Full wwPDB X-ray Structure Validation Report (i)

Sep 5, 2023 – 06:20 AM EDT

PDB ID	:	3VAV
Title	:	Crystal structure of 3-methyl-2-oxobutanoate hydroxymethyltransferase from Burkholderia thailandensis
Authors	:	Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on	:	2011-12-29
Resolution	:	1.80 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

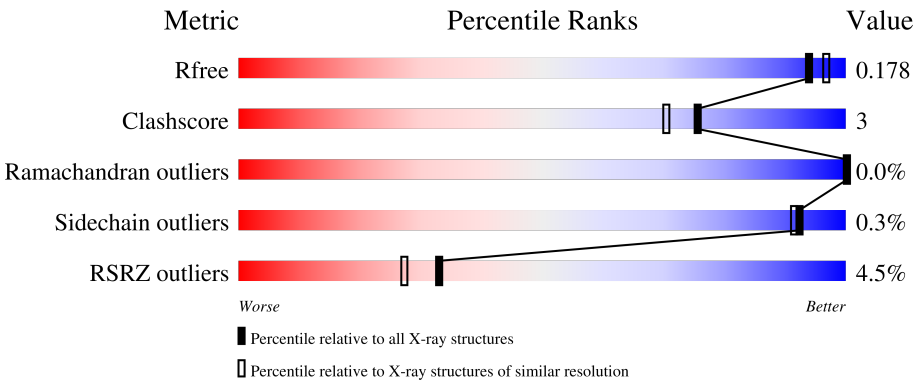
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	275	7% 89% 5% 5%
1	B	275	6% 88% 6% 5%
1	C	275	2% 83% 5% 12%
1	D	275	5% 91% • 6%
1	E	275	6% 87% • 9%

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Mol	Chain	Length	Quality of chain
1	F	275	6% 85% 6% 8%
1	G	275	% 83% 13%
1	H	275	3% 92%
1	I	275	2% 85% 11%
1	J	275	4% 91%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 21566 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 3-methyl-2-oxobutanoate hydroxymethyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	260	1947	1239	337	361	10	0	7	0
1	B	260	1955	1250	337	358	10	0	6	0
1	C	243	1828	1165	315	338	10	0	4	0
1	D	259	1958	1247	341	360	10	0	7	0
1	E	251	1897	1210	322	354	11	0	9	0
1	F	253	1899	1205	334	350	10	0	5	0
1	G	239	1793	1145	304	333	11	0	4	0
1	H	263	1966	1251	339	366	10	0	5	0
1	I	245	1861	1185	321	344	11	0	9	0
1	J	263	1959	1247	338	364	10	0	4	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP Q2SYZ1
A	-2	PRO	-	expression tag	UNP Q2SYZ1
A	-1	GLY	-	expression tag	UNP Q2SYZ1
A	0	SER	-	expression tag	UNP Q2SYZ1
B	-3	GLY	-	expression tag	UNP Q2SYZ1
B	-2	PRO	-	expression tag	UNP Q2SYZ1
B	-1	GLY	-	expression tag	UNP Q2SYZ1
B	0	SER	-	expression tag	UNP Q2SYZ1
C	-3	GLY	-	expression tag	UNP Q2SYZ1

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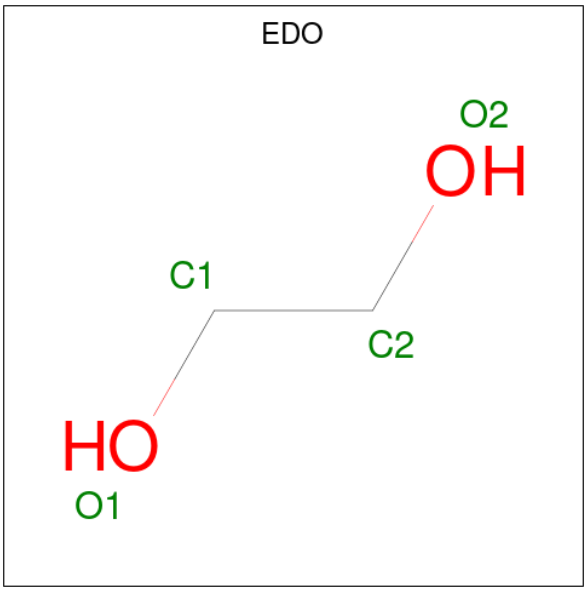
Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	PRO	-	expression tag	UNP Q2SYZ1
C	-1	GLY	-	expression tag	UNP Q2SYZ1
C	0	SER	-	expression tag	UNP Q2SYZ1
D	-3	GLY	-	expression tag	UNP Q2SYZ1
D	-2	PRO	-	expression tag	UNP Q2SYZ1
D	-1	GLY	-	expression tag	UNP Q2SYZ1
D	0	SER	-	expression tag	UNP Q2SYZ1
E	-3	GLY	-	expression tag	UNP Q2SYZ1
E	-2	PRO	-	expression tag	UNP Q2SYZ1
E	-1	GLY	-	expression tag	UNP Q2SYZ1
E	0	SER	-	expression tag	UNP Q2SYZ1
F	-3	GLY	-	expression tag	UNP Q2SYZ1
F	-2	PRO	-	expression tag	UNP Q2SYZ1
F	-1	GLY	-	expression tag	UNP Q2SYZ1
F	0	SER	-	expression tag	UNP Q2SYZ1
G	-3	GLY	-	expression tag	UNP Q2SYZ1
G	-2	PRO	-	expression tag	UNP Q2SYZ1
G	-1	GLY	-	expression tag	UNP Q2SYZ1
G	0	SER	-	expression tag	UNP Q2SYZ1
H	-3	GLY	-	expression tag	UNP Q2SYZ1
H	-2	PRO	-	expression tag	UNP Q2SYZ1
H	-1	GLY	-	expression tag	UNP Q2SYZ1
H	0	SER	-	expression tag	UNP Q2SYZ1
I	-3	GLY	-	expression tag	UNP Q2SYZ1
I	-2	PRO	-	expression tag	UNP Q2SYZ1
I	-1	GLY	-	expression tag	UNP Q2SYZ1
I	0	SER	-	expression tag	UNP Q2SYZ1
J	-3	GLY	-	expression tag	UNP Q2SYZ1
J	-2	PRO	-	expression tag	UNP Q2SYZ1
J	-1	GLY	-	expression tag	UNP Q2SYZ1
J	0	SER	-	expression tag	UNP Q2SYZ1

