



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:45 AM UTC

PDB ID : 1MAT / pdb_00001mat
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 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
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

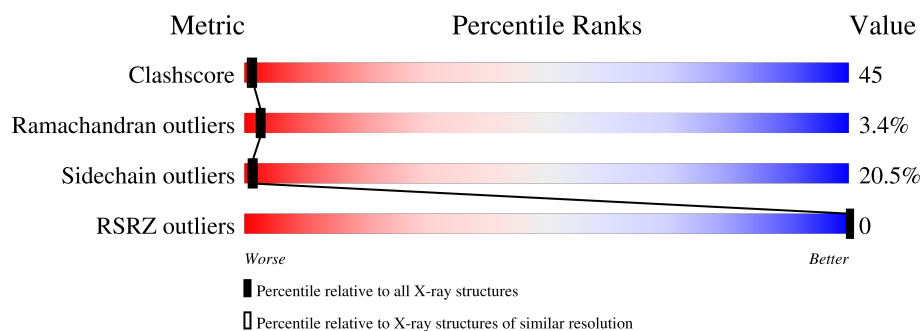
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 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	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 (CCD ID: CO) (formula: Co).

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

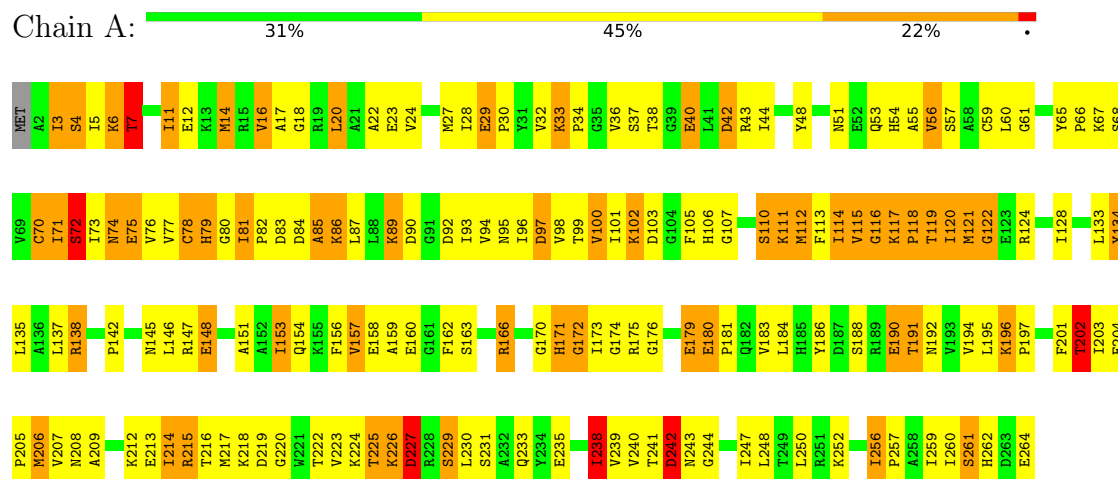
- Molecule 3 is water.

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	39.00Å 61.70Å 54.50Å 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) 85.8 (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 2.39Å)	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)	0.29 , 131.7	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	1.59	13/2000 (0.7%)	2.02	61/2714 (2.2%)

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 (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	20	LEU	CA-C	-7.12	1.43	1.52
1	A	120	ILE	N-CA	-5.74	1.39	1.46
1	A	40	GLU	CA-C	-5.56	1.45	1.52
1	A	176	GLY	CA-C	5.47	1.56	1.52
1	A	196	LYS	C-N	-5.26	1.27	1.33
1	A	227	ASP	CG-OD1	5.14	1.35	1.25
1	A	3	ILE	CA-CB	-5.11	1.48	1.54
1	A	171	HIS	ND1-CE1	5.11	1.37	1.32
1	A	119	THR	C-N	-5.10	1.27	1.33
1	A	179	GLU	CD-OE2	5.05	1.34	1.25
1	A	7	THR	CA-CB	5.04	1.59	1.53
1	A	33	LYS	CA-C	-5.04	1.46	1.52
1	A	76	VAL	CA-CB	-5.01	1.48	1.54

