Full wwPDB X-ray Structure Validation Report

Oct 23, 2023 – 01:30 AM EDT

PDB ID	:	3H63
Title	:	Catalytic domain of human Serine/Threonine Phosphatase 5 (PP5c) with two Mn2+ atoms originally soaked with cantharidin (which is present in the structure in the hydrolyzed form)
Authors	:	Bertini, I.; Calderone, V.; Fragai, M.; Luchinat, C.; Talluri, E.
Deposited on	:	2009-04-23
Resolution	:	1.30 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:

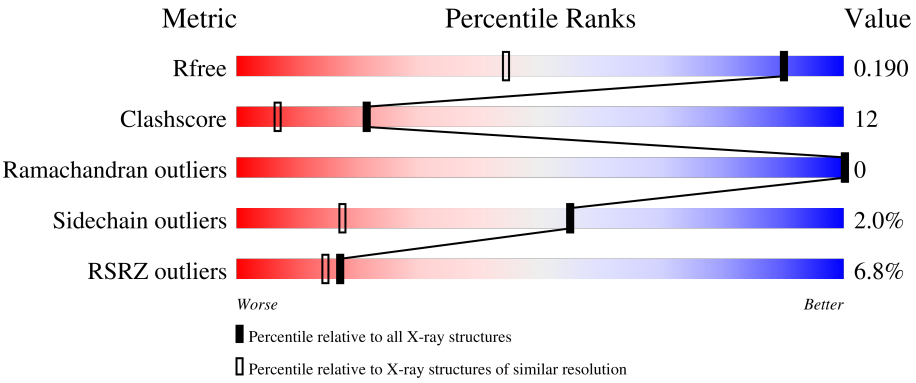
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.30 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}	130704	1058 (1.30-1.30)
Clashscore	141614	1101 (1.30-1.30)
Ramachandran outliers	138981	1058 (1.30-1.30)
Sidechain outliers	138945	1058 (1.30-1.30)
RSRZ outliers	127900	1029 (1.30-1.30)

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 <=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	4% 89% 10%
1	C	315	9% 88% 11%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NHC	A	1[A]	-	-	X	-
3	NHC	A	1[B]	-	-	X	-
3	NHC	C	1[A]	-	-	X	-
3	NHC	C	1[B]	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5932 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.

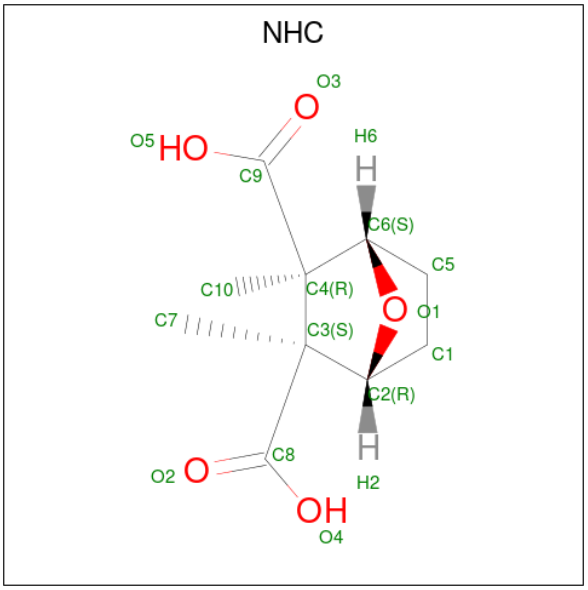
- Molecule 1 is a protein called Serine/threonine-protein phosphatase 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	315	Total	C	N	O	S	0	1	0
			2540	1624	426	475	15			
1	C	315	Total	C	N	O	S	0	1	0
			2540	1624	426	475	15			

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

- Molecule 3 is (1R,2S,3R,4S)-2,3-dimethyl-7-oxabicyclo[2.2.1]heptane-2,3-dicarboxylic acid (three-letter code: NHC) (formula: $C_{10}H_{14}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 30	C 20	O 10	0	1
3	C	1	Total 30	C 20	O 10	0	1

- Molecule 4 is water.

