



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2026 – 10:40 PM UTC

PDB ID : 4NJR / pdb_00004njr
Title : Structural and kinetic bases for the metal preference of the M18 aminopeptidase from *Pseudomonas aeruginosa*
Authors : Nguyen, D.D.; Pandian, R.; Kim, D.Y.; Ha, S.C.; Yun, K.H.; Kim, K.S.; Kim, J.H.; Kim, K.K.
Deposited on : 2013-11-11
Resolution : 2.30 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

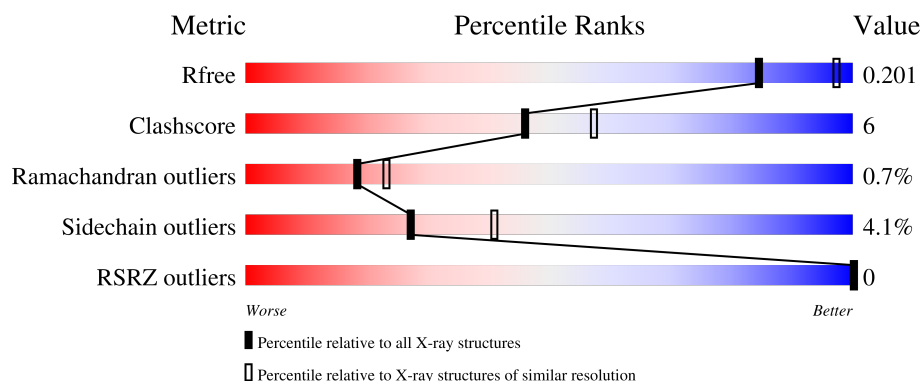
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	429	 84% 13% ...
1	B	429	 83% 12% ...
1	C	429	 84% 12% ..
1	D	429	 86% 11% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13955 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.

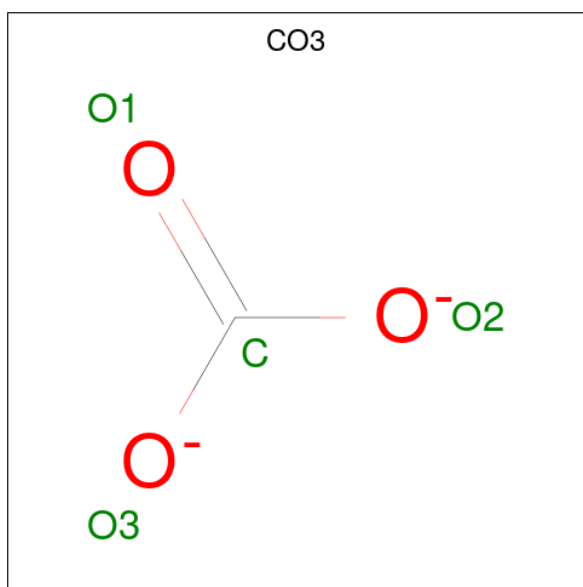
- Molecule 1 is a protein called Probable M18 family aminopeptidase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	425	Total	C	N	O	S	0	9	0
			3265	2043	598	614	10			
1	B	425	Total	C	N	O	S	0	9	0
			3260	2040	596	614	10			
1	C	424	Total	C	N	O	S	0	9	0
			3257	2037	597	613	10			
1	D	425	Total	C	N	O	S	0	9	0
			3265	2043	598	614	10			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		
2	C	2	Total	Zn	0	0
			2	2		
2	D	2	Total	Zn	0	0
			2	2		

- Molecule 3 is CARBONATE ION (CCD ID: CO3) (formula: CO₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	1	3		
3	B	1	Total	C	O	0	0
			4	1	3		
3	C	1	Total	C	O	0	0
			4	1	3		
3	D	1	Total	C	O	0	0
			4	1	3		

