



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 05:52 PM EDT

PDB ID : 4EME / pdb_00004eme
Title : X-ray crystal structure and specificity of the Plasmodium falciparum malaria aminopeptidase
Authors : McGowan, S.
Deposited on : 2012-04-11
Resolution : 2.60 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

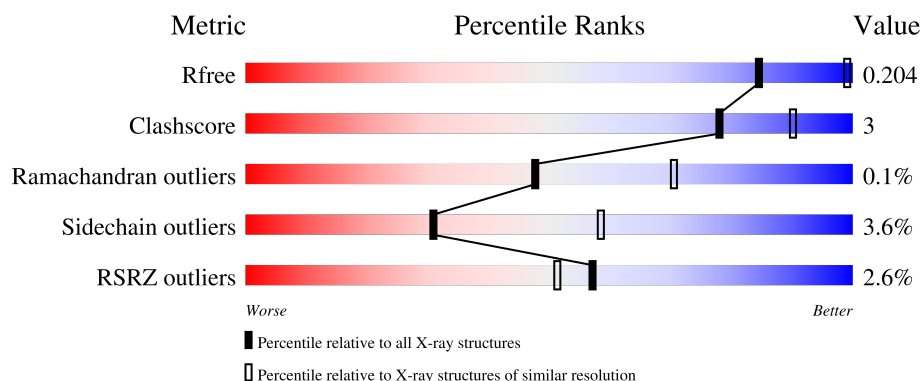
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	571	2% 72% 10% • 17%
1	B	571	2% 72% 9% • 17%
1	C	571	2% 74% 9% • 17%
1	D	571	2% 72% 9% 18%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15462 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 M18 aspartyl aminopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	474	Total	C	N	O	S	0	1	0
			3775	2416	635	703	21			
1	B	473	Total	C	N	O	S	0	2	0
			3779	2419	637	703	20			
1	C	475	Total	C	N	O	S	0	0	0
			3770	2410	635	705	20			
1	D	469	Total	C	N	O	S	0	1	0
			3686	2357	615	694	20			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	TYR	-	expression tag	UNP Q8I2J3
A	2	VAL	-	expression tag	UNP Q8I2J3
B	1	TYR	-	expression tag	UNP Q8I2J3
B	2	VAL	-	expression tag	UNP Q8I2J3
C	1	TYR	-	expression tag	UNP Q8I2J3
C	2	VAL	-	expression tag	UNP Q8I2J3
D	1	TYR	-	expression tag	UNP Q8I2J3
D	2	VAL	-	expression tag	UNP Q8I2J3

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

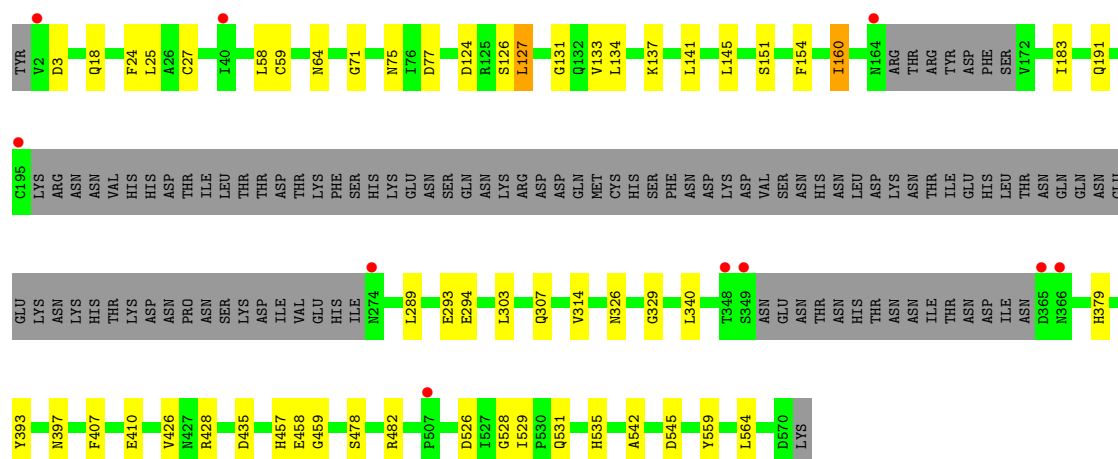
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		
2	C	2	Total	Zn	0	0
			2	2		
2	D	2	Total	Zn	0	0
			2	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	131	Total 131	O 131	0	0
3	B	141	Total 141	O 141	0	0
3	C	105	Total 105	O 105	0	0
3	D	67	Total 67	O 67	0	0

