



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:30 PM UTC

PDB ID : 5JR6 / pdb_00005jr6
Title : The Xray Crystal Structure of P. falciparum Aminopeptidase P in Complex With Apstatin
Authors : Drinkwater, N.; McGowan, S.
Deposited on : 2016-05-05
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

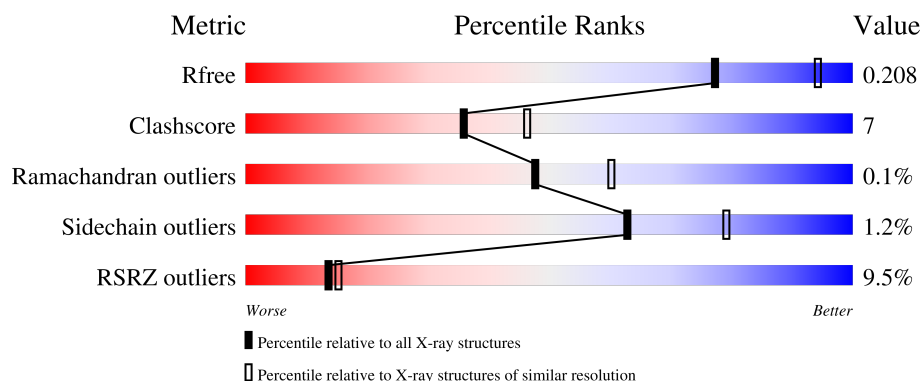
1 Overall quality at a glance

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	664	9% 78% 16% • 5%
1	B	664	8% 70% 12% 18%
2	F	5	20% 40% 60%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9214 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 Peptidase, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	628	Total	C	N	O	S	0	0	0
			4841	3120	794	911	16			
1	B	545	Total	C	N	O	S	0	0	0
			4138	2659	687	778	14			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	120	MET	-	initiating methionine	UNP Q8IKT5
A	778	HIS	-	expression tag	UNP Q8IKT5
A	779	HIS	-	expression tag	UNP Q8IKT5
A	780	HIS	-	expression tag	UNP Q8IKT5
A	781	HIS	-	expression tag	UNP Q8IKT5
A	782	HIS	-	expression tag	UNP Q8IKT5
A	783	HIS	-	expression tag	UNP Q8IKT5
B	120	MET	-	initiating methionine	UNP Q8IKT5
B	778	HIS	-	expression tag	UNP Q8IKT5
B	779	HIS	-	expression tag	UNP Q8IKT5
B	780	HIS	-	expression tag	UNP Q8IKT5
B	781	HIS	-	expression tag	UNP Q8IKT5
B	782	HIS	-	expression tag	UNP Q8IKT5
B	783	HIS	-	expression tag	UNP Q8IKT5

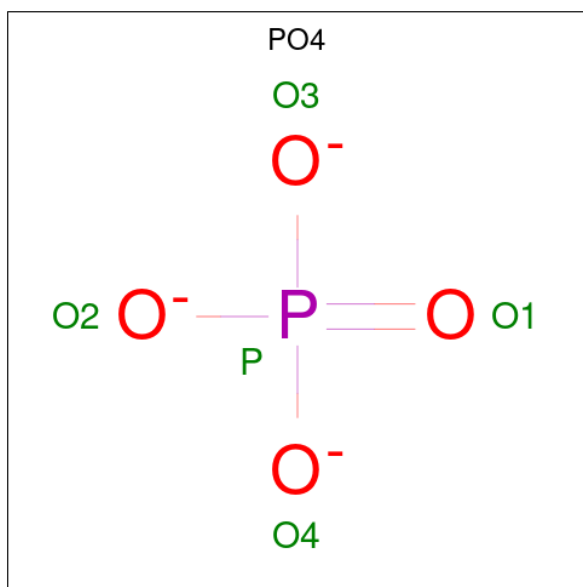
- Molecule 2 is a protein called Apstatin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	F	5	Total	C	N	O	0	0	1
			33	23	5	5			

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mn	0	0
			2	2		
3	B	2	Total	Mn	0	0
			2	2		

