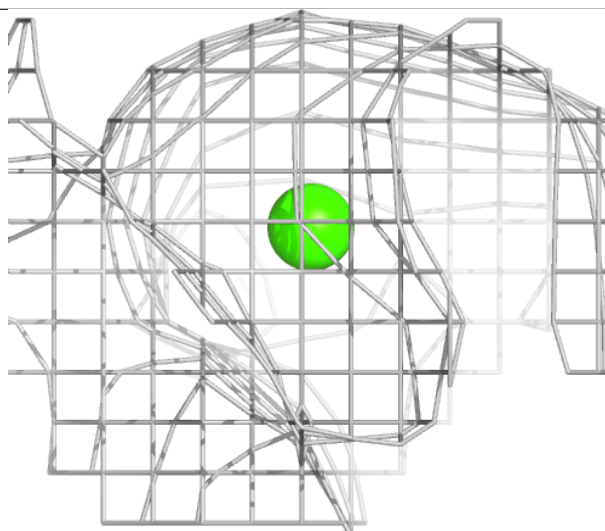
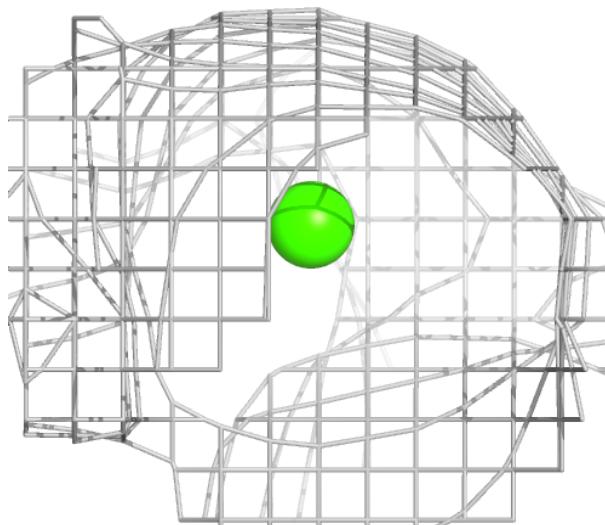
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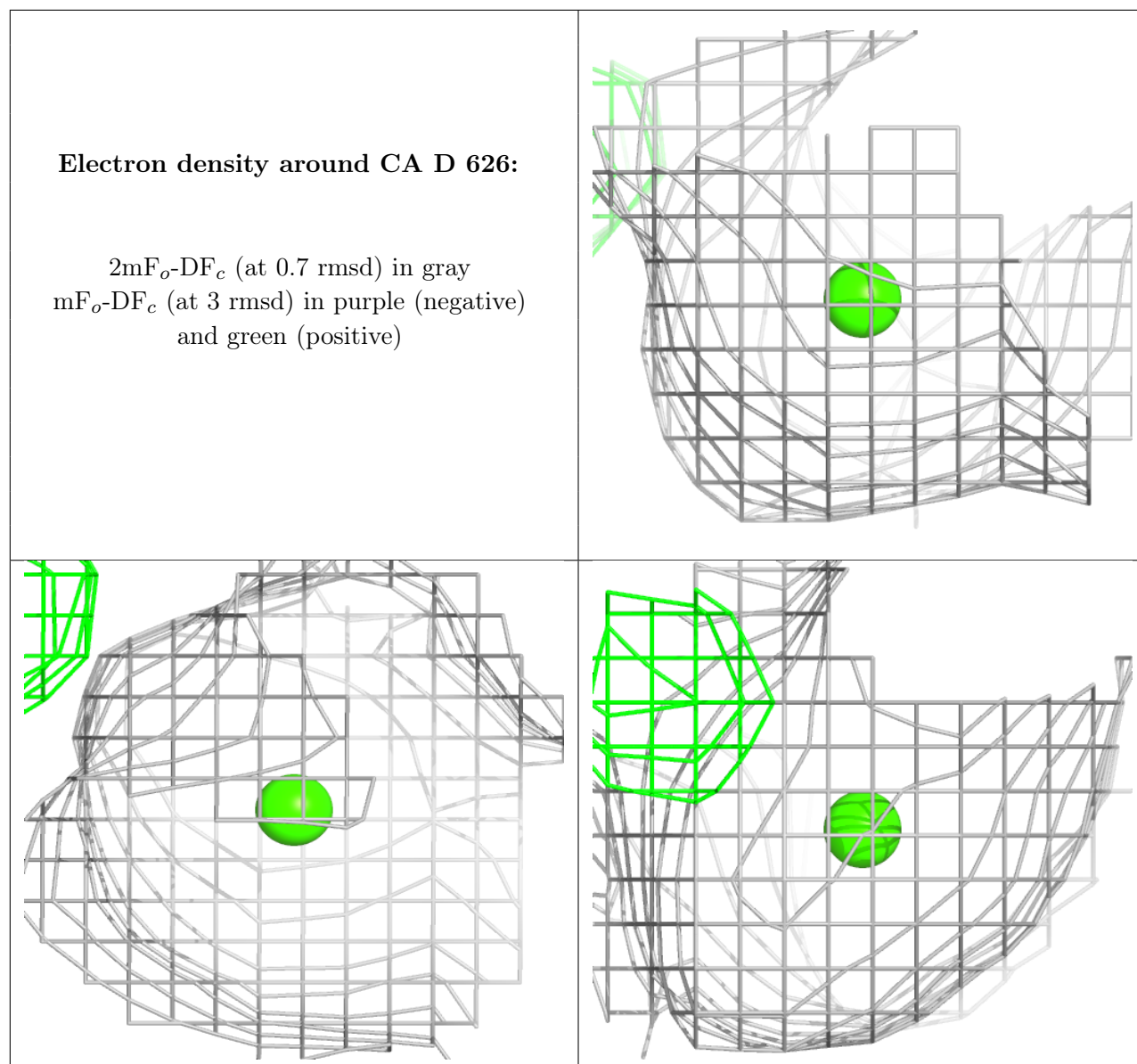
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	EDO	F	1709	4/4	0.99	0.06	55,64,66,68	0
8	GOL	C	602	6/6	0.99	0.09	58,70,73,73	0
9	PGE	B	612	10/10	0.99	0.05	58,72,77,79	0
8	GOL	C	607	6/6	0.99	0.06	53,67,71,75	0
7	EDO	F	1710	4/4	0.99	0.11	37,40,45,63	0
7	EDO	D	612	4/4	0.99	0.13	58,62,66,72	0
7	EDO	B	601	4/4	0.99	0.06	50,54,59,66	0
11	CL	C	619	1/1	0.99	0.03	58,58,58,58	0
11	CL	D	625	1/1	0.99	0.03	62,62,62,62	0
12	CA	F	1724	1/1	0.99	0.03	86,86,86,86	0
12	CA	D	626	1/1	1.00	0.02	55,55,55,55	0

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

Electron density around CA F 1724:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.