



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2020 – 01:42 PM BST

PDB ID : 1MAT
Title : STRUCTURE OF THE COBALT-DEPENDENT METHIONINE AMINOPEPTIDASE FROM ESCHERICHIA COLI: A NEW TYPE OF PROTEOLYTIC ENZYME
Authors : Roderick, S.L.; Matthews, B.W.
Deposited on : 1992-12-02
Resolution : 2.40 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.13
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)	:	2.13

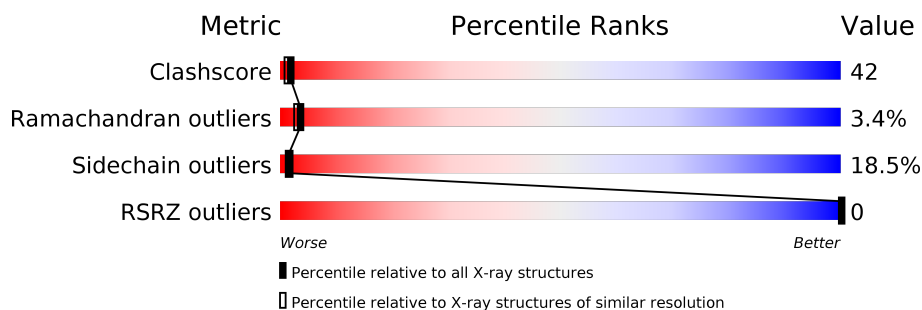
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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))
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 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	264	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1982 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 METHIONYL AMINOPEPTIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	S	0	0	0
			1965	1240	330	380	15			

- Molecule 2 is COBALT (II) ION (three-letter code: CO) (formula: Co).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Co	0	0
			2	2		

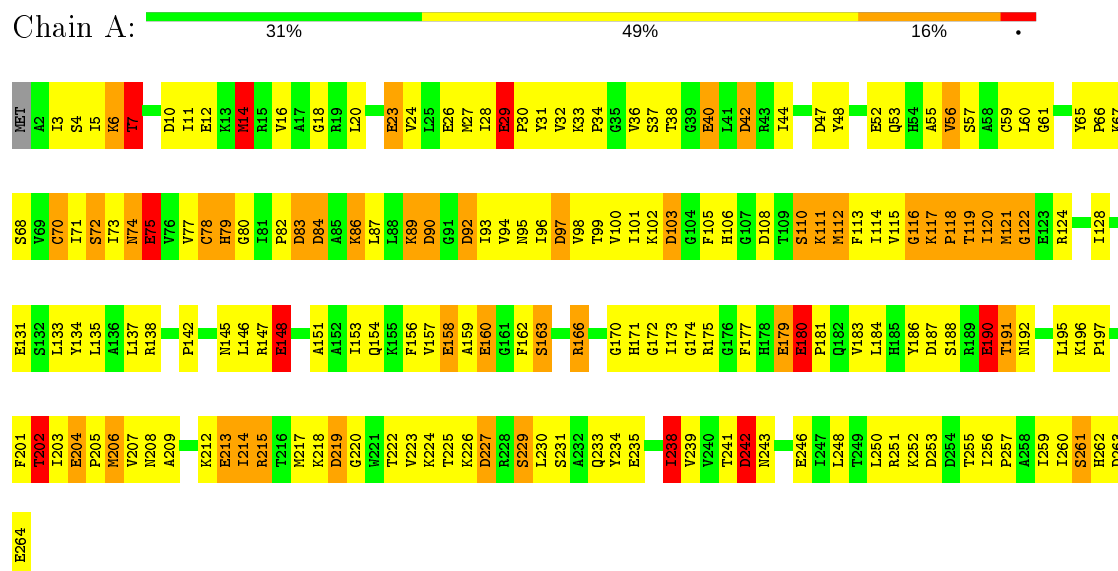
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	15	Total	O	0	0
			15	15		

3 Residue-property plots

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: METHIONYL AMINOPEPTIDASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	39.00 Å 61.70 Å 54.50 Å 90.00° 107.30° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.40 52.03 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.40) 85.7 (52.03-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 2.39 Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.182 , (Not available) 0.174 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	36.1	Xtriage
Anisotropy	0.811	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 114.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	1982	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.67% of the height of the origin peak. No significant pseudotranslation is detected.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CO

