



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:56 PM UTC

PDB ID : 3H60 / pdb_00003h60
Title : Catalytic domain of human Serine/Threonine Phosphatase 5 (PP5c) with two Mn²⁺ atoms
Authors : Bertini, I.; Calderone, V.; Fragai, M.; Luchinat, C.; Talluri, E.
Deposited on : 2009-04-23
Resolution : 2.00 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

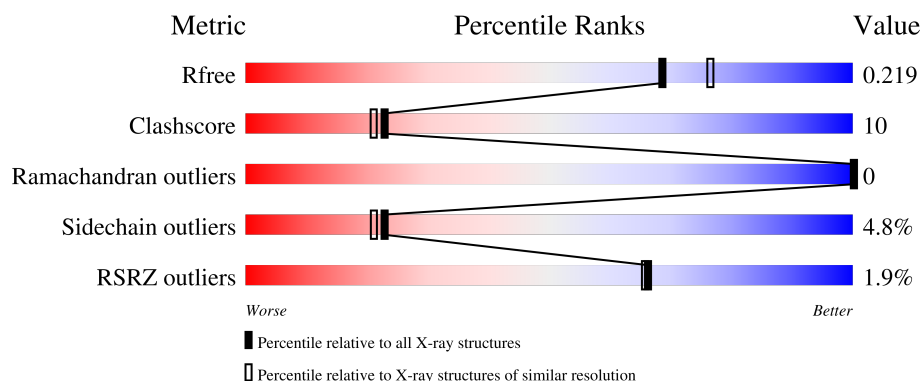
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	315	% 80% 16% ..
1	B	315	3% 79% 18% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5492 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 Serine/threonine-protein phosphatase 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	315	Total	C	N	O	S	0	0	0
			2528	1615	425	473	15			
1	B	315	Total	C	N	O	S	0	0	0
			2528	1615	425	473	15			

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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

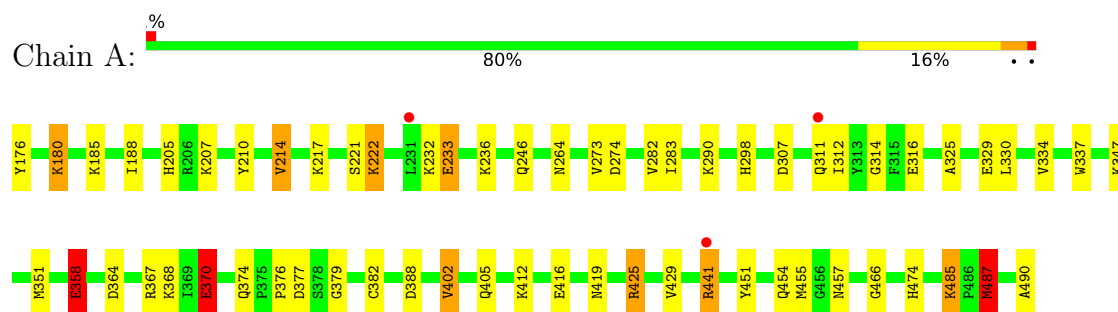
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	256	Total	O	0	0
			256	256		
3	B	176	Total	O	0	0
			176	176		