- Molecule 1: M18 aspartyl aminopeptidase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	200.38Å 200.38Å 200.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	55.58 – 2.60 55.58 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (55.58-2.60) 99.9 (55.58-2.60)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 2.61Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.159 , 0.196 0.168 , 0.204	Depositor DCC
R_{free} test set	4111 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	36.7	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 58.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.025 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15462	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 1.46% 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:
ZN

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	0.77	0/3856	1.30	21/5213 (0.4%)
1	B	0.78	0/3863	1.30	18/5219 (0.3%)
1	C	0.78	0/3849	1.32	13/5207 (0.2%)
1	D	0.75	0/3765	1.31	13/5101 (0.3%)
All	All	0.77	0/15333	1.31	65/20740 (0.3%)

There are no bond length outliers.

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	77	ASP	N-CA-C	6.95	120.23	111.69
1	C	178	ASN	N-CA-C	6.79	118.76	111.36
1	B	119	TRP	N-CA-C	6.66	119.37	111.71
1	A	379	HIS	N-CA-C	6.43	120.90	113.38
1	D	379	HIS	N-CA-C	6.29	120.53	112.86
1	B	469	ASN	N-CA-C	-6.22	104.95	112.54
1	A	459	GLY	N-CA-C	6.17	120.81	112.17
1	B	484	PHE	CA-CB-CG	6.13	119.93	113.80
1	D	160	ILE	CA-C-N	6.02	129.18	120.38
1	D	160	ILE	C-N-CA	6.02	129.18	120.38
1	B	542	ALA	CA-C-N	5.97	128.30	120.60
1	B	542	ALA	C-N-CA	5.97	128.30	120.60
1	A	9	TYR	CA-C-N	5.96	128.19	120.44
1	A	9	TYR	C-N-CA	5.96	128.19	120.44
1	A	418	VAL	CA-C-N	5.96	128.26	120.28
1	A	418	VAL	C-N-CA	5.96	128.26	120.28
1	C	469	ASN	N-CA-C	-5.82	105.44	112.54
1	B	559	TYR	N-CA-C	5.81	120.52	113.38
1	A	542	ALA	CA-C-N	5.79	127.86	120.56
1	A	542	ALA	C-N-CA	5.79	127.86	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	71	GLY	CA-C-N	5.72	128.27	120.54
1	B	71	GLY	C-N-CA	5.72	128.27	120.54
1	C	394	CYS	N-CA-C	5.71	117.96	111.11
1	A	506	THR	N-CA-C	5.69	116.98	109.93
1	A	559	TYR	N-CA-C	5.67	121.09	113.72
1	D	293	GLU	CA-C-N	5.66	128.43	120.28
1	D	293	GLU	C-N-CA	5.66	128.43	120.28
1	D	131	GLY	N-CA-C	5.61	118.42	110.74
1	B	77	ASP	N-CA-C	5.55	118.17	111.40
1	A	178	ASN	N-CA-C	5.52	118.48	111.69
1	C	303	LEU	N-CA-C	-5.52	102.31	110.48
1	D	559	TYR	N-CA-C	5.49	120.85	113.72
1	B	514	SER	CA-C-N	5.47	127.55	120.44
1	B	514	SER	C-N-CA	5.47	127.55	120.44
1	C	275	THR	CA-C-N	5.47	128.16	120.28
1	C	275	THR	C-N-CA	5.47	128.16	120.28
1	C	131	GLY	N-CA-C	5.45	117.79	110.43
1	C	542	ALA	CA-C-N	5.40	127.37	120.56
1	C	542	ALA	C-N-CA	5.40	127.37	120.56
1	A	172	VAL	N-CA-C	5.39	115.62	107.75
1	B	347	HIS	N-CA-C	-5.37	105.86	112.90
1	B	450	ASP	N-CA-C	5.36	118.61	111.75
1	D	58	LEU	N-CA-C	5.36	117.15	108.26
1	C	119	TRP	N-CA-C	5.34	118.59	111.75
1	A	459	GLY	CA-C-N	5.34	128.56	120.77
1	A	459	GLY	C-N-CA	5.34	128.56	120.77
1	A	119	TRP	N-CA-C	5.29	117.74	111.33
1	A	336	GLY	CA-C-N	5.25	127.31	120.28
1	A	336	GLY	C-N-CA	5.25	127.31	120.28
1	C	484	PHE	CA-CB-CG	5.23	119.03	113.80
1	A	160	ILE	CA-C-N	5.21	127.26	120.28
1	A	160	ILE	C-N-CA	5.21	127.26	120.28
1	C	559	TYR	N-CA-C	5.19	119.77	113.38
1	D	71	GLY	CA-C-N	5.19	127.55	120.54
1	D	71	GLY	C-N-CA	5.19	127.55	120.54
1	B	449	GLN	N-CA-C	-5.18	100.64	108.67
1	D	459	GLY	N-CA-C	5.14	120.42	112.45
1	D	77	ASP	N-CA-C	5.10	117.96	111.69
1	B	504	ASN	CA-CB-CG	5.09	117.69	112.60
1	B	459	GLY	CA-C-N	5.09	128.12	120.69
1	B	459	GLY	C-N-CA	5.09	128.12	120.69
1	B	472	THR	N-CA-C	5.05	117.66	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	TYR	CA-C-N	5.05	127.38	120.46
1	A	1	TYR	C-N-CA	5.05	127.38	120.46
1	D	127	LEU	N-CA-C	5.02	117.43	109.24

