Full wwPDB X-ray Structure Validation Report (i)

Jul 26, 2019 – 12:08 PM EDT

PDB ID	:	6PV4
Title	:	Structure of CpGH84A
Deposited on	:	2019-07-19
Resolution	:	2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

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

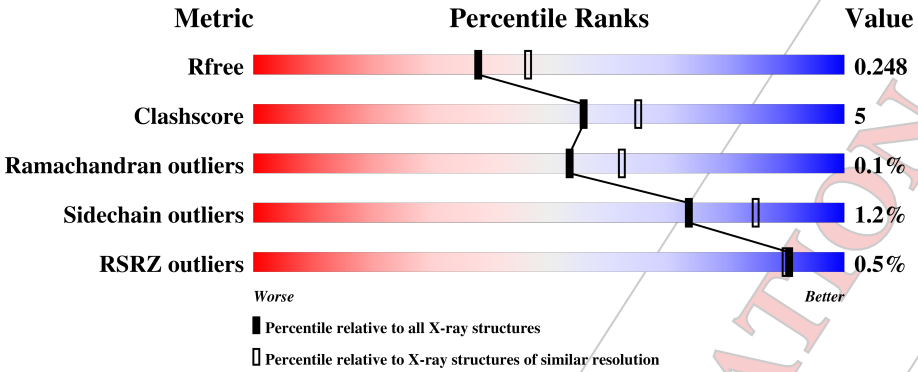
MolProbity	:	4.02b-467
Mogul	:	1.8.0 (224370), CSD as540be (2019)
Xtriage (Phenix)	:	1.13
EDS	:	2.4
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.4

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 2.20 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}	111664	4343 (2.20-2.20)
Clashscore	122126	5027 (2.20-2.20)
Ramachandran outliers	120053	4952 (2.20-2.20)
Sidechain outliers	120020	4953 (2.20-2.20)
RSRZ outliers	108989	4245 (2.20-2.20)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	653	79% 11% 10%
1	B	653	81% 12% • 7%
1	C	653	82% 11% 7%
1	D	653	% 81% 11% 8%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 20900 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 Glycoside Hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	589	Total	C	N	O	S	0	0	0
			4668	2951	776	923	18			
1	B	607	Total	C	N	O	S	0	1	0
			4820	3050	794	957	19			
1	C	608	Total	C	N	O	S	0	1	0
			4826	3055	796	956	19			
1	D	602	Total	C	N	O	S	0	1	0
			4757	3012	787	939	19			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	MET	-	initiating methionine	UNP A0A0H2YRL1
A	9	GLY	-	expression tag	UNP A0A0H2YRL1
A	10	SER	-	expression tag	UNP A0A0H2YRL1
A	11	SER	-	expression tag	UNP A0A0H2YRL1
A	12	HIS	-	expression tag	UNP A0A0H2YRL1
A	13	HIS	-	expression tag	UNP A0A0H2YRL1
A	14	HIS	-	expression tag	UNP A0A0H2YRL1
A	15	HIS	-	expression tag	UNP A0A0H2YRL1
A	16	HIS	-	expression tag	UNP A0A0H2YRL1
A	17	HIS	-	expression tag	UNP A0A0H2YRL1
A	18	SER	-	expression tag	UNP A0A0H2YRL1
A	19	SER	-	expression tag	UNP A0A0H2YRL1
A	20	GLY	-	expression tag	UNP A0A0H2YRL1
A	21	LEU	-	expression tag	UNP A0A0H2YRL1
A	22	VAL	-	expression tag	UNP A0A0H2YRL1
A	23	PRO	-	expression tag	UNP A0A0H2YRL1
A	24	ARG	-	expression tag	UNP A0A0H2YRL1
A	25	GLY	-	expression tag	UNP A0A0H2YRL1
A	26	SER	-	expression tag	UNP A0A0H2YRL1
A	27	HIS	-	expression tag	UNP A0A0H2YRL1
A	28	MET	-	expression tag	UNP A0A0H2YRL1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	29	ALA	-	expression tag	UNP A0A0H2YRL1
A	30	SER	-	expression tag	UNP A0A0H2YRL1
B	8	MET	-	initiating methionine	UNP A0A0H2YRL1
B	9	GLY	-	expression tag	UNP A0A0H2YRL1
B	10	SER	-	expression tag	UNP A0A0H2YRL1
B	11	SER	-	expression tag	UNP A0A0H2YRL1
B	12	HIS	-	expression tag	UNP A0A0H2YRL1
B	13	HIS	-	expression tag	UNP A0A0H2YRL1
B	14	HIS	-	expression tag	UNP A0A0H2YRL1
B	15	HIS	-	expression tag	UNP A0A0H2YRL1
B	16	HIS	-	expression tag	UNP A0A0H2YRL1
B	17	HIS	-	expression tag	UNP A0A0H2YRL1
B	18	SER	-	expression tag	UNP A0A0H2YRL1
B	19	SER	-	expression tag	UNP A0A0H2YRL1
B	20	GLY	-	expression tag	UNP A0A0H2YRL1
B	21	LEU	-	expression tag	UNP A0A0H2YRL1
B	22	VAL	-	expression tag	UNP A0A0H2YRL1
B	23	PRO	-	expression tag	UNP A0A0H2YRL1
B	24	ARG	-	expression tag	UNP A0A0H2YRL1
B	25	GLY	-	expression tag	UNP A0A0H2YRL1
B	26	SER	-	expression tag	UNP A0A0H2YRL1
B	27	HIS	-	expression tag	UNP A0A0H2YRL1
B	28	MET	-	expression tag	UNP A0A0H2YRL1
B	29	ALA	-	expression tag	UNP A0A0H2YRL1
B	30	SER	-	expression tag	UNP A0A0H2YRL1
C	8	MET	-	initiating methionine	UNP A0A0H2YRL1
C	9	GLY	-	expression tag	UNP A0A0H2YRL1
C	10	SER	-	expression tag	UNP A0A0H2YRL1
C	11	SER	-	expression tag	UNP A0A0H2YRL1
C	12	HIS	-	expression tag	UNP A0A0H2YRL1
C	13	HIS	-	expression tag	UNP A0A0H2YRL1
C	14	HIS	-	expression tag	UNP A0A0H2YRL1
C	15	HIS	-	expression tag	UNP A0A0H2YRL1
C	16	HIS	-	expression tag	UNP A0A0H2YRL1
C	17	HIS	-	expression tag	UNP A0A0H2YRL1
C	18	SER	-	expression tag	UNP A0A0H2YRL1
C	19	SER	-	expression tag	UNP A0A0H2YRL1
C	20	GLY	-	expression tag	UNP A0A0H2YRL1
C	21	LEU	-	expression tag	UNP A0A0H2YRL1
C	22	VAL	-	expression tag	UNP A0A0H2YRL1
C	23	PRO	-	expression tag	UNP A0A0H2YRL1
C	24	ARG	-	expression tag	UNP A0A0H2YRL1