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	4	2	2	0	0
2	B	1	4	2	2	0	0
2	C	1	4	2	2	0	0
2	D	1	4	2	2	0	0
2	E	1	4	2	2	0	0
2	G	1	4	2	2	0	0
2	G	1	4	2	2	0	0
2	H	1	4	2	2	0	0
2	I	1	4	2	2	0	0
2	J	1	4	2	2	0	0
2	J	1	4	2	2	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
3	I	1	1	1	0	0

- Molecule 4 is water.

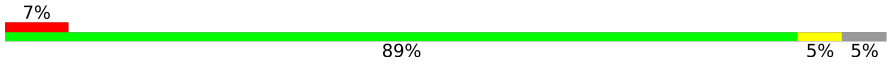
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	264	Total O 264 264	0	0
4	B	245	Total O 245 245	0	0
4	C	239	Total O 239 239	0	0
4	D	264	Total O 264 264	0	0
4	E	205	Total O 205 205	0	0
4	F	248	Total O 248 248	0	0
4	G	253	Total O 253 253	0	0
4	H	287	Total O 287 287	0	0
4	I	231	Total O 231 231	0	0
4	J	222	Total O 222 222	0	0

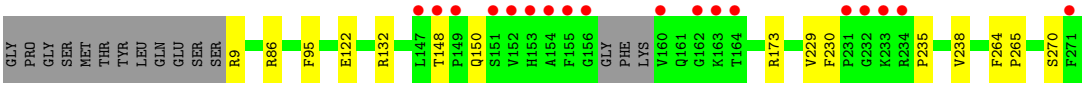
3 Residue-property plots (i)

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: 3-methyl-2-oxobutanoate hydroxymethyltransferase

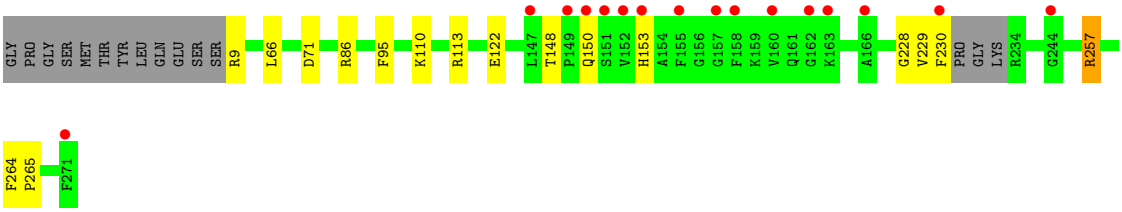
Chain A:





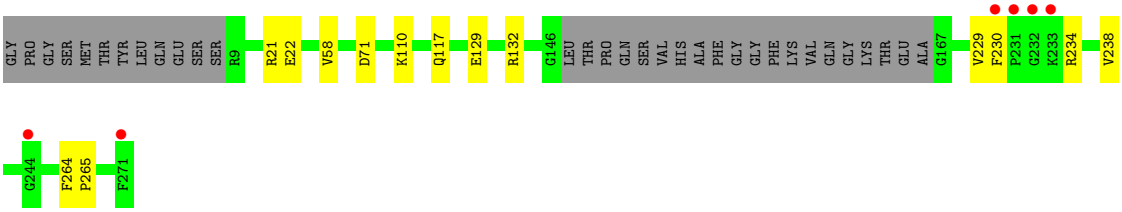
• Molecule 1: 3-methyl-2-oxobutanoate hydroxymethyltransferase

