



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 02:07 PM GMT

PDB ID : 1KD0
Title : Crystal Structure of beta-methylaspartase from Clostridium tetanomorphum.
Apo-structure.
Authors : Asuncion, M.; Blankenfeldt, W.; Barlow, J.N.; Gani, D.; Naismith, J.H.
Deposited on : 2001-11-12
Resolution : 1.90 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

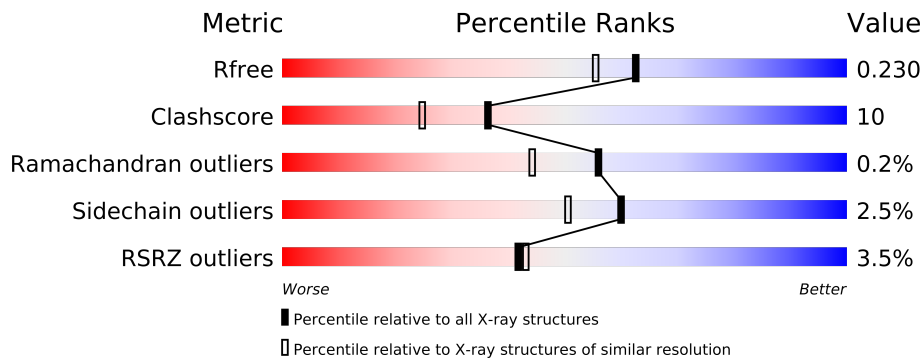
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.90 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}	66092	3684 (1.90-1.90)
Clashscore	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)
RSRZ outliers	66119	3686 (1.90-1.90)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	413	
1	B	413	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	EDO	A	701[A]	-	X
2	EDO	A	701[B]	-	X
2	EDO	B	702[A]	-	X
2	EDO	B	702[B]	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7136 atoms, of which 0 are hydrogen and 0 are deuterium.

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-methylaspartase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	413	Total	C	N	O	S	Se	0	5	0
			3226	2024	561	613	7	21			
1	B	413	Total	C	N	O	S	Se	0	6	0
			3235	2029	562	615	7	22			

There are 34 discrepancies between the modelled and reference sequences:

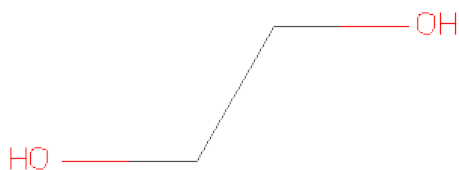
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q05514
A	112	MSE	MET	MODIFIED RESIDUE	UNP Q05514
A	119	MSE	MET	MODIFIED RESIDUE	UNP Q05514
A	150	MSE	MET	MODIFIED RESIDUE	UNP Q05514
A	184	MSE	MET	MODIFIED RESIDUE	UNP Q05514
A	254	MSE	MET	MODIFIED RESIDUE	UNP Q05514
A	276	MSE	MET	MODIFIED RESIDUE	UNP Q05514
A	285	MSE	MET	MODIFIED RESIDUE	UNP Q05514
A	288	MSE	MET	MODIFIED RESIDUE	UNP Q05514
A	327	MSE	MET	MODIFIED RESIDUE	UNP Q05514
A	346	MSE	MET	MODIFIED RESIDUE	UNP Q05514
A	353	MSE	MET	MODIFIED RESIDUE	UNP Q05514
A	376	MSE	MET	MODIFIED RESIDUE	UNP Q05514
A	389	MSE	MET	MODIFIED RESIDUE	UNP Q05514
A	395	MSE	MET	MODIFIED RESIDUE	UNP Q05514
A	396	MSE	MET	MODIFIED RESIDUE	UNP Q05514
A	402	MSE	MET	MODIFIED RESIDUE	UNP Q05514
B	1	MSE	MET	MODIFIED RESIDUE	UNP Q05514
B	112	MSE	MET	MODIFIED RESIDUE	UNP Q05514
B	119	MSE	MET	MODIFIED RESIDUE	UNP Q05514
B	150	MSE	MET	MODIFIED RESIDUE	UNP Q05514
B	184	MSE	MET	MODIFIED RESIDUE	UNP Q05514
B	254	MSE	MET	MODIFIED RESIDUE	UNP Q05514
B	276	MSE	MET	MODIFIED RESIDUE	UNP Q05514
B	285	MSE	MET	MODIFIED RESIDUE	UNP Q05514

