



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:55 PM UTC

PDB ID : 1KD0 / pdb_00001kd0
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 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

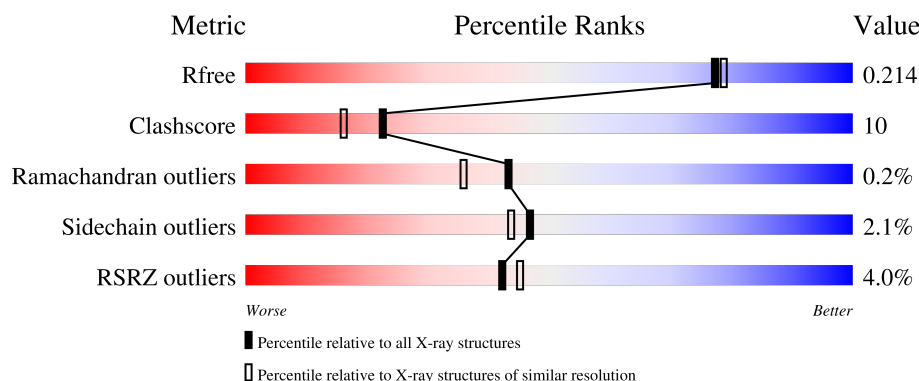
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (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 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 $\leq 5\%$. 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	413	5% 78% 19% .
1	B	413	3% 78% 20% .

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7136 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-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 (CCD ID: EDO) (formula: $C_2H_6O_2$).



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		

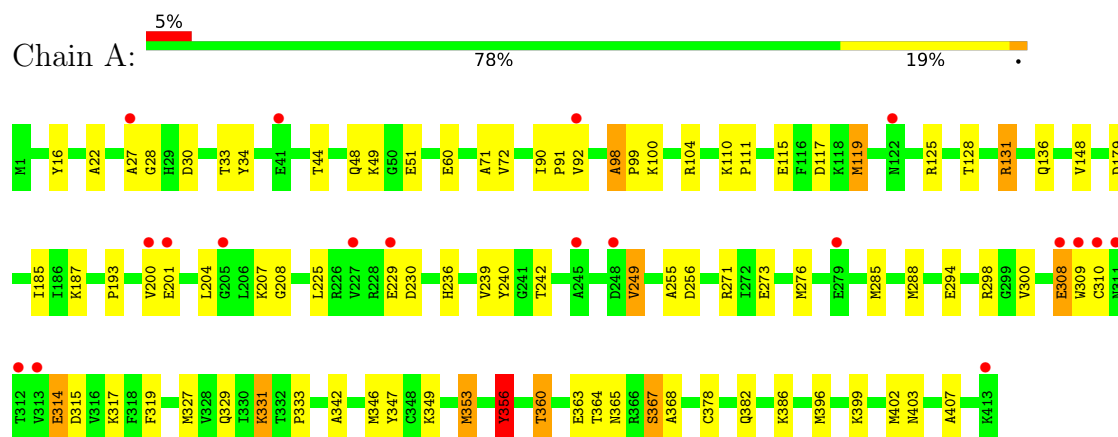
- Molecule 3 is water.

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

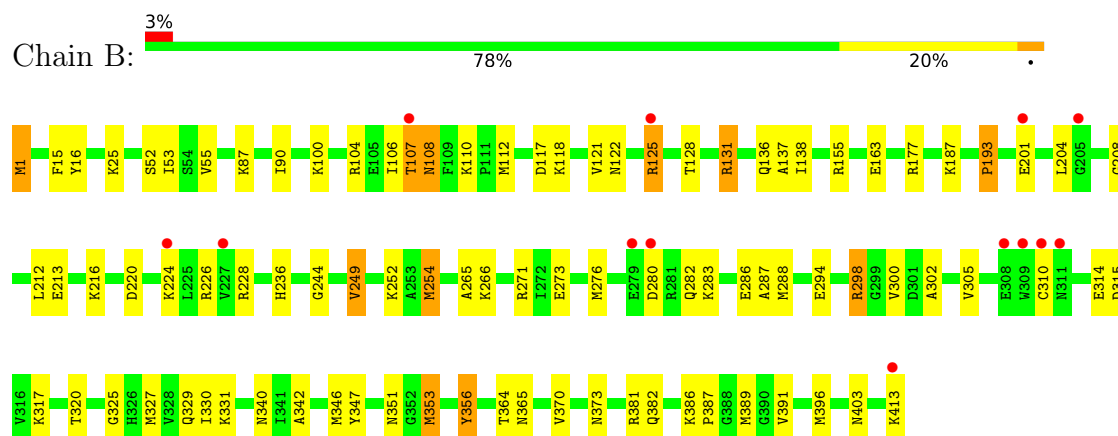
3 Residue-property plots [i](#)

