WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:13 AM GMT

PDB ID	:	2WC4
Title	:	Structure of family 1 beta-glucosidase from Thermotoga maritima in complex with 3-imino-2-thia-(+)-castanospermine
Authors	:	Aguilar, M.; Gloster, T.M.; Turkenburg, J.P.; Garcia-Moreno, M.I.; Ortiz Mellet, C.; Davies, G.J.; Garcia Fernandez, J.M.
Deposited on	:	2009-03-08
Resolution	:	1.70 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 1.70 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.
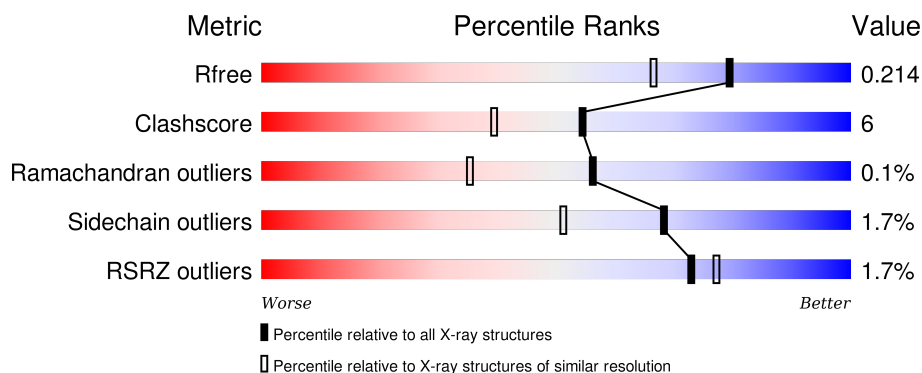
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (1.70-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	468	84% 10% · 5%
1	B	468	89% 5% 5%
1	C	468	86% 8% 5%
1	D	468	84% 10% 5%

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
3	EDO	A	1447	-	-	-	X
3	EDO	C	1448	-	-	-	X
3	EDO	D	1449	-	-	-	X
3	EDO	D	1450	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 16543 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 BETA-GLUCOSIDASE A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	443	Total	C	N	O	S	0	21	0
			3725	2432	625	661	7			
1	B	443	Total	C	N	O	S	0	11	0
			3653	2382	611	653	7			
1	C	443	Total	C	N	O	S	0	22	0
			3723	2428	622	666	7			
1	D	443	Total	C	N	O	S	0	16	0
			3674	2401	605	661	7			

- Molecule 2 is (3Z,5S,6R,7S,8R,8AS)-3-(OCTYLIMINO)HEXAHYDRO[1,3]THIAZOLO[3,4 -A]PYRIDINE-5,6,7,8-TETROL (three-letter code: AMF) (formula: $C_{15}H_{28}N_2O_4S$).
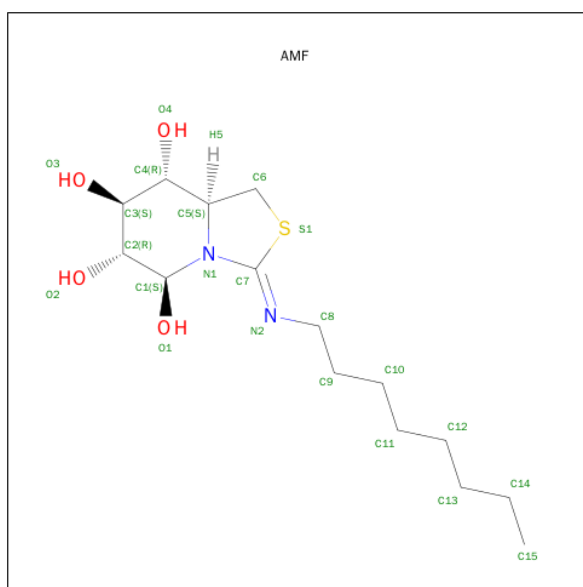
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			22	15	2	4	1		
2	B	1	Total	C	N	O	S	0	0
			22	15	2	4	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	S	0	0
			22	15	2	4	1		
2	D	1	Total	C	N	O	S	0	0
			22	15	2	4	1		

