



# Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 10:58 pm BST

PDB ID : 4F88  
Title : X-ray Crystal Structure of PlyC  
Authors : McGowan, S.; Buckle, A.M.; Fischetti, V.A.; Nelson, D.C.; Whisstock, J.C.  
Deposited on : 2012-05-17  
Resolution : 3.30 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](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.

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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	:	2.11
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)	:	2.11

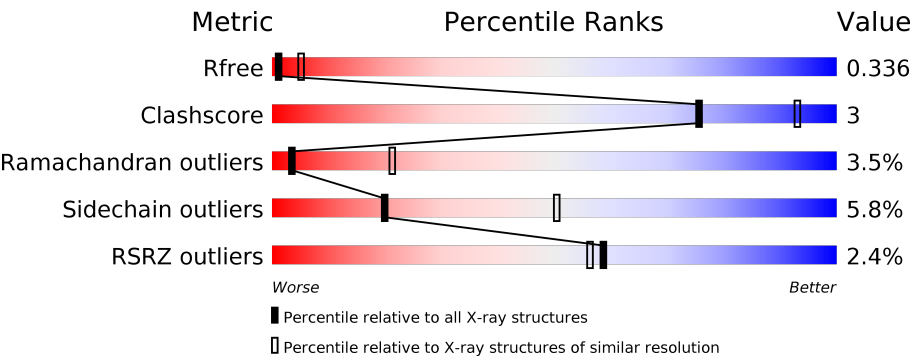
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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 on 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	1	465	<div><div>2%</div><div><div></div><div>78%</div><div>12%</div><div>•</div><div>8%</div></div></div>
1	2	465	<div><div>2%</div><div><div></div><div>74%</div><div>13%</div><div>•</div><div>10%</div></div></div>
2	A	72	<div><div>7%</div><div><div></div><div>86%</div><div>8%</div><div>6%</div></div></div>
2	B	72	<div><div>13%</div><div><div></div><div>89%</div><div>7%</div><div>•</div></div></div>
2	C	72	<div><div>•</div><div><div></div><div>89%</div><div>7%</div><div>•</div></div></div>
2	D	72	<div><div></div><div><div></div><div>85%</div><div>•</div><div>13%</div></div></div>

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Mol	Chain	Length	Quality of chain
2	E	72	<div><div>%</div><div><div></div><div>89%</div><div></div></div><div><div></div><div></div><div>10%</div></div></div>
2	F	72	<div><div></div><div><div></div><div>82%</div><div></div></div><div><div></div><div>7%</div><div></div></div><div><div></div><div></div><div>10%</div></div></div>
2	G	72	<div><div></div><div><div></div><div>82%</div><div></div></div><div><div></div><div>11%</div><div></div></div><div><div></div><div></div><div></div></div></div>
2	H	72	<div><div>3%</div><div><div></div><div>88%</div><div></div></div><div><div></div><div></div><div>7%</div></div></div>
2	I	72	<div><div>4%</div><div><div></div><div>68%</div><div></div></div><div><div></div><div></div><div>28%</div></div></div>
2	J	72	<div><div></div><div><div></div><div>47%</div><div></div></div><div><div></div><div></div><div>51%</div></div></div>
2	K	72	<div><div></div><div><div></div><div>65%</div><div></div></div><div><div></div><div>8%</div><div></div></div><div><div></div><div></div><div>26%</div></div></div>
2	L	72	<div><div></div><div><div></div><div>72%</div><div></div></div><div><div></div><div></div><div>24%</div></div></div>
2	M	72	<div><div>%</div><div><div></div><div>85%</div><div></div></div><div><div></div><div></div><div>10%</div></div></div>
2	N	72	<div><div>%</div><div><div></div><div>74%</div><div></div></div><div><div></div><div>7%</div><div></div></div><div><div></div><div></div><div>18%</div></div></div>
2	O	72	<div><div>3%</div><div><div></div><div>85%</div><div></div></div><div><div></div><div>6%</div><div></div></div><div><div></div><div></div><div>10%</div></div></div>
2	P	72	<div><div>4%</div><div><div></div><div>81%</div><div></div></div><div><div></div><div></div><div>17%</div></div></div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12281 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 PlyCA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	430	Total	C	N	O	S	0	0	0
			2858	1799	497	548	14			
1	2	418	Total	C	N	O	S	0	0	0
			2781	1752	471	545	13			

- Molecule 2 is a protein called PlyCB.

