Full wwPDB X-ray Structure Validation Report (i)

Jun 23, 2024 – 03:32 PM EDT

PDB ID	:	5LP5
Title	:	Complex between Penicillin-Binding Protein (PBP2) and MreC from Helicobacter pylori
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Deposited on	:	2016-08-11
Resolution	:	2.74 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 (i) 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 (1)) were used in the production of this report:

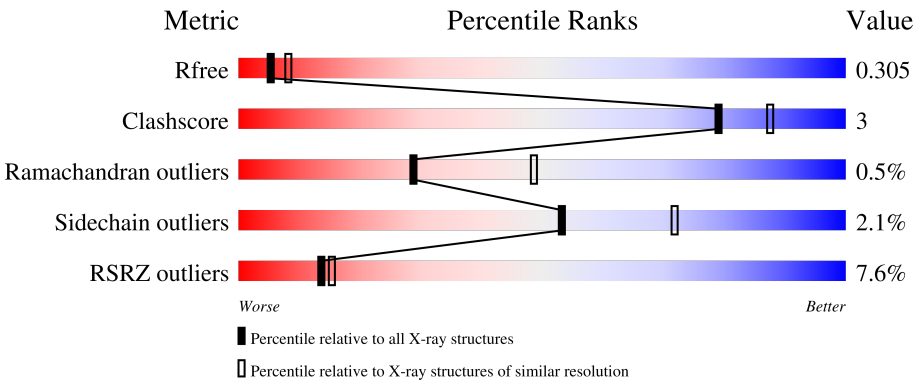
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.74 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	1271 (2.76-2.72)
Clashscore	141614	1322 (2.76-2.72)
Ramachandran outliers	138981	1297 (2.76-2.72)
Sidechain outliers	138945	1298 (2.76-2.72)
RSRZ outliers	127900	1243 (2.76-2.72)

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	594	7%, 80%, 10%, 10%
1	B	594	14%, 78%, 11%, 11%
2	C	248	58%, 6%, 37%
2	D	248	58%, 5%, 37%
2	E	248	2%, 60%, ·, 37%

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Mol	Chain	Length	Quality of chain
2	F	248	% 60% • 37%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 13381 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 Penicillin-binding protein 2 (Pbp2).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	535	4272	2755	722	785	10	0	0	0
1	B	530	4228	2730	712	777	9	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	589	HIS	-	expression tag	UNP O26085
A	590	HIS	-	expression tag	UNP O26085
A	591	HIS	-	expression tag	UNP O26085
A	592	HIS	-	expression tag	UNP O26085
A	593	HIS	-	expression tag	UNP O26085
A	594	HIS	-	expression tag	UNP O26085
B	589	HIS	-	expression tag	UNP O26085
B	590	HIS	-	expression tag	UNP O26085
B	591	HIS	-	expression tag	UNP O26085
B	592	HIS	-	expression tag	UNP O26085
B	593	HIS	-	expression tag	UNP O26085
B	594	HIS	-	expression tag	UNP O26085

- Molecule 2 is a protein called Rod shape-determining protein (MreC).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	157	1209	777	201	227	4	0	0	0
2	D	156	1201	773	199	225	4	0	0	0
2	E	156	1201	773	199	225	4	0	0	0
2	F	156	1201	773	199	225	4	0	0	0

- Molecule 3 is water.

