Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:10 AM GMT

PDB ID	:	3L4C
Title	:	Structural basis of membrane-targeting by Dock180
Authors	:	Premkumar, L.; Bobkov, A.A.; Patel, M.; Jaroszewski, L.; Bankston, L.A.; Stec, B.; Vuori, K.; Cote, J-.F.; Liddington, R.C.
Deposited on	:	2009-12-18
Resolution	:	2.37 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

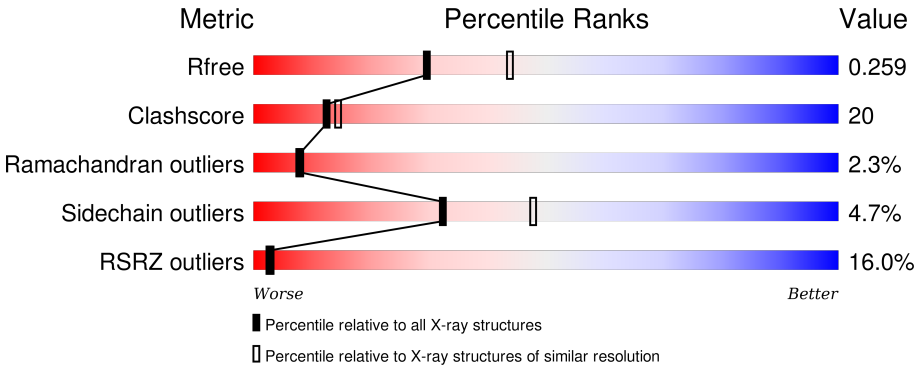
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.37 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}	91344	4019 (2.40-2.36)
Clashscore	102246	4595 (2.40-2.36)
Ramachandran outliers	100387	4520 (2.40-2.36)
Sidechain outliers	100360	4522 (2.40-2.36)
RSRZ outliers	91569	4034 (2.40-2.36)

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 >=3, 2, 1 and 0 types of geometric quality criteria. 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	220	15% 53% 23% 5% 19%
1	B	220	11% 61% 17% • • 19%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BME	A	2	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2924 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 Dedicator of cytokinesis protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	178	Total	C	N	O	S	0	0	0
			1424	900	240	280	4			
1	B	179	Total	C	N	O	S	0	0	0
			1428	901	240	283	4			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	400	MET	-	expression tag	UNP Q14185
A	401	GLY	-	expression tag	UNP Q14185
A	402	SER	-	expression tag	UNP Q14185
A	403	SER	-	expression tag	UNP Q14185
A	404	HIS	-	expression tag	UNP Q14185
A	405	HIS	-	expression tag	UNP Q14185
A	406	HIS	-	expression tag	UNP Q14185
A	407	HIS	-	expression tag	UNP Q14185
A	408	HIS	-	expression tag	UNP Q14185
A	409	HIS	-	expression tag	UNP Q14185
A	410	SER	-	expression tag	UNP Q14185
A	411	SER	-	expression tag	UNP Q14185
A	412	GLY	-	expression tag	UNP Q14185
A	413	LEU	-	expression tag	UNP Q14185
A	414	VAL	-	expression tag	UNP Q14185
A	415	PRO	-	expression tag	UNP Q14185
A	416	ARG	-	expression tag	UNP Q14185
A	417	GLY	-	expression tag	UNP Q14185
A	418	SER	-	expression tag	UNP Q14185
A	419	HIS	-	expression tag	UNP Q14185
A	420	MET	-	expression tag	UNP Q14185
A	421	PRO	-	expression tag	UNP Q14185
B	400	MET	-	expression tag	UNP Q14185
B	401	GLY	-	expression tag	UNP Q14185
B	402	SER	-	expression tag	UNP Q14185

