Full wwPDB X-ray Structure Validation Report (i)

Jun 22, 2024 – 11:11 PM EDT

PDB ID	:	6KXK
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 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 (1)) were used in the production of this report:

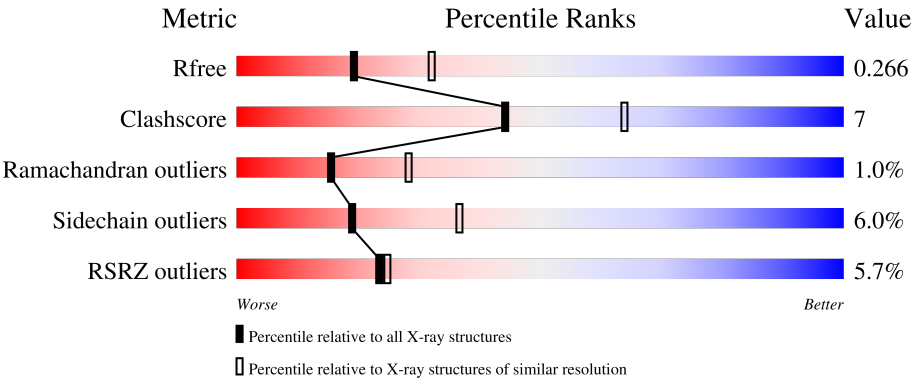
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 <=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	3% 83% 14% ·
1	C	553	2% 85% 13% ·
1	D	553	2% 84% 14% ·
1	F	553	5% 83% 14% ·
2	B	528	5% 82% 15% ··

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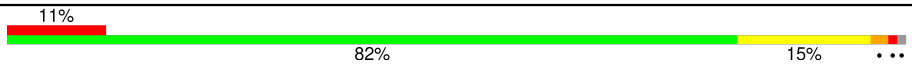
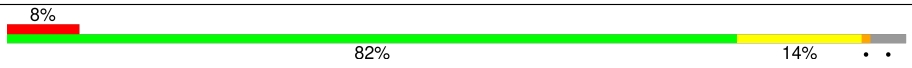
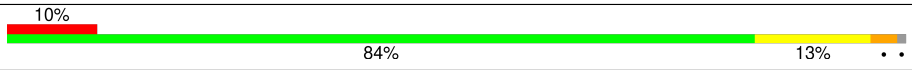
Mol	Chain	Length	Quality of chain
3	E	550	
4	G	527	
5	H	553	

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	A	807	-	-	-	X
6	PEG	D	611	-	-	X	X
6	PEG	D	614	-	-	X	-
7	EDO	A	804	-	-	X	-
7	EDO	A	805	-	-	X	-
7	EDO	A	813	-	-	-	X
7	EDO	A	817	-	-	X	-
7	EDO	B	601	-	-	-	X
7	EDO	B	603	-	-	-	X
7	EDO	B	608	-	-	X	-
7	EDO	B	609	-	-	X	-
7	EDO	B	616	-	-	-	X
7	EDO	D	612	-	-	X	-
7	EDO	D	621	-	-	-	X
7	EDO	F	1705	-	-	X	-
7	EDO	F	1707	-	-	-	X
7	EDO	F	1719	-	-	X	-
7	EDO	F	1720	-	-	-	X
8	GOL	B	607	-	-	-	X

2 Entry composition (i)

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			

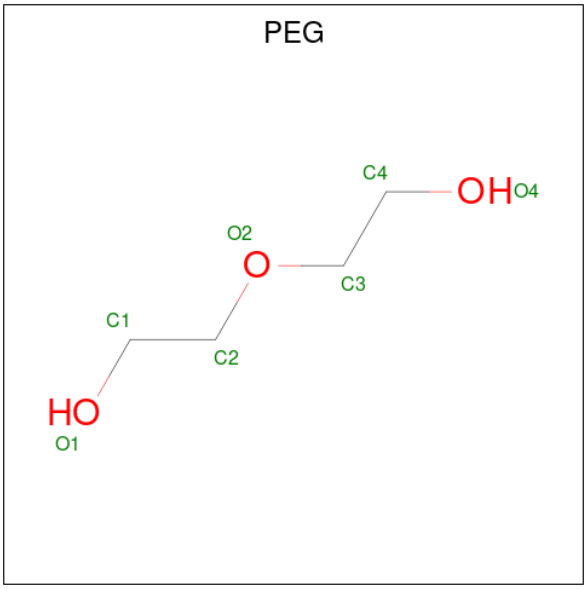
- Molecule 5 is a protein called Protein BONZAI 1.

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:

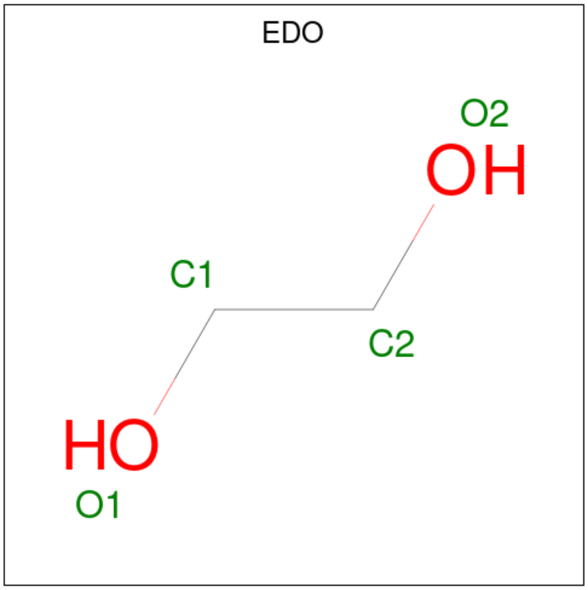
Chain	Residue	Modelled	Actual	Comment	Reference
H	-9	GLY	-	expression tag	UNP Q941L3
H	-8	THR	-	expression tag	UNP Q941L3
H	-7	SER	-	expression tag	UNP Q941L3
H	-6	SER	-	expression tag	UNP Q941L3
H	-5	MET	-	expression tag	UNP Q941L3
H	-4	ALA	-	expression tag	UNP Q941L3
H	-3	ASP	-	expression tag	UNP Q941L3
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 (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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

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

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

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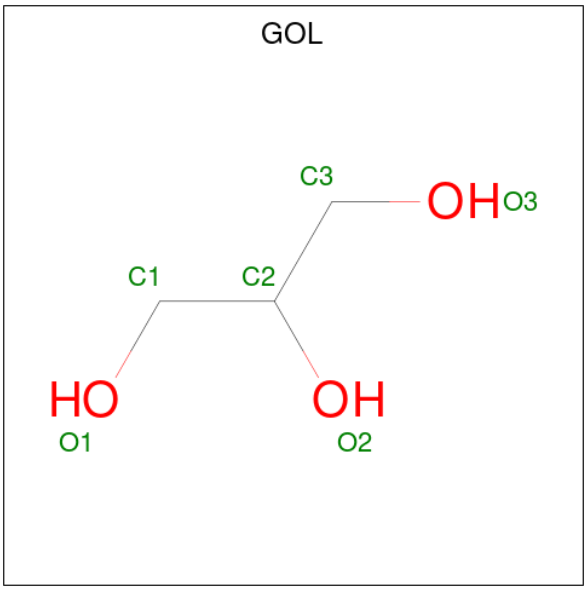
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	H	1	Total C O 4 2 2	0	0
7	H	1	Total C O 4 2 2	0	0
7	H	1	Total C O 4 2 2	0	0
7	H	1	Total C O 4 2 2	0	0

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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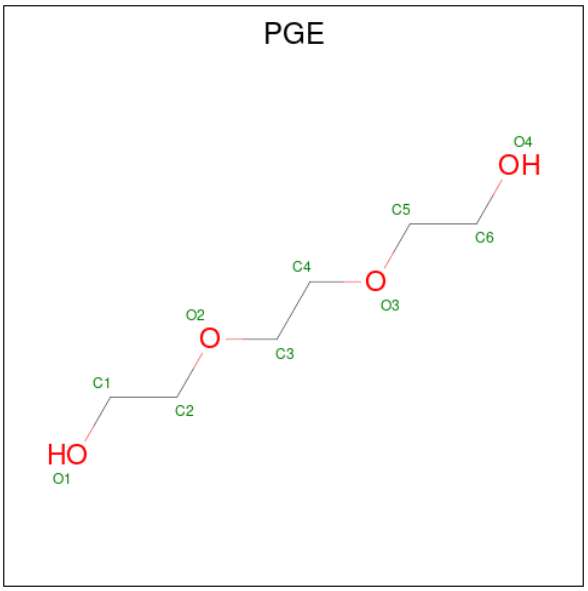
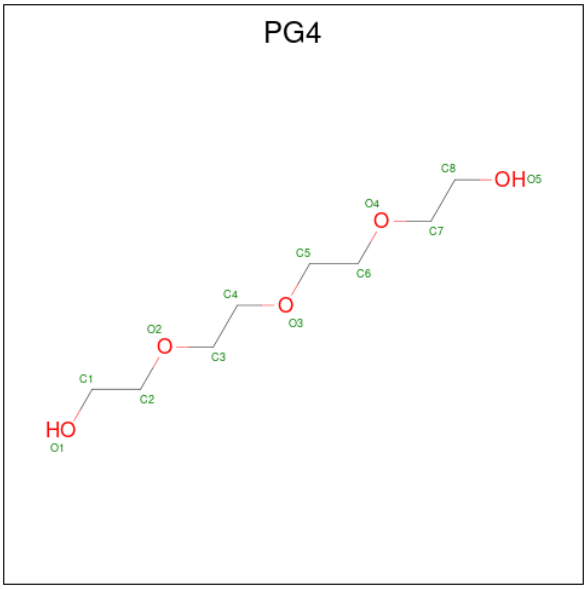
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	C	O	0	0
			6	3	3		
8	C	1	Total	C	O	0	0
			6	3	3		
8	C	1	Total	C	O	0	0
			6	3	3		
8	C	1	Total	C	O	0	0
			6	3	3		
8	D	1	Total	C	O	0	0
			6	3	3		
8	D	1	Total	C	O	0	0
			6	3	3		
8	D	1	Total	C	O	0	0
			6	3	3		
8	D	1	Total	C	O	0	0
			6	3	3		
8	E	1	Total	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 (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



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

- Molecule 10 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



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

- Molecule 11 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

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

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

- Molecule 13 is water.

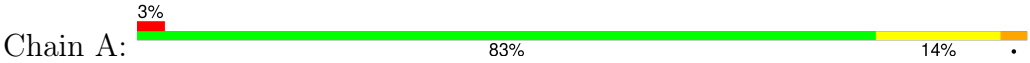
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	126	Total O 126 126	0	0
13	B	89	Total O 89 89	0	0
13	C	76	Total O 76 76	0	0
13	D	95	Total O 95 95	0	0
13	E	46	Total O 46 46	0	0
13	F	86	Total O 86 86	0	0
13	G	38	Total O 38 38	0	0
13	H	47	Total O 47 47	0	0

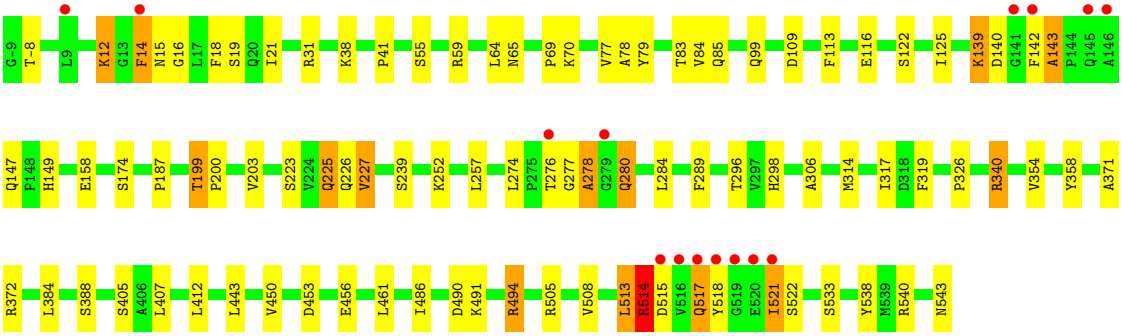
3 Residue-property plots (i)

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

• Molecule 1: Protein BONZAI 1

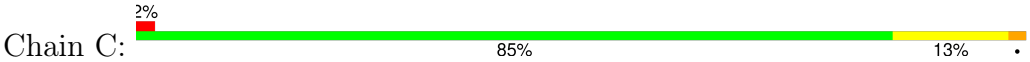
Chain A:

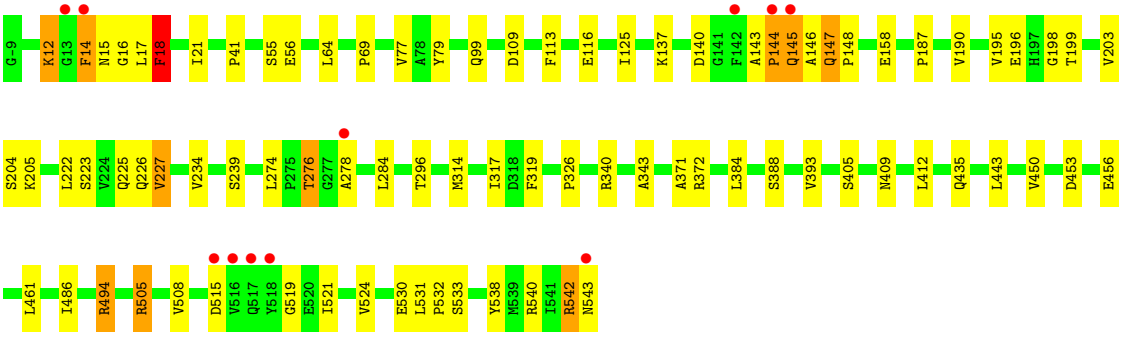




• Molecule 1: Protein BONZAI 1

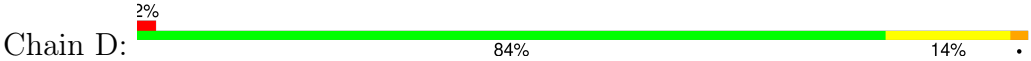
Chain C:

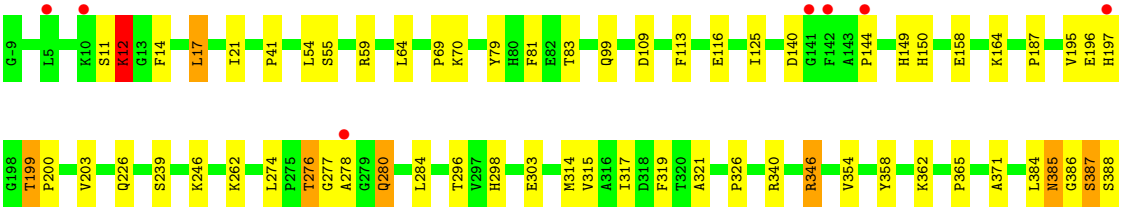


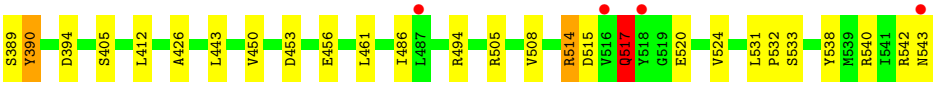


• Molecule 1: Protein BONZAI 1

Chain D:

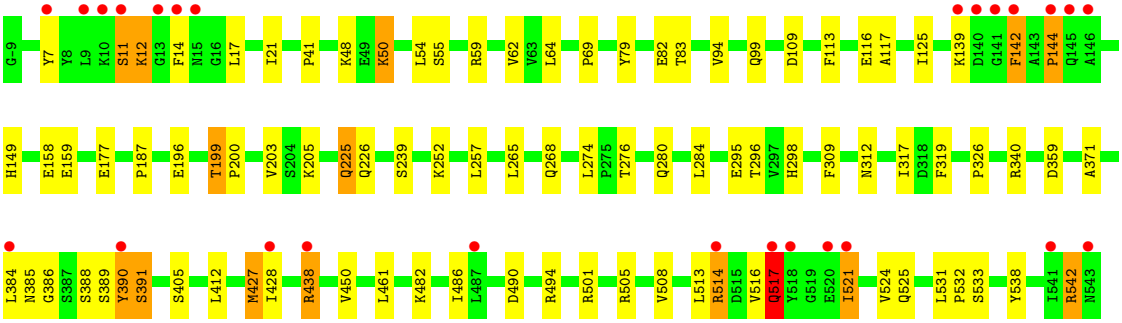






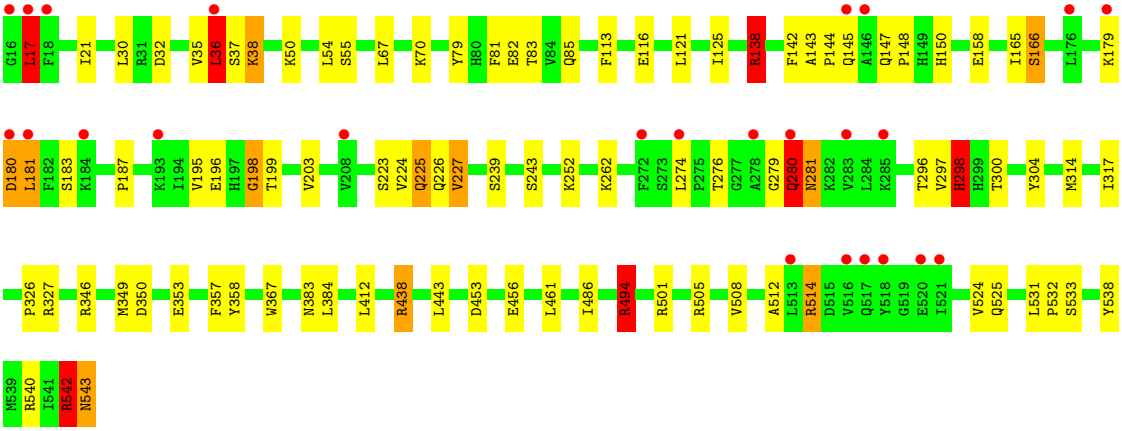
• Molecule 1: Protein BONZAI 1

Chain F:



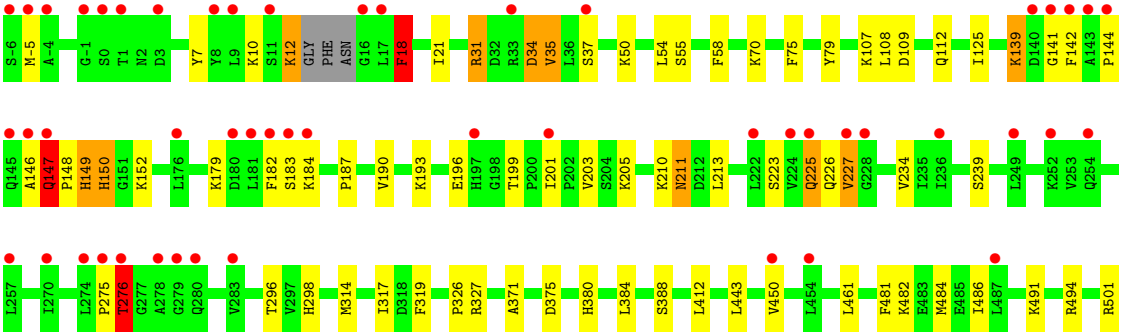
• Molecule 2: Protein BONZAI 1

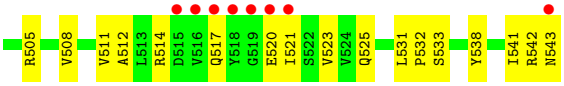
Chain B:



• Molecule 3: Protein BONZAI 1

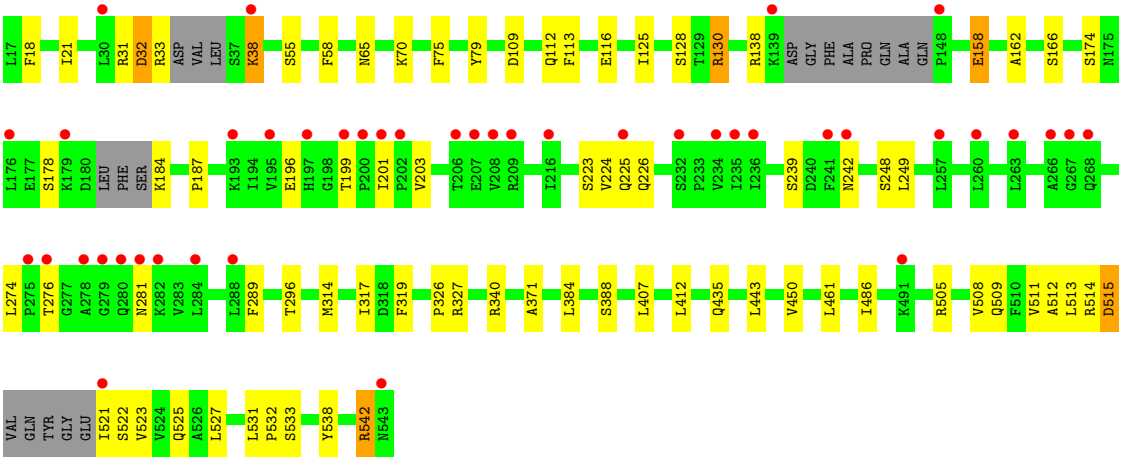
Chain E:





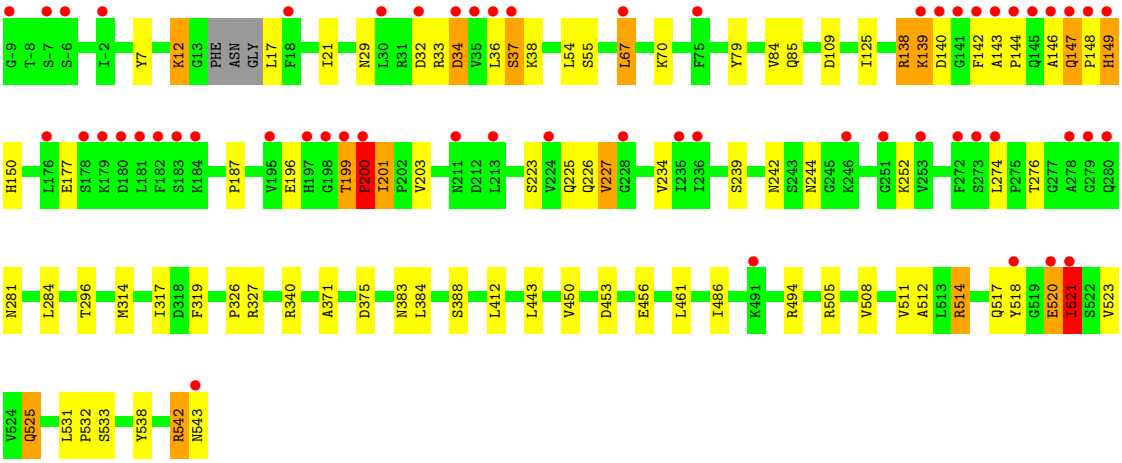
• Molecule 4: Protein BONZAI 1

Chain G:



• Molecule 5: Protein BONZAI 1

Chain H:



4 Data and refinement statistics (i)

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 48.16 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.0 (48.21-2.50) 97.1 (48.16-2.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 (5.04%)	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)	0.32 , 37.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	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	0.95	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.*

[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

5.1 Standard geometry

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

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	0.43	0/4382	0.78	5/5929 (0.1%)
1	C	0.42	0/4382	0.75	4/5929 (0.1%)
1	D	0.44	0/4382	0.81	6/5929 (0.1%)
1	F	0.43	0/4382	0.75	2/5929 (0.0%)
2	B	0.45	0/4194	0.85	13/5676 (0.2%)
3	E	0.43	0/4340	0.76	5/5871 (0.1%)
4	G	0.41	0/4035	0.74	1/5452 (0.0%)
5	H	0.41	0/4358	0.74	1/5896 (0.0%)
All	All	0.43	0/34455	0.77	37/46611 (0.1%)

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.

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	540	ARG	CG-CD-NE	-9.88	91.06	111.80
4	G	138	ARG	CB-CG-CD	-9.24	87.58	111.60
1	D	540	ARG	CG-CD-NE	-8.58	93.79	111.80
1	D	346	ARG	CG-CD-NE	8.24	129.12	111.80
1	A	340	ARG	CG-CD-NE	-7.75	95.53	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	514	ARG	CB-CA-C	-6.84	96.72	110.40
1	A	494	ARG	CB-CG-CD	6.61	128.77	111.60
2	B	298	HIS	CB-CA-C	6.60	123.61	110.40
3	E	150	HIS	N-CA-CB	6.59	122.45	110.60
2	B	542	ARG	CB-CG-CD	6.58	128.71	111.60
2	B	327	ARG	CG-CD-NE	-6.54	98.06	111.80
2	B	280	GLN	CB-CA-C	6.41	123.23	110.40
2	B	138	ARG	CG-CD-NE	-6.36	98.44	111.80
2	B	38	LYS	CB-CA-C	6.34	123.09	110.40
1	C	494	ARG	CB-CG-CD	6.31	128.00	111.60
2	B	501	ARG	CG-CD-NE	-5.97	99.27	111.80
2	B	279	GLY	C-N-CA	5.88	136.40	121.70
1	C	276	THR	CB-CA-C	-5.87	95.76	111.60
2	B	494	ARG	CB-CG-CD	5.81	126.70	111.60
1	D	298	HIS	CB-CA-C	5.74	121.88	110.40
3	E	147	GLN	CB-CA-C	5.69	121.78	110.40
5	H	200	PRO	CB-CA-C	-5.61	97.98	112.00
1	F	438	ARG	CG-CD-NE	5.59	123.54	111.80
2	B	438	ARG	CG-CD-NE	5.56	123.47	111.80
1	C	18	PHE	CB-CA-C	5.47	121.35	110.40
3	E	31	ARG	CB-CA-C	5.43	121.26	110.40
3	E	112	GLN	CB-CG-CD	-5.38	97.60	111.60
3	E	35	VAL	CA-CB-CG2	5.38	118.97	110.90
1	D	494	ARG	CB-CG-CD	5.38	125.58	111.60
2	B	148	PRO	N-CA-C	5.36	126.03	112.10
2	B	17	LEU	CB-CA-C	5.28	120.24	110.20
1	D	340	ARG	CG-CD-NE	-5.27	100.72	111.80
1	A	515	ASP	CB-CA-C	5.17	120.74	110.40
1	C	505	ARG	NE-CZ-NH1	-5.06	117.77	120.30
1	F	427	MET	CA-CB-CG	5.06	121.90	113.30
2	B	540	ARG	CG-CD-NE	5.04	122.39	111.80
1	A	18	PHE	CB-CA-C	5.03	120.47	110.40

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 (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	4299	0	4300	64	0
1	C	4299	0	4300	50	0
1	D	4299	0	4300	56	0
1	F	4299	0	4300	66	0
2	B	4114	0	4125	58	0
3	E	4259	0	4266	55	0
4	G	3963	0	3986	45	0
5	H	4277	0	4283	49	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	17	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	457	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.