Continued on next page...

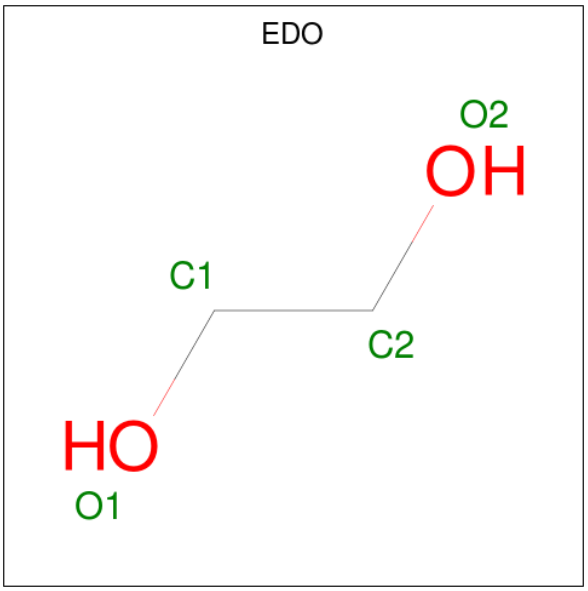
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	25	GLY	-	expression tag	UNP A0A0H2YRL1
C	26	SER	-	expression tag	UNP A0A0H2YRL1
C	27	HIS	-	expression tag	UNP A0A0H2YRL1
C	28	MET	-	expression tag	UNP A0A0H2YRL1
C	29	ALA	-	expression tag	UNP A0A0H2YRL1
C	30	SER	-	expression tag	UNP A0A0H2YRL1
D	8	MET	-	initiating methionine	UNP A0A0H2YRL1
D	9	GLY	-	expression tag	UNP A0A0H2YRL1
D	10	SER	-	expression tag	UNP A0A0H2YRL1
D	11	SER	-	expression tag	UNP A0A0H2YRL1
D	12	HIS	-	expression tag	UNP A0A0H2YRL1
D	13	HIS	-	expression tag	UNP A0A0H2YRL1
D	14	HIS	-	expression tag	UNP A0A0H2YRL1
D	15	HIS	-	expression tag	UNP A0A0H2YRL1
D	16	HIS	-	expression tag	UNP A0A0H2YRL1
D	17	HIS	-	expression tag	UNP A0A0H2YRL1
D	18	SER	-	expression tag	UNP A0A0H2YRL1
D	19	SER	-	expression tag	UNP A0A0H2YRL1
D	20	GLY	-	expression tag	UNP A0A0H2YRL1
D	21	LEU	-	expression tag	UNP A0A0H2YRL1
D	22	VAL	-	expression tag	UNP A0A0H2YRL1
D	23	PRO	-	expression tag	UNP A0A0H2YRL1
D	24	ARG	-	expression tag	UNP A0A0H2YRL1
D	25	GLY	-	expression tag	UNP A0A0H2YRL1
D	26	SER	-	expression tag	UNP A0A0H2YRL1
D	27	HIS	-	expression tag	UNP A0A0H2YRL1
D	28	MET	-	expression tag	UNP A0A0H2YRL1
D	29	ALA	-	expression tag	UNP A0A0H2YRL1
D	30	SER	-	expression tag	UNP A0A0H2YRL1

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	6	Total Ca 6 6	0	0
2	A	3	Total Ca 3 3	0	0
2	D	5	Total Ca 5 5	0	0
2	C	5	Total Ca 5 5	0	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

Continued on next page...

Continued from previous page...

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

- Molecule 4 is water.

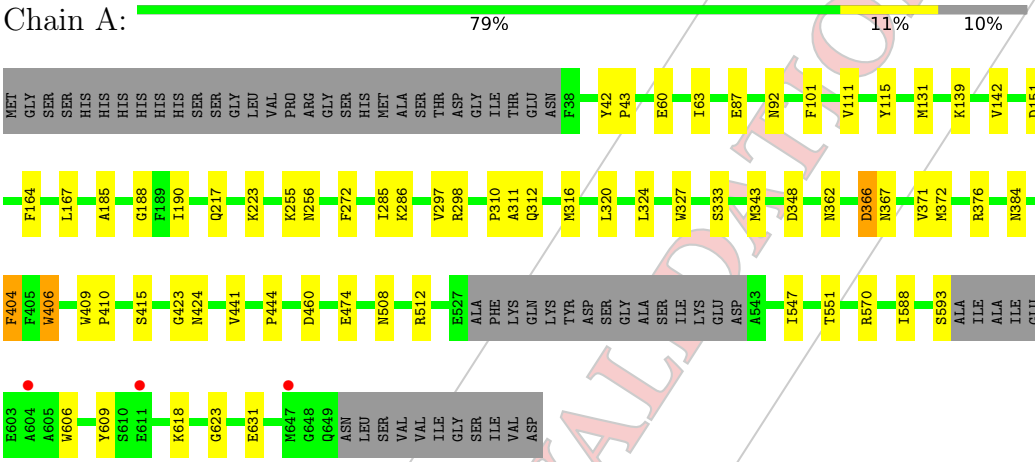
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	417	Total O 417 417	0	0
4	B	448	Total O 448 448	0	0
4	C	430	Total O 430 430	0	0
4	D	423	Total O 423 423	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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 geometryand 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.