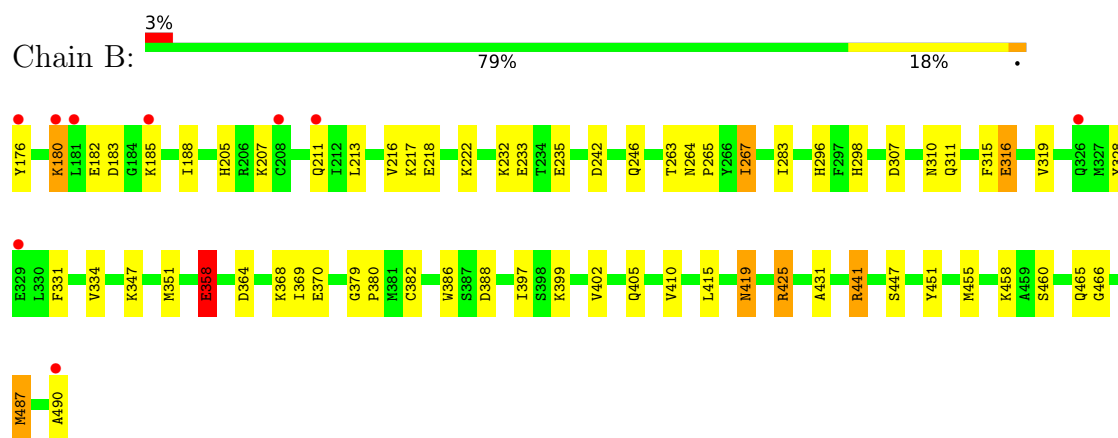
3 Residue-property plots

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: Serine/threonine-protein phosphatase 5



- Molecule 1: Serine/threonine-protein phosphatase 5



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	154.41Å 41.76Å 105.43Å 90.00° 97.07° 90.00°	Depositor
Resolution (Å)	65.80 – 2.00 65.80 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (65.80-2.00) 97.9 (65.80-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.57 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.4.0067	Depositor
R, R_{free}	0.161 , 0.219 0.160 , 0.219	Depositor DCC
R_{free} test set	4062 reflections (9.08%)	wwPDB-VP
Wilson B-factor (Å ²)	20.9	Xtriage
Anisotropy	0.355	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 49.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5492	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.04% 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: 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	1.41	7/2592 (0.3%)	1.21	12/3506 (0.3%)
1	B	1.19	7/2592 (0.3%)	1.14	10/3506 (0.3%)
All	All	1.30	14/5184 (0.3%)	1.17	22/7012 (0.3%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	283	ILE	CA-CB	7.07	1.63	1.54
1	A	358	GLU	CG-CD	6.61	1.68	1.52
1	B	358	GLU	CG-CD	6.21	1.67	1.52
1	A	264	ASN	C-O	-6.15	1.16	1.23
1	A	214	VAL	CA-CB	5.79	1.61	1.54
1	B	441	ARG	CZ-NH1	5.59	1.40	1.32
1	B	410	VAL	CA-CB	5.54	1.61	1.54
1	B	358	GLU	CB-CG	5.50	1.69	1.52
1	B	460	SER	CA-C	-5.48	1.45	1.52
1	A	441	ARG	CZ-NH1	5.44	1.40	1.32
1	B	382	CYS	CA-C	5.43	1.59	1.52
1	A	330	LEU	CA-C	5.11	1.59	1.52
1	B	431	ALA	CA-CB	5.09	1.61	1.53
1	A	282	VAL	C-O	-5.08	1.18	1.24

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	379	GLY	CA-C-N	8.42	128.40	119.05
1	A	379	GLY	C-N-CA	8.42	128.40	119.05
1	A	441	ARG	NE-CZ-NH2	-6.96	112.93	119.20
1	B	441	ARG	NE-CZ-NH2	-6.84	113.04	119.20
1	A	312	ILE	CB-CA-C	-6.59	103.63	111.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	379	GLY	CA-C-N	6.51	126.01	119.24
1	B	379	GLY	C-N-CA	6.51	126.01	119.24
1	B	316	GLU	CA-C-N	6.18	126.98	119.99
1	B	316	GLU	C-N-CA	6.18	126.98	119.99
1	A	314	GLY	N-CA-C	5.96	119.95	113.58
1	B	386	TRP	N-CA-C	5.72	121.69	114.31
1	A	374	GLN	CA-C-N	-5.47	115.67	119.66
1	A	374	GLN	C-N-CA	-5.47	115.67	119.66
1	B	370	GLU	CB-CA-C	5.41	120.39	111.31
1	A	370	GLU	CB-CG-CD	5.37	121.73	112.60
1	A	454	GLN	CB-CA-C	-5.36	100.76	109.13
1	A	487	MET	N-CA-C	5.34	119.37	112.86
1	B	267	ILE	CB-CA-C	-5.19	103.41	110.42
1	A	233	GLU	N-CA-C	5.11	117.75	111.82
1	B	283	ILE	N-CA-C	5.03	115.80	110.72
1	B	447	SER	N-CA-C	5.03	118.89	112.26
1	A	441	ARG	NE-CZ-NH1	5.02	126.52	121.50

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	2528	0	2462	61	0
1	B	2528	0	2462	43	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	256	0	0	27	0
3	B	176	0	0	14	0
All	All	5492	0	4924	104	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 10.