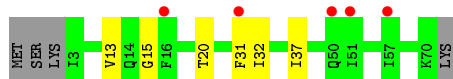
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	68	Total	C	N	O	S	0	0	0
			490	307	82	100	1			
2	B	69	Total	C	N	O	S	0	0	0
			509	319	87	102	1			
2	C	69	Total	C	N	O	S	0	0	0
			499	310	87	101	1			
2	D	63	Total	C	N	O	S	0	0	0
			455	287	76	91	1			
2	E	65	Total	C	N	O	S	0	0	0
			463	293	78	91	1			
2	F	65	Total	C	N	O	S	0	0	0
			473	299	80	93	1			
2	G	69	Total	C	N	O	S	0	0	0
			483	307	80	95	1			
2	H	67	Total	C	N	O	S	0	0	0
			485	306	83	95	1			
2	I	52	Total	C	N	O		0	0	0
			309	189	58	62				
2	J	35	Total	C	N	O		0	0	0
			185	110	36	39				
2	K	53	Total	C	N	O		0	0	0
			283	169	58	56				
2	L	55	Total	C	N	O		0	0	0
			300	178	58	64				

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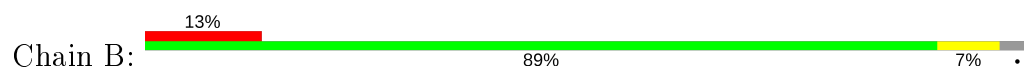
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	65	Total	C	N	O		0	0	0
			447	283	77	87				
2	N	59	Total	C	N	O		0	0	0
			435	277	73	85				
2	O	65	Total	C	N	O	S	0	0	0
			439	276	76	86	1			
2	P	60	Total	C	N	O	S	0	0	0
			387	237	70	79	1			

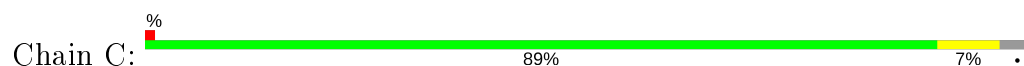




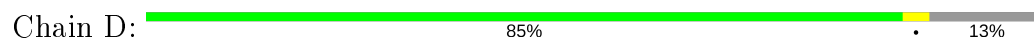
• Molecule 2: PlyCB



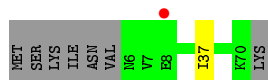
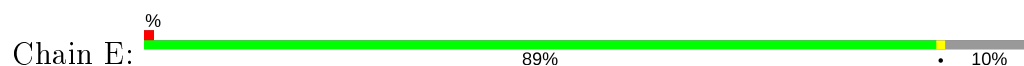
• Molecule 2: PlyCB