- 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	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).
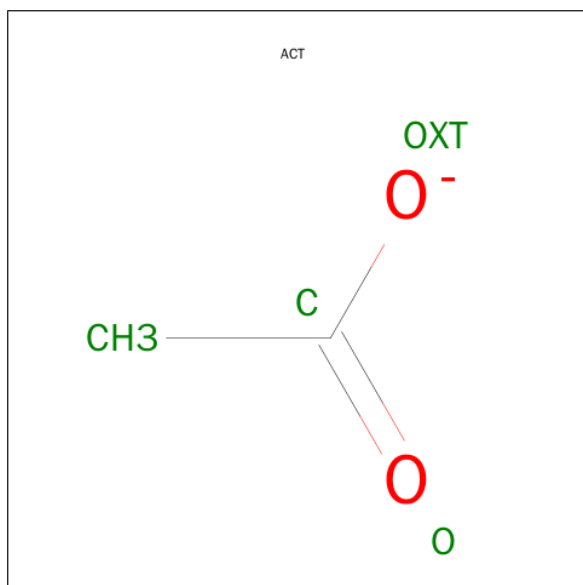
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total C O 4 2 2			0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	1	Total Ca 1 1		0	0
5	C	1	Total Ca 1 1		0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	414	Total O 414 414		0	0
6	B	347	Total O 347 347		0	0
6	C	478	Total O 478 478		0	0
6	D	411	Total O 411 411		0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: BETA-GLUCOSIDASE A
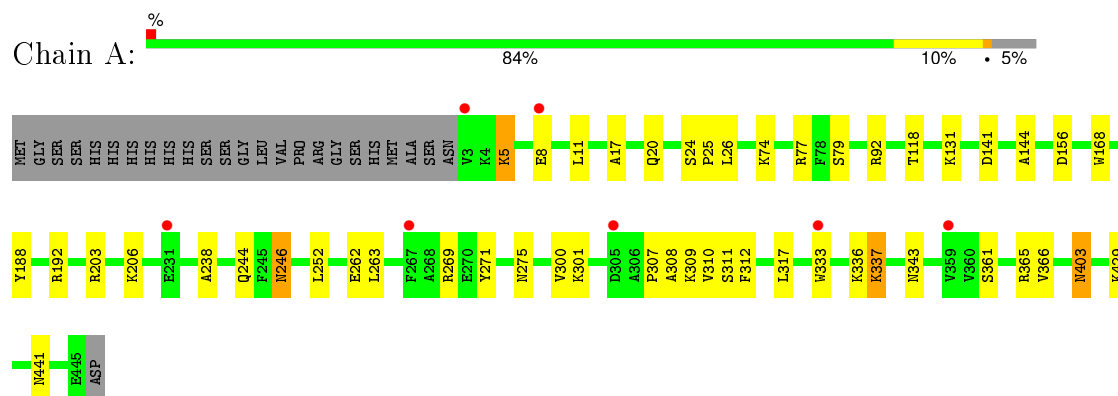
- Molecule 1: BETA-GLUCOSIDASE A

- Molecule 1: BETA-GLUCOSIDASE A

- Molecule 1: BETA-GLUCOSIDASE A

MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET ALA SER ASN V3 K4 K5 F6 P7 Q20 D99 R103 L109 E110 W134 D141 E145 F151 P167 W168 V169 V170 A171 M184 R185 D186 V189 A193

L197 R203 V207 T211 D214 K232 E233 I236 R240 F241 M242 N246 N247 Y248 P249 Y260 P261 L265 E266 F267 E270 H298 L299 V300 D303 P304 D305 A306 P307 A308 K309 V310 S311 F312 V313 A355 S361 N370 W383 Q387

