WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 27, 2014 – 08:15 AM GMT

PDB ID : 3TNF
Title : LidA from Legionella in complex with active Rab8a
Authors : Schoebel, S.; Cichy, A.L.; Goody, R.S.; Itzen, A.
Deposited on : 2011-09-01
Resolution : 2.50 Å(reported)

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

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance (i)

The reported resolution of this entry is 2.50 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	Percentile Ranks	Value
Rfree		0.270
Clashscore		15
Ramachandran outliers		0.9%
Sidechain outliers		16.4%
RSRZ outliers		5.4%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
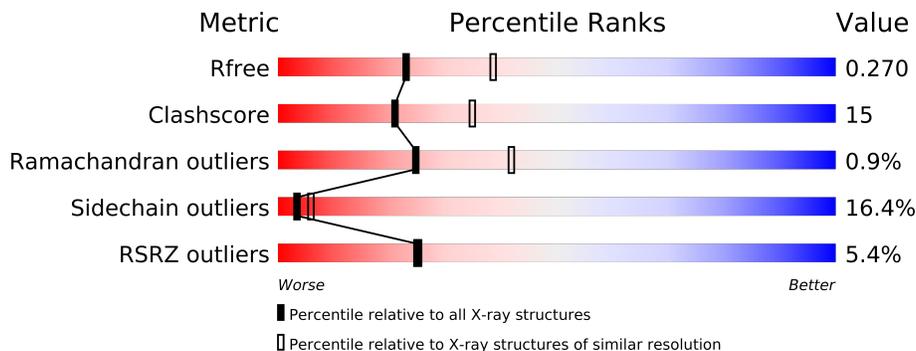
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	174	
2	B	384	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	MG	A	199	-	X
5	MPD	A	1	-	X
5	MPD	A	177	-	X
5	MPD	B	2	-	X
5	MPD	B	3	-	X

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 4590 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Ras-related protein Rab-8A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	170	Total	C	N	O	S	0	0	0
			1372	872	236	257	7			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	GLY	-	EXPRESSION TAG	UNP P61006
A	4	HIS	-	EXPRESSION TAG	UNP P61006
A	5	MET	-	EXPRESSION TAG	UNP P61006

- Molecule 2 is a protein called LidA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	379	Total	C	N	O	S	0	0	0
			3091	1935	536	613	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	200	GLY	-	EXPRESSION TAG	UNP Q5ZWZ3

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is PHOSPHOAMINOPHOSPHONICACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).
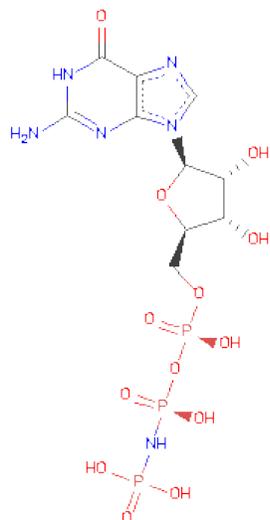
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			32	10	6	13	3		

- Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).
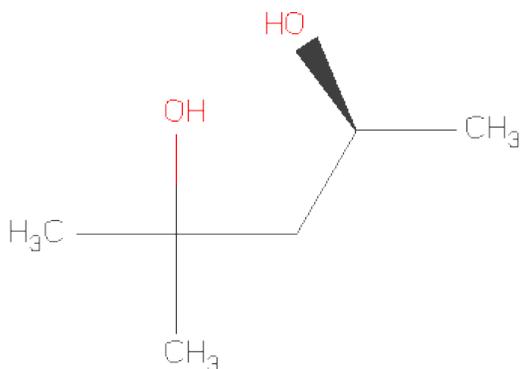
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			8	6	2		
5	A	1	Total	C	O	0	0
			8	6	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total 8	C 6	O 2	0	0
5	B	1	Total 8	C 6	O 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	26	Total 26	O 26	0	0
6	B	36	Total 36	O 36	0	0

3 Residue-property plots ⓘ

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: Ras-related protein Rab-8A