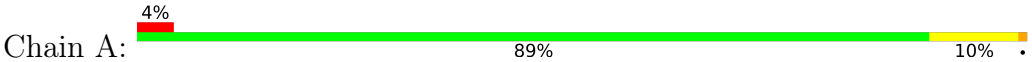
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	466	Total 466	O 466	0	0
4	C	322	Total 322	O 322	0	0

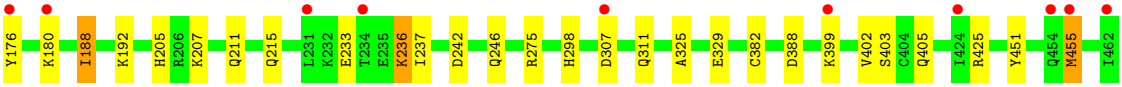
3 Residue-property plots (i)

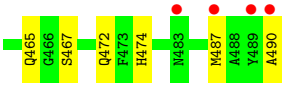
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

Chain A:

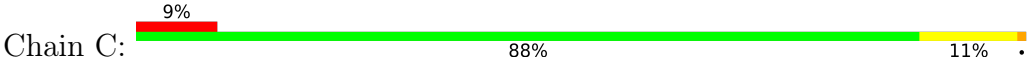


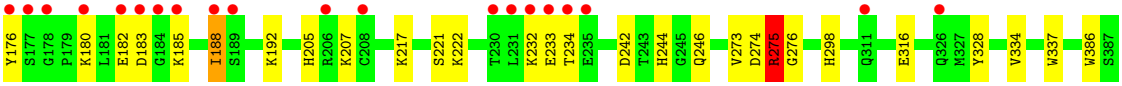


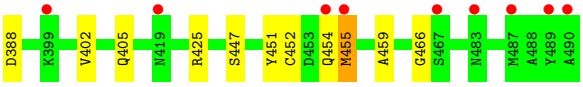


• Molecule 1: Serine/threonine-protein phosphatase 5

Chain C:







4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	154.46Å 41.78Å 105.83Å 90.00° 96.88° 90.00°	Depositor
Resolution (Å)	38.35 – 1.30 38.34 – 1.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (38.35-1.30) 99.7 (38.34-1.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.77 (at 1.30Å)	Xtriage
Refinement program	REFMAC 5.4.0067	Depositor
R, R_{free}	0.161 , 0.191 0.161 , 0.190	Depositor DCC
R_{free} test set	14953 reflections (9.07%)	wwPDB-VP
Wilson B-factor (Å^2)	11.5	Xtriage
Anisotropy	0.440	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 51.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	5932	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.60% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: MN, NHC

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	0.44	0/2605	0.62	0/3524
1	C	0.36	0/2605	0.56	1/3524 (0.0%)
All	All	0.40	0/5210	0.59	1/7048 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	275	ARG	CD-NE-CZ	6.84	133.18	123.60

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	2540	0	2470	51	0
1	C	2540	0	2470	51	0
2	A	2	0	0	0	0
2	C	2	0	0	0	0
3	A	30	0	24	22	0
3	C	30	0	24	29	0
4	A	466	0	0	8	0
4	C	322	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5932	0	4988	122	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 12.

