



# Full wwPDB X-ray Structure Validation Report i

Sep 10, 2014 – 12:37 PM EDT

PDB ID : 3WT4  
Title : Structural and kinetic bases for the metal preference of the M18 aminopeptidase from *Pseudomonas aeruginosa*  
Authors : Nguyen, D.D.; Pandian, R.; Kim, D.D.; Ha, S.C.; Yoon, H.J.; Kim, K.S.; Yun, K.H.; Kim, J.H.; Kim, K.K.  
Deposited on : 2014-04-07  
Resolution : 2.30 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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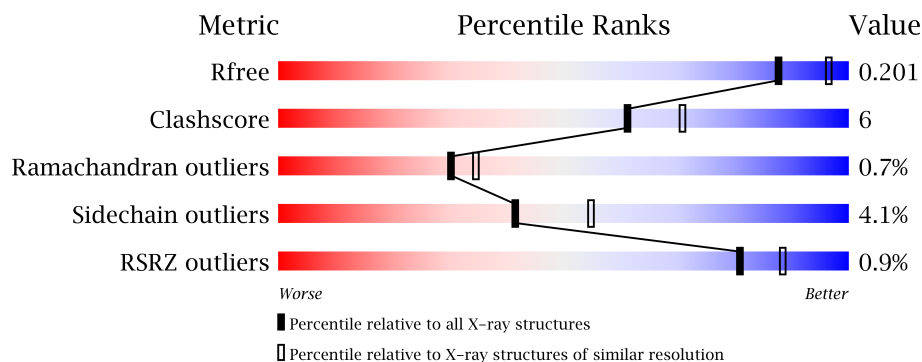
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1439  
EDS : stable23489  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable23489

# 1 Overall quality at a glance

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))
$R_{free}$	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	429	
1	B	429	
1	C	429	
1	D	429	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13955 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

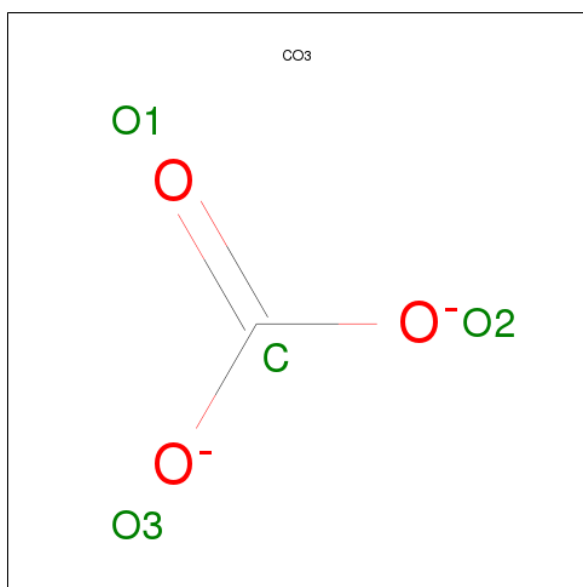
- Molecule 1 is a protein called Probable M18 family aminopeptidase 2.

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 (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is CARBONATE ION (three-letter code: CO3) (formula: CO<sub>3</sub>).



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.

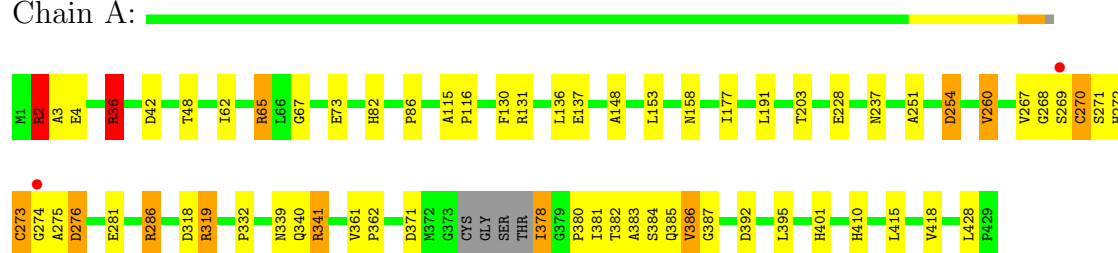
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	222	Total	O	0	0
			222	222		
4	B	220	Total	O	0	0
			220	220		
4	C	219	Total	O	0	0
			219	219		
4	D	223	Total	O	0	0
			223	223		

### 3 Residue-property plots

These plots are drawn for all protein, RNA 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.