Chain A:
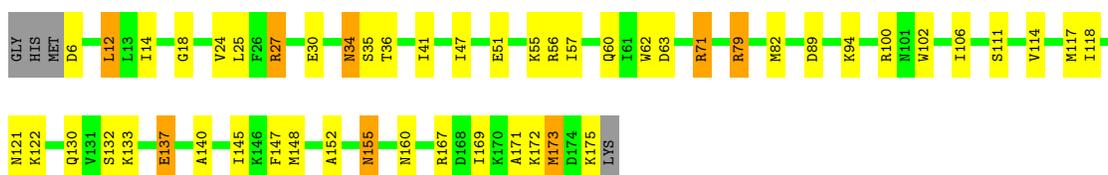
• Molecule 2: LidA

Chain B:
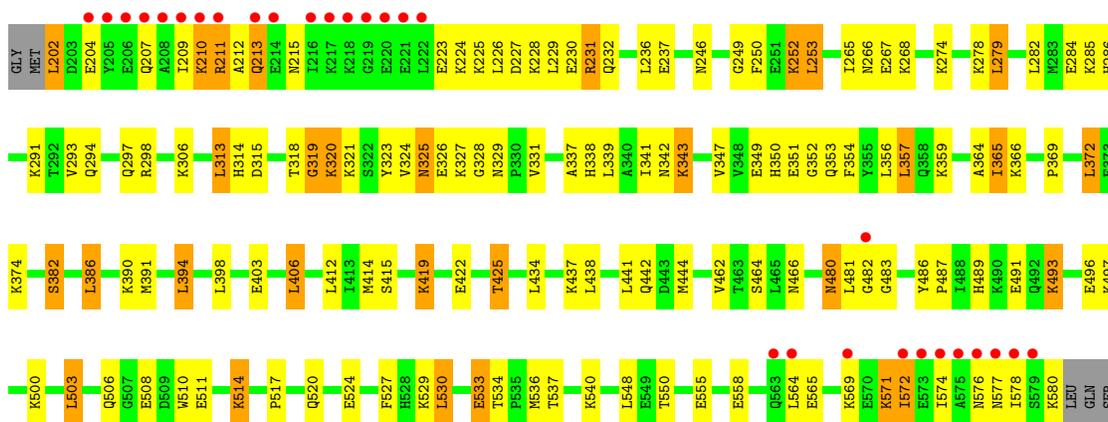
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	103.82Å 103.82Å 150.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.50 49.08 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (30.00-2.50) 99.8 (49.08-2.50)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.49 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.216 , 0.275 0.212 , 0.270	Depositor DCC
R_{free} test set	1457 reflections (5.00%)	DCC
Wilson B-factor (Å^2)	60.2	Xtriage
Anisotropy	0.352	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 49.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Outliers	1 of 29141 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4590	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, MPD, GNP

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	0.51	0/1392	0.58	0/1865
2	B	0.45	0/3138	0.54	0/4197
All	All	0.47	0/4530	0.55	0/6062

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1372	0	1385	32	0
2	B	3091	0	3082	109	0
3	A	1	0	0	0	0
4	A	32	0	13	1	0
5	A	16	0	28	2	0
5	B	16	0	28	4	0
6	A	26	0	0	3	0
6	B	36	0	0	0	0
All	All	4590	0	4536	140	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 15.