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Chain	Residue	Modelled	Actual	Comment	Reference
B	288	MSE	MET	MODIFIED RESIDUE	UNP Q05514
B	327	MSE	MET	MODIFIED RESIDUE	UNP Q05514
B	346	MSE	MET	MODIFIED RESIDUE	UNP Q05514
B	353	MSE	MET	MODIFIED RESIDUE	UNP Q05514
B	376	MSE	MET	MODIFIED RESIDUE	UNP Q05514
B	389	MSE	MET	MODIFIED RESIDUE	UNP Q05514
B	395	MSE	MET	MODIFIED RESIDUE	UNP Q05514
B	396	MSE	MET	MODIFIED RESIDUE	UNP Q05514
B	402	MSE	MET	MODIFIED RESIDUE	UNP Q05514

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	1
			8	4	4		
2	B	1	Total	C	O	0	1
			8	4	4		

- Molecule 3 is water.

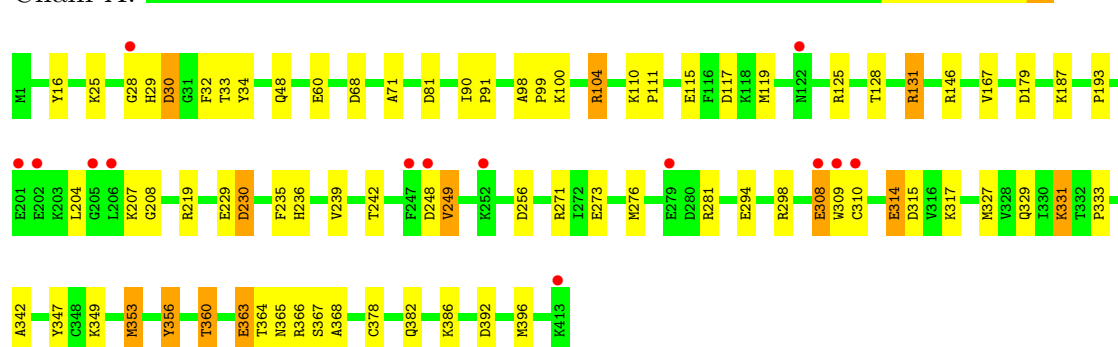
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	315	Total	O	0	0
			315	315		
3	B	344	Total	O	0	0
			344	344		

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.

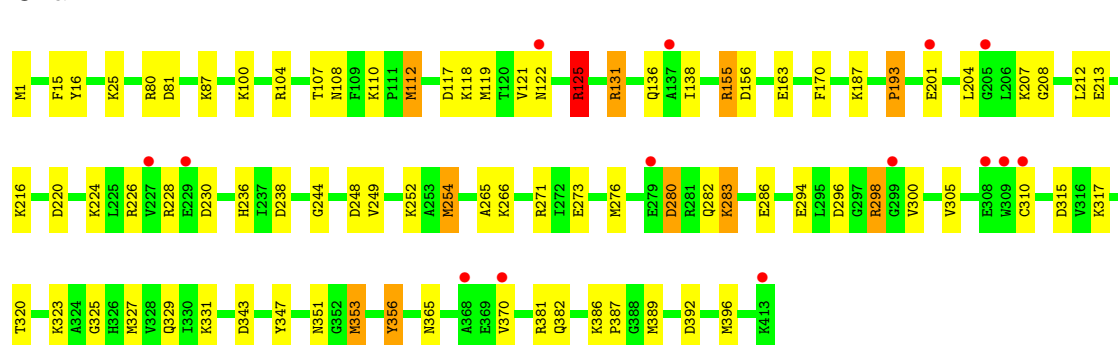
- Molecule 1: beta-methylaspartase

Chain A:



- Molecule 1: beta-methylaspartase

Chain B:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.28Å 109.26Å 108.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	57.74 – 1.90 30.84 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (57.74-1.90) 99.9 (30.84-1.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.71 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.175 , 0.222 0.181 , 0.230	Depositor DCC
R_{free} test set	3229 reflections (5.05%)	DCC
Wilson B-factor (Å ²)	19.2	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.1	EDS
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	2 of 63974 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7136	wwPDB-VP
Average B, all atoms (Å ²)	38.0	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 22.10 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 6.1040e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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: 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	1.21	7/3259 (0.2%)	1.14	21/4366 (0.5%)
1	B	1.24	8/3268 (0.2%)	1.22	19/4377 (0.4%)
All	All	1.22	15/6527 (0.2%)	1.18	40/8743 (0.5%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	353	MSE	SE-CE	-12.19	1.23	1.95
1	B	353[A]	MSE	SE-CE	-9.46	1.39	1.95
1	B	353[B]	MSE	SE-CE	-9.46	1.39	1.95
1	B	125	ARG	CB-CG	6.85	1.71	1.52
1	B	131	ARG	CD-NE	-6.58	1.35	1.46
1	A	363	GLU	CB-CG	-6.13	1.40	1.52
1	A	131	ARG	CD-NE	-5.90	1.36	1.46
1	A	342	ALA	CA-CB	5.75	1.64	1.52
1	B	254	MSE	SE-CE	-5.64	1.62	1.95
1	B	170	PHE	CG-CD2	5.60	1.47	1.38
1	A	71	ALA	CA-CB	5.45	1.64	1.52
1	A	167	VAL	CB-CG1	-5.39	1.41	1.52
1	B	283	LYS	CD-CE	5.26	1.64	1.51
1	A	60	GLU	CD-OE1	5.05	1.31	1.25
1	B	323	LYS	CE-NZ	5.01	1.61	1.49

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	131	ARG	NE-CZ-NH1	19.79	130.19	120.30
1	B	131	ARG	NE-CZ-NH2	-19.59	110.51	120.30
1	A	131	ARG	NE-CZ-NH1	13.18	126.89	120.30
1	A	131	ARG	NE-CZ-NH2	-10.71	114.94	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	104	ARG	CG-CD-NE	-9.11	92.67	111.80
1	B	104	ARG	NE-CZ-NH2	-8.67	115.96	120.30
1	A	30	ASP	CB-CG-OD2	7.62	125.16	118.30
1	A	392	ASP	CB-CG-OD2	7.51	125.06	118.30
1	B	343	ASP	CB-CG-OD1	7.17	124.75	118.30
1	B	131	ARG	CD-NE-CZ	7.03	133.44	123.60
1	A	366	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	A	235	PHE	CB-CG-CD1	6.94	125.66	120.80
1	A	235	PHE	CB-CG-CD2	-6.89	115.97	120.80
1	B	80	ARG	NE-CZ-NH1	-6.63	116.99	120.30
1	B	156	ASP	CB-CG-OD1	6.27	123.94	118.30
1	B	155	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	B	81	ASP	CB-CG-OD2	6.23	123.91	118.30
1	A	146	ARG	NE-CZ-NH2	-6.19	117.20	120.30
1	A	230	ASP	CB-CG-OD2	6.10	123.79	118.30
1	B	283	LYS	CD-CE-NZ	6.03	125.56	111.70
1	B	104	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	A	363	GLU	OE1-CD-OE2	5.84	130.31	123.30
1	A	366	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	A	68	ASP	CB-CG-OD1	5.74	123.47	118.30
1	A	131	ARG	CD-NE-CZ	5.65	131.51	123.60
1	A	248	ASP	CB-CG-OD2	5.64	123.37	118.30
1	A	179	ASP	CB-CG-OD1	5.55	123.29	118.30
1	A	353	MSE	CG-SE-CE	5.51	111.02	98.90
1	B	392	ASP	CB-CG-OD2	5.45	123.20	118.30
1	B	298	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	A	81	ASP	CB-CG-OD2	5.38	123.14	118.30
1	B	238	ASP	CB-CG-OD1	5.35	123.11	118.30
1	B	280	ASP	CB-CG-OD2	5.24	123.02	118.30
1	A	104	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	A	281	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	A	219	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	B	248	ASP	CB-CG-OD2	5.14	122.93	118.30
1	B	296	ASP	CB-CG-OD2	5.12	122.91	118.30
1	A	30	ASP	OD1-CG-OD2	-5.10	113.61	123.30
1	B	230	ASP	CB-CG-OD2	5.04	122.84	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3226	0	3229	61	0
1	B	3235	0	3234	78	0
2	A	8	0	12	0	0
2	B	8	0	12	0	0
3	A	315	0	0	12	3
3	B	344	0	0	18	4
All	All	7136	0	6487	134	4