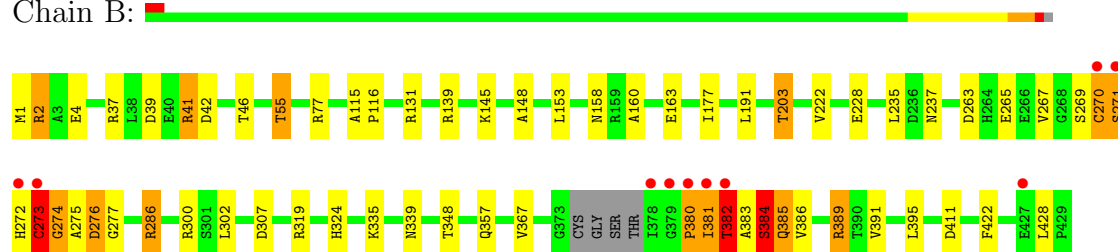
- Molecule 1: Probable M18 family aminopeptidase 2

Chain A:



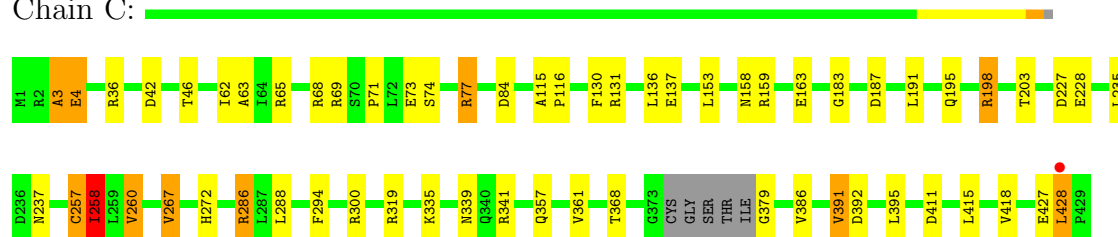
- Molecule 1: Probable M18 family aminopeptidase 2

Chain B:



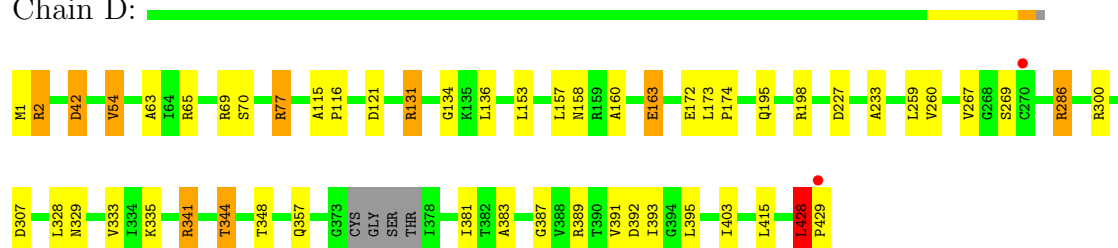
- Molecule 1: Probable M18 family aminopeptidase 2

Chain C:



- Molecule 1: Probable M18 family aminopeptidase 2

Chain D:



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.48 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.146 , 0.196 0.155 , 0.201	Depositor DCC
$R_{free}$ test set	4898 reflections (5.25%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.9	Xtriage
Anisotropy	0.005	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 44.2	EDS
Estimated twinning fraction	0.025 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
L-test for twinning	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 98152 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	13955	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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	0.92	2/3324 (0.1%)	0.98	10/4509 (0.2%)
1	B	0.93	3/3318 (0.1%)	1.02	10/4501 (0.2%)
1	C	0.93	2/3316 (0.1%)	1.05	15/4498 (0.3%)
1	D	0.91	1/3324 (0.0%)	1.00	13/4509 (0.3%)
All	All	0.92	8/13282 (0.1%)	1.01	48/18017 (0.3%)

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	0	1
1	C	0	1
1	D	0	1
All	All	0	6