All (122) 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:455:MET:HA	1:A:455:MET:CE	1.32	1.55
1:C:275:ARG:HH12	3:C:1[A]:NHC:C8	1.33	1.37
1:A:176:TYR:CE2	1:A:180:LYS:HE2	1.62	1.33
1:A:451[B]:TYR:OH	3:A:1[B]:NHC:H2	1.21	1.32
1:A:451[B]:TYR:CE2	3:A:1[B]:NHC:H1A	1.66	1.29
1:C:451[B]:TYR:CE2	3:C:1[B]:NHC:H1A	1.66	1.29
1:C:451[B]:TYR:OH	3:C:1[B]:NHC:H2	1.32	1.21
3:A:1[A]:NHC:O4	4:A:872:HOH:O	1.61	1.17
1:C:176:TYR:CE2	1:C:180:LYS:HE2	1.79	1.17
1:A:455:MET:CE	1:A:455:MET:CA	2.22	1.14
1:A:188:ILE:HD11	1:A:192:LYS:HE3	1.21	1.14
1:A:455:MET:CA	1:A:455:MET:HE3	1.78	1.13
3:C:1[A]:NHC:C8	3:C:1[A]:NHC:O5	1.97	1.12
1:C:275:ARG:NH1	3:C:1[A]:NHC:C8	2.16	1.09
1:A:451[B]:TYR:OH	3:A:1[B]:NHC:C2	2.00	1.07
3:A:1[B]:NHC:O4	4:A:871:HOH:O	1.72	1.06
1:A:176:TYR:CD2	1:A:180:LYS:HE2	1.94	1.02
1:A:455:MET:HA	1:A:455:MET:HE2	1.37	1.02
1:C:451[B]:TYR:OH	3:C:1[B]:NHC:C2	2.08	1.01
1:A:188:ILE:HD11	1:A:192:LYS:CE	1.93	0.99
1:C:176:TYR:CD2	1:C:180:LYS:HE2	1.98	0.97
1:A:176:TYR:HE2	1:A:180:LYS:HE2	1.14	0.95
1:C:275:ARG:NH2	3:C:1[A]:NHC:O4	2.02	0.93
1:A:451[B]:TYR:CZ	3:A:1[B]:NHC:H1A	2.03	0.93
1:C:451[B]:TYR:CZ	3:C:1[B]:NHC:H1A	2.03	0.92
1:A:451[B]:TYR:CE2	3:A:1[B]:NHC:C1	2.53	0.90
1:A:487:MET:HG3	1:A:490:ALA:HB3	1.52	0.90
1:C:176:TYR:HE2	1:C:180:LYS:HE2	1.34	0.90
3:A:1[B]:NHC:O4	3:A:1[B]:NHC:O5	1.90	0.89
1:C:451[B]:TYR:CE2	3:C:1[B]:NHC:C1	2.55	0.88
1:A:451[B]:TYR:HH	3:A:1[B]:NHC:H2	1.35	0.88
1:C:275:ARG:HH12	3:C:1[B]:NHC:C8	1.85	0.87
1:A:455:MET:HA	1:A:455:MET:HE3	0.87	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1[A]:NHC:O5	4:C:873:HOH:O	1.92	0.87
1:C:451[B]:TYR:HH	3:C:1[B]:NHC:H2	1.35	0.86
1:C:188:ILE:HD11	1:C:192:LYS:HE3	1.59	0.82
1:A:233:GLU:HG2	1:A:467:SER:HB3	1.62	0.82
1:A:176:TYR:CD2	1:A:180:LYS:CE	2.63	0.81
1:C:275:ARG:NH1	3:C:1[A]:NHC:O4	2.12	0.81
1:A:205:HIS:HD2	1:A:207:LYS:H	1.26	0.81
3:C:1[B]:NHC:O4	4:C:874:HOH:O	1.97	0.81
1:C:451[B]:TYR:HE2	3:C:1[B]:NHC:H1A	1.44	0.80
1:A:176:TYR:CE2	1:A:180:LYS:CE	2.56	0.80
3:C:1[B]:NHC:O4	3:C:1[B]:NHC:O5	2.03	0.76
1:A:451[B]:TYR:HE2	3:A:1[B]:NHC:H1A	1.48	0.76
3:C:1[A]:NHC:O5	3:C:1[A]:NHC:O2	2.02	0.75
3:A:1[A]:NHC:O5	3:A:1[A]:NHC:C8	2.35	0.75
1:A:455:MET:CA	1:A:455:MET:HE2	2.03	0.71
1:A:451[B]:TYR:CZ	3:A:1[B]:NHC:C1	2.74	0.70
1:C:205:HIS:HD2	1:C:207:LYS:H	1.38	0.70
1:A:487:MET:HG3	1:A:490:ALA:CB	2.21	0.70
1:A:188:ILE:HD13	1:A:188:ILE:O	1.92	0.69
1:C:275:ARG:CZ	3:C:1[A]:NHC:O4	2.39	0.69
1:C:176:TYR:CD2	1:C:180:LYS:CE	2.74	0.69
1:C:233:GLU:HG3	1:C:234:THR:HG23	1.75	0.68
1:A:188:ILE:HD13	1:A:188:ILE:C	2.13	0.68
1:C:452:CYS:O	1:C:454:GLN:HG3	1.94	0.68
3:A:1[A]:NHC:C8	4:A:852:HOH:O	2.42	0.67
1:A:205:HIS:CD2	1:A:207:LYS:H	2.13	0.66
3:A:1[A]:NHC:O5	3:A:1[A]:NHC:O2	2.15	0.64
1:C:451[B]:TYR:CZ	3:C:1[B]:NHC:C1	2.77	0.64
1:C:275:ARG:HH11	1:C:275:ARG:HG3	1.64	0.62
1:A:325:ALA:O	1:A:329:GLU:HG2	2.00	0.61
1:C:451[B]:TYR:OH	3:C:1[B]:NHC:C1	2.50	0.60
1:A:451[B]:TYR:OH	3:A:1[B]:NHC:C1	2.50	0.58