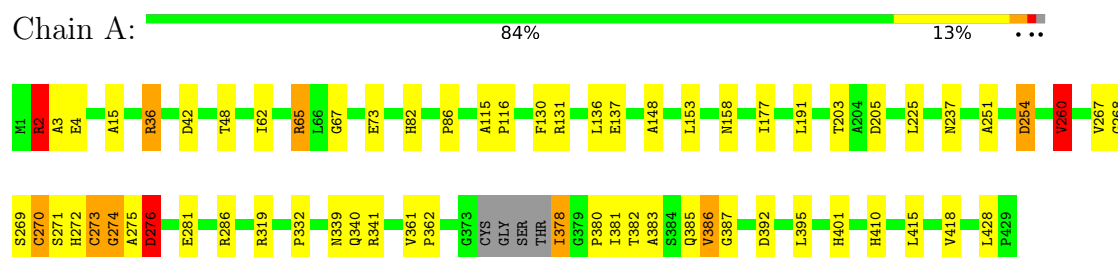
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	224	Total	O	0	0
			224	224		
4	B	218	Total	O	0	0
			218	218		
4	C	219	Total	O	0	0
			219	219		
4	D	223	Total	O	0	0
			223	223		

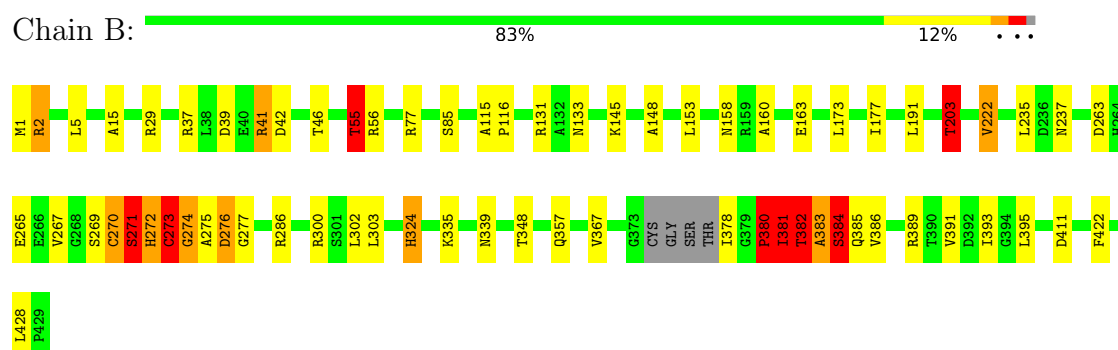
3 Residue-property plots

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.

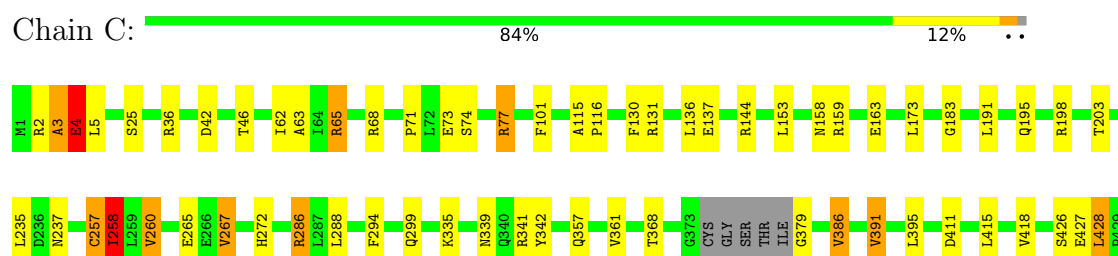
- Molecule 1: Probable M18 family aminopeptidase 2



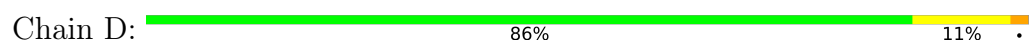
- Molecule 1: Probable M18 family aminopeptidase 2

