



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:37 AM UTC

PDB ID : 6CD2 / pdb\_00006cd2  
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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (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

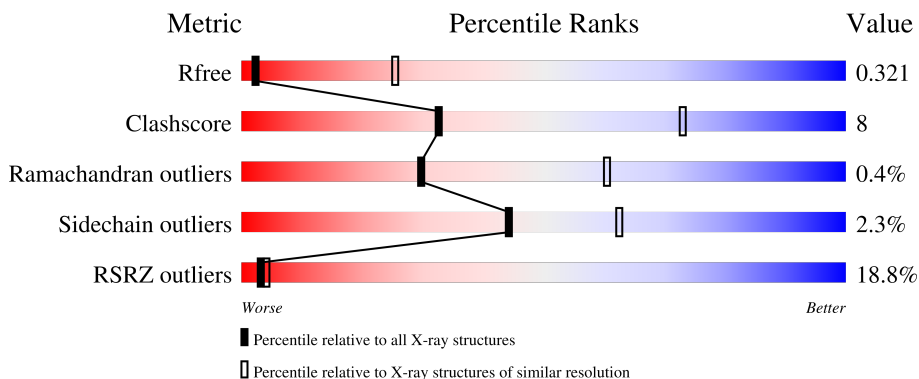
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	180053	1131 (3.80-3.60)
Clashscore	190562	1171 (3.80-3.60)
Ramachandran outliers	187476	1129 (3.80-3.60)
Sidechain outliers	187428	1126 (3.80-3.60)
RSRZ outliers	180081	1130 (3.80-3.60)

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  $\geq 3$ , 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	221	
2	B	316	
3	C	757	

## 2 Entry composition

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

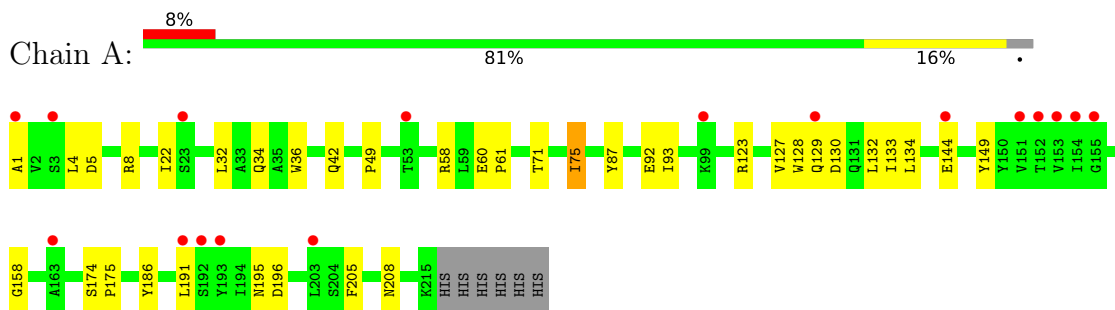
- Molecule 3 is a protein called Outer membrane usher protein PapC.

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

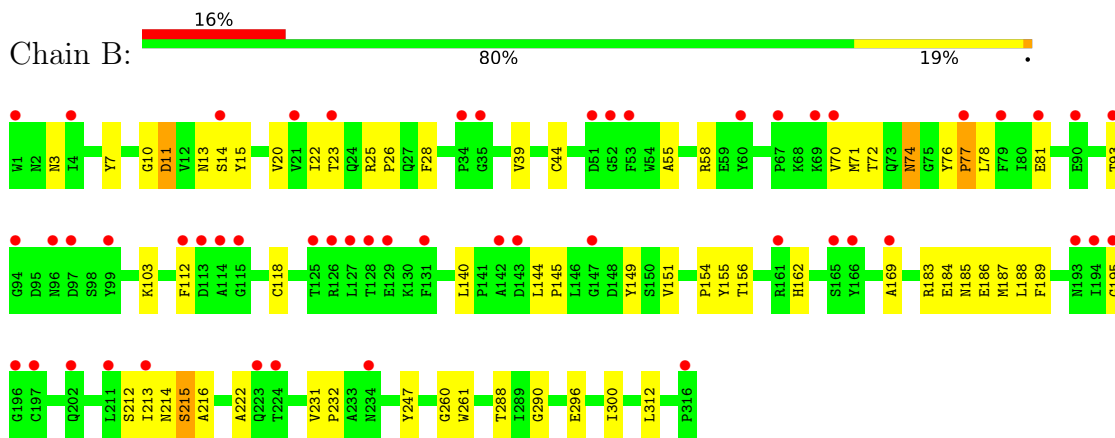
### 3 Residue-property plots [i](#)

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.