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	1.27	18/2000 (0.9%)	1.71	48/2714 (1.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	0

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	179	GLU	CD-OE2	8.46	1.34	1.25
1	A	40	GLU	CD-OE2	7.73	1.34	1.25
1	A	190	GLU	CD-OE2	7.40	1.33	1.25
1	A	29	GLU	CD-OE2	7.32	1.33	1.25
1	A	158	GLU	CD-OE2	7.07	1.33	1.25
1	A	23	GLU	CD-OE2	6.96	1.33	1.25
1	A	75	GLU	CD-OE2	6.77	1.33	1.25
1	A	204	GLU	CD-OE2	6.63	1.32	1.25
1	A	246	GLU	CD-OE2	6.39	1.32	1.25
1	A	148	GLU	CD-OE2	6.30	1.32	1.25
1	A	26	GLU	CD-OE2	5.92	1.32	1.25
1	A	160	GLU	CD-OE2	5.87	1.32	1.25
1	A	213	GLU	CD-OE2	5.86	1.32	1.25
1	A	52	GLU	CD-OE2	5.72	1.31	1.25
1	A	131	GLU	CD-OE1	5.70	1.31	1.25
1	A	75	GLU	CD-OE1	-5.45	1.19	1.25
1	A	180	GLU	CD-OE2	5.27	1.31	1.25
1	A	23	GLU	CD-OE1	-5.04	1.20	1.25

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	97	ASP	CB-CG-OD1	10.67	127.91	118.30
1	A	31	TYR	CB-CG-CD1	9.98	126.99	121.00
1	A	31	TYR	CB-CG-CD2	-9.75	115.15	121.00
1	A	253	ASP	CB-CG-OD2	-9.07	110.14	118.30
1	A	78	CYS	CB-CA-C	-8.86	92.69	110.40
1	A	103	ASP	CB-CG-OD2	-8.64	110.53	118.30
1	A	242	ASP	CB-CG-OD1	-8.35	110.79	118.30
1	A	187	ASP	CB-CG-OD2	-8.19	110.93	118.30
1	A	42	ASP	CB-CG-OD1	8.17	125.66	118.30
1	A	251	ARG	NE-CZ-NH1	8.16	124.38	120.30
1	A	187	ASP	CB-CG-OD1	8.16	125.64	118.30
1	A	42	ASP	CB-CG-OD2	-8.04	111.06	118.30
1	A	103	ASP	CB-CG-OD1	7.89	125.40	118.30
1	A	97	ASP	CB-CG-OD2	-7.89	111.20	118.30
1	A	263	ASP	CB-CG-OD2	-7.61	111.45	118.30
1	A	253	ASP	CB-CG-OD1	7.37	124.94	118.30
1	A	92	ASP	CB-CG-OD2	-7.06	111.95	118.30
1	A	90	ASP	CB-CG-OD1	6.90	124.51	118.30
1	A	83	ASP	CB-CG-OD2	-6.85	112.14	118.30
1	A	10	ASP	CB-CG-OD2	-6.84	112.15	118.30
1	A	86	LYS	N-CA-CB	6.69	122.65	110.60
1	A	40	GLU	N-CA-CB	6.58	122.44	110.60
1	A	14	MET	CG-SD-CE	-6.27	90.17	100.20
1	A	108	ASP	CB-CG-OD2	-6.21	112.71	118.30
1	A	219	ASP	CB-CG-OD2	-6.17	112.75	118.30
1	A	255	THR	CA-CB-CG2	-6.13	103.82	112.40
1	A	202	THR	N-CA-CB	-6.01	98.89	110.30
1	A	191	THR	CA-CB-CG2	-5.89	104.16	112.40
1	A	195	LEU	CB-CA-C	5.88	121.38	110.20
1	A	90	ASP	CB-CG-OD2	-5.85	113.04	118.30
1	A	229	SER	N-CA-CB	5.82	119.23	110.50
1	A	83	ASP	CB-CG-OD1	5.80	123.52	118.30
1	A	84	ASP	CB-CG-OD2	-5.78	113.09	118.30
1	A	84	ASP	CB-CG-OD1	5.75	123.47	118.30
1	A	119	THR	C-N-CA	-5.54	107.84	121.70
1	A	263	ASP	CB-CG-OD1	5.52	123.27	118.30
1	A	242	ASP	CB-CG-OD2	5.52	123.27	118.30
1	A	47	ASP	CB-CG-OD1	5.51	123.26	118.30
1	A	14	MET	CA-CB-CG	-5.41	104.10	113.30
1	A	7	THR	CA-CB-OG1	5.41	120.35	109.00
1	A	163	SER	N-CA-CB	5.35	118.53	110.50
1	A	120	ILE	CB-CA-C	5.27	122.14	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	179	GLU	N-CA-CB	5.23	120.01	110.60
1	A	97	ASP	N-CA-CB	5.14	119.85	110.60
1	A	7	THR	CA-CB-CG2	5.12	119.57	112.40
1	A	264	GLU	N-CA-CB	5.09	119.77	110.60
1	A	234	TYR	CB-CG-CD1	-5.01	117.99	121.00
1	A	238	ILE	CB-CA-C	-5.01	101.58	111.60

