Full wwPDB X-ray Structure Validation Report (i)

Dec 18, 2023 – 11:51 AM EST

PDB ID	:	1VKP
Title	:	X-RAY STRUCTURE OF GENE PRODUCT FROM ARABIDOPSIS THALIANA AT5G08170, AGMATINE IMINOHYDROLASE
Authors	:	Wesenberg, G.E.; Smith, D.W.; Phillips Jr., G.N.; Bingman, C.A.; Allard, S.T.M.; Center for Eukaryotic Structural Genomics (CESG)
Deposited on	:	2004-06-15
Resolution	:	1.53 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:

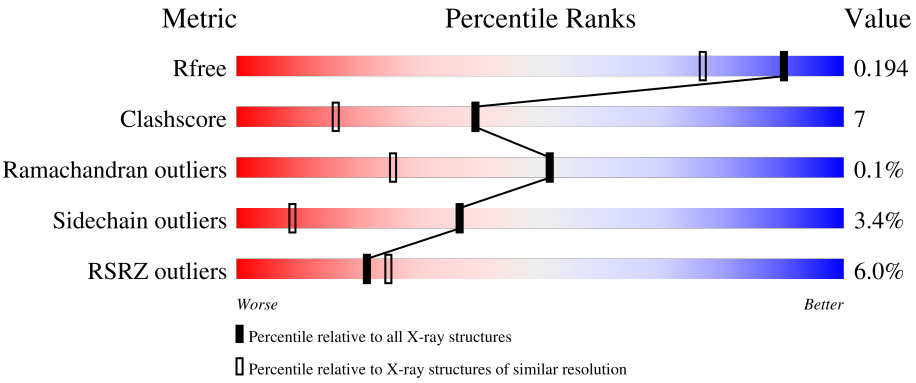
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.53 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	2556 (1.56-1.52)
Clashscore	141614	2634 (1.56-1.52)
Ramachandran outliers	138981	2580 (1.56-1.52)
Sidechain outliers	138945	2577 (1.56-1.52)
RSRZ outliers	127900	2524 (1.56-1.52)

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	383	4% 81% 13% • 5%
1	B	383	7% 77% 16% • 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	B	911	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6699 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 AGMATINE IMINOHYDROLASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	365	Total	C	N	O	S	Se	0	7	0
			2935	1845	523	553	7	7			
1	B	363	Total	C	N	O	S	Se	0	9	0
			2918	1835	517	552	7	7			

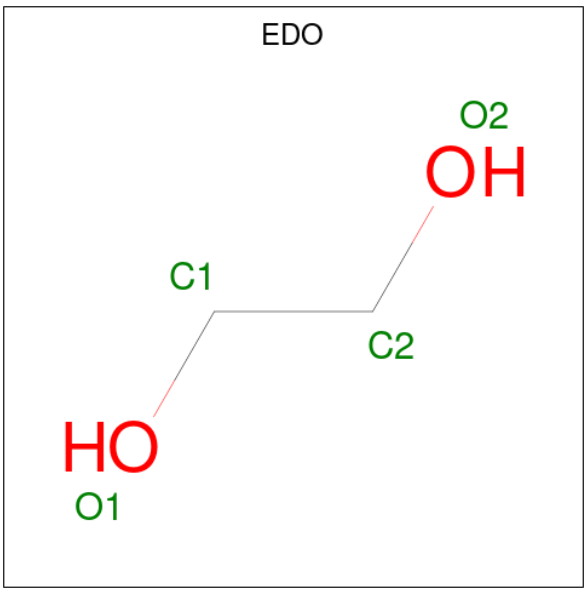
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP Q8GWW7
A	15	MSE	MET	modified residue	UNP Q8GWW7
A	85	MSE	MET	modified residue	UNP Q8GWW7
A	87	MSE	MET	modified residue	UNP Q8GWW7
A	159	MSE	MET	modified residue	UNP Q8GWW7
A	190	MSE	MET	modified residue	UNP Q8GWW7
A	228	MSE	MET	modified residue	UNP Q8GWW7
A	284	MSE	MET	modified residue	UNP Q8GWW7
B	1	MSE	MET	modified residue	UNP Q8GWW7
B	15	MSE	MET	modified residue	UNP Q8GWW7
B	85	MSE	MET	modified residue	UNP Q8GWW7
B	87	MSE	MET	modified residue	UNP Q8GWW7
B	159	MSE	MET	modified residue	UNP Q8GWW7
B	190	MSE	MET	modified residue	UNP Q8GWW7
B	228	MSE	MET	modified residue	UNP Q8GWW7
B	284	MSE	MET	modified residue	UNP Q8GWW7