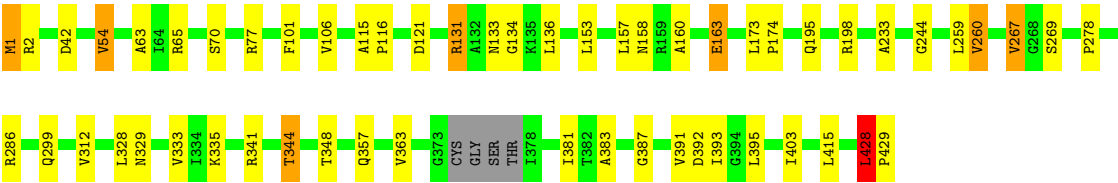


- Molecule 1: Probable M18 family aminopeptidase 2



- Molecule 1: Probable M18 family aminopeptidase 2





4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	134.19Å 134.19Å 328.76Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	27.40 – 2.30 27.40 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (27.40-2.30) 100.0 (27.40-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.146 , 0.196 0.155 , 0.201	Depositor DCC
R_{free} test set	4898 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	25.9	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 38.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.024 for $-1/3^*h+1/3^*k+1/3^*l, -k, 8/3^*h+4/3^*k+1/3^*l$ 0.026 for $-2/3^*h-1/3^*k-1/3^*l, -1/3^*h-2/3^*k+1/3^*l, -4/3^*h+4/3^*k+1/3^*l$ 0.024 for $-h, 1/3^*h-1/3^*k-1/3^*l, -4/3^*h-8/3^*k+1/3^*l$ 0.456 for $-h, 2/3^*h+1/3^*k+1/3^*l, 4/3^*h+8/3^*k-1/3^*l$ 0.457 for $1/3^*h+2/3^*k-1/3^*l, -k, -8/3^*h-4/3^*k-1/3^*l$ 0.457 for $-1/3^*h-2/3^*k+1/3^*l, -2/3^*h-1/3^*k-1/3^*l, 4/3^*h-4/3^*k-1/3^*l$ 0.030 for $-h-k, k, -l$	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	13955	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CO3

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	1.22	3/3324 (0.1%)	1.14	5/4509 (0.1%)
1	B	1.28	15/3318 (0.5%)	1.20	14/4501 (0.3%)
1	C	1.25	8/3316 (0.2%)	1.20	14/4498 (0.3%)
1	D	1.21	5/3324 (0.2%)	1.13	8/4509 (0.2%)
All	All	1.24	31/13282 (0.2%)	1.17	41/18017 (0.2%)

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	0	3
1	B	1	1
1	C	0	1
1	D	0	1
All	All	1	6

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	384	SER	N-CA	8.49	1.57	1.46
1	C	258	ILE	N-CA	8.40	1.56	1.46
1	D	363	VAL	C-O	-7.05	1.16	1.23
1	B	382	THR	N-CA	6.61	1.54	1.46
1	B	271	SER	N-CA	6.41	1.54	1.46
1	B	324	HIS	CA-CB	6.07	1.57	1.53
1	B	381	ILE	N-CA	5.95	1.53	1.46
1	C	286	ARG	C-O	-5.92	1.16	1.24
1	B	383	ALA	C-O	5.91	1.31	1.24
1	C	101	PHE	N-CA	5.77	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	342[H]	TYR	CA-C	5.74	1.59	1.52
1	B	273	CYS	C-O	5.72	1.34	1.23
1	B	272	HIS	N-CA	5.62	1.53	1.46
1	C	257	CYS	C-N	-5.62	1.25	1.33
1	B	85	SER	CA-C	5.62	1.58	1.52
1	B	56	ARG	C-O	5.59	1.30	1.23
1	B	303	LEU	C-O	-5.49	1.17	1.24
1	A	2	ARG	CA-C	5.49	1.60	1.52
1	C	299	GLN	C-O	-5.48	1.17	1.24
1	A	15	ALA	C-O	-5.42	1.16	1.24
1	C	25	SER	C-O	-5.41	1.17	1.24
1	C	4	GLU	C-O	-5.37	1.17	1.24
1	B	380	PRO	CA-C	5.29	1.59	1.52
1	B	15	ALA	C-O	-5.28	1.17	1.24
1	A	225	LEU	C-O	-5.19	1.18	1.24
1	B	273	CYS	CA-C	5.10	1.63	1.52
1	D	278	PRO	N-CA	-5.09	1.42	1.47
1	D	101	PHE	N-CA	5.05	1.51	1.45
1	D	299	GLN	C-O	-5.05	1.17	1.24
1	B	5	LEU	N-CA	-5.04	1.40	1.46
1	D	312	VAL	CA-C	5.03	1.58	1.52

