



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:27 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 X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) 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

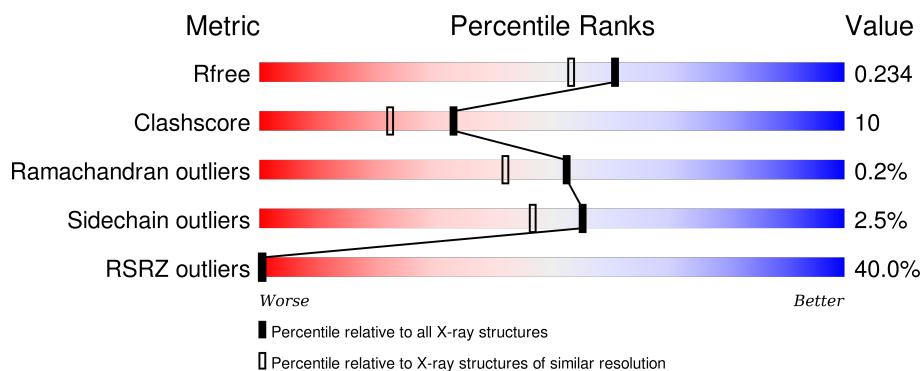
# 1 Overall quality at a glance

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))
$R_{free}$	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (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  $\geq 3$ , 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  $\leq 5\%$ . 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	<div> <div>40%</div> <div> <div></div> <div>81%</div> <div>16%</div> <div>•</div> </div> </div>
1	B	413	<div> <div>37%</div> <div> <div></div> <div>80%</div> <div>18%</div> <div>•</div> </div> </div>

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
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 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:

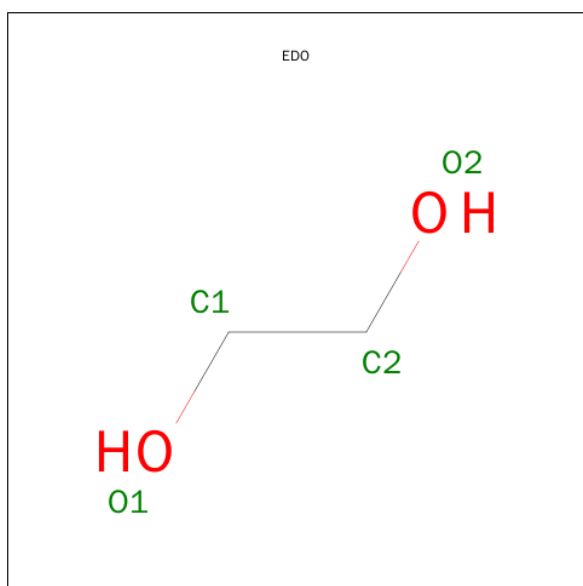
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q05514
A	112	MSE	MET	MODIFIED RESIDUE	UNP Q05514
A	119	MSE	MET	MODIFIED RESIDUE	UNP Q05514
A	150	MSE	MET	MODIFIED RESIDUE	UNP Q05514
A	184	MSE	MET	MODIFIED RESIDUE	UNP Q05514
A	254	MSE	MET	MODIFIED RESIDUE	UNP Q05514
A	276	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 (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