All (457) 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
7:B:608:EDO:H21	7:B:609:EDO:H11	1.43	0.99
4:G:435:GLN:HG3	4:G:435:GLN:O	1.65	0.97
1:A:85:GLN:H	7:A:805:EDO:C1	1.80	0.94
3:E:147:GLN:HG3	3:E:148:PRO:CD	2.01	0.90
4:G:249:LEU:CD1	4:G:274:LEU:CD2	2.50	0.90
2:B:85:GLN:N	7:B:609:EDO:H12	1.87	0.90
3:E:147:GLN:HE21	3:E:147:GLN:HA	1.37	0.88
3:E:147:GLN:HG3	3:E:148:PRO:HD2	1.55	0.87
1:F:513:LEU:O	1:F:514:ARG:O	1.92	0.86
1:F:94:VAL:CG1	7:F:1705:EDO:H22	2.08	0.82
1:F:94:VAL:HG12	7:F:1705:EDO:H22	1.59	0.82
1:D:394:ASP:HB2	13:D:705:HOH:O	1.79	0.81
1:A:16:GLY:O	1:A:225:GLN:HG2	1.81	0.81
3:E:380:HIS:H	7:E:2010:EDO:H11	1.44	0.81
10:D:613:PG4:H72	13:D:737:HOH:O	1.79	0.81
1:F:11:SER:O	1:F:12:LYS:HB2	1.81	0.80
1:C:205:LYS:NZ	6:C:603:PEG:H11	1.96	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:67:LEU:H	5:H:67:LEU:HD23	1.44	0.80
4:G:162:ALA:O	4:G:224:VAL:HG21	1.83	0.79
4:G:249:LEU:CD1	4:G:274:LEU:HD22	2.10	0.79
2:B:85:GLN:H	7:B:609:EDO:C1	1.96	0.78
1:D:303:GLU:HG3	6:D:614:PEG:H11	1.66	0.78
5:H:201:ILE:N	5:H:201:ILE:HD12	1.99	0.77
1:D:303:GLU:CG	6:D:614:PEG:H11	2.15	0.76
1:D:346:ARG:HG2	13:D:781:HOH:O	1.84	0.76
1:F:312:ASN:ND2	1:F:359:ASP:OD1	2.18	0.76
1:C:542:ARG:HG3	13:C:726:HOH:O	1.86	0.75
1:A:139:LYS:O	1:A:139:LYS:HG3	1.87	0.75
5:H:67:LEU:HD23	5:H:67:LEU:N	2.02	0.75
1:A:85:GLN:H	7:A:805:EDO:H12	1.51	0.74
1:D:453:ASP:HB2	1:D:456:GLU:HG2	1.68	0.74
5:H:453:ASP:HB2	5:H:456:GLU:HG2	1.70	0.74
1:A:354:VAL:HG13	7:A:817:EDO:H21	1.68	0.74
1:D:321:ALA:HB3	8:D:604:GOL:H32	1.70	0.73
4:G:249:LEU:HD13	4:G:274:LEU:HD21	1.70	0.73
1:A:453:ASP:HB2	1:A:456:GLU:HG2	1.69	0.72
1:C:453:ASP:HB2	1:C:456:GLU:HG2	1.71	0.71
1:F:514:ARG:HA	13:F:1874:HOH:O	1.89	0.71
2:B:179:LYS:HE3	2:B:274:LEU:HD13	1.73	0.71
2:B:453:ASP:HB2	2:B:456:GLU:HG2	1.70	0.71
5:H:33:ARG:NH1	5:H:150:HIS:ND1	2.38	0.71
1:F:139:LYS:HG3	7:F:1719:EDO:H12	1.71	0.70
2:B:166:SER:HB3	2:B:298:HIS:HB3	1.73	0.70
4:G:249:LEU:HD11	4:G:274:LEU:HD22	1.73	0.70
1:F:14:PHE:HZ	1:F:490:ASP:HB2	1.56	0.70
3:E:147:GLN:HG3	3:E:148:PRO:HD3	1.72	0.70
1:A:83:THR:O	7:A:817:EDO:H22	1.92	0.69
2:B:358:TYR:OH	7:B:608:EDO:H22	1.92	0.69
5:H:511:VAL:HG21	5:H:523:VAL:HG12	1.74	0.69
2:B:367:TRP:HE1	9:B:612:PGE:H42	1.58	0.69
1:C:18:PHE:HA	8:C:607:GOL:H32	1.74	0.69
1:F:14:PHE:CZ	1:F:490:ASP:HB2	2.28	0.69
1:C:17:LEU:HD12	1:C:17:LEU:N	2.08	0.69
1:C:393:VAL:HA	8:C:612:GOL:H2	1.75	0.68
1:D:362:LYS:HD2	10:D:613:PG4:H22	1.76	0.68
1:F:159:GLU:H	7:F:1721:EDO:H22	1.59	0.68
4:G:317:ILE:HD12	4:G:384:LEU:HD11	1.75	0.68
3:E:107:LYS:HA	6:E:2007:PEG:H22	1.73	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:108:LEU:HG	6:E:2007:PEG:H21	1.76	0.67
2:B:317:ILE:HD12	2:B:384:LEU:HD11	1.76	0.67
4:G:249:LEU:CD1	4:G:274:LEU:HD21	2.22	0.67
5:H:317:ILE:HD12	5:H:384:LEU:HD11	1.77	0.67
3:E:317:ILE:HD12	3:E:384:LEU:HD11	1.78	0.66
1:F:298:HIS:HB2	13:F:1869:HOH:O	1.95	0.66
1:C:409:ASN:HB2	7:C:611:EDO:H21	1.78	0.66
3:E:147:GLN:HA	3:E:147:GLN:NE2	2.06	0.66
1:D:59:ARG:HH22	6:D:611:PEG:C3	2.08	0.66
9:F:1718:PGE:H12	7:F:1719:EDO:H11	1.78	0.65
1:F:312:ASN:HB3	13:F:1864:HOH:O	1.96	0.65
3:E:211:ASN:O	3:E:211:ASN:ND2	2.29	0.65
1:A:78:ALA:H	7:A:804:EDO:H21	1.61	0.65
1:A:85:GLN:HB2	7:A:805:EDO:H12	1.77	0.65
1:C:77:VAL:HG23	7:C:614:EDO:H21	1.79	0.65
1:A:85:GLN:N	7:A:805:EDO:H12	2.11	0.65
1:C:278:ALA:HB1	5:H:177:GLU:OE1	1.96	0.64
9:F:1718:PGE:H12	7:F:1719:EDO:C1	2.28	0.64
1:A:317:ILE:HD12	1:A:384:LEU:HD11	1.79	0.64
1:D:362:LYS:HD2	10:D:613:PG4:C2	2.28	0.64
2:B:350:ASP:HB3	2:B:524:VAL:HG21	1.78	0.64
1:A:85:GLN:CB	7:A:805:EDO:H12	2.27	0.64
4:G:249:LEU:HD12	4:G:249:LEU:C	2.17	0.64
1:D:317:ILE:HD12	1:D:384:LEU:HD11	1.79	0.63
1:C:12:LYS:HE3	1:C:530:GLU:OE1	1.98	0.63
1:C:16:GLY:HA3	8:C:607:GOL:H11	1.80	0.63
1:C:205:LYS:HZ2	6:C:603:PEG:H11	1.60	0.63
1:F:389:SER:O	1:F:390:TYR:C	2.36	0.63
1:A:59:ARG:HH22	9:A:814:PGE:H3	1.63	0.62
1:A:517:GLN:HA	1:A:517:GLN:NE2	2.15	0.62
1:F:386:GLY:HA2	7:F:1723:EDO:H21	1.82	0.62
1:C:317:ILE:HD12	1:C:384:LEU:HD11	1.80	0.62
1:D:326:PRO:HD3	1:D:412:LEU:HD11	1.81	0.62
1:D:517:GLN:CG	1:D:520:GLU:HB2	2.30	0.62
9:F:1718:PGE:H12	7:F:1719:EDO:H22	1.82	0.61
1:C:203:VAL:HG11	1:C:226:GLN:HB3	1.82	0.61
5:H:34:ASP:OD1	5:H:37:SER:HB2	1.99	0.61
2:B:21:ILE:HD13	2:B:125:ILE:HG21	1.82	0.61
1:F:317:ILE:HD12	1:F:384:LEU:HD11	1.82	0.61
1:D:426:ALA:HB1	8:D:602:GOL:H11	1.82	0.61
1:A:85:GLN:N	7:A:805:EDO:C1	2.57	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:385:ASN:HD21	1:F:391:SER:CB	2.14	0.61
1:A:203:VAL:HG11	1:A:226:GLN:HB3	1.83	0.60
2:B:138:ARG:HD2	2:B:142:PHE:CD2	2.36	0.60
1:D:321:ALA:HB3	8:D:604:GOL:C3	2.32	0.60
1:C:205:LYS:HE3	9:C:617:PGE:H5	1.83	0.60
1:D:203:VAL:HG11	1:D:226:GLN:HB3	1.84	0.60
1:D:517:GLN:HG2	1:D:520:GLU:HB2	1.83	0.59
1:D:276:THR:O	1:D:278:ALA:N	2.34	0.59
2:B:147:GLN:O	2:B:147:GLN:HG2	2.01	0.59
1:C:205:LYS:HZ3	6:C:603:PEG:H11	1.65	0.59
1:C:326:PRO:HD3	1:C:412:LEU:HD11	1.85	0.59
1:D:389:SER:O	1:D:390:TYR:C	2.39	0.59
1:A:149:HIS:HB3	7:A:809:EDO:O2	2.01	0.59
1:D:59:ARG:HH22	6:D:611:PEG:H32	1.67	0.59
1:F:21:ILE:HD13	1:F:125:ILE:HG21	1.85	0.59
9:F:1718:PGE:H12	7:F:1719:EDO:C2	2.33	0.59
2:B:67:LEU:H	7:B:604:EDO:H11	1.68	0.59
5:H:203:VAL:HG11	5:H:226:GLN:HB3	1.85	0.59
1:A:122:SER:HB3	7:A:805:EDO:H22	1.85	0.58
3:E:542:ARG:HG3	3:E:543:ASN:N	2.18	0.58
1:A:-8:THR:HB	13:A:912:HOH:O	2.03	0.58
7:A:805:EDO:H22	7:A:817:EDO:O2	2.04	0.58
1:A:31:ARG:HH12	7:A:809:EDO:H11	1.68	0.58
2:B:67:LEU:HB2	7:B:604:EDO:H11	1.85	0.58
1:F:59:ARG:HH22	6:F:1712:PEG:H11	1.69	0.58
2:B:35:VAL:O	2:B:37:SER:N	2.37	0.57
4:G:274:LEU:O	4:G:281:ASN:HB3	2.04	0.57
5:H:227:VAL:HG12	5:H:234:VAL:HG11	1.85	0.57
2:B:349:MET:O	2:B:353:GLU:HB2	2.04	0.57
3:E:203:VAL:HG11	3:E:226:GLN:HB3	1.86	0.57
5:H:33:ARG:O	5:H:34:ASP:HB2	2.03	0.57
3:E:-5:MET:SD	3:E:210:LYS:HE2	2.45	0.57
7:B:608:EDO:H21	7:B:609:EDO:C1	2.29	0.57
1:A:203:VAL:CG1	1:A:226:GLN:HB3	2.35	0.56
3:E:275:PRO:O	3:E:276:THR:O	2.23	0.56
4:G:511:VAL:HG21	4:G:523:VAL:HG12	1.86	0.56
1:A:326:PRO:HD3	1:A:412:LEU:HD11	1.86	0.56
1:A:372:ARG:HD3	13:A:994:HOH:O	2.04	0.56
1:F:386:GLY:CA	7:F:1723:EDO:H21	2.35	0.56
5:H:85:GLN:H	7:H:603:EDO:H21	1.70	0.56
1:D:358:TYR:CE1	7:D:612:EDO:H22	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:142:PHE:C	1:F:144:PRO:HD3	2.25	0.56
5:H:201:ILE:N	5:H:201:ILE:CD1	2.67	0.56
1:F:203:VAL:HG11	1:F:226:GLN:HB3	1.88	0.56
1:A:21:ILE:HD13	1:A:125:ILE:HG21	1.87	0.56
3:E:108:LEU:H	6:E:2007:PEG:C2	2.19	0.56
4:G:21:ILE:HD13	4:G:125:ILE:HG21	1.88	0.56
4:G:509:GLN:HE22	4:G:527:LEU:HA	1.71	0.56
1:F:62:VAL:HG11	7:F:1705:EDO:H11	1.88	0.56
5:H:21:ILE:HD13	5:H:125:ILE:HG21	1.88	0.56
13:A:992:HOH:O	7:B:601:EDO:H11	2.06	0.55
1:D:203:VAL:CG1	1:D:226:GLN:HB3	2.36	0.55
1:F:326:PRO:HD3	1:F:412:LEU:HD11	1.87	0.55
1:A:513:LEU:O	1:A:514:ARG:C	2.44	0.55
1:C:203:VAL:CG1	1:C:226:GLN:HB3	2.37	0.55
5:H:85:GLN:H	7:H:603:EDO:C2	2.20	0.55
3:E:147:GLN:HE21	3:E:147:GLN:CA	2.15	0.55
3:E:31:ARG:HB3	3:E:34:ASP:CB	2.36	0.55
1:F:203:VAL:CG1	1:F:226:GLN:HB3	2.36	0.55
1:F:427:MET:HG3	4:G:184:LYS:N	2.22	0.55
4:G:326:PRO:HD3	4:G:412:LEU:HD11	1.88	0.55
2:B:346:ARG:HG2	13:B:724:HOH:O	2.06	0.55
1:F:177:GLU:HB2	7:F:1707:EDO:H21	1.89	0.55
5:H:542:ARG:O	5:H:543:ASN:HB2	2.07	0.55
1:A:143:ALA:O	1:A:147:GLN:HB2	2.07	0.55
1:C:227:VAL:HG12	1:C:234:VAL:HG11	1.89	0.55
1:D:21:ILE:HD13	1:D:125:ILE:HG21	1.88	0.55
10:B:610:PG4:H41	13:B:757:HOH:O	2.07	0.54
1:D:81:PHE:O	7:D:612:EDO:H12	2.07	0.54
1:A:16:GLY:O	1:A:225:GLN:CG	2.55	0.54
4:G:203:VAL:HG11	4:G:226:GLN:HB3	1.90	0.54
2:B:203:VAL:HG11	2:B:226:GLN:HB3	1.89	0.54
5:H:29:ASN:O	5:H:32:ASP:OD1	2.25	0.54
1:C:64:LEU:HD22	1:C:99:GLN:HG2	1.88	0.54
1:F:7:TYR:CZ	1:F:494:ARG:HG3	2.42	0.54
2:B:358:TYR:CZ	7:B:608:EDO:H22	2.42	0.54
3:E:21:ILE:HD13	3:E:125:ILE:HG21	1.90	0.54
1:F:389:SER:O	1:F:390:TYR:O	2.25	0.54
1:D:354:VAL:HG13	7:D:612:EDO:H21	1.90	0.53
3:E:326:PRO:HD3	3:E:412:LEU:HD11	1.91	0.53
4:G:509:GLN:NE2	4:G:527:LEU:HA	2.24	0.53
5:H:203:VAL:CG1	5:H:226:GLN:HB3	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:LEU:HD22	1:A:99:GLN:HG2	1.90	0.53
1:A:517:GLN:OE1	1:A:521:ILE:HG12	2.08	0.53
1:D:59:ARG:HH22	6:D:611:PEG:H31	1.74	0.53
1:F:276:THR:HG23	1:F:276:THR:O	2.08	0.53
1:F:54:LEU:HD11	8:F:1714:GOL:H11	1.90	0.53
4:G:18:PHE:HA	8:G:605:GOL:H11	1.91	0.53
9:A:824:PGE:H52	13:A:1012:HOH:O	2.07	0.53
4:G:203:VAL:CG1	4:G:226:GLN:HB3	2.39	0.53
1:A:59:ARG:H	6:A:802:PEG:H21	1.73	0.53
1:C:137:LYS:HD3	1:C:147:GLN:NE2	2.25	0.53
1:A:21:ILE:HD12	1:A:79:TYR:HB2	1.91	0.52
4:G:184:LYS:NZ	4:G:242:ASN:ND2	2.56	0.52
5:H:139:LYS:O	5:H:139:LYS:HG3	2.07	0.52
5:H:326:PRO:HD3	5:H:412:LEU:HD11	1.92	0.52
2:B:358:TYR:CE1	7:B:608:EDO:H22	2.44	0.52
2:B:461:LEU:HD13	2:B:508:VAL:HG21	1.92	0.52
4:G:223:SER:HB2	13:G:716:HOH:O	2.08	0.52
1:D:461:LEU:HD13	1:D:508:VAL:HG21	1.90	0.52
4:G:21:ILE:HD12	4:G:79:TYR:HB2	1.91	0.52
3:E:147:GLN:CG	3:E:148:PRO:CD	2.81	0.52
1:D:426:ALA:CB	8:D:602:GOL:H11	2.40	0.52
3:E:203:VAL:CG1	3:E:226:GLN:HB3	2.40	0.52
3:E:31:ARG:HG2	13:E:2115:HOH:O	2.08	0.52
2:B:326:PRO:HD3	2:B:412:LEU:HD11	1.92	0.52
3:E:147:GLN:CG	3:E:148:PRO:HD3	2.39	0.52
1:F:205:LYS:HE3	13:F:1871:HOH:O	2.09	0.52
1:A:358:TYR:HE1	7:A:817:EDO:HO1	1.58	0.52
1:F:64:LEU:HD22	1:F:99:GLN:HG2	1.91	0.51
4:G:521:ILE:HG23	4:G:522:SER:O	2.10	0.51
2:B:203:VAL:CG1	2:B:226:GLN:HB3	2.40	0.51
3:E:182:PHE:N	3:E:182:PHE:CD1	2.78	0.51
2:B:383:ASN:OD1	9:B:612:PGE:H32	2.09	0.51
5:H:21:ILE:HD12	5:H:79:TYR:HB2	1.93	0.51
1:D:389:SER:O	1:D:390:TYR:O	2.28	0.51
3:E:275:PRO:O	3:E:276:THR:C	2.49	0.51
7:D:608:EDO:H22	13:D:756:HOH:O	2.11	0.51
3:E:50:LYS:HE3	3:E:520:GLU:HA	1.93	0.50
1:C:17:LEU:HB3	1:C:225:GLN:HG3	1.92	0.50
1:D:54:LEU:HD12	6:D:601:PEG:H42	1.93	0.50
1:A:85:GLN:H	7:A:805:EDO:H11	1.74	0.50
2:B:297:VAL:HB	1:F:295:GLU:HB2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:17:LEU:N	1:C:17:LEU:CD1	2.74	0.50
1:C:21:ILE:HD13	1:C:125:ILE:HG21	1.93	0.50
3:E:18:PHE:HA	8:E:2005:GOL:H12	1.93	0.50
4:G:178:SER:HG	4:G:184:LYS:N	2.10	0.50
1:C:21:ILE:HD12	1:C:79:TYR:HB2	1.93	0.50
4:G:461:LEU:HD13	4:G:508:VAL:HG21	1.94	0.49
1:A:142:PHE:O	1:A:143:ALA:HB2	2.10	0.49
5:H:514:ARG:CZ	5:H:514:ARG:HB2	2.41	0.49