All (140) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:319:GLY:HA2	2:B:321:LYS:H	1.17	1.10
2:B:325:ASN:O	2:B:327:LYS:HA	1.67	0.94
2:B:391:MET:CE	2:B:444:MET:HB3	1.98	0.94
2:B:225:LYS:HA	2:B:228:LYS:HG2	1.48	0.93
2:B:391:MET:HE1	2:B:444:MET:HB3	1.55	0.87
2:B:237:GLU:HG3	5:B:3:MPD:HM1	1.57	0.86
2:B:481:LEU:HB2	2:B:486:TYR:HE2	1.40	0.86
1:A:71:ARG:HH21	5:A:1:MPD:H31	1.42	0.83
2:B:319:GLY:HA2	2:B:321:LYS:N	1.94	0.82
2:B:328:GLY:HA2	2:B:347:VAL:HB	1.62	0.81
2:B:480:ASN:HD21	2:B:483:GLY:H	1.27	0.81
2:B:319:GLY:CA	2:B:321:LYS:H	1.94	0.79
2:B:250:PHE:HZ	2:B:444:MET:CE	2.01	0.72
2:B:250:PHE:HZ	2:B:444:MET:HE1	1.53	0.72
2:B:391:MET:HE2	2:B:444:MET:HB3	1.72	0.70
2:B:480:ASN:HD21	2:B:483:GLY:N	1.89	0.69
1:A:14:ILE:HD11	1:A:106:ILE:HD11	1.76	0.67
1:A:34:ASN:HD22	1:A:36:THR:H	1.42	0.65
2:B:441:LEU:HA	2:B:444:MET:HE3	1.77	0.65
2:B:315:ASP:O	2:B:319:GLY:HA2	1.98	0.64
2:B:325:ASN:C	2:B:327:LYS:HA	2.17	0.64
2:B:441:LEU:HD23	2:B:444:MET:HE3	1.79	0.64
2:B:386:LEU:HD13	2:B:390:LYS:HE3	1.78	0.64
2:B:497:LYS:HE3	2:B:510:TRP:CD1	2.33	0.64
1:A:111:SER:O	1:A:114:VAL:HG22	1.97	0.63
2:B:250:PHE:CZ	2:B:444:MET:HE1	2.32	0.63
2:B:480:ASN:HD22	2:B:481:LEU:N	1.97	0.63
2:B:537:THR:HG22	2:B:540:LYS:HB3	1.80	0.62
2:B:481:LEU:HB2	2:B:486:TYR:CE2	2.28	0.62
2:B:339:LEU:HD23	2:B:382:SER:OG	2.01	0.61
2:B:250:PHE:CZ	2:B:444:MET:CE	2.83	0.60
2:B:537:THR:HG22	2:B:540:LYS:CB	2.31	0.60
1:A:14:ILE:CD1	1:A:106:ILE:HD11	2.31	0.60
1:A:47:ILE:HD13	1:A:60:GLN:HA	1.83	0.60
2:B:511:GLU:HA	2:B:514:LYS:HD2	1.82	0.59
1:A:79:ARG:HH11	1:A:79:ARG:HB2	1.66	0.59
2:B:441:LEU:HD23	2:B:444:MET:CE	2.33	0.59
2:B:246:ASN:OD1	2:B:437:LYS:HE3	2.03	0.58
1:A:14:ILE:HD12	1:A:102:TRP:CE3	2.38	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:253:LEU:HD22	2:B:437:LYS:HD3	1.84	0.58
2:B:537:THR:HG23	2:B:540:LYS:H	1.70	0.57
2:B:357:LEU:HD13	2:B:357:LEU:N	2.20	0.56
2:B:517:PRO:HA	2:B:520:GLN:HE21	1.69	0.56
2:B:210:LYS:HA	2:B:213:GLN:HB2	1.86	0.56
1:A:34:ASN:ND2	1:A:36:THR:H	2.03	0.56
1:A:140:ALA:HB1	1:A:145:ILE:O	2.06	0.56
2:B:550:THR:OG1	5:B:3:MPD:H12	2.05	0.56
2:B:215:ASN:OD1	2:B:571:LYS:HG2	2.05	0.55
2:B:364:ALA:O	2:B:365:ILE:HD13	2.07	0.54
1:A:130:GLN:HE22	2:B:529:LYS:HE2	1.72	0.54
1:A:89:ASP:OD2	1:A:122:LYS:HE3	2.06	0.54
1:A:27:ARG:HD2	1:A:152:ALA:O	2.06	0.53
2:B:285:LYS:NZ	2:B:286:HIS:HE1	2.06	0.53
1:A:12:LEU:HD23	1:A:62:TRP:HB2	1.91	0.53
6:A:204:HOH:O	2:B:534:THR:HG23	2.09	0.53
2:B:224:LYS:O	2:B:228:LYS:HB3	2.09	0.53
2:B:536:MET:HG2	2:B:540:LYS:HG2	1.91	0.53
2:B:223:GLU:HG3	2:B:564:LEU:HD11	1.91	0.52
2:B:207:GLN:O	2:B:211:ARG:HB2	2.08	0.52
2:B:318:THR:OG1	2:B:320:LYS:HG3	2.09	0.52
2:B:253:LEU:O	2:B:253:LEU:HG	2.05	0.52
2:B:326:GLU:CB	2:B:338:HIS:CE1	2.93	0.52
2:B:394:LEU:HD22	5:B:2:MPD:H11	1.92	0.51
2:B:228:LYS:HA	2:B:231:ARG:HE	1.75	0.50
1:A:71:ARG:NH2	5:A:1:MPD:H31	2.20	0.50
2:B:422:GLU:O	2:B:425:THR:HG23	2.12	0.50
2:B:325:ASN:OD1	2:B:329:ASN:HB2	2.12	0.50
2:B:324:VAL:HG21	2:B:341:ILE:HD11	1.94	0.50
2:B:569:LYS:O	2:B:572:ILE:HG12	2.12	0.50
2:B:209:ILE:HG13	2:B:210:LYS:HD3	1.94	0.50