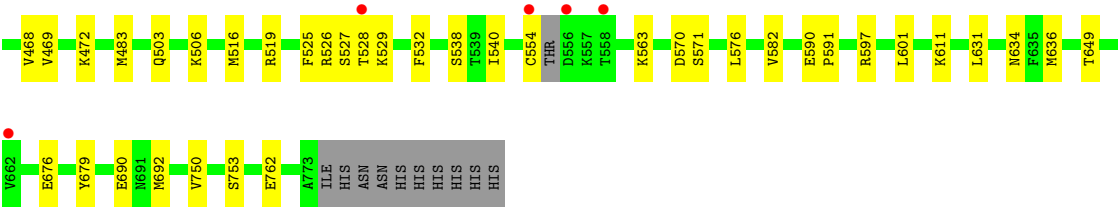
- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	105	Total	O	0	0
			105	105		
5	B	88	Total	O	0	0
			88	88		



● Molecule 2: Apstatin



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	147.22Å 99.93Å 105.17Å 90.00° 105.21° 90.00°	Depositor
Resolution (Å)	42.79 – 2.30 42.79 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.5 (42.79-2.30) 99.5 (42.79-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.197 , 0.241 0.209 , 0.208	Depositor DCC
R_{free} test set	3232 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	42.2	Xtriage
Anisotropy	0.499	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 71.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9214	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% 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: NH2, PO4, 01B, MN

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	0.52	0/4938	0.90	7/6706 (0.1%)
1	B	0.52	0/4218	0.86	2/5724 (0.0%)
2	F	4.19	2/20 (10.0%)	1.96	2/27 (7.4%)
All	All	0.55	2/9176 (0.0%)	0.89	11/12457 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	2	PRO	C-N	12.93	1.50	1.34
2	F	3	PRO	C-N	12.17	1.50	1.33

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	131	ASN	CA-C-N	11.71	132.04	119.05
1	A	131	ASN	C-N-CA	11.71	132.04	119.05
1	A	660	GLY	CA-C-N	7.05	126.67	119.19
1	A	660	GLY	C-N-CA	7.05	126.67	119.19
1	B	753	SER	CA-C-N	5.56	125.92	119.47
1	B	753	SER	C-N-CA	5.56	125.92	119.47
1	A	190	LYS	CA-C-N	5.44	125.44	119.89
1	A	190	LYS	C-N-CA	5.44	125.44	119.89
1	A	559	ASN	N-CA-C	5.42	118.08	109.96
2	F	2	PRO	CA-C-N	5.36	124.87	119.19
2	F	2	PRO	C-N-CA	5.36	124.87	119.19

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	4841	0	4574	77	0
1	B	4138	0	3835	51	0
2	F	33	0	24	3	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	B	5	0	0	0	0
5	A	105	0	0	2	0
5	B	88	0	0	4	0
All	All	9214	0	8433	128	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 7.