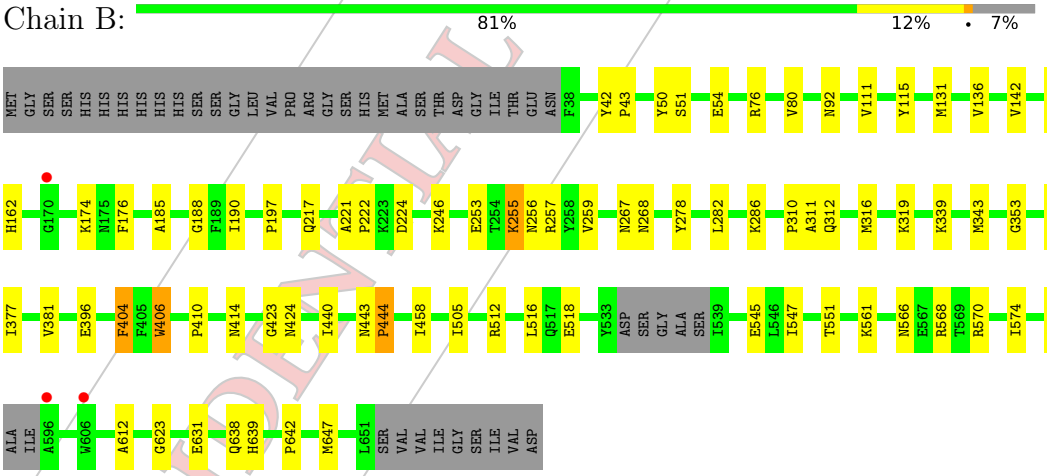
- Molecule 1: Glycoside Hydrolase

Chain A:



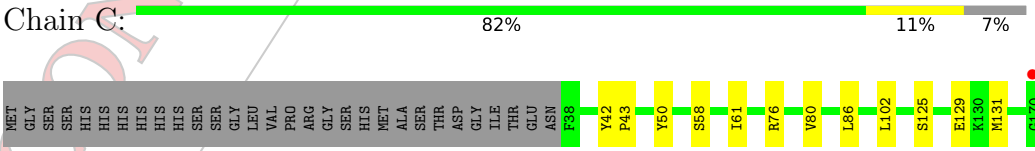
- Molecule 1: Glycoside Hydrolase

Chain B:

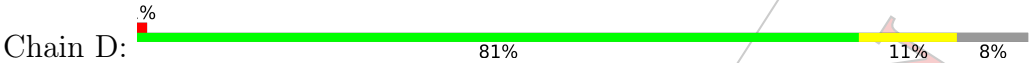


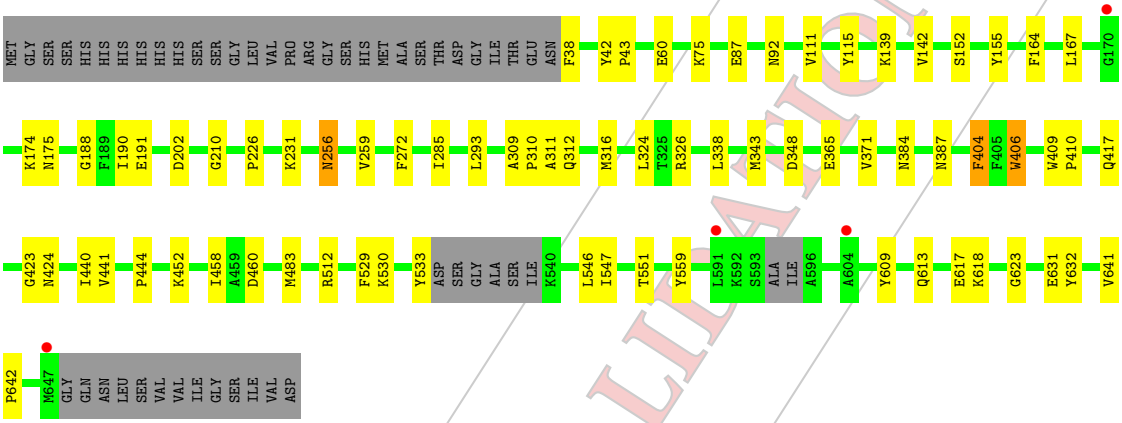
- Molecule 1: Glycoside Hydrolase

Chain C:



• Molecule 1: Glycoside Hydrolase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	92.09Å 92.11Å 103.08Å 95.74° 110.52° 119.71°	Depositor
Resolution (Å)	75.45 – 2.20 75.34 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.1 (75.45-2.20) 98.0 (75.34-2.20)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.14 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.202 , 0.248 0.202 , 0.248	Depositor DCC
R_{free} test set	6401 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	15.9	Xtriage
Anisotropy	0.684	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 23.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.438 for k,h,-h-k-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	20900	wwPDB-VP
Average B, all atoms (Å^2)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.77% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, EDO

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.33	0/4783	0.65	0/6494
1	B	0.33	0/4937	0.63	0/6703
1	C	0.32	0/4944	0.63	0/6711
1	D	0.32	0/4875	0.65	0/6623
All	All	0.33	0/19539	0.64	0/26531

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	4668	0	4316	48	0
1	B	4820	0	4449	51	0
1	C	4826	0	4452	51	0
1	D	4757	0	4354	51	0
2	A	3	0	0	0	0
2	B	6	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	28	0	42	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	20	0	30	1	0
3	C	28	0	42	4	0
3	D	16	0	24	4	0
4	A	417	0	0	5	0
4	B	448	0	0	6	0
4	C	430	0	0	4	0
4	D	423	0	0	6	0
All	All	20900	0	17709	202	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 5.