1:A:275:ARG:HG3	4:A:852:HOH:O	2.04	0.57
1:A:298:HIS:HD2	4:A:16:HOH:O	1.87	0.57
1:A:455:MET:HE1	1:C:454:GLN:HG2	1.86	0.57
1:C:188:ILE:HD11	1:C:192:LYS:CE	2.32	0.57
1:A:451[B]:TYR:CZ	3:A:1[B]:NHC:C2	2.87	0.56
1:C:451[B]:TYR:HE2	3:C:1[B]:NHC:C1	2.09	0.56
1:C:298:HIS:HD2	4:C:125:HOH:O	1.89	0.55
1:A:176:TYR:HD2	1:A:180:LYS:CE	2.19	0.54
1:A:211:GLN:HE21	1:A:215:GLN:HE21	1.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451[B]:TYR:HE2	3:A:1[B]:NHC:C1	2.12	0.54
1:C:246:GLN:HE22	1:C:451[B]:TYR:HA	1.74	0.53
1:A:246:GLN:HE22	1:A:451[A]:TYR:HA	1.73	0.52
1:A:474:HIS:HE1	4:A:627:HOH:O	1.93	0.51
1:C:246:GLN:HE22	1:C:451[A]:TYR:HA	1.75	0.51
1:C:217:LYS:HB2	1:C:334:VAL:HG22	1.93	0.51
3:A:1[A]:NHC:C8	4:A:872:HOH:O	2.33	0.51
1:A:246:GLN:HE22	1:A:451[B]:TYR:HA	1.75	0.51
1:C:451[B]:TYR:HB3	1:C:455:MET:HG3	1.92	0.51
1:C:232:LYS:O	1:C:466:GLY:HA3	2.11	0.50
1:C:273:VAL:O	1:C:274:ASP:HB2	2.12	0.50
1:A:388:ASP:O	1:A:405:GLN:HA	2.11	0.50
1:C:388:ASP:O	1:C:405:GLN:HA	2.12	0.49
1:A:307:ASP:O	1:A:311:GLN:HG3	2.11	0.49
1:C:188:ILE:C	1:C:188:ILE:HD13	2.33	0.49
1:C:182:GLU:O	1:C:183:ASP:HB2	2.11	0.49
1:C:316:GLU:HG3	1:C:328:TYR:CE2	2.48	0.49
1:C:176:TYR:HD2	1:C:180:LYS:CE	2.24	0.48
1:C:316:GLU:HG3	1:C:328:TYR:CZ	2.49	0.47
1:C:451[B]:TYR:CZ	3:C:1[B]:NHC:C2	2.97	0.47
1:A:382:CYS:SG	1:A:402:VAL:HG22	2.54	0.47
1:C:298:HIS:HE1	4:C:491:HOH:O	1.96	0.47
1:C:176:TYR:HD2	1:C:180:LYS:HE2	1.71	0.47
1:A:236:LYS:HG2	1:A:237:ILE:N	2.30	0.46
1:C:275:ARG:NH2	3:C:1[B]:NHC:H7B	2.30	0.46
1:A:298:HIS:HE1	4:A:77:HOH:O	1.99	0.46
1:A:382:CYS:SG	1:A:402:VAL:CG2	3.04	0.45
3:C:1[A]:NHC:H7	3:C:1[A]:NHC:H1	1.67	0.45
3:A:1[A]:NHC:H1	3:A:1[A]:NHC:H7	1.71	0.45
3:C:1[B]:NHC:H1	3:C:1[B]:NHC:H7	1.75	0.45
1:A:399:LYS:HE3	1:A:399:LYS:HB2	1.75	0.45
1:A:188:ILE:C	1:A:188:ILE:CD1	2.85	0.45
1:A:402:VAL:HG22	1:A:403:SER:N	2.32	0.44
1:C:222:LYS:HA	1:C:222:LYS:HD3	1.74	0.43
1:A:188:ILE:HD11	1:A:192:LYS:CD	2.44	0.43
3:A:1[B]:NHC:H5	3:A:1[B]:NHC:H10B	1.76	0.43
1:C:221:SER:HA	1:C:337:TRP:CE3	2.53	0.43
3:C:1[B]:NHC:C8	4:C:874:HOH:O	2.51	0.42
3:A:1[B]:NHC:H7	3:A:1[B]:NHC:H1	1.79	0.42
1:A:465:GLN:NE2	1:A:472:GLN:HE22	2.17	0.42
3:C:1[A]:NHC:H10B	3:C:1[A]:NHC:H5	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:205:HIS:CD2	1:C:207:LYS:H	2.27	0.42
3:A:1[A]:NHC:H5	3:A:1[A]:NHC:H10B	1.85	0.41
1:C:386:TRP:CE3	1:C:402:VAL:HG11	2.56	0.41
1:C:447:SER:HA	1:C:459:ALA:HB1	2.02	0.41
3:C:1[B]:NHC:H10B	3:C:1[B]:NHC:H5	1.74	0.41
1:C:275:ARG:NH1	3:C:1[B]:NHC:H2	2.36	0.40
1:C:244:HIS:O	1:C:276:GLY:HA3	2.20	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	314/315 (100%)	304 (97%)	10 (3%)	0	100	100
1	C	314/315 (100%)	305 (97%)	9 (3%)	0	100	100
All	All	628/630 (100%)	609 (97%)	19 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	280/279 (100%)	275 (98%)	5 (2%)	59	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	280/279 (100%)	274 (98%)	6 (2%)	53 16
All	All	560/558 (100%)	549 (98%)	11 (2%)	55 17