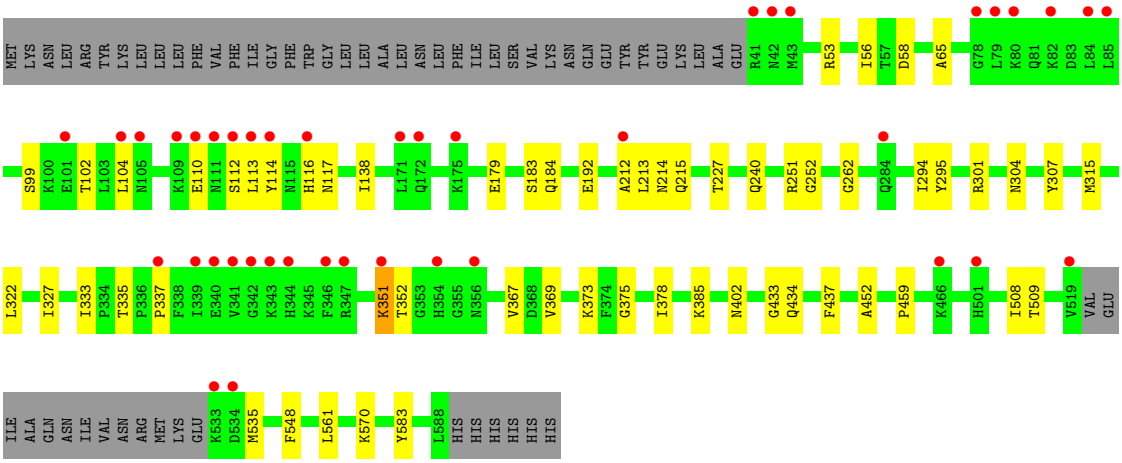
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	19	19	19	0	0
			Total	O		
3	B	5	5	5	0	0
			Total	O		
3	C	12	12	12	0	0
			Total	O		
3	D	18	18	18	0	0
			Total	O		
3	E	7	7	7	0	0
			Total	O		
3	F	8	8	8	0	0

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.

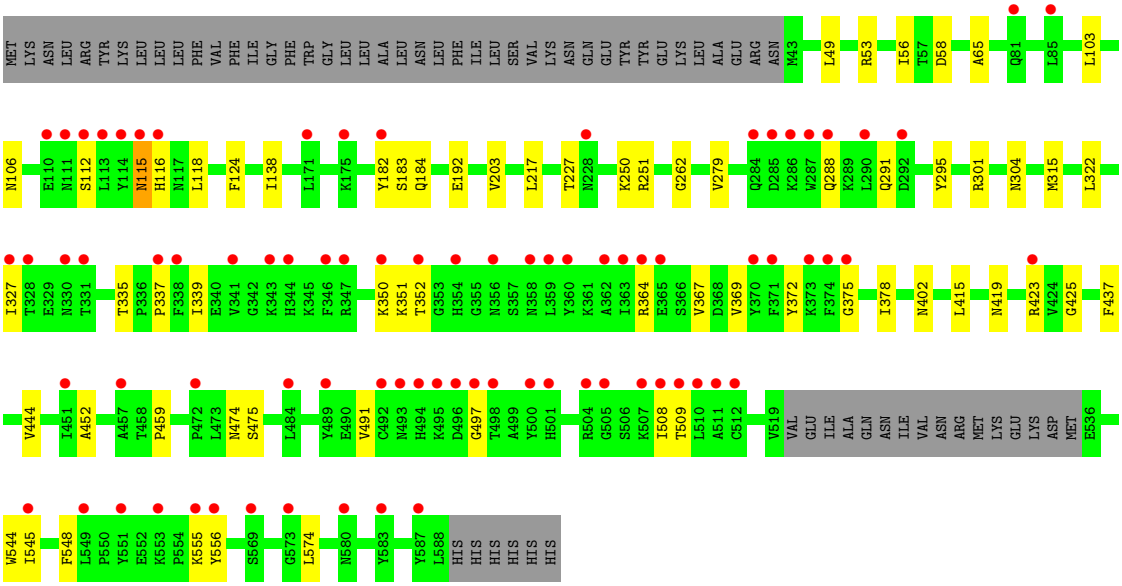
- Molecule 1: Penicillin-binding protein 2 (Pbp2)

Chain A:



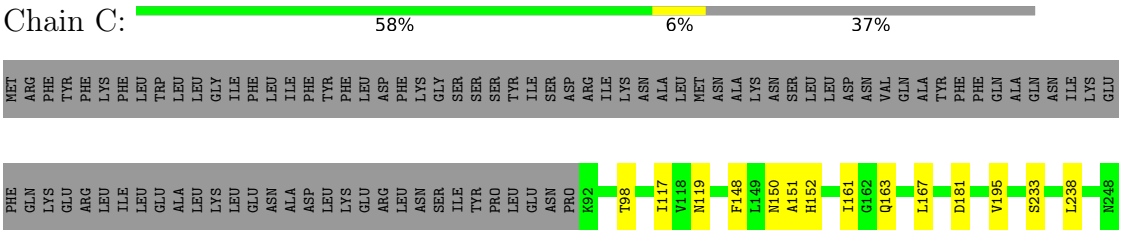
- Molecule 1: Penicillin-binding protein 2 (Pbp2)

Chain B:



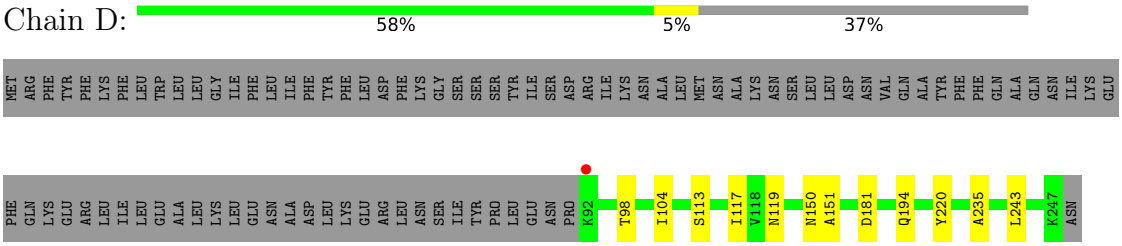
• Molecule 2: Rod shape-determining protein (MreC)

Chain C:



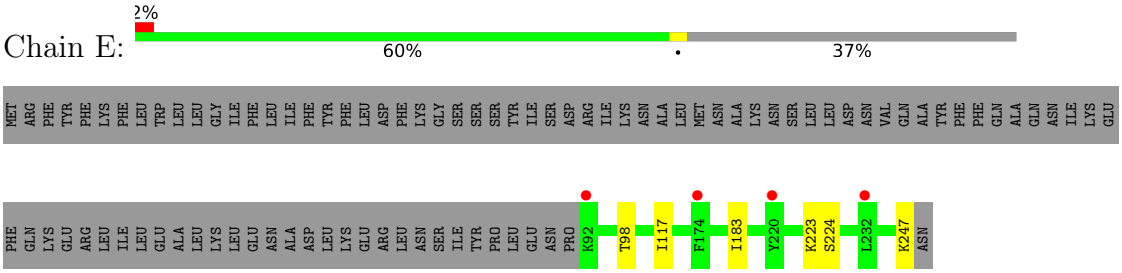
• Molecule 2: Rod shape-determining protein (MreC)

Chain D:



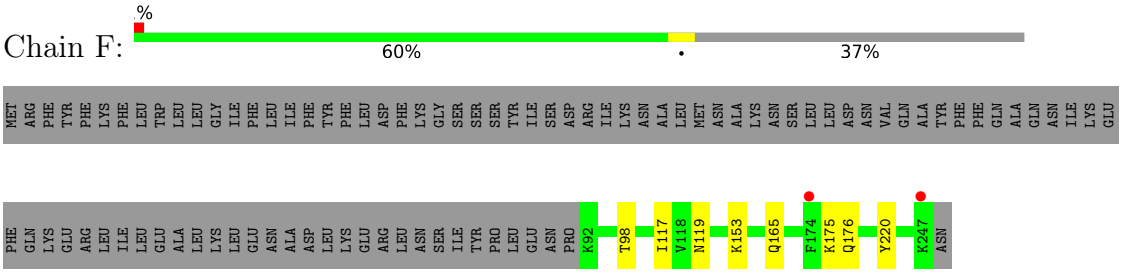
• Molecule 2: Rod shape-determining protein (MreC)

Chain E:



• Molecule 2: Rod shape-determining protein (MreC)

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	338.66Å 48.34Å 151.51Å 90.00° 113.02° 90.00°	Depositor
Resolution (Å)	43.94 – 2.74 43.94 – 2.74	Depositor EDS
% Data completeness (in resolution range)	86.6 (43.94-2.74) 86.6 (43.94-2.74)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.74 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.257 , 0.292 0.266 , 0.305	Depositor DCC
R_{free} test set	1307 reflections (2.49%)	wwPDB-VP
Wilson B-factor (Å^2)	39.3	Xtriage
Anisotropy	0.179	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 48.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	13381	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.41% 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 (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	0.46	0/4365	0.64	0/5900
1	B	0.42	0/4321	0.61	0/5843
2	C	0.54	0/1231	0.71	0/1665
2	D	0.52	0/1223	0.70	0/1654
2	E	0.50	0/1223	0.71	0/1654
2	F	0.50	0/1223	0.73	0/1654
All	All	0.47	0/13586	0.66	0/18370

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	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	117	ASN	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	4272	0	4326	26	0
1	B	4228	0	4281	34	0
2	C	1209	0	1216	8	0
2	D	1201	0	1210	5	0
2	E	1201	0	1210	2	0
2	F	1201	0	1210	4	0
3	A	19	0	0	1	0
3	B	5	0	0	0	0
3	C	12	0	0	0	0
3	D	18	0	0	0	0
3	E	7	0	0	0	0
3	F	8	0	0	0	0
All	All	13381	0	13453	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 3.