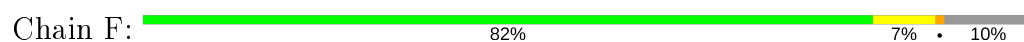
• Molecule 2: PlyCB



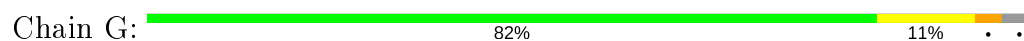
• Molecule 2: PlyCB



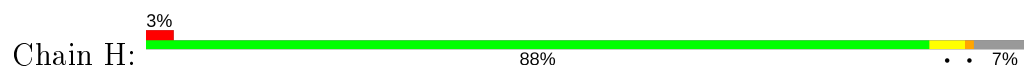
• Molecule 2: PlyCB

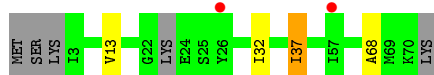


• Molecule 2: PlyCB

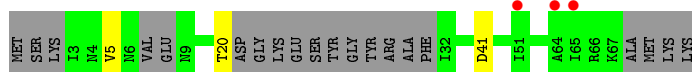


• Molecule 2: PlyCB

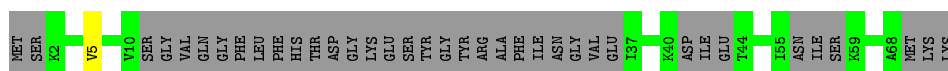




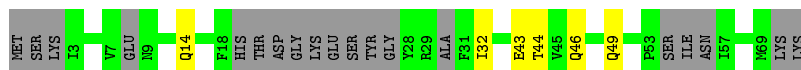
• Molecule 2: PlyCB



• Molecule 2: PlyCB



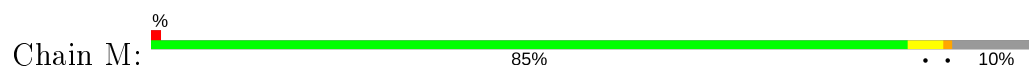
• Molecule 2: PlyCB



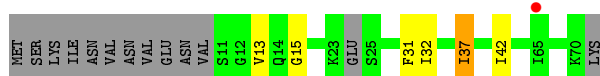
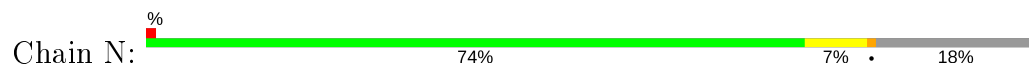
• Molecule 2: PlyCB



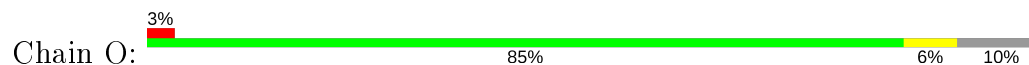
• Molecule 2: PlyCB



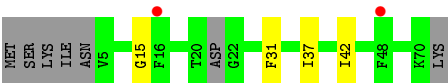
• Molecule 2: PlyCB



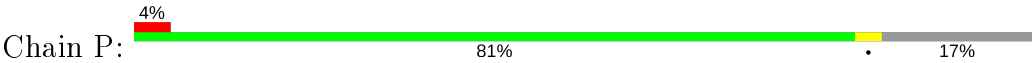
• Molecule 2: PlyCB







● Molecule 2: PlyCB



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.85Å 117.42Å 222.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.72 – 3.30 86.46 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.0 (46.72-3.30) 98.8 (86.46-3.30)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.94 (at 3.33Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, $R_{free}$	0.266 , 0.297 0.297 , 0.336	Depositor DCC
$R_{free}$ test set	1870 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	106.2	Xtriage
Anisotropy	0.168	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 79.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	12281	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% 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	1	0.42	0/2926	0.72	3/4021 (0.1%)
1	2	0.42	0/2850	0.70	1/3923 (0.0%)
2	A	0.39	0/496	0.60	0/675
2	B	0.44	0/515	0.57	0/696
2	C	0.36	0/506	0.57	0/686
2	D	0.38	0/462	0.57	0/626
2	E	0.36	0/470	0.56	0/638
2	F	0.38	0/480	0.61	0/651
2	G	0.39	0/490	0.67	1/666 (0.2%)
2	H	0.37	0/491	0.56	0/663
2	I	0.39	0/310	0.58	0/421
2	J	0.38	0/182	0.51	0/247
2	K	0.42	0/279	0.76	1/378 (0.3%)
2	L	0.37	0/299	0.58	0/406
2	M	0.39	0/453	0.58	0/616
2	N	0.45	0/441	0.58	0/595
2	O	0.37	0/444	0.55	0/603
2	P	0.37	0/390	0.55	0/530
All	All	0.40	0/12484	0.65	6/17041 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	376	TRP	C-N-CA	6.02	136.75	121.70
1	1	371	HIS	C-N-CA	5.56	135.59	121.70
2	K	43	GLU	C-N-CA	5.47	135.38	121.70
1	1	354	GLY	C-N-CA	5.24	134.79	121.70
1	1	382	GLY	C-N-CA	5.17	134.62	121.70
2	G	8	GLU	C-N-CA	5.01	134.23	121.70