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	7	THR	CB

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	1965	0	1875	161	0
2	A	2	0	0	0	0
3	A	15	0	0	3	0
All	All	1982	0	1875	161	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 42.

All (161) 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:119:THR:HG22	1:A:122:GLY:H	1.11	1.15
1:A:92:ASP:HB2	1:A:115:VAL:HG11	1.50	0.91
1:A:92:ASP:HB2	1:A:115:VAL:CG1	2.02	0.89
1:A:202:THR:HG23	1:A:204:GLU:HG3	1.54	0.88
1:A:166:ARG:HB3	1:A:186:TYR:CE2	2.16	0.80
1:A:119:THR:CG2	1:A:122:GLY:H	1.92	0.79
1:A:124:ARG:HH21	1:A:160:GLU:HB3	1.45	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:ASP:H	1:A:115:VAL:HG12	1.48	0.78
1:A:55:ALA:HB2	1:A:102:LYS:HD2	1.66	0.78
1:A:56:VAL:HG22	1:A:57:SER:H	1.49	0.77
1:A:124:ARG:NH2	1:A:160:GLU:HB3	1.99	0.77
1:A:121:MET:HE1	1:A:124:ARG:NH1	2.00	0.76
1:A:119:THR:HG22	1:A:122:GLY:N	1.96	0.76
1:A:7:THR:O	1:A:11:ILE:HG13	1.86	0.75
1:A:214:ILE:HG22	1:A:224:LYS:O	1.87	0.74
1:A:59:CYS:O	1:A:65:TYR:HB3	1.88	0.74
1:A:151:ALA:O	1:A:154:GLN:HB3	1.89	0.73
1:A:208:ASN:OD1	1:A:231:SER:HB2	1.87	0.73
1:A:111:LYS:HG2	1:A:112:MET:N	2.03	0.71
1:A:217:MET:HG2	1:A:222:THR:O	1.91	0.69
1:A:134:TYR:O	1:A:137:LEU:HB2	1.93	0.68
1:A:202:THR:HG23	1:A:204:GLU:CG	2.24	0.68
1:A:42:ASP:OD2	1:A:67:LYS:HD2	1.94	0.68
1:A:166:ARG:HD3	1:A:186:TYR:CD2	2.29	0.68
1:A:3:ILE:HG12	1:A:180:GLU:HB3	1.77	0.67
1:A:48:TYR:CE1	1:A:53:GLN:HG3	2.30	0.66
1:A:4:SER:C	1:A:5:ILE:HD12	2.16	0.66
1:A:202:THR:HG21	1:A:204:GLU:OE2	1.96	0.66
1:A:171:HIS:H	1:A:202:THR:HG22	1.62	0.64
1:A:56:VAL:HG22	1:A:57:SER:N	2.13	0.62
1:A:153:ILE:O	1:A:157:VAL:HG23	1.98	0.62
1:A:214:ILE:O	1:A:215:ARG:HD3	2.00	0.62
1:A:202:THR:CG2	1:A:204:GLU:HG3	2.27	0.61
1:A:243:ASN:ND2	1:A:261:SER:OG	2.33	0.61
1:A:37:SER:OG	1:A:40:GLU:N	2.27	0.61
1:A:34:PRO:HD3	1:A:115:VAL:CG2	2.31	0.60
1:A:28:ILE:O	1:A:28:ILE:HG13	2.02	0.60
1:A:48:TYR:HE1	1:A:53:GLN:NE2	1.99	0.60
1:A:156:PHE:O	1:A:159:ALA:HB3	2.01	0.59
1:A:12:GLU:O	1:A:16:VAL:HG23	2.02	0.59
1:A:33:LYS:O	1:A:36:VAL:HG22	2.03	0.59
1:A:97:ASP:HA	1:A:110:SER:HB2	1.85	0.58
1:A:6:LYS:N	1:A:6:LYS:HD2	2.17	0.58
1:A:92:ASP:HB2	1:A:115:VAL:HG12	1.83	0.58
1:A:213:GLU:C	1:A:226:LYS:HB2	2.24	0.58
1:A:205:PRO:O	1:A:233:GLN:HA	2.04	0.57
1:A:227:ASP:OD1	1:A:227:ASP:N	2.35	0.57