All (128) 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:377:ARG:O	1:B:380:GLN:CB	2.18	0.91
1:A:669:LYS:HD2	1:A:697:SER:HB2	1.58	0.85
1:B:634:ASN:HB2	1:B:636:MET:HE2	1.61	0.83
1:B:601:LEU:HD13	1:B:636:MET:HE1	1.60	0.83
1:B:468:VAL:O	5:B:901:HOH:O	1.98	0.82
1:A:132:PRO:HB3	1:A:174:ILE:O	1.81	0.80
1:B:380:GLN:O	1:B:381:ASP:HB2	1.80	0.80
1:A:634:ASN:HB2	1:A:636:MET:HE2	1.62	0.79
1:A:154:ILE:HG12	1:A:183:ILE:HG23	1.67	0.77
1:A:272:ASN:HA	1:A:294:LYS:HE2	1.69	0.75
1:A:348:ASP:OD2	1:A:472:LYS:NZ	2.20	0.74
1:B:376:ASP:O	1:B:377:ARG:C	2.32	0.71
1:A:378:GLU:O	1:A:380:GLN:N	2.23	0.71
1:A:631:LEU:HD23	1:A:636:MET:HE3	1.72	0.70
1:A:291:VAL:HG21	1:A:454:LYS:HG3	1.74	0.69
1:A:601:LEU:HD13	1:A:636:MET:HE1	1.73	0.69
1:A:225:ILE:O	1:A:229:ILE:HG12	1.93	0.69
1:B:472:LYS:N	5:B:901:HOH:O	2.04	0.68
1:A:273:ASN:N	1:A:294:LYS:HZ1	1.91	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:519:ARG:NH2	1:B:538:SER:OG	2.26	0.67
1:A:629:GLU:OE2	5:A:901:HOH:O	2.13	0.66
1:A:714:MET:HE1	1:A:741:THR:HG22	1.80	0.64
1:B:154:ILE:HG23	1:B:183:ILE:HG12	1.81	0.63
1:A:519:ARG:NH2	1:A:538:SER:OG	2.31	0.62
1:B:516:MET:SD	1:B:554:CYS:HB3	2.41	0.61
1:A:549:VAL:HB	1:A:552:TYR:HB2	1.83	0.61
1:A:453:TYR:CE1	1:A:461:VAL:HG21	2.38	0.59
1:B:360:ASP:HB2	1:B:367:PHE:HA	1.84	0.58
1:B:324:LYS:NZ	1:B:355:ASN:OD1	2.38	0.56
1:A:634:ASN:CB	1:A:636:MET:HE2	2.32	0.55
1:A:759:GLU:HA	1:A:762:GLU:HG2	1.89	0.55
1:A:320:CYS:SG	5:A:1004:HOH:O	2.58	0.54
1:B:313:ASP:OD1	1:B:314:ARG:N	2.40	0.54
1:A:207:LEU:HD11	1:A:212:PHE:HB2	1.90	0.54
1:B:324:LYS:HE2	1:B:352:TYR:CZ	2.43	0.53
1:B:365:PRO:HG3	1:B:649:THR:HG22	1.92	0.52
1:B:293:GLU:HA	1:B:451:MET:HE3	1.90	0.52
1:A:253:ARG:HH21	1:A:254:LYS:HZ2	1.58	0.52
1:B:611:LYS:NZ	5:B:907:HOH:O	2.43	0.52
1:B:540:ILE:HB	1:B:570:ASP:HB3	1.91	0.52
1:A:329:LYS:NZ	1:A:380:GLN:O	2.39	0.52
1:A:453:TYR:HE1	1:A:461:VAL:HG21	1.75	0.52
1:A:659:ILE:HG13	1:A:673:LEU:HD22	1.91	0.51
1:A:640:HIS:CG	2:F:2:PRO:HB3	2.46	0.51
1:B:527:SER:HA	1:B:532:PHE:CD2	2.45	0.50
1:A:273:ASN:H	1:A:294:LYS:HZ1	1.59	0.50
1:A:597:ARG:NH2	1:A:634:ASN:OD1	2.45	0.50
1:B:246:VAL:HG13	1:B:448:ILE:O	2.11	0.50
1:A:356:LEU:O	1:A:357:ARG:HD3	2.12	0.50
1:B:402:LEU:HD13	1:B:409:VAL:HG21	1.95	0.49
1:A:250:GLU:OE2	1:A:254:LYS:NZ	2.45	0.49
1:A:332:LEU:O	1:A:377:ARG:NH1	2.35	0.49
1:A:259:ALA:C	1:A:260:TYR:HD1	2.20	0.49
1:B:158:GLU:HA	1:B:242:LYS:O	2.13	0.49
1:A:513:GLU:OE1	1:A:517:SER:OG	2.28	0.49
1:B:438:LYS:HE3	1:B:440:TYR:CE1	2.48	0.48
1:A:527:SER:HA	1:A:532:PHE:CD2	2.49	0.48
1:A:250:GLU:OE1	1:A:458:ARG:NH2	2.46	0.48
1:B:315:LYS:HE3	1:B:316:TYR:CZ	2.48	0.47
1:A:507:THR:O	1:A:508:LYS:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:ASN:HD22	1:A:275:PHE:HE2	1.63	0.47
1:A:229:ILE:CD1	1:A:252:LEU:HD13	2.44	0.47
1:A:183:ILE:O	1:A:193:LEU:HD12	2.15	0.47
1:A:250:GLU:HB3	1:A:254:LYS:HZ3	1.80	0.46
1:B:339:VAL:HG22	1:B:341:ASN:H	1.80	0.46
1:B:503:GLN:HA	1:B:506:LYS:HE2	1.96	0.46