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	271	SER	N-CA-C	13.02	138.52	110.80
1	C	3	ALA	N-CA-C	-10.77	95.32	110.50
1	C	391	VAL	CB-CA-C	-10.68	94.58	110.81
1	B	272	HIS	N-CA-C	10.51	124.01	111.82
1	A	260	VAL	CB-CA-C	-10.44	97.42	110.99
1	C	260	VAL	CB-CA-C	-9.03	97.95	110.77
1	D	260	VAL	CB-CA-C	-8.89	97.97	110.96
1	C	258	ILE	N-CA-C	8.84	127.72	109.34
1	B	274	GLY	N-CA-C	-7.68	99.78	112.83
1	D	54	VAL	CB-CA-C	-7.63	97.06	110.71
1	B	173	LEU	CA-C-N	-7.26	112.90	120.38
1	B	173	LEU	C-N-CA	-7.26	112.90	120.38
1	B	2	ARG	N-CA-C	6.95	125.60	110.80
1	D	267	VAL	N-CA-CB	-6.92	103.16	112.16
1	A	273	CYS	N-CA-CB	-6.72	100.77	110.65
1	B	384	SER	N-CA-C	6.67	125.00	110.80
1	C	257	CYS	CA-C-N	-6.67	109.97	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	257	CYS	C-N-CA	-6.67	109.97	121.97
1	D	65	ARG	CB-CA-C	-6.30	100.52	110.79
1	D	267	VAL	CB-CA-C	6.27	119.30	111.65
1	C	257	CYS	O-C-N	-5.97	114.37	122.19
1	B	203	THR	CB-CA-C	5.84	119.49	110.14
1	D	133	ASN	CB-CA-C	-5.77	103.69	111.89
1	C	426	SER	N-CA-C	5.73	117.21	110.97
1	B	55	THR	N-CA-CB	-5.67	101.05	111.37
1	A	274	GLY	CA-C-O	-5.66	117.52	122.16
1	B	133	ASN	CB-CA-C	-5.64	103.88	111.89
1	C	65	ARG	CB-CA-C	-5.60	101.72	110.74
1	C	391	VAL	N-CA-C	-5.60	100.41	108.53
1	C	386	VAL	N-CA-CB	-5.57	102.35	111.98
1	A	276	ASP	N-CA-CB	5.55	118.02	110.42
1	B	380	PRO	N-CA-C	5.33	123.45	112.47
1	B	222	VAL	CB-CA-C	5.30	118.94	111.63
1	B	29	ARG	N-CA-C	5.27	117.02	111.28
1	D	244	GLY	N-CA-C	-5.20	106.12	112.77
1	C	391	VAL	N-CA-CB	5.16	120.75	111.21
1	C	5	LEU	N-CA-C	-5.13	105.58	111.07
1	D	106	VAL	N-CA-C	5.10	116.05	108.46
1	B	270	CYS	CA-C-O	-5.04	115.39	120.84
1	C	173	LEU	N-CA-C	5.01	120.88	109.81
1	A	205	ASP	N-CA-C	-5.01	105.53	111.69

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	271	SER	CA

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2	ARG	Peptide
1	A	272	HIS	Peptide
1	A	276	ASP	Peptide
1	B	1	MET	Peptide
1	C	183	GLY	Peptide
1	D	428	LEU	Peptide

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	3265	0	3124	43	0
1	B	3260	0	3119	51	0
1	C	3257	0	3113	32	0
1	D	3265	0	3124	30	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
3	C	4	0	0	0	0
3	D	4	0	0	0	0
4	A	224	0	0	6	0
4	B	218	0	0	9	0
4	C	219	0	0	6	0
4	D	223	0	0	5	0
All	All	13955	0	12480	150	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 6.