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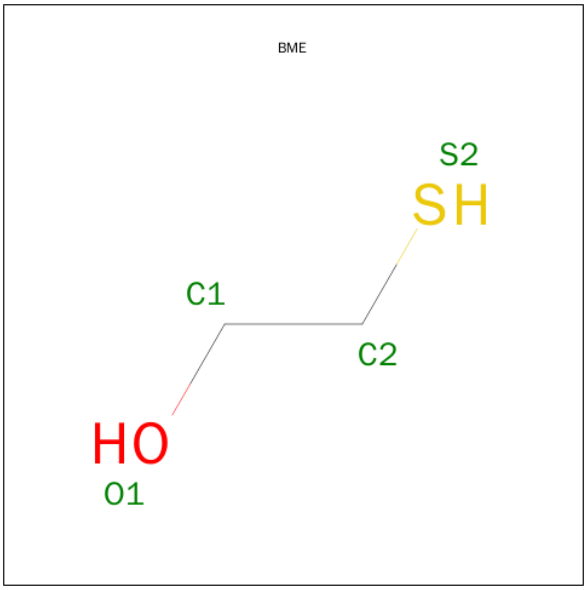
Chain	Residue	Modelled	Actual	Comment	Reference
B	403	SER	-	expression tag	UNP Q14185
B	404	HIS	-	expression tag	UNP Q14185
B	405	HIS	-	expression tag	UNP Q14185
B	406	HIS	-	expression tag	UNP Q14185
B	407	HIS	-	expression tag	UNP Q14185
B	408	HIS	-	expression tag	UNP Q14185
B	409	HIS	-	expression tag	UNP Q14185
B	410	SER	-	expression tag	UNP Q14185
B	411	SER	-	expression tag	UNP Q14185
B	412	GLY	-	expression tag	UNP Q14185
B	413	LEU	-	expression tag	UNP Q14185
B	414	VAL	-	expression tag	UNP Q14185
B	415	PRO	-	expression tag	UNP Q14185
B	416	ARG	-	expression tag	UNP Q14185
B	417	GLY	-	expression tag	UNP Q14185
B	418	SER	-	expression tag	UNP Q14185
B	419	HIS	-	expression tag	UNP Q14185
B	420	MET	-	expression tag	UNP Q14185
B	421	PRO	-	expression tag	UNP Q14185

- Molecule 2 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total S 1 1	0	0
2	B	1	Total S 1 1	0	0

- Molecule 3 is water.

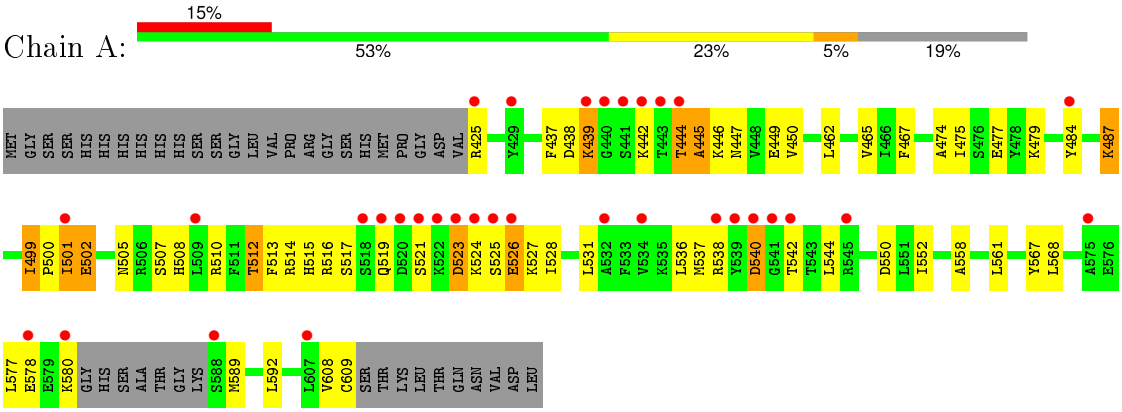
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	27	Total O 27 27	0	0
3	B	43	Total O 43 43	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