2:B:391:MET:HE2	2:B:444:MET:CB	2.43	0.49
1:A:147:PHE:CG	1:A:148:MET:N	2.80	0.49
2:B:357:LEU:HD13	2:B:357:LEU:H	1.78	0.49
2:B:224:LYS:HB2	2:B:224:LYS:HE3	1.43	0.48
2:B:517:PRO:HA	2:B:520:GLN:NE2	2.27	0.48
2:B:500:LYS:HD3	2:B:524:GLU:OE2	2.14	0.48
2:B:323:TYR:HB3	2:B:337:ALA:HB2	1.96	0.48
1:A:140:ALA:CB	1:A:147:PHE:HB2	2.44	0.48
2:B:250:PHE:CZ	2:B:444:MET:HE2	2.49	0.47
2:B:209:ILE:HG13	2:B:210:LYS:N	2.29	0.47
2:B:493:LYS:HG3	2:B:506:GLN:HA	1.96	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:285:LYS:HG2	2:B:286:HIS:CE1	2.50	0.47
2:B:293:VAL:O	2:B:297:GLN:HG3	2.15	0.47
1:A:25:LEU:HD22	1:A:63:ASP:HB2	1.97	0.46
1:A:47:ILE:CD1	1:A:60:GLN:HA	2.45	0.46
2:B:369:PRO:HA	2:B:372:LEU:HB2	1.97	0.46
2:B:419:LYS:HD2	2:B:419:LYS:HA	1.55	0.46
2:B:319:GLY:CA	2:B:321:LYS:N	2.67	0.46
2:B:274:LYS:O	2:B:278:LYS:HG3	2.14	0.46
2:B:326:GLU:CB	2:B:338:HIS:ND1	2.79	0.46
2:B:226:LEU:HD13	2:B:564:LEU:HD22	1.98	0.45
2:B:349:GLU:HG3	2:B:354:PHE:CE1	2.52	0.45
2:B:266:ASN:HD21	2:B:314:HIS:CE1	2.33	0.45
2:B:487:PRO:CG	2:B:533:GLU:HG2	2.47	0.45
2:B:285:LYS:HZ3	2:B:286:HIS:HE1	1.65	0.45
2:B:250:PHE:HZ	2:B:444:MET:HE2	1.80	0.45
1:A:18:GLY:H	4:A:200:GNP:HNB3	1.64	0.45
2:B:386:LEU:CD1	2:B:390:LYS:HE3	2.45	0.45
2:B:480:ASN:C	2:B:480:ASN:HD22	2.20	0.44
2:B:212:ALA:HB2	2:B:574:ILE:CG2	2.46	0.44
2:B:394:LEU:HA	2:B:394:LEU:HD13	1.80	0.44
2:B:527:PHE:O	2:B:530:LEU:HB2	2.18	0.44
2:B:503:LEU:HA	2:B:503:LEU:HD23	1.89	0.44
2:B:357:LEU:CD1	2:B:357:LEU:N	2.81	0.44
2:B:487:PRO:HG2	2:B:533:GLU:HG2	1.99	0.44
6:A:189:HOH:O	2:B:534:THR:HG22	2.18	0.44
1:A:147:PHE:O	1:A:148:MET:HB2	2.18	0.44
1:A:34:ASN:HD22	1:A:35:SER:N	2.16	0.43
2:B:493:LYS:CG	2:B:506:GLN:HA	2.48	0.43
1:A:169:ILE:O	1:A:173:MET:HB2	2.19	0.43
2:B:343:LYS:HG3	2:B:343:LYS:H	1.44	0.43
2:B:325:ASN:C	2:B:325:ASN:HD22	2.22	0.43
2:B:537:THR:HG22	2:B:540:LYS:HB2	2.01	0.43
2:B:489:HIS:ND1	2:B:491:GLU:HG2	2.33	0.43
1:A:147:PHE:CD2	1:A:148:MET:N	2.87	0.42
2:B:353:GLN:HE21	2:B:353:GLN:HB2	1.62	0.42
2:B:578:ILE:C	2:B:580:LYS:H	2.21	0.42
2:B:351:GLU:HG2	2:B:352:GLY:N	2.34	0.42
1:A:133:LYS:O	1:A:137:GLU:HG2	2.20	0.42
1:A:117:MET:HE3	1:A:117:MET:HB2	1.83	0.42
1:A:118:ILE:HD11	1:A:145:ILE:HD11	2.02	0.42
2:B:223:GLU:HG3	2:B:564:LEU:HD21	2.01	0.42
1:A:155:ASN:ND2	6:A:190:HOH:O	2.52	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:278:LYS:O	2:B:282:LEU:HG	2.19	0.41
2:B:249:GLY:HA2	2:B:252:LYS:HG3	2.02	0.41
2:B:279:LEU:HA	2:B:279:LEU:HD12	1.75	0.41
1:A:121:ASN:CG	1:A:122:LYS:H	2.24	0.41
2:B:202:LEU:HB3	2:B:204:GLU:H	1.85	0.41
2:B:438:LEU:O	2:B:442:GLN:HG2	2.21	0.41
1:A:175:LYS:HB3	1:A:175:LYS:HE2	1.80	0.41
1:A:56:ARG:O	1:A:57:ILE:HD13	2.21	0.41
2:B:354:PHE:N	2:B:354:PHE:CD2	2.89	0.40
2:B:265:ILE:HD13	2:B:313:LEU:HB3	2.03	0.40
1:A:47:ILE:HA	1:A:47:ILE:HD13	1.88	0.40
2:B:394:LEU:CD2	5:B:2:MPD:H11	2.51	0.40
2:B:228:LYS:HE2	2:B:232:GLN:NE2	2.36	0.40
2:B:225:LYS:CA	2:B:228:LYS:HG2	2.36	0.40
2:B:403:GLU:HA	2:B:406:LEU:HD22	2.04	0.40
2:B:414:MET:O	2:B:415:SER:C	2.60	0.40
2:B:228:LYS:HG3	2:B:228:LYS:O	2.20	0.40