All (202) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:613:GLN:O	1:D:617:GLU:HG2	1.65	0.94
1:B:590:TYR:HB3	1:B:647:MET:HG2	1.53	0.90
1:D:547:ILE:O	1:D:551:THR:HG23	1.80	0.81
1:B:561:LYS:HE3	1:B:574:ILE:HD11	1.68	0.76
1:B:154:PHE:CD2	1:B:255:LYS:HG2	2.20	0.76
1:A:43:PRO:HB3	1:A:460:ASP:HA	1.71	0.71
1:A:547:ILE:O	1:A:551:THR:HG23	1.90	0.71
1:C:547:ILE:O	1:C:551:THR:HG23	1.92	0.69
1:D:311:ALA:O	1:D:312:GLN:HB2	1.93	0.68
1:B:547:ILE:O	1:B:551:THR:HG23	1.96	0.64
1:B:638:GLN:O	1:B:642:PRO:HG2	1.96	0.64
1:B:51:SER:HB3	4:B:1042:HOH:O	1.98	0.63
1:A:362:ASN:HB2	1:A:393:ILE:HG12	1.80	0.63
1:A:311:ALA:O	1:A:312:GLN:HB2	1.99	0.63
1:C:311:ALA:O	1:C:312:GLN:HB2	1.99	0.62
1:C:362:ASN:HB2	1:C:393:ILE:HG12	1.82	0.62
1:D:417:GLN:HG2	1:D:632:TYR:O	2.00	0.62
1:C:371:VAL:HA	1:C:404:PHE:O	2.00	0.61
1:A:371:VAL:HA	1:A:404:PHE:O	2.00	0.61
1:D:190:ILE:HD13	1:D:406:TRP:CZ3	2.36	0.61
1:B:259:VAL:HG11	1:B:343[A]:MET:HE1	1.84	0.60
1:A:618:LYS:HE3	4:A:921:HOH:O	2.01	0.60
1:D:43:PRO:HB3	1:D:460:ASP:HA	1.84	0.60
1:D:202:ASP:OD2	4:D:801:HOH:O	2.17	0.59
1:D:152:SER:HA	1:D:155:TYR:CD2	2.37	0.58
1:A:190:ILE:HD13	1:A:406:TRP:CZ3	2.39	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:VAL:HG11	1:B:343[A]:MET:CE	2.33	0.58
1:C:190:ILE:HD13	1:C:406:TRP:CZ3	2.38	0.58
1:D:164:PHE:HA	1:D:167:LEU:HG	1.85	0.57
1:A:310:PRO:HG2	1:A:316:MET:HB2	1.87	0.57
1:C:282:LEU:HG	1:C:286:LYS:HE3	1.85	0.57
1:D:559:TYR:CG	3:D:709:EDO:H12	2.40	0.57
1:A:223:LYS:HE3	4:A:1156:HOH:O	2.05	0.57
1:C:639:HIS:C	1:C:642:PRO:HD2	2.26	0.56
1:B:190:ILE:HD13	1:B:406:TRP:CZ3	2.40	0.56
1:D:440:ILE:CG2	1:D:458:ILE:HD11	2.36	0.56
1:C:440:ILE:CG2	1:C:458:ILE:HD11	2.36	0.55
1:A:606:TRP:HH2	4:A:1214:HOH:O	1.89	0.55
1:B:311:ALA:O	1:B:312:GLN:HB2	2.06	0.55
3:A:706:EDO:H12	1:B:377:ILE:CG1	2.37	0.54
1:C:343[D]:MET:HE2	1:C:371:VAL:HG21	1.88	0.54
1:A:152:SER:HA	1:A:155:TYR:CD2	2.42	0.54
1:C:343[D]:MET:CE	1:C:371:VAL:HG21	2.37	0.54
1:A:343:MET:HG3	1:A:371:VAL:CG2	2.37	0.54
1:B:310:PRO:HG2	1:B:316:MET:HB2	1.91	0.53
1:B:343[B]:MET:HG3	1:B:371:VAL:CG2	2.38	0.53
1:C:609:TYR:HD1	1:C:651:LEU:CD1	2.22	0.53
1:C:61:ILE:HD13	1:C:86:LEU:HB3	1.89	0.53
1:C:589:GLY:HA3	1:C:612:ALA:HB2	1.90	0.53
1:C:410:PRO:HD2	1:C:444:PRO:HA	1.91	0.53
1:A:188:GLY:O	1:A:441:VAL:HA	2.09	0.52
1:D:115:TYR:CZ	1:D:142:VAL:HG11	2.44	0.52
1:D:191:GLU:HG2	3:D:708:EDO:H12	1.92	0.52
1:B:371:VAL:HA	1:B:404:PHE:O	2.09	0.52
1:B:154:PHE:CG	1:B:255:LYS:HG2	2.44	0.52
1:A:609:TYR:CD2	1:A:609:TYR:C	2.83	0.52
1:C:309:ALA:HB3	4:D:964:HOH:O	2.10	0.52
1:A:474:GLU:HG3	4:A:1026:HOH:O	2.09	0.52
1:C:424:ASN:HB2	4:C:1136:HOH:O	2.09	0.52
1:B:589:GLY:HA3	1:B:612:ALA:HB2	1.92	0.52
1:C:353:GLY:HA2	1:C:358:LEU:HD13	1.92	0.52
1:A:320:LEU:O	1:A:324:LEU:HD23	2.10	0.51
1:D:618:LYS:HE3	4:D:1003:HOH:O	2.10	0.51
1:C:440:ILE:HG21	1:C:458:ILE:HD11	1.93	0.51
1:C:351:GLY:HA2	3:C:708:EDO:H12	1.92	0.51
1:C:61:ILE:CD1	1:C:86:LEU:HB3	2.41	0.51
1:D:512:ARG:NH1	3:D:706:EDO:H11	2.26	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:551:THR:HG22	1:A:588:ILE:HD11	1.93	0.51