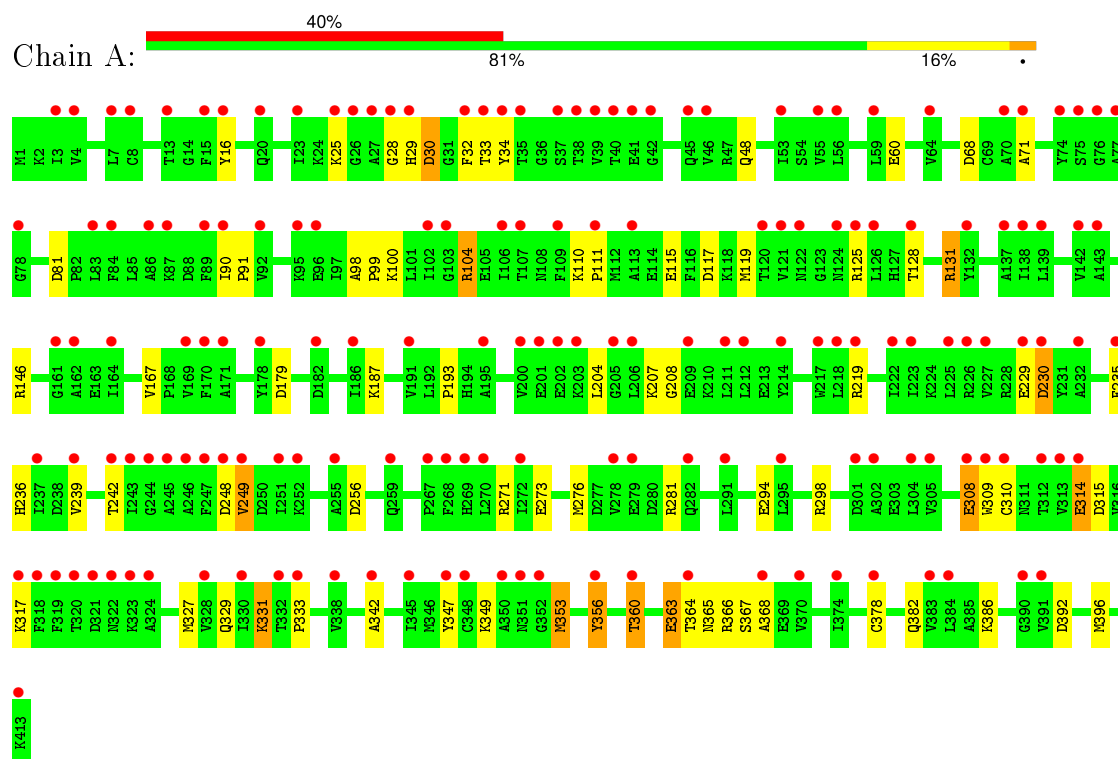
- Molecule 3 is water.

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

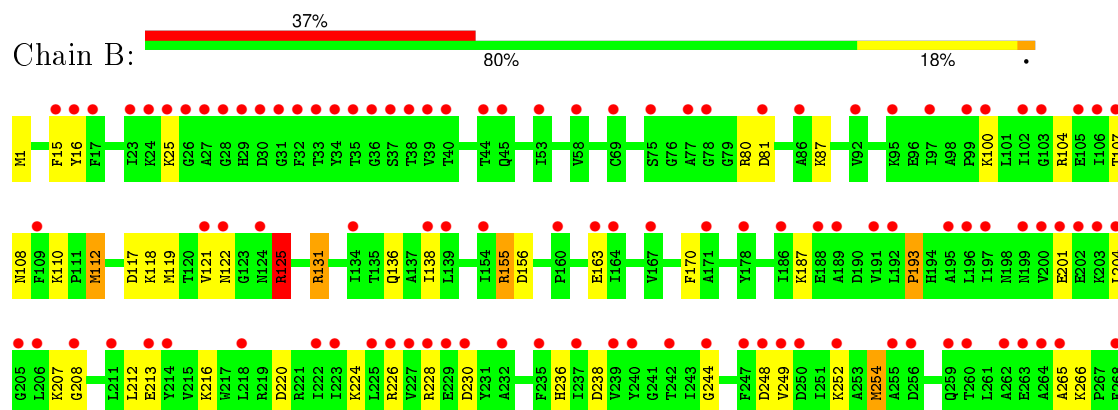
### 3 Residue-property plots [i](#)

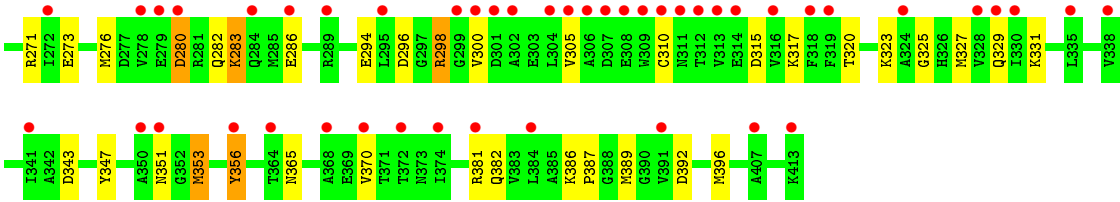
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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



- Molecule 1: beta-methylaspartase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.71 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, $R_{free}$	0.175 , 0.222 0.185 , 0.234	Depositor DCC
$R_{free}$ test set	3228 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	19.2	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 74.1	EDS
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	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 <sup>2</sup> )	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.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: 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 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	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