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	1	2858	0	2235	20	0
1	2	2781	0	2169	24	0
2	A	490	0	444	2	0
2	B	509	0	471	2	0
2	C	499	0	439	1	0
2	D	455	0	408	1	0
2	E	463	0	411	0	0
2	F	473	0	430	3	0
2	G	483	0	426	6	0
2	H	485	0	437	3	0
2	I	309	0	213	1	0
2	J	185	0	97	1	0
2	K	283	0	164	2	0
2	L	300	0	171	1	0
2	M	447	0	394	2	0
2	N	435	0	404	3	0
2	O	439	0	372	1	0
2	P	387	0	307	1	0
All	All	12281	0	9992	70	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 3.

All (70) 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)
1:2:442:SER:HB3	1:2:443:PRO:HA	1.55	0.88
2:N:32:ILE:HD12	2:N:37:ILE:HD11	1.72	0.71
2:H:32:ILE:HD12	2:H:37:ILE:HD11	1.74	0.69
2:M:32:ILE:HD12	2:M:37:ILE:HD11	1.73	0.69
2:G:8:GLU:HA	2:G:10:VAL:H	1.61	0.65
1:1:383:ILE:HG13	1:1:384:VAL:H	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:86:ILE:HG22	1:2:87:ASN:H	1.70	0.55
2:F:37:ILE:HG12	2:G:64:ALA:HB1	1.88	0.55
2:G:8:GLU:HA	2:G:10:VAL:N	2.21	0.54
2:B:13:VAL:HG13	2:B:32:ILE:HG23	1.88	0.54
2:A:13:VAL:HG13	2:A:32:ILE:HG23	1.89	0.54
2:N:13:VAL:HG13	2:N:32:ILE:HG23	1.90	0.53
1:1:376:TRP:HB2	1:1:381:THR:HG23	1.91	0.53
1:2:325:GLY:HA2	1:2:444:VAL:HB	1.91	0.53
1:2:58:ILE:HD11	1:2:72:LEU:HD11	1.90	0.53
1:1:442:SER:CB	1:1:443:PRO:HA	2.38	0.53
1:2:368:HIS:HD2	1:2:419:GLY:H	1.58	0.51
1:2:37:ALA:HA	1:2:39:ALA:N	2.25	0.51
2:H:13:VAL:HG13	2:H:32:ILE:HG23	1.91	0.51
1:1:37:ALA:HA	1:1:39:ALA:N	2.26	0.51
1:1:368:HIS:HD2	1:1:419:GLY:H	1.58	0.50
1:2:129:THR:O	1:2:130:GLU:HB2	2.11	0.50
1:1:261:LYS:HG3	1:1:262:TYR:H	1.76	0.50
1:2:271:THR:HG23	1:2:274:GLY:H	1.76	0.50
2:C:15:GLY:HA3	2:C:31:PHE:O	2.11	0.50
2:G:13:VAL:HG13	2:G:32:ILE:HG23	1.94	0.49
1:2:361:ILE:HG12	1:2:375:ASP:HB2	1.94	0.49
1:2:37:ALA:HA	1:2:39:ALA:H	1.78	0.49
1:1:313:VAL:HG11	1:1:400:GLY:H	1.77	0.48
1:1:37:ALA:HA	1:1:39:ALA:H	1.78	0.48
2:F:13:VAL:HG13	2:F:32:ILE:HG23	1.94	0.48
1:2:442:SER:HB3	1:2:443:PRO:CA	2.36	0.47
1:1:399:VAL:HA	1:1:400:GLY:HA2	1.77	0.46
2:G:37:ILE:HD13	2:H:68:ALA:HB2	1.98	0.46
1:1:119:ALA:HB1	1:1:157:MET:HA	1.99	0.45
1:1:329:GLY:HA3	1:1:331:GLY:H	1.82	0.45
1:2:437:GLN:O	1:2:442:SER:HA	2.16	0.45
1:2:119:ALA:HB1	1:2:157:MET:HA	1.99	0.45
1:2:173:GLN:HA	1:2:174:GLY:HA3	1.73	0.44
1:2:86:ILE:HG22	1:2:87:ASN:N	2.31	0.44