3:E:227:VAL:HG12	3:E:234:VAL:HG11	1.93	0.49
1:A:65:ASN:HD22	7:A:816:EDO:H21	1.78	0.49
1:A:306:ALA:HB2	13:A:979:HOH:O	2.12	0.49
1:C:144:PRO:O	1:C:145:GLN:CB	2.61	0.49
1:D:262:LYS:NZ	4:G:128:SER:O	2.46	0.49
4:G:32:ASP:O	4:G:33:ARG:C	2.52	0.49
5:H:201:ILE:HD12	5:H:201:ILE:H	1.75	0.49
1:F:521:ILE:HB	1:F:525:GLN:OE1	2.13	0.48
1:D:385:ASN:ND2	1:D:387:SER:H	2.11	0.48
1:C:542:ARG:HG2	1:C:543:ASN:N	2.27	0.48
13:A:992:HOH:O	7:B:601:EDO:C1	2.62	0.48
1:F:385:ASN:HD21	1:F:391:SER:HB3	1.76	0.48
1:F:427:MET:HE3	13:F:1881:HOH:O	2.14	0.48
5:H:223:SER:O	5:H:227:VAL:HG22	2.13	0.48
1:A:84:VAL:HA	7:A:805:EDO:H11	1.95	0.48
3:E:21:ILE:HD12	3:E:79:TYR:HB2	1.96	0.48
5:H:521:ILE:HA	5:H:525:GLN:OE1	2.13	0.48
1:C:319:PHE:HB3	1:C:371:ALA:HB2	1.95	0.47
1:A:505:ARG:HD2	13:A:930:HOH:O	2.14	0.47
1:A:59:ARG:N	6:A:802:PEG:H21	2.30	0.47
10:B:610:PG4:H61	13:B:775:HOH:O	2.13	0.47
1:D:64:LEU:HD22	1:D:99:GLN:HG2	1.95	0.47
3:E:184:LYS:HG2	3:E:213:LEU:HG	1.96	0.47
1:A:280:GLN:HE21	1:A:280:GLN:HA	1.80	0.47
1:F:21:ILE:HD12	1:F:79:TYR:HB2	1.96	0.47
2:B:223:SER:O	2:B:227:VAL:HG12	2.14	0.47
1:D:83:THR:O	7:D:612:EDO:H11	2.15	0.47
3:E:139:LYS:HA	3:E:139:LYS:HD3	1.50	0.47
1:C:461:LEU:HD13	1:C:508:VAL:HG21	1.96	0.47
1:D:517:GLN:HG3	1:D:520:GLU:HB2	1.96	0.47
5:H:33:ARG:HH12	5:H:150:HIS:CE1	2.32	0.47
5:H:461:LEU:HD13	5:H:508:VAL:HG21	1.97	0.47
5:H:520:GLU:O	5:H:521:ILE:C	2.52	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:17:LEU:HG	5:H:225:GLN:HE22	1.79	0.47
1:D:358:TYR:HE1	7:D:612:EDO:C2	2.28	0.47
5:H:138:ARG:HG3	5:H:139:LYS:H	1.80	0.47
2:B:298:HIS:CE1	2:B:300:THR:HG22	2.50	0.47
4:G:184:LYS:HZ2	4:G:242:ASN:ND2	2.13	0.47
1:A:14:PHE:CG	1:A:298:HIS:CE1	3.03	0.46
1:D:314:MET:HG2	1:D:365:PRO:HG2	1.96	0.46
1:F:390:TYR:HE2	1:F:428:ILE:CD1	2.28	0.46
5:H:453:ASP:HB2	5:H:456:GLU:CG	2.43	0.46
3:E:7:TYR:CZ	3:E:494:ARG:HG3	2.51	0.46
8:E:2012:GOL:H2	13:E:2126:HOH:O	2.16	0.46
2:B:180:ASP:O	2:B:181:LEU:HB2	2.16	0.46
1:F:225:GLN:H	1:F:225:GLN:HG2	1.53	0.46
1:F:532:PRO:HD2	13:F:1802:HOH:O	2.14	0.46
3:E:223:SER:O	3:E:227:VAL:HG22	2.14	0.46
1:F:142:PHE:O	1:F:144:PRO:HD3	2.16	0.46
5:H:314:MET:HB2	5:H:443:LEU:HA	1.98	0.46
1:A:319:PHE:HB3	1:A:371:ALA:HB2	1.97	0.46
1:F:319:PHE:HB3	1:F:371:ALA:HB2	1.96	0.46
1:F:513:LEU:O	1:F:514:ARG:C	2.54	0.46
3:E:461:LEU:HD13	3:E:508:VAL:HG21	1.98	0.46
1:C:343:ALA:H	7:C:610:EDO:H22	1.79	0.46
3:E:314:MET:HB2	3:E:443:LEU:HA	1.98	0.46
3:E:511:VAL:HG21	3:E:523:VAL:HG12	1.97	0.46
1:F:50:LYS:HD3	1:F:50:LYS:HA	1.72	0.46
1:A:77:VAL:HA	7:A:804:EDO:H21	1.98	0.46
1:D:319:PHE:HB3	1:D:371:ALA:HB2	1.97	0.46
1:A:453:ASP:HB2	1:A:456:GLU:CG	2.44	0.45
1:A:461:LEU:HD13	1:A:508:VAL:HG21	1.97	0.45
2:B:195:VAL:HG23	2:B:198:GLY:H	1.80	0.45
2:B:21:ILE:HD12	2:B:79:TYR:HB2	1.97	0.45
2:B:314:MET:HB2	2:B:443:LEU:HA	1.99	0.45
1:C:140:ASP:OD2	1:C:148:PRO:HD2	2.17	0.45
1:C:223:SER:O	1:C:227:VAL:HG22	2.17	0.45
5:H:319:PHE:HB3	5:H:371:ALA:HB2	1.98	0.45
1:C:77:VAL:HG23	7:C:614:EDO:C2	2.46	0.45
2:B:179:LYS:CE	2:B:274:LEU:HD13	2.43	0.45
1:F:284:LEU:HB3	7:F:1707:EDO:H22	1.98	0.45
1:A:77:VAL:HG23	7:A:804:EDO:H21	1.97	0.45
2:B:145:GLN:OE1	2:B:145:GLN:HA	2.17	0.45
1:C:276:THR:O	1:C:276:THR:HG22	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:11:SER:O	1:D:12:LYS:HD2	2.16	0.45
3:E:511:VAL:HG21	3:E:523:VAL:CG1	2.47	0.45
4:G:511:VAL:HG21	4:G:523:VAL:CG1	2.47	0.45
5:H:7:TYR:CZ	5:H:494:ARG:HG3	2.51	0.45
2:B:121:LEU:HB3	7:B:609:EDO:H21	1.99	0.44
2:B:438:ARG:NH2	1:F:268:GLN:OE1	2.50	0.44
1:F:117:ALA:HB1	9:F:1718:PGE:H42	1.99	0.44
1:D:195:VAL:HG12	1:D:197:HIS:H	1.81	0.44
1:D:385:ASN:HD22	1:D:386:GLY:N	2.15	0.44
1:D:453:ASP:HB2	1:D:456:GLU:CG	2.43	0.44
3:E:12:LYS:HB3	3:E:12:LYS:HE3	1.76	0.44
1:F:7:TYR:CE2	1:F:494:ARG:HG3	2.52	0.44
1:D:41:PRO:HG2	1:D:69:PRO:HG3	2.00	0.44
3:E:225:GLN:H	3:E:225:GLN:HG3	1.62	0.44
5:H:199:THR:HA	5:H:200:PRO:HD3	1.82	0.44
3:E:319:PHE:HB3	3:E:371:ALA:HB2	1.99	0.44
4:G:319:PHE:HB3	4:G:371:ALA:HB2	1.98	0.44
5:H:84:VAL:HA	7:H:603:EDO:H21	1.99	0.44
2:B:81:PHE:O	7:B:608:EDO:O2	2.36	0.44
3:E:542:ARG:HG3	3:E:543:ASN:H	1.82	0.44
1:A:223:SER:O	1:A:227:VAL:HG12	2.18	0.44
1:D:274:LEU:HG	1:D:284:LEU:HD11	1.99	0.44
6:A:825:PEG:H32	6:A:825:PEG:H11	1.57	0.44
2:B:524:VAL:CG2	2:B:525:GLN:N	2.81	0.44
1:D:21:ILE:HD12	1:D:79:TYR:HB2	2.00	0.44
1:D:59:ARG:NH2	6:D:611:PEG:H32	2.33	0.44
1:F:41:PRO:HG2	1:F:69:PRO:HG3	2.00	0.44
1:A:85:GLN:HA	6:A:801:PEG:H32	2.00	0.43
6:A:802:PEG:H31	13:A:1011:HOH:O	2.17	0.43
2:B:223:SER:OG	2:B:225:GLN:HG2	2.18	0.43
1:D:14:PHE:O	1:D:17:LEU:HB2	2.18	0.43
1:F:82:GLU:HG2	1:F:83:THR:HG23	2.00	0.43
1:C:195:VAL:HG23	1:C:198:GLY:O	2.18	0.43
6:D:620:PEG:H11	13:D:784:HOH:O	2.17	0.43
3:E:149:HIS:CE1	3:E:152:LYS:HE2	2.53	0.43
4:G:505:ARG:CZ	4:G:538:TYR:HB2	2.48	0.43
5:H:242:ASN:HB3	5:H:244:ASN:OD1	2.18	0.43
3:E:520:GLU:HB3	3:E:521:ILE:H	1.66	0.43
1:A:314:MET:HB2	1:A:443:LEU:HA	2.01	0.43
1:C:41:PRO:HG2	1:C:69:PRO:HG3	2.00	0.43
3:E:505:ARG:CZ	3:E:538:TYR:HB2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:314:MET:HB2	4:G:443:LEU:HA	2.01	0.43
1:A:274:LEU:HG	1:A:284:LEU:HD11	2.00	0.43
1:A:505:ARG:CZ	1:A:538:TYR:HB2	2.49	0.43
1:A:12:LYS:HA	1:A:12:LYS:HD3	1.69	0.43
1:A:12:LYS:HB3	1:A:15:ASN:HB2	2.00	0.43
1:A:277:GLY:O	1:A:278:ALA:C	2.56	0.43
2:B:453:ASP:HB2	2:B:456:GLU:CG	2.44	0.43
2:B:494:ARG:H	2:B:494:ARG:HG2	1.29	0.43
3:E:31:ARG:HB3	3:E:34:ASP:HB3	2.00	0.43
1:F:113:PHE:HZ	1:F:116:GLU:HB2	1.84	0.43
5:H:140:ASP:O	5:H:147:GLN:NE2	2.51	0.43
1:C:195:VAL:CG2	1:C:198:GLY:O	2.66	0.43
1:C:274:LEU:HG	1:C:284:LEU:HD11	2.00	0.43
1:F:516:VAL:O	1:F:517:GLN:HB2	2.17	0.43
5:H:505:ARG:CZ	5:H:538:TYR:HB2	2.48	0.43
2:B:30:LEU:O	2:B:67:LEU:HD22	2.18	0.43
2:B:280:GLN:C	2:B:281:ASN:HD22	2.22	0.43
1:F:48:LYS:HE3	8:F:1714:GOL:O2	2.19	0.43
4:G:201:ILE:HD12	4:G:201:ILE:HA	1.96	0.43
1:A:38:LYS:HD2	7:B:601:EDO:H11	2.00	0.43
2:B:505:ARG:CZ	2:B:538:TYR:HB2	2.49	0.43
1:F:159:GLU:HB3	7:F:1721:EDO:H11	2.00	0.43
1:F:461:LEU:HD13	1:F:508:VAL:HG21	2.00	0.43
5:H:32:ASP:OD2	5:H:149:HIS:HB2	2.19	0.43
5:H:142:PHE:HB3	5:H:143:ALA:H	1.65	0.43
1:A:78:ALA:H	7:A:804:EDO:C2	2.31	0.42
1:D:17:LEU:O	7:D:622:EDO:H12	2.19	0.42
1:A:41:PRO:HG2	1:A:69:PRO:HG3	2.01	0.42
1:C:314:MET:HB2	1:C:443:LEU:HA	2.01	0.42
1:D:187:PRO:HA	1:D:239:SER:O	2.19	0.42
8:D:602:GOL:H2	13:D:776:HOH:O	2.19	0.42
4:G:113:PHE:HZ	4:G:116:GLU:HB2	1.85	0.42
2:B:143:ALA:HB2	2:B:150:HIS:CE1	2.55	0.42
1:D:199:THR:HA	1:D:200:PRO:HD3	1.81	0.42
4:G:187:PRO:HA	4:G:239:SER:O	2.19	0.42
1:C:14:PHE:O	1:C:540:ARG:NH1	2.53	0.42
1:C:453:ASP:HB2	1:C:456:GLU:CG	2.45	0.42
2:B:113:PHE:HZ	2:B:116:GLU:HB2	1.85	0.42
1:C:113:PHE:HZ	1:C:116:GLU:HB2	1.85	0.42
1:C:187:PRO:HA	1:C:239:SER:O	2.20	0.42
5:H:383:ASN:HD21	8:H:601:GOL:H32	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:187:PRO:HA	2:B:239:SER:O	2.19	0.42
1:C:17:LEU:HD21	1:C:223:SER:HB2	2.01	0.42
5:H:33:ARG:NH1	5:H:150:HIS:CE1	2.87	0.42
1:D:113:PHE:HZ	1:D:116:GLU:HB2	1.85	0.42
1:F:64:LEU:HD21	7:F:1705:EDO:H11	2.02	0.42
1:D:164:LYS:NZ	6:D:614:PEG:H22	2.35	0.42
3:E:187:PRO:HA	3:E:239:SER:O	2.20	0.42
1:F:187:PRO:HA	1:F:239:SER:O	2.20	0.42
1:F:274:LEU:HG	1:F:284:LEU:HD11	2.01	0.42
1:F:309:PHE:HE1	1:F:438:ARG:HH21	1.68	0.42
1:A:85:GLN:HA	6:A:801:PEG:C3	2.50	0.42
1:A:113:PHE:HZ	1:A:116:GLU:HB2	1.85	0.42
5:H:274:LEU:HG	5:H:284:LEU:HD11	2.02	0.41
1:A:187:PRO:HA	1:A:239:SER:O	2.20	0.41
3:E:193:LYS:HE3	3:E:201:ILE:HD12	2.02	0.41
5:H:187:PRO:HA	5:H:239:SER:O	2.20	0.41
3:E:7:TYR:CE2	3:E:494:ARG:HG3	2.55	0.41
4:G:531:LEU:N	4:G:532:PRO:CD	2.83	0.41
3:E:380:HIS:N	7:E:2010:EDO:H11	2.22	0.41
4:G:407:LEU:HD23	4:G:407:LEU:HA	1.95	0.41
1:A:77:VAL:HG23	7:A:804:EDO:C2	2.51	0.41
1:A:407:LEU:HD23	1:A:407:LEU:HA	1.95	0.41
2:B:35:VAL:HG13	2:B:36:LEU:HD23	2.02	0.41
2:B:304:TYR:CZ	1:F:265:LEU:HD22	2.56	0.41
1:C:56:GLU:HG2	6:C:605:PEG:H21	2.01	0.41
1:C:505:ARG:CZ	1:C:538:TYR:HB2	2.50	0.41
1:D:280:GLN:HE21	1:D:280:GLN:HB3	1.73	0.41
1:D:505:ARG:CZ	1:D:538:TYR:HB2	2.50	0.41
2:B:512:ALA:O	2:B:514:ARG:N	2.49	0.41
1:F:505:ARG:CZ	1:F:538:TYR:HB2	2.50	0.41
4:G:58:PHE:CD1	4:G:75:PHE:HB2	2.56	0.41
1:C:143:ALA:HB3	1:C:144:PRO:HD3	2.02	0.41
5:H:531:LEU:N	5:H:532:PRO:CD	2.83	0.41
2:B:82:GLU:HG2	2:B:83:THR:HG23	2.03	0.41
2:B:357:PHE:CD1	10:B:610:PG4:H22	2.55	0.41
2:B:531:LEU:N	2:B:532:PRO:CD	2.84	0.41
2:B:542:ARG:HG3	2:B:543:ASN:N	2.35	0.41
1:C:204:SER:HB2	1:C:222:LEU:HD21	2.02	0.41
3:E:190:VAL:HG22	3:E:205:LYS:HG3	2.03	0.41
3:E:531:LEU:N	3:E:532:PRO:CD	2.83	0.41
1:F:199:THR:HA	1:F:200:PRO:HD3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:531:LEU:N	1:F:532:PRO:CD	2.84	0.41
4:G:174:SER:HB2	4:G:289:PHE:HE2	1.85	0.41
4:G:512:ALA:C	4:G:514:ARG:H	2.23	0.41
2:B:165:ILE:O	2:B:224:VAL:HG23	2.21	0.41
1:C:531:LEU:N	1:C:532:PRO:CD	2.84	0.41
1:D:531:LEU:N	1:D:532:PRO:CD	2.84	0.41
3:E:481:PHE:O	3:E:484:MET:HB2	2.21	0.41
1:F:59:ARG:NH2	6:F:1712:PEG:H11	2.33	0.41
4:G:38:LYS:HB2	4:G:65:ASN:OD1	2.21	0.41
1:A:199:THR:HA	1:A:200:PRO:HD3	1.84	0.40
1:D:140:ASP:OD2	1:D:150:HIS:HE1	2.03	0.40
1:D:314:MET:HB2	1:D:443:LEU:HA	2.02	0.40
3:E:512:ALA:O	3:E:514:ARG:N	2.48	0.40
4:G:515:ASP:C	4:G:523:VAL:HG21	2.42	0.40
2:B:32:ASP:OD1	2:B:38:LYS:HE3	2.21	0.40
6:D:614:PEG:H21	13:D:783:HOH:O	2.21	0.40
1:F:99:GLN:HA	7:F:1705:EDO:C1	2.29	0.40
1:C:190:VAL:HG12	13:C:702:HOH:O	2.21	0.40
4:G:130:ARG:NH2	4:G:158:GLU:HA	2.36	0.40
5:H:201:ILE:CD1	5:H:201:ILE:H	2.32	0.40
5:H:512:ALA:HB3	5:H:514:ARG:HH21	1.85	0.40
1:A:174:SER:HB2	1:A:289:PHE:HE2	1.87	0.40
2:B:85:GLN:HB2	7:B:609:EDO:H21	2.04	0.40
2:B:147:GLN:O	2:B:147:GLN:CG	2.68	0.40
3:E:58:PHE:CD1	3:E:75:PHE:HB2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	551/553 (100%)	525 (95%)	22 (4%)	4 (1%)	22 39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	551/553 (100%)	521 (95%)	24 (4%)	6 (1%)	14	26
1	D	551/553 (100%)	524 (95%)	21 (4%)	6 (1%)	14	26
1	F	551/553 (100%)	524 (95%)	21 (4%)	6 (1%)	14	26
2	B	526/528 (100%)	501 (95%)	20 (4%)	5 (1%)	15	28
3	E	543/550 (99%)	505 (93%)	31 (6%)	7 (1%)	12	21
4	G	498/527 (94%)	477 (96%)	19 (4%)	2 (0%)	34	54
5	H	546/553 (99%)	514 (94%)	25 (5%)	7 (1%)	12	21
All	All	4317/4370 (99%)	4091 (95%)	183 (4%)	43 (1%)	15	28