Chain B:



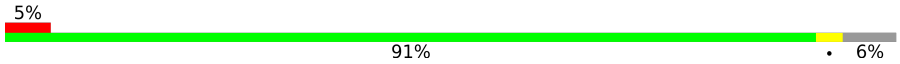
• Molecule 1: 3-methyl-2-oxobutanoate hydroxymethyltransferase

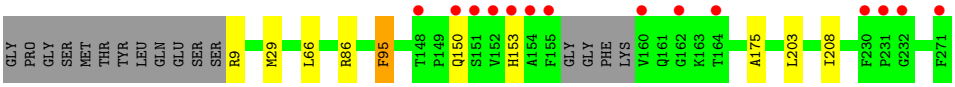
Chain C:



• Molecule 1: 3-methyl-2-oxobutanoate hydroxymethyltransferase

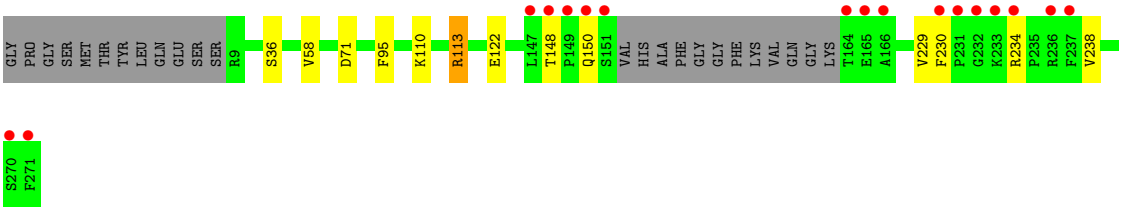
Chain D:





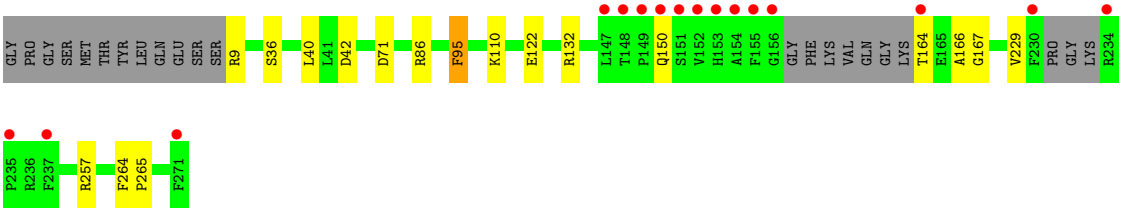
• Molecule 1: 3-methyl-2-oxobutanoate hydroxymethyltransferase

Chain E:



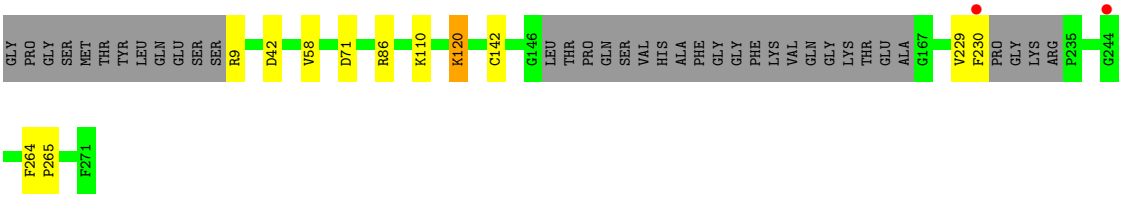
• Molecule 1: 3-methyl-2-oxobutanoate hydroxymethyltransferase

Chain F:



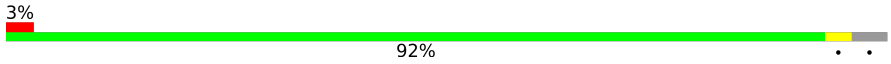
• Molecule 1: 3-methyl-2-oxobutanoate hydroxymethyltransferase

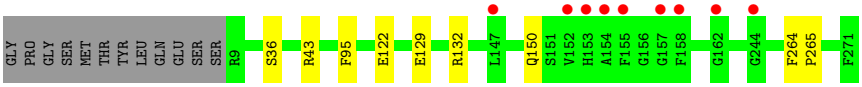
Chain G:



• Molecule 1: 3-methyl-2-oxobutanoate hydroxymethyltransferase

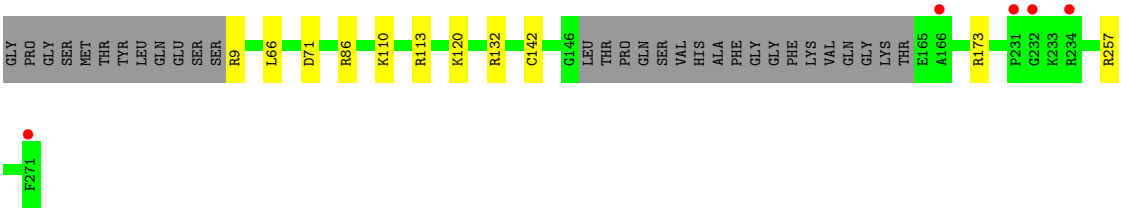
Chain H:





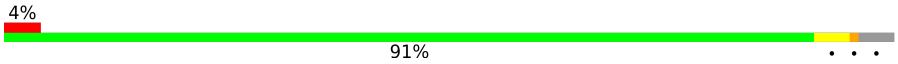
• Molecule 1: 3-methyl-2-oxobutanoate hydroxymethyltransferase

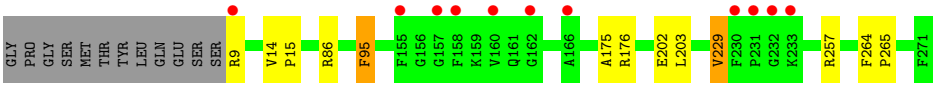
Chain I:



• Molecule 1: 3-methyl-2-oxobutanoate hydroxymethyltransferase

Chain J:


4%
91%


GLY
PRO
GLY
SER
MET
THR
TYR
LEU
GLN
GLU
SER
SER
R9
V14
P15
R86
F95
F155
G156
G157
F158
K159
V160
Q161
G162
A166
A175
R176
E202
L203
V229
F230
P231
G232
K233
R257
F264
P265
F271

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	81.71Å 174.75Å 104.58Å 90.00° 108.71° 90.00°	Depositor
Resolution (Å)	50.00 – 1.80 47.67 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-1.80) 100.0 (47.67-1.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.91 (at 1.79Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.154 , 0.180 0.153 , 0.178	Depositor DCC
R_{free} test set	12850 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	15.0	Xtriage
Anisotropy	0.216	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 48.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	21566	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, 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	0.65	0/2001	0.66	0/2723
1	B	0.65	0/2003	0.70	2/2723 (0.1%)
1	C	0.68	0/1868	0.73	1/2541 (0.0%)
1	D	0.66	0/2010	0.66	0/2734
1	E	0.57	0/1953	0.63	1/2657 (0.0%)
1	F	0.65	0/1944	0.69	0/2640
1	G	0.66	0/1833	0.69	0/2488
1	H	0.69	0/2019	0.69	1/2746 (0.0%)
1	I	0.64	0/1917	0.69	2/2601 (0.1%)
1	J	0.61	0/2006	0.65	0/2731
All	All	0.65	0/19554	0.68	7/26584 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	257	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	B	257[A]	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	B	257[B]	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	H	43	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	C	21	ARG	NE-CZ-NH2	-5.47	117.57	120.30
1	E	113	ARG	NE-CZ-NH2	5.38	122.99	120.30
1	I	257	ARG	NE-CZ-NH2	-5.14	117.73	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1947	0	1957	22	0
1	B	1955	0	1971	14	0
1	C	1828	0	1842	9	0
1	D	1958	0	1966	12	0
1	E	1897	0	1908	12	0
1	F	1899	0	1913	20	0
1	G	1793	0	1806	7	0
1	H	1966	0	1970	9	0
1	I	1861	0	1889	14	0
1	J	1959	0	1960	10	0
2	A	4	0	6	0	0
2	B	4	0	6	0	0
2	C	4	0	6	0	0
2	D	4	0	6	0	0
2	E	4	0	6	0	0
2	G	8	0	12	0	0
2	H	4	0	6	0	0
2	I	4	0	6	0	0
2	J	8	0	12	0	0
3	I	1	0	0	0	0
4	A	264	0	0	4	0
4	B	245	0	0	2	0
4	C	239	0	0	2	0
4	D	264	0	0	2	0
4	E	205	0	0	3	0
4	F	248	0	0	2	0
4	G	253	0	0	0	0
4	H	287	0	0	4	0
4	I	231	0	0	2	0
4	J	222	0	0	1	0
All	All	21566	0	19248	120	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 3.