1:C:381:VAL:HG21	1:C:440:ILE:HD13	1.92	0.51
1:C:523:ALA:N	1:C:524:PRO:HD2	2.27	0.50
1:D:371:VAL:HA	1:D:404:PHE:O	2.12	0.50
1:A:115:TYR:CZ	1:A:142:VAL:HG11	2.46	0.50
1:B:54:GLU:HG3	1:B:174:LYS:HD3	1.94	0.50
1:C:239:GLU:CD	1:C:239:GLU:H	2.14	0.50
1:C:343[D]:MET:HG3	1:C:371:VAL:CG2	2.42	0.50
1:D:285:ILE:HG21	1:D:324:LEU:HD21	1.94	0.50
1:B:162:HIS:HE1	4:B:812:HOH:O	1.95	0.49
1:B:396:GLU:OE1	1:C:396:GLU:HB2	2.12	0.49
1:D:139:LYS:HA	1:D:175:ASN:OD1	2.12	0.49
1:C:547:ILE:HD12	1:C:588:ILE:HG23	1.95	0.49
1:D:326:ARG:NH2	1:D:365:GLU:OE2	2.46	0.49
1:D:609:TYR:CD2	1:D:609:TYR:C	2.86	0.49
1:A:512:ARG:HA	3:A:710:EDO:H11	1.95	0.49
1:C:125:SER:O	1:C:129:GLU:HG2	2.12	0.49
1:D:311:ALA:O	1:D:312:GLN:CB	2.60	0.49
1:D:188:GLY:O	1:D:441:VAL:HA	2.12	0.49
1:C:221:ALA:N	1:C:222:PRO:CD	2.76	0.48
1:D:259:VAL:HG11	1:D:343[A]:MET:CE	2.43	0.48
1:A:508:ASN:ND2	4:A:801:HOH:O	2.25	0.48
1:B:162:HIS:CE1	4:B:812:HOH:O	2.66	0.48
1:B:440:ILE:CG2	1:B:458:ILE:HD11	2.44	0.48
1:C:543:ALA:O	1:C:547:ILE:HG12	2.14	0.48
1:A:42:TYR:HA	1:A:43:PRO:C	2.34	0.48
1:B:50:TYR:CD1	1:B:176:PHE:HB3	2.49	0.47
1:D:423:GLY:O	1:D:424:ASN:C	2.52	0.47
1:D:440:ILE:HG21	1:D:458:ILE:HD11	1.97	0.47
1:B:253:GLU:HG2	4:B:1224:HOH:O	2.13	0.47
1:D:529:PHE:O	1:D:533:TYR:HB2	2.14	0.47
1:A:343:MET:HG3	1:A:371:VAL:HG23	1.97	0.47
1:B:566:ASN:OD1	1:B:568:ARG:HB2	2.15	0.47
1:D:38:PHE:CZ	1:D:174:LYS:HE3	2.50	0.47
1:A:372:MET:HG3	1:A:389:PHE:CE1	2.49	0.47
1:C:411:CYS:HB2	1:C:443:ASN:O	2.15	0.47
1:A:131:MET:SD	1:A:185:ALA:HB2	2.55	0.46
1:D:42:TYR:HA	1:D:43:PRO:C	2.35	0.46
1:C:609:TYR:CD1	1:C:651:LEU:HD12	2.51	0.46
1:A:297:VAL:O	1:A:298:ARG:NH1	2.46	0.46
1:B:423:GLY:O	1:B:424:ASN:C	2.54	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:638:GLN:O	1:C:642:PRO:HG2	2.15	0.46
1:D:530:LYS:O	1:D:533:TYR:HB3	2.15	0.46
1:A:311:ALA:O	1:A:312:GLN:CB	2.61	0.46
1:D:272:PHE:CD1	1:D:310:PRO:HB3	2.51	0.46
1:B:381:VAL:HG21	1:B:440:ILE:HD13	1.98	0.45
3:C:711:EDO:O1	1:D:348:ASP:HB3	2.15	0.45
1:B:623:GLY:HA2	1:B:631:GLU:O	2.15	0.45
1:D:343[B]:MET:HG3	1:D:371:VAL:CG2	2.45	0.45
1:A:623:GLY:HA2	1:A:631:GLU:O	2.16	0.45
1:A:60:GLU:HA	1:A:87:GLU:O	2.16	0.45
1:B:278:TYR:CE2	1:B:319:LYS:HE3	2.52	0.45
1:A:423:GLY:O	1:A:424:ASN:C	2.54	0.45
1:C:423:GLY:O	1:C:424:ASN:C	2.55	0.45
1:B:406:TRP:CD1	1:B:406:TRP:C	2.90	0.45
1:B:92:ASN:O	1:B:111:VAL:HG21	2.16	0.45
1:C:505:ILE:HB	1:C:518:GLU:HB3	1.98	0.45
1:C:551:THR:HG22	1:C:588:ILE:HD13	1.99	0.45
1:A:384:ASN:HB3	4:C:1051:HOH:O	2.16	0.45
1:B:410:PRO:HD2	1:B:444:PRO:HA	1.99	0.45
1:C:423:GLY:HA2	1:C:516:LEU:HD22	1.99	0.45
1:A:367:ASN:HA	3:A:704:EDO:H11	1.98	0.45
1:B:136:VAL:HG22	1:B:145:VAL:HG22	1.98	0.45
1:A:151:ASP:O	1:A:154:PHE:HB3	2.17	0.45
1:B:197:PRO:HG3	1:B:224:ASP:OD2	2.17	0.45
1:B:423:GLY:HA2	1:B:516:LEU:HD22	1.99	0.45
1:A:151:ASP:OD1	1:A:255:LYS:NZ	2.44	0.44
1:B:76:ARG:O	1:B:80:VAL:HG23	2.17	0.44
3:A:710:EDO:H12	4:B:1036:HOH:O	2.16	0.44
1:D:38:PHE:CE1	1:D:174:LYS:HE3	2.52	0.44
1:D:60:GLU:HA	1:D:87:GLU:O	2.17	0.44
1:C:50:TYR:CD1	1:C:176:PHE:HB3	2.53	0.44