All (150) 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:2:ARG:HD3	1:A:2:ARG:C	1.75	1.06
1:B:273:CYS:SG	1:B:274:GLY:N	2.32	0.95
1:B:276:ASP:OD1	1:B:276:ASP:N	2.00	0.92
1:D:344:THR:HG22	1:D:392:ASP:H	1.35	0.91
1:A:276:ASP:HB3	1:A:381:ILE:HG23	1.57	0.84
1:B:357:GLN:HB3	4:B:731:HOH:O	1.79	0.82
1:B:272:HIS:N	1:B:273:CYS:HA	1.94	0.82
1:D:1:MET:HE2	1:D:1:MET:HA	1.59	0.81
1:B:381:ILE:HD13	1:B:382:THR:N	1.94	0.81
1:C:3:ALA:O	1:C:4:GLU:CB	2.25	0.81
1:A:382:THR:O	1:A:385:GLN:O	2.00	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:379:GLY:N	4:C:764:HOH:O	2.17	0.78
1:C:77:ARG:O	1:C:257:CYS:O	2.04	0.76
1:B:270:CYS:O	1:B:271:SER:CB	2.35	0.75
1:B:37:ARG:HH21	1:B:55:THR:HG21	1.53	0.74
1:A:378:ILE:HD12	4:A:822:HOH:O	1.86	0.74
1:B:39:ASP:OD1	1:B:41:ARG:HD3	1.88	0.72
1:B:275:ALA:C	1:B:276:ASP:OD1	2.36	0.69
1:B:382:THR:O	1:B:382:THR:HG23	1.93	0.68
1:D:341:ARG:HD2	4:D:767:HOH:O	1.97	0.65
1:A:2:ARG:HD3	1:A:3:ALA:N	2.12	0.65
1:B:37:ARG:NH2	1:B:55:THR:HG21	2.12	0.64
1:C:195:GLN:OE1	1:C:198:ARG:NH1	2.30	0.64
1:D:1:MET:HA	1:D:1:MET:CE	2.26	0.63
1:C:77:ARG:NH2	1:C:428:LEU:HD22	2.14	0.62
1:B:270:CYS:O	1:B:271:SER:HB3	1.99	0.62
1:B:389:ARG:NE	4:B:721:HOH:O	2.32	0.62
1:B:276:ASP:HA	1:B:277:GLY:O	1.99	0.61
1:C:3:ALA:O	1:C:4:GLU:HB3	2.01	0.61
1:D:198:ARG:NH1	4:D:707:HOH:O	2.32	0.61
1:C:3:ALA:O	1:C:4:GLU:HB2	2.01	0.60
1:B:160:ALA:HB1	1:B:163:GLU:HG3	1.84	0.60
1:B:41:ARG:HD2	4:B:667:HOH:O	2.00	0.60
1:A:378:ILE:HG13	1:A:380:PRO:HD2	1.84	0.59
1:B:274:GLY:O	1:B:275:ALA:HB3	2.00	0.59
1:B:55:THR:CG2	4:B:655:HOH:O	2.51	0.59
1:A:269:SER:O	1:A:270:CYS:CB	2.50	0.58
1:A:2:ARG:C	1:A:4:GLU:N	2.59	0.58
1:B:381:ILE:HD13	1:B:382:THR:HA	1.85	0.58
1:B:37:ARG:HH21	1:B:55:THR:CG2	2.16	0.58
1:A:341:ARG:CZ	4:A:777:HOH:O	2.53	0.57
1:B:275:ALA:CA	1:B:276:ASP:OD1	2.52	0.57
1:B:384:SER:HA	1:B:386:VAL:N	2.20	0.56
1:A:340:GLN:HB3	1:B:271:SER:OG	2.06	0.56
1:D:195:GLN:OE1	1:D:198:ARG:NH1	2.39	0.56
1:A:271:SER:C	1:A:273:CYS:H	2.14	0.56
1:B:55:THR:HG23	4:B:655:HOH:O	2.05	0.56
1:D:348:THR:HB	1:D:391:VAL:HB	1.87	0.56
1:B:384:SER:HA	1:B:386:VAL:H	1.70	0.55
1:B:275:ALA:HA	1:B:276:ASP:OD1	2.06	0.55
1:A:36:ARG:HG2	1:A:36:ARG:HH11	1.71	0.55
1:A:42:ASP:O	1:A:286:ARG:NH2	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:153:LEU:HD23	1:D:158:ASN:HB2	1.87	0.54