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

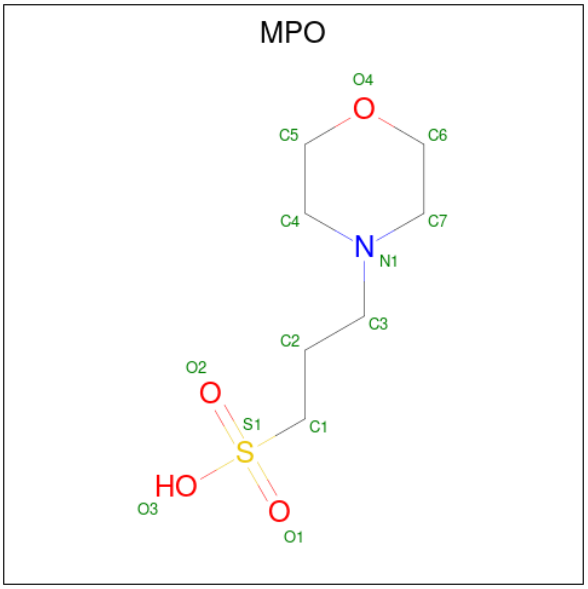
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		

- 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 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	B	1	Total C O 4 2 2	0	0

- Molecule 4 is 3[N-MORPHOLINO]PROPANE SULFONIC ACID (three-letter code: MPO) (formula: $C_7H_{15}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			13	7	1	4	1		

- Molecule 5 is water.

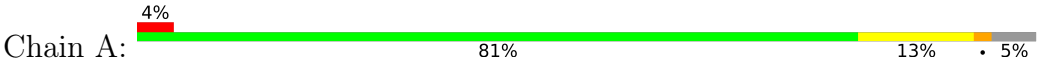
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	406	Total	O	0	0
			406	406		
5	B	373	Total	O	0	0
			373	373		

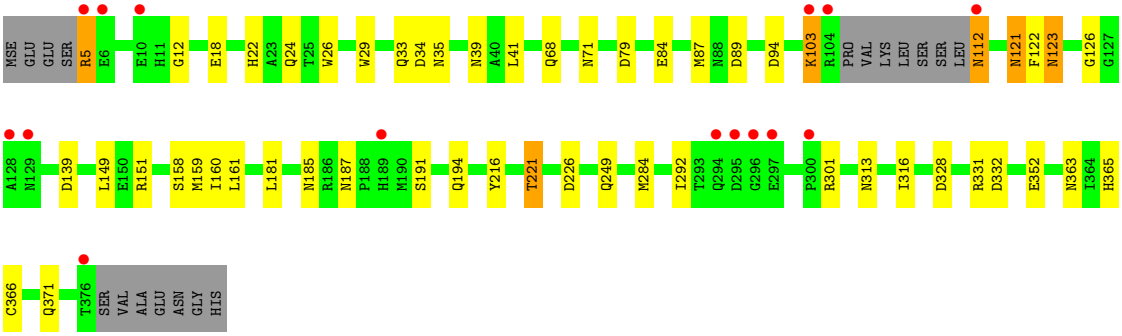
3 Residue-property plots (i)

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: AGMATINE IMINOHYDROLASE

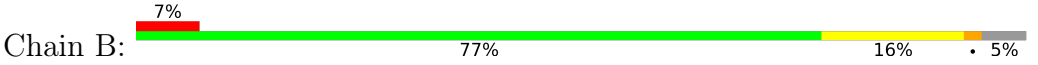
Chain A:

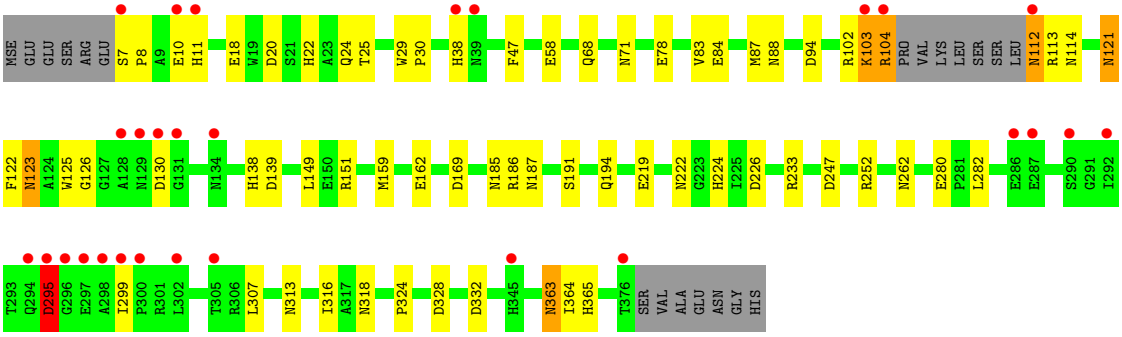




• Molecule 1: AGMATINE IMINOHYDROLASE

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	58.02Å 115.81Å 66.63Å 90.00° 97.10° 90.00°	Depositor
Resolution (Å)	19.88 – 1.53 19.87 – 1.53	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.88-1.53) 91.9 (19.87-1.53)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.11 (at 1.53Å)	Xtriage
Refinement program	REFMAC refmac_5.1.24	Depositor
R, R_{free}	0.146 , 0.174 0.177 , 0.194	Depositor DCC
R_{free} test set	6038 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	14.6	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 49.2	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	6699	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.66% 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: EDO, MG, MPO

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	0.79	2/3034 (0.1%)	0.88	8/4110 (0.2%)
1	B	0.81	4/3022 (0.1%)	0.88	9/4095 (0.2%)
All	All	0.80	6/6056 (0.1%)	0.88	17/8205 (0.2%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	159	MSE	SE-CE	-9.98	1.36	1.95
1	B	159	MSE	SE-CE	-8.19	1.47	1.95
1	B	87	MSE	SE-CE	-7.26	1.52	1.95
1	B	78[A]	GLU	CD-OE1	6.96	1.33	1.25
1	B	78[B]	GLU	CD-OE1	6.96	1.33	1.25
1	A	87	MSE	SE-CE	-5.46	1.63	1.95