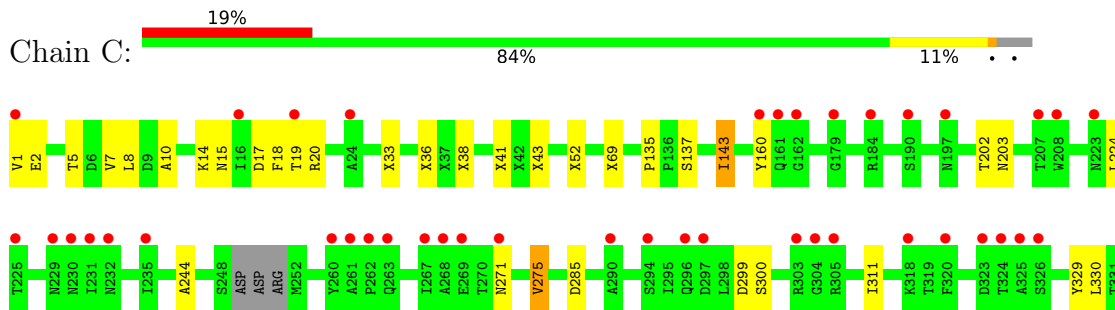
- Molecule 1: Chaperone protein PapD

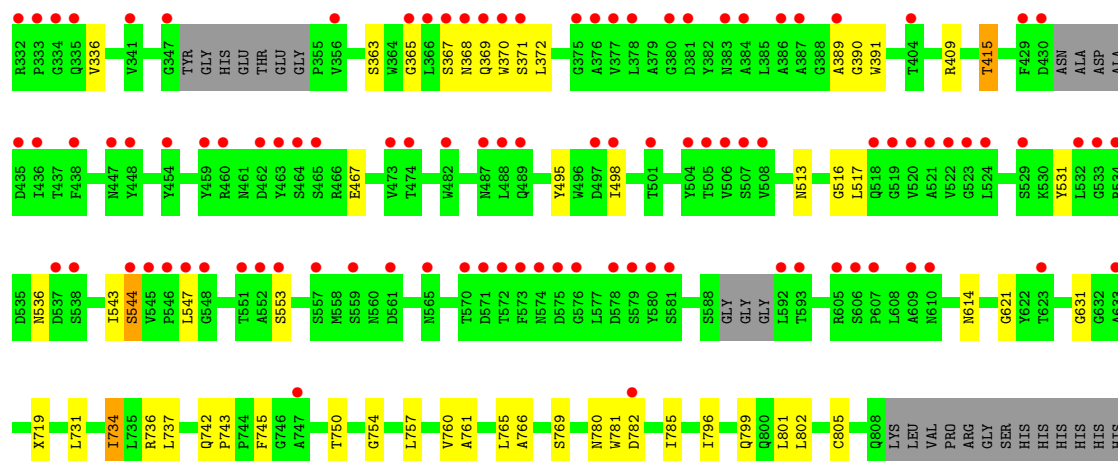


- Molecule 2: PapGII adhesin protein



- Molecule 3: Outer membrane usher protein PapC





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	204.30Å 300.71Å 100.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.01 – 3.70 50.01 – 3.70	Depositor EDS
% Data completeness (in resolution range)	81.0 (50.01-3.70) 81.0 (50.01-3.70)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.63 (at 3.67Å)	Xtrriage
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 (4.13%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	100.5	Xtrriage
Anisotropy	0.670	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 128.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.84	EDS
Total number of atoms	8640	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	147.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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](#)

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	0.77	1/1671 (0.1%)	0.95	1/2279 (0.0%)
2	B	0.60	0/2418	0.83	1/3309 (0.0%)
3	C	0.65	0/4052	0.86	4/5545 (0.1%)
All	All	0.66	1/8141 (0.0%)	0.87	6/11133 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	191	LEU	N-CA	6.03	1.53	1.46

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	137	SER	N-CA-C	6.13	118.82	110.55
3	C	544	SER	N-CA-C	5.94	117.88	108.79
1	A	36	TRP	N-CA-C	5.92	117.78	108.96
3	C	498	ILE	N-CA-C	5.51	116.24	110.62
2	B	11	ASP	N-CA-C	5.19	117.55	110.24
3	C	631	GLY	N-CA-C	5.14	120.42	110.66

There are no chirality outliers.

There are no planarity outliers.