1:A:20:LEU:O	1:A:23:GLU:HB2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:LYS:NZ	1:A:213:GLU:OE2	2.38	0.57
1:A:256:ILE:HG12	1:A:257:PRO:HD2	1.87	0.57
1:A:34:PRO:HD3	1:A:115:VAL:HG23	1.87	0.56
1:A:121:MET:HE1	1:A:124:ARG:HH11	1.67	0.56
1:A:61:GLY:N	1:A:65:TYR:O	2.29	0.56
1:A:90:ASP:HA	1:A:115:VAL:HG13	1.87	0.56
1:A:218:LYS:O	1:A:220:GLY:N	2.37	0.56
1:A:227:ASP:HB2	1:A:229:SER:H	1.70	0.56
1:A:67:LYS:HG3	1:A:82:PRO:HG2	1.88	0.55
1:A:93:ILE:O	1:A:93:ILE:HG13	2.06	0.55
1:A:243:ASN:N	1:A:243:ASN:OD1	2.38	0.55
1:A:204:GLU:HG2	1:A:235:GLU:HG3	1.87	0.55
1:A:172:GLY:HA2	1:A:201:PHE:HB3	1.90	0.54
1:A:201:PHE:CE2	1:A:238:ILE:HD11	2.43	0.54
1:A:89:LYS:O	1:A:90:ASP:OD1	2.26	0.54
1:A:92:ASP:N	1:A:115:VAL:HG12	2.19	0.53
1:A:133:LEU:O	1:A:137:LEU:HG	2.09	0.53
1:A:27:MET:O	1:A:30:PRO:HD2	2.09	0.53
1:A:70:CYS:C	1:A:71:ILE:HG13	2.29	0.53
1:A:135:LEU:C	1:A:135:LEU:HD23	2.30	0.53
1:A:171:HIS:CD2	1:A:202:THR:HG21	2.43	0.52
1:A:6:LYS:HG2	1:A:14:MET:CE	2.39	0.52
1:A:37:SER:HA	1:A:86:LYS:O	2.10	0.52
1:A:48:TYR:HE1	1:A:53:GLN:HE21	1.57	0.52
1:A:93:ILE:HD11	1:A:230:LEU:HD22	1.92	0.52
1:A:92:ASP:H	1:A:115:VAL:CG1	2.18	0.52
1:A:11:ILE:HD13	1:A:239:VAL:HG21	1.91	0.52
1:A:157:VAL:O	1:A:162:PHE:HB2	2.09	0.52
1:A:142:PRO:HG3	1:A:241:THR:O	2.09	0.52
1:A:28:ILE:C	1:A:30:PRO:HD2	2.30	0.52
1:A:48:TYR:CE1	1:A:53:GLN:NE2	2.78	0.51
1:A:96:ILE:HD12	1:A:113:PHE:CE1	2.46	0.51
1:A:121:MET:CE	1:A:124:ARG:HH11	2.23	0.50
1:A:24:VAL:HG23	1:A:53:GLN:HE22	1.76	0.50
1:A:100:VAL:O	1:A:106:HIS:HA	2.11	0.50
1:A:36:VAL:O	1:A:87:LEU:HA	2.12	0.50
1:A:37:SER:OG	1:A:37:SER:O	2.29	0.49
1:A:184:LEU:HD23	1:A:186:TYR:CE1	2.48	0.49
1:A:111:LYS:CG	1:A:112:MET:N	2.75	0.49
1:A:213:GLU:O	1:A:226:LYS:HB2	2.13	0.49
1:A:238:ILE:O	1:A:238:ILE:HG12	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:VAL:HG22	1:A:116:GLY:N	2.27	0.48
1:A:145:ASN:OD1	1:A:147:ARG:HB3	2.14	0.48
1:A:218:LYS:C	1:A:220:GLY:H	2.18	0.47
1:A:207:VAL:O	1:A:231:SER:HA	2.14	0.47
1:A:137:LEU:HA	1:A:137:LEU:HD23	1.53	0.47
1:A:162:PHE:HD1	1:A:209:ALA:O	1.98	0.47
1:A:188:SER:OG	1:A:190:GLU:HB2	2.15	0.47
1:A:121:MET:CE	1:A:124:ARG:NH1	2.75	0.47
1:A:196:LYS:HB3	1:A:197:PRO:HD2	1.96	0.47
1:A:135:LEU:O	1:A:135:LEU:HD23	2.14	0.47
1:A:18:GLY:HA3	1:A:248:LEU:O	2.14	0.47
1:A:83:ASP:OD1	1:A:84:ASP:N	2.48	0.47
1:A:94:VAL:HG22	1:A:95:ASN:N	2.30	0.46
1:A:121:MET:HE1	1:A:162:PHE:CZ	2.51	0.46
1:A:75:GLU:H	1:A:75:GLU:HG3	1.24	0.46