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 10.

All (134) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:353:MSE:CE	1:A:353:MSE:SE	1.23	1.42
1:B:353[B]:MSE:CE	1:B:353[B]:MSE:SE	1.22	1.42
1:B:1:MSE:SE	1:B:1:MSE:CE	2.22	1.38
1:B:244:GLY:HA2	1:B:254:MSE:CE	1.53	1.38
1:A:353:MSE:HE1	1:A:353:MSE:SE	1.80	1.12
1:B:353[B]:MSE:HE3	1:B:353[B]:MSE:SE	1.80	1.09
1:B:353[B]:MSE:SE	1:B:353[B]:MSE:HE1	1.80	1.06
1:A:353:MSE:HE2	1:A:353:MSE:SE	1.80	1.05
1:A:353:MSE:HE3	1:A:353:MSE:SE	1.80	1.05
1:B:353[B]:MSE:HE2	1:B:353[B]:MSE:SE	1.80	1.04
1:B:25:LYS:HE2	3:B:937:HOH:O	1.58	1.04
1:B:244:GLY:HA2	1:B:254:MSE:HE2	1.36	1.02
1:B:244:GLY:CA	1:B:254:MSE:CE	2.37	1.01
1:B:244:GLY:HA2	1:B:254:MSE:HE3	1.47	0.94
1:B:244:GLY:CA	1:B:254:MSE:HE2	1.97	0.91
1:B:353[B]:MSE:CE	1:B:353[B]:MSE:CG	2.52	0.87
1:A:294:GLU:O	1:A:298:ARG:HG3	1.75	0.85
1:B:201:GLU:HB3	3:B:881:HOH:O	1.78	0.82
1:B:107:THR:HG22	1:B:108:ASN:H	1.43	0.82
1:B:325:GLY:O	1:B:353[B]:MSE:HE1	1.81	0.79
1:B:117:ASP:O	1:B:131:ARG:HD3	1.81	0.79