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: beta-methylaspartase



- Molecule 1: beta-methylaspartase



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 57.74 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (57.74-1.90) 99.9 (57.74-1.90)	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 5.0	Depositor
R, R_{free}	0.175 , 0.222 (Not available) , 0.214	Depositor DCC
R_{free} test set	3228 reflections (5.05%)	wwPDB-VP
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 , 70.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	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.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: 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	1.56	28/3259 (0.9%)	1.26	8/4366 (0.2%)
1	B	1.59	23/3268 (0.7%)	1.31	11/4377 (0.3%)
All	All	1.58	51/6527 (0.8%)	1.28	19/8743 (0.2%)

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	353	MSE	SE-CE	-23.97	1.23	1.95
1	B	353[A]	MSE	SE-CE	-18.61	1.39	1.95
1	B	353[B]	MSE	SE-CE	-18.61	1.39	1.95
1	B	254	MSE	SE-CE	-11.09	1.62	1.95
1	B	107	THR	CA-C	10.31	1.59	1.53
1	B	1	MSE	SE-CE	8.90	2.22	1.95
1	A	98	ALA	CA-CB	-8.16	1.44	1.53
1	B	131	ARG	CD-NE	-7.85	1.35	1.46
1	B	346	MSE	SE-CE	-7.49	1.73	1.95
1	A	342	ALA	CA-CB	7.12	1.64	1.53
1	B	90	ILE	CA-CB	-7.10	1.50	1.54
1	A	131	ARG	CD-NE	-7.03	1.36	1.46
1	A	22	ALA	CA-CB	-6.83	1.42	1.53
1	B	53	ILE	CA-CB	6.77	1.63	1.54
1	A	276	MSE	SE-CE	-6.69	1.75	1.95
1	A	119	MSE	SE-CE	-6.51	1.75	1.95
1	A	185	ILE	C-O	-6.50	1.16	1.24
1	A	148	VAL	C-O	6.28	1.31	1.23
1	A	346	MSE	SE-CE	-6.22	1.76	1.95
1	B	125	ARG	CB-CG	6.20	1.71	1.52
1	A	60	GLU	C-O	-6.12	1.16	1.24
1	A	255	ALA	CA-CB	-6.09	1.43	1.53
1	B	403	ASN	C-O	-6.09	1.17	1.24
1	B	373	ASN	C-O	-6.07	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	391	VAL	N-CA	6.01	1.53	1.46
1	A	200	VAL	N-CA	-5.91	1.39	1.46
1	B	52	SER	N-CA	-5.89	1.38	1.45
1	A	356	TYR	C-O	-5.86	1.17	1.24
1	A	49	LYS	C-O	-5.86	1.16	1.23
1	A	71	ALA	CA-CB	5.80	1.64	1.54
1	B	287	ALA	CA-CB	-5.79	1.44	1.53
1	B	364	THR	CA-C	-5.59	1.45	1.52
1	A	319	PHE	C-O	-5.55	1.17	1.24
1	A	399	LYS	C-O	-5.55	1.17	1.24
1	A	407	ALA	CA-C	5.49	1.59	1.52
1	B	340	ASN	C-O	5.32	1.30	1.24
1	B	330	ILE	CA-CB	-5.31	1.47	1.53
1	B	55	VAL	C-O	5.24	1.29	1.24
1	B	107	THR	CA-CB	5.23	1.61	1.53
1	A	288	MSE	SE-CE	-5.22	1.79	1.95
1	B	128	THR	CA-CB	5.22	1.61	1.53
1	A	72	VAL	CA-CB	5.22	1.61	1.54
1	A	92	VAL	C-O	5.17	1.29	1.24
1	A	27	ALA	CA-CB	5.13	1.61	1.53
1	A	403	ASN	C-O	-5.10	1.18	1.24
1	A	179	ASP	C-O	-5.10	1.18	1.24
1	A	402	MSE	SE-CE	-5.07	1.80	1.95
1	A	367	SER	CA-C	5.05	1.59	1.52
1	A	51	GLU	C-O	5.05	1.30	1.23
1	B	342	ALA	CA-CB	5.02	1.61	1.53
1	B	137	ALA	CA-CB	5.00	1.61	1.53

