Full wwPDB X-ray Structure Validation Report ⓘ

Sep 26, 2023 – 09:50 PM EDT

PDB ID	:	6CD2
Title	:	Crystal structure of the PapC usher bound to the chaperone-adhesin PapD-PapG
Authors	:	Omattage, N.S.; Deng, Z.; Yuan, P.; Hultgren, S.J.
Deposited on	:	2018-02-07
Resolution	:	3.70 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:

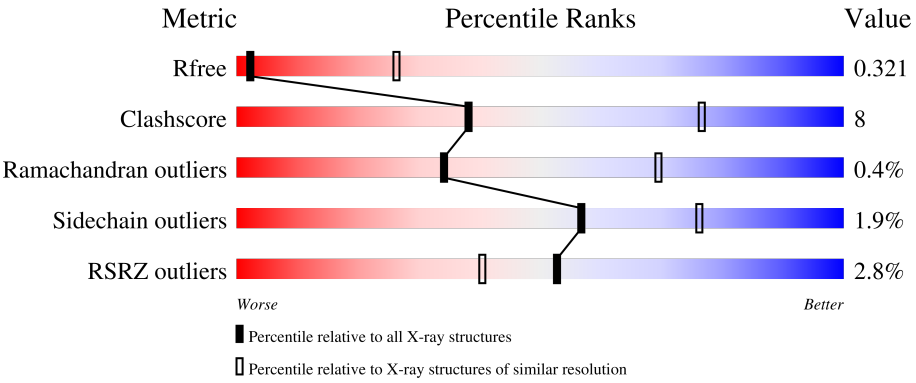
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.70 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	1049 (3.88-3.52)
Clashscore	141614	1027 (3.86-3.54)
Ramachandran outliers	138981	1069 (3.88-3.52)
Sidechain outliers	138945	1065 (3.88-3.52)
RSRZ outliers	127900	1578 (3.90-3.50)

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	221	2% 81% 16%
2	B	316	81% 18%
3	C	757	3% 85% 10%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8640 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 Chaperone protein PapD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	215	1637	1029	285	319	4	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	216	HIS	-	expression tag	UNP P15319
A	217	HIS	-	expression tag	UNP P15319
A	218	HIS	-	expression tag	UNP P15319
A	219	HIS	-	expression tag	UNP P15319
A	220	HIS	-	expression tag	UNP P15319
A	221	HIS	-	expression tag	UNP P15319

- Molecule 2 is a protein called PapGII adhesin protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	316	2353	1495	405	446	7	0	0	0

- Molecule 3 is a protein called Outer membrane usher protein PapC.

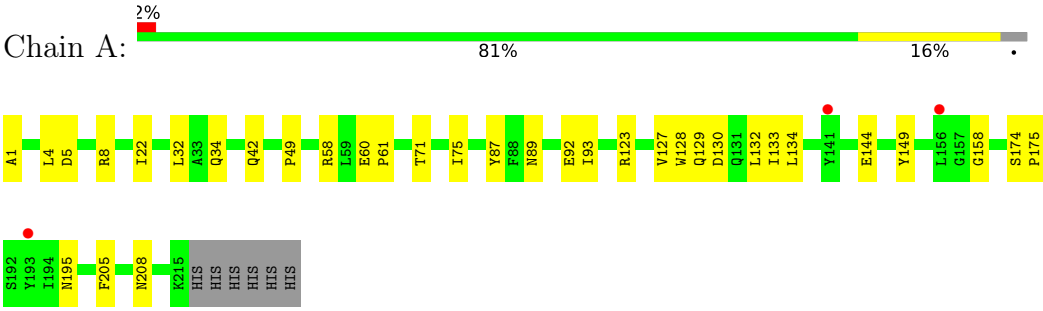
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	727	4650	2844	830	968	8	0	0	0

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.