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:385:LYS:HE3	1:B:419:ASN:HD21	1.47	0.77
1:B:337:PRO:HB3	1:B:351:LYS:O	1.92	0.69
1:B:335:THR:HG21	1:B:367:VAL:HG11	1.83	0.60
1:B:304:ASN:ND2	1:B:402:ASN:O	2.34	0.59
1:B:350:LYS:HG3	1:B:352:THR:HG22	1.87	0.57
1:A:179:GLU:O	1:A:179:GLU:HG2	2.06	0.56
1:B:335:THR:HG23	1:B:369:VAL:HB	1.88	0.55
2:C:150:ASN:O	2:C:151:ALA:HB3	2.06	0.54
1:A:337:PRO:HB3	1:A:351:LYS:O	2.07	0.54
1:B:474:ASN:OD1	1:B:475:SER:N	2.41	0.54
2:D:150:ASN:O	2:D:151:ALA:HB3	2.08	0.54
1:A:99:SER:OG	1:A:102:THR:HG23	2.09	0.53
1:A:304:ASN:ND2	1:A:402:ASN:O	2.36	0.53
1:A:56:ILE:HB	1:A:65:ALA:HB3	1.91	0.52
1:B:452:ALA:HB2	1:B:548:PHE:CG	2.45	0.52
1:A:335:THR:HG21	1:A:367:VAL:HG11	1.92	0.51
1:A:322:LEU:HD23	1:A:327:ILE:HD12	1.93	0.51
1:B:56:ILE:HB	1:B:65:ALA:HB3	1.92	0.51
1:B:555:LYS:HD2	1:B:556:TYR:CE2	2.45	0.51
1:B:288:GLN:HA	1:B:291:GLN:HE21	1.76	0.50
1:A:508:ILE:HG22	1:A:509:THR:N	2.26	0.50
1:A:295:TYR:O	1:A:301:ARG:NH2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:508:ILE:HD11	1:A:583:TYR:CD1	2.48	0.49
1:B:335:THR:HG21	1:B:367:VAL:CG1	2.41	0.49
2:D:194:GLN:O	2:D:194:GLN:HG2	2.12	0.49
1:A:335:THR:HG23	1:A:369:VAL:HB	1.93	0.49
2:C:98:THR:HB	2:C:117:ILE:HD11	1.95	0.49
1:B:115:ASN:O	1:B:116:HIS:HB2	2.14	0.48
3:A:611:HOH:O	2:C:167:LEU:HB3	2.12	0.48
1:B:508:ILE:HG22	1:B:509:THR:N	2.29	0.48
2:C:148:PHE:CD1	2:C:152:HIS:CD2	3.02	0.47
2:C:148:PHE:HB3	2:C:152:HIS:HD2	1.80	0.47
1:A:213:LEU:HD22	1:A:215:GLN:HE21	1.80	0.47
1:A:53:ARG:NH2	1:A:192:GLU:OE1	2.41	0.46
1:A:452:ALA:HB2	1:A:548:PHE:CG	2.51	0.46
1:B:124:PHE:HE2	1:B:279:VAL:HG12	1.80	0.46
1:A:433:GLY:O	1:A:434:GLN:HG2	2.16	0.46
1:A:113:LEU:HG	1:A:114:TYR:H	1.81	0.45
1:B:118:LEU:HD12	1:B:118:LEU:N	2.31	0.45
1:B:217:LEU:HA	2:F:220:TYR:CE2	2.51	0.45
1:B:262:GLY:O	1:B:459:PRO:HA	2.17	0.45
1:A:333:ILE:HD12	1:A:373:LYS:HD2	1.98	0.45
2:E:98:THR:HB	2:E:117:ILE:HD11	1.99	0.45
2:F:175:LYS:O	2:F:176:GLN:HG2	2.17	0.44
1:B:295:TYR:O	1:B:301:ARG:NH2	2.46	0.44
1:B:444:VAL:HG21	1:B:544:TRP:CZ3	2.53	0.44
2:F:98:THR:HB	2:F:117:ILE:HD11	2.00	0.43
1:A:307:TYR:CE1	1:A:561:LEU:HD21	2.53	0.43
2:E:183:ILE:HB	2:E:223:LYS:HG3	2.01	0.43
1:A:262:GLY:O	1:A:459:PRO:HA	2.19	0.42
1:B:322:LEU:HD23	1:B:327:ILE:HD12	2.00	0.42
1:B:182:TYR:CD2	1:B:203:VAL:HG11	2.54	0.42
2:C:161:ILE:HG12	2:C:195:VAL:HG22	2.01	0.42
1:B:250:LYS:HE3	1:B:574:LEU:HD21	2.01	0.42
2:D:235:ALA:HB3	2:F:165:GLN:HB3	2.01	0.42
1:B:364:ARG:HG2	1:B:497:GLY:HA2	2.01	0.42
2:D:98:THR:HB	2:D:117:ILE:HD11	2.01	0.42
1:A:138:ILE:HD13	1:A:138:ILE:HA	1.85	0.41
1:B:49:LEU:HD22	2:D:220:TYR:HE2	1.85	0.41
1:B:444:VAL:HG21	1:B:544:TRP:CH2	2.55	0.41
1:A:212:ALA:C	1:A:214:ASN:H	2.24	0.41
1:B:350:LYS:CG	1:B:352:THR:HG22	2.50	0.41
1:B:423:ARG:HG3	1:B:425:GLY:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:375:GLY:HA2	1:B:378:ILE:HG22	2.03	0.41
2:C:150:ASN:O	2:C:151:ALA:CB	2.69	0.41
1:A:252:GLY:HA3	1:A:561:LEU:O	2.20	0.41
1:B:103:LEU:HA	1:B:106:ASN:HD22	1.86	0.41
1:B:138:ILE:HD13	1:B:138:ILE:HA	1.86	0.41
1:B:339:ILE:HD11	1:B:372:TYR:HB3	2.02	0.41
2:C:238:LEU:HD23	2:C:238:LEU:HA	1.98	0.41
1:A:294:ILE:HD12	1:A:294:ILE:O	2.21	0.41
1:B:53:ARG:NH2	1:B:192:GLU:OE1	2.43	0.40
1:B:364:ARG:HA	1:B:491:VAL:HG22	2.03	0.40
1:A:335:THR:HG21	1:A:367:VAL:CG1	2.51	0.40
1:A:375:GLY:HA2	1:A:378:ILE:HG22	2.04	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	531/594 (89%)	496 (93%)	32 (6%)	3 (1%)	25	44
1	B	526/594 (89%)	491 (93%)	32 (6%)	3 (1%)	25	44
2	C	155/248 (62%)	147 (95%)	7 (4%)	1 (1%)	25	44
2	D	154/248 (62%)	147 (96%)	6 (4%)	1 (1%)	25	44
2	E	154/248 (62%)	149 (97%)	5 (3%)	0	100	100
2	F	154/248 (62%)	148 (96%)	5 (3%)	1 (1%)	25	44
All	All	1674/2180 (77%)	1578 (94%)	87 (5%)	9 (0%)	29	48