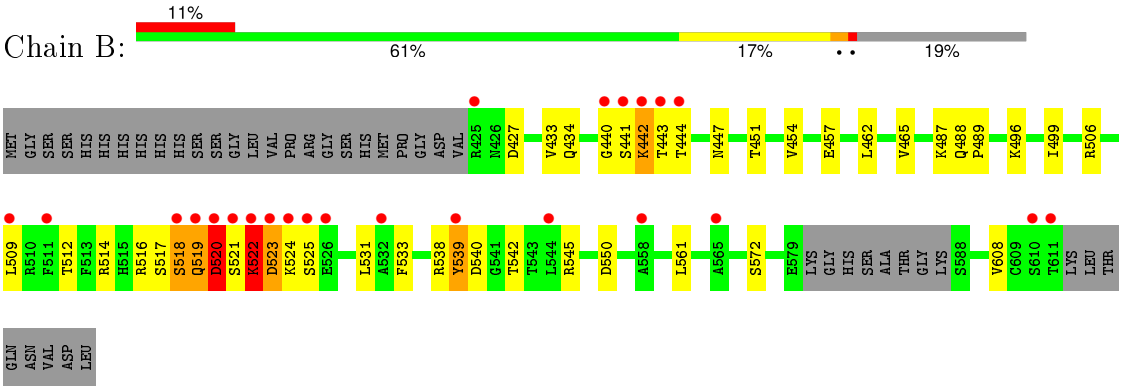
- Molecule 1: Dedicator of cytokinesis protein 1

Chain A:



- Molecule 1: Dedicator of cytokinesis protein 1

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	46.99Å 63.53Å 63.42Å 90.00° 109.28° 90.00°	Depositor
Resolution (Å)	50.00 – 2.37 22.18 – 2.37	Depositor EDS
% Data completeness (in resolution range)	96.6 (50.00-2.37) 96.6 (22.18-2.37)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	0.86 (at 2.36Å)	Xtriage
Refinement program	Refmac5 & CNS	Depositor
R, R_{free}	0.216 , 0.269 0.212 , 0.259	Depositor DCC
R_{free} test set	699 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	34.6	Xtriage
Anisotropy	0.681	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 51.9	EDS
Estimated twinning fraction	0.035 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 14379 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	2924	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.84% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BME

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	0.34	0/1448	0.60	0/1949
1	B	0.39	0/1452	0.74	2/1956 (0.1%)
All	All	0.36	0/2900	0.67	2/3905 (0.1%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	519	GLN	N-CA-C	7.75	131.92	111.00
1	B	518	SER	N-CA-C	-6.22	94.19	111.00

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	1424	0	1415	60	0
1	B	1428	0	1414	51	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	27	0	0	1	0
3	B	43	0	0	1	0
All	All	2924	0	2829	111	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 20.