1:A:540:ILE:HB	1:A:570:ASP:HB3	1.98	0.46
1:B:315:LYS:HE3	1:B:316:TYR:CE2	2.50	0.46
1:A:314:ARG:HA	1:A:317:ASN:OD1	2.16	0.46
1:A:352:TYR:CD2	1:A:472:LYS:HG2	2.51	0.46
1:A:653:HIS:NE2	2:F:1:O1B:O	2.39	0.46
1:A:519:ARG:HG3	1:A:539:THR:HB	1.98	0.45
1:A:177:TYR:CZ	1:A:179:GLY:HA3	2.52	0.45
1:A:339:VAL:CG1	1:A:440:TYR:HB2	2.47	0.45
1:B:246:VAL:HG12	1:B:450:LEU:HD23	1.97	0.45
1:A:151:TYR:CE2	1:A:153:LEU:HG	2.51	0.45
1:A:246:VAL:HG13	1:A:448:ILE:O	2.16	0.45
1:B:416:VAL:HB	1:B:417:PRO:HD3	1.98	0.45
1:A:223:ASP:HA	1:A:226:PHE:HD2	1.81	0.44
1:A:497:PHE:CE2	1:A:569:LEU:HD22	2.52	0.44
1:B:631:LEU:HD23	1:B:636:MET:HE3	1.98	0.44
1:B:636:MET:HB3	1:B:679:TYR:CE1	2.52	0.44
1:A:310:TYR:CZ	1:A:357:ARG:HB2	2.51	0.44
1:A:293:GLU:HA	1:A:451:MET:HE3	2.00	0.44
1:A:329:LYS:HG2	1:A:333:MET:HE2	1.99	0.44
1:A:675:ASN:O	1:A:690:GLU:HA	2.18	0.44
1:B:267:GLU:HA	1:B:289:PHE:O	2.18	0.43
1:B:246:VAL:HG22	1:B:446:PRO:O	2.18	0.43
1:B:308:THR:HG22	1:B:309:LEU:O	2.18	0.43
1:B:676:GLU:HB3	1:B:690:GLU:HG3	1.99	0.43
1:A:190:LYS:HA	1:A:191:PRO:HD2	1.84	0.43
1:B:529:LYS:HA	1:B:529:LYS:HD3	1.83	0.43
1:A:468:VAL:O	1:A:472:LYS:HG3	2.18	0.43
1:B:526:ARG:HH12	1:B:571:SER:HB2	1.83	0.43
1:A:714:MET:HE3	1:A:742:ILE:HA	2.01	0.43
1:B:380:GLN:O	1:B:381:ASP:CB	2.55	0.43
1:B:519:ARG:HH11	1:B:554:CYS:HB2	1.84	0.43
1:A:644:HIS:HB3	2:F:3:PRO:HB3	2.00	0.43
1:A:759:GLU:HA	1:A:762:GLU:CG	2.49	0.43
1:A:166:GLU:HA	1:A:169:LYS:HG3	2.01	0.43
1:B:525:PHE:O	1:B:528:THR:HG22	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:684:LYS:HB3	1:A:684:LYS:HE3	1.90	0.42
1:A:253:ARG:NH2	1:A:254:LYS:HZ2	2.15	0.42
1:A:631:LEU:CD2	1:A:636:MET:HE3	2.47	0.42
1:B:469:VAL:C	5:B:901:HOH:O	2.62	0.42
1:A:413:GLU:H	1:A:413:GLU:CD	2.28	0.42
1:A:544:GLY:HA3	1:A:545:PRO:HD3	1.88	0.42
1:A:192:ILE:HG13	1:A:213:THR:HB	2.02	0.42
1:A:264:LYS:O	1:A:287:LEU:N	2.53	0.42
1:A:352:TYR:HB2	1:A:650:LEU:HD11	2.01	0.41
1:B:590:GLU:HA	1:B:591:PRO:HD3	1.90	0.41
1:B:750:VAL:HG12	1:B:762:GLU:HG2	2.01	0.41
1:A:340:ASP:OD1	1:A:377:ARG:NE	2.50	0.41
1:A:601:LEU:CD1	1:A:636:MET:HE1	2.47	0.41
1:B:442:ILE:HG13	1:B:443:SER:N	2.35	0.41
1:B:611:LYS:HD3	1:B:611:LYS:HA	1.86	0.41
1:A:131:ASN:O	1:A:134:ALA:HB3	2.21	0.41
1:B:316:TYR:CE2	1:B:576:LEU:HD13	2.55	0.41
1:A:352:TYR:CG	1:A:472:LYS:HG2	2.55	0.41
1:B:597:ARG:NH2	1:B:634:ASN:OD1	2.52	0.41
1:B:422:VAL:C	1:B:425:PRO:HD2	2.47	0.40
1:B:307:LYS:HE2	1:B:359:TYR:HB3	2.03	0.40
1:B:399:LYS:HA	1:B:402:LEU:HD12	2.03	0.40
1:B:483:MET:HE3	1:B:692:MET:HE1	2.03	0.40
1:A:272:ASN:HA	1:A:294:LYS:CE	2.44	0.40
1:A:273:ASN:H	1:A:294:LYS:NZ	2.19	0.40
1:A:324:LYS:HB3	1:A:353:LEU:HD12	2.04	0.40
1:A:394:LEU:HD12	1:A:394:LEU:HA	1.92	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	616/664 (93%)	602 (98%)	14 (2%)	0	100	100
1	B	525/664 (79%)	511 (97%)	13 (2%)	1 (0%)	43	55
2	F	3/5 (60%)	1 (33%)	2 (67%)	0	100	100
All	All	1144/1333 (86%)	1114 (97%)	29 (2%)	1 (0%)	48	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	381	ASP