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	112	SER

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Mol	Chain	Res	Type
1	A	58	ASP
1	B	58	ASP
1	B	112	SER
2	C	119	ASN
2	D	119	ASN
2	F	119	ASN
1	B	545	ILE
1	A	351	LYS

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	464/518 (90%)	451 (97%)	13 (3%)	43	63
1	B	459/518 (89%)	451 (98%)	8 (2%)	60	76
2	C	134/217 (62%)	131 (98%)	3 (2%)	52	71
2	D	133/217 (61%)	129 (97%)	4 (3%)	41	61
2	E	133/217 (61%)	131 (98%)	2 (2%)	65	79
2	F	133/217 (61%)	132 (99%)	1 (1%)	81	89
All	All	1456/1904 (76%)	1425 (98%)	31 (2%)	53	72

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

Mol	Chain	Res	Type
1	A	104	LEU
1	A	110	GLU
1	A	116	HIS
1	A	183	SER
1	A	184	GLN
1	A	227	THR
1	A	240	GLN
1	A	251	ARG
1	A	315	MET
1	A	352	THR

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Mol	Chain	Res	Type
1	A	437	PHE
1	A	535	MET
1	A	570	LYS
1	B	115	ASN
1	B	183	SER
1	B	184	GLN
1	B	227	THR
1	B	251	ARG
1	B	315	MET
1	B	415	LEU
1	B	437	PHE
2	C	163	GLN
2	C	181	ASP
2	C	233	SER
2	D	104	ILE
2	D	113	SER
2	D	181	ASP
2	D	243	LEU
2	E	224	SER
2	E	247	LYS
2	F	153	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	184	GLN
1	A	200	GLN
1	A	215	GLN
1	A	467	GLN
1	B	106	ASN
1	B	155	ASN
1	B	200	GLN
1	B	291	GLN
1	B	354	HIS
1	B	419	ASN
1	B	467	GLN
2	C	133	GLN
2	C	152	HIS
2	E	110	HIS
2	E	146	ASN
2	F	133	GLN
2	F	146	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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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	535/594 (90%)	0.27	41 (7%) 13 15	26, 54, 104, 150	0
1	B	530/594 (89%)	0.87	81 (15%) 2 2	34, 81, 134, 170	0
2	C	157/248 (63%)	-0.34	0 100 100	21, 32, 54, 69	0
2	D	156/248 (62%)	-0.14	1 (0%) 89 91	20, 32, 57, 87	0
2	E	156/248 (62%)	-0.07	4 (2%) 56 63	25, 41, 73, 116	0
2	F	156/248 (62%)	-0.01	2 (1%) 77 82	26, 46, 75, 102	0
All	All	1690/2180 (77%)	0.31	129 (7%) 13 15	20, 52, 120, 170	0