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	247	ASP	CB-CG-OD2	7.11	124.70	118.30
1	B	328	ASP	CB-CG-OD2	7.02	124.62	118.30
1	A	331	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	B	169	ASP	CB-CG-OD2	6.27	123.94	118.30
1	B	94	ASP	CB-CG-OD2	6.18	123.86	118.30
1	A	139	ASP	CB-CG-OD2	6.11	123.80	118.30
1	A	79	ASP	CB-CG-OD2	5.95	123.66	118.30
1	A	328	ASP	CB-CG-OD2	5.88	123.59	118.30
1	A	332	ASP	CB-CG-OD1	5.87	123.58	118.30
1	B	295	ASP	CB-CG-OD2	5.64	123.38	118.30
1	A	89	ASP	CB-CG-OD2	5.61	123.35	118.30
1	B	252	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	A	331	ARG	NE-CZ-NH1	5.58	123.09	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	332	ASP	CB-CG-OD2	5.33	123.09	118.30
1	A	34	ASP	CB-CG-OD2	5.24	123.02	118.30
1	B	20	ASP	CB-CG-OD2	5.11	122.89	118.30
1	B	233	ARG	NE-CZ-NH2	5.01	122.81	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	2935	0	2829	40	0
1	B	2918	0	2800	51	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	28	0	42	6	0
3	B	24	0	36	8	0
4	A	13	0	15	0	0
5	A	406	0	0	3	0
5	B	373	0	0	2	0
All	All	6699	0	5722	86	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (86) 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:B:22:HIS:H	1:B:318:ASN:HD21	1.16	0.89
1:A:160:ILE:H	1:A:187:ASN:HD21	1.25	0.84
1:A:191:SER:H	1:A:194:GLN:HE21	1.25	0.84
1:A:68:GLN:HE22	1:A:71:ASN:HD22	1.26	0.81
1:B:219:GLU:O	3:B:911:EDO:H22	1.83	0.79
1:B:186:ARG:HH12	1:B:222:ASN:HD22	1.30	0.79
1:A:26:TRP:HE1	1:A:371:GLN:HE21	1.30	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:SER:H	1:B:194:GLN:HE21	1.31	0.76
1:A:94:ASP:OD2	3:A:903:EDO:H12	1.90	0.72
1:B:18:GLU:OE2	1:B:365:HIS:HE1	1.73	0.71
1:A:18:GLU:OE1	1:A:365:HIS:HE1	1.73	0.71
1:B:7:SER:N	1:B:8:PRO:CD	2.55	0.70
1:B:222:ASN:HD21	3:B:911:EDO:C1	2.04	0.69
1:B:226:ASP:OD2	1:B:365:HIS:HD2	1.75	0.69
1:B:68:GLN:HE22	1:B:71:ASN:HD22	1.39	0.69
1:B:222:ASN:ND2	3:B:911:EDO:H11	2.08	0.69
1:A:313:ASN:HD22	1:A:363:ASN:HB3	1.57	0.67
1:B:138:HIS:HD2	5:B:1083:HOH:O	1.76	0.67
1:A:226:ASP:OD2	1:A:365:HIS:HD2	1.78	0.66
1:A:216:TYR:H	1:A:249:GLN:HE22	1.43	0.64
1:B:7:SER:N	1:B:8:PRO:HD3	2.12	0.64
1:B:125:TRP:O	3:B:911:EDO:C1	2.47	0.63
1:A:216:TYR:H	1:A:249:GLN:NE2	1.99	0.61
1:B:103:LYS:H	1:B:103:LYS:NZ	1.98	0.60
1:A:313:ASN:ND2	1:A:363:ASN:HB3	2.17	0.59
1:A:112:ASN:HD22	1:A:112:ASN:N	2.01	0.59
1:B:88:ASN:HD21	1:B:138:HIS:H	1.52	0.58
1:B:162:GLU:OE2	1:B:224:HIS:HE1	1.86	0.58
1:A:12:GLY:O	1:A:103:LYS:NZ	2.40	0.55
1:B:280:GLU:O	1:B:282:LEU:HD13	2.07	0.55
1:B:102:ARG:HA	1:B:103:LYS:HZ2	1.71	0.55
