Full wwPDB X-ray Structure Validation Report ⓘ

Nov 1, 2023 – 08:25 PM EDT

PDB ID	:	3NMZ
Title	:	Crystal structure of APC complexed with Asef
Authors	:	Zhang, Z.; Chen, L.; Gao, L.; Lin, K.; Wu, G.
Deposited on	:	2010-06-23
Resolution	:	3.01 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:

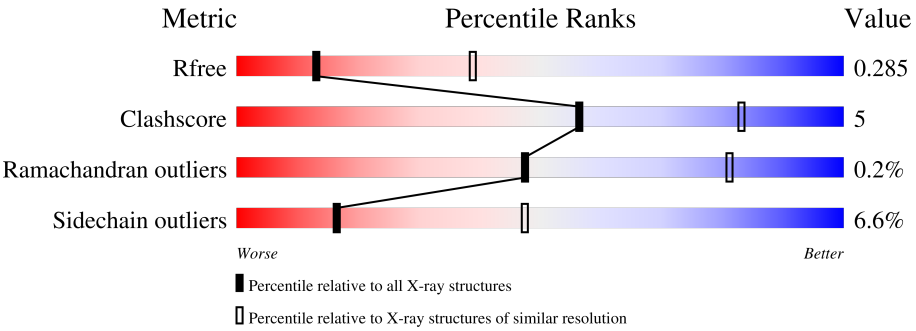
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 3.01 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	2399 (3.04-3.00)
Clashscore	141614	2734 (3.04-3.00)
Ramachandran outliers	138981	2640 (3.04-3.00)
Sidechain outliers	138945	2643 (3.04-3.00)

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	458	76% 12% • 11%
1	B	458	73% 14% • 13%
2	C	116	60% 11% • 27%
2	D	116	59% 12% • 28%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7673 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 APC variant protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	406	Total	C	N	O	S	0	0	0
			3130	1929	576	595	30			
1	B	400	Total	C	N	O	S	0	0	0
			3088	1901	570	587	30			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	282	MET	-	expression tag	UNP Q4LE70
A	283	GLY	-	expression tag	UNP Q4LE70
A	284	SER	-	expression tag	UNP Q4LE70
A	285	SER	-	expression tag	UNP Q4LE70
A	286	HIS	-	expression tag	UNP Q4LE70
A	287	HIS	-	expression tag	UNP Q4LE70
A	288	HIS	-	expression tag	UNP Q4LE70
A	289	HIS	-	expression tag	UNP Q4LE70
A	290	HIS	-	expression tag	UNP Q4LE70
A	291	HIS	-	expression tag	UNP Q4LE70
A	292	SER	-	expression tag	UNP Q4LE70
A	293	SER	-	expression tag	UNP Q4LE70
A	294	GLY	-	expression tag	UNP Q4LE70
A	295	LEU	-	expression tag	UNP Q4LE70
A	296	VAL	-	expression tag	UNP Q4LE70
A	297	PRO	-	expression tag	UNP Q4LE70
A	298	ARG	-	expression tag	UNP Q4LE70
A	299	GLY	-	expression tag	UNP Q4LE70
A	300	SER	-	expression tag	UNP Q4LE70
A	301	HIS	-	expression tag	UNP Q4LE70
A	302	MET	-	expression tag	UNP Q4LE70
B	282	MET	-	expression tag	UNP Q4LE70
B	283	GLY	-	expression tag	UNP Q4LE70
B	284	SER	-	expression tag	UNP Q4LE70
B	285	SER	-	expression tag	UNP Q4LE70

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Chain	Residue	Modelled	Actual	Comment	Reference
B	286	HIS	-	expression tag	UNP Q4LE70
B	287	HIS	-	expression tag	UNP Q4LE70
B	288	HIS	-	expression tag	UNP Q4LE70
B	289	HIS	-	expression tag	UNP Q4LE70
B	290	HIS	-	expression tag	UNP Q4LE70
B	291	HIS	-	expression tag	UNP Q4LE70
B	292	SER	-	expression tag	UNP Q4LE70
B	293	SER	-	expression tag	UNP Q4LE70
B	294	GLY	-	expression tag	UNP Q4LE70
B	295	LEU	-	expression tag	UNP Q4LE70
B	296	VAL	-	expression tag	UNP Q4LE70
B	297	PRO	-	expression tag	UNP Q4LE70
B	298	ARG	-	expression tag	UNP Q4LE70
B	299	GLY	-	expression tag	UNP Q4LE70
B	300	SER	-	expression tag	UNP Q4LE70
B	301	HIS	-	expression tag	UNP Q4LE70
B	302	MET	-	expression tag	UNP Q4LE70