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

Mol	Chain	Res	Type
1	A	188	ILE
1	A	236	LYS
1	A	242	ASP
1	A	425	ARG
1	A	455	MET
1	C	185	LYS
1	C	188	ILE
1	C	242	ASP
1	C	275	ARG
1	C	425	ARG
1	C	455	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	205	HIS
1	A	211	GLN
1	A	246	GLN
1	A	264	ASN
1	A	298	HIS
1	A	405	GLN
1	A	419	ASN
1	A	465	GLN
1	A	474	HIS
1	C	205	HIS
1	C	211	GLN
1	C	246	GLN
1	C	264	ASN
1	C	298	HIS
1	C	405	GLN
1	C	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 monosaccharides in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 4 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	NHC	C	1[A]	2	16,16,16	1.33	3 (18%)	17,27,27	1.42	2 (11%)
3	NHC	C	1[B]	2	16,16,16	1.47	3 (18%)	17,27,27	1.40	2 (11%)
3	NHC	A	1[A]	2	16,16,16	1.36	3 (18%)	17,27,27	1.40	2 (11%)
3	NHC	A	1[B]	2	16,16,16	1.45	3 (18%)	17,27,27	1.44	3 (17%)

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	NHC	C	1[A]	2	-	2/12/42/42	0/3/2/2
3	NHC	C	1[B]	2	-	0/12/42/42	0/3/2/2
3	NHC	A	1[A]	2	-	2/12/42/42	0/3/2/2
3	NHC	A	1[B]	2	-	0/12/42/42	0/3/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1[B]	NHC	C4-C3	-3.37	1.51	1.57
3	C	1[B]	NHC	C4-C3	-3.33	1.51	1.57
3	C	1[B]	NHC	C4-C6	-2.79	1.52	1.55
3	C	1[A]	NHC	C4-C6	-2.68	1.52	1.55
3	A	1[A]	NHC	C4-C3	-2.60	1.52	1.57
3	C	1[A]	NHC	C4-C3	-2.60	1.52	1.57
3	A	1[A]	NHC	C4-C6	-2.59	1.52	1.55
3	A	1[B]	NHC	C4-C6	-2.57	1.52	1.55
3	C	1[B]	NHC	C3-C2	-2.50	1.52	1.55
3	C	1[A]	NHC	C3-C2	-2.46	1.52	1.55
3	A	1[B]	NHC	C3-C2	-2.38	1.52	1.55
3	A	1[A]	NHC	C3-C2	-2.22	1.52	1.55