All (104) 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:441:ARG:HG3	3:A:628:HOH:O	1.25	1.28
1:B:441:ARG:HG3	3:B:600:HOH:O	1.14	1.24
1:B:267:ILE:HG13	3:B:598:HOH:O	1.44	1.14
1:A:307:ASP:O	1:A:311:GLN:HG2	1.47	1.13
1:A:236:LYS:HD3	3:A:632:HOH:O	1.47	1.12
1:A:485:LYS:HD2	3:A:617:HOH:O	1.52	1.09
1:A:176:TYR:CE2	1:A:180:LYS:HE3	1.88	1.09
1:A:311:GLN:HG3	3:A:633:HOH:O	1.53	1.07
1:A:416:GLU:HG3	3:A:139:HOH:O	1.57	1.05
1:B:307:ASP:O	1:B:311:GLN:HG2	1.64	0.96
1:A:416:GLU:HB3	3:A:585:HOH:O	1.66	0.94
1:B:267:ILE:CD1	3:B:598:HOH:O	2.17	0.93
1:A:176:TYR:CD2	1:A:180:LYS:HE3	2.05	0.90
1:A:205:HIS:HD2	1:A:207:LYS:H	1.16	0.89
1:A:441:ARG:CG	3:A:628:HOH:O	1.89	0.89
1:A:176:TYR:HE2	1:A:180:LYS:HE3	1.39	0.84
1:A:487:MET:HG2	1:A:490:ALA:HB2	1.60	0.83
1:B:298:HIS:HD2	3:B:56:HOH:O	1.61	0.83
1:B:205:HIS:HD2	1:B:207:LYS:H	1.28	0.80
1:A:185:LYS:CD	3:A:506:HOH:O	2.28	0.80
1:A:311:GLN:OE1	1:A:316:GLU:OE1	2.04	0.75
1:A:358:GLU:CG	3:A:2:HOH:O	2.35	0.75
1:B:176:TYR:CE2	1:B:180:LYS:HE2	2.23	0.73
1:A:311:GLN:OE1	1:A:316:GLU:CD	2.33	0.72
1:A:358:GLU:HG3	3:A:2:HOH:O	1.90	0.71
1:B:490:ALA:HA	3:B:547:HOH:O	1.92	0.70
1:A:176:TYR:CE2	1:A:180:LYS:CE	2.70	0.70
1:B:205:HIS:CD2	1:B:207:LYS:H	2.10	0.70
1:B:232:LYS:HD2	1:B:235:GLU:OE2	1.92	0.69
1:A:185:LYS:HD2	3:A:506:HOH:O	1.90	0.65
1:A:307:ASP:HB3	1:A:311:GLN:HE21	1.62	0.65
1:A:205:HIS:CD2	1:A:207:LYS:H	2.08	0.64
1:A:176:TYR:HE2	1:A:180:LYS:CE	2.06	0.63
1:A:487:MET:HG2	1:A:490:ALA:CB	2.28	0.63
1:B:176:TYR:HE2	1:B:180:LYS:HE2	1.64	0.62
1:A:185:LYS:HD3	3:A:506:HOH:O	1.94	0.61
1:A:474:HIS:HE1	3:A:518:HOH:O	1.85	0.59
1:A:441:ARG:NH2	3:A:139:HOH:O	2.36	0.58
1:B:397:ILE:HD12	3:B:577:HOH:O	2.04	0.58
1:B:182:GLU:O	1:B:183:ASP:HB2	2.03	0.57
1:A:347:LYS:NZ	3:A:586:HOH:O	2.38	0.57
1:A:298:HIS:HD2	3:A:23:HOH:O	1.88	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:HIS:HE1	3:A:109:HOH:O	1.86	0.57
1:B:176:TYR:HD2	1:B:180:LYS:NZ	2.03	0.55
1:A:388:ASP:O	1:A:405:GLN:HA	2.06	0.55
1:A:217:LYS:HB2	1:A:334:VAL:HG22	1.89	0.55
1:A:364:ASP:OD2	1:A:368:LYS:NZ	2.19	0.55
1:A:441:ARG:NE	3:A:628:HOH:O	2.08	0.54
1:B:364:ASP:OD2	1:B:368:LYS:NZ	2.36	0.53
1:A:474:HIS:CE1	3:A:518:HOH:O	2.60	0.53
1:A:367:ARG:NH2	3:A:596:HOH:O	2.37	0.53
1:B:298:HIS:HE1	3:B:504:HOH:O	1.90	0.52
1:B:388:ASP:O	1:B:405:GLN:HA	2.10	0.52
1:A:176:TYR:CD2	1:A:180:LYS:CE	2.89	0.51
1:A:412:LYS:NZ	1:A:416:GLU:OE2	2.44	0.51
1:A:429:VAL:HG11	1:A:455:MET:HE3	1.94	0.50