1:C:74:SER:O	1:C:77:ARG:NH2	2.41	0.54
1:B:382:THR:O	1:B:382:THR:CG2	2.54	0.54
1:D:160:ALA:O	1:D:163:GLU:HB2	2.08	0.54
1:B:339:ASN:HA	1:C:267:VAL:HG21	1.90	0.54
1:C:357:GLN:HB3	4:C:709:HOH:O	2.08	0.53
1:C:288:LEU:HD13	1:C:294:PHE:HA	1.90	0.53
1:B:145:LYS:HE2	4:B:758:HOH:O	2.07	0.52
1:D:121:ASP:OD2	4:D:718:HOH:O	2.19	0.52
1:B:381:ILE:HD13	1:B:382:THR:CA	2.39	0.52
1:C:159:ARG:NH2	4:C:813:HOH:O	2.42	0.52
1:D:233:ALA:HB2	1:D:403:ILE:O	2.10	0.52
1:C:65:ARG:HB2	1:C:257:CYS:HB2	1.91	0.52
1:D:77:ARG:HG2	1:D:77:ARG:HH11	1.75	0.51
1:A:385:GLN:NE2	4:A:757:HOH:O	2.38	0.50
1:D:344:THR:CG2	1:D:392:ASP:H	2.15	0.50
1:A:153:LEU:HD23	1:A:158:ASN:HB2	1.93	0.50
1:C:395:LEU:HD22	1:C:411:ASP:HB3	1.94	0.50
1:D:115:ALA:N	1:D:116:PRO:CD	2.74	0.50
1:D:395:LEU:HD21	1:D:415:LEU:HB2	1.93	0.50
1:B:265:GLU:OE2	1:B:380:PRO:HB2	2.12	0.50
1:A:395:LEU:HD21	1:A:415:LEU:HB2	1.93	0.49
1:A:115:ALA:N	1:A:116:PRO:CD	2.75	0.49
1:D:131:ARG:HE	1:D:134:GLY:HA2	1.77	0.49
1:A:269:SER:O	1:A:270:CYS:HB3	2.13	0.49
1:A:339:ASN:HA	1:B:267:VAL:HG11	1.95	0.48
1:D:42:ASP:O	1:D:286:ARG:NH2	2.47	0.48
1:D:70:SER:HB2	4:D:698:HOH:O	2.13	0.48
1:C:62:ILE:HG12	1:C:260:VAL:HG13	1.95	0.48
1:C:361:VAL:HG11	1:C:418:VAL:HG21	1.95	0.48
1:A:2:ARG:NH2	1:A:410:HIS:HA	2.29	0.47
1:A:36:ARG:HH11	1:A:36:ARG:CG	2.26	0.47
1:C:71:PRO:HB2	1:C:288:LEU:HD21	1.95	0.47
1:A:267:VAL:HG11	1:C:339:ASN:HA	1.97	0.47
1:B:77:ARG:CD	1:B:428:LEU:HD21	2.45	0.47
1:C:153:LEU:HD23	1:C:158:ASN:HB2	1.97	0.47
1:C:335:LYS:HE3	4:C:738:HOH:O	2.15	0.47
1:A:276:ASP:HB3	1:A:381:ILE:CG2	2.37	0.47
1:A:361:VAL:HG21	1:A:418:VAL:HG13	1.96	0.47
1:C:63:ALA:O	1:C:258:ILE:HA	2.15	0.46
1:D:428:LEU:HB2	1:D:429:PRO:CD	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:63:ALA:HB3	1:D:259:LEU:HB3	1.96	0.46
1:B:269:SER:O	1:B:275:ALA:HB1	2.16	0.46
1:B:274:GLY:O	1:B:275:ALA:CB	2.64	0.46
1:C:77:ARG:HH21	1:C:428:LEU:HD22	1.80	0.46
1:A:268:GLY:C	1:A:269:SER:O	2.56	0.46
1:B:381:ILE:CD1	1:B:382:THR:N	2.74	0.46
4:B:620:HOH:O	1:C:272:HIS:HE1	1.99	0.45
1:A:269:SER:HB3	1:A:275:ALA:N	2.32	0.45
1:C:42:ASP:O	1:C:286:ARG:NH2	2.50	0.45
1:D:335:LYS:O	1:D:344:THR:CG2	2.65	0.45
1:D:335:LYS:O	1:D:344:THR:HG23	2.17	0.45