- Molecule 2 is a protein called Rho guanine nucleotide exchange factor 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	84	Total	C	N	O	S	0	0	0
			661	414	116	128	3			
2	C	85	Total	C	N	O	S	0	0	0
			667	417	117	130	3			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	161	MET	-	expression tag	UNP Q9NR80
D	162	GLY	-	expression tag	UNP Q9NR80
D	163	HIS	-	expression tag	UNP Q9NR80
D	164	HIS	-	expression tag	UNP Q9NR80
D	165	HIS	-	expression tag	UNP Q9NR80
D	166	HIS	-	expression tag	UNP Q9NR80
D	167	HIS	-	expression tag	UNP Q9NR80
D	168	HIS	-	expression tag	UNP Q9NR80
D	169	MET	-	expression tag	UNP Q9NR80
C	161	MET	-	expression tag	UNP Q9NR80
C	162	GLY	-	expression tag	UNP Q9NR80
C	163	HIS	-	expression tag	UNP Q9NR80
C	164	HIS	-	expression tag	UNP Q9NR80

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Chain	Residue	Modelled	Actual	Comment	Reference
C	165	HIS	-	expression tag	UNP Q9NR80
C	166	HIS	-	expression tag	UNP Q9NR80
C	167	HIS	-	expression tag	UNP Q9NR80
C	168	HIS	-	expression tag	UNP Q9NR80
C	169	MET	-	expression tag	UNP Q9NR80

- Molecule 3 is water.

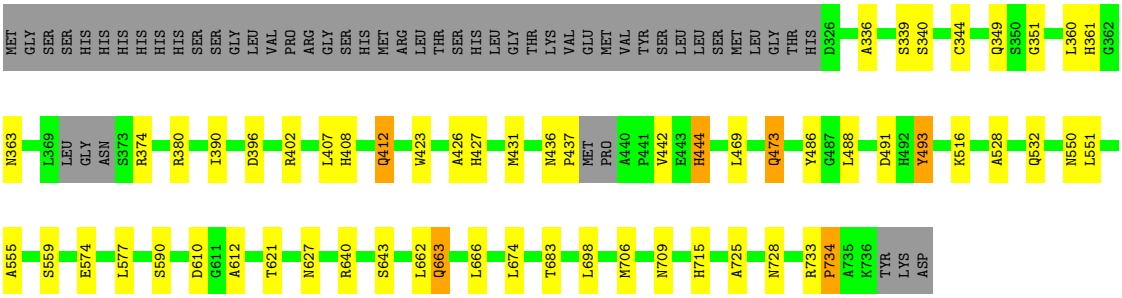
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	50	Total O 50 50	0	0
3	B	56	Total O 56 56	0	0
3	D	11	Total O 11 11	0	0
3	C	10	Total O 10 10	0	0

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. 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. 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.

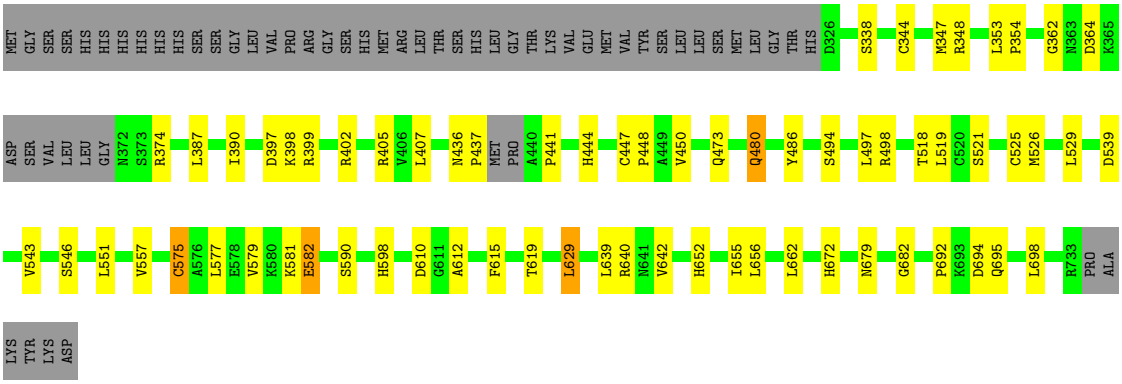
• Molecule 1: APC variant protein

Chain A:



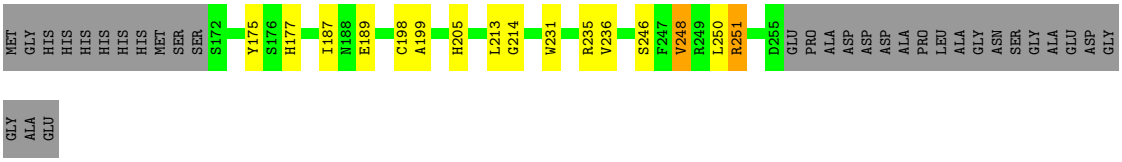
• Molecule 1: APC variant protein

Chain B:



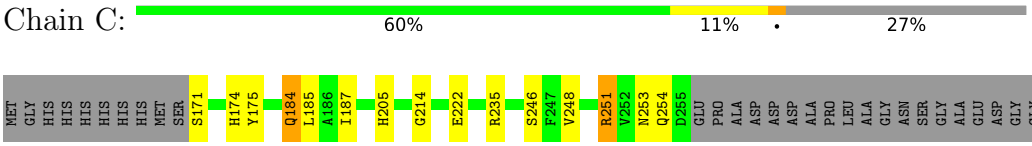
• Molecule 2: Rho guanine nucleotide exchange factor 4

Chain D:



• Molecule 2: Rho guanine nucleotide exchange factor 4

Chain C:


60%
11%
27%
MET GLY HIS HIS HIS HIS HIS HIS MET SER S171 H174 Y175 Q184 L185 A186 I187 H205 G214 E222 R235 S246 F247 V248 R251 V252 N253 Q254 D255 GLU PRO ALA ASP ASP ALA PRO LEU ALA GLY ASN SER GLY ALA GLU ASP GLY GLY ALA GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	163.18Å 163.18Å 242.59Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.01 40.70 – 3.01	Depositor EDS
% Data completeness (in resolution range)	90.2 (50.00-3.01) 90.7 (40.70-3.01)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	9.62 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.249 , 0.284 0.248 , 0.285	Depositor DCC
R_{free} test set	2202 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	76.2	Xtriage
Anisotropy	0.004	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 34.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	0.298 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7673	wwPDB-VP
Average B, all atoms (Å^2)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% 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	0.27	0/3170	0.46	0/4273
1	B	0.28	0/3127	0.47	0/4214
2	C	0.32	0/686	0.50	0/933
2	D	0.30	0/680	0.47	0/925
All	All	0.28	0/7663	0.47	0/10345

There are no bond length outliers.

There are no bond angle outliers.

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	3130	0	3160	29	0
1	B	3088	0	3112	32	0
2	C	667	0	600	8	0
2	D	661	0	595	7	0
3	A	50	0	0	1	0
3	B	56	0	0	2	0
3	C	10	0	0	0	0
3	D	11	0	0	0	0
All	All	7673	0	7467	75	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 5.