There are no symmetry-related clashes.

5.3   Torsion angles

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	168/174 (97%)	161 (96%)	6 (4%)	1 (1%)	33	55
2	B	377/384 (98%)	353 (94%)	20 (5%)	4 (1%)	21	34
All	All	545/558 (98%)	514 (94%)	26 (5%)	5 (1%)	25	42

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	319	GLY
2	B	231	ARG
2	B	320	LYS

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Mol	Chain	Res	Type
1	A	171	ALA
2	B	482	GLY

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	147/150 (98%)	126 (86%)	21 (14%)	5	8
2	B	340/346 (98%)	281 (83%)	59 (17%)	3	5
All	All	487/496 (98%)	407 (84%)	80 (16%)	3	6

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ASP
1	A	12	LEU
1	A	24	VAL
1	A	27	ARG
1	A	30	GLU
1	A	34	ASN
1	A	41	ILE
1	A	51	GLU
1	A	55	LYS
1	A	71	ARG
1	A	79	ARG
1	A	82	MET
1	A	94	LYS
1	A	100	ARG
1	A	132	SER
1	A	137	GLU
1	A	155	ASN
1	A	160	ASN
1	A	167	ARG
1	A	172	LYS
1	A	173	MET
2	B	202	LEU
2	B	210	LYS

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Mol	Chain	Res	Type
2	B	211	ARG
2	B	213	GLN
2	B	227	ASP
2	B	229	LEU
2	B	230	GLU
2	B	236	LEU
2	B	252	LYS
2	B	253	LEU
2	B	267	GLU
2	B	268	LYS
2	B	279	LEU
2	B	284	GLU
2	B	291	LYS
2	B	294	GLN
2	B	298	ARG
2	B	306	LYS
2	B	313	LEU
2	B	325	ASN
2	B	331	VAL
2	B	342	ASN
2	B	343	LYS
2	B	350	HIS
2	B	356	LEU
2	B	357	LEU
2	B	359	LYS
2	B	365	ILE
2	B	366	LYS
2	B	372	LEU
2	B	374	LYS
2	B	382	SER
2	B	386	LEU
2	B	394	LEU
2	B	398	LEU
2	B	406	LEU
2	B	412	LEU
2	B	419	LYS
2	B	425	THR
2	B	434	LEU
2	B	462	VAL
2	B	464	SER
2	B	466	ASN
2	B	480	ASN