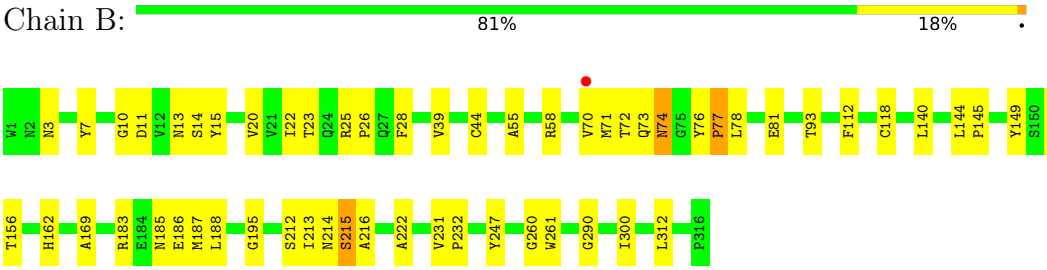
• Molecule 1: Chaperone protein PapD

Chain A:



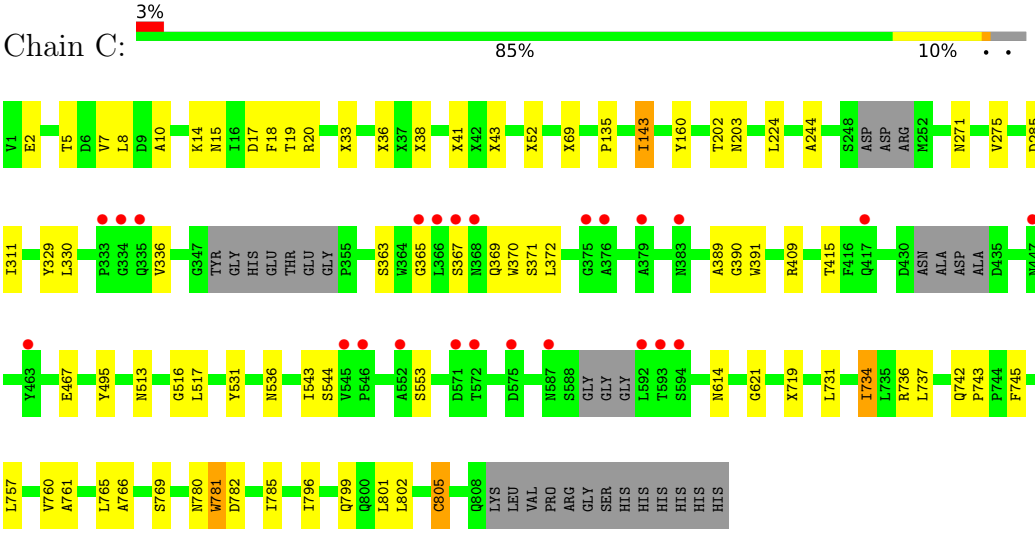
• Molecule 2: PapGII adhesin protein

Chain B:



• Molecule 3: Outer membrane usher protein PapC

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	204.30Å 300.71Å 100.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.01 – 3.70 49.14 – 3.70	Depositor EDS
% Data completeness (in resolution range)	81.0 (50.01-3.70) 81.0 (49.14-3.70)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.63 (at 3.67Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.282 , 0.329 0.276 , 0.321	Depositor DCC
R_{free} test set	1384 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	100.5	Xtriage
Anisotropy	0.670	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.23 , 99.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	8640	wwPDB-VP
Average B, all atoms (Å^2)	147.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% 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	0/1671	0.75	0/2279
2	B	0.42	0/2418	0.63	0/3309
3	C	0.43	0/4052	0.60	0/5545
All	All	0.46	0/8141	0.65	0/11133

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	1637	0	1568	20	0
2	B	2353	0	2131	40	0
3	C	4650	0	3451	63	0
All	All	8640	0	7150	120	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 8.