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3775	0	3682	23	0
1	B	3779	0	3702	28	0
1	C	3770	0	3650	25	0
1	D	3686	0	3523	17	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	131	0	0	1	0
3	B	141	0	0	1	0
3	C	105	0	0	1	0
3	D	67	0	0	0	0
All	All	15462	0	14557	84	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 3.

All (84) 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:B:63:ARG:HD2	1:B:388:VAL:HG21	1.58	0.83
1:B:340:LEU:HD13	1:B:557:TYR:HB3	1.69	0.74
1:C:134:LEU:HD21	1:C:141:LEU:HD23	1.73	0.68
1:C:340:LEU:HD13	1:C:557:TYR:HB3	1.76	0.66
1:B:457:HIS:CE1	1:B:542:ALA:HB1	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:VAL:HG11	1:B:289:LEU:HD11	1.80	0.63
1:D:59:CYS:HA	1:D:64:ASN:O	1.99	0.62
1:A:134:LEU:HD11	1:B:475:LEU:HD12	1.81	0.61
1:A:120:HIS:HB3	1:A:174:ILE:HD11	1.83	0.61
1:C:307:GLN:HG3	1:D:307:GLN:HG3	1.85	0.59
1:B:340:LEU:HD13	1:B:557:TYR:CB	2.35	0.57
1:A:323:ARG:NH2	3:A:1169:HOH:O	2.38	0.56
1:A:457:HIS:CE1	1:A:542:ALA:HB1	2.39	0.56
1:C:457:HIS:CE1	1:C:542:ALA:HB1	2.41	0.56
1:C:533:ALA:O	1:C:536:SER:HB3	2.06	0.55
1:B:63:ARG:CD	1:B:388:VAL:HG21	2.34	0.55
1:B:63:ARG:HD3	1:B:378:ASP:OD2	2.07	0.55
1:B:66:CYS:HB2	1:B:375:ILE:HD12	1.89	0.55
1:C:323:ARG:HB3	1:C:327:LEU:HD22	1.89	0.54
1:A:70:VAL:HG11	1:A:406:VAL:HG21	1.91	0.53
1:A:63:ARG:O	1:A:378:ASP:HB2	2.08	0.52
1:A:176:TYR:HA	1:A:180:ILE:HD12	1.91	0.52
1:C:124:ASP:HA	1:C:154:PHE:CZ	2.44	0.52
1:D:457:HIS:CE1	1:D:542:ALA:HB1	2.45	0.51
1:B:134:LEU:HD11	1:C:475:LEU:HD12	1.92	0.51
1:A:53:ASN:HB2	1:A:72:LYS:HG3	1.95	0.49
1:B:393:TYR:CE2	1:B:397:ASN:HB2	2.47	0.49
1:B:63:ARG:O	1:B:88:ILE:HD11	2.13	0.49
1:C:133:VAL:HG11	1:C:289:LEU:HD11	1.95	0.48
1:B:502:VAL:HG21	1:B:508:CYS:HB2	1.94	0.48
1:A:340:LEU:HD13	1:A:557:TYR:HB3	1.96	0.47
1:C:63:ARG:O	1:C:378:ASP:HB2	2.15	0.47
1:C:114:TYR:OH	1:C:379:HIS:HA	2.14	0.47
1:A:66:CYS:HB2	1:A:375:ILE:HD12	1.97	0.46
1:B:141:LEU:HD11	1:C:482:ARG:HG2	1.97	0.46
1:A:141:LEU:HD21	1:B:482:ARG:HG2	1.98	0.46
1:A:14:LEU:HD22	1:A:309:PRO:HB2	1.97	0.46
1:A:42:LEU:HD23	1:A:58:LEU:HD22	1.97	0.45
1:A:160:ILE:HG12	1:A:165:ARG:HD2	1.99	0.45
1:A:133:VAL:HG11	1:A:289:LEU:HD11	1.98	0.45