1:1:382:GLY:HA3	1:1:463:THR:H	1.82	0.44
2:K:44:THR:H	2:L:58:SER:HB2	1.83	0.44
1:1:366:ASN:HA	1:1:418:TYR:HB3	2.01	0.43
1:2:363:ASP:HA	1:2:364:GLY:HA3	1.74	0.43
1:1:173:GLN:HA	1:1:174:GLY:HA3	1.72	0.43
1:2:329:GLY:HA3	1:2:331:GLY:H	1.83	0.43
1:2:366:ASN:HA	1:2:418:TYR:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:207:GLY:HA3	1:2:208:ASP:HA	1.86	0.43
2:I:5:VAL:HG23	2:J:5:VAL:HB	2.01	0.43
2:A:15:GLY:HA3	2:A:31:PHE:O	2.19	0.42
1:2:399:VAL:HA	1:2:400:GLY:HA2	1.71	0.42
1:2:411:ALA:HB3	1:2:412:PRO:HD3	2.01	0.42
1:2:173:GLN:HB3	1:2:179:VAL:HG13	2.00	0.42
2:F:15:GLY:HA3	2:F:31:PHE:O	2.20	0.42
1:1:207:GLY:HA2	1:1:208:ASP:HA	1.74	0.42
2:N:15:GLY:HA3	2:N:31:PHE:O	2.20	0.42
2:G:15:GLY:HA3	2:G:31:PHE:O	2.21	0.41
1:1:411:ALA:HB3	1:1:412:PRO:HD3	2.02	0.41
1:1:363:ASP:HA	1:1:364:GLY:HA3	1.75	0.41
1:2:26:PRO:HB2	1:2:27:GLN:H	1.71	0.41
1:1:360:LEU:HD11	1:1:364:GLY:HA2	2.01	0.41
1:1:371:HIS:NE2	1:1:460:GLY:HA3	2.36	0.41
1:2:47:GLY:HA2	1:2:48:VAL:HA	1.91	0.41
2:B:15:GLY:HA3	2:B:31:PHE:O	2.21	0.40
2:K:46:GLN:O	2:K:49:GLN:HG2	2.21	0.40
2:M:15:GLY:HA3	2:M:31:PHE:O	2.21	0.40
2:D:15:GLY:HA3	2:D:31:PHE:O	2.22	0.40
2:P:15:GLY:HA3	2:P:31:PHE:O	2.21	0.40
1:1:214:VAL:HG13	1:1:440:LEU:HD21	2.02	0.40
2:O:15:GLY:HA3	2:O:31:PHE:O	2.21	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	1	412/465 (89%)	327 (79%)	59 (14%)	26 (6%)	<a href="#">1</a> <a href="#">9</a>
1	2	400/465 (86%)	315 (79%)	55 (14%)	30 (8%)	<a href="#">1</a> <a href="#">7</a>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	66/72 (92%)	65 (98%)	1 (2%)	0	100	100
2	B	65/72 (90%)	64 (98%)	1 (2%)	0	100	100
2	C	67/72 (93%)	66 (98%)	1 (2%)	0	100	100
2	D	61/72 (85%)	60 (98%)	1 (2%)	0	100	100
2	E	63/72 (88%)	62 (98%)	1 (2%)	0	100	100
2	F	63/72 (88%)	59 (94%)	4 (6%)	0	100	100
2	G	67/72 (93%)	62 (92%)	5 (8%)	0	100	100
2	H	63/72 (88%)	62 (98%)	1 (2%)	0	100	100
2	I	46/72 (64%)	44 (96%)	2 (4%)	0	100	100
2	J	27/72 (38%)	26 (96%)	1 (4%)	0	100	100
2	K	43/72 (60%)	34 (79%)	7 (16%)	2 (5%)	2	14
2	L	47/72 (65%)	45 (96%)	0	2 (4%)	2	16
2	M	63/72 (88%)	60 (95%)	3 (5%)	0	100	100
2	N	55/72 (76%)	55 (100%)	0	0	100	100
2	O	61/72 (85%)	59 (97%)	2 (3%)	0	100	100
2	P	56/72 (78%)	54 (96%)	2 (4%)	0	100	100
All	All	1725/2082 (83%)	1519 (88%)	146 (8%)	60 (4%)	3	21