N403 R413 E445 ASP

Full wwPDB X-ray Structure Validation Report
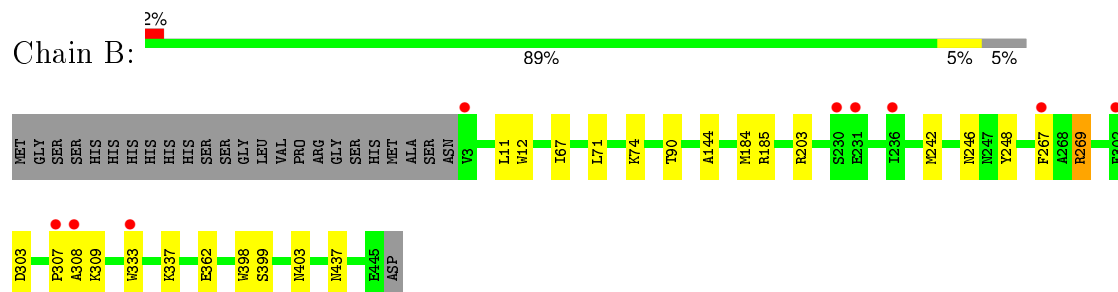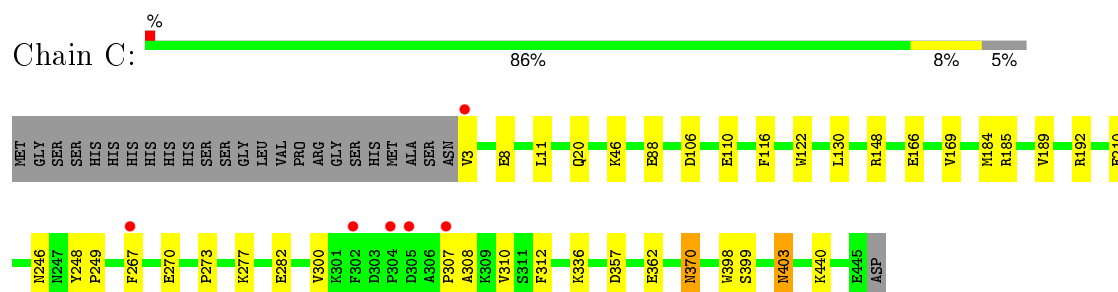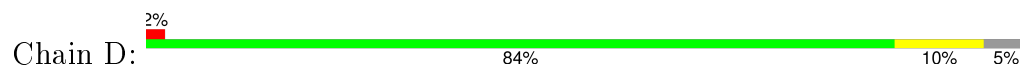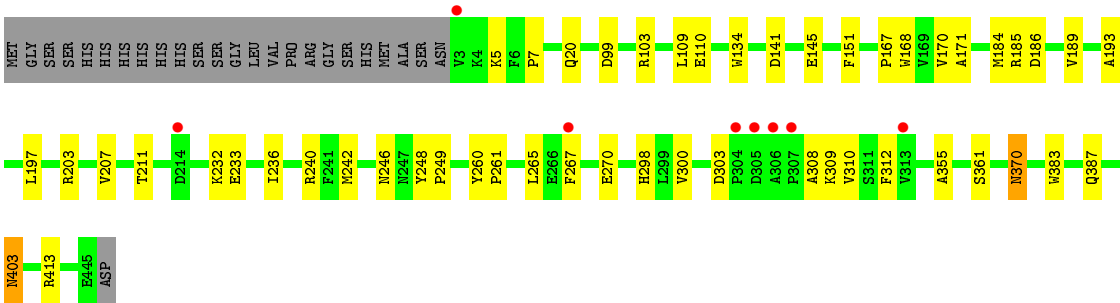
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	89.87Å 73.29Å 137.98Å 90.00° 94.17° 90.00°	Depositor
Resolution (Å)	137.36 – 1.70 29.88 – 1.70	Depositor EDS
% Data completeness (in resolution range)	92.5 (137.36-1.70) 92.5 (29.88-1.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.89 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.4.0077	Depositor
R, R_{free}	0.167 , 0.213 0.167 , 0.214	Depositor DCC
R_{free} test set	9088 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	13.4	Xtriage
Anisotropy	0.431	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 56.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 181264 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	16543	wwPDB-VP
Average B, all atoms (Å^2)	19.0	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 31.99 % 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 1.0109e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: CA, ACT, EDO, AMF

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	0.73	1/3901 (0.0%)	0.74	0/5301
1	B	0.65	0/3799	0.69	0/5165
1	C	0.79	0/3899	0.78	0/5294
1	D	0.71	0/3838	0.74	0/5220
All	All	0.72	1/15437 (0.0%)	0.74	0/20980

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	188	TYR	CD2-CE2	-5.08	1.31	1.39

There are no bond angle outliers.

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	3725	0	3647	54	0
1	B	3653	0	3523	26	0
1	C	3723	0	3633	43	0
1	D	3674	0	3546	71	0
2	A	22	0	28	0	0
2	B	22	0	28	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	22	0	28	0	0
2	D	22	0	28	1	0
3	A	4	0	6	0	0
3	C	4	0	6	0	0
3	D	16	0	24	0	0
4	C	4	0	3	1	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	414	0	0	13	0
6	B	347	0	0	8	0
6	C	478	0	0	16	0
6	D	411	0	0	8	0
All	All	16543	0	14500	189	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 6.