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 (134) 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: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	Interatomic distance (Å)	Clash overlap (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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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	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

### 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%)	52	42
1	B	417/413 (101%)	402 (96%)	14 (3%)	1 (0%)	52	42
All	All	833/826 (101%)	801 (96%)	30 (4%)	2 (0%)	52	42

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%)	43	31
1	B	340/317 (107%)	334 (98%)	6 (2%)	66	61
All	All	679/634 (107%)	661 (97%)	18 (3%)	55	43

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

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Mol	Chain	Res	Type
1	A	193	PRO
1	A	229	GLU
1	A	276	MSE
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 [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](#)

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	0.75	0	2,2,2	0.28	0
2	EDO	A	701[B]	-	3,3,3	0.49	0	2,2,2	0.30	0
2	EDO	B	702[A]	-	3,3,3	0.60	0	2,2,2	0.49	0
2	EDO	B	702[B]	-	3,3,3	0.36	0	2,2,2	0.39	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.

No monomer is involved in short contacts.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	396/413 (95%)	1.99	166 (41%) 0 0	29, 35, 48, 59	0
1	B	396/413 (95%)	1.92	151 (38%) 0 0	28, 35, 48, 58	0
All	All	792/826 (95%)	1.95	317 (40%) 0 0	28, 35, 48, 59	0

All (317) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	310	CYS	9.6
1	A	310	CYS	9.3
1	B	122	ASN	8.4
1	B	308	GLU	8.1
1	A	201	GLU	7.9
1	B	309	TRP	7.1
1	B	227	VAL	7.1
1	A	248	ASP	6.9
1	B	229	GLU	6.9
1	A	347	TYR	6.9
1	A	28	GLY	6.6
1	A	27	ALA	6.5
1	A	247	PHE	6.0
1	A	35	THR	5.9
1	B	279	GLU	5.9
1	A	37	SER	5.7
1	B	107	THR	5.7
1	B	37	SER	5.7
1	A	308	GLU	5.7
1	B	201	GLU	5.5
1	A	202	GLU	5.4
1	A	122	ASN	5.4
1	B	248	ASP	5.3
1	A	230	ASP	5.3