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:236:HIS:CD2	1:B:382:GLN:HE22	2.03	0.76
1:A:308:GLU:HG2	3:A:976:HOH:O	1.87	0.74
1:B:110:LYS:NZ	3:B:1016:HOH:O	2.06	0.74
1:A:310:CYS:N	3:A:1009:HOH:O	2.21	0.73
1:A:236:HIS:HE1	1:A:273:GLU:OE1	1.72	0.73
1:B:125:ARG:HG2	3:B:712:HOH:O	1.90	0.71
1:B:244:GLY:N	1:B:254:MSE:HE2	2.06	0.71
1:A:349:LYS:HD2	1:A:378:CYS:O	1.89	0.71
1:A:104:ARG:NH2	1:A:115:GLU:OE1	2.24	0.70
1:A:353:MSE:CE	1:A:353:MSE:CG	2.70	0.69
1:A:117:ASP:O	1:A:131:ARG:HD3	1.94	0.68
1:A:331:LYS:NZ	3:A:1009:HOH:O	2.23	0.68
1:A:294:GLU:OE2	1:A:298:ARG:HD3	1.94	0.68
1:A:273:GLU:OE2	1:A:329:GLN:NE2	2.28	0.67
1:B:112[A]:MSE:HG2	1:B:138:ILE:HD13	1.77	0.67
1:A:349:LYS:NZ	3:A:994:HOH:O	2.28	0.66
1:B:244:GLY:HA2	1:B:254:MSE:HE1	1.71	0.65
1:A:236:HIS:CD2	1:A:382:GLN:HE22	2.14	0.65
1:B:305:VAL:CG2	1:B:327[B]:MSE:HE2	2.26	0.65
1:A:396[B]:MSE:SE	1:B:365:ASN:OD1	2.64	0.65
1:B:236:HIS:HD2	1:B:382:GLN:HE22	1.41	0.65
1:A:314:GLU:HG2	1:A:315:ASP:N	2.11	0.64
1:A:310:CYS:O	3:A:1009:HOH:O	2.15	0.64
1:B:305:VAL:HG22	1:B:327[B]:MSE:HE2	1.79	0.63
1:B:320:THR:HG23	1:B:353[B]:MSE:HG3	1.81	0.63
1:A:100:LYS:HD3	3:A:869:HOH:O	2.00	0.61
1:A:360:THR:CG2	1:A:363:GLU:HG3	2.30	0.61
1:B:249:VAL:HA	1:B:254:MSE:HE3	1.82	0.60
1:A:249:VAL:HG12	1:A:249:VAL:O	2.02	0.60
1:B:294:GLU:OE2	1:B:298:ARG:HD3	2.00	0.60
1:B:273:GLU:OE2	1:B:329:GLN:OE1	2.20	0.58
1:A:104:ARG:HH22	1:A:115:GLU:CD	2.05	0.58
1:A:360:THR:HG23	1:A:363:GLU:HG3	1.85	0.58
1:A:310:CYS:C	3:A:1009:HOH:O	2.41	0.58
1:A:365:ASN:OD1	1:B:396[B]:MSE:SE	2.71	0.58
1:B:317:LYS:HE3	1:B:347:TYR:OH	2.02	0.57
1:A:30:ASP:O	1:A:33:THR:HG22	2.04	0.57
1:B:283:LYS:HE3	3:B:932:HOH:O	2.02	0.57
1:A:207:LYS:NZ	3:A:875:HOH:O	2.34	0.57
1:B:317:LYS:HG3	1:B:347:TYR:CZ	2.40	0.57
1:B:121:VAL:O	1:B:122:ASN:HB2	2.05	0.57
1:A:308:GLU:O	1:A:309:TRP:HB2	2.05	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:163:GLU:HG2	3:B:987:HOH:O	2.04	0.56
1:A:294:GLU:O	1:A:298:ARG:CG	2.51	0.55
1:A:236:HIS:HD2	1:A:382:GLN:HE22	1.55	0.55
1:A:117:ASP:OD1	1:A:131:ARG:HD2	2.06	0.54
1:A:236:HIS:CE1	1:A:273:GLU:OE1	2.59	0.54
1:A:363:GLU:HB3	1:A:367:SER:OG	2.07	0.54
1:A:28:GLY:O	1:A:34:TYR:HA	2.08	0.54
1:B:244:GLY:CA	1:B:254:MSE:HE1	2.33	0.53
1:B:155:ARG:HD2	1:B:155:ARG:C	2.28	0.53
1:B:204:LEU:HG	1:B:208:GLY:HA2	1.92	0.52
1:A:110:LYS:HB3	1:A:111:PRO:HD3	1.92	0.51
1:B:226:ARG:HD2	1:B:228:ARG:O	2.11	0.51
1:B:118:LYS:NZ	3:B:944:HOH:O	2.22	0.51
1:B:327[B]:MSE:HE3	1:B:356:TYR:HB2	1.92	0.51
1:A:271:ARG:HD3	1:A:327[A]:MSE:SE	2.61	0.50
1:A:98:ALA:HB3	1:A:99:PRO:HD3	1.92	0.50