All (120) 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)
3:C:544:SER:HA	3:C:553:SER:HB2	1.42	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:154:PRO:HA	2:B:186:GLU:CB	1.97	0.93
3:C:745:PHE:HB3	3:C:761:ALA:O	1.73	0.88
2:B:3:ASN:ND2	2:B:118:CYS:SG	2.49	0.86
3:C:544:SER:HA	3:C:553:SER:CB	2.07	0.83
3:C:330:LEU:HD23	3:C:371:SER:HB2	1.60	0.83
2:B:7:TYR:CE2	2:B:39:VAL:HG13	2.24	0.71
2:B:72:THR:HG22	2:B:76:TYR:O	1.92	0.70
2:B:15:TYR:CD2	2:B:28:PHE:HA	2.27	0.69
2:B:71:MET:HA	2:B:77:PRO:HA	1.75	0.69
3:C:513:ASN:HB3	3:C:516:GLY:C	2.14	0.68
3:C:544:SER:CA	3:C:553:SER:HB2	2.23	0.67
3:C:513:ASN:ND2	3:C:517:LEU:O	2.28	0.67
3:C:15:ASN:O	3:C:18:PHE:HB3	1.96	0.65
3:C:745:PHE:HB2	3:C:760:VAL:O	1.97	0.64
2:B:144:LEU:HD11	2:B:149:TYR:CZ	2.33	0.64
2:B:3:ASN:OD1	2:B:44:CYS:HA	1.99	0.63
3:C:543:ILE:O	3:C:553:SER:HB2	1.99	0.62
3:C:17:ASP:CB	3:C:781:TRP:HB2	2.30	0.61
2:B:14:SER:HA	2:B:188:LEU:O	2.01	0.61
3:C:36:UNK:O	3:C:43:UNK:N	2.34	0.61
3:C:2:GLU:HA	3:C:19:THR:HG23	1.82	0.59
3:C:409:ARG:NE	3:C:415:THR:OG1	2.36	0.59
2:B:13:ASN:O	2:B:187:MET:CB	2.51	0.59
3:C:737:LEU:HD23	3:C:805:CYS:HB3	1.85	0.59
3:C:757:LEU:HD22	3:C:769:SER:O	2.04	0.58
1:A:32:LEU:HB2	1:A:93:ILE:HB	1.84	0.58
1:A:34:GLN:OE1	3:C:8:LEU:HD12	2.03	0.57
3:C:7:VAL:O	3:C:7:VAL:HG12	2.03	0.57
1:A:32:LEU:HD23	1:A:58:ARG:HA	1.87	0.57
3:C:52:UNK:HA	3:C:69:UNK:HA	1.85	0.57
3:C:299:ASP:OD1	3:C:300:SER:N	2.38	0.57
3:C:780:ASN:OD1	3:C:785:ILE:HG12	2.04	0.57
3:C:20:ARG:HD3	3:C:782:ASP:HA	1.85	0.57
2:B:74:ASN:HD22	2:B:74:ASN:N	2.03	0.56
3:C:33:UNK:N	3:C:754:GLY:O	2.39	0.56
3:C:796:ILE:HG12	3:C:799:GLN:NE2	2.20	0.56
2:B:78:LEU:CD1	2:B:151:VAL:HG21	2.36	0.55
3:C:38:UNK:N	3:C:41:UNK:O	2.41	0.54
2:B:11:ASP:N	2:B:185:ASN:CB	2.71	0.54
1:A:130:ASP:C	1:A:132:LEU:HD12	2.29	0.53
3:C:271:ASN:ND2	3:C:614:ASN:HD22	2.06	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:513:ASN:HB3	3:C:516:GLY:O	2.07	0.53
1:A:149:TYR:C	1:A:175:PRO:HG3	2.30	0.52
3:C:367:SER:O	3:C:370:TRP:N	2.41	0.52
3:C:544:SER:CA	3:C:553:SER:CB	2.84	0.51
2:B:145:PRO:HD2	2:B:149:TYR:OH	2.10	0.51
2:B:261:TRP:CZ2	2:B:300:ILE:HD12	2.45	0.51
3:C:531:TYR:HB3	3:C:536:ASN:OD1	2.10	0.51
2:B:13:ASN:OD1	2:B:187:MET:CB	2.59	0.51
2:B:162:HIS:CE1	2:B:169:ALA:HB1	2.46	0.51
2:B:70:VAL:HG13	2:B:78:LEU:HB2	1.92	0.50
3:C:5:THR:O	3:C:8:LEU:HB3	2.12	0.50
1:A:58:ARG:NH1	1:A:60:GLU:OE1	2.36	0.50
1:A:60:GLU:CD	1:A:61:PRO:HD2	2.31	0.50
3:C:143:ILE:HD11	3:C:719:UNK:C	2.42	0.49
3:C:365:GLY:HA2	3:C:371:SER:HA	1.93	0.49
2:B:155:TYR:O	2:B:185:ASN:O	2.30	0.48
3:C:224:LEU:HD21	3:C:244:ALA:HB1	1.95	0.48
2:B:13:ASN:O	2:B:187:MET:CA	2.61	0.48
1:A:4:LEU:HD23	1:A:22:ILE:HG22	1.96	0.48
2:B:212:SER:HB3	2:B:216:ALA:HB2	1.96	0.48