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1[A]	NHC	O1-C2-C1	-3.11	98.94	104.06
3	C	1[B]	NHC	C10-C4-C3	-2.82	111.84	116.74
3	C	1[A]	NHC	O1-C2-C3	2.65	103.32	101.23
3	A	1[B]	NHC	C10-C4-C3	-2.34	112.67	116.74
3	C	1[B]	NHC	C1-C5-C6	-2.26	100.93	104.69
3	A	1[B]	NHC	O1-C2-C1	-2.17	100.49	104.06
3	A	1[B]	NHC	C1-C5-C6	-2.14	101.13	104.69
3	A	1[A]	NHC	C1-C5-C6	-2.13	101.15	104.69
3	C	1[A]	NHC	O1-C2-C1	-2.12	100.56	104.06

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1[A]	NHC	C7-C3-C8-O2
3	A	1[A]	NHC	C7-C3-C8-O4
3	C	1[A]	NHC	C7-C3-C8-O2
3	C	1[A]	NHC	C7-C3-C8-O4

There are no ring outliers.

4 monomers are involved in 51 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1[A]	NHC	10	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1[B]	NHC	19	0
3	A	1[A]	NHC	7	0
3	A	1[B]	NHC	15	0

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, 95^{th} 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%)	0.15	14 (4%)	34	32	7, 12, 22, 29	2 (0%)
1	C	315/315 (100%)	0.49	29 (9%)	9	6	9, 18, 30, 41	1 (0%)
All	All	630/630 (100%)	0.32	43 (6%)	17	14	7, 15, 27, 41	3 (0%)

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	176	TYR	6.0
1	C	177	SER	5.7
1	C	490	ALA	5.7
1	A	176	TYR	5.3
1	C	184	GLY	5.2
1	C	183	ASP	5.1
1	C	234	THR	4.5
1	C	233	GLU	4.3
1	C	230	THR	4.1
1	C	185	LYS	4.0
1	C	232	LYS	3.9
1	C	182	GLU	3.8
1	A	399	LYS	3.7
1	A	490	ALA	3.7
1	C	487	MET	3.1
1	C	231	LEU	3.1
1	C	489	TYR	3.0
1	C	467	SER	2.9
1	C	208	CYS	2.9
1	A	231	LEU	2.9
1	A	489	TYR	2.8
1	A	455	MET	2.8
1	C	326	GLN	2.8
1	C	311	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	487	MET	2.7
1	C	454	GLN	2.7
1	C	455	MET	2.6
1	C	399	LYS	2.6
1	A	454	GLN	2.5
1	C	188	ILE	2.5
1	A	234	THR	2.5
1	C	178	GLY	2.4
1	A	180	LYS	2.3
1	C	235	GLU	2.2
1	C	419	ASN	2.1
1	A	307	ASP	2.1
1	C	483	ASN	2.0
1	C	189	SER	2.0
1	C	180	LYS	2.0
1	C	206	ARG	2.0
1	A	424	ILE	2.0
1	A	462	ILE	2.0
1	A	483	ASN	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 monosaccharides 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, 95^{th} 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	NHC	C	1[A]	15/15	0.87	0.19	8,13,14,15	15
3	NHC	C	1[B]	15/15	0.87	0.19	13,16,17,17	15
3	NHC	A	1[A]	15/15	0.88	0.19	4,7,9,10	15
3	NHC	A	1[B]	15/15	0.88	0.19	6,12,15,15	15

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MN	A	500	1/1	1.00	0.07	6,6,6,6	0
2	MN	A	501	1/1	1.00	0.07	9,9,9,9	0
2	MN	C	500	1/1	1.00	0.06	10,10,10,10	0
2	MN	C	501	1/1	1.00	0.11	9,9,9,9	1

6.5 Other polymers (i)

There are no such residues in this entry.