1:A:79:HIS:CD2	1:A:79:HIS:N	2.81	0.46
1:A:124:ARG:O	1:A:128:ILE:HG12	2.17	0.45
1:A:203:ILE:HG22	1:A:205:PRO:HD3	1.98	0.45
1:A:29:GLU:N	1:A:30:PRO:HD2	2.31	0.45
1:A:33:LYS:HB2	1:A:34:PRO:HD2	1.98	0.45
1:A:98:VAL:HG12	1:A:99:THR:N	2.30	0.45
1:A:242:ASP:N	1:A:242:ASP:OD1	2.42	0.45
1:A:78:CYS:O	1:A:80:GLY:N	2.50	0.45
1:A:173:ILE:HG12	1:A:174:GLY:N	2.32	0.45
1:A:77:VAL:HG21	1:A:214:ILE:CG2	2.47	0.45
1:A:73:ILE:CG2	1:A:74:ASN:ND2	2.80	0.45
1:A:158:GLU:HA	1:A:162:PHE:O	2.17	0.45
1:A:213:GLU:O	1:A:226:LYS:N	2.43	0.45
1:A:98:VAL:CG1	1:A:99:THR:N	2.80	0.45
1:A:180:GLU:HB2	3:A:510:HOH:O	2.16	0.45
1:A:119:THR:CG2	1:A:120:ILE:N	2.79	0.44
1:A:94:VAL:CG2	1:A:95:ASN:N	2.80	0.44
1:A:243:ASN:O	1:A:262:HIS:HB2	2.16	0.44
1:A:48:TYR:HE1	1:A:53:GLN:HG3	1.79	0.44
1:A:4:SER:O	1:A:5:ILE:HD12	2.17	0.44
1:A:171:HIS:H	1:A:202:THR:CG2	2.30	0.44
1:A:214:ILE:C	1:A:215:ARG:HD3	2.38	0.44
1:A:65:TYR:HA	1:A:66:PRO:HD3	1.81	0.44
1:A:72:SER:HA	3:A:513:HOH:O	2.18	0.44
1:A:146:LEU:HD21	1:A:183:VAL:HG22	2.00	0.43
1:A:6:LYS:HG2	1:A:14:MET:HE1	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:GLU:N	1:A:30:PRO:CD	2.81	0.43
1:A:105:PHE:CE1	1:A:175:ARG:HG3	2.54	0.43
1:A:78:CYS:HB2	1:A:223:VAL:CG2	2.49	0.42
1:A:6:LYS:CD	1:A:6:LYS:N	2.81	0.42
1:A:32:VAL:O	1:A:32:VAL:HG12	2.18	0.42
1:A:172:GLY:HA2	1:A:201:PHE:CB	2.50	0.42
1:A:218:LYS:C	1:A:220:GLY:N	2.74	0.42
1:A:206:MET:HB2	3:A:515:HOH:O	2.18	0.41
1:A:252:LYS:HD3	1:A:252:LYS:HA	1.83	0.41
1:A:78:CYS:HB2	1:A:223:VAL:HB	2.02	0.41
1:A:78:CYS:HB3	1:A:79:HIS:CG	2.55	0.41
1:A:138:ARG:HD2	1:A:138:ARG:HH11	1.61	0.41
1:A:166:ARG:CB	1:A:186:TYR:CE2	2.98	0.41
1:A:75:GLU:HB3	1:A:229:SER:O	2.20	0.41
1:A:148:GLU:HG3	1:A:148:GLU:H	1.65	0.41
1:A:89:LYS:CG	1:A:90:ASP:N	2.78	0.41
1:A:208:ASN:HA	1:A:230:LEU:O	2.20	0.41
1:A:71:ILE:CG2	1:A:94:VAL:HG21	2.51	0.41
1:A:117:LYS:HA	1:A:118:PRO:HD2	1.74	0.41
1:A:204:GLU:HB3	1:A:233:GLN:NE2	2.36	0.41
1:A:89:LYS:CG	1:A:90:ASP:H	2.25	0.41
1:A:170:GLY:CA	1:A:202:THR:HG22	2.51	0.41
1:A:217:MET:CG	1:A:222:THR:HG22	2.51	0.41
1:A:204:GLU:HG2	1:A:235:GLU:CG	2.49	0.41
1:A:5:ILE:CD1	1:A:5:ILE:N	2.84	0.41
1:A:217:MET:HG2	1:A:222:THR:HG22	2.04	0.40
1:A:38:THR:OG1	1:A:82:PRO:HA	2.21	0.40
1:A:171:HIS:HA	1:A:181:PRO:O	2.21	0.40
1:A:171:HIS:N	1:A:202:THR:HG22	2.33	0.40
1:A:119:THR:HG22	1:A:121:MET:N	2.36	0.40
1:A:44:ILE:HD13	1:A:44:ILE:HG21	1.79	0.40