All (111) 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:439:LYS:HG2	1:A:442:LYS:HB2	1.10	1.04
1:A:439:LYS:HD3	1:A:446:LYS:HE2	1.46	0.97
1:A:439:LYS:HG2	1:A:442:LYS:CB	1.95	0.96
1:A:439:LYS:CG	1:A:442:LYS:HB2	1.99	0.91
1:B:442:LYS:HG3	1:B:443:THR:H	1.32	0.89
1:B:519:GLN:HG3	1:B:524:LYS:HE3	1.62	0.81
1:A:445:ALA:HB2	1:A:487:LYS:NZ	1.94	0.81
1:A:512:THR:HG21	1:A:528:ILE:HD13	1.63	0.80
1:A:524:LYS:NZ	1:A:526:GLU:HA	1.95	0.80
1:B:540:ASP:OD2	1:B:542:THR:HG22	1.84	0.78
1:A:501:ILE:HD13	1:A:501:ILE:H	1.52	0.75
1:A:439:LYS:HE3	1:A:442:LYS:HG3	1.71	0.73
1:A:515:HIS:O	1:A:526:GLU:HB3	1.89	0.72
1:B:427:ASP:OD2	1:B:496:LYS:HD2	1.93	0.69
1:B:443:THR:HG22	1:B:444:THR:HG23	1.74	0.68
1:A:524:LYS:HZ3	1:A:526:GLU:HA	1.59	0.67
1:A:589:MET:HE1	1:A:592:LEU:HD13	1.76	0.67
1:B:517:SER:OG	1:B:524:LYS:HA	1.96	0.66
1:B:519:GLN:CD	1:B:524:LYS:HG2	2.15	0.66
1:A:445:ALA:HB2	1:A:487:LYS:HZ2	1.61	0.64
1:B:519:GLN:CG	1:B:524:LYS:HE3	2.28	0.63
1:A:501:ILE:N	1:A:501:ILE:HD13	2.13	0.62
1:A:512:THR:HG21	1:A:528:ILE:CD1	2.28	0.62
1:A:524:LYS:HZ2	1:A:526:GLU:HA	1.63	0.62
1:B:539:TYR:CD2	1:B:539:TYR:N	2.69	0.61
1:A:462:LEU:HD11	1:A:507:SER:OG	2.01	0.61
1:B:531:LEU:HD13	1:B:561:LEU:O	2.01	0.61
1:B:442:LYS:HG3	1:B:443:THR:N	2.11	0.61
1:B:443:THR:HG22	1:B:444:THR:N	2.16	0.60
1:B:517:SER:HB2	1:B:519:GLN:HE21	1.66	0.60
1:A:589:MET:CE	1:A:592:LEU:HD13	2.32	0.60
1:B:517:SER:HB2	1:B:519:GLN:NE2	2.16	0.59
1:B:433:VAL:HG12	1:B:434:GLN:HG2	1.85	0.59
1:B:518:SER:O	1:B:519:GLN:NE2	2.36	0.59
1:A:500:PRO:HB2	1:A:502:GLU:HG3	1.86	0.58
1:A:475:ILE:HD12	1:A:477:GLU:O	2.04	0.58
1:B:533:PHE:O	1:B:572:SER:HB2	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:520:ASP:OD1	1:B:520:ASP:O	2.22	0.57
1:B:441:SER:HB3	1:B:487:LYS:NZ	2.20	0.57
1:B:441:SER:HB3	1:B:487:LYS:HZ1	1.70	0.56
1:A:519:GLN:C	1:A:521:SER:H	2.08	0.56
1:A:487:LYS:HB2	1:A:487:LYS:NZ	2.21	0.55
1:A:501:ILE:H	1:A:501:ILE:CD1	2.20	0.55
1:A:467:PHE:CE1	1:A:474:ALA:HB2	2.42	0.55
1:A:438:ASP:O	1:A:446:LYS:HE3	2.07	0.55
1:A:538:ARG:C	1:A:540:ASP:H	2.10	0.54
1:A:447:ASN:HB2	1:A:516:ARG:O	2.08	0.53
1:B:454:VAL:HG22	1:B:509:LEU:HD23	1.89	0.53
1:A:487:LYS:HB2	1:A:487:LYS:HZ2	1.75	0.52
1:A:578:GLU:C	1:A:580:LYS:H	2.13	0.52
1:B:519:GLN:CG	1:B:524:LYS:HG2	2.38	0.52
1:B:487:LYS:C	1:B:489:PRO:HD3	2.31	0.52
1:B:539:TYR:HD2	1:B:539:TYR:N	2.06	0.51
1:B:519:GLN:NE2	1:B:523:ASP:O	2.43	0.51
1:B:516:ARG:HH11	1:B:525:SER:HB3	1.76	0.51
1:A:531:LEU:HD13	1:A:561:LEU:O	2.12	0.50
1:B:457:GLU:OE2	1:B:506:ARG:HD2	2.11	0.50