3:A:908:EDO:H11	1:B:83:VAL:HB	1.90	0.54
1:B:112:ASN:ND2	5:B:1252:HOH:O	2.40	0.54
1:A:161:LEU:HD11	1:A:181[B]:LEU:HD11	1.89	0.54
1:A:29:TRP:HE1	1:A:68:GLN:HE21	1.55	0.53
1:A:352:GLU:OE2	5:A:1271:HOH:O	2.19	0.53
1:A:185:ASN:HA	3:A:906:EDO:H12	1.90	0.53
1:A:35:ASN:HD21	1:A:301:ARG:HH21	1.56	0.53
1:A:35:ASN:ND2	1:A:301:ARG:HE	2.07	0.53
1:B:222:ASN:HD21	3:B:911:EDO:H11	1.68	0.52
1:B:88:ASN:ND2	1:B:139:ASP:H	2.08	0.52
1:A:103:LYS:HZ2	1:A:103:LYS:H	1.58	0.51
1:B:125:TRP:O	3:B:911:EDO:H12	2.12	0.51
1:B:324:PRO:HB3	1:B:363:ASN:HD21	1.76	0.51
1:B:186:ARG:HH12	1:B:222:ASN:ND2	2.05	0.50
1:B:313:ASN:OD1	1:B:363:ASN:HB3	2.12	0.49
1:B:121:ASN:HD22	1:B:122:PHE:H	1.59	0.49
1:A:149[B]:LEU:HD23	1:B:83:VAL:HG12	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:ARG:CB	1:B:114:ASN:HD21	2.25	0.49
1:A:84:GLU:O	3:A:908:EDO:H22	2.12	0.49
1:B:88:ASN:HD22	1:B:139:ASP:H	1.59	0.48
1:A:68:GLN:NE2	1:A:71:ASN:HD22	2.03	0.48
1:B:68:GLN:NE2	1:B:71:ASN:HD22	2.09	0.48
1:B:88:ASN:HD21	1:B:138:HIS:N	2.12	0.48
1:A:149[A]:LEU:HD23	5:A:1315:HOH:O	2.14	0.48
1:A:149[B]:LEU:HD22	1:B:149:LEU:HD11	1.95	0.48
1:B:112:ASN:HD22	1:B:113:ARG:H	1.61	0.47
1:B:185:ASN:HD21	1:B:222:ASN:ND2	2.12	0.47
1:B:104:ARG:HB3	1:B:114:ASN:HD21	1.79	0.47
1:A:26:TRP:HE1	1:A:371:GLN:NE2	2.05	0.46
1:B:22:HIS:HE1	1:B:316:ILE:O	1.99	0.46
1:A:123:ASN:ND2	1:A:126:GLY:H	2.14	0.45
1:B:222:ASN:ND2	3:B:911:EDO:C1	2.71	0.45
1:B:123:ASN:ND2	1:B:126:GLY:H	2.15	0.44
1:A:24:GLN:HE22	1:B:151:ARG:HH22	1.65	0.44
1:A:161:LEU:CD1	1:A:181[B]:LEU:HD11	2.47	0.44
1:A:5:ARG:HH12	1:A:158:SER:H	1.65	0.43
1:A:151:ARG:HH22	1:B:24:GLN:HE22	1.66	0.43
1:A:22:HIS:HE1	1:A:316:ILE:O	2.01	0.43
1:A:33:GLN:HG2	1:A:39:ASN:HD22	1.84	0.43
1:B:58:GLU:CA	3:B:909:EDO:H22	2.49	0.43
1:A:35:ASN:HD21	1:A:301:ARG:NH2	2.15	0.42
1:B:103:LYS:H	1:B:103:LYS:HZ3	1.65	0.42
1:B:185:ASN:HD21	1:B:222:ASN:HD21	1.66	0.42
1:A:121:ASN:HD22	1:A:122:PHE:H	1.67	0.42
1:B:363:ASN:ND2	1:B:364:ILE:H	2.18	0.42
1:A:284:MSE:HE1	1:A:292:ILE:CD1	2.50	0.42
1:A:24:GLN:NE2	1:B:151:ARG:HH22	2.17	0.42
3:A:908:EDO:H21	1:B:84:GLU:O	2.19	0.42
1:A:191:SER:H	1:A:194:GLN:NE2	2.05	0.41
1:A:221[A]:THR:CG2	5:A:1295:HOH:O	2.68	0.41
1:A:366:CYS:HB3	3:A:903:EDO:H11	2.02	0.41
1:B:29:TRP:HE1	1:B:68:GLN:HE21	1.69	0.41
1:B:30:PRO:HD3	1:B:47:PHE:CD2	2.55	0.40
1:B:25:THR:OG1	1:B:58:GLU:OE1	2.36	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	369/383 (96%)	357 (97%)	12 (3%)	0	100 100
1	B	368/383 (96%)	358 (97%)	9 (2%)	1 (0%)	41 19
All	All	737/766 (96%)	715 (97%)	21 (3%)	1 (0%)	51 26