2:B:22:ILE:HG23	2:B:195:GLY:HA2	1.96	0.48
3:C:371:SER:O	3:C:390:GLY:N	2.47	0.47
2:B:231:VAL:HB	2:B:232:PRO:HD2	1.97	0.47
2:B:155:TYR:CD1	2:B:186:GLU:HA	2.51	0.47
2:B:156:THR:OG1	2:B:183:ARG:HD3	2.15	0.47
2:B:10:GLY:HA2	2:B:185:ASN:N	2.30	0.46
2:B:78:LEU:HD11	2:B:151:VAL:HG21	1.97	0.46
2:B:20:VAL:HG11	2:B:26:PRO:HB3	1.97	0.46
3:C:17:ASP:HA	3:C:20:ARG:HD2	1.98	0.46
3:C:369:GLN:O	3:C:391:TRP:HA	2.16	0.46
3:C:467:GLU:HA	3:C:495:TYR:HA	1.97	0.46
3:C:160:TYR:N	3:C:621:GLY:O	2.49	0.45
3:C:330:LEU:HD23	3:C:371:SER:CB	2.41	0.45
3:C:543:ILE:O	3:C:553:SER:CB	2.64	0.45
3:C:745:PHE:CB	3:C:761:ALA:O	2.56	0.45
3:C:365:GLY:CA	3:C:371:SER:HA	2.48	0.44
3:C:2:GLU:HA	3:C:19:THR:CG2	2.47	0.44
3:C:202:THR:HG22	3:C:203:ASN:N	2.33	0.44
2:B:70:VAL:O	2:B:78:LEU:N	2.51	0.44
3:C:731:LEU:HD13	3:C:801:LEU:HD12	2.00	0.44
2:B:25:ARG:NH2	2:B:81:GLU:CB	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:144:LEU:HD12	2:B:145:PRO:HD2	2.00	0.43
2:B:222:ALA:HB2	2:B:290:GLY:HA2	2.00	0.43
3:C:38:UNK:O	3:C:41:UNK:N	2.51	0.43
3:C:275:VAL:HG23	3:C:285:ASP:HB3	2.01	0.43
3:C:736:ARG:NH1	3:C:742:GLN:HG2	2.34	0.43
3:C:743:PRO:O	3:C:760:VAL:HG11	2.19	0.43
1:A:128:TRP:CD1	1:A:129:GLN:N	2.87	0.43
1:A:5:ASP:O	2:B:23:THR:HG23	2.18	0.43
1:A:133:ILE:HB	1:A:144:GLU:HB2	2.01	0.43
3:C:734:ILE:HB	3:C:802:LEU:HD23	2.01	0.43
1:A:123:ARG:HB2	1:A:127:VAL:CG2	2.49	0.42
1:A:8:ARG:NH2	1:A:195:ASN:O	2.53	0.42
1:A:71:THR:HB	1:A:75:ILE:HD12	2.01	0.42
1:A:1:ALA:HA	1:A:92:GLU:OE1	2.19	0.42
2:B:214:ASN:OD1	2:B:215:SER:N	2.53	0.42
1:A:34:GLN:OE1	3:C:8:LEU:CD1	2.67	0.42
3:C:365:GLY:HA3	3:C:370:TRP:O	2.20	0.41
3:C:796:ILE:CG1	3:C:799:GLN:NE2	2.83	0.41
2:B:55:ALA:HB2	2:B:112:PHE:CZ	2.54	0.41
2:B:155:TYR:CE1	2:B:186:GLU:HA	2.55	0.41
1:A:134:LEU:HD13	1:A:205:PHE:CE2	2.55	0.41
3:C:365:GLY:CA	3:C:370:TRP:O	2.68	0.41
3:C:10:ALA:HB2	3:C:745:PHE:HZ	1.85	0.41
3:C:14:LYS:O	3:C:14:LYS:HG3	2.20	0.41
3:C:745:PHE:HB2	3:C:760:VAL:C	2.40	0.41
1:A:158:GLY:CA	1:A:186:TYR:CD1	3.03	0.41
1:A:42:GLN:HG2	1:A:87:TYR:CE1	2.56	0.41
2:B:72:THR:N	2:B:76:TYR:O	2.52	0.41
2:B:78:LEU:HD22	2:B:140:LEU:HD23	2.03	0.41
3:C:745:PHE:HA	3:C:760:VAL:HB	2.02	0.41
3:C:765:LEU:HG	3:C:766:ALA:N	2.35	0.41
2:B:7:TYR:CD2	2:B:39:VAL:HG13	2.55	0.40
3:C:311:ILE:HD12	3:C:311:ILE:N	2.36	0.40
1:A:49:PRO:HB3	1:A:75:ILE:HG13	2.03	0.40
2:B:247:TYR:OH	2:B:260:GLY:O	2.31	0.40
3:C:329:TYR:CD2	3:C:363:SER:HB2	2.57	0.40
3:C:372:LEU:HA	3:C:389:ALA:HA	2.02	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	213/221 (96%)	195 (92%)	18 (8%)	0	100	100
2	B	314/316 (99%)	292 (93%)	20 (6%)	2 (1%)	25	62
3	C	583/757 (77%)	527 (90%)	54 (9%)	2 (0%)	41	74
All	All	1110/1294 (86%)	1014 (91%)	92 (8%)	4 (0%)	34	69