All (120) 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:F:229[A]:VAL:HG12	1:F:229[A]:VAL:O	1.63	0.96
1:H:129[A]:GLU:OE1	1:H:132[A]:ARG:NH2	2.01	0.93
1:I:173[B]:ARG:HH21	1:I:173[B]:ARG:CG	1.87	0.86
1:J:229[B]:VAL:O	1:J:229[B]:VAL:HG12	1.84	0.78
1:I:173[B]:ARG:HH21	1:I:173[B]:ARG:HG2	1.49	0.76
1:G:229:VAL:O	1:G:230[B]:PHE:CD2	2.38	0.76
1:F:229[A]:VAL:O	1:F:229[A]:VAL:CG1	2.37	0.72
1:I:9:ARG:HE	1:I:86:ARG:HE	1.37	0.72
4:H:1492:HOH:O	1:I:66:LEU:HD22	1.89	0.71
1:F:9:ARG:HE	1:F:86:ARG:HE	1.36	0.70
1:H:150:GLN:HG2	4:H:697:HOH:O	1.92	0.68
1:A:150:GLN:HG2	4:A:1283:HOH:O	1.94	0.66
1:I:113:ARG:NH1	1:J:95:PHE:O	2.26	0.66
1:J:9:ARG:HE	1:J:86:ARG:HE	1.46	0.64
1:E:71:ASP:OD2	1:E:110[B]:LYS:HE2	1.98	0.64
1:G:229:VAL:O	1:G:230[B]:PHE:CG	2.52	0.62
1:I:173[B]:ARG:CG	1:I:173[B]:ARG:NH2	2.53	0.61
1:C:132[A]:ARG:NH1	4:C:2104:HOH:O	2.33	0.61
1:A:9:ARG:HE	1:A:86:ARG:HE	1.47	0.61
1:G:71:ASP:OD2	1:G:110:LYS:HE2	2.01	0.61
1:D:9:ARG:HE	1:D:86:ARG:HE	1.47	0.61
1:B:150:GLN:HG2	4:B:1039:HOH:O	1.99	0.60
1:A:95:PHE:HB2	1:A:150:GLN:HB3	1.83	0.60
1:C:129[A]:GLU:OE2	1:C:132[A]:ARG:NH2	2.35	0.59
1:F:164:THR:HG22	1:F:167:GLY:H	1.67	0.59
1:A:229[B]:VAL:HG12	1:A:229[B]:VAL:O	2.00	0.59
1:E:229[B]:VAL:O	1:E:230[B]:PHE:CG	2.56	0.59
1:B:95:PHE:HB2	1:B:150:GLN:HB3	1.84	0.58
1:C:22:GLU:OE1	4:C:299:HOH:O	2.17	0.58
1:E:229[B]:VAL:O	1:E:229[B]:VAL:HG12	2.04	0.58
1:H:95:PHE:HB2	1:H:150:GLN:HB3	1.86	0.58
1:E:229[B]:VAL:O	1:E:230[B]:PHE:CD2	2.58	0.57
1:B:257[B]:ARG:HB2	1:B:257[B]:ARG:CZ	2.34	0.57
1:E:234:ARG:NE	1:E:238:VAL:O	2.37	0.56
1:A:229[B]:VAL:HG13	1:F:40:LEU:HD12	1.87	0.55
1:E:122:GLU:OE1	1:E:148:THR:HB	2.06	0.55
1:F:164:THR:HG22	1:F:166:ALA:N	2.21	0.55
1:A:270:SER:CB	4:A:2071:HOH:O	2.55	0.55
1:E:150:GLN:NE2	4:E:2034:HOH:O	2.40	0.55
1:E:36:SER:HB3	1:J:229[A]:VAL:HG11	1.89	0.54
1:F:257[A]:ARG:CZ	1:F:257[A]:ARG:HB2	2.37	0.53
1:I:173[B]:ARG:NH2	1:I:173[B]:ARG:HG3	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:71:ASP:OD2	1:I:110[A]:LYS:HE2	2.09	0.53
1:D:95:PHE:O	1:E:113:ARG:NH1	2.38	0.53
1:B:122:GLU:HB3	1:B:148:THR:HB	1.91	0.52
1:A:173[A]:ARG:NH2	4:A:2064:HOH:O	2.34	0.51
1:A:229[A]:VAL:HG11	1:F:36:SER:HB3	1.93	0.51
1:F:164:THR:HG22	1:F:166:ALA:H	1.74	0.50
1:J:229[B]:VAL:O	1:J:229[B]:VAL:CG1	2.56	0.50
1:E:58:VAL:HG12	1:E:230[B]:PHE:CZ	2.46	0.50
1:I:173[B]:ARG:HH21	1:I:173[B]:ARG:HG3	1.74	0.50
1:A:95:PHE:O	1:B:113:ARG:NH1	2.42	0.50
1:B:229[B]:VAL:O	1:B:229[B]:VAL:HG12	2.12	0.50
1:J:176:ARG:NH2	1:J:202:GLU:OE1	2.41	0.50
1:D:29:MET:HE3	1:D:208:ILE:HG13	1.94	0.49
1:F:122:GLU:HG3	4:F:1696:HOH:O	2.10	0.49
1:D:95:PHE:HB2	1:D:150:GLN:HB3	1.95	0.49
1:F:257[A]:ARG:HB2	1:F:257[A]:ARG:NH1	2.28	0.49
1:B:153:HIS:CE1	1:C:117:GLN:HG2	2.48	0.48
1:A:9:ARG:HG2	1:A:86:ARG:NE	2.29	0.48
1:B:71:ASP:OD2	1:B:110[A]:LYS:HE2	2.12	0.48
1:D:150:GLN:NE2	4:D:1924:HOH:O	2.46	0.48
1:A:132[A]:ARG:HD3	4:A:1331:HOH:O	2.14	0.48
1:F:95:PHE:HB2	1:F:150:GLN:HB3	1.94	0.48
1:D:153:HIS:CD2	4:E:1061:HOH:O	2.65	0.48