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	131	ARG	NE-CZ-NH2	-9.66	110.51	119.20
1	B	104	ARG	CG-CD-NE	-8.79	92.67	112.00
1	B	131	ARG	NE-CZ-NH1	8.69	130.19	121.50
1	B	107	THR	CA-C-O	7.99	122.57	117.94
1	B	302	ALA	N-CA-C	-7.03	97.50	109.24
1	B	131	ARG	CD-NE-CZ	6.46	133.44	124.40
1	A	288	MSE	N-CA-C	-5.95	104.71	111.14
1	B	106	ILE	CA-C-N	5.92	129.43	123.04
1	B	106	ILE	C-N-CA	5.92	129.43	123.04
1	A	300	VAL	CB-CA-C	-5.72	105.05	111.23
1	B	177	ARG	N-CA-C	5.63	120.02	113.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	353	MSE	CG-SE-CE	5.50	111.02	98.92
1	A	131	ARG	NE-CZ-NH1	5.39	126.89	121.50
1	A	240	TYR	N-CA-CB	-5.39	103.92	111.62
1	B	288	MSE	N-CA-C	-5.29	105.59	111.36
1	A	225	LEU	N-CA-C	5.14	119.82	113.50
1	A	131	ARG	CD-NE-CZ	5.08	131.51	124.40
1	B	108	ASN	N-CA-C	-5.08	103.01	110.52
1	A	136	GLN	CB-CA-C	-5.01	103.01	110.88

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3226	0	3229	62	0
1	B	3235	0	3234	79	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	136	4

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 10.

All (136) 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:A:353:MSE:SE	1:A:353:MSE:CE	1.23	1.42
1:B:353[B]:MSE:SE	1:B:353[B]:MSE:CE	1.22	1.42
1:B:1:MSE:CE	1:B:1:MSE:SE	2.22	1.38
1:B:244:GLY:HA2	1:B:254:MSE:CE	1.53	1.38
1:A:353:MSE:SE	1:A:353:MSE:HE1	1.80	1.12
1:B:353[B]:MSE:SE	1:B:353[B]:MSE:HE3	1.80	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:353[B]:MSE:SE	1:B:353[B]:MSE:HE1	1.80	1.06
1:A:353:MSE:SE	1:A:353:MSE:HE2	1.80	1.05
1:A:353:MSE:SE	1:A:353:MSE:HE3	1.80	1.05
1:B:25:LYS:HE2	3:B:937:HOH:O	1.58	1.04
1:B:353[B]:MSE:SE	1:B:353[B]:MSE:HE2	1.80	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:B:110:LYS:NZ	3:B:1016:HOH:O	2.06	0.86
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:117:ASP:O	1:B:131:ARG:HD3	1.81	0.79
1:B:325:GLY:O	1:B:353[B]:MSE:HE1	1.81	0.79
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: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:A:349:LYS:HD2	1:A:378:CYS:O	1.89	0.71
1:B:244:GLY:N	1:B:254:MSE:HE2	2.06	0.71
1:A:104:ARG:NH2	1:A:115:GLU:OE1	2.24	0.70
1:B:118:LYS:NZ	3:B:944:HOH:O	2.22	0.69
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:B:413:LYS:NZ	3:B:791:HOH:O	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:ARG:HH22	1:A:115:GLU:CD	2.05	0.63
1:B:320:THR:HG23	1:B:353[B]:MSE:HG3	1.81	0.63
1:A:310:CYS:C	3:A:1009:HOH:O	2.41	0.62
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:O	1:A:249:VAL:HG12	2.02	0.60
1:B:294:GLU:OE2	1:B:298:ARG:HD3	2.00	0.60
1:B:155:ARG:HD2	1:B:155:ARG:C	2.28	0.58
1:B:273:GLU:OE2	1:B:329:GLN:OE1	2.20	0.58
1:A:360:THR:HG23	1:A:363:GLU:HG3	1.85	0.58
1:A:365:ASN:OD1	1:B:396[B]:MSE:SE	2.71	0.58
1:A:30:ASP:O	1:A:33:THR:HG22	2.04	0.57
1:B:317:LYS:HE3	1:B:347:TYR:OH	2.02	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:121:VAL:O	1:B:122:ASN:HB2	2.05	0.57
1:B:317:LYS:HG3	1:B:347:TYR:CZ	2.40	0.57
1:A:308:GLU:O	1:A:309:TRP:HB2	2.05	0.56
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: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: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:213:GLU:CD	3:B:802:HOH:O	2.54	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:MSE:HE1	1:B:276:MSE:HB3	1.95	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:OD1	1:A:230:ASP:N	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:265:ALA:O	1:B:266:LYS:C	2.56	0.46
1:B:356:TYR:CD1	1:B:356:TYR:C	2.94	0.46
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: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
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:HD3	1:B:252:LYS:HA	1.72	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:A:201:GLU:CD	3:A:961:HOH:O	2.63	0.42
1:B:314:GLU:H	1:B:314:GLU:CD	2.28	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:A:360:THR:HG22	1:A:363:GLU:HG3	2.02	0.41
1:A:285:MSE:SE	1:A:285:MSE:C	3.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:ASP:OD2	1:B:282:GLN:HB3	2.21	0.41
1:B:298:ARG:HB2	1:B:300:VAL:HG23	2.03	0.41
1:A:363:GLU:HB3	1:A:364:THR:H	1.76	0.40
1:A:204:LEU:HG	1:A:208:GLY:HA2	2.03	0.40
1:B:15:PHE:CD1	1:B:389[B]:MSE:HG3	2.56	0.40
1:B:201:GLU:CA	3:B:881:HOH:O	2.69	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	Interatomic distance (Å)	Clash overlap (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 [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	416/413 (101%)	399 (96%)	16 (4%)	1 (0%)	43	36
1	B	417/413 (101%)	402 (96%)	14 (3%)	1 (0%)	43	36
All	All	833/826 (101%)	801 (96%)	30 (4%)	2 (0%)	43	36

