Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2022 – 10:05 AM EDT

PDB ID	:	7RQF
Title	:	Crystal Structure of LbcA (lipoprotein binding partner of CtpA) of Pseudomonas aeruginosa
Authors	:	Hsu, H.C.; Li, H.
Deposited on	:	2021-08-06
Resolution	:	3.50 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 following versions of software and data (see references ⓘ) were used in the production of this report:

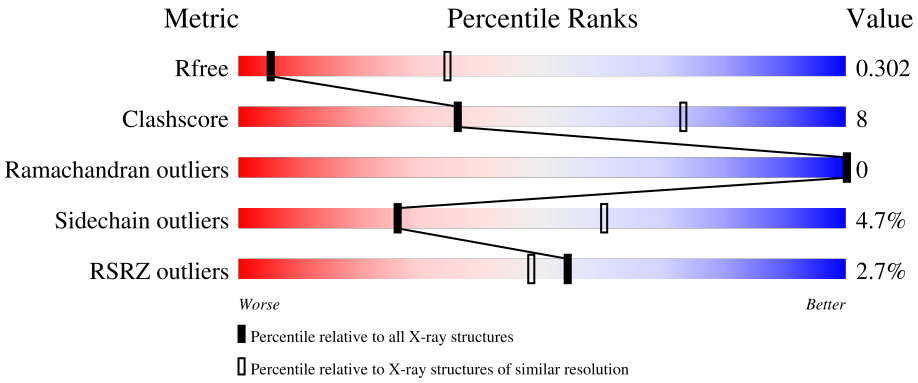
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.27
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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 3.50 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	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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	540	4% 74% 22%
1	B	540	% 76% 20%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 8352 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 TPR repeat-containing protein PA4667.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	523	Total	C	N	O	S	Se	0	0	0
			4176	2603	757	808	1	7			
1	B	523	Total	C	N	O	S	Se	0	0	0
			4176	2603	757	808	1	7			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	49	MSE	-	initiating methionine	UNP P42810
A	576	LYS	-	expression tag	UNP P42810
A	577	LEU	-	expression tag	UNP P42810
A	578	ALA	-	expression tag	UNP P42810
A	579	ALA	-	expression tag	UNP P42810
A	580	ALA	-	expression tag	UNP P42810
A	581	LEU	-	expression tag	UNP P42810
A	582	GLU	-	expression tag	UNP P42810
A	583	HIS	-	expression tag	UNP P42810
A	584	HIS	-	expression tag	UNP P42810
A	585	HIS	-	expression tag	UNP P42810
A	586	HIS	-	expression tag	UNP P42810
A	587	HIS	-	expression tag	UNP P42810
A	588	HIS	-	expression tag	UNP P42810
B	49	MSE	-	initiating methionine	UNP P42810
B	576	LYS	-	expression tag	UNP P42810
B	577	LEU	-	expression tag	UNP P42810
B	578	ALA	-	expression tag	UNP P42810
B	579	ALA	-	expression tag	UNP P42810
B	580	ALA	-	expression tag	UNP P42810
B	581	LEU	-	expression tag	UNP P42810
B	582	GLU	-	expression tag	UNP P42810
B	583	HIS	-	expression tag	UNP P42810
B	584	HIS	-	expression tag	UNP P42810
B	585	HIS	-	expression tag	UNP P42810