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	295	ASP

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	318/318 (100%)	310 (98%)	8 (2%)	47 17
1	B	317/318 (100%)	302 (95%)	15 (5%)	26 3
All	All	635/636 (100%)	612 (96%)	23 (4%)	37 8

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

Mol	Chain	Res	Type
1	A	5	ARG
1	A	41	LEU
1	A	103	LYS
1	A	112	ASN
1	A	121	ASN

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Mol	Chain	Res	Type
1	A	123	ASN
1	A	221[A]	THR
1	A	221[B]	THR
1	B	10	GLU
1	B	11	HIS
1	B	38	HIS
1	B	103	LYS
1	B	104	ARG
1	B	112	ASN
1	B	121	ASN
1	B	123	ASN
1	B	130	ASP
1	B	262[A]	ASN
1	B	262[B]	ASN
1	B	295	ASP
1	B	299	ILE
1	B	307	LEU
1	B	363	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	35	ASN
1	A	39	ASN
1	A	44	GLN
1	A	68	GLN
1	A	75	GLN
1	A	121	ASN
1	A	123	ASN
1	A	187	ASN
1	A	194	GLN
1	A	249	GLN
1	A	313	ASN
1	A	353	ASN
1	A	365	HIS
1	A	371	GLN
1	B	24	GLN
1	B	39	ASN
1	B	68	GLN
1	B	75	GLN
1	B	88	ASN

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Mol	Chain	Res	Type
1	B	112	ASN
1	B	114	ASN
1	B	121	ASN
1	B	123	ASN
1	B	134	ASN
1	B	138	HIS
1	B	156	GLN
1	B	187	ASN
1	B	194	GLN
1	B	222	ASN
1	B	224	HIS
1	B	318	ASN
1	B	325	GLN
1	B	363	ASN
1	B	365	HIS

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 16 ligands modelled in this entry, 2 are monoatomic - leaving 14 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	910	-	3,3,3	0.28	0	2,2,2	0.34	0
3	EDO	B	909	-	3,3,3	0.29	0	2,2,2	0.51	0
3	EDO	B	911	-	3,3,3	0.56	0	2,2,2	0.73	0
3	EDO	B	904	-	3,3,3	0.27	0	2,2,2	0.54	0
3	EDO	A	902	-	3,3,3	0.33	0	2,2,2	0.54	0
3	EDO	B	913	-	3,3,3	0.31	0	2,2,2	0.52	0
3	EDO	A	907	-	3,3,3	0.32	0	2,2,2	0.67	0
3	EDO	B	912	-	3,3,3	0.28	0	2,2,2	0.71	0
3	EDO	A	908	-	3,3,3	0.19	0	2,2,2	0.43	0
4	MPO	A	1000	-	13,13,13	1.48	3 (23%)	17,17,17	1.69	3 (17%)
3	EDO	A	906	-	3,3,3	0.22	0	2,2,2	0.53	0
3	EDO	A	901	-	3,3,3	0.23	0	2,2,2	0.47	0
3	EDO	B	905	-	3,3,3	0.20	0	2,2,2	0.67	0
3	EDO	A	903	-	3,3,3	0.28	0	2,2,2	1.00	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	910	-	-	1/1/1/1	-
3	EDO	B	909	-	-	1/1/1/1	-
3	EDO	B	911	-	-	1/1/1/1	-
3	EDO	B	904	-	-	1/1/1/1	-
3	EDO	A	902	-	-	0/1/1/1	-
3	EDO	B	913	-	-	0/1/1/1	-
3	EDO	A	907	-	-	0/1/1/1	-
3	EDO	B	912	-	-	1/1/1/1	-
3	EDO	A	908	-	-	0/1/1/1	-
4	MPO	A	1000	-	-	7/7/15/15	0/1/1/1
3	EDO	A	906	-	-	1/1/1/1	-
3	EDO	A	901	-	-	0/1/1/1	-
3	EDO	B	905	-	-	0/1/1/1	-
3	EDO	A	903	-	-	1/1/1/1	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1000	MPO	C1-S1	3.88	1.83	1.77
4	A	1000	MPO	O1-S1	2.27	1.51	1.45
4	A	1000	MPO	O2-S1	2.24	1.51	1.45

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1000	MPO	O3-S1-C1	3.77	111.87	105.77
4	A	1000	MPO	C2-C1-S1	3.33	118.36	113.25
4	A	1000	MPO	C6-C7-N1	2.08	113.26	110.10