All (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
1	D	144	PRO
1	D	390	TYR
1	D	514	ARG
1	D	542	ARG
3	E	146	ALA
3	E	276	THR
1	F	144	PRO
1	F	390	TYR
1	F	514	ARG
1	F	517	GLN
4	G	542	ARG
5	H	34	ASP
1	A	143	ALA
1	C	146	ALA
1	D	277	GLY
3	E	18	PHE
3	E	144	PRO
1	F	12	LYS
1	F	542	ARG
5	H	146	ALA
2	B	17	LEU
3	E	141	GLY
3	E	150	HIS

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Mol	Chain	Res	Type
5	H	144	PRO
5	H	200	PRO
2	B	181	LEU
1	C	15	ASN
1	C	147	GLN
1	C	519	GLY
1	D	517	GLN
3	E	149	HIS
4	G	513	LEU
5	H	12	LYS
5	H	148	PRO
1	A	513	LEU
2	B	280	GLN
5	H	521	ILE
1	C	144	PRO

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	481/481 (100%)	449 (93%)	32 (7%)	16	31
1	C	481/481 (100%)	458 (95%)	23 (5%)	25	48
1	D	481/481 (100%)	456 (95%)	25 (5%)	23	44
1	F	481/481 (100%)	454 (94%)	27 (6%)	21	40
2	B	461/461 (100%)	433 (94%)	28 (6%)	18	36
3	E	477/479 (100%)	444 (93%)	33 (7%)	15	30
4	G	446/461 (97%)	421 (94%)	25 (6%)	21	40
5	H	479/481 (100%)	444 (93%)	35 (7%)	14	27
All	All	3787/3806 (100%)	3559 (94%)	228 (6%)	19	37

All (228) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LYS
1	A	14	PHE
1	A	19	SER
1	A	55	SER
1	A	70	LYS
1	A	109	ASP
1	A	139	LYS
1	A	140	ASP
1	A	158	GLU
1	A	199	THR
1	A	225	GLN
1	A	227	VAL
1	A	252	LYS
1	A	257	LEU
1	A	276	THR
1	A	280	GLN
1	A	296	THR
1	A	340	ARG
1	A	388	SER
1	A	405	SER
1	A	450	VAL
1	A	486	ILE
1	A	490	ASP
1	A	491	LYS
1	A	494	ARG
1	A	514	ARG
1	A	517	GLN
1	A	518	TYR
1	A	521	ILE
1	A	522	SER
1	A	533	SER
1	A	543	ASN
2	B	17	LEU
2	B	36	LEU
2	B	50	LYS
2	B	54	LEU
2	B	55	SER
2	B	70	LYS
2	B	138	ARG
2	B	158	GLU
2	B	166	SER
2	B	180	ASP
2	B	183	SER

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Mol	Chain	Res	Type
2	B	196	GLU
2	B	199	THR
2	B	225	GLN
2	B	227	VAL
2	B	243	SER
2	B	252	LYS
2	B	262	LYS
2	B	276	THR
2	B	280	GLN
2	B	281	ASN
2	B	296	THR
2	B	298	HIS
2	B	486	ILE
2	B	494	ARG
2	B	533	SER
2	B	542	ARG
2	B	543	ASN
1	C	12	LYS
1	C	14	PHE
1	C	18	PHE
1	C	55	SER
1	C	109	ASP
1	C	158	GLU
1	C	196	GLU
1	C	199	THR
1	C	227	VAL
1	C	296	THR
1	C	340	ARG
1	C	372	ARG
1	C	388	SER
1	C	405	SER
1	C	435	GLN
1	C	450	VAL
1	C	486	ILE
1	C	494	ARG
1	C	515	ASP
1	C	521	ILE
1	C	524	VAL
1	C	533	SER
1	C	542	ARG
1	D	12	LYS
1	D	17	LEU

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Mol	Chain	Res	Type
1	D	55	SER
1	D	70	LYS
1	D	109	ASP
1	D	149	HIS
1	D	158	GLU
1	D	196	GLU
1	D	199	THR
1	D	246	LYS
1	D	276	THR
1	D	280	GLN
1	D	296	THR
1	D	315	VAL
1	D	385	ASN
1	D	387	SER
1	D	388	SER
1	D	405	SER
1	D	450	VAL
1	D	486	ILE
1	D	515	ASP
1	D	517	GLN
1	D	524	VAL
1	D	533	SER
1	D	543	ASN
3	E	12	LYS
3	E	18	PHE
3	E	34	ASP
3	E	35	VAL
3	E	37	SER
3	E	54	LEU
3	E	55	SER
3	E	70	LYS
3	E	109	ASP
3	E	139	LYS
3	E	142	PHE
3	E	147	GLN
3	E	179	LYS
3	E	183	SER
3	E	196	GLU
3	E	199	THR
3	E	211	ASN
3	E	225	GLN
3	E	227	VAL

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Mol	Chain	Res	Type
3	E	276	THR
3	E	296	THR
3	E	298	HIS
3	E	327	ARG
3	E	375	ASP
3	E	388	SER
3	E	450	VAL
3	E	482	LYS
3	E	486	ILE
3	E	491	LYS
3	E	501	ARG
3	E	517	GLN
3	E	525	GLN
3	E	533	SER
1	F	17	LEU
1	F	50	LYS
1	F	55	SER
1	F	109	ASP
1	F	142	PHE
1	F	149	HIS
1	F	158	GLU
1	F	196	GLU
1	F	199	THR
1	F	225	GLN
1	F	252	LYS
1	F	257	LEU
1	F	280	GLN
1	F	296	THR
1	F	340	ARG
1	F	388	SER
1	F	391	SER
1	F	405	SER
1	F	450	VAL
1	F	482	LYS
1	F	486	ILE
1	F	501	ARG
1	F	517	GLN
1	F	521	ILE
1	F	524	VAL
1	F	533	SER
1	F	542	ARG
4	G	31	ARG

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Mol	Chain	Res	Type
4	G	32	ASP
4	G	38	LYS
4	G	55	SER
4	G	70	LYS
4	G	109	ASP
4	G	112	GLN
4	G	130	ARG
4	G	158	GLU
4	G	166	SER
4	G	196	GLU
4	G	199	THR
4	G	225	GLN
4	G	248	SER
4	G	276	THR
4	G	296	THR
4	G	327	ARG
4	G	340	ARG
4	G	388	SER
4	G	450	VAL
4	G	486	ILE
4	G	515	ASP
4	G	525	GLN
4	G	533	SER
4	G	542	ARG
5	H	12	LYS
5	H	36	LEU
5	H	37	SER
5	H	38	LYS
5	H	54	LEU
5	H	55	SER
5	H	67	LEU
5	H	70	LYS
5	H	109	ASP
5	H	138	ARG
5	H	139	LYS
5	H	147	GLN
5	H	149	HIS
5	H	196	GLU
5	H	199	THR
5	H	201	ILE
5	H	227	VAL
5	H	252	LYS

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Mol	Chain	Res	Type
5	H	276	THR
5	H	281	ASN
5	H	296	THR
5	H	327	ARG
5	H	340	ARG
5	H	375	ASP
5	H	388	SER
5	H	450	VAL
5	H	486	ILE
5	H	514	ARG
5	H	517	GLN
5	H	518	TYR
5	H	520	GLU
5	H	521	ILE
5	H	525	GLN
5	H	533	SER
5	H	542	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	ASN
1	A	225	GLN
1	A	280	GLN
1	A	281	ASN
1	A	409	ASN
1	A	455	GLN
1	A	534	GLN
2	B	150	HIS
2	B	175	ASN
2	B	280	GLN
2	B	298	HIS
2	B	525	GLN
2	B	534	GLN
2	B	543	ASN
1	C	15	ASN
1	C	65	ASN
1	C	147	GLN
1	C	150	HIS
1	C	281	ASN
1	C	298	HIS
1	C	409	ASN

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Mol	Chain	Res	Type
1	C	435	GLN
1	D	15	ASN
1	D	29	ASN
1	D	65	ASN
1	D	99	GLN
1	D	147	GLN
1	D	150	HIS
1	D	280	GLN
1	D	281	ASN
1	D	385	ASN
1	D	534	GLN
3	E	147	GLN
3	E	280	GLN
3	E	281	ASN
1	F	15	ASN
1	F	65	ASN
1	F	99	GLN
1	F	150	HIS
1	F	281	ASN
1	F	409	ASN
1	F	455	GLN
4	G	242	ASN
4	G	268	GLN
4	G	281	ASN
4	G	509	GLN
4	G	534	GLN
5	H	99	GLN
5	H	225	GLN
5	H	281	ASN
5	H	409	ASN
5	H	455	GLN
5	H	534	GLN