1:C:58:SER:HA	4:C:838:HOH:O	2.18	0.44
1:D:452:LYS:HB2	1:D:483:MET:HG3	1.99	0.44
1:B:188:GLY:HA3	1:B:217:GLN:O	2.18	0.44
1:B:443:ASN:HA	1:B:444:PRO:HD3	1.85	0.44
1:A:63:ILE:HA	1:A:101:PHE:O	2.18	0.44
1:C:593:SER:O	1:C:596:ALA:HB3	2.17	0.44
1:D:226:PRO:HB2	1:D:231:LYS:HD3	2.00	0.44
1:A:188:GLY:HA3	1:A:217:GLN:O	2.18	0.44
1:A:286:LYS:HE3	1:A:327:TRP:CD1	2.53	0.44
1:B:639:HIS:C	1:B:642:PRO:HD2	2.37	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:410:PRO:HD2	1:D:444:PRO:HA	2.00	0.44
1:A:139:LYS:HG3	1:A:139:LYS:O	2.18	0.44
1:B:131:MET:SD	1:B:185:ALA:HB2	2.58	0.44
1:B:512:ARG:HH11	3:B:711:EDO:H21	1.83	0.43
1:A:348:ASP:HB3	3:A:706:EDO:O2	2.19	0.43
1:D:310:PRO:HG2	1:D:316:MET:HB2	2.00	0.43
1:D:343[B]:MET:CG	1:D:371:VAL:CG2	2.97	0.43
1:A:551:THR:HG22	1:A:588:ILE:CD1	2.47	0.43
1:A:164:PHE:HA	1:A:167:LEU:HG	1.99	0.43
1:A:376:ARG:HH11	3:A:710:EDO:H11	1.83	0.43
1:B:154:PHE:CE2	1:B:255:LYS:HG2	2.53	0.43
1:D:259:VAL:HG11	1:D:343[A]:MET:HE1	2.01	0.43
1:B:221:ALA:N	1:B:222:PRO:CD	2.81	0.43
1:D:293:LEU:HD21	1:D:338:LEU:HD13	2.01	0.43
3:D:706:EDO:C2	4:D:902:HOH:O	2.67	0.43
1:A:285:ILE:HG21	1:A:324:LEU:HD11	2.00	0.42
1:D:641:VAL:N	1:D:642:PRO:CD	2.82	0.42
1:D:75:LYS:HD2	1:D:75:LYS:HA	1.80	0.42
1:B:343[A]:MET:CE	4:B:951:HOH:O	2.67	0.42
1:C:76:ARG:O	1:C:80:VAL:HG23	2.20	0.42
1:D:623:GLY:HA2	1:D:631:GLU:O	2.19	0.42
1:A:406:TRP:CD1	1:A:406:TRP:C	2.93	0.42
1:C:243:GLU:OE1	3:C:707:EDO:O2	2.36	0.42
1:C:351:GLY:CA	3:C:708:EDO:H12	2.50	0.42
1:D:92:ASN:O	1:D:111:VAL:HG21	2.20	0.42
1:C:623:GLY:HA2	1:C:631:GLU:O	2.20	0.42
1:C:547:ILE:HD11	1:C:591:LEU:CB	2.49	0.42
1:A:320:LEU:HD13	1:A:320:LEU:C	2.40	0.41
1:B:353:GLY:HA2	1:B:358:LEU:HD13	2.02	0.41
1:C:42:TYR:HA	1:C:43:PRO:C	2.39	0.41
4:C:1000:HOH:O	1:D:309:ALA:HB3	2.19	0.41
1:D:387:ASN:HB3	4:D:978:HOH:O	2.20	0.41
1:B:267:ASN:O	1:B:268:ASN:C	2.58	0.41
1:A:409:TRP:CD1	1:A:410:PRO:HA	2.55	0.41
1:B:505:ILE:HB	1:B:518:GLU:HB3	2.02	0.41
1:C:417:GLN:HG2	1:C:632:TYR:O	2.21	0.41
1:A:366:ASP:O	3:A:704:EDO:H11	2.21	0.41
1:A:92:ASN:O	1:A:111:VAL:HG21	2.20	0.41
1:C:131:MET:SD	1:C:185:ALA:HB2	2.61	0.41
1:B:115:TYR:CZ	1:B:142:VAL:HG11	2.56	0.41
1:C:188:GLY:O	1:C:441:VAL:HA	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:546:LEU:HA	1:D:546:LEU:HD23	1.88	0.41
1:C:311:ALA:O	1:C:312:GLN:CB	2.68	0.41
1:D:384:ASN:HB3	4:D:935:HOH:O	2.20	0.41
1:B:282:LEU:HG	1:B:286:LYS:HE3	2.01	0.40
1:C:267:ASN:O	1:C:268:ASN:C	2.59	0.40
1:C:522:LEU:HG	1:C:522:LEU:O	2.20	0.40
1:D:409:TRP:CD1	1:D:410:PRO:HA	2.57	0.40
1:A:272:PHE:CD1	1:A:310:PRO:HB3	2.57	0.40
1:B:545:GLU:OE1	1:B:545:GLU:HA	2.19	0.40
1:D:210:GLY:HA3	1:D:256:ASN:OD1	2.21	0.40
1:B:257:ARG:CZ	1:B:339:LYS:HE2	2.52	0.40
1:B:42:TYR:HA	1:B:43:PRO:C	2.41	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	583/653 (89%)	561 (96%)	21 (4%)	1 (0%)	49	57
1	B	602/653 (92%)	577 (96%)	24 (4%)	1 (0%)	49	57
1	C	603/653 (92%)	575 (95%)	28 (5%)	0	100	100
1	D	597/653 (91%)	570 (96%)	27 (4%)	0	100	100
All	All	2385/2612 (91%)	2283 (96%)	100 (4%)	2 (0%)	53	62