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	213	ILE
2	B	77	PRO
3	C	135	PRO
3	C	336	VAL

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	173/197 (88%)	170 (98%)	3 (2%)	60	79
2	B	232/269 (86%)	226 (97%)	6 (3%)	46	69
3	C	342/514 (66%)	337 (98%)	5 (2%)	65	81
All	All	747/980 (76%)	733 (98%)	14 (2%)	57	76

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	ASN
1	A	174	SER
1	A	208	ASN
2	B	58	ARG
2	B	73	GLN
2	B	74	ASN
2	B	93	THR
2	B	215	SER
2	B	312	LEU
3	C	143	ILE
3	C	734	ILE
3	C	750	THR
3	C	781	TRP
3	C	805	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	74	ASN
2	B	162	HIS
2	B	242	ASN
3	C	271	ASN
3	C	453	GLN

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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	C	4

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	633:ALA	C	651:UNK	N	11.72
1	C	662:UNK	C	672:UNK	N	8.12
1	C	687:UNK	C	714:UNK	N	8.01
1	C	54:UNK	C	67:UNK	N	5.42

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	215/221 (97%)	-0.22	4 (1%)	66	55	57, 88, 129, 170	0
2	B	316/316 (100%)	-0.38	1 (0%)	94	90	74, 142, 191, 221	0
3	C	594/757 (78%)	-0.17	26 (4%)	34	25	60, 189, 246, 285	0
All	All	1125/1294 (86%)	-0.23	31 (2%)	53	40	57, 154, 236, 285	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	366	LEU	4.6
3	C	334	GLY	4.0
3	C	552	ALA	3.9
3	C	572	THR	3.7
3	C	335	GLN	3.4
3	C	333	PRO	3.4
3	C	592	LEU	3.4
3	C	367	SER	3.3
3	C	545	VAL	3.2
3	C	593	THR	3.1
3	C	447	ASN	3.1
3	C	463	TYR	3.1
1	A	191	LEU	3.0
3	C	368	ASN	2.8
3	C	571	ASP	2.8
3	C	594	SER	2.7
3	C	575	ASP	2.6
3	C	375	GLY	2.6
3	C	383	ASN	2.5
3	C	379	ALA	2.5
3	C	546	PRO	2.4
1	A	193	TYR	2.3
3	C	376	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	156	LEU	2.2
3	C	365	GLY	2.2
3	C	417	GLN	2.2
3	C	449	MET	2.1
1	A	141	TYR	2.1
2	B	70	VAL	2.0
3	C	454	TYR	2.0
3	C	587	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.