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	119	THR	CA-C-N	-10.69	107.84	120.88
1	A	119	THR	C-N-CA	-10.69	107.84	120.88
1	A	157	VAL	N-CA-C	9.01	120.89	110.62
1	A	40	GLU	N-CA-CB	8.38	122.44	110.12
1	A	172	GLY	N-CA-C	-8.37	103.13	112.33
1	A	78	CYS	CB-CA-C	-7.90	92.69	111.65
1	A	202	THR	N-CA-CB	-7.77	98.89	110.85
1	A	120	ILE	CB-CA-C	7.73	122.14	111.94
1	A	86	LYS	N-CA-CB	7.43	122.65	110.17
1	A	7	THR	CA-CB-OG1	7.17	120.35	109.60
1	A	195	LEU	CB-CA-C	6.57	121.38	109.62
1	A	115	VAL	N-CA-C	6.57	118.05	108.53
1	A	119	THR	N-CA-C	-6.51	100.33	110.42
1	A	229	SER	N-CA-CB	6.46	119.23	110.38
1	A	226	LYS	CA-C-N	6.43	128.90	120.28
1	A	226	LYS	C-N-CA	6.43	128.90	120.28
1	A	76	VAL	N-CA-CB	6.34	118.11	110.31
1	A	191	THR	N-CA-CB	6.31	119.34	109.69
1	A	54	HIS	CA-CB-CG	6.29	120.09	113.80
1	A	40	GLU	O-C-N	6.28	128.77	122.12
1	A	226	LYS	O-C-N	6.25	128.50	122.07
1	A	242	ASP	CA-CB-CG	-6.24	106.36	112.60
1	A	20	LEU	O-C-N	6.16	129.17	122.15
1	A	4	SER	CA-C-N	-5.94	115.29	122.90
1	A	4	SER	C-N-CA	-5.94	115.29	122.90
1	A	97	ASP	N-CA-CB	5.79	119.85	110.42
1	A	153	ILE	CA-C-O	5.72	126.90	120.95
1	A	17	ALA	N-CA-C	-5.72	105.04	111.28
1	A	3	ILE	N-CA-CB	5.70	117.33	110.95
1	A	43	ARG	N-CA-CB	5.69	118.22	109.91
1	A	81	ILE	N-CA-C	5.69	114.14	107.77
1	A	196	LYS	N-CA-CB	5.68	119.26	111.25
1	A	42	ASP	CB-CA-C	5.67	120.20	110.79
1	A	71	ILE	O-C-N	5.58	127.99	122.97
1	A	85	ALA	CA-C-N	-5.57	114.78	122.30
1	A	85	ALA	C-N-CA	-5.57	114.78	122.30
1	A	22	ALA	CA-C-N	5.55	127.66	120.44
1	A	22	ALA	C-N-CA	5.55	127.66	120.44
1	A	138	ARG	CD-NE-CZ	-5.53	116.65	124.40
1	A	179	GLU	N-CA-CB	5.49	120.01	110.07
1	A	134	TYR	CA-C-O	5.48	126.36	120.55
1	A	264	GLU	N-CA-CB	5.45	119.77	110.50
1	A	7	THR	N-CA-C	-5.36	102.25	110.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	114	ILE	CA-C-N	-5.35	116.19	123.10
1	A	114	ILE	C-N-CA	-5.35	116.19	123.10
1	A	7	THR	CA-CB-CG2	5.33	119.57	110.50
1	A	51	ASN	CA-C-O	5.24	126.39	120.89
1	A	107	GLY	N-CA-C	-5.24	100.77	113.18
1	A	225	THR	CA-C-N	-5.23	113.64	120.44
1	A	225	THR	C-N-CA	-5.23	113.64	120.44
1	A	72	SER	N-CA-C	5.20	117.86	107.62
1	A	54	HIS	N-CA-C	-5.16	106.93	113.23
1	A	256	ILE	CA-C-N	-5.16	114.92	120.03
1	A	256	ILE	C-N-CA	-5.16	114.92	120.03
1	A	238	ILE	CB-CA-C	-5.16	101.58	110.30
1	A	16	VAL	N-CA-C	5.11	115.78	110.82
1	A	194	VAL	N-CA-CB	5.11	117.19	111.21
1	A	240	VAL	N-CA-CB	5.10	116.08	110.53
1	A	3	ILE	N-CA-C	5.08	116.06	108.54
1	A	244	GLY	CA-C-N	-5.03	114.32	122.36
1	A	244	GLY	C-N-CA	-5.03	114.32	122.36