1:B:224:LYS:HG2	3:B:779:HOH:O	2.12	0.50
1:B:224:LYS:CG	3:B:779:HOH:O	2.59	0.49
1:B:317:LYS:HG3	1:B:347:TYR:CE2	2.46	0.49
1:B:294:GLU:O	1:B:298:ARG:HG3	2.14	0.48
1:B:117:ASP:OD1	1:B:131:ARG:HD2	2.13	0.48
1:B:254:MSE:HE1	1:B:276:MSE:HB3	1.95	0.48
1:A:100:LYS:HD2	1:A:119:MSE:HE3	1.95	0.48
1:B:212:LEU:O	1:B:216:LYS:HG3	2.14	0.48
1:A:90:ILE:N	1:A:91:PRO:CD	2.77	0.47
1:A:187:LYS:HE3	1:B:16:TYR:CZ	2.50	0.47
1:A:230:ASP:N	1:A:230:ASP:OD1	2.44	0.47
1:A:314:GLU:HB3	3:A:823:HOH:O	2.14	0.47
1:B:87:LYS:HE3	3:B:960:HOH:O	2.15	0.47
1:B:100:LYS:HE2	3:B:970:HOH:O	2.14	0.46
1:B:136:GLN:HG2	1:B:370:VAL:HG11	1.98	0.46
1:B:282:GLN:O	1:B:286:GLU:HG3	2.15	0.46
1:A:16:TYR:CE2	1:B:187:LYS:HE3	2.51	0.46
1:B:271:ARG:HD3	1:B:327[A]:MSE:SE	2.66	0.45
1:B:107:THR:HG22	1:B:108:ASN:N	2.21	0.45
1:A:128[A]:THR:HG22	1:A:333:PRO:O	2.17	0.45
1:B:305:VAL:HG21	1:B:327[B]:MSE:HE2	1.99	0.45
1:B:252:LYS:HB2	3:B:940:HOH:O	2.16	0.45
1:B:207:LYS:NZ	3:B:871:HOH:O	2.43	0.45
1:B:201:GLU:CB	3:B:881:HOH:O	2.49	0.45
1:A:98:ALA:N	1:A:99:PRO:CD	2.80	0.44
1:A:239:VAL:O	1:A:242:THR:HG23	2.17	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:117:ASP:O	1:B:131:ARG:CD	2.61	0.44
1:A:331:LYS:HA	3:A:899:HOH:O	2.17	0.44
1:B:252:LYS:HA	1:B:252:LYS:HD3	1.72	0.44
1:B:213:GLU:CD	3:B:802:HOH:O	2.54	0.44
1:A:368:ALA:HA	1:A:386:LYS:HE3	1.98	0.44
1:A:256:ASP:OD1	1:A:298:ARG:NH2	2.41	0.44
1:B:310:CYS:HA	1:B:315:ASP:HB3	1.99	0.43
1:B:381:ARG:NH1	3:B:1046:HOH:O	2.50	0.43
1:A:317:LYS:HG3	1:A:347:TYR:CZ	2.54	0.42
1:B:25:LYS:CE	3:B:937:HOH:O	2.39	0.42
1:B:386:LYS:HB2	1:B:387:PRO:HA	2.02	0.42
1:B:265:ALA:O	1:B:266:LYS:C	2.56	0.42
1:A:353:MSE:CE	1:A:353:MSE:CB	2.97	0.41
1:B:320:THR:CG2	1:B:351:ASN:HB2	2.50	0.41
1:A:329:GLN:HG3	1:A:356:TYR:CD2	2.55	0.41
1:B:356:TYR:CD1	1:B:356:TYR:C	2.94	0.41
1:A:360:THR:HG22	1:A:363:GLU:HG3	2.02	0.41
1:A:25:LYS:NZ	3:A:874:HOH:O	2.31	0.41
1:A:329:GLN:HG3	1:A:356:TYR:CE2	2.55	0.41
1:B:310:CYS:O	1:B:331:LYS:HE3	2.21	0.41
1:A:187:LYS:HE3	1:B:16:TYR:CE2	2.55	0.41
1:B:220:ASP:O	1:B:224:LYS:HG3	2.21	0.41
1:B:298:ARG:HB2	1:B:300:VAL:HG23	2.03	0.41
1:B:280:ASP:OD2	1:B:282:GLN:HB3	2.21	0.41
1:A:363:GLU:HB3	1:A:364:THR:H	1.76	0.40
1:B:201:GLU:CA	3:B:881:HOH:O	2.69	0.40
1:B:15:PHE:CD1	1:B:389[B]:MSE:HG3	2.56	0.40
1:A:204:LEU:HG	1:A:208:GLY:HA2	2.03	0.40
1:A:314:GLU:HG3	3:A:821:HOH:O	2.20	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:986:HOH:O	3:B:1025:HOH:O[1_455]	1.84	0.36
3:A:949:HOH:O	3:B:1024:HOH:O[1_455]	2.00	0.20
3:A:1016:HOH:O	3:B:797:HOH:O[2_554]	2.06	0.14
3:B:960:HOH:O	3:B:962:HOH:O[3_655]	2.15	0.05