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	228	GLU	CD-OE1	6.88	1.33	1.25
1	B	273	CYS	C-O	6.13	1.34	1.23
1	A	228	GLU	CD-OE1	5.89	1.32	1.25
1	C	228	GLU	CD-OE1	5.59	1.31	1.25
1	B	384	SER	N-CA	5.40	1.57	1.46
1	A	273	CYS	CB-SG	-5.32	1.73	1.81
1	D	172	GLU	CD-OE2	-5.29	1.19	1.25
1	C	258	ILE	N-CA	5.25	1.56	1.46

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	391	VAL	CB-CA-C	-8.85	94.58	111.40
1	D	389	ARG	NE-CZ-NH2	-8.83	115.89	120.30
1	B	41	ARG	NE-CZ-NH1	8.20	124.40	120.30
1	A	36	ARG	NE-CZ-NH1	8.05	124.33	120.30
1	D	54	VAL	CB-CA-C	-7.55	97.06	111.40
1	A	2	ARG	NE-CZ-NH1	7.52	124.06	120.30
1	C	300	ARG	NE-CZ-NH1	7.47	124.03	120.30
1	A	260	VAL	CB-CA-C	-7.36	97.42	111.40
1	C	260	VAL	CB-CA-C	-7.08	97.95	111.40
1	D	260	VAL	CB-CA-C	-7.07	97.97	111.40
1	D	286	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	C	69	ARG	NE-CZ-NH2	-6.65	116.98	120.30
1	C	227	ASP	CB-CG-OD1	6.57	124.21	118.30
1	D	77	ARG	NE-CZ-NH1	6.57	123.58	120.30
1	C	187	ASP	CB-CG-OD2	-6.53	112.42	118.30
1	B	41	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	B	307	ASP	CB-CG-OD1	6.28	123.95	118.30
1	B	389	ARG	NE-CZ-NH1	6.27	123.44	120.30
1	C	258	ILE	N-CA-C	6.20	127.72	111.00
1	B	139	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	D	69	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	A	318	ASP	CB-CG-OD1	6.09	123.78	118.30
1	C	319	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	C	286	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	D	65	ARG	NE-CZ-NH2	-5.89	117.35	120.30
1	A	260	VAL	CG1-CB-CG2	5.89	120.32	110.90
1	C	3	ALA	N-CA-C	-5.81	95.32	111.00
1	D	300	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	A	286	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	D	227	ASP	CB-CG-OD1	5.66	123.40	118.30
1	C	300	ARG	NE-CZ-NH2	-5.65	117.48	120.30
1	C	187	ASP	CB-CG-OD1	5.59	123.33	118.30
1	D	42	ASP	CB-CG-OD1	5.57	123.31	118.30
1	A	273	CYS	N-CA-CB	-5.46	100.77	110.60
1	B	2	ARG	N-CA-C	5.41	125.60	111.00
1	C	198	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	B	274	GLY	N-CA-C	-5.33	99.78	113.10
1	D	307	ASP	CB-CG-OD1	5.31	123.08	118.30
1	B	319	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	A	36	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	C	257	CYS	O-C-N	-5.21	114.37	122.70
1	D	260	VAL	CG1-CB-CG2	5.20	119.22	110.90
1	A	371	ASP	CB-CG-OD1	5.19	122.97	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	384	SER	N-CA-C	5.19	125.00	111.00
1	C	84	ASP	CB-CG-OD2	-5.14	113.67	118.30
1	B	286	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	D	69	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	A	319	ARG	NE-CZ-NH1	5.09	122.85	120.30

There are no chirality outliers.