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Mol	Chain	Res	Type
2	B	493	LYS
2	B	496	GLU
2	B	503	LEU
2	B	508	GLU
2	B	514	LYS
2	B	530	LEU
2	B	533	GLU
2	B	548	LEU
2	B	555	GLU
2	B	558	GLU
2	B	565	GLU
2	B	571	LYS
2	B	572	ILE
2	B	576	ASN
2	B	577	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	105	ASN
1	A	130	GLN
1	A	155	ASN
2	B	232	GLN
2	B	266	ASN
2	B	281	GLN
2	B	286	HIS
2	B	314	HIS
2	B	353	GLN
2	B	480	ASN
2	B	563	GLN
2	B	577	ASN

5.3.3 RNA (i)

There are no RNA chains 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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
5	MPD	A	1	-	7,7,7	0.35	0	10,10,10	0.46	0
5	MPD	A	177	-	7,7,7	0.29	0	10,10,10	0.35	0
4	GNP	A	200	3	34,34,34	1.37	4 (11%)	50,54,54	5.06	8 (16%)
5	MPD	B	2	-	7,7,7	0.32	0	10,10,10	0.31	0
5	MPD	B	3	-	7,7,7	0.27	0	10,10,10	0.38	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MPD	A	1	-	-	0/5/5/5	0/0/0/0
5	MPD	A	177	-	-	0/5/5/5	0/0/0/0
4	GNP	A	200	3	-	0/18/38/38	0/1/3/3
5	MPD	B	2	-	-	0/5/5/5	0/0/0/0
5	MPD	B	3	-	-	0/5/5/5	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	200	GNP	PG-O1G	3.82	1.50	1.46
4	A	200	GNP	PB-O3A	-2.86	1.55	1.59
4	A	200	GNP	PA-O3A	-2.58	1.55	1.59
4	A	200	GNP	PB-O1B	2.57	1.49	1.46

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	200	GNP	C6-C5-N7	-34.04	129.56	134.14
4	A	200	GNP	O2B-PB-O1B	5.02	121.47	109.89
4	A	200	GNP	O3G-PG-O1G	-3.54	104.51	113.60
4	A	200	GNP	PB-N3B-PG	-2.99	125.04	130.07
4	A	200	GNP	O3G-PG-O2G	2.87	115.89	107.66
4	A	200	GNP	C6-N1-C2	2.75	124.32	119.51
4	A	200	GNP	O1G-PG-N3B	-2.25	108.43	111.83
4	A	200	GNP	C2-N3-C4	-2.16	112.06	115.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 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	170/174 (97%)	-0.07	0	100	100	43, 61, 90, 98	0
2	B	379/384 (98%)	0.31	29 (7%)	13	13	40, 72, 125, 137	0
All	All	549/558 (98%)	0.19	29 (5%)	25	26	40, 67, 121, 137	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	221	GLU	6.8
2	B	574	ILE	6.4
2	B	578	ILE	6.2
2	B	209	ILE	6.2
2	B	575	ALA	6.0
2	B	217	LYS	6.0
2	B	564	LEU	5.2
2	B	216	ILE	5.1
2	B	210	LYS	4.4
2	B	211	ARG	4.3
2	B	208	ALA	4.2
2	B	572	ILE	4.2
2	B	218	LYS	4.1
2	B	220	GLU	4.0
2	B	576	ASN	3.6
2	B	214	GLU	3.5
2	B	222	LEU	3.5
2	B	207	GLN	3.5
2	B	204	GLU	3.4
2	B	579	SER	3.3
2	B	206	GLU	3.2
2	B	577	ASN	3.2
2	B	563	GLN	3.2
2	B	213	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	573	GLU	2.4
2	B	205	TYR	2.2
2	B	569	LYS	2.2
2	B	219	GLY	2.2
2	B	482	GLY	2.0

6.2   Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3   Carbohydrates ⓘ

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, 95th 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	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	MG	A	199	1/1	0.25	6.38	50,50,50,50	0
5	MPD	B	3	8/8	0.34	4.51	84,89,90,91	0
5	MPD	A	1	8/8	0.26	4.25	54,65,72,75	0
5	MPD	B	2	8/8	0.24	4.06	52,66,69,71	0
5	MPD	A	177	8/8	0.21	2.91	59,66,78,83	0
4	GNP	A	200	32/32	0.19	1.01	40,50,61,64	0

6.5   Other polymers ⓘ

There are no such residues in this entry.