



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 02:52 AM GMT

PDB ID : 3RKO
Title : Crystal structure of the membrane domain of respiratory complex I from E. coli at 3.0 angstrom resolution
Authors : Efremov, R.G.; Sazanov, L.A.
Deposited on : 2011-04-18
Resolution : 3.00 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

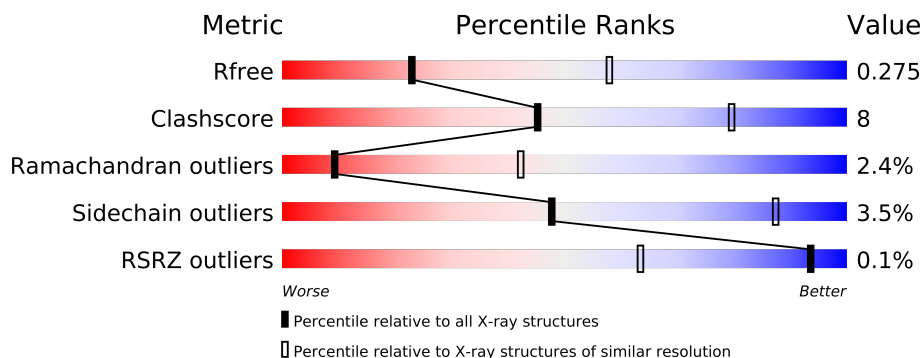
The following versions of software and data (see [references](#)) were used in the production of this report:

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

The reported resolution of this entry is 3.00 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}	66092	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)

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	B	613	
1	L	613	
2	C	509	
2	M	509	
3	D	485	
3	N	485	
4	G	100	
4	K	100	
5	A	147	
5	E	147	
6	F	184	
6	J	184	

The following table lists non-polymeric compounds that are outliers for geometric or electron-

density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
7	LFA	C	512	-	X
7	LFA	C	513	-	X
7	LFA	D	487	-	X
7	LFA	D	488	-	X
7	LFA	L	614	-	X
7	LFA	N	488	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 30310 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 NADH-QUINONE OXIDOREDUCTASE SUBUNIT L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	612	Total	C	N	O	S	0	0	0
			4676	3108	749	787	32			
1	B	612	Total	C	N	O	S	0	0	0
			4676	3108	749	787	32			

- Molecule 2 is a protein called NADH-QUINONE OXIDOREDUCTASE SUBUNIT M.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	504	Total	C	N	O	S	0	0	0
			3953	2661	617	646	29			
2	C	504	Total	C	N	O	S	0	0	0
			3953	2661	617	646	29			

- Molecule 3 is a protein called NADH-QUINONE OXIDOREDUCTASE SUBUNIT N.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	N	473	Total	C	N	O	S	0	0	0
			3590	2399	566	606	19			
3	D	473	Total	C	N	O	S	0	0	0
			3590	2399	566	606	19			

- Molecule 4 is a protein called NADH-QUINONE OXIDOREDUCTASE SUBUNIT K.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	K	100	Total	C	N	O	S	0	0	0
			760	494	132	129	5			
4	G	100	Total	C	N	O	S	0	0	0
			760	494	132	129	5			

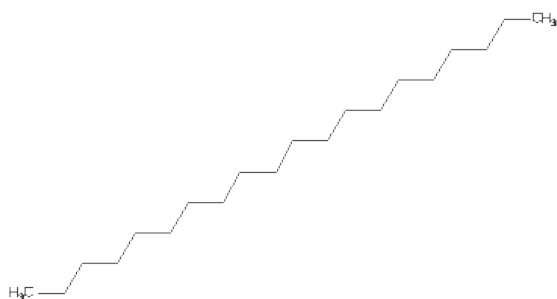
- Molecule 5 is a protein called NADH-QUINONE OXIDOREDUCTASE SUBUNIT A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	A	95	Total	C	N	O	S	0	0	0
			752	516	118	114	4			
5	E	95	Total	C	N	O	S	0	0	0
			752	516	118	114	4			

- Molecule 6 is a protein called NADH-QUINONE OXIDOREDUCTASE SUBUNIT J.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	J	168	Total	C	N	O	S	0	0	0
			1270	851	197	215	7			
6	F	168	Total	C	N	O	S	0	0	0
			1270	851	197	215	7			

- Molecule 7 is EICOSANE (three-letter code: LFA) (formula: C₂₀H₄₂).