All (189) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88[A]:GLU:HG2	6:C:2127:HOH:O	1.27	1.33
1:D:193:ALA:O	1:D:197[B]:LEU:HD13	1.43	1.18
1:B:437[A]:ASN:OD1	6:B:2342:HOH:O	1.67	1.13
1:A:366[B]:VAL:HG21	1:A:429:LYS:HG2	1.21	1.12
1:D:260:TYR:HB2	1:D:265[B]:LEU:HD11	1.19	1.10
1:B:437[A]:ASN:CG	6:B:2342:HOH:O	1.92	1.06
1:A:131[B]:LYS:NZ	6:A:2167:HOH:O	1.74	1.05
1:C:88[A]:GLU:CG	6:C:2127:HOH:O	1.92	1.04
1:C:148[C]:ARG:NH1	6:C:2206:HOH:O	1.60	1.04
1:D:141:ASP:O	1:D:145[C]:GLU:HG2	1.60	1.01
1:C:246[B]:ASN:ND2	6:C:2291:HOH:O	1.63	1.01
1:D:370:ASN:HB3	6:D:2354:HOH:O	1.62	0.98
1:C:88[B]:GLU:OE2	6:C:2127:HOH:O	1.83	0.96
1:D:167:PRO:HA	1:D:170[B]:VAL:CG2	1.99	0.93
1:C:357[B]:ASP:OD2	6:C:2385:HOH:O	1.86	0.93
1:A:144:ALA:HB2	1:A:203[A]:ARG:HG2	1.50	0.90
1:D:260:TYR:HB2	1:D:265[B]:LEU:CD1	2.02	0.90
1:C:357[A]:ASP:OD1	6:C:2384:HOH:O	1.91	0.88
1:A:131[B]:LYS:NZ	6:A:2166:HOH:O	2.09	0.86
1:D:260:TYR:CB	1:D:265[B]:LEU:HD11	2.05	0.85
1:D:167:PRO:HA	1:D:170[B]:VAL:HG22	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:148[C]:ARG:HD2	6:C:2206:HOH:O	1.75	0.84
1:A:92[B]:ARG:NH1	6:A:2120:HOH:O	1.77	0.83
1:A:366[B]:VAL:CG2	1:A:429:LYS:HG2	2.06	0.82
1:D:167:PRO:O	1:D:170[B]:VAL:CG2	2.28	0.81
1:D:186:ASP:HB3	1:D:189[B]:VAL:HG22	1.62	0.81
1:B:307:PRO:O	1:B:308:ALA:HB3	1.82	0.78
1:A:144:ALA:HB2	1:A:203[A]:ARG:CG	2.12	0.78
1:C:166:GLU:O	1:C:169[A]:VAL:HG22	1.85	0.77
1:C:357[B]:ASP:OD1	6:C:2386:HOH:O	2.01	0.76
1:C:185:ARG:HD2	6:C:2229:HOH:O	1.84	0.76
1:B:246[B]:ASN:ND2	6:B:2196:HOH:O	1.71	0.76
1:A:156[B]:ASP:OD1	6:A:2197:HOH:O	2.03	0.76
1:A:307:PRO:O	1:A:308:ALA:HB3	1.85	0.76
1:D:211[A]:THR:HG22	6:D:2193:HOH:O	1.86	0.75
1:C:166:GLU:HB3	1:C:169[A]:VAL:HG22	1.68	0.75
1:B:144:ALA:HB2	1:B:203[A]:ARG:HG2	1.68	0.75
1:A:366[B]:VAL:CG2	1:A:429:LYS:HA	2.19	0.73
1:D:211[A]:THR:CG2	6:D:2193:HOH:O	2.36	0.73
1:C:88[A]:GLU:OE2	6:C:2127:HOH:O	2.06	0.73
1:D:167:PRO:HA	1:D:170[B]:VAL:HG21	1.69	0.71
1:D:99:ASP:O	1:D:103[A]:ARG:HG3	1.92	0.70
1:D:186:ASP:HB3	1:D:189[B]:VAL:CG2	2.22	0.70
1:A:366[B]:VAL:HG21	1:A:429:LYS:CG	2.13	0.69
1:A:74:LYS:HE2	6:A:2103:HOH:O	1.91	0.69
1:D:167:PRO:O	1:D:170[B]:VAL:HG22	1.92	0.68
1:D:151:PHE:HB3	1:D:211[B]:THR:CG2	2.24	0.68
1:D:167:PRO:CA	1:D:170[B]:VAL:HG22	2.23	0.68
1:C:166:GLU:O	1:C:169[A]:VAL:CG2	2.42	0.68
1:B:307:PRO:O	1:B:308:ALA:CB	2.41	0.67
1:A:366[B]:VAL:HG23	1:A:429:LYS:HA	1.76	0.67
1:D:167:PRO:C	1:D:170[B]:VAL:HG22	2.15	0.66
1:D:167:PRO:O	1:D:170[B]:VAL:HG23	1.93	0.66
1:D:151:PHE:HB3	1:D:211[B]:THR:HG23	1.78	0.65
1:B:269:ARG:NH2	6:B:2211:HOH:O	2.29	0.65
1:C:192[A]:ARG:HG3	1:C:192[A]:ARG:HH11	1.61	0.64
1:B:144:ALA:HB2	1:B:203[A]:ARG:CG	2.28	0.62
1:D:185:ARG:HD2	6:D:2207:HOH:O	2.00	0.61
1:A:141:ASP:OD1	1:A:203[A]:ARG:NH1	2.31	0.60
1:D:151:PHE:CB	1:D:211[B]:THR:HG21	2.32	0.59
1:C:166:GLU:CB	1:C:169[A]:VAL:HG22	2.33	0.59
1:A:307:PRO:O	1:A:308:ALA:CB	2.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:ILE:O	1:B:71[B]:LEU:HD13	2.03	0.58