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1965	0	1875	171	0
2	A	2	0	0	0	0
3	A	15	0	0	3	0
All	All	1982	0	1875	171	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 45.

All (171) 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:216:THR:C	1:A:217:MET:HE2	2.00	0.87
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:121:MET:HE1	1:A:124:ARG:NH1	1.97	0.79
1:A:124:ARG:HH21	1:A:160:GLU:HB3	1.45	0.79
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: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:59:CYS:O	1:A:65:TYR:HB3	1.88	0.74
1:A:214:ILE:HG22	1:A:224:LYS:O	1.87	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:4:SER:C	1:A:5:ILE:HD12	2.16	0.71
1:A:217:MET:HG2	1:A:222:THR:O	1.91	0.69
1:A:42:ASP:OD2	1:A:67:LYS:HD2	1.94	0.68
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: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: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:217:MET:HE2	1:A:217:MET:N	2.13	0.63
1:A:121:MET:HE1	1:A:124:ARG:HH11	1.62	0.63
1:A:213:GLU:C	1:A:226:LYS:HB2	2.24	0.62
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:TYR:HE1	1:A:53:GLN:NE2	1.99	0.60
1:A:28:ILE:O	1:A:28:ILE:HG13	2.02	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:70:CYS:C	1:A:71:ILE:HG13	2.29	0.58
1:A:135:LEU:C	1:A:135:LEU:HD23	2.30	0.57
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
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:28:ILE:C	1:A:30:PRO:HD2	2.30	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:206:MET:HE2	1:A:233:GLN:NE2	2.22	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:93:ILE:HG13	1:A:93:ILE:O	2.06	0.54
1:A:89:LYS:O	1:A:90:ASP:OD1	2.26	0.54
1:A:201:PHE:CE2	1:A:238:ILE:HD11	2.43	0.54
1:A:92:ASP:N	1:A:115:VAL:HG12	2.19	0.53
1:A:27:MET:O	1:A:30:PRO:HD2	2.09	0.53
1:A:133:LEU:O	1:A:137:LEU:HG	2.09	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:218:LYS:C	1:A:220:GLY:H	2.18	0.52
1:A:48:TYR:HE1	1:A:53:GLN:HE21	1.57	0.52
1:A:92:ASP:H	1:A:115:VAL:CG1	2.18	0.52
1:A:93:ILE:HD11	1:A:230:LEU:HD22	1.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:PRO:HG3	1:A:241:THR:O	2.09	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: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:121:MET:CE	1:A:124:ARG:HH11	2.23	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:214:ILE:C	1:A:215:ARG:HD3	2.38	0.49
1:A:238:ILE:O	1:A:238:ILE:HG12	2.13	0.48
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: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:HD23	1:A:135:LEU:O	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:218:LYS:C	1:A:220:GLY:N	2.74	0.46
1:A:94:VAL:HG22	1:A:95:ASN:N	2.30	0.46
1:A:75:GLU:H	1:A:75:GLU:HG3	1.24	0.46
1:A:79:HIS:N	1:A:79:HIS:CD2	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:OD1	1:A:242:ASP:N	2.42	0.45
1:A:78:CYS:O	1:A:80:GLY:N	2.50	0.45
1:A:77:VAL:HG21	1:A:214:ILE:CG2	2.47	0.45
1:A:173:ILE:HG12	1:A:174:GLY:N	2.32	0.45
1:A:73:ILE:CG2	1:A:74:ASN:ND2	2.80	0.45