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Mol	Chain	Res	Type	RSRZ
1	A	252	LYS	5.1
1	B	29	HIS	5.1
1	B	413	LYS	5.1
1	B	247	PHE	5.0
1	B	230	ASP	4.9
1	A	413	LYS	4.8
1	B	28	GLY	4.7
1	A	309	TRP	4.7
1	B	31	GLY	4.6
1	A	124	ASN	4.6
1	B	121	VAL	4.6
1	B	316	VAL	4.4
1	A	351	ASN	4.3
1	B	312	THR	4.3
1	A	243	ILE	4.3
1	A	161	GLY	4.3
1	B	206	LEU	4.2
1	B	25	LYS	4.2
1	A	55	VAL	4.2
1	A	34	TYR	4.1
1	A	182	ASP	4.1
1	B	307	ASP	4.1
1	B	24	LYS	4.1
1	A	178	TYR	4.0
1	A	244	GLY	4.0
1	B	105	GLU	4.0
1	B	30	ASP	3.9
1	A	384	LEU	3.9
1	B	223	ILE	3.9
1	B	202	GLU	3.9
1	A	200	VAL	3.9
1	B	86	ALA	3.9
1	B	299	GLY	3.9
1	B	263	GLU	3.9
1	A	304	LEU	3.8
1	B	199	ASN	3.8
1	B	313	VAL	3.8
1	B	33	THR	3.8
1	B	278	VAL	3.7
1	A	186	ILE	3.7
1	B	222	ILE	3.7
1	A	279	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	38	THR	3.7
1	B	272	ILE	3.7
1	A	92	VAL	3.7
1	A	314	GLU	3.6
1	A	225	LEU	3.6
1	A	319	PHE	3.6
1	A	169	VAL	3.6
1	A	278	VAL	3.6
1	A	211	LEU	3.5
1	A	33	THR	3.5
1	B	249	VAL	3.5
1	A	322	ASN	3.5
1	A	324	ALA	3.5
1	B	200	VAL	3.4
1	A	272	ILE	3.4
1	B	23	ILE	3.4
1	B	226	ARG	3.4
1	A	212	LEU	3.4
1	A	128[A]	THR	3.4
1	A	249	VAL	3.4
1	B	34	TYR	3.4
1	B	32	PHE	3.3
1	A	323	LYS	3.3
1	B	242	THR	3.3
1	A	218	LEU	3.3
1	B	39	VAL	3.3
1	B	235	PHE	3.3
1	B	225	LEU	3.3
1	A	143	ALA	3.3
1	A	245	ALA	3.3
1	A	102	ILE	3.3
1	A	350	ALA	3.2
1	B	44	THR	3.2
1	A	227	VAL	3.2
1	A	242	THR	3.2
1	B	35	THR	3.2
1	A	223	ILE	3.2
1	B	341	ILE	3.2
1	A	312	THR	3.2
1	B	228	ARG	3.2
1	A	205	GLY	3.1
1	B	99	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	370	VAL	3.1
1	A	107	THR	3.1
1	A	229	GLU	3.1
1	B	268	PHE	3.1
1	B	103	GLY	3.1
1	B	109	PHE	3.1
1	B	302	ALA	3.1
1	B	124	ASN	3.1
1	B	319	PHE	3.0
1	A	29	HIS	3.0
1	B	264	ALA	3.0
1	A	86	ALA	3.0
1	B	27	ALA	3.0
1	A	301	ASP	3.0
1	B	384	LEU	3.0
1	B	95	LYS	3.0
1	B	214	TYR	3.0
1	B	305	VAL	3.0
1	B	244	GLY	3.0
1	B	301[A]	ASP	3.0
1	B	295	LEU	2.9
1	B	300	VAL	2.9
1	A	214	TYR	2.9
1	B	311	ASN	2.9
1	A	64	VAL	2.9
1	A	121	VAL	2.9
1	B	45	GLN	2.9
1	A	125	ARG	2.9
1	A	171	ALA	2.9
1	B	350	ALA	2.9
1	A	84	PHE	2.8
1	B	318	PHE	2.8
1	A	75	SER	2.8
1	A	270	LEU	2.8
1	B	26	GLY	2.8
1	A	246	ALA	2.8
1	A	217	TRP	2.8
1	A	318	PHE	2.8
1	A	206	LEU	2.8
1	B	306	ALA	2.8
1	B	328	VAL	2.8
1	B	205	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	222	ILE	2.8
1	A	42	GLY	2.8
1	A	162	ALA	2.7
1	B	192	LEU	2.7
1	A	96	GLU	2.7
1	B	97	ILE	2.7
1	B	239	VAL	2.7
1	A	70	ALA	2.7
1	B	171	ALA	2.7
1	A	345	ILE	2.7
1	A	313	VAL	2.7
1	B	324	ALA	2.7
1	B	36	GLY	2.7
1	A	295	LEU	2.7
1	B	314	GLU	2.7
1	B	255	ALA	2.7
1	A	268	PHE	2.7
1	A	106	ILE	2.7
1	A	237	ILE	2.7
1	A	16	TYR	2.7
1	A	89	PHE	2.7
1	A	39	VAL	2.6
1	A	74	TYR	2.6
1	A	126	LEU	2.6
1	A	282	GLN	2.6
1	A	352	GLY	2.6
1	B	284	GLN	2.6
1	B	139	LEU	2.6
1	A	364	THR	2.6