1:B:127:LEU:HD13	1:B:303:LEU:HD23	1.99	0.45
1:C:454:LEU:HD21	1:C:500:PHE:HB2	1.98	0.45
1:C:439:CYS:HB2	1:C:530:PRO:HB2	1.99	0.45
1:D:133:VAL:HG11	1:D:289:LEU:HD11	1.99	0.45
1:B:124:ASP:HA	1:B:154:PHE:CZ	2.51	0.44
1:D:407:PHE:HB3	1:D:410:GLU:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:79:GLY:HA2	1:C:369:ASN:HD22	1.83	0.43
1:D:24:PHE:HB3	1:D:145:LEU:HD22	2.00	0.43
1:A:124:ASP:HA	1:A:154:PHE:CZ	2.53	0.43
1:C:323:ARG:O	1:C:327:LEU:HB2	2.19	0.43
1:B:99:ASN:HA	1:B:110:ASN:HB2	2.00	0.43
1:D:529:ILE:HG21	1:D:545:ASP:O	2.19	0.43
1:B:506:THR:HG21	3:B:1202:HOH:O	2.19	0.43
1:D:393:TYR:CE2	1:D:397:ASN:HB2	2.54	0.43
1:A:59:CYS:HA	1:A:64:ASN:O	2.19	0.42
1:C:27:CYS:SG	1:C:59:CYS:SG	3.02	0.42
1:B:503:LYS:O	1:B:506:THR:HB	2.20	0.42
1:A:108:GLN:HG2	1:A:183:ILE:HG22	2.01	0.42
1:C:110:ASN:ND2	3:C:1160:HOH:O	2.53	0.42
1:B:114:TYR:OH	1:B:379:HIS:HA	2.19	0.42
1:B:118:LEU:HD12	1:B:118:LEU:HA	1.91	0.42
1:D:326:ASN:OD1	1:D:329:GLY:HA3	2.20	0.42
1:B:134:LEU:HD21	1:C:475:LEU:HG	2.02	0.42
1:A:27[A]:CYS:SG	1:A:59:CYS:SG	3.14	0.41
1:B:63:ARG:HH22	1:B:300:GLU:CD	2.26	0.41
1:C:63:ARG:O	1:C:88:ILE:HD11	2.20	0.41
1:B:14:LEU:HD21	1:B:319:ILE:HB	2.02	0.41
1:A:344:ILE:C	1:A:346:ASN:H	2.28	0.41
1:C:116:SER:O	1:D:160:ILE:HG21	2.20	0.41
1:D:124:ASP:HA	1:D:154:PHE:CZ	2.55	0.41
1:B:304:MET:HE2	1:B:304:MET:HB3	1.95	0.41
1:D:428:ARG:HA	1:D:564:LEU:HD21	2.03	0.41
1:B:27[B]:CYS:SG	1:B:88:ILE:HG12	2.61	0.41
1:C:70:VAL:HG11	1:C:406:VAL:HG21	2.02	0.41
1:D:435:ASP:O	1:D:528:GLY:HA3	2.20	0.41
1:D:482:ARG:HD3	1:D:482:ARG:HA	1.92	0.41
1:A:410:GLU:HA	1:A:414:LYS:HB2	2.03	0.40
1:A:59:CYS:SG	1:A:65:ILE:HD12	2.61	0.40
1:C:540:ILE:HD13	1:D:183:ILE:HD11	2.03	0.40
1:D:127:LEU:HD13	1:D:303:LEU:HD23	2.02	0.40
1:A:482:ARG:HG2	1:C:141:LEU:HD21	2.03	0.40
1:B:24:PHE:HB3	1:B:145:LEU:HD22	2.03	0.40
1:C:14:LEU:HD22	1:C:309:PRO:HB2	2.03	0.40
1:D:126:SER:HB3	1:D:151:SER:HB2	2.04	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	467/571 (82%)	453 (97%)	14 (3%)	0	100	100
1	B	467/571 (82%)	457 (98%)	10 (2%)	0	100	100
1	C	467/571 (82%)	451 (97%)	16 (3%)	0	100	100
1	D	462/571 (81%)	444 (96%)	17 (4%)	1 (0%)	43	66
All	All	1863/2284 (82%)	1805 (97%)	57 (3%)	1 (0%)	48	70