All (60) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	119	ALA
1	1	354	GLY
1	1	383	ILE
1	1	388	VAL
1	1	411	ALA
1	1	438	ASN
1	2	50	ALA
1	2	119	ALA
1	2	130	GLU
1	2	144	PRO
1	2	388	VAL
2	L	33	ASN
1	1	26	PRO
1	1	37	ALA
1	1	85	TRP

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Mol	Chain	Res	Type
1	1	86	ILE
1	1	121	SER
1	1	144	PRO
1	1	222	SER
1	1	442	SER
1	2	26	PRO
1	2	37	ALA
1	2	49	ASN
1	2	85	TRP
1	2	86	ILE
1	2	88	HIS
1	2	91	TYR
1	2	121	SER
1	2	411	ALA
1	2	442	SER
2	K	32	ILE
1	1	122	ALA
1	1	126	TYR
1	1	173	GLN
1	1	412	PRO
1	2	122	ALA
1	2	201	THR
1	2	375	ASP
1	2	379	ALA
1	2	398	ARG
1	2	412	PRO
1	2	417	GLN
1	1	20	ASN
1	1	124	GLU
1	1	355	ASP
1	1	375	ASP
1	1	393	ARG
1	1	398	ARG
1	1	409	SER
1	1	417	GLN
1	2	20	ASN
1	2	173	GLN
1	2	393	ARG
1	2	438	ASN
2	K	14	GLN
1	2	260	MET
1	2	383	ILE

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Mol	Chain	Res	Type
2	L	32	ILE
1	2	325	GLY
1	2	384	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	1	205/375 (55%)	186 (91%)	19 (9%)	9	30
1	2	204/375 (54%)	187 (92%)	17 (8%)	11	36
2	A	49/62 (79%)	47 (96%)	2 (4%)	30	61
2	B	52/62 (84%)	51 (98%)	1 (2%)	57	77
2	C	48/62 (77%)	45 (94%)	3 (6%)	18	47
2	D	44/62 (71%)	44 (100%)	0	100	100
2	E	43/62 (69%)	42 (98%)	1 (2%)	50	73
2	F	46/62 (74%)	44 (96%)	2 (4%)	29	59
2	G	44/62 (71%)	41 (93%)	3 (7%)	16	44
2	H	46/62 (74%)	45 (98%)	1 (2%)	52	74
2	I	18/62 (29%)	16 (89%)	2 (11%)	6	23
2	J	5/62 (8%)	5 (100%)	0	100	100
2	K	8/62 (13%)	8 (100%)	0	100	100
2	L	11/62 (18%)	11 (100%)	0	100	100
2	M	39/62 (63%)	38 (97%)	1 (3%)	46	71
2	N	43/62 (69%)	41 (95%)	2 (5%)	26	57
2	O	37/62 (60%)	35 (95%)	2 (5%)	22	53
2	P	30/62 (48%)	30 (100%)	0	100	100
All	All	972/1742 (56%)	916 (94%)	56 (6%)	20	50

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	78	GLU
1	1	104	ASP
1	1	112	TRP
1	1	126	TYR
1	1	131	ASP
1	1	156	THR
1	1	200	PHE
1	1	218	ASN
1	1	220	THR
1	1	232	LEU
1	1	261	LYS
1	1	264	THR
1	1	281	LEU
1	1	317	LEU
1	1	343	ARG
1	1	381	THR
1	1	418	TYR
1	1	423	ILE
1	1	440	LEU
1	2	25	SER
1	2	42	VAL
1	2	78	GLU
1	2	89	TYR
1	2	90	MET
1	2	104	ASP
1	2	112	TRP
1	2	123	PRO
1	2	129	THR
1	2	130	GLU
1	2	156	THR
1	2	232	LEU
1	2	376	TRP
1	2	381	THR
1	2	418	TYR
1	2	424	ILE
1	2	440	LEU
2	A	20	THR
2	A	37	ILE
2	B	20	THR
2	C	3	ILE
2	C	4	ASN
2	C	42	ILE
2	E	37	ILE