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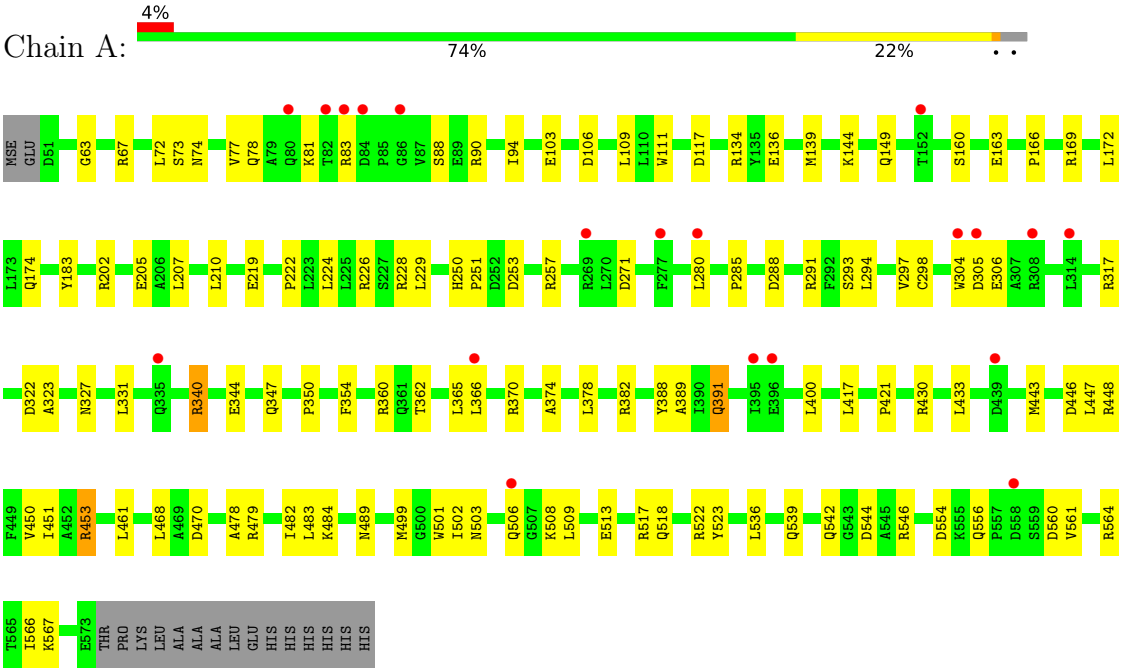
Chain	Residue	Modelled	Actual	Comment	Reference
B	586	HIS	-	expression tag	UNP P42810
B	587	HIS	-	expression tag	UNP P42810
B	588	HIS	-	expression tag	UNP P42810

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.

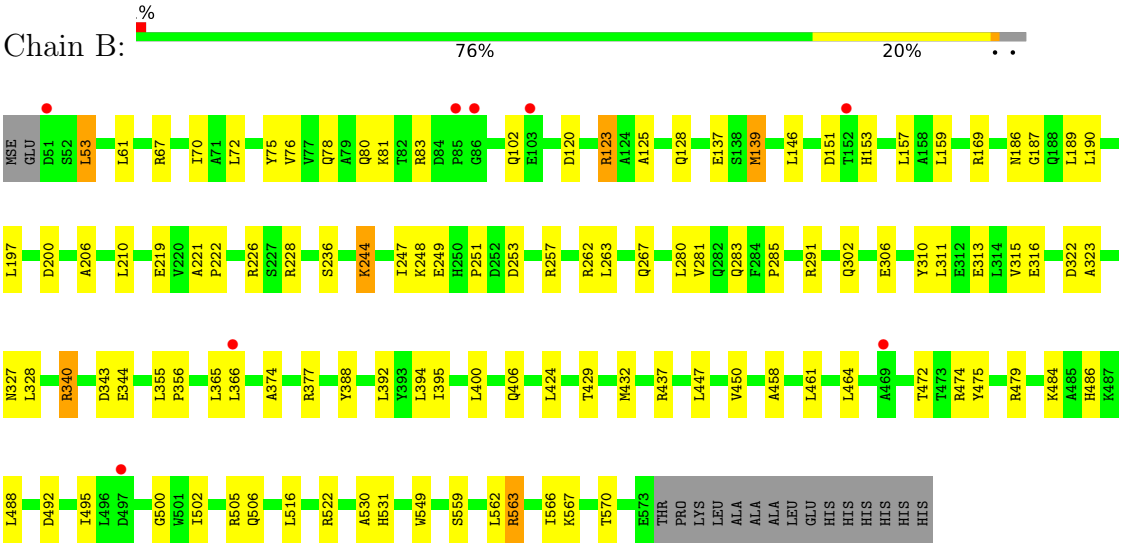
• Molecule 1: TPR repeat-containing protein PA4667