1:B:232:LYS:O	1:B:466:GLY:HA3	2.12	0.50
1:A:451:TYR:HB3	1:A:455:MET:HG3	1.94	0.50
1:B:246:GLN:HE22	1:B:451:TYR:HA	1.77	0.49
1:B:217:LYS:HB2	1:B:334:VAL:HG22	1.93	0.49
1:B:176:TYR:CD2	1:B:180:LYS:HE2	2.47	0.49
1:B:351:MET:O	1:B:425:ARG:HA	2.13	0.49
1:A:246:GLN:HE22	1:A:451:TYR:HA	1.78	0.48
1:B:176:TYR:CD2	1:B:180:LYS:CE	2.96	0.48
1:B:451:TYR:HB3	1:B:455:MET:HG3	1.96	0.48
1:A:358:GLU:HG2	3:A:2:HOH:O	2.10	0.47
1:B:213:LEU:HD21	1:B:331:PHE:CE1	2.50	0.47
1:A:351:MET:O	1:A:425:ARG:HA	2.15	0.46
1:A:221:SER:HA	1:A:337:TRP:CE3	2.50	0.46
1:B:415:LEU:CD1	1:B:441:ARG:HD2	2.46	0.46
1:B:358:GLU:CG	3:B:9:HOH:O	2.63	0.46
1:B:419:ASN:HB3	3:B:602:HOH:O	2.15	0.45
1:A:376:PRO:HG2	3:A:629:HOH:O	2.16	0.45
1:A:273:VAL:O	1:A:274:ASP:HB2	2.17	0.45
1:B:265:PRO:HB3	1:B:296:HIS:HB3	1.99	0.44
1:B:458:LYS:NZ	3:B:590:HOH:O	2.50	0.44
1:A:307:ASP:O	1:A:311:GLN:CG	2.40	0.44
1:B:487:MET:HE2	1:B:487:MET:HB2	1.69	0.44
1:B:267:ILE:HD13	1:B:298:HIS:HB2	2.00	0.43
1:B:267:ILE:HD11	3:B:598:HOH:O	2.01	0.43
1:A:232:LYS:O	1:A:466:GLY:HA3	2.18	0.43
1:A:233:GLU:HB2	3:A:88:HOH:O	2.17	0.43
1:A:325:ALA:O	1:A:329:GLU:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:441:ARG:CG	3:B:600:HOH:O	2.01	0.43
1:A:367:ARG:HD3	3:A:41:HOH:O	2.18	0.43
1:A:176:TYR:HD2	1:A:180:LYS:HE3	1.73	0.42
1:A:236:LYS:CD	3:A:632:HOH:O	2.30	0.42
1:B:211:GLN:HG2	3:B:559:HOH:O	2.19	0.42
1:A:487:MET:HE3	1:A:487:MET:HB2	1.41	0.42
1:A:487:MET:HA	3:A:79:HOH:O	2.19	0.42
1:B:347:LYS:HD3	1:B:347:LYS:HA	1.80	0.42
1:A:455:MET:HB2	1:A:457:ASN:OD1	2.21	0.41
1:A:382:CYS:SG	1:A:402:VAL:HG23	2.60	0.41
1:B:310:ASN:HB2	1:B:328:TYR:OH	2.21	0.41
1:A:222:LYS:HA	1:A:222:LYS:HD2	1.69	0.40
1:A:370:GLU:OE2	3:A:621:HOH:O	2.22	0.40
1:B:311:GLN:OE1	1:B:316:GLU:OE1	2.39	0.40
1:A:210:TYR:CZ	1:A:214:VAL:HG11	2.56	0.40
1:B:419:ASN:CG	3:B:602:HOH:O	2.64	0.40
1:A:351:MET:HB3	1:A:351:MET:HE3	1.88	0.40
1:B:369:ILE:HD11	1:B:380:PRO:HB2	2.04	0.40
1:B:264:ASN:HD22	1:B:264:ASN:HA	1.75	0.40
1:B:315:PHE:O	1:B:319:VAL:HG23	2.22	0.40
1:B:263:THR:C	1:B:265:PRO:HD3	2.45	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	313/315 (99%)	300 (96%)	13 (4%)	0	100	100
1	B	313/315 (99%)	299 (96%)	14 (4%)	0	100	100
All	All	626/630 (99%)	599 (96%)	27 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	279/279 (100%)	267 (96%)	12 (4%)	26	25
1	B	279/279 (100%)	264 (95%)	15 (5%)	20	17
All	All	558/558 (100%)	531 (95%)	27 (5%)	23	21