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	444	PRO
1	B	444	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	487/560 (87%)	479 (98%)	8 (2%)	65	79
1	B	501/560 (90%)	494 (99%)	7 (1%)	69	82
1	C	501/560 (90%)	496 (99%)	5 (1%)	78	88
1	D	487/560 (87%)	484 (99%)	3 (1%)	87	94
All	All	1976/2240 (88%)	1953 (99%)	23 (1%)	74	85

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	256	ASN
1	A	333	SER
1	A	366	ASP
1	A	404	PHE
1	A	406	TRP
1	A	415	SER
1	A	570	ARG
1	A	593	SER
1	B	246	LYS
1	B	255	LYS
1	B	256	ASN
1	B	404	PHE
1	B	406	TRP
1	B	414	ASN
1	B	570	ARG
1	C	102	LEU
1	C	256	ASN
1	C	404	PHE
1	C	406	TRP
1	C	570	ARG
1	D	256	ASN
1	D	404	PHE
1	D	406	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no

such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 42 ligands modelled in this entry, 19 are monoatomic - leaving 23 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	$\#\|Z\| > 2$
3	EDO	A	704	-	3,3,3	0.16	0	2,2,2	0.33	0
3	EDO	A	705	-	3,3,3	0.07	0	2,2,2	0.27	0
3	EDO	A	706	-	3,3,3	0.08	0	2,2,2	0.09	0
3	EDO	A	707	-	3,3,3	0.11	0	2,2,2	0.23	0
3	EDO	A	708	-	3,3,3	0.28	0	2,2,2	0.71	0
3	EDO	A	709	-	3,3,3	0.10	0	2,2,2	0.28	0
3	EDO	A	710	-	3,3,3	0.06	0	2,2,2	0.33	0
3	EDO	B	707	-	3,3,3	0.13	0	2,2,2	0.32	0
3	EDO	B	708	-	3,3,3	0.11	0	2,2,2	0.50	0
3	EDO	B	709	-	3,3,3	0.12	0	2,2,2	0.30	0
3	EDO	B	710	-	3,3,3	0.04	0	2,2,2	0.25	0
3	EDO	B	711	-	3,3,3	0.07	0	2,2,2	0.21	0
3	EDO	C	706	-	3,3,3	0.14	0	2,2,2	0.57	0
3	EDO	C	707	-	3,3,3	0.14	0	2,2,2	0.09	0
3	EDO	C	708	-	3,3,3	0.26	0	2,2,2	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	EDO	C	709	-	3,3,3	0.18	0	2,2,2	0.31	0
3	EDO	C	710	-	3,3,3	0.10	0	2,2,2	0.38	0
3	EDO	C	711	-	3,3,3	0.13	0	2,2,2	0.09	0
3	EDO	C	712	-	3,3,3	0.27	0	2,2,2	0.56	0
3	EDO	D	706	-	3,3,3	0.10	0	2,2,2	0.10	0
3	EDO	D	707	-	3,3,3	0.21	0	2,2,2	0.46	0
3	EDO	D	708	-	3,3,3	0.08	0	2,2,2	0.37	0
3	EDO	D	709	-	3,3,3	0.05	0	2,2,2	0.23	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	704	-	-	1/1/1/1	-
3	EDO	A	705	-	-	0/1/1/1	-
3	EDO	A	706	-	-	1/1/1/1	-
3	EDO	A	707	-	-	1/1/1/1	-
3	EDO	A	708	-	-	1/1/1/1	-
3	EDO	A	709	-	-	0/1/1/1	-
3	EDO	A	710	-	-	0/1/1/1	-
3	EDO	B	707	-	-	0/1/1/1	-
3	EDO	B	708	-	-	1/1/1/1	-
3	EDO	B	709	-	-	0/1/1/1	-
3	EDO	B	710	-	-	1/1/1/1	-
3	EDO	B	711	-	-	1/1/1/1	-
3	EDO	C	706	-	-	1/1/1/1	-
3	EDO	C	707	-	-	1/1/1/1	-
3	EDO	C	708	-	-	0/1/1/1	-
3	EDO	C	709	-	-	1/1/1/1	-
3	EDO	C	710	-	-	1/1/1/1	-
3	EDO	C	711	-	-	0/1/1/1	-
3	EDO	C	712	-	-	1/1/1/1	-
3	EDO	D	706	-	-	0/1/1/1	-
3	EDO	D	707	-	-	1/1/1/1	-
3	EDO	D	708	-	-	1/1/1/1	-
3	EDO	D	709	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	707	EDO	O1-C1-C2-O2
3	A	706	EDO	O1-C1-C2-O2
3	D	709	EDO	O1-C1-C2-O2
3	C	707	EDO	O1-C1-C2-O2
3	C	709	EDO	O1-C1-C2-O2
3	B	710	EDO	O1-C1-C2-O2
3	D	708	EDO	O1-C1-C2-O2
3	C	710	EDO	O1-C1-C2-O2
3	B	708	EDO	O1-C1-C2-O2
3	A	704	EDO	O1-C1-C2-O2
3	D	707	EDO	O1-C1-C2-O2
3	C	712	EDO	O1-C1-C2-O2
3	C	706	EDO	O1-C1-C2-O2
3	A	708	EDO	O1-C1-C2-O2
3	B	711	EDO	O1-C1-C2-O2

