Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2024 – 11:24 AM EDT

PDB ID	:	5BPW
Title	:	Atomic-resolution structures of the APC/C subunits Apc4 and the Apc5 N-terminal domain
Authors	:	Kulkarni, K.; Yang, J.; Zhang, Z.; Barford, D.
Deposited on	:	2015-05-28
Resolution	:	3.40 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:

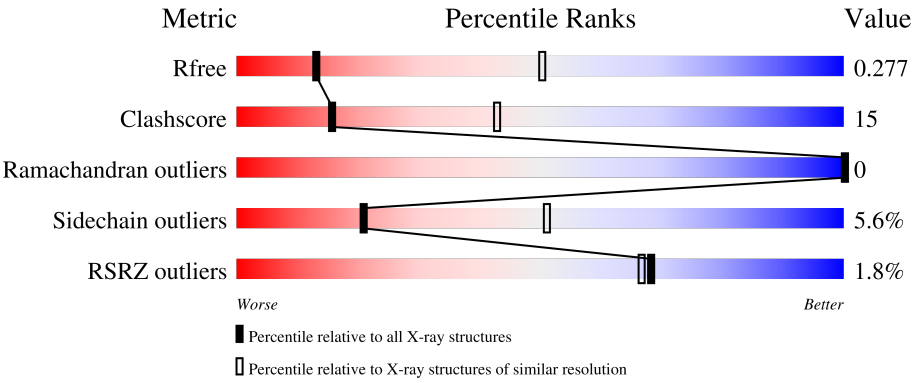
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.40 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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	843	% 55% 21% · 22%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 5091 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 Anaphase-promoting complex subunit 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	659	5091	3251	847	964	29	0	0	0

There are 35 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	809	GLU	-	expression tag	UNP Q9UJX5
A	810	ASN	-	expression tag	UNP Q9UJX5
A	811	LEU	-	expression tag	UNP Q9UJX5
A	812	TYR	-	expression tag	UNP Q9UJX5
A	813	PHE	-	expression tag	UNP Q9UJX5
A	814	GLN	-	expression tag	UNP Q9UJX5
A	815	SER	-	expression tag	UNP Q9UJX5
A	816	TRP	-	expression tag	UNP Q9UJX5
A	817	SER	-	expression tag	UNP Q9UJX5
A	818	HIS	-	expression tag	UNP Q9UJX5
A	819	PRO	-	expression tag	UNP Q9UJX5
A	820	GLN	-	expression tag	UNP Q9UJX5
A	821	PHE	-	expression tag	UNP Q9UJX5
A	822	GLU	-	expression tag	UNP Q9UJX5
A	823	LYS	-	expression tag	UNP Q9UJX5
A	824	GLY	-	expression tag	UNP Q9UJX5
A	825	GLY	-	expression tag	UNP Q9UJX5
A	826	GLY	-	expression tag	UNP Q9UJX5
A	827	SER	-	expression tag	UNP Q9UJX5
A	828	GLY	-	expression tag	UNP Q9UJX5
A	829	GLY	-	expression tag	UNP Q9UJX5
A	830	GLY	-	expression tag	UNP Q9UJX5
A	831	SER	-	expression tag	UNP Q9UJX5
A	832	GLY	-	expression tag	UNP Q9UJX5
A	833	GLY	-	expression tag	UNP Q9UJX5
A	834	GLY	-	expression tag	UNP Q9UJX5
A	835	SER	-	expression tag	UNP Q9UJX5