1:A:98:VAL:CG1	1:A:99:THR:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:GLU:HB2	3:A:510:HOH:O	2.16	0.45
1:A:94:VAL:CG2	1:A:95:ASN:N	2.80	0.44
1:A:119:THR:CG2	1:A:120:ILE:N	2.79	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:65:TYR:HA	1:A:66:PRO:HD3	1.81	0.44
1:A:171:HIS:H	1:A:202:THR:CG2	2.30	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	1.99	0.43
1:A:121:MET:HE1	1:A:162:PHE:CZ	2.54	0.43
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:78:CYS:C	1:A:80:GLY:N	2.76	0.42
1:A:27:MET:HE3	1:A:27:MET:HB3	1.95	0.42
1:A:6:LYS:N	1:A:6:LYS:CD	2.81	0.42
1:A:32:VAL:HG12	1:A:32:VAL:O	2.18	0.42
1:A:172:GLY:HA2	1:A:201:PHE:CB	2.50	0.42
1:A:48:TYR:C	1:A:48:TYR:CD1	2.98	0.42
1:A:94:VAL:C	1:A:112:MET:HE3	2.45	0.41
1:A:206:MET:HB2	3:A:515:HOH:O	2.18	0.41
1:A:252:LYS:HA	1:A:252:LYS:HD3	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:75:GLU:HB3	1:A:229:SER:O	2.20	0.41
1:A:138:ARG:HH11	1:A:138:ARG:HD2	1.61	0.41
1:A:166:ARG:CB	1:A:186:TYR:CE2	2.98	0.41
1:A:148:GLU:H	1:A:148:GLU:HG3	1.65	0.41
1:A:71:ILE:CG2	1:A:94:VAL:HG21	2.51	0.41
1:A:208:ASN:HA	1:A:230:LEU:O	2.20	0.41
1:A:89:LYS:CG	1:A:90:ASP:H	2.25	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:145:ASN:C	1:A:147:ARG:N	2.78	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:5:ILE:N	1:A:5:ILE:CD1	2.84	0.41
1:A:78:CYS:C	1:A:80:GLY:H	2.29	0.41
1:A:83:ASP:C	1:A:85:ALA:H	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:LYS:CG	1:A:90:ASP:N	2.78	0.41
1:A:204:GLU:HG2	1:A:235:GLU:CG	2.49	0.41
1:A:38:THR:OG1	1:A:82:PRO:HA	2.21	0.40
1:A:217:MET:HG2	1:A:222:THR:HG22	2.04	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:44:ILE:HD13	1:A:44:ILE:HG21	1.79	0.40
1:A:119:THR:HG22	1:A:121:MET:N	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	261/264 (99%)	230 (88%)	22 (8%)	9 (3%)	3 2

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%)	159 (80%)	41 (20%)	1 1

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LYS
1	A	7	THR
1	A	11	ILE
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
1	A	81	ILE
1	A	100	VAL
1	A	101	ILE
1	A	102	LYS
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	179	GLU
1	A	180	GLU
1	A	190	GLU
1	A	191	THR
1	A	202	THR
1	A	206	MET

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Mol	Chain	Res	Type
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	247	ILE
1	A	250	LEU
1	A	259	ILE
1	A	260	ILE
1	A	261	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	HIS
1	A	182	GLN
1	A	233	GLN
1	A	243	ASN

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 oligosaccharides 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

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 [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%)	-0.35	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 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(Å ²)	Q<0.9
2	CO	A	401	1/1	0.99	0.01	27,27,27,27	0
2	CO	A	402	1/1	0.99	0.02	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.