1	A	25	LYS	2.6
1	A	95	LYS	2.6
1	B	289	ARG	2.6
1	B	78	GLY	2.6
1	A	45	GLN	2.6
1	A	109	PHE	2.6
1	A	195	ALA	2.6
1	A	330	ILE	2.6
1	A	103	GLY	2.5
1	A	32	PHE	2.5
1	A	56	LEU	2.5
1	B	407	ALA	2.5
1	A	139	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	53	ILE	2.5
1	B	364	THR	2.5
1	B	265	ALA	2.5
1	A	332	THR	2.5
1	B	372	THR	2.5
1	B	250	ASP	2.5
1	A	255	ALA	2.5
1	B	368	ALA	2.5
1	B	188	GLU	2.5
1	B	58	VAL	2.5
1	A	164	ILE	2.5
1	A	137	ALA	2.5
1	B	178	TYR	2.5
1	A	219	ARG	2.4
1	B	204	LEU	2.4
1	B	17	PHE	2.4
1	A	3	ILE	2.4
1	A	23	ILE	2.4
1	A	76	GLY	2.4
1	A	251	ILE	2.4
1	A	348	CYS	2.4
1	A	120	THR	2.4
1	A	191	VAL	2.4
1	B	167	VAL	2.4
1	A	77	ALA	2.4
1	A	138	ILE	2.4
1	A	226	ARG	2.4
1	A	374	ILE	2.4
1	B	374	ILE	2.4
1	A	20	GLN	2.4
1	B	102	ILE	2.3
1	B	164	ILE	2.3
1	A	267	PRO	2.3
1	A	83	LEU	2.3
1	B	77	ALA	2.3
1	A	38	THR	2.3
1	A	142	VAL	2.3
1	B	256	ASP	2.3
1	B	134	ILE	2.3
1	B	330	ILE	2.3
1	B	351	ASN	2.3
1	A	13	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	321	ASP	2.3
1	B	280	ASP	2.3
1	A	78	GLY	2.3
1	A	305	VAL	2.3
1	B	92	VAL	2.3
1	A	390	GLY	2.3
1	A	26	GLY	2.3
1	A	90	ILE	2.3
1	B	208	GLY	2.3
1	A	232	ALA	2.3
1	A	8	CYS	2.2
1	A	338	VAL	2.2
1	B	335	LEU	2.2
1	A	391	VAL	2.2
1	B	338	VAL	2.2
1	A	235	PHE	2.2
1	A	87	LYS	2.2
1	B	53	ILE	2.2
1	B	197	ILE	2.2
1	B	160	PRO	2.2
1	B	213	GLU	2.2
1	B	240	TYR	2.2
1	B	356	TYR	2.2
1	B	203	LYS	2.2
1	B	391	VAL	2.2
1	A	259	GLN	2.2
1	A	356	TYR	2.2
1	B	286	GLU	2.2
1	A	46	VAL	2.2
1	A	239	VAL	2.2
1	A	342	ALA	2.2
1	A	111	PRO	2.2
1	A	378	CYS	2.2
1	B	100	LYS	2.2
1	B	106	ILE	2.2
1	A	132	TYR	2.2
1	A	40	THR	2.2
1	A	370	VAL	2.2
1	A	71	ALA	2.1
1	B	81	ASP	2.1
1	A	170	PHE	2.1
1	B	138	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	381	ARG	2.1
1	A	291	LEU	2.1
1	A	368	ALA	2.1
1	B	211	LEU	2.1
1	B	218	LEU	2.1
1	B	304	LEU	2.1
1	B	259	GLN	2.1
1	A	113	ALA	2.1
1	B	252	LYS	2.1
1	A	360	THR	2.1
1	A	15	PHE	2.1
1	B	189	ALA	2.1
1	B	232	ALA	2.1
1	A	209	GLU	2.1
1	A	383	VAL	2.1
1	B	40	THR	2.1
1	B	163	GLU	2.0
1	B	15	PHE	2.0
1	B	262	ALA	2.0
1	A	7	LEU	2.0
1	A	59	LEU	2.0
1	B	16	TYR	2.0
1	B	75	SER	2.0
1	B	69	CYS	2.0
1	A	4	VAL	2.0
1	A	320	THR	2.0
1	A	328	VAL	2.0
1	A	269	HIS	2.0
1	B	260	THR	2.0
1	A	333	PRO	2.0
1	A	302	ALA	2.0
1	B	154	ILE	2.0
1	A	41	GLU	2.0
1	B	196	LEU	2.0
1	B	191	VAL	2.0
1	A	203	LYS	2.0
1	A	317	LYS	2.0
1	B	195	ALA	2.0
1	B	329	GLN	2.0
1	B	186	ILE	2.0
1	B	237	ILE	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 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	EDO	A	701[B]	4/4	0.62	0.35	16.49	36,36,38,38	4
2	EDO	B	702[A]	4/4	0.57	0.46	14.32	33,37,38,41	4
2	EDO	B	702[B]	4/4	0.57	0.46	8.74	53,56,56,56	4
2	EDO	A	701[A]	4/4	0.62	0.35	6.20	29,33,34,39	4

## 6.5 Other polymers [i](#)

There are no such residues in this entry.