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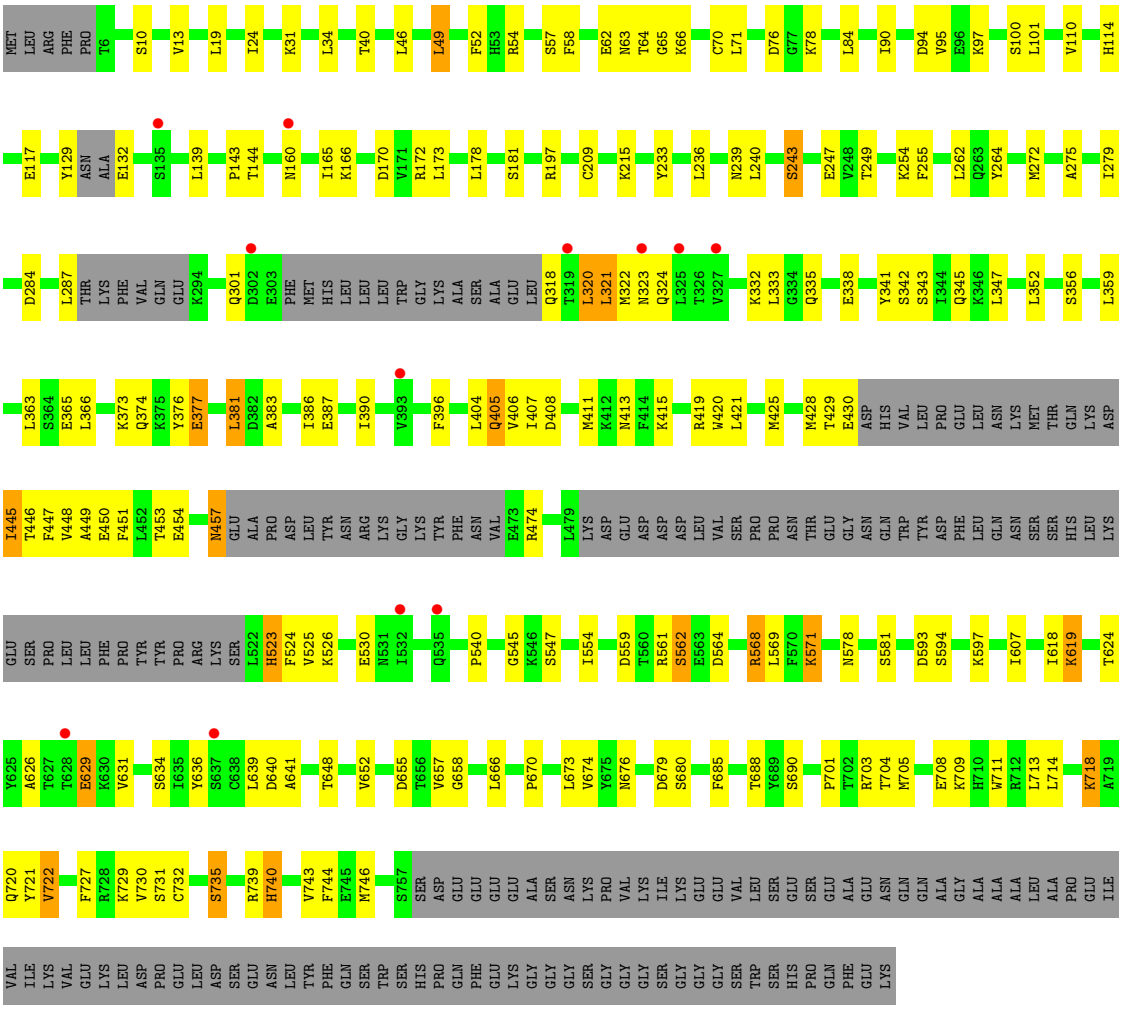
Chain	Residue	Modelled	Actual	Comment	Reference
A	836	TRP	-	expression tag	UNP Q9UJX5
A	837	SER	-	expression tag	UNP Q9UJX5
A	838	HIS	-	expression tag	UNP Q9UJX5
A	839	PRO	-	expression tag	UNP Q9UJX5
A	840	GLN	-	expression tag	UNP Q9UJX5
A	841	PHE	-	expression tag	UNP Q9UJX5
A	842	GLU	-	expression tag	UNP Q9UJX5
A	843	LYS	-	expression tag	UNP Q9UJX5