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	180	LYS
1	A	188	ILE
1	A	222	LYS
1	A	290	LYS
1	A	358	GLU
1	A	370	GLU
1	A	377	ASP
1	A	402	VAL
1	A	419	ASN
1	A	425	ARG
1	A	485	LYS
1	A	487	MET
1	B	180	LYS
1	B	185	LYS
1	B	188	ILE
1	B	216	VAL
1	B	218	GLU
1	B	222	LYS
1	B	233	GLU
1	B	242	ASP
1	B	358	GLU
1	B	399	LYS
1	B	402	VAL
1	B	419	ASN
1	B	425	ARG

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Mol	Chain	Res	Type
1	B	465	GLN
1	B	487	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	205	HIS
1	A	246	GLN
1	A	264	ASN
1	A	298	HIS
1	A	310	ASN
1	A	311	GLN
1	A	390	GLN
1	A	393	ASN
1	A	405	GLN
1	A	454	GLN
1	A	474	HIS
1	B	201	GLN
1	B	205	HIS
1	B	246	GLN
1	B	264	ASN
1	B	296	HIS
1	B	298	HIS
1	B	310	ASN
1	B	390	GLN
1	B	393	ASN
1	B	472	GLN
1	B	474	HIS

5.3.3 RNA ⓘ

There are no RNA molecules 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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	315/315 (100%)	-0.50	3 (0%) 79 79	9, 18, 32, 41	4 (1%)
1	B	315/315 (100%)	-0.09	9 (2%) 53 52	12, 25, 48, 61	4 (1%)
All	All	630/630 (100%)	-0.30	12 (1%) 66 66	9, 21, 39, 61	8 (1%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	490	ALA	3.1
1	A	441	ARG	2.7
1	B	181	LEU	2.6
1	B	211	GLN	2.5
1	A	231	LEU	2.5
1	B	326	GLN	2.5
1	B	176	TYR	2.3
1	B	180	LYS	2.3
1	B	329	GLU	2.3
1	A	311	GLN	2.1
1	B	185	LYS	2.1
1	B	208	CYS	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(Å ²)	Q<0.9
2	MN	A	501	1/1	0.92	0.19	7,7,7,7	0
2	MN	B	501	1/1	0.96	0.22	8,8,8,8	1
2	MN	A	500	1/1	0.97	0.19	3,3,3,3	0
2	MN	B	500	1/1	0.98	0.20	4,4,4,4	0

6.5 Other polymers [i](#)

There are no such residues in this entry.