Chain A:



• Molecule 1: TPR repeat-containing protein PA4667

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	120.70Å 120.70Å 221.94Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	60.39 – 3.50 60.39 – 3.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (60.39-3.50) 100.0 (60.39-3.50)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.66 (at 3.49Å)	Xtriage
Refinement program	PHENIX (1.19_4092)	Depositor
R, R_{free}	0.245 , 0.281 0.277 , 0.302	Depositor DCC
R_{free} test set	1198 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	137.7	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 95.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.045 for -h,-k,l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	8352	wwPDB-VP
Average B, all atoms (Å^2)	135.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% 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	0.28	0/4238	0.54	0/5721
1	B	0.28	0/4238	0.53	0/5721
All	All	0.28	0/8476	0.54	0/11442

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	4176	0	4110	73	0
1	B	4176	0	4110	61	0
All	All	8352	0	8220	132	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 (132) 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:482:ILE:HG22	1:A:499:MSE:SE	2.29	0.82
1:B:328:LEU:HB3	1:B:344:GLU:HG2	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:447:LEU:HD23	1:B:464:LEU:HB2	1.69	0.74
1:A:210:LEU:HD23	1:A:226:ARG:HB2	1.71	0.72
1:A:354:PHE:CD2	1:A:388:TYR:OH	2.42	0.71
1:A:354:PHE:HD2	1:A:388:TYR:OH	1.75	0.69
1:B:366:LEU:HD21	1:B:400:LEU:HD23	1.76	0.68
1:A:479:ARG:NH2	1:A:503:ASN:OD1	2.27	0.67
1:B:123:ARG:HD3	1:B:123:ARG:H	1.60	0.66
1:A:117:ASP:OD2	1:B:228:ARG:NH1	2.28	0.65
1:A:354:PHE:HD2	1:A:388:TYR:HH	1.40	0.65
1:A:461:LEU:HD11	1:A:484:LYS:HD3	1.80	0.64
1:B:424:LEU:HD13	1:B:450:VAL:HG23	1.79	0.64
1:B:257:ARG:NH2	1:B:283:GLN:OE1	2.31	0.62
1:A:340:ARG:NH1	1:A:344:GLU:OE1	2.32	0.62
1:A:365:LEU:HB3	1:A:374:ALA:HB2	1.82	0.61
1:B:72:LEU:O	1:B:76:VAL:HG23	1.99	0.61
1:A:323:ALA:O	1:A:327:ASN:ND2	2.28	0.60
1:A:388:TYR:HB2	1:A:391:GLN:HG3	1.83	0.60
1:A:202:ARG:HG2	1:A:205:GLU:HB2	1.84	0.60
1:B:251:PRO:O	1:B:257:ARG:NH1	2.35	0.60
1:B:187:GLY:HA3	1:B:219:GLU:HG3	1.83	0.60
1:A:251:PRO:O	1:A:257:ARG:NH1	2.35	0.60
1:A:366:LEU:HD21	1:A:400:LEU:HD23	1.84	0.59
1:A:74:ASN:O	1:A:78:GLN:HG2	2.01	0.59
1:A:509:LEU:HD12	1:A:539:GLN:HB2	1.85	0.59
1:B:285:PRO:O	1:B:291:ARG:NH2	2.28	0.59
1:B:236:SER:HB3	1:B:263:LEU:HD11	1.86	0.58