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: Anaphase-promoting complex subunit 4

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α, β, γ	139.18Å 139.18Å 156.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	51.94 – 3.40 57.82 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.6 (51.94-3.40) 99.6 (57.82-3.40)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.76 (at 3.40Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.220 , 0.275 0.227 , 0.277	Depositor DCC
R_{free} test set	702 reflections (3.24%)	wwPDB-VP
Wilson B-factor (Å^2)	82.5	Xtriage
Anisotropy	0.664	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 74.9	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	0.92	EDS
Total number of atoms	5091	wwPDB-VP
Average B, all atoms (Å^2)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% 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

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	0.56	0/5183	0.86	4/7025 (0.1%)

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	5

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	381	LEU	CA-CB-CG	6.97	131.33	115.30
1	A	321	LEU	CA-CB-CG	6.50	130.25	115.30
1	A	236	LEU	CB-CG-CD2	-6.36	100.19	111.00
1	A	71	LEU	CA-CB-CG	5.51	127.98	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	320	LEU	Peptide
1	A	377	GLU	Peptide
1	A	523	HIS	Peptide
1	A	629	GLU	Peptide
1	A	658	GLY	Peptide

5.2 Too-close contacts (i)

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	5091	0	4991	148	1
All	All	5091	0	4991	148	1

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 15.