There are no symmetry-related clashes.

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	261/264 (99%)	230 (88%)	22 (8%)	9 (3%)	3	3

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	79	HIS
1	A	89	LYS
1	A	192	ASN
1	A	219	ASP
1	A	117	LYS
1	A	118	PRO
1	A	116	GLY
1	A	74	ASN
1	A	122	GLY

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	200/228 (88%)	163 (82%)	37 (18%)	1	2

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LYS
1	A	7	THR
1	A	14	MET
1	A	29	GLU
1	A	56	VAL
1	A	60	LEU
1	A	68	SER
1	A	70	CYS
1	A	72	SER
1	A	75	GLU

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Mol	Chain	Res	Type
1	A	101	ILE
1	A	103	ASP
1	A	110	SER
1	A	111	LYS
1	A	112	MET
1	A	114	ILE
1	A	121	MET
1	A	148	GLU
1	A	163	SER
1	A	166	ARG
1	A	177	PHE
1	A	179	GLU
1	A	180	GLU
1	A	190	GLU
1	A	191	THR
1	A	202	THR
1	A	206	MET
1	A	214	ILE
1	A	215	ARG
1	A	225	THR
1	A	227	ASP
1	A	238	ILE
1	A	242	ASP
1	A	250	LEU
1	A	259	ILE
1	A	260	ILE
1	A	261	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
1	A	53	GLN
1	A	79	HIS
1	A	233	GLN
1	A	243	ASN

5.3.3 RNA ⓘ

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 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	263/264 (99%)	-0.70	0 100 100	13, 41, 72, 98	0

There are no RSRZ outliers to report.

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, 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(Å ²)	Q<0.9
2	CO	A	402	1/1	0.98	0.07	28,28,28,28	0
2	CO	A	401	1/1	1.00	0.09	27,27,27,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.