1:H:95:PHE:HB2	1:H:150:GLN:CG	2.44	0.47
1:E:95:PHE:HB2	1:E:150:GLN:HB3	1.97	0.47
1:F:150:GLN:HG2	4:F:926:HOH:O	2.14	0.47
1:J:175:ALA:HB1	1:J:203:LEU:HD11	1.96	0.47
1:J:257:ARG:NH1	4:J:1579:HOH:O	2.47	0.47
1:D:150:GLN:HG2	4:D:1505:HOH:O	2.14	0.46
1:E:58:VAL:HG12	1:E:230[B]:PHE:HZ	1.80	0.46
1:G:264:PHE:CD1	1:G:265:PRO:HA	2.51	0.46
1:F:9:ARG:HG3	1:F:86:ARG:HD2	1.98	0.45
1:C:234:ARG:HD3	1:C:238:VAL:O	2.16	0.45
1:H:122:GLU:HG3	4:H:2396:HOH:O	2.16	0.45
1:B:66[A]:LEU:HD22	4:B:1039:HOH:O	2.16	0.45
1:C:71:ASP:OD2	1:C:110:LYS:NZ	2.45	0.45
1:A:229[B]:VAL:HG13	1:F:40:LEU:CD1	2.47	0.45
1:C:58:VAL:HG12	1:C:230[B]:PHE:CZ	2.51	0.45
1:B:264:PHE:CD1	1:B:265:PRO:HA	2.52	0.44
1:F:9:ARG:HG2	1:F:86:ARG:NE	2.32	0.44
1:H:95:PHE:HB2	1:H:150:GLN:CB	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:264:PHE:CD1	1:C:265:PRO:HA	2.52	0.44
1:J:264:PHE:CD1	1:J:265:PRO:HA	2.53	0.44
1:A:9:ARG:HG3	1:A:86:ARG:HD2	1.99	0.43
1:D:9:ARG:HG3	1:D:86:ARG:HD2	1.99	0.43
1:D:9:ARG:CG	1:D:86:ARG:HE	2.30	0.43
1:C:229[B]:VAL:HG11	1:H:36:SER:HB3	1.99	0.43
1:F:132[B]:ARG:NH2	1:F:132[B]:ARG:HG2	2.32	0.43
1:D:66:LEU:HD22	4:E:1061:HOH:O	2.18	0.43
1:A:264:PHE:CD1	1:A:265:PRO:HA	2.54	0.43
1:A:229[B]:VAL:O	1:A:230:PHE:CG	2.72	0.43
1:I:173[B]:ARG:NH2	4:I:1879:HOH:O	2.52	0.43
1:H:264:PHE:CD1	1:H:265:PRO:HA	2.53	0.43
1:I:120:LYS:HA	1:I:142:CYS:O	2.19	0.42
1:A:9:ARG:NE	1:A:86:ARG:HE	2.14	0.42
1:A:9:ARG:O	1:A:86:ARG:HD2	2.19	0.42
1:B:95:PHE:HB2	1:B:150:GLN:CB	2.49	0.42
1:D:175:ALA:HB1	1:D:203:LEU:HD11	2.00	0.42
1:B:66[A]:LEU:HD13	1:B:95:PHE:CD2	2.55	0.42
1:D:9:ARG:O	1:D:86:ARG:HD2	2.19	0.42
1:G:58:VAL:HG12	1:G:230[B]:PHE:CZ	2.55	0.42
1:H:122:GLU:HG3	4:H:1068:HOH:O	2.21	0.41
1:B:9:ARG:O	1:B:86:ARG:HD2	2.21	0.41
1:J:14:VAL:HB	1:J:15:PRO:HD3	2.02	0.41
1:B:228:GLY:HA2	1:B:230[A]:PHE:CE2	2.55	0.41
1:A:235:PRO:O	1:A:238[B]:VAL:HG22	2.20	0.41
1:G:9:ARG:O	1:G:86:ARG:HD2	2.20	0.41
1:A:95:PHE:HB2	1:A:150:GLN:CG	2.50	0.41
1:F:164:THR:CG2	1:F:167:GLY:H	2.31	0.41
1:F:264:PHE:CD1	1:F:265:PRO:HA	2.56	0.41
1:G:120:LYS:HA	1:G:142:CYS:O	2.21	0.41
1:I:9:ARG:O	1:I:86:ARG:HD2	2.21	0.41
1:F:71:ASP:OD2	1:F:110[A]:LYS:HE2	2.22	0.40
1:A:95:PHE:HB2	1:A:150:GLN:CB	2.48	0.40
1:A:122:GLU:HB3	1:A:148:THR:HB	2.03	0.40
1:A:229[A]:VAL:O	1:A:229[A]:VAL:CG1	2.68	0.40
1:I:132:ARG:NH1	4:I:1865:HOH:O	2.39	0.40
1:I:9:ARG:NE	1:I:86:ARG:HE	2.14	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	263/275 (96%)	256 (97%)	7 (3%)	0	100	100
1	B	261/275 (95%)	259 (99%)	2 (1%)	0	100	100
1	C	243/275 (88%)	238 (98%)	5 (2%)	0	100	100
1	D	262/275 (95%)	259 (99%)	3 (1%)	0	100	100
1	E	256/275 (93%)	249 (97%)	7 (3%)	0	100	100
1	F	252/275 (92%)	248 (98%)	4 (2%)	0	100	100
1	G	236/275 (86%)	230 (98%)	6 (2%)	0	100	100
1	H	266/275 (97%)	263 (99%)	3 (1%)	0	100	100
1	I	249/275 (90%)	246 (99%)	3 (1%)	0	100	100
1	J	265/275 (96%)	259 (98%)	4 (2%)	2 (1%)	19	7
All	All	2553/2750 (93%)	2507 (98%)	44 (2%)	2 (0%)	100	36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	229[A]	VAL
1	J	229[B]	VAL