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Mol	Chain	Res	Type
2	F	37	ILE
2	F	41	ASP
2	G	37	ILE
2	G	41	ASP
2	G	70	LYS
2	H	37	ILE
2	I	20	THR
2	I	41	ASP
2	M	37	ILE
2	N	37	ILE
2	N	42	ILE
2	O	37	ILE
2	O	42	ILE

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

Mol	Chain	Res	Type
1	1	103	HIS

### 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 carbohydrates 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 ⓘ

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<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	1	430/465 (92%)	0.17	8 (1%) 66 65	61, 97, 138, 172	0
1	2	418/465 (89%)	0.21	7 (1%) 70 68	69, 98, 156, 184	0
2	A	68/72 (94%)	0.29	5 (7%) 14 14	65, 94, 110, 122	0
2	B	69/72 (95%)	0.63	9 (13%) 3 3	73, 92, 112, 142	0
2	C	69/72 (95%)	-0.08	1 (1%) 75 75	74, 86, 100, 108	0
2	D	63/72 (87%)	0.18	0 100 100	73, 84, 100, 114	0
2	E	65/72 (90%)	0.31	1 (1%) 73 72	66, 80, 114, 123	0
2	F	65/72 (90%)	0.21	0 100 100	62, 78, 112, 123	0
2	G	69/72 (95%)	0.15	0 100 100	72, 88, 106, 137	0
2	H	67/72 (93%)	0.27	2 (2%) 50 49	76, 89, 105, 132	0
2	I	52/72 (72%)	0.43	3 (5%) 23 22	99, 122, 138, 149	0
2	J	35/72 (48%)	-0.18	0 100 100	103, 122, 142, 161	0
2	K	53/72 (73%)	-0.10	0 100 100	103, 118, 145, 161	0
2	L	55/72 (76%)	-0.34	0 100 100	98, 111, 140, 158	0
2	M	65/72 (90%)	0.15	1 (1%) 73 72	78, 98, 117, 125	0
2	N	59/72 (81%)	0.28	1 (1%) 70 68	81, 96, 107, 139	0
2	O	65/72 (90%)	0.19	2 (3%) 49 48	94, 104, 119, 129	0
2	P	60/72 (83%)	0.50	3 (5%) 28 27	105, 116, 129, 140	0
All	All	1827/2082 (87%)	0.19	43 (2%) 59 56	61, 97, 138, 184	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	64	ALA	4.6
1	2	93	THR	4.1
2	B	16	PHE	4.0

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Mol	Chain	Res	Type	RSRZ
1	1	106	GLN	3.4
2	O	48	PHE	3.3
2	M	68	ALA	3.3
2	I	65	ILE	3.2
2	A	31	PHE	3.1
1	2	206	THR	3.1
2	B	55	ILE	3.0
2	B	25	SER	3.0
1	1	421	THR	3.0
2	A	51	ILE	3.0
2	N	65	ILE	2.9
2	B	53	PRO	2.9
1	2	374	TRP	2.8
2	B	33	ASN	2.7
2	H	26	TYR	2.7
2	H	57	ILE	2.7
2	P	51	ILE	2.7
2	C	18	PHE	2.7
2	B	51	ILE	2.6
2	E	8	GLU	2.6
1	2	411	ALA	2.6
1	1	461	LEU	2.5
1	1	402	ILE	2.4
2	B	57	ILE	2.4
2	B	52	ILE	2.4
2	B	32	ILE	2.4
1	1	336	TRP	2.3
2	P	52	ILE	2.3
1	2	128	ALA	2.3
1	2	349	ILE	2.3
2	A	16	PHE	2.3
2	A	57	ILE	2.3
1	1	340	TRP	2.1
2	I	51	ILE	2.1
2	A	50	GLN	2.1
2	P	32	ILE	2.1
2	O	16	PHE	2.1
1	2	89	TYR	2.0
1	1	407	ALA	2.0
1	1	240	PHE	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 carbohydrates 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.