1:A:281:GLU:HB2	1:A:386:VAL:HG12	1.99	0.45
1:A:67:GLY:HA3	1:A:254:ASP:O	2.17	0.44
1:C:130:PHE:CZ	1:C:137:GLU:HG3	2.52	0.44
1:A:271:SER:C	1:A:273:CYS:N	2.74	0.44
1:D:173:LEU:N	1:D:174:PRO:CD	2.81	0.44
1:B:115:ALA:N	1:B:116:PRO:CD	2.81	0.44
1:B:235:LEU:O	1:B:237:ASN:HA	2.18	0.44
1:C:36:ARG:NH1	4:C:797:HOH:O	2.24	0.44
1:A:383:ALA:O	1:A:387:GLY:HA2	2.18	0.44
1:A:383:ALA:HB1	1:B:271:SER:O	2.18	0.44
1:A:130:PHE:CZ	1:A:137:GLU:HG3	2.52	0.43
1:A:319:ARG:NH2	4:A:624:HOH:O	2.51	0.43
1:A:86:PRO:HG2	1:A:401:HIS:CG	2.54	0.43
1:A:2:ARG:CA	1:A:4:GLU:H	2.31	0.43
1:A:148:ALA:HB2	1:A:177:ILE:HG22	2.00	0.43
1:B:300:ARG:O	1:B:428:LEU:HD12	2.18	0.43
1:C:115:ALA:N	1:C:116:PRO:CD	2.81	0.43
1:D:383:ALA:O	1:D:387:GLY:HA2	2.18	0.43
1:B:270:CYS:O	1:B:271:SER:OG	2.36	0.43
1:A:65:ARG:NH2	1:A:251:ALA:HB3	2.34	0.42
1:C:361:VAL:HG21	1:C:418:VAL:HG23	2.00	0.42
1:D:2:ARG:HD2	4:D:798:HOH:O	2.18	0.42
1:B:263:ASP:O	1:B:275:ALA:HB2	2.20	0.42
1:B:302:LEU:HD23	1:B:422:PHE:CE1	2.54	0.42
1:D:333:VAL:O	1:D:393:ILE:HA	2.19	0.42
1:B:395:LEU:HD22	1:B:411:ASP:HB3	2.02	0.42
1:A:378:ILE:HB	4:A:822:HOH:O	2.19	0.42
1:B:335:LYS:HE2	4:B:675:HOH:O	2.20	0.42
1:C:368:THR:HG22	4:C:686:HOH:O	2.19	0.42
1:D:269:SER:HB2	1:D:381:ILE:HD13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:HIS:NE2	1:A:237:ASN:HB2	2.35	0.41
1:A:332:PRO:HD2	1:A:362:PRO:O	2.20	0.41
1:D:77:ARG:CD	1:D:428:LEU:HD21	2.49	0.41
1:B:42:ASP:O	1:B:286:ARG:NH2	2.53	0.41
1:C:265:GLU:CD	1:C:265:GLU:C	2.89	0.41
1:B:148:ALA:HB2	1:B:177:ILE:HG22	2.02	0.41
1:B:324:HIS:CG	1:B:367:VAL:HG12	2.56	0.41
1:C:395:LEU:HD21	1:C:415:LEU:HB2	2.02	0.41
1:A:62:ILE:HG12	1:A:260:VAL:HG13	2.03	0.41
1:A:274:GLY:HA2	4:A:675:HOH:O	2.21	0.41
1:A:319:ARG:NH1	1:D:157:LEU:O	2.54	0.41
1:B:153:LEU:HD23	1:B:158:ASN:HB2	2.01	0.41
1:D:328:LEU:O	1:D:329:ASN:HB2	2.21	0.41
1:B:203:THR:HA	4:B:763:HOH:O	2.20	0.41
1:C:235:LEU:O	1:C:237:ASN:HA	2.20	0.40
1:B:348:THR:HB	1:B:391:VAL:HB	2.02	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	421/429 (98%)	398 (94%)	21 (5%)	2 (0%)	24	31
1	B	421/429 (98%)	391 (93%)	23 (6%)	7 (2%)	7	7
1	C	420/429 (98%)	403 (96%)	15 (4%)	2 (0%)	24	31
1	D	421/429 (98%)	403 (96%)	17 (4%)	1 (0%)	43	55
All	All	1683/1716 (98%)	1595 (95%)	76 (4%)	12 (1%)	18	23