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3265	0	3124	45	0
1	B	3260	0	3119	54	0
1	C	3257	0	3113	31	0
1	D	3265	0	3124	29	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	222	0	0	6	0
4	B	220	0	0	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	219	0	0	6	0
4	D	223	0	0	5	0
All	All	13955	0	12480	151	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (151) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:340:GLN:NE2	1:B:271:SER:O	1.83	1.11
1:A:2:ARG:C	1:A:2:ARG:HD3	1.75	1.03
1:B:272:HIS:H	1:B:273:CYS:HA	1.23	1.02
1:B:273:CYS:SG	1:B:274:GLY:N	2.32	1.02
1:B:270:CYS:O	4:B:728:HOH:O	1.81	0.97
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:733:HOH:O	1.79	0.82
1:B:272:HIS:N	1:B:273:CYS:HA	1.94	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
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:37:ARG:HH21	1:B:55:THR:HG21	1.53	0.74
1:A:378:ILE:HD12	4:A:821:HOH:O	1.86	0.74
1:B:39:ASP:OD1	1:B:41:ARG:HD3	1.88	0.72
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:275:ALA:C	1:B:276:ASP:OD1	2.36	0.64
1:B:37:ARG:NH2	1:B:55:THR:HG21	2.12	0.64
1:D:1:MET:CE	1:D:1:MET:HA	2.26	0.64
1:C:195:GLN:OE1	1:C:198:ARG:NH1	2.30	0.64
1:C:77:ARG:NH2	1:C:428:LEU:HD22	2.14	0.62
1:B:389:ARG:NE	4:B:722: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:668:HOH:O	2.00	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:656:HOH:O	2.51	0.59
1:A:269:SER:O	1:A:270:CYS:CB	2.50	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:776: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:D:195:GLN:OE1	1:D:198:ARG:NH1	2.39	0.56
1:B:55:THR:HG23	4:B:656: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
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:A:2:ARG:C	1:A:4:GLU:N	2.59	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:760:HOH:O	2.07	0.52
1:D:121:ASP:OD2	4:D:718:HOH:O	2.19	0.52
1:A:340:GLN:HE21	1:B:271:SER:C	2.09	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:271:SER:C	1:A:273:CYS:H	2.14	0.51
1:A:385:GLN:NE2	4:A:756: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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:B:270:CYS:HA	1:B:271:SER:HB3	1.93	0.48
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:361:VAL:HG11	1:C:418:VAL:HG21	1.95	0.48
1:C:62:ILE:HG12	1:C:260:VAL:HG13	1.95	0.48
1:A:2:ARG:NH2	1:A:410:HIS:HA	2.29	0.47
1:A:36:ARG:CG	1:A:36:ARG:HH11	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
1:D:63:ALA:HB3	1:D:259:LEU:HB3	1.96	0.46
1:B:274:GLY:O	1:B:275:ALA:CB	2.64	0.46
1:B:269:SER:O	1:B:275:ALA:HB1	2.16	0.46
1:C:77:ARG:HH21	1:C:428:LEU:HD22	1.80	0.46
1:B:270:CYS:HA	1:B:271:SER:CB	2.46	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:HG23	2.17	0.45
1:D:335:LYS:O	1:D:344:THR:CG2	2.65	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: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: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:340:GLN:NE2	1:B:271:SER:C	2.63	0.43
1:A:86:PRO:HG2	1:A:401:HIS:CG	2.54	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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: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:821:HOH:O	2.19	0.42
1:B:335:LYS:HE2	4:B:676: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
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: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:A:268:GLY:C	1:A:269:SER:O	2.56	0.41
1:A:271:SER:C	1:A:273:CYS:N	2.74	0.41
1:C:395:LEU:HD21	1:C:415:LEU:HB2	2.02	0.41
1:A:274:GLY:HA2	4:A:675:HOH:O	2.21	0.41
1:B:153:LEU:HD23	1:B:158:ASN:HB2	2.01	0.41
1:A:319:ARG:NH1	1:D:157:LEU:O	2.54	0.41
1:A:62:ILE:HG12	1:A:260:VAL:HG13	2.03	0.41
1:D:328:LEU:O	1:D:329:ASN:HB2	2.21	0.41
1:B:203:THR:HA	4:B:765:HOH:O	2.20	0.41
1:A:384:SER:CB	1:B:270:CYS:HB3	2.51	0.40
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

### 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	421/429 (98%)	398 (94%)	21 (5%)	2 (0%)	38	45
1	B	421/429 (98%)	390 (93%)	25 (6%)	6 (1%)	16	15
1	C	420/429 (98%)	403 (96%)	15 (4%)	2 (0%)	38	45
1	D	421/429 (98%)	403 (96%)	17 (4%)	1 (0%)	56	68
All	All	1683/1716 (98%)	1594 (95%)	78 (5%)	11 (1%)	30	34