All (148) 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:453:THR:O	1:A:457:ASN:ND2	1.83	1.10
1:A:457:ASN:OD1	1:A:474:ARG:HD3	1.54	1.07
1:A:445:ILE:N	1:A:448:VAL:HG23	1.76	0.99
1:A:445:ILE:HG12	1:A:446:THR:H	1.27	0.99
1:A:450:GLU:O	1:A:453:THR:HG22	1.78	0.84
1:A:688:THR:HG22	1:A:690:SER:H	1.39	0.84
1:A:445:ILE:CA	1:A:448:VAL:HG23	2.08	0.83
1:A:446:THR:O	1:A:449:ALA:HB3	1.79	0.82
1:A:255:PHE:HE2	1:A:540:PRO:HG2	1.46	0.80
1:A:448:VAL:HA	1:A:451:PHE:CG	2.16	0.80
1:A:457:ASN:OD1	1:A:474:ARG:CD	2.33	0.76
1:A:445:ILE:HG12	1:A:446:THR:N	2.01	0.76
1:A:445:ILE:N	1:A:445:ILE:HD13	2.03	0.74
1:A:404:LEU:HA	1:A:407:ILE:HD12	1.70	0.73
1:A:674:VAL:O	1:A:703:ARG:NH1	2.22	0.73
1:A:94:ASP:HB2	1:A:101:LEU:HD13	1.71	0.72
1:A:562:SER:HB3	1:A:568:ARG:HH21	1.55	0.71
1:A:447:PHE:HA	1:A:450:GLU:CB	2.22	0.70
1:A:445:ILE:O	1:A:448:VAL:HB	1.92	0.69
1:A:457:ASN:N	1:A:457:ASN:HD22	1.91	0.69
1:A:381:LEU:HD22	1:A:386:ILE:HD11	1.74	0.68
1:A:255:PHE:HE1	1:A:366:LEU:HD21	1.59	0.68
1:A:454:GLU:O	1:A:457:ASN:HB2	1.95	0.66
1:A:445:ILE:HA	1:A:448:VAL:HG23	1.77	0.66
1:A:377:GLU:OE1	1:A:381:LEU:N	2.28	0.65
1:A:76:ASP:HB3	1:A:78:LYS:HG3	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:LYS:HA	1:A:335:GLN:OE1	1.96	0.64
1:A:377:GLU:CD	1:A:381:LEU:HB2	2.18	0.64
1:A:666:LEU:HD21	1:A:746:MET:HE1	1.80	0.64
1:A:129:TYR:O	1:A:132:GLU:N	2.32	0.63
1:A:445:ILE:HA	1:A:448:VAL:CG2	2.29	0.62
1:A:342:SER:HA	1:A:345:GLN:OE1	2.00	0.61
1:A:376:TYR:HB3	1:A:377:GLU:OE2	2.01	0.61
1:A:619:LYS:HE3	1:A:704:THR:OG1	1.99	0.61
1:A:65:GLY:N	1:A:84:LEU:HG	2.16	0.60
1:A:446:THR:CG2	1:A:447:PHE:CE2	2.86	0.59
1:A:173:LEU:HB2	1:A:249:THR:HG23	1.84	0.59
1:A:343:SER:O	1:A:347:LEU:HB2	2.02	0.58
1:A:679:ASP:OD1	1:A:703:ARG:NH2	2.37	0.58
1:A:49:LEU:HD13	1:A:730:VAL:HG21	1.84	0.58
1:A:447:PHE:HA	1:A:450:GLU:H	1.67	0.58
1:A:457:ASN:HD22	1:A:457:ASN:H	1.52	0.57
1:A:363:LEU:HB3	1:A:390:ILE:HG12	1.86	0.57
1:A:254:LYS:NZ	1:A:365:GLU:OE1	2.24	0.57
1:A:413:ASN:HD21	1:A:453:THR:CG2	2.18	0.57
1:A:405:GLN:HE21	1:A:408:ASP:HB2	1.69	0.57
1:A:65:GLY:H	1:A:84:LEU:HG	1.70	0.56
1:A:19:LEU:N	1:A:739:ARG:O	2.35	0.56
1:A:447:PHE:CA	1:A:450:GLU:CB	2.85	0.55
1:A:404:LEU:O	1:A:407:ILE:HB	2.06	0.55
1:A:718:LYS:HG2	1:A:735:SER:HB3	1.90	0.53
1:A:447:PHE:HB3	1:A:450:GLU:CB	2.38	0.53
1:A:578:ASN:ND2	1:A:581:SER:OG	2.40	0.53
1:A:373:LYS:HG3	1:A:374:GLN:N	2.24	0.53
1:A:415:LYS:HZ3	1:A:419:ARG:NH2	2.06	0.53
1:A:421:LEU:O	1:A:425:MET:HG3	2.09	0.53
1:A:110:VAL:HG11	1:A:178:LEU:HD22	1.90	0.53
1:A:13:VAL:HG22	1:A:744:PHE:CE2	2.44	0.53
1:A:735:SER:OG	1:A:740:HIS:O	2.25	0.52
1:A:523:HIS:ND1	1:A:524:PHE:HD1	2.07	0.52
1:A:377:GLU:HG3	1:A:381:LEU:O	2.08	0.52
1:A:413:ASN:ND2	1:A:453:THR:CG2	2.73	0.52
1:A:429:THR:HG23	1:A:430:GLU:H	1.75	0.52
1:A:445:ILE:N	1:A:445:ILE:CD1	2.73	0.52
1:A:624:THR:HB	1:A:631:VAL:HG23	1.92	0.51
1:A:10:SER:OG	1:A:711:TRP:O	2.28	0.51
1:A:239:ASN:O	1:A:243:SER:OG	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:ARG:O	1:A:545:GLY:HA3	2.11	0.50
1:A:335:GLN:HA	1:A:338:GLU:OE1	2.10	0.50
1:A:676:ASN:O	1:A:680:SER:HB3	2.12	0.50
1:A:457:ASN:ND2	1:A:457:ASN:N	2.60	0.50
1:A:607:ILE:H	1:A:607:ILE:HD12	1.77	0.49
1:A:640:ASP:OD1	1:A:641:ALA:N	2.45	0.49
1:A:356:SER:O	1:A:359:LEU:HB2	2.13	0.49