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	198/209 (95%)	198 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	198/209 (95%)	198 (100%)	0	100	100
1	C	186/209 (89%)	186 (100%)	0	100	100
1	D	198/209 (95%)	197 (100%)	1 (0%)	88	87
1	E	194/209 (93%)	194 (100%)	0	100	100
1	F	192/209 (92%)	190 (99%)	2 (1%)	76	71
1	G	183/209 (88%)	181 (99%)	2 (1%)	73	68
1	H	199/209 (95%)	199 (100%)	0	100	100
1	I	190/209 (91%)	190 (100%)	0	100	100
1	J	198/209 (95%)	197 (100%)	1 (0%)	88	87
All	All	1936/2090 (93%)	1930 (100%)	6 (0%)	92	91

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	95	PHE
1	F	42	ASP
1	F	95	PHE
1	G	42	ASP
1	G	120	LYS
1	J	95	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	184	GLN
1	D	243	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 12 ligands modelled in this entry, 1 is monoatomic - leaving 11 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	$\#\|Z\| > 2$
2	EDO	J	273	-	3,3,3	0.50	0	2,2,2	0.52	0
2	EDO	J	272	-	3,3,3	0.66	0	2,2,2	0.10	0
2	EDO	B	272	-	3,3,3	0.62	0	2,2,2	0.11	0
2	EDO	A	272	-	3,3,3	0.39	0	2,2,2	0.20	0
2	EDO	E	272	-	3,3,3	0.52	0	2,2,2	0.22	0
2	EDO	H	272	-	3,3,3	0.61	0	2,2,2	0.44	0
2	EDO	G	273	-	3,3,3	0.48	0	2,2,2	0.31	0
2	EDO	D	272	-	3,3,3	0.50	0	2,2,2	0.22	0
2	EDO	C	272	-	3,3,3	0.44	0	2,2,2	0.06	0
2	EDO	G	272	-	3,3,3	0.35	0	2,2,2	0.36	0
2	EDO	I	272	-	3,3,3	0.45	0	2,2,2	0.13	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
2	EDO	J	273	-	-	0/1/1/1	-
2	EDO	J	272	-	-	1/1/1/1	-
2	EDO	B	272	-	-	0/1/1/1	-
2	EDO	A	272	-	-	1/1/1/1	-
2	EDO	E	272	-	-	1/1/1/1	-
2	EDO	H	272	-	-	0/1/1/1	-
2	EDO	G	273	-	-	0/1/1/1	-
2	EDO	D	272	-	-	0/1/1/1	-
2	EDO	C	272	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	G	272	-	-	0/1/1/1	-
2	EDO	I	272	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	272	EDO	O1-C1-C2-O2
2	A	272	EDO	O1-C1-C2-O2
2	E	272	EDO	O1-C1-C2-O2
2	J	272	EDO	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	260/275 (94%)	-0.26	18 (6%)	16	13	8, 13, 37, 48	0
1	B	260/275 (94%)	-0.30	16 (6%)	20	16	8, 14, 37, 52	0
1	C	243/275 (88%)	-0.52	6 (2%)	57	52	7, 12, 27, 53	0
1	D	259/275 (94%)	-0.38	14 (5%)	25	20	8, 14, 41, 57	0
1	E	251/275 (91%)	-0.20	17 (6%)	17	13	9, 18, 42, 67	0
1	F	253/275 (92%)	-0.31	16 (6%)	20	15	8, 15, 37, 55	0
1	G	239/275 (86%)	-0.67	2 (0%)	86	84	7, 12, 24, 40	0
1	H	263/275 (95%)	-0.40	9 (3%)	45	39	7, 12, 31, 43	0
1	I	245/275 (89%)	-0.52	5 (2%)	65	61	8, 14, 29, 51	0
1	J	263/275 (95%)	-0.31	11 (4%)	36	30	9, 17, 36, 49	0
All	All	2536/2750 (92%)	-0.38	114 (4%)	33	27	7, 14, 35, 67	0