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 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	$\#\|Z\| > 2$
7	EDO	F	1709	-	3,3,3	0.09	0	2,2,2	0.30	0
7	EDO	D	605	-	3,3,3	0.14	0	2,2,2	0.32	0
7	EDO	F	1715	-	3,3,3	0.08	0	2,2,2	0.28	0
6	PEG	C	606	-	6,6,6	0.17	0	5,5,5	0.11	0
8	GOL	C	612	-	5,5,5	0.15	0	5,5,5	0.47	0
7	EDO	F	1713	-	3,3,3	0.14	0	2,2,2	0.42	0
7	EDO	A	813	-	3,3,3	0.07	0	2,2,2	0.09	0
7	EDO	B	601	-	3,3,3	0.25	0	2,2,2	0.85	0
6	PEG	E	2001	-	6,6,6	0.12	0	5,5,5	0.12	0
7	EDO	G	603	-	3,3,3	0.10	0	2,2,2	0.17	0
7	EDO	C	609	-	3,3,3	0.15	0	2,2,2	0.39	0
7	EDO	C	604	-	3,3,3	0.19	0	2,2,2	0.33	0
7	EDO	F	1723	-	3,3,3	0.10	0	2,2,2	0.23	0
7	EDO	B	602	-	3,3,3	0.06	0	2,2,2	0.11	0
8	GOL	E	2005	-	5,5,5	0.16	0	5,5,5	0.47	0
7	EDO	G	602	-	3,3,3	0.15	0	2,2,2	0.15	0
7	EDO	D	623	-	3,3,3	0.07	0	2,2,2	0.04	0
8	GOL	F	1714	-	5,5,5	0.14	0	5,5,5	0.67	0
7	EDO	A	804	-	3,3,3	0.11	0	2,2,2	0.40	0
7	EDO	A	812	-	3,3,3	0.17	0	2,2,2	0.47	0
8	GOL	F	1716	-	5,5,5	0.07	0	5,5,5	0.40	0
9	PGE	A	824	-	9,9,9	0.22	0	8,8,8	0.13	0
7	EDO	F	1719	-	3,3,3	0.18	0	2,2,2	0.27	0
7	EDO	F	1706	-	3,3,3	0.14	0	2,2,2	0.28	0
7	EDO	F	1704	-	3,3,3	0.04	0	2,2,2	0.10	0
8	GOL	D	609	-	5,5,5	0.11	0	5,5,5	0.51	0
7	EDO	H	603	-	3,3,3	0.05	0	2,2,2	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	GOL	E	2004	-	5,5,5	0.17	0	5,5,5	0.48	0
8	GOL	B	607	-	5,5,5	0.17	0	5,5,5	0.48	0
7	EDO	E	2003	-	3,3,3	0.09	0	2,2,2	0.04	0
7	EDO	D	603	-	3,3,3	0.07	0	2,2,2	0.12	0
7	EDO	B	613	-	3,3,3	0.13	0	2,2,2	0.43	0
7	EDO	C	608	-	3,3,3	0.17	0	2,2,2	0.21	0
7	EDO	A	817	-	3,3,3	0.24	0	2,2,2	0.23	0
8	GOL	H	601	-	5,5,5	0.09	0	5,5,5	0.25	0
7	EDO	B	605	-	3,3,3	0.10	0	2,2,2	0.13	0
6	PEG	F	1712	-	6,6,6	0.17	0	5,5,5	0.14	0
7	EDO	D	619	-	3,3,3	0.12	0	2,2,2	0.54	0
6	PEG	C	605	-	6,6,6	0.18	0	5,5,5	0.12	0
10	PG4	B	610	-	12,12,12	0.35	0	11,11,11	0.26	0
7	EDO	G	604	-	3,3,3	0.14	0	2,2,2	0.11	0
6	PEG	D	614	-	6,6,6	0.11	0	5,5,5	0.10	0
7	EDO	F	1701	-	3,3,3	0.10	0	2,2,2	0.48	0
9	PGE	B	612	-	9,9,9	0.29	0	8,8,8	0.29	0
7	EDO	D	624	-	3,3,3	0.09	0	2,2,2	0.13	0
7	EDO	F	1717	-	3,3,3	0.10	0	2,2,2	0.10	0
6	PEG	C	603	-	6,6,6	0.33	0	5,5,5	0.26	0
7	EDO	E	2011	-	3,3,3	0.15	0	2,2,2	0.26	0
6	PEG	B	611	-	6,6,6	0.36	0	5,5,5	0.24	0
7	EDO	B	604	-	3,3,3	0.09	0	2,2,2	0.28	0
7	EDO	B	616	-	3,3,3	0.12	0	2,2,2	0.20	0
7	EDO	F	1711	-	3,3,3	0.14	0	2,2,2	0.27	0
7	EDO	A	803	-	3,3,3	0.61	0	2,2,2	1.87	1 (50%)
6	PEG	D	611	-	6,6,6	0.15	0	5,5,5	0.10	0
7	EDO	D	612	-	3,3,3	0.29	0	2,2,2	0.99	0
8	GOL	H	606	-	5,5,5	0.18	0	5,5,5	0.55	0
6	PEG	A	807	-	6,6,6	0.16	0	5,5,5	0.09	0
6	PEG	A	825	-	6,6,6	0.16	0	5,5,5	0.08	0
7	EDO	A	809	-	3,3,3	0.06	0	2,2,2	0.19	0
9	PGE	C	617	-	9,9,9	0.20	0	8,8,8	0.19	0
7	EDO	D	606	-	3,3,3	0.15	0	2,2,2	0.35	0
7	EDO	E	2009	-	3,3,3	0.13	0	2,2,2	0.12	0
7	EDO	D	608	-	3,3,3	0.11	0	2,2,2	0.05	0
7	EDO	F	1710	-	3,3,3	0.10	0	2,2,2	1.00	0
7	EDO	B	609	-	3,3,3	0.28	0	2,2,2	0.11	0
7	EDO	D	607	-	3,3,3	0.12	0	2,2,2	0.24	0
7	EDO	F	1707	-	3,3,3	0.32	0	2,2,2	0.89	0
8	GOL	E	2012	-	5,5,5	0.10	0	5,5,5	0.35	0
10	PG4	D	613	-	12,12,12	0.24	0	11,11,11	0.21	0
6	PEG	D	617	-	6,6,6	0.20	0	5,5,5	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	EDO	A	823	-	3,3,3	0.15	0	2,2,2	0.20	0
8	GOL	A	821	-	5,5,5	0.09	0	5,5,5	0.40	0
8	GOL	D	610	-	5,5,5	0.07	0	5,5,5	0.29	0
7	EDO	A	819	-	3,3,3	0.08	0	2,2,2	0.33	0
7	EDO	A	806	-	3,3,3	0.06	0	2,2,2	0.20	0
7	EDO	C	610	-	3,3,3	0.11	0	2,2,2	0.41	0
7	EDO	B	608	-	3,3,3	0.11	0	2,2,2	0.81	0
8	GOL	A	810	-	5,5,5	0.10	0	5,5,5	0.37	0
8	GOL	A	820	-	5,5,5	0.17	0	5,5,5	0.56	0
6	PEG	A	801	-	6,6,6	0.25	0	5,5,5	0.21	0
7	EDO	B	617	-	3,3,3	0.10	0	2,2,2	0.15	0
7	EDO	B	615	-	3,3,3	0.02	0	2,2,2	0.24	0
7	EDO	A	816	-	3,3,3	0.12	0	2,2,2	0.20	0
7	EDO	C	616	-	3,3,3	0.12	0	2,2,2	0.18	0
6	PEG	E	2007	-	6,6,6	0.18	0	5,5,5	0.13	0
7	EDO	F	1703	-	3,3,3	0.13	0	2,2,2	0.25	0
6	PEG	A	811	-	6,6,6	0.16	0	5,5,5	0.07	0
8	GOL	E	2006	-	5,5,5	0.14	0	5,5,5	0.41	0
7	EDO	A	805	-	3,3,3	0.57	0	2,2,2	0.29	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
7	EDO	D	616	-	3,3,3	0.07	0	2,2,2	0.06	0
8	GOL	C	618	-	5,5,5	0.10	0	5,5,5	0.42	0
7	EDO	C	614	-	3,3,3	0.08	0	2,2,2	0.26	0
7	EDO	D	622	-	3,3,3	0.15	0	2,2,2	0.05	0
8	GOL	F	1708	-	5,5,5	0.08	0	5,5,5	0.34	0
7	EDO	C	601	-	3,3,3	0.19	0	2,2,2	0.40	0
7	EDO	H	602	-	3,3,3	0.06	0	2,2,2	0.18	0
9	PGE	F	1718	-	9,9,9	0.27	0	8,8,8	0.13	0
7	EDO	H	607	-	3,3,3	0.11	0	2,2,2	0.53	0
7	EDO	H	608	-	3,3,3	0.09	0	2,2,2	0.02	0
8	GOL	G	605	-	5,5,5	0.11	0	5,5,5	0.40	0
7	EDO	B	606	-	3,3,3	0.16	0	2,2,2	0.30	0
7	EDO	F	1720	-	3,3,3	0.14	0	2,2,2	0.15	0
7	EDO	E	2010	-	3,3,3	0.08	0	2,2,2	0.18	0
9	PGE	A	814	-	9,9,9	0.25	0	8,8,8	0.11	0
7	EDO	D	621	-	3,3,3	0.20	0	2,2,2	0.35	0
8	GOL	C	602	-	5,5,5	0.16	0	5,5,5	0.49	0
8	GOL	C	607	-	5,5,5	0.13	0	5,5,5	0.77	0
8	GOL	A	822	-	5,5,5	0.13	0	5,5,5	0.41	0
7	EDO	B	614	-	3,3,3	0.14	0	2,2,2	0.41	0
7	EDO	F	1702	-	3,3,3	0.08	0	2,2,2	0.20	0
6	PEG	D	601	-	6,6,6	0.11	0	5,5,5	0.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	GOL	A	815	-	5,5,5	0.18	0	5,5,5	0.29	0
6	PEG	D	620	-	6,6,6	0.20	0	5,5,5	0.24	0
8	GOL	D	604	-	5,5,5	0.11	0	5,5,5	0.39	0
7	EDO	A	808	-	3,3,3	0.05	0	2,2,2	0.17	0
7	EDO	E	2002	-	3,3,3	0.07	0	2,2,2	0.20	0
8	GOL	A	818	-	5,5,5	0.12	0	5,5,5	0.53	0
7	EDO	D	615	-	3,3,3	0.12	0	2,2,2	0.27	0
7	EDO	D	618	-	3,3,3	0.09	0	2,2,2	0.09	0
8	GOL	F	1722	-	5,5,5	0.09	0	5,5,5	0.35	0
8	GOL	E	2008	-	5,5,5	0.10	0	5,5,5	0.35	0
8	GOL	D	602	-	5,5,5	0.13	0	5,5,5	0.43	0
7	EDO	H	605	-	3,3,3	0.21	0	2,2,2	0.71	0
7	EDO	H	604	-	3,3,3	0.10	0	2,2,2	0.26	0
7	EDO	C	611	-	3,3,3	0.07	0	2,2,2	0.06	0
7	EDO	F	1705	-	3,3,3	0.11	0	2,2,2	0.69	0
7	EDO	F	1721	-	3,3,3	0.08	0	2,2,2	0.09	0
7	EDO	G	601	-	3,3,3	0.28	0	2,2,2	0.49	0
6	PEG	A	802	-	6,6,6	0.21	0	5,5,5	0.11	0
7	EDO	B	603	-	3,3,3	0.19	0	2,2,2	0.64	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
7	EDO	F	1709	-	-	1/1/1/1	-
7	EDO	D	605	-	-	0/1/1/1	-
7	EDO	F	1715	-	-	1/1/1/1	-
6	PEG	C	606	-	-	3/4/4/4	-
8	GOL	C	612	-	-	0/4/4/4	-
7	EDO	F	1713	-	-	1/1/1/1	-
7	EDO	A	813	-	-	0/1/1/1	-
7	EDO	B	601	-	-	1/1/1/1	-
6	PEG	E	2001	-	-	1/4/4/4	-
7	EDO	G	603	-	-	0/1/1/1	-
7	EDO	C	609	-	-	1/1/1/1	-
7	EDO	C	604	-	-	1/1/1/1	-
7	EDO	F	1723	-	-	0/1/1/1	-
7	EDO	B	602	-	-	0/1/1/1	-
8	GOL	E	2005	-	-	2/4/4/4	-
7	EDO	G	602	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	D	623	-	-	0/1/1/1	-
8	GOL	F	1714	-	-	4/4/4/4	-
7	EDO	A	804	-	-	1/1/1/1	-
7	EDO	A	812	-	-	0/1/1/1	-
8	GOL	F	1716	-	-	2/4/4/4	-
9	PGE	A	824	-	-	7/7/7/7	-
7	EDO	F	1719	-	-	0/1/1/1	-
7	EDO	F	1706	-	-	0/1/1/1	-
7	EDO	F	1704	-	-	1/1/1/1	-
8	GOL	D	609	-	-	4/4/4/4	-
7	EDO	H	603	-	-	1/1/1/1	-
8	GOL	E	2004	-	-	2/4/4/4	-
8	GOL	B	607	-	-	0/4/4/4	-
7	EDO	E	2003	-	-	1/1/1/1	-
7	EDO	D	603	-	-	0/1/1/1	-
7	EDO	B	613	-	-	1/1/1/1	-
7	EDO	C	608	-	-	0/1/1/1	-
7	EDO	A	817	-	-	0/1/1/1	-
8	GOL	H	601	-	-	4/4/4/4	-
7	EDO	B	605	-	-	1/1/1/1	-
6	PEG	F	1712	-	-	2/4/4/4	-
7	EDO	D	619	-	-	0/1/1/1	-
6	PEG	C	605	-	-	2/4/4/4	-
10	PG4	B	610	-	-	6/10/10/10	-
7	EDO	G	604	-	-	1/1/1/1	-
6	PEG	D	614	-	-	2/4/4/4	-
7	EDO	F	1701	-	-	1/1/1/1	-
9	PGE	B	612	-	-	4/7/7/7	-
7	EDO	D	624	-	-	1/1/1/1	-
7	EDO	F	1717	-	-	1/1/1/1	-
6	PEG	C	603	-	-	2/4/4/4	-
7	EDO	E	2011	-	-	1/1/1/1	-
6	PEG	B	611	-	-	4/4/4/4	-
7	EDO	B	604	-	-	0/1/1/1	-
7	EDO	B	616	-	-	1/1/1/1	-
7	EDO	F	1711	-	-	0/1/1/1	-
7	EDO	A	803	-	-	1/1/1/1	-
6	PEG	D	611	-	-	2/4/4/4	-
7	EDO	D	612	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	GOL	H	606	-	-	4/4/4/4	-
6	PEG	A	807	-	-	2/4/4/4	-
6	PEG	A	825	-	-	3/4/4/4	-
7	EDO	A	809	-	-	0/1/1/1	-
9	PGE	C	617	-	-	4/7/7/7	-
7	EDO	D	606	-	-	1/1/1/1	-
7	EDO	E	2009	-	-	1/1/1/1	-
7	EDO	D	608	-	-	1/1/1/1	-
7	EDO	F	1710	-	-	1/1/1/1	-
7	EDO	B	609	-	-	0/1/1/1	-
7	EDO	D	607	-	-	0/1/1/1	-
7	EDO	F	1707	-	-	0/1/1/1	-
8	GOL	E	2012	-	-	2/4/4/4	-
10	PG4	D	613	-	-	4/10/10/10	-
6	PEG	D	617	-	-	3/4/4/4	-
7	EDO	A	823	-	-	1/1/1/1	-
8	GOL	A	821	-	-	4/4/4/4	-
8	GOL	D	610	-	-	2/4/4/4	-
7	EDO	A	819	-	-	1/1/1/1	-
7	EDO	A	806	-	-	0/1/1/1	-
7	EDO	C	610	-	-	0/1/1/1	-
7	EDO	B	608	-	-	1/1/1/1	-
8	GOL	A	810	-	-	0/4/4/4	-
8	GOL	A	820	-	-	0/4/4/4	-
6	PEG	A	801	-	-	4/4/4/4	-
7	EDO	B	617	-	-	1/1/1/1	-
7	EDO	B	615	-	-	0/1/1/1	-
7	EDO	A	816	-	-	1/1/1/1	-
7	EDO	C	616	-	-	1/1/1/1	-
6	PEG	E	2007	-	-	2/4/4/4	-
7	EDO	F	1703	-	-	1/1/1/1	-
6	PEG	A	811	-	-	2/4/4/4	-
8	GOL	E	2006	-	-	1/4/4/4	-
7	EDO	A	805	-	-	0/1/1/1	-
7	EDO	C	613	-	-	0/1/1/1	-
7	EDO	C	615	-	-	1/1/1/1	-
7	EDO	D	616	-	-	0/1/1/1	-
8	GOL	C	618	-	-	2/4/4/4	-
7	EDO	C	614	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	D	622	-	-	0/1/1/1	-
8	GOL	F	1708	-	-	2/4/4/4	-
7	EDO	C	601	-	-	1/1/1/1	-
7	EDO	H	602	-	-	0/1/1/1	-
9	PGE	F	1718	-	-	4/7/7/7	-
7	EDO	H	607	-	-	1/1/1/1	-
7	EDO	H	608	-	-	1/1/1/1	-
8	GOL	G	605	-	-	2/4/4/4	-
7	EDO	B	606	-	-	0/1/1/1	-
7	EDO	F	1720	-	-	1/1/1/1	-
7	EDO	E	2010	-	-	1/1/1/1	-
9	PGE	A	814	-	-	5/7/7/7	-
7	EDO	D	621	-	-	1/1/1/1	-
8	GOL	C	602	-	-	2/4/4/4	-
8	GOL	C	607	-	-	1/4/4/4	-
8	GOL	A	822	-	-	2/4/4/4	-
7	EDO	B	614	-	-	1/1/1/1	-
7	EDO	F	1702	-	-	0/1/1/1	-
6	PEG	D	601	-	-	2/4/4/4	-
8	GOL	A	815	-	-	2/4/4/4	-
6	PEG	D	620	-	-	2/4/4/4	-
8	GOL	D	604	-	-	4/4/4/4	-
7	EDO	A	808	-	-	0/1/1/1	-
7	EDO	E	2002	-	-	0/1/1/1	-
8	GOL	A	818	-	-	2/4/4/4	-
7	EDO	D	615	-	-	1/1/1/1	-
7	EDO	D	618	-	-	0/1/1/1	-
8	GOL	F	1722	-	-	2/4/4/4	-
8	GOL	E	2008	-	-	4/4/4/4	-
8	GOL	D	602	-	-	2/4/4/4	-
7	EDO	H	605	-	-	0/1/1/1	-
7	EDO	H	604	-	-	0/1/1/1	-
7	EDO	C	611	-	-	1/1/1/1	-
7	EDO	F	1705	-	-	1/1/1/1	-
7	EDO	F	1721	-	-	1/1/1/1	-
7	EDO	G	601	-	-	1/1/1/1	-
6	PEG	A	802	-	-	2/4/4/4	-
7	EDO	B	603	-	-	0/1/1/1	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

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

There are no chirality outliers.

All (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
8	C	618	GOL	C1-C2-C3-O3
8	D	602	GOL	C1-C2-C3-O3
8	D	604	GOL	O1-C1-C2-O2
8	D	604	GOL	O1-C1-C2-C3
8	D	604	GOL	C1-C2-C3-O3
8	D	609	GOL	O1-C1-C2-C3
8	D	609	GOL	C1-C2-C3-O3
8	D	610	GOL	C1-C2-C3-O3
8	E	2004	GOL	O1-C1-C2-C3
8	E	2008	GOL	O1-C1-C2-C3
8	E	2008	GOL	C1-C2-C3-O3
8	E	2012	GOL	O1-C1-C2-C3
8	F	1714	GOL	O1-C1-C2-O2
8	F	1714	GOL	O1-C1-C2-C3
8	H	601	GOL	C1-C2-C3-O3
8	H	601	GOL	O2-C2-C3-O3
6	A	825	PEG	C1-C2-O2-C3
10	B	610	PG4	O3-C5-C6-O4
9	B	612	PGE	C6-C5-O3-C4
9	C	617	PGE	O2-C3-C4-O3
10	B	610	PG4	O2-C3-C4-O3
9	A	824	PGE	O2-C3-C4-O3
8	C	618	GOL	O2-C2-C3-O3
8	D	609	GOL	O2-C2-C3-O3
8	D	610	GOL	O2-C2-C3-O3
8	F	1708	GOL	O1-C1-C2-O2
8	G	605	GOL	O1-C1-C2-O2
6	D	620	PEG	O1-C1-C2-O2
9	F	1718	PGE	O3-C5-C6-O4

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Mol	Chain	Res	Type	Atoms
6	A	801	PEG	O1-C1-C2-O2
6	B	611	PEG	O2-C3-C4-O4
6	D	601	PEG	O1-C1-C2-O2
6	E	2007	PEG	O2-C3-C4-O4
9	F	1718	PGE	O1-C1-C2-O2
10	D	613	PG4	O4-C7-C8-O5
8	C	602	GOL	O1-C1-C2-C3
8	C	607	GOL	O1-C1-C2-C3
8	E	2005	GOL	C1-C2-C3-O3
8	F	1708	GOL	O1-C1-C2-C3
8	F	1714	GOL	C1-C2-C3-O3
8	F	1722	GOL	O1-C1-C2-C3
8	G	605	GOL	O1-C1-C2-C3
8	H	601	GOL	O1-C1-C2-C3
8	H	606	GOL	O1-C1-C2-C3
8	H	606	GOL	C1-C2-C3-O3
6	C	603	PEG	O1-C1-C2-O2
9	A	814	PGE	O1-C1-C2-O2
9	A	824	PGE	O3-C5-C6-O4
8	A	818	GOL	O2-C2-C3-O3
8	A	821	GOL	O1-C1-C2-O2
8	C	602	GOL	O1-C1-C2-O2
8	D	604	GOL	O2-C2-C3-O3
8	E	2004	GOL	O1-C1-C2-O2
8	E	2008	GOL	O1-C1-C2-O2
6	A	825	PEG	O1-C1-C2-O2
6	B	611	PEG	O1-C1-C2-O2
6	C	603	PEG	O2-C3-C4-O4
6	C	605	PEG	O2-C3-C4-O4
6	D	611	PEG	O2-C3-C4-O4
7	B	605	EDO	O1-C1-C2-O2
7	B	617	EDO	O1-C1-C2-O2
7	C	616	EDO	O1-C1-C2-O2
7	F	1721	EDO	O1-C1-C2-O2
7	G	602	EDO	O1-C1-C2-O2
6	C	606	PEG	O1-C1-C2-O2
9	B	612	PGE	O2-C3-C4-O3
8	A	822	GOL	O2-C2-C3-O3
8	D	602	GOL	O2-C2-C3-O3
8	D	609	GOL	O1-C1-C2-O2
8	E	2008	GOL	O2-C2-C3-O3
8	F	1714	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
8	H	606	GOL	O2-C2-C3-O3
6	D	614	PEG	O2-C3-C4-O4
7	A	804	EDO	O1-C1-C2-O2
7	A	823	EDO	O1-C1-C2-O2
7	B	616	EDO	O1-C1-C2-O2
7	C	601	EDO	O1-C1-C2-O2
7	C	611	EDO	O1-C1-C2-O2
7	G	601	EDO	O1-C1-C2-O2
7	H	603	EDO	O1-C1-C2-O2
10	B	610	PG4	C8-C7-O4-C6
6	A	825	PEG	O2-C3-C4-O4
9	C	617	PGE	O3-C5-C6-O4
6	A	801	PEG	O2-C3-C4-O4
6	A	801	PEG	C4-C3-O2-C2
7	F	1703	EDO	O1-C1-C2-O2
9	C	617	PGE	C4-C3-O2-C2
9	A	824	PGE	O1-C1-C2-O2
8	E	2006	GOL	O2-C2-C3-O3
9	A	824	PGE	C4-C3-O2-C2
6	B	611	PEG	C4-C3-O2-C2
6	D	620	PEG	C1-C2-O2-C3
9	A	814	PGE	C4-C3-O2-C2
6	C	605	PEG	C4-C3-O2-C2
6	E	2007	PEG	C1-C2-O2-C3
10	B	610	PG4	C5-C6-O4-C7
6	D	611	PEG	C4-C3-O2-C2
10	D	613	PG4	C6-C5-O3-C4
6	A	807	PEG	O2-C3-C4-O4
7	F	1720	EDO	O1-C1-C2-O2
6	A	811	PEG	C1-C2-O2-C3
6	D	614	PEG	O1-C1-C2-O2
8	F	1722	GOL	O1-C1-C2-O2
9	A	814	PGE	C3-C4-O3-C5
10	B	610	PG4	C3-C4-O3-C5
6	C	606	PEG	O2-C3-C4-O4
9	C	617	PGE	C6-C5-O3-C4
9	A	824	PGE	C1-C2-O2-C3
7	D	624	EDO	O1-C1-C2-O2
7	F	1713	EDO	O1-C1-C2-O2
8	F	1716	GOL	O1-C1-C2-O2
8	H	606	GOL	O1-C1-C2-O2
8	F	1716	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
6	C	606	PEG	C1-C2-O2-C3
9	B	612	PGE	C1-C2-O2-C3
6	F	1712	PEG	O1-C1-C2-O2
7	A	803	EDO	O1-C1-C2-O2
7	B	614	EDO	O1-C1-C2-O2
7	C	615	EDO	O1-C1-C2-O2
7	E	2003	EDO	O1-C1-C2-O2
7	F	1704	EDO	O1-C1-C2-O2
7	F	1710	EDO	O1-C1-C2-O2
6	A	802	PEG	O2-C3-C4-O4
6	D	601	PEG	C4-C3-O2-C2
6	A	802	PEG	C1-C2-O2-C3
9	F	1718	PGE	O2-C3-C4-O3
8	A	822	GOL	C1-C2-C3-O3
7	D	621	EDO	O1-C1-C2-O2
7	F	1709	EDO	O1-C1-C2-O2
7	H	607	EDO	O1-C1-C2-O2
6	B	611	PEG	C1-C2-O2-C3
8	A	821	GOL	O2-C2-C3-O3
8	E	2005	GOL	O2-C2-C3-O3
8	E	2012	GOL	O1-C1-C2-O2
10	B	610	PG4	O1-C1-C2-O2
10	D	613	PG4	O1-C1-C2-O2
6	A	801	PEG	C1-C2-O2-C3
6	E	2001	PEG	C1-C2-O2-C3
9	A	824	PGE	C3-C4-O3-C5
6	D	617	PEG	O2-C3-C4-O4
9	A	814	PGE	O3-C5-C6-O4
6	F	1712	PEG	C4-C3-O2-C2
9	F	1718	PGE	C4-C3-O2-C2
8	H	601	GOL	O1-C1-C2-O2
7	A	816	EDO	O1-C1-C2-O2
7	A	819	EDO	O1-C1-C2-O2
7	B	608	EDO	O1-C1-C2-O2
7	C	604	EDO	O1-C1-C2-O2
7	D	606	EDO	O1-C1-C2-O2
7	D	615	EDO	O1-C1-C2-O2
7	E	2009	EDO	O1-C1-C2-O2
7	F	1701	EDO	O1-C1-C2-O2
7	F	1717	EDO	O1-C1-C2-O2
7	G	604	EDO	O1-C1-C2-O2
6	D	617	PEG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
7	B	601	EDO	O1-C1-C2-O2
7	B	613	EDO	O1-C1-C2-O2
7	D	608	EDO	O1-C1-C2-O2
7	F	1715	EDO	O1-C1-C2-O2
7	H	608	EDO	O1-C1-C2-O2
6	D	617	PEG	C1-C2-O2-C3
10	D	613	PG4	C3-C4-O3-C5
7	C	609	EDO	O1-C1-C2-O2
7	E	2010	EDO	O1-C1-C2-O2
7	E	2011	EDO	O1-C1-C2-O2
6	A	811	PEG	O2-C3-C4-O4
9	B	612	PGE	C4-C3-O2-C2
9	A	814	PGE	O2-C3-C4-O3
6	A	807	PEG	O1-C1-C2-O2
9	A	824	PGE	C6-C5-O3-C4
7	F	1705	EDO	O1-C1-C2-O2