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	416/413 (101%)	399 (96%)	16 (4%)	1 (0%)	56	44
1	B	417/413 (101%)	402 (96%)	14 (3%)	1 (0%)	56	44
All	All	833/826 (101%)	801 (96%)	30 (4%)	2 (0%)	56	44

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	249	VAL
1	B	193	PRO

5.3.2 Protein sidechains ⓘ

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	339/317 (107%)	327 (96%)	12 (4%)	48	34
1	B	340/317 (107%)	334 (98%)	6 (2%)	71	66
All	All	679/634 (107%)	661 (97%)	18 (3%)	60	47

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	HIS
1	A	32	PHE
1	A	48	GLN
1	A	125	ARG
1	A	193	PRO
1	A	229	GLU
1	A	276	MSE

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Mol	Chain	Res	Type
1	A	308	GLU
1	A	314	GLU
1	A	331	LYS
1	A	356	TYR
1	A	360	THR
1	B	112[A]	MSE
1	B	112[B]	MSE
1	B	119	MSE
1	B	125	ARG
1	B	193	PRO
1	B	356	TYR

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

Mol	Chain	Res	Type
1	A	236	HIS
1	B	236	HIS

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

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	A	701[A]	-	3,3,3	0.83	0	2,2,2	0.24	0
2	EDO	A	701[B]	-	3,3,3	0.58	0	2,2,2	0.24	0
2	EDO	B	702[A]	-	3,3,3	0.68	0	2,2,2	0.54	0
2	EDO	B	702[B]	-	3,3,3	0.43	0	2,2,2	0.34	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	A	701[A]	-	-	0/1/1/1	0/0/0/0
2	EDO	A	701[B]	-	-	0/1/1/1	0/0/0/0
2	EDO	B	702[A]	-	-	0/1/1/1	0/0/0/0
2	EDO	B	702[B]	-	-	0/1/1/1	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	413/413 (100%)	0.23	14 (3%) 43 44	29, 35, 48, 59	0
1	B	413/413 (100%)	0.25	14 (3%) 43 44	28, 35, 48, 58	0
All	All	826/826 (100%)	0.24	28 (3%) 42 44	28, 35, 48, 59	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	201	GLU	4.5
1	B	227	VAL	4.1
1	A	279	GLU	3.5
1	B	201	GLU	3.4
1	B	279	GLU	3.4
1	A	122	ASN	3.3
1	B	309	TRP	3.2
1	A	248	ASP	3.0
1	B	308	GLU	2.7
1	A	206	LEU	2.6
1	B	122	ASN	2.5
1	B	310	CYS	2.5
1	A	413	LYS	2.5
1	B	299	GLY	2.5
1	A	205	GLY	2.4
1	A	309	TRP	2.4
1	B	368	ALA	2.3
1	B	205	GLY	2.3
1	A	252	LYS	2.3
1	A	308	GLU	2.2
1	A	247	PHE	2.2
1	A	310	CYS	2.2
1	B	137	ALA	2.1
1	A	28	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	229	GLU	2.1
1	B	413	LYS	2.1
1	A	202	GLU	2.1
1	B	370	VAL	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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	EDO	B	702[B]	4/4	0.37	11.89	53,56,56,56	4
2	EDO	B	702[A]	4/4	0.37	11.39	33,37,38,41	4
2	EDO	A	701[B]	4/4	0.33	10.17	36,36,38,38	4
2	EDO	A	701[A]	4/4	0.33	7.19	29,33,34,39	4

6.5 Other polymers ⓘ

There are no such residues in this entry.