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	491/613 (80%)	483 (98%)	8 (2%)	55	73
1	B	409/613 (67%)	406 (99%)	3 (1%)	76	87
2	F	2/2 (100%)	2 (100%)	0	100	100
All	All	902/1228 (74%)	891 (99%)	11 (1%)	63	79

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	201	LEU
1	A	244	THR
1	A	293	GLU
1	A	294	LYS
1	A	490	ASP
1	A	696	ILE
1	A	759	GLU
1	A	774	ILE
1	B	222	ARG
1	B	563	LYS
1	B	582	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	ASN
1	A	374	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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
2	01B	F	1	2,3	11,13,14	4.21	4 (36%)	12,16,18	0.81	0

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
2	01B	F	1	2,3	-	8/9/10/12	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1	01B	C9-C8	8.74	1.53	1.38
2	F	1	01B	C12-C7	7.87	1.54	1.38
2	F	1	01B	C11-C10	6.37	1.52	1.38
2	F	1	01B	C6-C7	2.62	1.57	1.51

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	1	01B	O2-CA-CB-N
2	F	1	01B	C-CA-CB-N
2	F	1	01B	O2-CA-CB-C6
2	F	1	01B	C-CA-CB-C6
2	F	1	01B	CB-C6-C7-C8
2	F	1	01B	CB-C6-C7-C12
2	F	1	01B	C7-C6-CB-N
2	F	1	01B	C7-C6-CB-CA

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	1	01B	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 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	$\# Z > 2$
4	PO4	B	803	3	4,4,4	0.86	0	6,6,6	0.67	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

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, 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	628/664 (94%)	0.43	60 (9%)	13 15	26, 60, 124, 163	3 (0%)
1	B	545/664 (82%)	0.48	51 (9%)	14 15	31, 69, 124, 168	1 (0%)
2	F	3/5 (60%)	1.98	1 (33%)	1 1	82, 82, 101, 106	0
All	All	1176/1333 (88%)	0.46	112 (9%)	14 15	26, 65, 124, 168	4 (0%)