### 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	1637	0	1568	21	0
2	B	2353	0	2131	43	0
3	C	4650	0	3451	64	0
All	All	8640	0	7150	125	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 (125) 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
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
3:C:513:ASN:HB3	3:C:516:GLY:C	2.14	0.73
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: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
1:A:130:ASP:C	1:A:132:LEU:HD12	2.29	0.58
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:TYR:C	1:A:175:PRO:HG3	2.30	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
1:A:60:GLU:CD	1:A:61:PRO:HD2	2.31	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
3:C:271:ASN:ND2	3:C:614:ASN:HD22	2.06	0.53
3:C:513:ASN:HB3	3:C:516:GLY:O	2.07	0.53
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:467:GLU:HA	3:C:495:TYR:HA	1.97	0.46
3:C:745:PHE:HB2	3:C:760:VAL:C	2.40	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:296:GLU:C	2:B:300:ILE:HG12	2.43	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
1:A:195:ASN:O	1:A:196:ASP:C	2.60	0.43
2:B:10:GLY:HA2	2:B:184:GLU:C	2.43	0.43
2:B:25:ARG:NH2	2:B:81:GLU:CB	2.82	0.43
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:367:SER:O	3:C:368:ASN:C	2.63	0.41
1:A:158:GLY:CA	1:A:186:TYR:CD1	3.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:189:PHE:CD1	2:B:189:PHE:C	2.97	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%)	21	52
3	C	583/757 (77%)	527 (90%)	54 (9%)	2 (0%)	36	65
All	All	1110/1294 (86%)	1014 (91%)	92 (8%)	4 (0%)	30	60

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

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%)	53	67
2	B	232/269 (86%)	225 (97%)	7 (3%)	36	57
3	C	342/514 (66%)	335 (98%)	7 (2%)	48	64
All	All	747/980 (76%)	730 (98%)	17 (2%)	44	62

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	ILE
1	A	174	SER
1	A	208	ASN
2	B	58	ARG
2	B	74	ASN
2	B	93	THR
2	B	103	LYS
2	B	215	SER
2	B	288	THR
2	B	312	LEU
3	C	1	VAL
3	C	143	ILE
3	C	275	VAL
3	C	415	THR
3	C	547	LEU
3	C	734	ILE
3	C	750	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	74	ASN
2	B	162	HIS
2	B	242	ASN
2	B	259	HIS

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Mol	Chain	Res	Type
3	C	453	GLN
3	C	597	GLN
3	C	614	ASN
3	C	800	GLN
3	C	808	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 oligosaccharides 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

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	215/221 (97%)	0.44	17 (7%) 18 15	57, 88, 129, 170	0
2	B	316/316 (100%)	0.78	52 (16%) 4 6	74, 142, 191, 221	0
3	C	594/757 (78%)	1.19	142 (23%) 2 2	60, 189, 246, 285	0
All	All	1125/1294 (86%)	0.93	211 (18%) 3 4	57, 154, 236, 285	0