1:D:134:TRP:CE3	1:D:197[B]:LEU:HD12	2.40	0.57
1:B:12:TRP:H	1:B:74[B]:LYS:HZ3	1.53	0.57
1:D:151:PHE:CB	1:D:211[B]:THR:CG2	2.83	0.57
1:D:170[B]:VAL:HG23	1:D:171:ALA:N	2.20	0.57
1:A:92[A]:ARG:NH1	6:A:2118:HOH:O	2.37	0.56
1:B:333:TRP:CZ2	1:B:337:LYS:HG3	2.40	0.56
1:A:77:ARG:HH21	1:A:118[B]:THR:HG21	1.71	0.56
1:C:166:GLU:HB3	1:C:169[A]:VAL:CG2	2.33	0.55
1:A:300[B]:VAL:HG12	1:A:312:PHE:HD2	1.71	0.55
1:C:270[B]:GLU:H	1:C:270[B]:GLU:CD	2.09	0.55
1:D:260:TYR:CB	1:D:265[B]:LEU:CD1	2.78	0.55
1:D:242:MET:CE	1:D:246[A]:ASN:ND2	2.70	0.55
1:D:7:PRO:HG2	6:D:2370:HOH:O	2.08	0.54
1:C:166:GLU:CB	1:C:169[A]:VAL:CG2	2.86	0.54
1:D:207:VAL:O	1:D:211[B]:THR:HB	2.08	0.54
1:A:192[B]:ARG:NH1	6:A:2213:HOH:O	1.73	0.54
1:D:170[B]:VAL:CG2	1:D:197[B]:LEU:HD21	2.37	0.54
1:B:184[A]:MET:HE2	1:D:184[A]:MET:CE	2.39	0.53
1:D:186:ASP:O	1:D:189[B]:VAL:HG22	2.08	0.53
1:A:300[A]:VAL:HG13	1:A:310[A]:VAL:HG13	1.91	0.52
1:D:167:PRO:CA	1:D:170[B]:VAL:CG2	2.79	0.52
1:D:186:ASP:CB	1:D:189[B]:VAL:HG22	2.37	0.52
1:C:300[A]:VAL:CG1	1:C:310:VAL:HG13	2.40	0.52
1:A:5:LYS:HE2	1:A:441:ASN:O	2.10	0.52
1:C:106:ASP:O	1:C:110:GLU:HG3	2.10	0.52
1:A:77:ARG:NH2	1:A:118[B]:THR:HG21	2.26	0.51
1:D:383:TRP:O	1:D:387:GLN:HG2	2.11	0.51
1:D:170[B]:VAL:HG23	1:D:197[B]:LEU:HD21	1.93	0.50
1:A:300[A]:VAL:HG13	1:A:310[A]:VAL:CG1	2.41	0.50
1:A:366[B]:VAL:HG23	1:A:429:LYS:CA	2.42	0.50
1:C:307:PRO:O	1:C:308:ALA:HB3	2.12	0.50
1:D:141:ASP:O	1:D:145[C]:GLU:CG	2.46	0.50
1:A:206:LYS:HG2	6:A:2223:HOH:O	2.12	0.49
1:A:333:TRP:CZ2	1:A:337:LYS:HD2	2.47	0.49
1:C:11[A]:LEU:HD21	1:C:116:PHE:CE1	2.48	0.48
1:A:77:ARG:HE	1:A:118[B]:THR:CG2	2.26	0.48
1:D:261:PRO:O	1:D:265[B]:LEU:HD13	2.13	0.48
1:D:236:ILE:O	1:D:240:ARG:HG3	2.13	0.48
1:A:79:SER:CB	1:A:118[B]:THR:OG1	2.61	0.48
1:A:300[B]:VAL:HG12	1:A:312:PHE:CD2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:248:TYR:CD1	1:D:249:PRO:HD3	2.48	0.48
1:D:170[B]:VAL:CG2	1:D:197[B]:LEU:CD2	2.91	0.48
1:A:192[B]:ARG:HD3	1:C:130:LEU:HD21	1.96	0.48
1:C:300[A]:VAL:HG13	1:C:310:VAL:CG1	2.44	0.48
1:D:170[B]:VAL:HG23	1:D:171:ALA:H	1.79	0.48
1:A:262:GLU:HG2	6:A:2263:HOH:O	2.14	0.47
1:B:362:GLU:HG2	6:B:2284:HOH:O	2.15	0.47
1:B:184[B]:MET:HG2	1:D:184[B]:MET:HB3	1.96	0.47
1:C:300[A]:VAL:HG13	1:C:310:VAL:HG13	1.97	0.47
1:C:210:GLU:HG2	6:C:2256:HOH:O	2.14	0.47
1:D:298:HIS:CE1	2:D:1446:AMF:H142	2.50	0.47
1:C:192[B]:ARG:HG2	1:C:273:PRO:HG3	1.96	0.46
1:D:303:ASP:O	1:D:309:LYS:HA	2.16	0.46
1:A:238:ALA:HB1	1:A:310[B]:VAL:HG12	1.97	0.46
1:D:168:TRP:CZ2	1:D:246[A]:ASN:OD1	2.68	0.46
1:B:248:TYR:OH	1:B:337:LYS:HB3	2.15	0.46
1:B:184[A]:MET:CE	1:D:184[A]:MET:CE	2.94	0.46
1:C:300[B]:VAL:HG12	1:C:312:PHE:CD1	2.51	0.46
1:A:366[B]:VAL:HG23	1:A:429:LYS:CB	2.46	0.45
1:A:333:TRP:CZ2	1:A:337:LYS:CD	2.99	0.45
1:A:300[A]:VAL:CG1	1:A:310[A]:VAL:HG13	2.46	0.45
1:B:184[A]:MET:HE2	1:D:184[A]:MET:HE3	1.98	0.45
1:C:248:TYR:CD1	1:C:249:PRO:HD3	2.52	0.45