There are no ring outliers.

49 monomers are involved in 121 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	612	GOL	1	0
7	B	601	EDO	3	0
7	F	1723	EDO	2	0
8	E	2005	GOL	1	0
8	F	1714	GOL	2	0
7	A	804	EDO	5	0
9	A	824	PGE	1	0
7	F	1719	EDO	5	0
7	H	603	EDO	3	0
7	A	817	EDO	4	0
8	H	601	GOL	1	0
6	F	1712	PEG	2	0
6	C	605	PEG	1	0
10	B	610	PG4	3	0
6	D	614	PEG	4	0
9	B	612	PGE	2	0
6	C	603	PEG	3	0
7	B	604	EDO	2	0
6	D	611	PEG	4	0
7	D	612	EDO	5	0
6	A	825	PEG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	809	EDO	2	0
9	C	617	PGE	1	0
7	D	608	EDO	1	0
7	B	609	EDO	7	0
7	F	1707	EDO	2	0
8	E	2012	GOL	1	0
10	D	613	PG4	3	0
7	C	610	EDO	1	0
7	B	608	EDO	6	0
6	A	801	PEG	2	0
7	A	816	EDO	1	0
6	E	2007	PEG	3	0
7	A	805	EDO	10	0
7	C	614	EDO	2	0
7	D	622	EDO	1	0
9	F	1718	PGE	5	0
8	G	605	GOL	1	0
7	E	2010	EDO	2	0
9	A	814	PGE	1	0
8	C	607	GOL	2	0
6	D	601	PEG	1	0
6	D	620	PEG	1	0
8	D	604	GOL	2	0
8	D	602	GOL	3	0
7	C	611	EDO	1	0
7	F	1705	EDO	6	0
7	F	1721	EDO	2	0
6	A	802	PEG	3	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	0.13	15 (2%) 54 58	27, 53, 112, 173	0
1	C	553/553 (100%)	0.13	11 (1%) 65 68	35, 56, 118, 183	0
1	D	553/553 (100%)	0.11	11 (1%) 65 68	25, 55, 123, 163	0
1	F	553/553 (100%)	0.25	26 (4%) 31 33	27, 58, 128, 200	0
2	B	528/528 (100%)	0.32	25 (4%) 31 33	27, 54, 130, 173	0
3	E	547/550 (99%)	0.53	59 (10%) 5 5	29, 60, 154, 199	0
4	G	508/527 (96%)	0.41	43 (8%) 10 10	35, 65, 144, 187	0
5	H	550/553 (99%)	0.56	57 (10%) 6 6	39, 66, 165, 204	0
All	All	4345/4370 (99%)	0.31	247 (5%) 23 25	25, 58, 143, 204	0

All (247) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	H	35	VAL	17.2
2	B	16	GLY	12.0
3	E	143	ALA	10.7
5	H	198	GLY	10.6
2	B	521	ILE	10.0
5	H	179	LYS	9.1
5	H	182	PHE	8.3
1	C	518	TYR	8.3
5	H	146	ALA	8.2
3	E	144	PRO	8.1
3	E	-5	MET	7.9
5	H	518	TYR	7.5
5	H	144	PRO	7.2
5	H	145	GLN	7.2
4	G	543	ASN	7.1
1	F	14	PHE	7.1

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Mol	Chain	Res	Type	RSRZ
2	B	278	ALA	7.1
3	E	516	VAL	7.0
5	H	143	ALA	7.0
3	E	227	VAL	7.0
1	F	518	TYR	6.9
4	G	275	PRO	6.9
4	G	195	VAL	6.9
5	H	148	PRO	6.8
3	E	518	TYR	6.8
1	F	144	PRO	6.8
5	H	180	ASP	6.6
1	A	521	ILE	6.6
1	F	15	ASN	6.4
3	E	142	PHE	6.4
3	E	515	ASP	6.4
5	H	36	LEU	6.3
1	F	140	ASP	6.3
5	H	181	LEU	6.1
5	H	176	LEU	6.1
4	G	148	PRO	6.0
3	E	279	GLY	5.8
1	C	516	VAL	5.8
1	A	142	PHE	5.8
3	E	278	ALA	5.7
2	B	516	VAL	5.6
5	H	147	GLN	5.6
3	E	146	ALA	5.6
4	G	282	LYS	5.4
3	E	145	GLN	5.4
1	C	144	PRO	5.4
2	B	179	LYS	5.3
3	E	17	LEU	5.1
3	E	16	GLY	5.1
5	H	178	SER	5.1
4	G	197	HIS	5.1
5	H	149	HIS	5.1
1	A	518	TYR	5.0
1	D	518	TYR	5.0
4	G	521	ILE	5.0
1	A	515	ASP	5.0
5	H	278	ALA	4.9
5	H	197	HIS	4.8

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Mol	Chain	Res	Type	RSRZ
3	E	274	LEU	4.7
1	F	146	ALA	4.7
1	A	516	VAL	4.7
1	A	519	GLY	4.6
4	G	208	VAL	4.6
4	G	139	LYS	4.5
5	H	-2	ILE	4.5
1	C	517	GLN	4.3
5	H	272	PHE	4.3
3	E	147	GLN	4.3
3	E	141	GLY	4.3
5	H	32	ASP	4.3
1	F	142	PHE	4.2
1	A	146	ALA	4.1
3	E	228	GLY	4.1
2	B	517	GLN	4.0
1	F	521	ILE	4.0
4	G	257	LEU	4.0
4	G	176	LEU	3.9
1	F	517	GLN	3.9
4	G	235	ILE	3.9
1	C	14	PHE	3.9
5	H	34	ASP	3.9
1	A	14	PHE	3.9
1	D	141	GLY	3.9
2	B	180	ASP	3.9
5	H	142	PHE	3.9
2	B	146	ALA	3.8
5	H	200	PRO	3.8
2	B	145	GLN	3.7
3	E	280	GLN	3.7
4	G	179	LYS	3.7
4	G	491	LYS	3.6
1	F	141	GLY	3.6
5	H	195	VAL	3.6
1	C	13	GLY	3.6
3	E	180	ASP	3.6
4	G	234	VAL	3.6
2	B	520	GLU	3.5
5	H	520	GLU	3.5
3	E	543	ASN	3.5
5	H	199	THR	3.5