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	270	CYS
1	B	2	ARG
1	B	271	SER
1	B	382	THR
1	B	383	ALA
1	C	4	GLU
1	B	380	PRO
1	B	384	SER
1	D	428	LEU
1	B	385	GLN
1	C	258	ILE

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	341/344 (99%)	326 (96%)	15 (4%)	25	38
1	B	340/344 (99%)	326 (96%)	14 (4%)	27	41
1	C	340/344 (99%)	323 (95%)	17 (5%)	22	33
1	D	341/344 (99%)	331 (97%)	10 (3%)	37	55
All	All	1362/1376 (99%)	1306 (96%)	56 (4%)	27	41

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	36	ARG
1	A	48	THR
1	A	65	ARG
1	A	73	GLU
1	A	131	ARG
1	A	136	LEU
1	A	191	LEU
1	A	203	THR
1	A	254	ASP

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Mol	Chain	Res	Type
1	A	260	VAL
1	A	378	ILE
1	A	386	VAL
1	A	392	ASP
1	A	428	LEU
1	B	41	ARG
1	B	46	THR
1	B	55	THR
1	B	131	ARG
1	B	191	LEU
1	B	203	THR
1	B	222	VAL
1	B	273	CYS
1	B	276	ASP
1	B	378	ILE
1	B	381	ILE
1	B	382	THR
1	B	384	SER
1	B	393	ILE
1	C	2	ARG
1	C	46	THR
1	C	68	ARG
1	C	73	GLU
1	C	77	ARG
1	C	131	ARG
1	C	136	LEU
1	C	144	ARG
1	C	163	GLU
1	C	191	LEU
1	C	203	THR
1	C	267	VAL
1	C	341	ARG
1	C	386	VAL
1	C	391	VAL
1	C	427	GLU
1	C	428	LEU
1	D	1	MET
1	D	54	VAL
1	D	131	ARG
1	D	136	LEU
1	D	163	GLU
1	D	260	VAL

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Mol	Chain	Res	Type
1	D	267	VAL
1	D	344	THR
1	D	357	GLN
1	D	428	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	ASN
1	A	340	GLN
1	A	354	HIS
1	B	264	HIS
1	B	385	GLN
1	C	323	ASN
1	C	357	GLN
1	C	410	HIS
1	D	93	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 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

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	$\# Z > 2$
3	CO3	D	503	2	3,3,3	1.03	0	2,3,3	0.71	0
3	CO3	A	503	2	3,3,3	1.03	0	2,3,3	0.84	0
3	CO3	C	503	2	3,3,3	1.13	0	2,3,3	0.50	0
3	CO3	B	503	2	3,3,3	1.25	0	2,3,3	0.91	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 [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	425/429 (99%)	-1.37	0 100 100	15, 24, 50, 76	0
1	B	425/429 (99%)	-1.34	0 100 100	15, 24, 54, 131	0
1	C	424/429 (98%)	-1.36	0 100 100	16, 24, 47, 81	0
1	D	425/429 (99%)	-1.37	0 100 100	16, 24, 47, 113	0
All	All	1699/1716 (99%)	-1.36	0 100 100	15, 24, 51, 131	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
3	CO3	A	503	4/4	0.99	0.03	35,51,52,54	0
3	CO3	C	503	4/4	0.99	0.05	45,51,57,57	0
3	CO3	D	503	4/4	0.99	0.04	33,51,53,58	0
2	ZN	B	502	1/1	1.00	0.01	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	C	501	1/1	1.00	0.02	26,26,26,26	0
2	ZN	C	502	1/1	1.00	0.02	29,29,29,29	0
2	ZN	D	501	1/1	1.00	0.02	25,25,25,25	0
2	ZN	D	502	1/1	1.00	0.01	28,28,28,28	0
2	ZN	A	501	1/1	1.00	0.01	25,25,25,25	0
3	CO3	B	503	4/4	1.00	0.04	38,48,51,55	0
2	ZN	A	502	1/1	1.00	0.03	29,29,29,29	0
2	ZN	B	501	1/1	1.00	0.03	29,29,29,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.