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	232	GLY	6.3
1	E	231	PRO	6.0
1	F	155	PHE	5.6
1	F	271	PHE	5.5
1	A	160	VAL	5.5
1	E	271	PHE	5.4
1	A	232	GLY	5.2
1	B	158	PHE	5.1
1	G	230[A]	PHE	5.0
1	B	162	GLY	4.9
1	I	232	GLY	4.9
1	E	230[A]	PHE	4.7
1	D	160	VAL	4.6

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Mol	Chain	Res	Type	RSRZ
1	E	166	ALA	4.6
1	B	155	PHE	4.4
1	B	160	VAL	4.4
1	B	271	PHE	4.3
1	F	154	ALA	4.3
1	E	147	LEU	4.3
1	D	232	GLY	4.2
1	F	152	VAL	4.0
1	A	155	PHE	3.9
1	H	155	PHE	3.9
1	D	152	VAL	3.8
1	E	151	SER	3.8
1	D	154	ALA	3.7
1	F	235	PRO	3.7
1	D	231	PRO	3.7
1	J	158	PHE	3.7
1	J	166	ALA	3.6
1	F	147	LEU	3.6
1	F	156	GLY	3.6
1	D	230[A]	PHE	3.5
1	A	271	PHE	3.5
1	A	147	LEU	3.5
1	I	166	ALA	3.5
1	G	244	GLY	3.4
1	H	147	LEU	3.4
1	I	231	PRO	3.4
1	H	157	GLY	3.4
1	E	150	GLN	3.4
1	D	151	SER	3.3
1	A	151	SER	3.3
1	A	148	THR	3.3
1	F	230	PHE	3.2
1	J	233	LYS	3.2
1	E	270	SER	3.2
1	C	230[A]	PHE	3.2
1	D	271	PHE	3.2
1	E	164	THR	3.2
1	F	151	SER	3.2
1	E	149	PRO	3.1
1	F	150	GLN	3.1
1	H	162	GLY	3.1
1	A	233	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	153	HIS	3.1
1	A	152	VAL	3.1
1	B	151	SER	3.1
1	C	232	GLY	3.1
1	J	157	GLY	3.1
1	F	149	PRO	3.0
1	D	148	THR	3.0
1	A	163	LYS	3.0
1	B	230[A]	PHE	3.0
1	J	232	GLY	3.0
1	A	231	PRO	3.0
1	I	271	PHE	3.0
1	E	148	THR	3.0
1	J	162	GLY	2.9
1	F	164	THR	2.9
1	A	154	ALA	2.9
1	J	155	PHE	2.8
1	A	162	GLY	2.8
1	B	149	PRO	2.8
1	D	153	HIS	2.8
1	J	160	VAL	2.8
1	D	164	THR	2.7
1	E	233	LYS	2.7
1	H	153	HIS	2.7
1	B	152	VAL	2.7
1	A	153	HIS	2.7
1	A	156	GLY	2.6
1	D	162	GLY	2.6
1	H	154	ALA	2.6
1	C	244	GLY	2.6
1	B	147	LEU	2.6
1	C	231	PRO	2.6
1	C	233	LYS	2.6
1	D	155	PHE	2.6
1	H	244	GLY	2.6
1	B	163	LYS	2.5
1	D	150	GLN	2.5
1	E	165	GLU	2.5
1	B	157	GLY	2.5
1	B	166	ALA	2.4
1	F	234	ARG	2.4
1	J	9	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	J	231	PRO	2.4
1	A	149	PRO	2.4
1	E	236	ARG	2.3
1	A	164	THR	2.3
1	A	234	ARG	2.2
1	I	234	ARG	2.2
1	B	153	HIS	2.2
1	E	237	PHE	2.2
1	F	237	PHE	2.2
1	E	234	ARG	2.1
1	H	158	PHE	2.1
1	J	230	PHE	2.1
1	B	244	GLY	2.1
1	F	148	THR	2.1
1	C	271	PHE	2.1
1	B	150	GLN	2.0
1	H	152	VAL	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	EDO	E	272	4/4	0.84	0.10	29,30,31,35	0
2	EDO	B	272	4/4	0.87	0.12	23,26,27,28	0
2	EDO	I	272	4/4	0.91	0.23	8,8,8,9	0
2	EDO	J	272	4/4	0.91	0.12	15,17,17,20	0
2	EDO	J	273	4/4	0.91	0.15	15,15,15,17	0
2	EDO	D	272	4/4	0.92	0.11	22,24,25,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	EDO	A	272	4/4	0.92	0.11	22,24,27,30	0
2	EDO	H	272	4/4	0.92	0.10	22,23,24,26	0
2	EDO	G	273	4/4	0.95	0.08	21,22,24,25	0
2	EDO	G	272	4/4	0.96	0.11	21,24,25,29	0
3	CL	I	273	1/1	0.96	0.10	46,46,46,46	0
2	EDO	C	272	4/4	0.97	0.09	22,23,23,25	0

6.5 Other polymers (i)

There are no such residues in this entry.