All (129) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	114	TYR	9.1
1	B	113	LEU	6.6
1	A	341	VAL	6.4
1	A	112	SER	6.2
1	B	359	LEU	6.0
1	A	110	GLU	6.0
1	B	510	LEU	6.0
2	E	174	PHE	6.0
1	A	111	ASN	5.9
1	B	330	ASN	5.8
1	B	111	ASN	5.8
1	B	110	GLU	5.7
1	B	494	HIS	5.7
1	A	114	TYR	5.7
1	A	116	HIS	5.5
1	A	84	LEU	5.0
1	A	41	ARG	4.8
1	B	352	THR	4.8
1	B	116	HIS	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	115	ASN	4.6
1	B	373	LYS	4.5
1	B	504	ARG	4.4
1	A	534	ASP	4.3
1	B	497	GLY	4.3
1	A	113	LEU	4.2
1	B	338	PHE	4.1
1	B	371	PHE	4.0
1	B	498	THR	3.9
1	B	343	LYS	3.8
1	A	346	PHE	3.8
1	B	341	VAL	3.8
1	B	508	ILE	3.7
1	B	511	ALA	3.6
1	B	112	SER	3.6
1	B	493	ASN	3.6
1	A	79	LEU	3.6
1	B	492	CYS	3.6
1	B	580	ASN	3.6
1	B	85	LEU	3.5
2	E	92	LYS	3.4
1	B	350	LYS	3.4
1	B	507	LYS	3.4
1	B	285	ASP	3.4
1	A	85	LEU	3.4
1	B	374	PHE	3.3
2	E	232	LEU	3.3
1	B	451	ILE	3.3
1	B	556	TYR	3.2
1	B	495	LYS	3.2
1	A	101	GLU	3.2
1	A	344	HIS	3.1
1	A	356	ASN	3.1
1	A	533	LYS	3.1
2	E	220	TYR	3.0
1	B	583	TYR	3.0
1	B	346	PHE	3.0
1	B	423	ARG	3.0
2	D	92	LYS	3.0
1	A	339	ILE	2.9
1	B	370	TYR	2.9
1	B	549	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	284	GLN	2.9
1	B	360	TYR	2.9
1	A	175	LYS	2.8
1	A	284	GLN	2.8
1	B	328	THR	2.8
1	A	109	LYS	2.8
1	B	364	ARG	2.8
1	B	354	HIS	2.7
2	F	174	PHE	2.7
1	B	509	THR	2.7
1	A	78	GLY	2.7
1	A	347	ARG	2.7
1	B	500	TYR	2.6
1	A	354	HIS	2.6
1	B	496	ASP	2.6
1	A	82	LYS	2.6
1	B	175	LYS	2.6
1	A	172	GLN	2.5
1	B	327	ILE	2.5
1	B	501	HIS	2.5
2	F	247	LYS	2.5
1	A	42	ASN	2.5
1	B	81	GLN	2.5
1	B	545	ILE	2.5
1	B	472	PRO	2.4
1	B	356	ASN	2.4
1	A	80	LYS	2.4
1	B	363	ILE	2.4
1	A	104	LEU	2.4
1	B	290	LEU	2.4
1	A	105	ASN	2.4
1	B	228	ASN	2.4
1	A	43	MET	2.4
1	A	342	GLY	2.3
1	B	512	CYS	2.3
1	A	343	LYS	2.3
1	B	344	HIS	2.3
1	B	569	SER	2.3
1	A	337	PRO	2.3
1	B	489	TYR	2.3
1	B	551	TYR	2.3
1	A	212	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	171	LEU	2.3
1	B	505	GLY	2.3
1	B	288	GLN	2.3
1	B	484	LEU	2.3
1	B	358	ASN	2.2
1	B	287	TRP	2.2
1	B	553	LYS	2.2
1	B	337	PRO	2.2
1	A	501	HIS	2.2
1	B	375	GLY	2.2
1	A	519	VAL	2.1
1	B	292	ASP	2.1
1	B	362	ALA	2.1
1	A	171	LEU	2.1
1	A	466	LYS	2.1
1	B	286	LYS	2.1
1	B	365	GLU	2.1
1	B	182	TYR	2.0
1	B	573	GLY	2.0
1	A	340	GLU	2.0
1	B	587	TYR	2.0
1	B	457	ALA	2.0
1	A	351	LYS	2.0
1	B	331	THR	2.0
1	B	555	LYS	2.0
1	B	347	ARG	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.