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	403	GLU	7.3
1	B	302	TYR	4.9
1	B	427	ILE	4.4
1	B	405	ASN	4.4
1	B	401	LEU	4.2
1	A	212	PHE	4.1
1	B	229	ILE	4.1
1	A	296	LEU	4.0
1	B	380	GLN	3.9
1	B	436	ASP	3.8
1	A	234	PHE	3.8
1	A	260	TYR	3.8
1	A	236	THR	3.7
1	A	194	TYR	3.7
1	B	216	ILE	3.7
1	B	415	ILE	3.7
1	A	229	ILE	3.6
1	A	235	ASN	3.6
1	A	427	ILE	3.6
1	A	400	ASN	3.5
1	A	150	VAL	3.4
1	B	397	ASP	3.4
1	A	437	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	299	ILE	3.3
1	B	558	THR	3.2
1	A	278	VAL	3.2
1	B	258	ASN	3.2
1	A	232	LEU	3.1
1	A	208	ASP	3.1
1	B	260	TYR	3.1
1	A	237	ILE	3.1
1	B	398	VAL	3.0
1	A	201	LEU	3.0
1	A	222	ARG	3.0
2	F	4	ALA	3.0
1	A	199	TYR	2.9
1	A	176	ASN	2.9
1	A	151	TYR	2.8
1	B	296	LEU	2.8
1	A	398	VAL	2.8
1	B	297	VAL	2.8
1	B	556	ASP	2.8
1	A	397	ASP	2.8
1	A	193	LEU	2.8
1	A	186	VAL	2.8
1	B	238	ALA	2.8
1	A	405	ASN	2.7
1	B	421	ASP	2.7
1	A	396	ALA	2.7
1	B	423	VAL	2.7
1	A	170	LYS	2.7
1	A	211	LEU	2.7
1	B	437	PHE	2.6
1	A	269	ILE	2.6
1	B	163	ILE	2.6
1	B	261	PRO	2.6
1	A	152	ILE	2.6
1	A	175	THR	2.6
1	B	662	VAL	2.6
1	A	274	ASN	2.5
1	A	134	ALA	2.5
1	A	428	PRO	2.5
1	B	382	PHE	2.5
1	A	404	ILE	2.5
1	A	174	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	429	LYS	2.4
1	A	133	ALA	2.4
1	B	295	SER	2.4
1	B	239	PHE	2.4
1	B	384	LYS	2.4
1	B	455	LEU	2.4
1	A	168	ASP	2.3
1	A	182	GLY	2.3
1	A	426	SER	2.3
1	B	334	TYR	2.3
1	A	172	VAL	2.3
1	B	554	CYS	2.3
1	B	308	THR	2.3
1	B	215	ARG	2.2
1	B	266	VAL	2.2
1	A	129	ASP	2.2
1	B	181	ASP	2.2
1	B	528	THR	2.2
1	A	171	ILE	2.2
1	A	136	LEU	2.2
1	B	402	LEU	2.2
1	A	507	THR	2.2
1	B	332	LEU	2.2
1	B	376	ASP	2.2
1	A	241	GLY	2.2
1	A	558	THR	2.2
1	B	259	ALA	2.2
1	A	177	TYR	2.1
1	B	366	LEU	2.1
1	B	391	VAL	2.1
1	A	230	SER	2.1
1	B	377	ARG	2.1
1	B	269	ILE	2.1
1	B	403	GLU	2.1
1	B	386	VAL	2.1
1	A	436	ASP	2.1
1	A	209	GLN	2.1
1	B	182	GLY	2.1
1	A	219	ILE	2.1
1	B	373	PHE	2.1
1	B	309	LEU	2.0
1	B	265	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	289	PHE	2.0
1	A	238	ALA	2.0
1	A	130	ASN	2.0
1	A	207	LEU	2.0
1	B	222	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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	01B	F	1	13/14	0.91	0.19	35,72,82,82	6

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
4	PO4	B	803	5/5	0.92	0.10	66,73,79,82	0
3	MN	B	801	1/1	0.98	0.08	74,74,74,74	0
3	MN	A	801	1/1	0.98	0.05	62,62,62,62	0
3	MN	B	802	1/1	0.99	0.03	57,57,57,57	0
3	MN	A	802	1/1	1.00	0.03	42,42,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.