There are no ring outliers.

10 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	704	EDO	2	0
3	A	706	EDO	2	0
3	A	710	EDO	3	0
3	B	711	EDO	1	0
3	C	707	EDO	1	0
3	C	708	EDO	2	0
3	C	711	EDO	1	0
3	D	706	EDO	2	0
3	D	708	EDO	1	0
3	D	709	EDO	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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	589/653 (90%)	-0.60	3 (0%)	90	90	2, 12, 33, 54	0
1	B	607/653 (92%)	-0.54	3 (0%)	90	90	2, 12, 35, 49	0
1	C	608/653 (93%)	-0.53	3 (0%)	90	90	2, 12, 36, 51	0
1	D	602/653 (92%)	-0.55	4 (0%)	87	86	2, 12, 38, 55	0
All	All	2406/2612 (92%)	-0.55	13 (0%)	90	90	2, 12, 36, 55	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	604	ALA	4.2
1	B	596	ALA	3.3
1	A	611	GLU	3.2
1	C	170	GLY	3.0
1	C	606	TRP	2.9
1	D	170	GLY	2.6
1	D	591	LEU	2.6
1	B	606	TRP	2.5
1	A	647	MET	2.4
1	D	647	MET	2.2
1	A	604	ALA	2.1
1	B	170	GLY	2.1
1	C	406	TRP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates (i)

There are no carbohydrates 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
3	EDO	D	709	4/4	0.82	0.16	32,34,34,37	0
3	EDO	A	708	4/4	0.87	0.10	10,11,11,11	0
3	EDO	C	712	4/4	0.87	0.14	9,9,10,10	0
3	EDO	C	706	4/4	0.89	0.14	27,28,28,29	0
3	EDO	A	705	4/4	0.89	0.14	36,37,38,39	0
3	EDO	B	708	4/4	0.90	0.14	27,27,28,29	0
3	EDO	A	709	4/4	0.90	0.14	30,31,32,32	0
3	EDO	C	709	4/4	0.90	0.11	17,18,19,20	0
3	EDO	C	707	4/4	0.91	0.12	36,38,38,39	0
3	EDO	C	708	4/4	0.92	0.11	20,21,22,22	0
2	CA	C	703	1/1	0.93	0.04	30,30,30,30	0
3	EDO	B	710	4/4	0.93	0.12	13,15,16,18	0
3	EDO	B	707	4/4	0.93	0.09	27,28,28,28	0
3	EDO	D	706	4/4	0.93	0.09	26,27,28,28	0
3	EDO	C	711	4/4	0.93	0.08	38,40,40,41	0
3	EDO	D	708	4/4	0.94	0.10	16,17,18,19	0
3	EDO	C	710	4/4	0.94	0.10	10,11,12,13	0
3	EDO	D	707	4/4	0.94	0.12	19,20,21,22	0
3	EDO	A	706	4/4	0.95	0.16	34,36,37,39	0
3	EDO	B	709	4/4	0.95	0.12	10,11,11,11	0
3	EDO	A	710	4/4	0.95	0.14	19,20,20,21	0
3	EDO	A	704	4/4	0.95	0.07	10,12,12,13	0
3	EDO	A	707	4/4	0.96	0.09	14,14,14,15	0
2	CA	B	706	1/1	0.96	0.08	33,33,33,33	0
2	CA	C	705	1/1	0.96	0.05	29,29,29,29	0
3	EDO	B	711	4/4	0.96	0.11	13,15,17,18	0
2	CA	D	702	1/1	0.96	0.04	30,30,30,30	0
2	CA	D	705	1/1	0.96	0.05	28,28,28,28	0
2	CA	B	701	1/1	0.97	0.04	30,30,30,30	0
2	CA	A	701	1/1	0.97	0.04	34,34,34,34	0
2	CA	B	704	1/1	0.98	0.05	35,35,35,35	0
2	CA	C	701	1/1	0.98	0.03	33,33,33,33	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CA	B	703	1/1	0.98	0.06	28,28,28,28	0
2	CA	B	705	1/1	0.98	0.03	24,24,24,24	0
2	CA	C	704	1/1	0.98	0.04	32,32,32,32	0
2	CA	B	702	1/1	0.98	0.05	26,26,26,26	0
2	CA	D	704	1/1	0.98	0.06	29,29,29,29	0
2	CA	D	703	1/1	0.99	0.04	33,33,33,33	0
2	CA	D	701	1/1	0.99	0.05	20,20,20,20	0
2	CA	A	702	1/1	0.99	0.05	29,29,29,29	0
2	CA	A	703	1/1	0.99	0.05	27,27,27,27	0
2	CA	C	702	1/1	0.99	0.07	26,26,26,26	0

6.5 Other polymers (i)

There are no such residues in this entry.