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%)	329 (97%)	10 (3%)	37	31
1	B	340/317 (107%)	336 (99%)	4 (1%)	63	63
All	All	679/634 (107%)	665 (98%)	14 (2%)	47	44

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	THR
1	A	48	GLN
1	A	125	ARG
1	A	193	PRO
1	A	229	GLU
1	A	308	GLU
1	A	314	GLU
1	A	331	LYS
1	A	356	TYR
1	A	360	THR
1	B	193	PRO
1	B	249	VAL
1	B	298	ARG
1	B	356	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	236	HIS
1	B	20	GLN
1	B	45	GLN
1	B	124	ASN
1	B	236	HIS
1	B	311	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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 oligosaccharides 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	0.70	0	2,2,2	0.25	0
2	EDO	A	701[B]	-	3,3,3	0.43	0	2,2,2	0.26	0
2	EDO	B	702[B]	-	3,3,3	0.31	0	2,2,2	0.34	0
2	EDO	B	702[A]	-	3,3,3	0.54	0	2,2,2	0.48	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]	-	-	1/1/1/1	-
2	EDO	A	701[B]	-	-	1/1/1/1	-
2	EDO	B	702[B]	-	-	1/1/1/1	-
2	EDO	B	702[A]	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701[B]	EDO	O1-C1-C2-O2
2	B	702[B]	EDO	O1-C1-C2-O2
2	A	701[A]	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 ⓘ

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	396/413 (95%)	0.66	19 (4%) 35 38	17, 35, 48, 59	1 (0%)
1	B	396/413 (95%)	0.57	13 (3%) 49 52	23, 35, 48, 58	1 (0%)
All	All	792/826 (95%)	0.62	32 (4%) 42 45	17, 35, 48, 59	2 (0%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	309	TRP	4.1
1	B	310	CYS	4.1
1	A	309	TRP	4.0
1	B	227	VAL	3.4
1	A	308	GLU	3.2
1	B	308	GLU	3.2
1	A	201	GLU	3.1
1	A	279	GLU	3.1
1	A	310	CYS	3.0
1	A	227	VAL	2.9
1	A	313	VAL	2.8
1	A	413	LYS	2.7
1	B	205	GLY	2.6
1	B	279	GLU	2.5
1	B	201	GLU	2.5
1	B	107	THR	2.5
1	B	311	ASN	2.4
1	A	200	VAL	2.4
1	A	248	ASP	2.3
1	A	229	GLU	2.3
1	A	41	GLU	2.3
1	B	280	ASP	2.3
1	B	125	ARG	2.2
1	A	122	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	312	THR	2.2
1	B	224	LYS	2.1
1	A	245	ALA	2.1
1	A	92	VAL	2.1
1	B	413	LYS	2.1
1	A	311	ASN	2.1
1	A	27	ALA	2.1
1	A	205	GLY	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	EDO	B	702[A]	4/4	0.93	0.12	33,37,38,41	4
2	EDO	B	702[B]	4/4	0.93	0.12	53,56,56,56	4
2	EDO	A	701[A]	4/4	0.94	0.13	29,33,34,39	4
2	EDO	A	701[B]	4/4	0.94	0.13	36,36,38,38	4

6.5 Other polymers [i](#)

There are no such residues in this entry.