All (75) 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:473:GLN:HE21	1:A:473:GLN:H	1.20	0.84
2:D:199:ALA:HB1	2:D:248:VAL:HG13	1.61	0.83
1:B:629:LEU:H	1:B:629:LEU:HD23	1.45	0.80
2:C:251:ARG:HD3	2:C:253:ASN:H	1.48	0.78
1:B:692:PRO:HA	1:B:695:GLN:HG2	1.68	0.75
1:A:663:GLN:H	1:A:663:GLN:HE21	1.39	0.71
1:A:423:TRP:O	1:A:427:HIS:HB3	1.96	0.66
2:C:251:ARG:HA	2:C:251:ARG:HE	1.63	0.64
1:A:444:HIS:HA	1:A:493:TYR:CE2	2.34	0.63
1:B:546:SER:N	3:B:60:HOH:O	2.32	0.63
1:B:344:CYS:HA	1:B:347:MET:HG3	1.81	0.62
2:D:213:LEU:HD11	2:D:236:VAL:HG22	1.88	0.56
1:B:629:LEU:HD23	1:B:629:LEU:N	2.16	0.56
1:B:398:LYS:O	1:B:402:ARG:HG2	2.05	0.56
2:D:175:TYR:HA	2:D:231:TRP:CD1	2.41	0.55
1:A:473:GLN:H	1:A:473:GLN:NE2	1.99	0.52
2:C:251:ARG:HD3	2:C:253:ASN:N	2.22	0.52
1:A:408:HIS:O	1:A:412:GLN:HG2	2.09	0.52
1:B:639:LEU:HA	1:B:642:VAL:HG22	1.92	0.52
1:B:640:ARG:HE	1:B:682:GLY:HA3	1.74	0.51
1:B:582:GLU:H	1:B:582:GLU:CD	2.12	0.51
1:B:695:GLN:HA	1:B:698:LEU:HD12	1.94	0.50
1:B:402:ARG:HD3	1:B:405:ARG:HH22	1.76	0.50
1:B:575:CYS:O	1:B:579:VAL:HG13	2.12	0.50
1:A:396:ASP:HA	3:A:91:HOH:O	2.11	0.50
1:A:351:GLY:HA2	1:B:557:VAL:HG11	1.94	0.50
2:C:185:LEU:HB2	2:C:187:ILE:HD12	1.94	0.50
1:B:480:GLN:HB3	1:B:525:CYS:HA	1.95	0.49
1:A:516:LYS:HD3	1:A:550:ASN:O	2.13	0.48
1:A:344:CYS:HB3	1:A:390:ILE:HA	1.95	0.47
1:B:447:CYS:N	1:B:448:PRO:HD2	2.30	0.47
1:B:543:VAL:C	3:B:60:HOH:O	2.52	0.47
2:D:199:ALA:HB1	2:D:248:VAL:CG1	2.41	0.47
2:C:184:GLN:HE21	2:C:185:LEU:H	1.63	0.47
1:A:725:ALA:HA	1:A:728:ASN:HD22	1.80	0.46
1:A:442:VAL:HG12	1:A:444:HIS:H	1.80	0.46
1:A:528:ALA:O	1:A:532:GLN:HG2	2.16	0.45
1:B:662:LEU:HD22	1:B:698:LEU:HD21	1.97	0.45
1:B:494:SER:O	1:B:498:ARG:HG2	2.17	0.45
1:B:348:ARG:HB2	1:B:390:ILE:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:364:ASP:OD2	1:B:364:ASP:N	2.50	0.44
1:B:519:LEU:HD23	1:B:551:LEU:HD21	1.98	0.44
1:A:336:ALA:O	1:A:339:SER:HB3	2.18	0.44
1:A:423:TRP:O	1:A:427:HIS:CB	2.63	0.44
1:A:407:LEU:HD13	1:A:469:LEU:HD22	2.00	0.43
2:D:251:ARG:HD2	2:D:251:ARG:HA	1.81	0.43
1:A:516:LYS:HG2	1:A:551:LEU:HD23	1.98	0.43
1:A:674:LEU:HD21	1:A:715:HIS:CE1	2.53	0.43
1:A:733:ARG:HA	1:A:734:PRO:HD3	1.82	0.43
1:B:539:ASP:O	1:B:543:VAL:HG23	2.17	0.43
1:B:353:LEU:HB2	1:B:354:PRO:HD3	1.99	0.43
1:B:436:ASN:HA	1:B:437:PRO:HD3	1.82	0.43
2:C:222:GLU:HB3	2:C:235:ARG:HG2	2.01	0.42
2:D:187:ILE:HG12	2:D:250:LEU:HD21	2.01	0.42
1:B:447:CYS:HA	1:B:450:VAL:HG12	2.00	0.42
1:A:360:LEU:HB3	1:A:361:HIS:CD2	2.55	0.42
1:A:374:ARG:HD3	1:A:380:ARG:HD3	2.02	0.42
1:A:577:LEU:HD21	1:A:612:ALA:HA	2.02	0.41
1:B:577:LEU:HD21	1:B:612:ALA:HA	2.02	0.41
1:A:555:ALA:HB1	1:A:559:SER:HB2	2.02	0.41
1:B:518:THR:O	1:B:521:SER:OG	2.38	0.41
1:B:652:HIS:HA	1:B:655:ILE:HD12	2.02	0.41
1:A:473:GLN:HE21	1:A:473:GLN:N	2.00	0.41
1:B:615:PHE:O	1:B:619:THR:HG23	2.21	0.41
1:A:436:ASN:HA	1:A:437:PRO:HD3	1.85	0.41
1:B:526:MET:HA	1:B:529:LEU:HD12	2.01	0.41
1:A:426:ALA:HA	1:A:431:MET:SD	2.61	0.41
1:A:643:SER:HB3	1:A:683:THR:HG23	2.02	0.41
1:A:662:LEU:HD22	1:A:698:LEU:HD21	2.03	0.40
1:A:666:LEU:HD12	1:A:706:MET:SD	2.62	0.40
1:B:629:LEU:N	1:B:629:LEU:CD2	2.83	0.40
2:C:171:SER:HB3	2:C:174:HIS:NE2	2.36	0.40
2:C:205:HIS:HD2	2:C:214:GLY:HA2	1.87	0.40
1:B:640:ARG:HG3	1:B:679:ASN:HA	2.04	0.40
2:D:205:HIS:CD2	2:D:214:GLY:HA2	2.57	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	400/458 (87%)	385 (96%)	14 (4%)	1 (0%)	41 75
1	B	394/458 (86%)	379 (96%)	14 (4%)	1 (0%)	41 75
2	C	83/116 (72%)	73 (88%)	10 (12%)	0	100 100
2	D	82/116 (71%)	77 (94%)	5 (6%)	0	100 100
All	All	959/1148 (84%)	914 (95%)	43 (4%)	2 (0%)	47 81