1:D:242:MET:HE3	1:D:246[A]:ASN:ND2	2.31	0.45
1:D:170[B]:VAL:HG21	1:D:197[B]:LEU:CD2	2.47	0.45
1:C:11[A]:LEU:CD2	1:C:116:PHE:CE1	3.00	0.45
1:A:307:PRO:C	1:A:309:LYS:H	2.20	0.44
1:D:151:PHE:CD2	1:D:211[B]:THR:HG21	2.51	0.44
1:A:275:ASN:N	6:A:2280:HOH:O	2.36	0.44
1:D:300[A]:VAL:HG13	1:D:310:VAL:HG13	1.99	0.44
1:A:366[B]:VAL:CG2	1:A:429:LYS:CG	2.85	0.44
1:A:269[B]:ARG:NH1	6:A:2276:HOH:O	2.51	0.43
1:D:308:ALA:O	1:D:309:LYS:HB2	2.18	0.43
1:D:355:ALA:HA	1:D:413:ARG:O	2.18	0.43
1:D:298:HIS:HB3	1:D:312:PHE:HD2	1.84	0.43
1:A:17:ALA:HB3	1:A:20:GLN:HE21	1.83	0.43
1:D:298:HIS:HB3	1:D:312:PHE:CD2	2.54	0.43
1:C:192[A]:ARG:HG3	1:C:192[A]:ARG:NH1	2.27	0.43
1:C:440:LYS:HB2	1:C:440:LYS:HE3	1.79	0.43
1:A:275:ASN:HB2	6:A:2280:HOH:O	2.18	0.43
1:A:192[A]:ARG:NH1	1:A:271:TYR:O	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:240:ARG:HD3	6:D:2252:HOH:O	2.19	0.43
1:B:184[A]:MET:CE	1:D:184[A]:MET:HE2	2.49	0.42
1:C:336:LYS:HE2	1:C:336:LYS:HB3	1.82	0.42
1:A:24:SER:N	1:A:25:PRO:CD	2.82	0.42
1:B:11:LEU:HD12	1:B:74[B]:LYS:HE2	2.00	0.42
1:D:151:PHE:HB2	1:D:211[B]:THR:HG21	2.00	0.42
1:D:20:GLN:O	1:D:403:ASN:HB2	2.20	0.42
1:C:20:GLN:O	1:C:403:ASN:HB2	2.19	0.42
1:C:184[A]:MET:SD	1:C:189:VAL:HG11	2.59	0.42
1:A:144:ALA:CB	1:A:203[A]:ARG:CG	2.92	0.42
1:A:252:LEU:HD23	1:A:252:LEU:HA	1.88	0.42
1:A:336:LYS:HE3	6:A:2370:HOH:O	2.19	0.42
1:D:110[B]:GLU:HG3	6:D:2142:HOH:O	2.19	0.42
1:B:303:ASP:O	1:B:309:LYS:HA	2.19	0.42
1:C:282:GLU:OE2	6:C:2327:HOH:O	2.22	0.42
1:B:398:TRP:HA	1:B:399:SER:HA	1.81	0.42
1:D:170[B]:VAL:HG23	1:D:197[B]:LEU:CD2	2.50	0.41
1:B:437[B]:ASN:HB2	6:B:2342:HOH:O	2.21	0.41
1:A:144:ALA:HB2	1:A:203[A]:ARG:HG3	1.97	0.41
1:D:248:TYR:N	1:D:249:PRO:CD	2.84	0.41
1:B:90:THR:HG22	6:B:2138:HOH:O	2.20	0.41
1:D:193:ALA:O	1:D:197[A]:LEU:HD12	2.21	0.41
1:C:184[A]:MET:HG2	1:C:185:ARG:N	2.36	0.41
1:B:184[A]:MET:HE2	1:B:184[A]:MET:HB2	1.81	0.41
1:D:184[A]:MET:HB2	1:D:184[A]:MET:HE3	1.84	0.41
1:A:301:LYS:HE3	1:A:311[A]:SER:OG	2.21	0.41
1:B:185:ARG:HD2	6:B:2152:HOH:O	2.19	0.41
1:A:262:GLU:HG3	1:A:263:LEU:N	2.36	0.41
1:C:398:TRP:HA	1:C:399:SER:HA	1.87	0.41
1:A:244:GLN:OE1	1:A:263:LEU:HB2	2.20	0.41
1:C:46:LYS:HE3	6:C:2063:HOH:O	2.19	0.41
4:C:1447:ACT:H2	6:C:2022:HOH:O	2.21	0.41
1:D:248:TYR:CG	1:D:249:PRO:HD3	2.56	0.41
1:D:232:LYS:O	1:D:233:GLU:C	2.59	0.41
1:A:26:LEU:HD23	1:A:26:LEU:HA	1.77	0.41
1:C:362:GLU:HG2	6:C:2396:HOH:O	2.21	0.40
1:C:11[A]:LEU:HD21	1:C:116:PHE:HE1	1.87	0.40
1:A:20:GLN:O	1:A:403:ASN:HB2	2.22	0.40
1:B:242:MET:O	1:B:246[A]:ASN:HB2	2.21	0.40
1:D:270:GLU:HB3	6:D:2273:HOH:O	2.20	0.40
1:A:168:TRP:CZ2	1:A:246[A]:ASN:OD1	2.75	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	462/468 (99%)	451 (98%)	11 (2%)	0	100	100
1	B	452/468 (97%)	444 (98%)	8 (2%)	0	100	100
1	C	464/468 (99%)	455 (98%)	8 (2%)	1 (0%)	52	32
1	D	458/468 (98%)	448 (98%)	10 (2%)	0	100	100
All	All	1836/1872 (98%)	1798 (98%)	37 (2%)	1 (0%)	56	35