1:B:519:GLN:HG3	1:B:524:LYS:HG2	1.93	0.50
1:A:425:ARG:NH2	1:A:465:VAL:HG12	2.27	0.50
1:A:519:GLN:C	1:A:521:SER:N	2.64	0.49
1:A:445:ALA:HB2	1:A:487:LYS:HZ1	1.70	0.49
1:A:514:ARG:HD2	1:A:516:ARG:CZ	2.43	0.49
1:B:514:ARG:HG3	1:B:514:ARG:HH11	1.78	0.49
1:A:467:PHE:CZ	1:A:474:ALA:HB2	2.48	0.48
1:B:447:ASN:HB2	1:B:516:ARG:O	2.14	0.48
1:A:449:GLU:OE1	1:A:479:LYS:HD3	2.14	0.48
1:B:538:ARG:NH2	1:B:545:ARG:HG3	2.29	0.48
1:B:443:THR:HG22	1:B:444:THR:H	1.78	0.48
1:B:608:VAL:HG23	3:B:737:HOH:O	2.12	0.48
1:A:439:LYS:HD3	1:A:446:LYS:CE	2.31	0.47
1:A:589:MET:HE1	1:A:592:LEU:HB2	1.97	0.47
1:B:517:SER:CB	1:B:519:GLN:HE21	2.28	0.47
1:A:437:PHE:O	1:A:487:LYS:HG3	2.15	0.47
1:A:512:THR:CG2	1:A:528:ILE:HD13	2.40	0.47
1:A:538:ARG:HB3	1:A:540:ASP:OD2	2.14	0.47
1:A:608:VAL:HG22	1:A:609:CYS:N	2.30	0.47
1:B:519:GLN:HG3	1:B:524:LYS:CE	2.37	0.47
1:A:508:HIS:HE1	1:A:567:TYR:OH	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:VAL:HG11	1:A:499:ILE:HG22	1.98	0.46
1:A:442:LYS:O	1:A:444:THR:N	2.40	0.46
1:A:536:LEU:O	1:A:544:LEU:N	2.49	0.45
1:A:538:ARG:HD3	1:A:542:THR:HB	1.98	0.45
1:A:523:ASP:CG	1:A:524:LYS:N	2.69	0.45
1:A:484:TYR:HB2	3:A:713:HOH:O	2.16	0.45
1:B:539:TYR:HD2	1:B:540:ASP:H	1.64	0.44
1:B:442:LYS:CG	1:B:443:THR:N	2.77	0.44
1:B:454:VAL:HG12	1:B:462:LEU:HD13	2.00	0.44
1:B:441:SER:OG	1:B:442:LYS:N	2.51	0.43
1:B:442:LYS:CG	1:B:443:THR:H	2.08	0.43
1:B:521:SER:O	1:B:522:LYS:HB2	2.17	0.43
1:A:524:LYS:C	1:A:526:GLU:H	2.20	0.43
1:A:517:SER:HB2	1:A:519:GLN:HG3	2.00	0.43
1:B:451:THR:HB	1:B:512:THR:OG1	2.18	0.43
1:B:465:VAL:HB	1:B:499:ILE:HD13	2.01	0.43
1:A:510:ARG:HD2	1:A:531:LEU:HD11	2.01	0.43
1:B:514:ARG:HG3	1:B:514:ARG:NH1	2.34	0.43
1:B:531:LEU:C	1:B:531:LEU:HD23	2.39	0.42
1:B:441:SER:CB	1:B:487:LYS:NZ	2.83	0.42
1:A:450:VAL:HG22	1:A:513:PHE:CE1	2.54	0.42
1:B:516:ARG:NH1	1:B:525:SER:HB3	2.34	0.42
1:A:552:ILE:HD11	1:A:577:LEU:HB2	2.00	0.42
1:B:488:GLN:HE21	1:B:488:GLN:HB3	1.72	0.42
1:A:516:ARG:HA	1:A:526:GLU:OE2	2.20	0.42
1:A:538:ARG:C	1:A:540:ASP:N	2.74	0.42
1:A:508:HIS:CD2	1:A:568:LEU:HD21	2.56	0.41
1:A:505:ASN:HB2	1:A:537:MET:SD	2.60	0.41
1:B:443:THR:HG22	1:B:444:THR:CG2	2.48	0.41
1:A:527:LYS:HD2	1:A:527:LYS:HA	1.78	0.41
1:B:441:SER:CB	1:B:487:LYS:HZ3	2.34	0.40
1:A:528:ILE:HG22	1:A:561:LEU:HD23	2.02	0.40
1:B:443:THR:CG2	1:B:444:THR:H	2.34	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	174/220 (79%)	154 (88%)	17 (10%)	3 (2%)	11 13
1	B	175/220 (80%)	156 (89%)	14 (8%)	5 (3%)	6 4
All	All	349/440 (79%)	310 (89%)	31 (9%)	8 (2%)	8 8