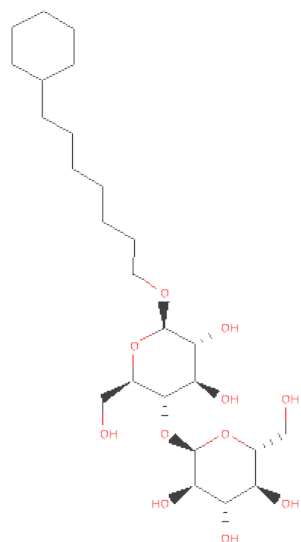
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	L	1	Total	C	0	0
			12	12		
7	L	1	Total	C	0	0
			14	14		
7	L	1	Total	C	0	0
			8	8		
7	M	1	Total	C	0	0
			14	14		
7	M	1	Total	C	0	0
			12	12		
7	N	1	Total	C	0	0
			12	12		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	N	1	Total C 14 14	0	0
7	N	1	Total C 12 12	0	0
7	N	1	Total C 12 12	0	0
7	B	1	Total C 12 12	0	0
7	B	1	Total C 14 14	0	0
7	B	1	Total C 8 8	0	0
7	C	1	Total C 14 14	0	0
7	C	1	Total C 12 12	0	0
7	C	1	Total C 12 12	0	0
7	D	1	Total C 14 14	0	0
7	D	1	Total C 12 12	0	0
7	D	1	Total C 12 12	0	0

- Molecule 8 is 7-CYCLOHEXYLHEPTYL 4-O-ALPHA-D-GLUCOPYRANOSYL-BETA-D-GLUCOPYRANOSIDE (three-letter code: CA7) (formula: C₂₅H₄₆O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	M	1	Total	C	O	0	0
			36	25	11		
8	C	1	Total	C	O	0	0
			36	25	11		

- Molecule 9 is water.

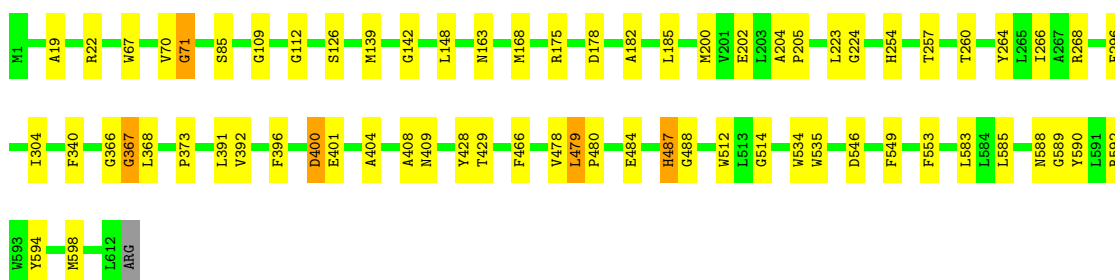
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	L	2	Total	O	0	0
			2	2		
9	M	2	Total	O	0	0
			2	2		
9	N	3	Total	O	0	0
			3	3		
9	K	1	Total	O	0	0
			1	1		
9	B	2	Total	O	0	0
			2	2		
9	C	2	Total	O	0	0
			2	2		
9	D	3	Total	O	0	0
			3	3		
9	G	1	Total	O	0	0
			1	1		

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.

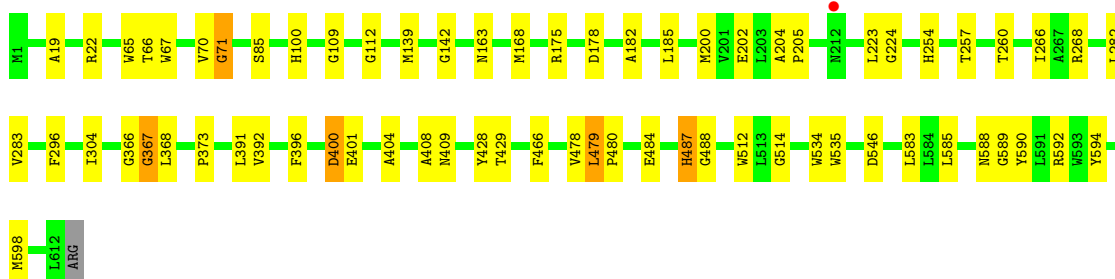
• Molecule 1: NADH-QUINONE OXIDOREDUCTASE SUBUNIT L

Chain L: 



• Molecule 1: NADH-QUINONE OXIDOREDUCTASE SUBUNIT L

Chain B: 



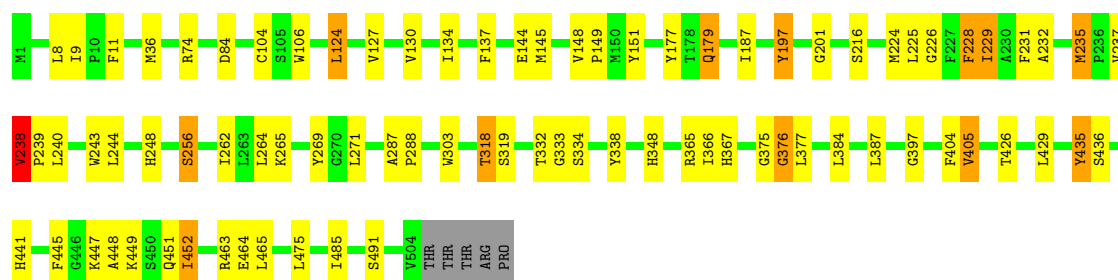
• Molecule 2: NADH-QUINONE OXIDOREDUCTASE SUBUNIT M