All (211) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	545	VAL	11.2
3	C	572	THR	11.2
2	B	52	GLY	10.7
3	C	575	ASP	9.4
3	C	366	LEU	8.7
3	C	546	PRO	8.2
3	C	552	ALA	7.9
2	B	114	ALA	7.8
1	A	193	TYR	7.5
3	C	325	ALA	7.5
3	C	576	GLY	6.9
2	B	96	ASN	6.9
3	C	368	ASN	6.2
3	C	522	VAL	6.1
2	B	128	THR	6.0
3	C	334	GLY	5.9
3	C	473	VAL	5.8
2	B	126	ARG	5.6
2	B	97	ASP	5.6
3	C	318	LYS	5.6
3	C	592	LEU	5.5
3	C	269	GLU	5.5
3	C	430	ASP	5.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	C	497	ASP	5.3
3	C	262	PRO	5.2
3	C	326	SER	5.2
3	C	383	ASN	5.2
3	C	197	ASN	5.1
3	C	367	SER	5.1
3	C	376	ALA	4.8
1	A	153	VAL	4.8
1	A	191	LEU	4.8
3	C	333	PRO	4.6
3	C	389	ALA	4.5
3	C	324	THR	4.5
3	C	465	SER	4.4
2	B	70	VAL	4.4
3	C	559	SER	4.4
3	C	294	SER	4.3
3	C	375	GLY	4.3
3	C	544	SER	4.3
3	C	474	THR	4.2
3	C	384	ALA	4.2
3	C	551	THR	4.2
3	C	335	GLN	4.2
1	A	152	THR	4.1
3	C	518	GLN	4.1
3	C	571	ASP	3.9
2	B	112	PHE	3.9
2	B	53	PHE	3.9
2	B	69	LYS	3.9
2	B	51	ASP	3.9
3	C	232	ASN	3.8
3	C	553	SER	3.8
3	C	508	VAL	3.8
2	B	166	TYR	3.7
3	C	304	GLY	3.7
2	B	196	GLY	3.6
3	C	377	VAL	3.6
1	A	192	SER	3.6
2	B	34	PRO	3.6
3	C	267	ILE	3.6
1	A	155	GLY	3.6
2	B	79	PHE	3.6
3	C	459	TYR	3.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	C	263	GLN	3.5
3	C	579	SER	3.5
3	C	436	ILE	3.5
3	C	260	TYR	3.5
2	B	143	ASP	3.5
3	C	561	ASP	3.5
3	C	261	ALA	3.5
2	B	113	ASP	3.4
3	C	463	TYR	3.3
3	C	488	LEU	3.3
3	C	610	ASN	3.3
3	C	523	GLY	3.3
2	B	93	THR	3.2
2	B	77	PRO	3.2
3	C	529	SER	3.2
3	C	381	ASP	3.2
3	C	305	ARG	3.2
2	B	197	CYS	3.1
2	B	94	GLY	3.1
2	B	60	TYR	3.1
3	C	323	ASP	3.1
3	C	547	LEU	3.1
2	B	202	GLN	3.1
3	C	489	GLN	3.1
2	B	67	PRO	3.1
2	B	316	PRO	3.1
3	C	507	SER	3.0
2	B	194	ILE	3.0
3	C	570	THR	3.0
2	B	1	TRP	3.0
2	B	81	GLU	3.0
3	C	404	THR	3.0
2	B	23	THR	3.0
3	C	464	SER	3.0
3	C	782	ASP	3.0
3	C	447	ASN	3.0
3	C	231	ILE	2.9
1	A	3	SER	2.9
1	A	203	LEU	2.9
2	B	115	GLY	2.9
3	C	574	ASN	2.9
3	C	341	VAL	2.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	B	224	THR	2.8
3	C	207	THR	2.8
3	C	369	GLN	2.8
3	C	429	PHE	2.8
3	C	356	VAL	2.8
3	C	462	ASP	2.7
3	C	225	THR	2.7
3	C	506	VAL	2.7
3	C	229	ASN	2.7
3	C	386	ALA	2.7
2	B	147	GLY	2.7
3	C	332	ARG	2.7
3	C	633	ALA	2.7
3	C	24	ALA	2.7
3	C	521	ALA	2.7
1	A	99	LYS	2.7
2	B	14	SER	2.6
3	C	387	ALA	2.6
2	B	211	LEU	2.6
3	C	505	THR	2.6
3	C	534	ARG	2.6
2	B	195	GLY	2.6
3	C	160	TYR	2.6
3	C	320	PHE	2.6
3	C	498	ILE	2.6
3	C	504	TYR	2.6
3	C	593	THR	2.6
1	A	151	VAL	2.6
3	C	290	ALA	2.6
2	B	129	GLU	2.5
2	B	142	ALA	2.5
2	B	165	SER	2.5
3	C	435	ASP	2.5
2	B	99	TYR	2.5
3	C	271	ASN	2.5
3	C	380	GLY	2.5
3	C	519	GLY	2.5
3	C	501	THR	2.5
2	B	4	ILE	2.5
2	B	234	ASN	2.5
3	C	578	ASP	2.5
3	C	19	THR	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	163	ALA	2.4
3	C	565	ASN	2.4
3	C	548	GLY	2.4
3	C	537	ASP	2.4
3	C	448	TYR	2.4
3	C	223	ASN	2.4
2	B	21	VAL	2.4
1	A	53	THR	2.4
3	C	538	SER	2.4
1	A	144	GLU	2.4
2	B	90	GLU	2.4
1	A	1	ALA	2.4
3	C	460	ARG	2.4
2	B	223	GLN	2.4
3	C	532	LEU	2.4
3	C	580	TYR	2.4
3	C	605	ARG	2.4
2	B	161	ARG	2.4
1	A	154	ILE	2.3
3	C	438	PHE	2.3
3	C	573	PHE	2.3
3	C	609	ALA	2.3
3	C	297	ASP	2.3
2	B	35	GLY	2.3
3	C	365	GLY	2.3
3	C	378	LEU	2.3
2	B	169	ALA	2.3
3	C	747	ALA	2.3
1	A	23	SER	2.3
2	B	125	THR	2.2
3	C	161	GLN	2.2
3	C	557	SER	2.2
2	B	193	ASN	2.2
3	C	268	ALA	2.2
3	C	520	VAL	2.2
2	B	127	LEU	2.2
3	C	370	TRP	2.2
3	C	482	TRP	2.2
3	C	524	LEU	2.2
3	C	607	PRO	2.2
3	C	16	ILE	2.2
3	C	208	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
3	C	184	ARG	2.2
3	C	1	VAL	2.2
3	C	162	GLY	2.2
3	C	235	ILE	2.1
3	C	347	GLY	2.1
3	C	533	GLY	2.1
3	C	190	SER	2.1
3	C	606	SER	2.1
3	C	296	GLN	2.1
3	C	623	THR	2.1
3	C	230	ASN	2.1
3	C	371	SER	2.1
2	B	131	PHE	2.1
3	C	454	TYR	2.1
3	C	581	SER	2.1
3	C	303	ARG	2.1
2	B	213	ILE	2.1
1	A	129	GLN	2.1
3	C	487	ASN	2.1
3	C	179	GLY	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.