1:A:111:TRP:O	1:B:262:ARG:NH1	2.37	0.57
1:B:365:LEU:HD23	1:B:374:ALA:HA	1.86	0.57
1:B:81:LYS:O	1:B:83:ARG:NE	2.39	0.56
1:A:106:ASP:HB3	1:A:109:LEU:HB3	1.87	0.56
1:B:244:LYS:O	1:B:247:ILE:HG22	2.06	0.55
1:A:90:ARG:O	1:A:94:ILE:HD12	2.06	0.54
1:A:518:GLN:O	1:A:522:ARG:HG2	2.06	0.54
1:B:502:ILE:O	1:B:506:GLN:HG2	2.08	0.54
1:A:554:ASP:HB3	1:A:556:GLN:HG2	1.91	0.53
1:B:281:VAL:HG21	1:B:310:TYR:CE1	2.44	0.53
1:A:344:GLU:OE2	1:A:347:GLN:NE2	2.42	0.52
1:A:482:ILE:CG2	1:A:499:MSE:SE	3.06	0.52
1:B:120:ASP:OD1	1:B:123:ARG:NH1	2.43	0.52
1:B:169:ARG:NE	1:B:200:ASP:OD1	2.40	0.52
1:B:472:THR:HG21	1:B:474:ARG:HD2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:559:SER:HB2	1:B:562:LEU:HB3	1.92	0.52
1:A:163:GLU:HG3	1:A:174:GLN:HG3	1.91	0.52
1:B:67:ARG:HA	1:B:70:ILE:HG22	1.94	0.50
1:A:136:GLU:HA	1:A:139:MSE:HE3	1.94	0.50
1:B:549:TRP:CG	1:B:566:ILE:HD11	2.46	0.50
1:A:250:HIS:HB3	1:A:253:ASP:HB2	1.92	0.50
1:A:502:ILE:O	1:A:506:GLN:HB2	2.13	0.49
1:B:322:ASP:N	1:B:322:ASP:OD1	2.44	0.49
1:B:340:ARG:HA	1:B:343:ASP:OD2	2.12	0.49
1:A:285:PRO:O	1:A:291:ARG:NH2	2.42	0.49
1:A:354:PHE:HD2	1:A:388:TYR:CE1	2.30	0.49
1:A:482:ILE:HG21	1:A:499:MSE:HA	1.94	0.49
1:A:166:PRO:O	1:A:172:LEU:HG	2.13	0.49
1:A:483:LEU:HD23	1:A:499:MSE:HE1	1.95	0.48
1:A:470:ASP:OD1	1:A:501:TRP:NE1	2.46	0.48
1:A:354:PHE:HD2	1:A:388:TYR:CZ	2.31	0.48
1:A:322:ASP:N	1:A:322:ASP:OD1	2.46	0.48
1:A:350:PRO:HA	1:A:354:PHE:HB2	1.96	0.47
1:B:458:ALA:HB2	1:B:488:LEU:HD23	1.95	0.47
1:B:221:ALA:HB3	1:B:222:PRO:HD3	1.96	0.47
1:A:378:LEU:HB3	1:A:382:ARG:HH21	1.79	0.47
1:B:492:ASP:HB3	1:B:495:ILE:HD12	1.97	0.47
1:A:304:TRP:HB3	1:A:331:LEU:HD21	1.96	0.47
1:B:530:ALA:HB2	1:B:562:LEU:HD12	1.95	0.47
1:B:197:LEU:HB2	1:B:206:ALA:HB2	1.96	0.47
1:B:186:ASN:O	1:B:190:LEU:HG	2.15	0.46
1:B:75:TYR:HB2	1:B:128:GLN:HB3	1.97	0.46
1:B:486:HIS:HA	1:B:495:ILE:HG21	1.97	0.46
1:A:288:ASP:OD1	1:A:317:ARG:HD2	2.16	0.46
1:A:382:ARG:HG2	1:A:389:ALA:HB1	1.98	0.46
1:B:461:LEU:HD23	1:B:484:LYS:HB3	1.98	0.46
1:A:354:PHE:CD2	1:A:388:TYR:CE1	3.03	0.45
1:B:447:LEU:HA	1:B:450:VAL:HG12	1.98	0.45
1:A:489:ASN:N	1:A:489:ASN:OD1	2.49	0.45
1:B:206:ALA:O	1:B:210:LEU:HD23	2.17	0.45
1:B:186:ASN:HB3	1:B:189:LEU:HD12	1.99	0.45
1:A:430:ARG:NH2	1:A:446:ASP:HB3	2.32	0.45
1:A:73:SER:O	1:A:77:VAL:HG22	2.17	0.44
1:A:453:ARG:HD3	1:A:453:ARG:HA	1.79	0.44
1:A:305:ASP:N	1:A:305:ASP:OD1	2.49	0.44
1:A:417:LEU:HD23	1:A:421:PRO:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:LEU:HD23	1:B:159:LEU:HD23	1.98	0.44