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	122	TRP

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	392/399 (98%)	380 (97%)	12 (3%)	47	25
1	B	378/399 (95%)	375 (99%)	3 (1%)	86	79
1	C	393/399 (98%)	386 (98%)	7 (2%)	66	49
1	D	382/399 (96%)	375 (98%)	7 (2%)	66	49
All	All	1545/1596 (97%)	1516 (98%)	29 (2%)	68	46

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	8	GLU
1	A	11	LEU
1	A	246[A]	ASN
1	A	246[B]	ASN
1	A	317[A]	LEU
1	A	317[B]	LEU
1	A	337	LYS
1	A	361	SER
1	A	365[A]	ARG
1	A	365[B]	ARG
1	A	403	ASN
1	B	267	PHE
1	B	269	ARG
1	B	403	ASN
1	C	3	VAL
1	C	8	GLU
1	C	267	PHE
1	C	277	LYS
1	C	370[A]	ASN
1	C	370[B]	ASN
1	C	403	ASN
1	D	5	LYS
1	D	109	LEU
1	D	203	ARG
1	D	267	PHE
1	D	361	SER
1	D	370	ASN
1	D	403	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	275	ASN
1	A	403	ASN
1	A	437	ASN
1	B	403	ASN
1	C	403	ASN
1	D	403	ASN

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 13 ligands modelled in this entry, 2 are 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	AMF	A	1446	-	21,23,23	1.30	2 (9%)	20,31,31	1.70	4 (20%)
3	EDO	A	1447	-	3,3,3	0.51	0	2,2,2	0.65	0
2	AMF	B	1446	-	21,23,23	1.01	2 (9%)	20,31,31	1.83	4 (20%)
2	AMF	C	1446	-	21,23,23	1.20	2 (9%)	20,31,31	2.28	5 (25%)
4	ACT	C	1447	-	1,3,3	0.86	0	0,3,3	0.00	-
3	EDO	C	1448	-	3,3,3	0.54	0	2,2,2	0.52	0
2	AMF	D	1446	-	21,23,23	1.32	3 (14%)	20,31,31	2.21	4 (20%)
3	EDO	D	1447	-	3,3,3	0.68	0	2,2,2	0.11	0
3	EDO	D	1448	-	3,3,3	0.54	0	2,2,2	0.52	0
3	EDO	D	1449	-	3,3,3	0.40	0	2,2,2	0.47	0
3	EDO	D	1450	-	3,3,3	0.52	0	2,2,2	0.36	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	AMF	A	1446	-	-	0/8/42/42	0/2/2/2
3	EDO	A	1447	-	-	0/1/1/1	0/0/0/0
2	AMF	B	1446	-	-	0/8/42/42	0/2/2/2
2	AMF	C	1446	-	-	0/8/42/42	0/2/2/2
4	ACT	C	1447	-	-	0/0/0/0	0/0/0/0
3	EDO	C	1448	-	-	0/1/1/1	0/0/0/0
2	AMF	D	1446	-	-	0/8/42/42	0/2/2/2
3	EDO	D	1447	-	-	0/1/1/1	0/0/0/0
3	EDO	D	1448	-	-	0/1/1/1	0/0/0/0
3	EDO	D	1449	-	-	0/1/1/1	0/0/0/0
3	EDO	D	1450	-	-	0/1/1/1	0/0/0/0