1:A:618:ILE:HD12	1:A:705:MET:HE1	1.95	0.48
1:A:639:LEU:HB2	1:A:652:VAL:HG12	1.94	0.48
1:A:673:LEU:HA	1:A:676:ASN:HB2	1.95	0.48
1:A:341:TYR:HE2	1:A:411:MET:HA	1.78	0.48
1:A:377:GLU:OE2	1:A:381:LEU:HB2	2.14	0.48
1:A:52:PHE:HD1	1:A:743:VAL:HG21	1.79	0.48
1:A:352:LEU:HD21	1:A:396:PHE:CE2	2.49	0.48
1:A:655:ASP:OD1	1:A:657:VAL:HG22	2.14	0.47
1:A:729:LYS:O	1:A:746:MET:HB2	2.14	0.47
1:A:275:ALA:O	1:A:279:ILE:HG23	2.15	0.47
1:A:571:LYS:HB3	1:A:571:LYS:HE2	1.41	0.47
1:A:84:LEU:HD13	1:A:84:LEU:HA	1.73	0.47
1:A:117:GLU:OE2	1:A:172:ARG:NH2	2.47	0.47
1:A:321:LEU:HD23	1:A:322:MET:HG3	1.97	0.47
1:A:139:LEU:HB2	1:A:165:ILE:HG23	1.97	0.47
1:A:166:LYS:HG3	1:A:170:ASP:OD2	2.15	0.47
1:A:94:ASP:OD1	1:A:95:VAL:N	2.48	0.46
1:A:114:HIS:ND1	1:A:209:CYS:HA	2.29	0.46
1:A:54:ARG:HE	1:A:57:SER:HB3	1.81	0.46
1:A:255:PHE:CE1	1:A:366:LEU:HD21	2.45	0.46
1:A:413:ASN:HD21	1:A:453:THR:HG22	1.81	0.46
1:A:144:THR:HG21	1:A:160:ASN:H	1.79	0.46
1:A:405:GLN:NE2	1:A:408:ASP:HB2	2.31	0.46
1:A:415:LYS:O	1:A:419:ARG:HG3	2.16	0.46
1:A:457:ASN:OD1	1:A:474:ARG:CG	2.62	0.46
1:A:255:PHE:CE2	1:A:540:PRO:HG2	2.38	0.45
1:A:324:GLN:N	1:A:324:GLN:OE1	2.49	0.45
1:A:24:ILE:HD13	1:A:40:THR:HG22	1.98	0.45
1:A:446:THR:CG2	1:A:447:PHE:CD2	2.99	0.45
1:A:562:SER:HB3	1:A:568:ARG:NH2	2.26	0.45
1:A:272:MET:HE3	1:A:347:LEU:HD22	1.99	0.45
1:A:363:LEU:HD23	1:A:363:LEU:HA	1.67	0.45
1:A:559:ASP:OD1	1:A:561:ARG:HG2	2.16	0.45
1:A:233:TYR:CD1	1:A:554:ILE:HD12	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:ALA:O	1:A:387:GLU:HG2	2.17	0.45
1:A:526:LYS:O	1:A:530:GLU:HG2	2.18	0.44
1:A:731:SER:HB2	1:A:746:MET:HE2	1.99	0.44
1:A:215:LYS:O	1:A:607:ILE:HD11	2.17	0.44
1:A:143:PRO:O	1:A:264:TYR:OH	2.26	0.44
1:A:247:GLU:HB3	1:A:376:TYR:CE2	2.53	0.44
1:A:685:PHE:HA	1:A:701:PRO:HD3	1.98	0.44
1:A:272:MET:H	1:A:272:MET:HG2	1.62	0.43
1:A:387:GLU:HA	1:A:390:ILE:HD12	2.00	0.43
1:A:284:ASP:O	1:A:287:LEU:HD13	2.19	0.43
1:A:593:ASP:O	1:A:594:SER:OG	2.29	0.43
1:A:708:GLU:C	1:A:709:LYS:HD2	2.38	0.43
1:A:64:THR:HG22	1:A:65:GLY:H	1.83	0.43
1:A:523:HIS:O	1:A:525:VAL:N	2.52	0.43
1:A:262:LEU:HA	1:A:262:LEU:HD23	1.65	0.42
1:A:377:GLU:CD	1:A:381:LEU:H	2.18	0.42
1:A:446:THR:HG23	1:A:447:PHE:CD1	2.54	0.42
1:A:571:LYS:NZ	1:A:722:VAL:H	2.17	0.42
1:A:730:VAL:HG22	1:A:731:SER:N	2.35	0.42
1:A:31:LYS:HA	1:A:727:PHE:CD2	2.55	0.42
1:A:34:LEU:HD13	1:A:46:LEU:HD21	2.01	0.42
1:A:720:GLN:HG2	1:A:721:TYR:CZ	2.54	0.42
1:A:333:LEU:HD23	1:A:333:LEU:HA	1.84	0.42
1:A:446:THR:CG2	1:A:447:PHE:CZ	3.03	0.42
1:A:523:HIS:ND1	1:A:524:PHE:HA	2.34	0.42
1:A:626:ALA:H	1:A:709:LYS:HZ1	1.68	0.42
1:A:445:ILE:CA	1:A:448:VAL:CG2	2.86	0.41
1:A:634:SER:HB3	1:A:636:TYR:CZ	2.55	0.41
1:A:320:LEU:HD22	1:A:323:ASN:CG	2.40	0.41
1:A:454:GLU:O	1:A:457:ASN:O	2.38	0.41
1:A:24:ILE:HD12	1:A:24:ILE:HA	1.77	0.41
1:A:445:ILE:CG1	1:A:446:THR:H	2.06	0.41
1:A:406:VAL:H	1:A:406:VAL:HG23	1.66	0.41
1:A:446:THR:HG23	1:A:447:PHE:CG	2.56	0.41
1:A:648:THR:HG22	1:A:670:PRO:HA	2.02	0.41
1:A:322:MET:HE1	1:A:428:MET:CB	2.51	0.40
1:A:447:PHE:CA	1:A:450:GLU:H	2.32	0.40
1:A:318:GLN:O	1:A:321:LEU:HB3	2.21	0.40
1:A:445:ILE:C	1:A:448:VAL:H	2.24	0.40
1:A:713:LEU:HD23	1:A:714:LEU:N	2.36	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:THR:OG1	1:A:446:THR:OG1[7_737]	1.81	0.39