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	526	GLU
1	A	445	ALA
1	B	440	GLY
1	B	520	ASP
1	B	522	LYS
1	B	442	LYS
1	B	523	ASP
1	A	558	ALA

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	159/194 (82%)	148 (93%)	11 (7%)	19 27
1	B	160/194 (82%)	156 (98%)	4 (2%)	55 74
All	All	319/388 (82%)	304 (95%)	15 (5%)	32 48

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	439	LYS
1	A	444	THR
1	A	487	LYS
1	A	499	ILE
1	A	501	ILE
1	A	502	GLU
1	A	512	THR
1	A	523	ASP
1	A	525	SER
1	A	540	ASP
1	A	550	ASP
1	B	520	ASP
1	B	522	LYS
1	B	539	TYR
1	B	550	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	426	ASN
1	A	508	HIS
1	A	549	HIS
1	B	488	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are modelled with single atom - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

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^{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	178/220 (80%)	1.09	33 (18%)	2	2	23, 44, 82, 98	0
1	B	179/220 (81%)	0.91	24 (13%)	4	5	19, 35, 73, 96	0
All	All	357/440 (81%)	1.00	57 (15%)	3	3	19, 39, 81, 98	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	521	SER	11.1
1	A	523	ASP	8.0
1	A	441	SER	7.2
1	B	523	ASP	6.7
1	A	443	THR	6.5
1	B	539	TYR	6.3
1	A	520	ASP	6.2
1	B	521	SER	5.6
1	B	522	LYS	5.6
1	B	525	SER	5.4
1	A	518	SER	5.0
1	B	442	LYS	5.0
1	A	440	GLY	4.7
1	A	539	TYR	4.6
1	B	519	GLN	4.6
1	A	588	SER	4.5
1	A	525	SER	4.2
1	B	524	LYS	4.2
1	A	542	THR	4.0
1	B	611	THR	4.0
1	B	526	GLU	3.9
1	A	540	ASP	3.9
1	B	443	THR	3.8
1	B	520	ASP	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	441	SER	3.7
1	A	442	LYS	3.6
1	A	580	LYS	3.6
1	A	575	ALA	3.5
1	A	444	THR	3.4
1	A	524	LYS	3.4
1	B	558	ALA	3.2
1	B	440	GLY	3.2
1	A	578	GLU	3.2
1	A	522	LYS	2.9
1	A	541	GLY	2.9
1	A	439	LYS	2.9
1	A	484	TYR	2.9
1	A	532	ALA	2.8
1	B	518	SER	2.8
1	B	565	ALA	2.6
1	A	526	GLU	2.5
1	A	501	ILE	2.5
1	B	610	SER	2.4
1	B	544	LEU	2.4
1	A	429	TYR	2.4
1	A	534	VAL	2.4
1	B	444	THR	2.3
1	A	607	LEU	2.3
1	A	538	ARG	2.3
1	B	532	ALA	2.3
1	B	511	PHE	2.3
1	A	545	ARG	2.2
1	B	425	ARG	2.1
1	B	509	LEU	2.1
1	A	425	ARG	2.1
1	A	519	GLN	2.1
1	A	509	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 carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	BME	A	2	1/4	0.94	0.26	2.83	43,43,43,43	0
2	BME	B	1	1/4	0.92	0.14	-0.32	39,39,39,39	0

6.5 Other polymers

There are no such residues in this entry.