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1000	MPO	C1-C2-C3-N1
3	B	909	EDO	O1-C1-C2-O2
4	A	1000	MPO	C2-C3-N1-C4
4	A	1000	MPO	C2-C3-N1-C7
4	A	1000	MPO	C2-C1-S1-O3
3	B	911	EDO	O1-C1-C2-O2
4	A	1000	MPO	C2-C1-S1-O1
4	A	1000	MPO	C2-C1-S1-O2
3	B	912	EDO	O1-C1-C2-O2
3	A	903	EDO	O1-C1-C2-O2
4	A	1000	MPO	S1-C1-C2-C3
3	A	906	EDO	O1-C1-C2-O2
3	A	910	EDO	O1-C1-C2-O2
3	B	904	EDO	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	909	EDO	1	0
3	B	911	EDO	7	0
3	A	908	EDO	3	0
3	A	906	EDO	1	0
3	A	903	EDO	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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	358/383 (93%)	-0.06	15 (4%)	36	41	10, 16, 33, 57	0
1	B	356/383 (92%)	0.10	28 (7%)	12	14	10, 17, 47, 73	0
All	All	714/766 (93%)	0.02	43 (6%)	21	25	10, 16, 40, 73	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	296	GLY	8.4
1	B	295	ASP	6.7
1	B	300	PRO	6.3
1	A	294	GLN	6.2
1	B	299	ILE	5.5
1	A	296	GLY	5.4
1	B	376	THR	5.2
1	B	294	GLN	5.2
1	A	295	ASP	5.1
1	A	376	THR	4.9
1	B	298	ALA	4.7
1	B	297	GLU	4.7
1	B	129	ASN	4.5
1	A	104	ARG	4.3
1	B	128	ALA	4.3
1	B	11	HIS	4.2
1	B	112	ASN	4.1
1	A	5	ARG	4.1
1	A	112	ASN	3.9
1	A	297	GLU	3.9
1	B	10	GLU	3.9
1	B	38	HIS	3.6
1	A	10	GLU	3.6
1	B	290	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	286	GLU	3.3
1	A	6	GLU	3.2
1	A	129	ASN	3.2
1	B	302	LEU	3.1
1	B	287	GLU	3.0
1	A	128	ALA	3.0
1	B	134	ASN	2.9
1	B	39	ASN	2.9
1	B	130	ASP	2.8
1	B	104	ARG	2.8
1	B	7	SER	2.7
1	A	103	LYS	2.4
1	A	300	PRO	2.4
1	B	103	LYS	2.3
1	A	189	HIS	2.3
1	B	292	ILE	2.3
1	B	305	THR	2.1
1	B	131	GLY	2.1
1	B	345	HIS	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MPO	A	1000	13/13	0.72	0.26	32,46,54,56	13
3	EDO	B	913	4/4	0.78	0.19	25,31,35,40	0
3	EDO	B	909	4/4	0.86	0.20	37,41,47,49	0
3	EDO	A	903	4/4	0.87	0.17	39,42,50,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	EDO	A	910	4/4	0.88	0.10	39,48,48,49	0
3	EDO	A	906	4/4	0.88	0.18	39,41,43,46	0
3	EDO	A	901	4/4	0.89	0.11	31,32,34,37	0
3	EDO	B	911	4/4	0.90	0.22	17,26,33,40	0
3	EDO	B	912	4/4	0.90	0.21	27,33,38,41	0
3	EDO	A	908	4/4	0.91	0.23	21,29,31,49	0
3	EDO	A	907	4/4	0.93	0.12	24,29,33,34	0
3	EDO	A	902	4/4	0.93	0.14	24,27,30,33	0
3	EDO	B	905	4/4	0.95	0.07	33,34,40,40	0
3	EDO	B	904	4/4	0.95	0.09	33,37,38,43	0
2	MG	A	802	1/1	0.97	0.07	20,20,20,20	0
2	MG	B	801	1/1	0.97	0.06	19,19,19,19	0

6.5 Other polymers (i)

There are no such residues in this entry.