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Mol	Chain	Res	Type	RSRZ
3	E	520	GLU	3.4
5	H	184	LYS	3.4
2	B	513	LEU	3.4
3	E	197	HIS	3.4
3	E	249	LEU	3.3
1	C	543	ASN	3.3
1	D	5	LEU	3.3
4	G	241	PHE	3.3
3	E	181	LEU	3.3
5	H	-9	GLY	3.3
3	E	182	PHE	3.3
1	C	142	PHE	3.3
3	E	-1	GLY	3.3
5	H	253	VAL	3.3
4	G	267	GLY	3.3
5	H	274	LEU	3.2
3	E	33	ARG	3.2
1	D	144	PRO	3.2
1	F	139	LYS	3.2
3	E	222	LEU	3.2
2	B	193	LYS	3.2
2	B	518	TYR	3.2
3	E	283	VAL	3.2
1	F	543	ASN	3.1
3	E	521	ILE	3.1
3	E	8	TYR	3.1
2	B	181	LEU	3.1
5	H	211	ASN	3.1
3	E	3	ASP	3.1
5	H	183	SER	3.1
4	G	200	PRO	3.0
5	H	228	GLY	3.0
4	G	263	LEU	3.0
4	G	266	ALA	3.0
3	E	236	ILE	3.0
3	E	519	GLY	3.0
3	E	276	THR	3.0
5	H	521	ILE	3.0
2	B	285	LYS	3.0
1	D	10	LYS	2.9
1	D	516	VAL	2.9
3	E	517	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	278	ALA	2.9
4	G	199	THR	2.9
1	A	517	GLN	2.9
1	F	10	LYS	2.9
3	E	1	THR	2.9
2	B	272	PHE	2.8
1	A	9	LEU	2.8
5	H	491	LYS	2.8
3	E	270	ILE	2.8
2	B	17	LEU	2.8
1	F	520	GLU	2.8
4	G	236	ILE	2.8
3	E	9	LEU	2.8
4	G	216	ILE	2.7
1	F	7	TYR	2.7
1	F	541	ILE	2.7
5	H	18	PHE	2.7
4	G	278	ALA	2.7
1	F	9	LEU	2.7
1	C	145	GLN	2.7
5	H	140	ASP	2.7
3	E	224	VAL	2.7
5	H	279	GLY	2.7
4	G	281	ASN	2.6
5	H	251	GLY	2.6
1	D	278	ALA	2.6
2	B	176	LEU	2.6
1	D	543	ASN	2.6
1	C	515	ASP	2.6
4	G	288	LEU	2.6
3	E	454	LEU	2.6
5	H	235	ILE	2.5
1	F	13	GLY	2.5
1	A	520	GLU	2.5
5	H	-6	SER	2.5
1	A	141	GLY	2.5
3	E	-4	ALA	2.5
4	G	276	THR	2.5
1	F	145	GLN	2.5
4	G	268	GLN	2.5
1	F	390	TYR	2.5
5	H	280	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
3	E	37	SER	2.5
4	G	232	SER	2.5
3	E	487	LEU	2.4
5	H	67	LEU	2.4
2	B	274	LEU	2.4
5	H	30	LEU	2.4
3	E	201	ILE	2.4
1	A	145	GLN	2.4
3	E	0	SER	2.4
5	H	543	ASN	2.4
3	E	252	LYS	2.4
1	D	142	PHE	2.4
4	G	279	GLY	2.4
5	H	139	LYS	2.3
3	E	257	LEU	2.3
4	G	201	ILE	2.3
5	H	246	LYS	2.3
4	G	280	GLN	2.3
5	H	37	SER	2.3
1	A	279	GLY	2.3
2	B	36	LEU	2.3
1	F	514	ARG	2.2
4	G	30	LEU	2.2
3	E	275	PRO	2.2
3	E	450	VAL	2.2
4	G	225	GLN	2.2
2	B	184	LYS	2.2
1	F	438	ARG	2.2
1	A	276	THR	2.2
4	G	38	LYS	2.2
4	G	202	PRO	2.2
5	H	141	GLY	2.2
2	B	283	VAL	2.2
1	F	11	SER	2.2
5	H	236	ILE	2.2
4	G	260	LEU	2.1
3	E	225	GLN	2.1
1	D	197	HIS	2.1
1	F	428	ILE	2.1
3	E	-6	SER	2.1
3	E	11	SER	2.1
5	H	-7	SER	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	280	GLN	2.1
1	D	487	LEU	2.1
1	F	384	LEU	2.1
5	H	224	VAL	2.1
2	B	18	PHE	2.1
5	H	75	PHE	2.1
4	G	193	LYS	2.1
3	E	140	ASP	2.1
1	F	487	LEU	2.1
4	G	207	GLU	2.1
4	G	209	ARG	2.1
3	E	183	SER	2.0
3	E	176	LEU	2.0
3	E	254	GLN	2.0
4	G	284	LEU	2.0
5	H	213	LEU	2.0
4	G	242	ASN	2.0
5	H	273	SER	2.0
4	G	206	THR	2.0
2	B	208	VAL	2.0
3	E	184	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides 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, 95^{th} 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
6	PEG	A	811	7/7	0.60	0.33	59,71,82,83	7
7	EDO	C	615	4/4	0.60	0.26	76,79,79,80	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	GOL	A	820	6/6	0.62	0.32	66,81,84,84	0
12	CA	F	1724	1/1	0.62	0.13	86,86,86,86	0
7	EDO	C	616	4/4	0.65	0.27	67,71,77,78	0
7	EDO	A	812	4/4	0.67	0.28	76,81,82,87	0
8	GOL	C	618	6/6	0.68	0.20	70,78,80,82	0
10	PG4	D	613	13/13	0.68	0.39	57,85,95,100	13
7	EDO	H	605	4/4	0.68	0.24	56,61,65,66	0
8	GOL	B	607	6/6	0.69	0.40	62,70,80,80	6
7	EDO	D	621	4/4	0.69	0.40	54,55,63,64	4
7	EDO	C	609	4/4	0.70	0.29	71,72,73,74	4
6	PEG	D	620	7/7	0.70	0.26	60,66,69,69	7
7	EDO	F	1702	4/4	0.71	0.23	78,88,92,94	0
7	EDO	B	616	4/4	0.72	0.41	79,84,93,95	0
6	PEG	C	606	7/7	0.72	0.27	59,70,77,79	7
7	EDO	E	2009	4/4	0.73	0.29	67,75,77,80	4
7	EDO	B	613	4/4	0.73	0.33	78,88,92,96	0
6	PEG	A	807	7/7	0.73	0.44	57,63,68,74	7
9	PGE	A	824	10/10	0.73	0.36	85,88,93,95	0
7	EDO	H	608	4/4	0.73	0.16	77,79,80,81	4
8	GOL	A	810	6/6	0.73	0.29	79,82,88,88	0
10	PG4	B	610	13/13	0.74	0.24	73,84,88,90	13
7	EDO	F	1720	4/4	0.74	0.40	72,76,83,87	0
7	EDO	B	603	4/4	0.74	0.48	59,69,72,75	0
7	EDO	C	604	4/4	0.75	0.22	90,92,93,104	4
7	EDO	F	1707	4/4	0.75	0.40	63,65,68,72	0
6	PEG	D	601	7/7	0.75	0.28	81,85,97,99	0
8	GOL	D	609	6/6	0.75	0.18	82,91,97,100	0
7	EDO	C	610	4/4	0.76	0.37	72,73,78,80	0
8	GOL	D	610	6/6	0.76	0.33	60,68,77,78	6
7	EDO	D	618	4/4	0.76	0.27	79,86,88,90	0
9	PGE	F	1718	10/10	0.76	0.34	63,78,80,84	10
7	EDO	A	813	4/4	0.76	0.73	72,74,74,79	4
7	EDO	D	624	4/4	0.76	0.24	66,78,79,82	4
7	EDO	E	2002	4/4	0.76	0.22	63,68,68,72	4
6	PEG	A	801	7/7	0.77	0.21	61,69,71,76	7
8	GOL	E	2005	6/6	0.78	0.35	61,71,75,77	0
6	PEG	D	614	7/7	0.78	0.37	75,80,89,92	7
7	EDO	C	611	4/4	0.78	0.21	74,85,91,95	0
7	EDO	F	1701	4/4	0.79	0.26	94,97,104,109	0
7	EDO	B	601	4/4	0.79	0.41	50,54,59,66	0
7	EDO	B	617	4/4	0.80	0.29	60,70,72,73	4
6	PEG	D	611	7/7	0.80	0.41	72,77,85,89	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	EDO	A	819	4/4	0.80	0.24	53,53,61,61	4
8	GOL	C	612	6/6	0.80	0.21	53,61,62,66	6
8	GOL	H	606	6/6	0.80	0.25	71,75,85,89	0
7	EDO	A	804	4/4	0.81	0.40	64,74,76,76	0
7	EDO	D	606	4/4	0.81	0.65	67,75,76,85	0
6	PEG	C	605	7/7	0.81	0.19	56,64,71,71	7
7	EDO	D	619	4/4	0.81	0.47	69,79,80,81	0
7	EDO	H	607	4/4	0.82	0.81	79,81,84,87	0
7	EDO	F	1713	4/4	0.82	0.18	71,77,84,92	0
7	EDO	C	613	4/4	0.82	0.15	64,73,74,78	4
7	EDO	D	623	4/4	0.82	0.29	64,65,66,67	4
7	EDO	B	605	4/4	0.83	0.20	77,78,82,85	0
7	EDO	E	2010	4/4	0.83	0.21	67,68,71,71	4
6	PEG	D	617	7/7	0.83	0.50	82,84,93,94	0
6	PEG	E	2001	7/7	0.83	0.21	74,85,93,93	0
7	EDO	F	1704	4/4	0.84	0.23	61,63,66,66	4
7	EDO	A	808	4/4	0.85	0.34	77,77,86,88	0
7	EDO	F	1719	4/4	0.85	0.40	80,81,81,83	4
7	EDO	B	604	4/4	0.85	0.49	91,92,94,102	0
7	EDO	E	2003	4/4	0.85	0.15	96,96,103,103	0
8	GOL	A	821	6/6	0.86	0.25	69,86,92,93	0
8	GOL	F	1708	6/6	0.86	0.25	74,80,81,86	0
8	GOL	H	601	6/6	0.86	0.13	62,70,73,74	0
6	PEG	B	611	7/7	0.86	0.29	65,77,81,86	0
7	EDO	B	615	4/4	0.86	0.18	78,82,82,89	0
7	EDO	F	1715	4/4	0.86	0.12	73,78,81,82	0
8	GOL	D	602	6/6	0.86	0.29	78,85,87,92	0
6	PEG	E	2007	7/7	0.86	0.39	55,72,76,76	0
6	PEG	F	1712	7/7	0.86	0.22	58,77,83,87	7
8	GOL	A	822	6/6	0.87	0.17	78,81,87,88	0
8	GOL	F	1716	6/6	0.87	0.24	72,82,84,86	0
7	EDO	G	604	4/4	0.87	0.25	64,65,75,75	0
7	EDO	B	614	4/4	0.87	0.24	76,91,91,96	0
7	EDO	D	605	4/4	0.87	0.23	55,69,70,79	0
9	PGE	B	612	10/10	0.87	0.29	58,72,77,79	0
9	PGE	C	617	10/10	0.87	0.16	56,68,74,78	10
7	EDO	C	614	4/4	0.87	0.23	76,82,83,88	0
7	EDO	E	2011	4/4	0.87	0.14	59,68,73,76	0
7	EDO	D	615	4/4	0.87	0.26	68,72,80,82	0
6	PEG	A	802	7/7	0.87	0.28	75,86,92,93	0
7	EDO	F	1723	4/4	0.88	0.41	76,80,80,81	0
7	EDO	F	1706	4/4	0.88	0.23	57,63,70,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	PGE	A	814	10/10	0.88	0.21	56,73,82,83	10
7	EDO	A	816	4/4	0.88	0.42	64,73,73,77	0
8	GOL	F	1722	6/6	0.88	0.27	67,90,92,96	0
8	GOL	A	818	6/6	0.89	0.17	54,61,67,69	0
7	EDO	C	608	4/4	0.89	0.17	51,53,58,61	4
8	GOL	E	2012	6/6	0.89	0.39	66,69,73,76	0
7	EDO	F	1717	4/4	0.89	0.24	61,69,71,73	4
7	EDO	B	606	4/4	0.90	0.40	66,70,82,86	0
8	GOL	E	2008	6/6	0.90	0.37	62,73,76,77	0
7	EDO	D	622	4/4	0.90	0.21	62,69,70,72	0
7	EDO	F	1709	4/4	0.90	0.17	55,64,66,68	0
7	EDO	F	1721	4/4	0.90	0.17	75,78,80,87	0
7	EDO	D	616	4/4	0.90	0.46	67,68,73,74	0
7	EDO	F	1705	4/4	0.90	0.59	52,59,59,64	0
7	EDO	H	604	4/4	0.90	0.22	82,92,93,95	0
8	GOL	E	2004	6/6	0.91	0.27	75,85,91,93	0
7	EDO	D	607	4/4	0.91	0.13	70,71,72,74	0
8	GOL	E	2006	6/6	0.91	0.15	90,94,96,103	0
7	EDO	A	809	4/4	0.91	0.22	68,77,90,94	0
8	GOL	C	607	6/6	0.91	0.30	53,67,71,75	0
7	EDO	F	1703	4/4	0.91	0.19	88,90,90,91	0
7	EDO	A	806	4/4	0.92	0.16	64,65,70,71	0
7	EDO	F	1710	4/4	0.92	0.33	37,40,45,63	0
7	EDO	A	803	4/4	0.92	0.19	43,45,48,49	0
7	EDO	B	602	4/4	0.92	0.24	71,71,78,82	0
7	EDO	H	602	4/4	0.92	0.11	63,68,73,75	0
7	EDO	H	603	4/4	0.92	0.44	68,70,73,74	0
6	PEG	C	603	7/7	0.92	0.30	66,79,88,90	0
7	EDO	D	612	4/4	0.92	0.51	58,62,66,72	0
8	GOL	A	815	6/6	0.93	0.16	52,56,59,64	0
7	EDO	G	601	4/4	0.93	0.12	60,61,62,63	0
7	EDO	G	603	4/4	0.93	0.32	66,83,85,86	0
7	EDO	B	608	4/4	0.93	0.42	66,67,69,71	0
8	GOL	D	604	6/6	0.93	0.28	76,89,92,92	0
7	EDO	F	1711	4/4	0.93	0.09	67,71,72,75	0
7	EDO	A	823	4/4	0.93	0.15	64,65,69,69	0
8	GOL	G	605	6/6	0.93	0.12	60,69,69,71	0
8	GOL	C	602	6/6	0.93	0.28	58,70,73,73	0
7	EDO	D	603	4/4	0.94	0.15	77,80,81,84	0
7	EDO	D	608	4/4	0.94	0.25	53,64,65,69	0
8	GOL	F	1714	6/6	0.94	0.17	61,66,68,70	0
7	EDO	G	602	4/4	0.94	0.14	71,73,73,75	0

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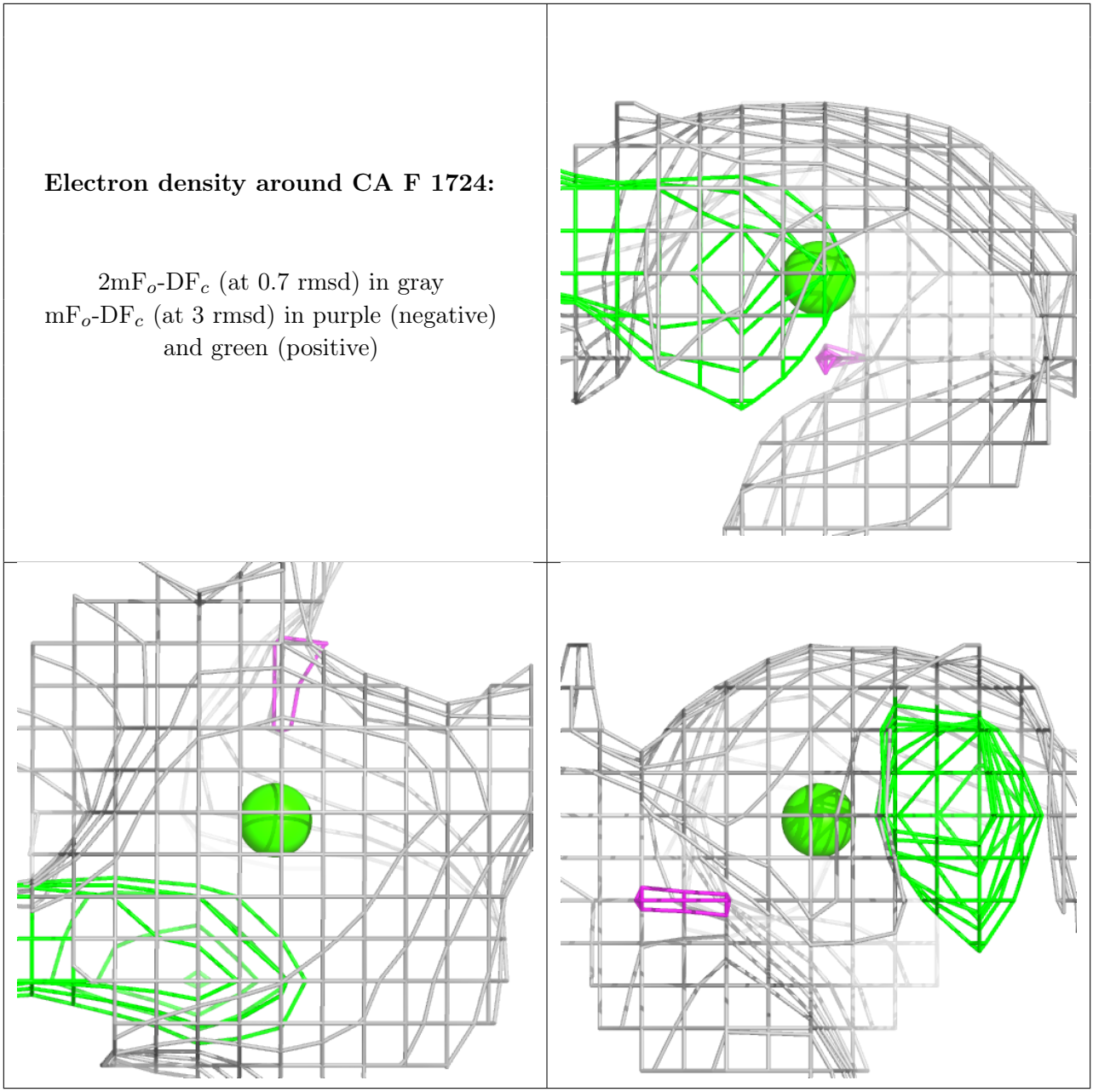
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	EDO	A	817	4/4	0.96	0.30	33,49,50,57	0
11	CL	D	625	1/1	0.96	0.13	62,62,62,62	0
7	EDO	C	601	4/4	0.96	0.11	62,62,63,64	0
7	EDO	A	805	4/4	0.97	0.33	40,41,44,47	0
11	CL	C	619	1/1	0.97	0.14	58,58,58,58	0
7	EDO	B	609	4/4	0.97	0.41	52,52,55,58	0
12	CA	D	626	1/1	0.97	0.17	55,55,55,55	0
6	PEG	A	825	7/7	0.97	0.28	56,58,63,68	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.

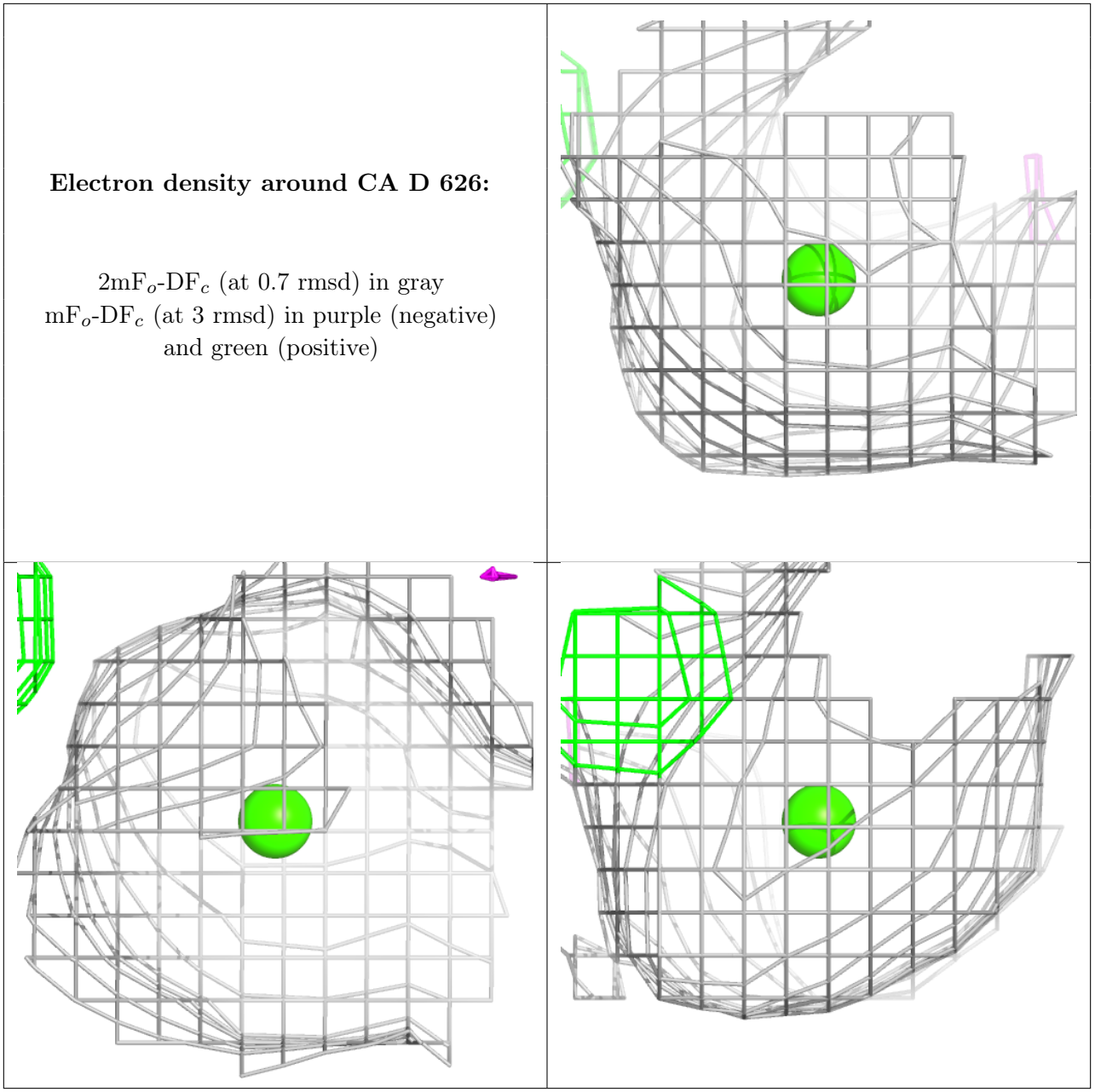
Electron density around CA F 1724:

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



Electron density around CA D 626:

$2mF_o$-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.