1:B:313:GLU:HA	1:B:316:GLU:HG2	1.99	0.44
1:A:536:LEU:HD21	1:A:544:ASP:HB2	2.00	0.44
1:B:306:GLU:HG2	1:B:310:TYR:CE2	2.53	0.44
1:B:365:LEU:HD21	1:B:377:ARG:HD2	2.01	0.43
1:B:247:ILE:HD11	1:B:257:ARG:HG2	2.00	0.43
1:A:468:LEU:HB3	1:A:478:ALA:HB2	2.00	0.43
1:A:542:GLN:O	1:A:546:ARG:HD3	2.19	0.43
1:A:72:LEU:HD12	1:A:72:LEU:HA	1.78	0.43
1:B:566:ILE:O	1:B:570:THR:OG1	2.28	0.43
1:B:394:LEU:HD22	1:B:429:THR:HG21	2.00	0.43
1:A:224:LEU:O	1:A:228:ARG:HG2	2.19	0.42
1:B:210:LEU:HB3	1:B:226:ARG:HD2	2.01	0.42
1:B:323:ALA:O	1:B:327:ASN:ND2	2.38	0.42
1:A:144:LYS:HD3	1:A:144:LYS:HA	1.65	0.42
1:A:362:THR:OG1	1:A:378:LEU:HD21	2.20	0.42
1:A:447:LEU:HA	1:A:450:VAL:HG12	2.01	0.42
1:B:522:ARG:HA	1:B:522:ARG:HD2	1.80	0.42
1:A:298:CYS:SG	1:A:306:GLU:HB3	2.59	0.42
1:B:61:LEU:HD12	1:B:146:LEU:HD12	2.02	0.42
1:B:500:GLY:HA3	1:B:516:LEU:HD22	2.02	0.42
1:B:75:TYR:CE1	1:B:125:ALA:HB1	2.54	0.42
1:B:139:MSE:HE2	1:B:139:MSE:HB2	1.87	0.42
1:A:293:SER:O	1:A:297:VAL:HG22	2.20	0.42
1:A:513:GLU:OE2	1:A:517:ARG:NH1	2.52	0.42
1:A:354:PHE:CD2	1:A:388:TYR:HE1	2.38	0.42
1:A:566:ILE:H	1:A:566:ILE:HG12	1.66	0.42
1:B:248:LYS:HD3	1:B:248:LYS:HA	1.81	0.41
1:A:219:GLU:HB2	1:A:222:PRO:HD2	2.02	0.41
1:A:370:ARG:HG3	1:A:370:ARG:O	2.21	0.41
1:B:311:LEU:O	1:B:315:VAL:HG23	2.21	0.41
1:A:508:LYS:HD2	1:A:508:LYS:HA	1.87	0.41
1:B:475:TYR:CE2	1:B:505:ARG:HB3	2.55	0.41
1:A:561:VAL:HG13	1:A:564:ARG:HH21	1.86	0.41
1:B:280:LEU:HD23	1:B:280:LEU:HA	1.94	0.41
1:A:63:GLY:O	1:A:67:ARG:HG3	2.21	0.41
1:A:103:GLU:H	1:A:103:GLU:HG3	1.71	0.41
1:A:567:LYS:HB3	1:A:567:LYS:HE3	1.55	0.41
1:B:61:LEU:HD23	1:B:61:LEU:HA	1.88	0.40
1:B:355:LEU:HB2	1:B:356:PRO:HD3	2.02	0.40
1:B:472:THR:HG23	1:B:474:ARG:H	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:LEU:HD12	1:A:294:LEU:HD21	2.02	0.40
1:A:433:LEU:HD23	1:A:433:LEU:HA	1.90	0.40
1:B:559:SER:O	1:B:563:ARG:N	2.48	0.40
1:A:207:LEU:HD23	1:A:229:LEU:HB3	2.04	0.40
1:A:448:ARG:HA	1:A:451:ILE:HG12	2.04	0.40
1:A:536:LEU:O	1:A:539:GLN:HG2	2.21	0.40
1:B:392:LEU:HD13	1:B:395:ILE:HD12	2.03	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	521/540 (96%)	511 (98%)	10 (2%)	0	100	100
1	B	521/540 (96%)	511 (98%)	10 (2%)	0	100	100
All	All	1042/1080 (96%)	1022 (98%)	20 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	428/434 (99%)	412 (96%)	16 (4%)	34	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	428/434 (99%)	404 (94%)	24 (6%)	21 54
All	All	856/868 (99%)	816 (95%)	40 (5%)	26 60