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	270	CYS
1	B	2	ARG
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%)	39	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	340/344 (99%)	325 (96%)	15 (4%)	39	51
1	C	340/344 (99%)	324 (95%)	16 (5%)	36	47
1	D	341/344 (99%)	331 (97%)	10 (3%)	55	71
All	All	1362/1376 (99%)	1306 (96%)	56 (4%)	41	55

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
1	A	341	ARG
1	A	378	ILE
1	A	386	VAL
1	A	392	ASP
1	A	428	LEU
1	B	4	GLU
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	270	CYS
1	B	271	SER
1	B	273	CYS
1	B	276	ASP
1	B	381	ILE
1	B	382	THR
1	B	384	SER
1	B	385	GLN
1	C	46	THR
1	C	68	ARG
1	C	73	GLU

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Mol	Chain	Res	Type
1	C	77	ARG
1	C	131	ARG
1	C	136	LEU
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	392	ASP
1	C	427	GLU
1	C	428	LEU
1	D	2	ARG
1	D	54	VAL
1	D	131	ARG
1	D	136	LEU
1	D	163	GLU
1	D	267	VAL
1	D	341	ARG
1	D	344	THR
1	D	357	GLN
1	D	428	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.



## 5.6 Ligand geometry ⓘ

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	A	503	2	0,3,3	0.00	-	0,3,3	0.00	-
3	CO3	B	503	2	0,3,3	0.00	-	0,3,3	0.00	-
3	CO3	C	503	2	0,3,3	0.00	-	0,3,3	0.00	-
3	CO3	D	503	2	0,3,3	0.00	-	0,3,3	0.00	-

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
3	CO3	A	503	2	-	0/0/0/0	0/0/0/0
3	CO3	B	503	2	-	0/0/0/0	0/0/0/0
3	CO3	C	503	2	-	0/0/0/0	0/0/0/0
3	CO3	D	503	2	-	0/0/0/0	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.

## 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	425/429 (99%)	-0.36	2 (0%) 88 94	15, 24, 50, 76	0
1	B	425/429 (99%)	-0.26	10 (2%) 56 66	15, 24, 54, 131	0
1	C	424/429 (98%)	-0.36	1 (0%) 93 97	16, 24, 47, 81	0
1	D	425/429 (99%)	-0.37	2 (0%) 88 94	16, 24, 47, 113	0
All	All	1699/1716 (99%)	-0.34	15 (0%) 81 88	15, 24, 51, 131	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	378	ILE	9.6
1	B	380	PRO	8.0
1	B	272	HIS	6.8
1	B	379	GLY	6.3
1	D	429	PRO	6.0
1	B	271	SER	3.9
1	B	270	CYS	3.9
1	B	381	ILE	3.0
1	D	270	CYS	2.7
1	B	273	CYS	2.6
1	C	428	LEU	2.5
1	A	269	SER	2.5
1	B	382	THR	2.3
1	B	427	GLU	2.2
1	A	274	GLY	2.1

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates

There are no carbohydrates in this entry.

### 6.4 Ligands

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	ZN	D	502	1/1	0.10	0.03	28,28,28,28	0
3	CO3	B	503	4/4	0.11	-0.33	38,48,51,55	0
3	CO3	C	503	4/4	0.11	-0.47	45,51,57,57	0
3	CO3	D	503	4/4	0.10	-0.67	33,51,53,58	0
2	ZN	B	502	1/1	0.10	-0.68	26,26,26,26	0
3	CO3	A	503	4/4	0.09	-0.72	35,51,52,54	0
2	ZN	A	501	1/1	0.09	-0.77	25,25,25,25	0
2	ZN	C	501	1/1	0.08	-1.20	26,26,26,26	0
2	ZN	C	502	1/1	0.08	-1.61	29,29,29,29	0
2	ZN	A	502	1/1	0.07	-1.93	29,29,29,29	0
2	ZN	D	501	1/1	0.08	-2.06	25,25,25,25	0
2	ZN	B	501	1/1	0.07	-2.45	29,29,29,29	0

### 6.5 Other polymers

There are no such residues in this entry.