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	645/843 (76%)	611 (95%)	34 (5%)	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	553/756 (73%)	522 (94%)	31 (6%)	21 51

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	LEU
1	A	58	PHE
1	A	62	GLU
1	A	63	ASN
1	A	66	LYS
1	A	70	CYS

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Mol	Chain	Res	Type
1	A	90	ILE
1	A	97	LYS
1	A	100	SER
1	A	181	SER
1	A	240	LEU
1	A	243	SER
1	A	301	GLN
1	A	405	GLN
1	A	420	TRP
1	A	445	ILE
1	A	457	ASN
1	A	547	SER
1	A	562	SER
1	A	564	ASP
1	A	568	ARG
1	A	569	LEU
1	A	571	LYS
1	A	597	LYS
1	A	619	LYS
1	A	629	GLU
1	A	718	LYS
1	A	722	VAL
1	A	732	CYS
1	A	735	SER
1	A	740	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	578	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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	659/843 (78%)	0.19	12 (1%) 68 67	47, 84, 159, 206	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	160	ASN	2.8
1	A	323	ASN	2.6
1	A	302	ASP	2.6
1	A	393	VAL	2.5
1	A	637	SER	2.4
1	A	135	SER	2.3
1	A	327	VAL	2.3
1	A	535	GLN	2.2
1	A	325	LEU	2.1
1	A	628	THR	2.1
1	A	532	ILE	2.1
1	A	319	THR	2.0

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 monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.