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1446	AMF	C6-S1	-2.77	1.75	1.81
2	B	1446	AMF	O1-C1	2.23	1.44	1.41
2	C	1446	AMF	O1-C1	2.46	1.44	1.41
2	D	1446	AMF	O1-C1	2.67	1.44	1.41
2	B	1446	AMF	C7-N2	2.84	1.32	1.26
2	A	1446	AMF	O1-C1	3.07	1.45	1.41
2	C	1446	AMF	C7-N2	3.62	1.34	1.26
2	D	1446	AMF	C7-N2	3.73	1.34	1.26
2	A	1446	AMF	C7-N2	4.37	1.35	1.26

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1446	AMF	C3-C4-C5	-5.62	103.81	111.39
2	D	1446	AMF	C3-C4-C5	-5.50	103.97	111.39
2	B	1446	AMF	C3-C4-C5	-4.67	105.08	111.39
2	C	1446	AMF	C6-C5-C4	-3.88	111.65	115.73
2	D	1446	AMF	O3-C3-C2	-3.37	102.75	110.34
2	A	1446	AMF	O3-C3-C2	-3.29	102.94	110.34
2	A	1446	AMF	C3-C4-C5	-3.11	107.19	111.39
2	C	1446	AMF	O3-C3-C2	-2.78	104.08	110.34
2	B	1446	AMF	O3-C3-C2	-2.51	104.67	110.34
2	A	1446	AMF	C3-C2-C1	2.79	113.56	109.13
2	B	1446	AMF	C3-C2-C1	2.95	113.81	109.13
2	B	1446	AMF	C8-N2-C7	4.00	124.49	117.86
2	C	1446	AMF	C8-N2-C7	4.12	124.70	117.86
2	A	1446	AMF	C8-N2-C7	4.28	124.96	117.86
2	D	1446	AMF	C8-N2-C7	4.33	125.04	117.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1446	AMF	C3-C2-C1	4.47	116.23	109.13
2	C	1446	AMF	C3-C2-C1	4.98	117.05	109.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1447	ACT	1	0
2	D	1446	AMF	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	443/468 (94%)	-0.26	7 (1%)	74	79	10, 16, 30, 42	0
1	B	443/468 (94%)	-0.17	9 (2%)	68	73	12, 20, 34, 45	0
1	C	443/468 (94%)	-0.37	6 (1%)	78	82	7, 13, 28, 43	0
1	D	443/468 (94%)	-0.25	8 (1%)	71	76	9, 16, 31, 49	0
All	All	1772/1872 (94%)	-0.26	30 (1%)	73	77	7, 16, 31, 49	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	306	ALA	5.2
1	D	307	PRO	4.6
1	D	3	VAL	3.8
1	D	304	PRO	3.8
1	D	267	PHE	3.6
1	D	305	ASP	3.5
1	B	307	PRO	3.5
1	C	267	PHE	3.3
1	A	3	VAL	3.2
1	C	304	PRO	3.0
1	B	267	PHE	2.8
1	A	305	ASP	2.7
1	B	302	PHE	2.6
1	A	267	PHE	2.6
1	B	3	VAL	2.6
1	C	307	PRO	2.5
1	C	3	VAL	2.5
1	A	359	VAL	2.4
1	A	8	GLU	2.4
1	B	236	ILE	2.3
1	D	214	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	305	ASP	2.2
1	B	333	TRP	2.2
1	B	230	SER	2.2
1	D	313	VAL	2.2
1	B	231	GLU	2.2
1	A	333	TRP	2.1
1	C	302	PHE	2.1
1	B	308	ALA	2.1
1	A	231	GLU	2.1

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 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
3	EDO	C	1448	4/4	0.87	0.12	3.75	35,35,35,35	0
3	EDO	A	1447	4/4	0.94	0.12	2.96	15,24,24,28	0
3	EDO	D	1450	4/4	0.82	0.14	2.90	43,43,43,44	0
3	EDO	D	1449	4/4	0.94	0.17	2.17	32,32,34,34	0
2	AMF	D	1446	22/22	0.94	0.12	0.62	10,14,28,34	0
2	AMF	A	1446	22/22	0.96	0.10	0.52	9,13,30,34	0
3	EDO	D	1447	4/4	0.95	0.07	0.01	20,22,23,25	0
2	AMF	B	1446	22/22	0.97	0.09	-0.16	10,16,32,38	0
2	AMF	C	1446	22/22	0.97	0.09	-0.25	8,11,24,28	0
3	EDO	D	1448	4/4	0.97	0.07	-0.42	25,27,30,31	0
5	CA	C	1449	1/1	0.98	0.17	-	37,37,37,37	0
5	CA	D	1451	1/1	0.97	0.13	-	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	ACT	C	1447	4/4	0.91	0.13	-	27,29,29,30	0

6.5 Other polymers (i)

There are no such residues in this entry.