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	535	HIS

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	417/527 (79%)	402 (96%)	15 (4%)	31	58
1	B	418/527 (79%)	402 (96%)	16 (4%)	29	56
1	C	414/527 (79%)	402 (97%)	12 (3%)	37	65
1	D	399/527 (76%)	381 (96%)	18 (4%)	24	50
All	All	1648/2108 (78%)	1587 (96%)	61 (4%)	31	57

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	VAL
1	A	65	ILE
1	A	109	ILE
1	A	118	LEU
1	A	141	LEU
1	A	191	GLN
1	A	195	CYS
1	A	294	GLU
1	A	314	VAL
1	A	369	ASN
1	A	375	ILE
1	A	426	VAL
1	A	440	SER
1	A	478	SER
1	A	526	ASP
1	B	2	VAL
1	B	18	GLN
1	B	110	ASN
1	B	118	LEU
1	B	141	LEU
1	B	146	ILE
1	B	173	LYS
1	B	191	GLN
1	B	193	ASN
1	B	294	GLU
1	B	340	LEU
1	B	409	LYS
1	B	426	VAL
1	B	478	SER
1	B	482	ARG
1	B	506	THR
1	C	3	ASP
1	C	181	LYS
1	C	191	GLN
1	C	290	ASN
1	C	327	LEU
1	C	340	LEU
1	C	367	ILE
1	C	426	VAL
1	C	466	THR
1	C	482	ARG
1	C	536	SER
1	C	569	HIS