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	LYS
1	A	83	ARG
1	A	88	SER
1	A	134	ARG
1	A	149	GLN
1	A	160	SER
1	A	169	ARG
1	A	183	TYR
1	A	271	ASP
1	A	340	ARG
1	A	360	ARG
1	A	391	GLN
1	A	443	MSE
1	A	453	ARG
1	A	523	TYR
1	A	560	ASP
1	B	53	LEU
1	B	78	GLN
1	B	80	GLN
1	B	102	GLN
1	B	123	ARG
1	B	137	GLU
1	B	139	MSE
1	B	151	ASP
1	B	153	HIS
1	B	157	LEU
1	B	244	LYS
1	B	249	GLU
1	B	253	ASP
1	B	267	GLN
1	B	302	GLN
1	B	340	ARG
1	B	388	TYR
1	B	406	GLN
1	B	432	MSE
1	B	437	ARG

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Mol	Chain	Res	Type
1	B	479	ARG
1	B	531	HIS
1	B	563	ARG
1	B	567	LYS

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

Mol	Chain	Res	Type
1	A	347	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)

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^{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	516/540 (95%)	0.38	20 (3%) 39 35	80, 138, 179, 242	0
1	B	516/540 (95%)	0.22	8 (1%) 72 66	77, 131, 174, 224	0
All	All	1032/1080 (95%)	0.30	28 (2%) 54 48	77, 135, 177, 242	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	82	THR	5.0
1	A	395	ILE	3.5
1	B	51	ASP	3.2
1	A	439	ASP	3.1
1	B	85	PRO	3.1
1	B	469	ALA	3.0
1	B	103	GLU	3.0
1	A	152	THR	3.0
1	A	304	TRP	2.8
1	A	80	GLN	2.7
1	A	396	GLU	2.6
1	A	86	GLY	2.6
1	A	314	LEU	2.5
1	B	86	GLY	2.4
1	A	308	ARG	2.4
1	A	84	ASP	2.4
1	B	366	LEU	2.4
1	A	277	PHE	2.2
1	A	558	ASP	2.2
1	A	83	ARG	2.1
1	A	366	LEU	2.1
1	A	506	GLN	2.1
1	A	269	ARG	2.1
1	A	305	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	497	ASP	2.1
1	A	335	GLN	2.1
1	B	152	THR	2.0
1	A	280	LEU	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.