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	362	GLY
1	A	734	PRO

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	345/391 (88%)	326 (94%)	19 (6%)	21 55
1	B	340/391 (87%)	318 (94%)	22 (6%)	17 48
2	C	68/89 (76%)	62 (91%)	6 (9%)	10 34
2	D	67/89 (75%)	60 (90%)	7 (10%)	7 26
All	All	820/960 (85%)	766 (93%)	54 (7%)	16 47

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	340	SER
1	A	349	GLN
1	A	363	ASN
1	A	402	ARG
1	A	412	GLN
1	A	444	HIS
1	A	473	GLN
1	A	486	TYR
1	A	488	LEU
1	A	491	ASP
1	A	493	TYR
1	A	574	GLU
1	A	590	SER
1	A	610	ASP
1	A	621	THR
1	A	627	ASN
1	A	640	ARG
1	A	663	GLN
1	A	709	ASN
1	B	338	SER
1	B	374	ARG
1	B	387	LEU
1	B	397	ASP
1	B	399	ARG
1	B	407	LEU
1	B	441	PRO
1	B	444	HIS
1	B	473	GLN
1	B	480	GLN
1	B	486	TYR
1	B	497	LEU
1	B	575	CYS
1	B	581	LYS
1	B	582	GLU
1	B	590	SER
1	B	598	HIS
1	B	610	ASP
1	B	629	LEU
1	B	656	LEU
1	B	672	HIS
1	B	694	ASP
2	D	177	HIS
2	D	189	GLU

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Mol	Chain	Res	Type
2	D	198	CYS
2	D	235	ARG
2	D	246	SER
2	D	248	VAL
2	D	251	ARG
2	C	175	TYR
2	C	184	GLN
2	C	246	SER
2	C	248	VAL
2	C	251	ARG
2	C	254	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	433	GLN
1	A	473	GLN
1	A	627	ASN
1	A	652	HIS
1	A	663	GLN
1	A	728	ASN
1	B	372	ASN
1	B	388	HIS
1	B	427	HIS
1	B	433	GLN
1	B	480	GLN
1	B	541	GLN
1	B	558	ASN
1	B	663	GLN
2	D	173	HIS
2	D	205	HIS
2	C	184	GLN
2	C	205	HIS

5.3.3 RNA

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.