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Mol	Chain	Res	Type
1	D	3	ASP
1	D	18	GLN
1	D	25	LEU
1	D	27[A]	CYS
1	D	27[C]	CYS
1	D	75	ASN
1	D	134	LEU
1	D	137	LYS
1	D	141	LEU
1	D	191	GLN
1	D	294	GLU
1	D	314	VAL
1	D	340	LEU
1	D	426	VAL
1	D	458	GLU
1	D	478	SER
1	D	526	ASP
1	D	531	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	98	ASN
1	A	368	HIS
1	A	370	ASN
1	A	469	ASN
1	A	493	GLN
1	A	499	ASN
1	B	18	GLN
1	B	193	ASN
1	B	465	ASN
1	B	467	ASN
1	B	499	ASN
1	C	49	ASN
1	C	369	ASN
1	C	412	HIS
1	C	415	ASN
1	C	465	ASN
1	C	467	ASN
1	C	469	ASN
1	C	499	ASN

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Mol	Chain	Res	Type
1	D	178	ASN
1	D	290	ASN
1	D	368	HIS
1	D	561	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 8 ligands modelled in this entry, 8 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 ⓘ

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, 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	474/571 (83%)	-0.53	13 (2%)	56 50	21, 34, 64, 103	1 (0%)
1	B	473/571 (82%)	-0.52	13 (2%)	56 50	20, 34, 62, 99	2 (0%)
1	C	475/571 (83%)	-0.36	13 (2%)	56 50	26, 40, 68, 114	0
1	D	469/571 (82%)	-0.05	10 (2%)	63 58	34, 53, 79, 117	1 (0%)
All	All	1891/2284 (82%)	-0.37	49 (2%)	57 51	20, 40, 73, 117	4 (0%)

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	349	SER	6.7
1	D	195	CYS	6.7
1	B	195	CYS	5.3
1	B	170	PHE	5.0
1	C	170	PHE	5.0
1	A	347	HIS	4.7
1	B	1	TYR	4.6
1	B	274	ASN	4.5
1	B	346	ASN	4.4
1	D	274	ASN	4.2
1	C	274	ASN	4.2
1	D	349	SER	4.1
1	D	365	ASP	3.9
1	A	364	ASN	3.8
1	A	196	LYS	3.8
1	C	352	ASN	3.7
1	C	171	SER	3.7
1	D	164	ASN	3.5
1	C	172	VAL	3.5
1	C	349	SER	3.4
1	B	172	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	172	VAL	3.4
1	A	1	TYR	3.3
1	B	2	VAL	3.3
1	D	348	THR	3.2
1	C	510	SER	3.2
1	B	365	ASP	3.1
1	B	273	ILE	3.1
1	A	366	ASN	3.1
1	C	365	ASP	3.0
1	B	164	ASN	3.0
1	D	2	VAL	3.0
1	A	170	PHE	3.0
1	C	196	LYS	2.8
1	D	366	ASN	2.8
1	C	164	ASN	2.7
1	A	165	ARG	2.7
1	A	273	ILE	2.7
1	A	508	CYS	2.5
1	A	365	ASP	2.4
1	C	507	PRO	2.4
1	A	2	VAL	2.4
1	C	505	ASP	2.3
1	B	412	HIS	2.2
1	B	366	ASN	2.2
1	A	195	CYS	2.2
1	C	570	ASP	2.2
1	D	507	PRO	2.0
1	D	40	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no 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($\text{\AA}^2$)	Q<0.9
2	ZN	A	1002	1/1	0.98	0.07	40,40,40,40	0
2	ZN	B	1002	1/1	0.98	0.06	41,41,41,41	0
2	ZN	C	1001	1/1	0.98	0.05	44,44,44,44	0
2	ZN	D	1002	1/1	0.98	0.06	54,54,54,54	0
2	ZN	B	1001	1/1	0.99	0.05	36,36,36,36	0
2	ZN	C	1002	1/1	0.99	0.06	47,47,47,47	0
2	ZN	D	1001	1/1	0.99	0.04	57,57,57,57	0
2	ZN	A	1001	1/1	0.99	0.06	42,42,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.