Chain M: 



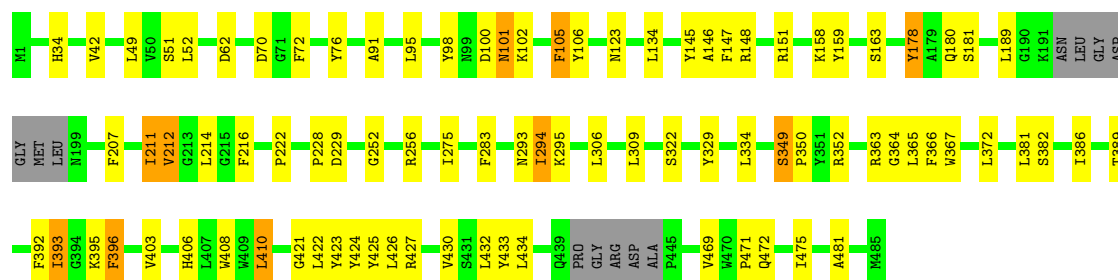
• Molecule 2: NADH-QUINONE OXIDOREDUCTASE SUBUNIT M

Chain C: 



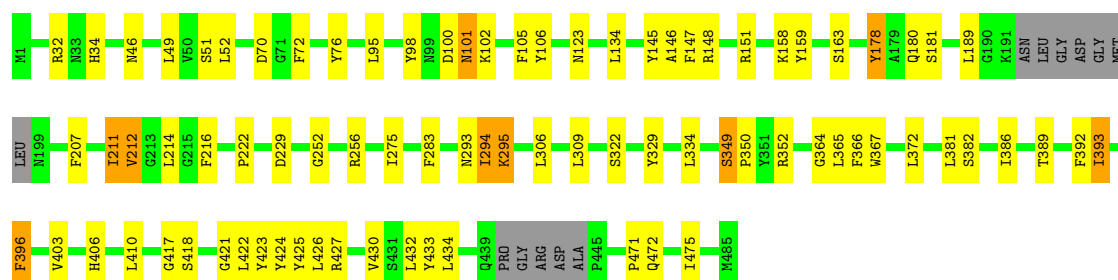
• Molecule 3: NADH-QUINONE OXIDOREDUCTASE SUBUNIT N

Chain N:



• Molecule 3: NADH-QUINONE OXIDOREDUCTASE SUBUNIT N

Chain D:



• Molecule 4: NADH-QUINONE OXIDOREDUCTASE SUBUNIT K

Chain K:



• Molecule 4: NADH-QUINONE OXIDOREDUCTASE SUBUNIT K

Chain G:



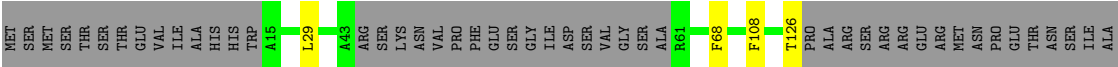
• Molecule 5: NADH-QUINONE OXIDOREDUCTASE SUBUNIT A

Chain A:



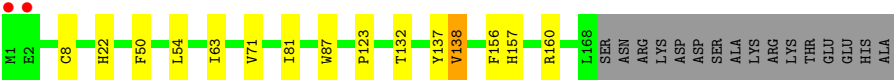
• Molecule 5: NADH-QUINONE OXIDOREDUCTASE SUBUNIT A

Chain E:



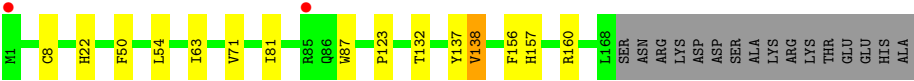
• Molecule 6: NADH-QUINONE OXIDOREDUCTASE SUBUNIT J

Chain J:



• Molecule 6: NADH-QUINONE OXIDOREDUCTASE SUBUNIT J

Chain F:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	94.98Å 116.57Å 191.37Å 98.51° 104.08° 108.51°	Depositor
Resolution (Å)	19.99 – 3.00 29.98 – 3.00	Depositor EDS
% Data completeness (in resolution range)	86.5 (19.99-3.00) 86.5 (29.98-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 3.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.232 , 0.282 0.228 , 0.275	Depositor DCC
R_{free} test set	2557 reflections (2.02%)	DCC
Wilson B-factor (Å ²)	58.1	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 39.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 126659 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	30310	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.29% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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: LFA, CA7

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	B	0.31	0/4797	0.49	0/6538
1	L	0.31	0/4797	0.49	0/6538
2	C	0.39	0/4074	0.58	1/5546 (0.0%)
2	M	0.39	0/4074	0.58	1/5546 (0.0%)
3	D	0.37	0/3678	0.58	0/5018
3	N	0.37	0/3678	0.58	0/5018
4	G	0.31	0/769	0.49	0/1040
4	K	0.31	0/769	0.49	0/1040
5	A	0.30	0/772	0.45	0/1046
5	E	0.30	0/772	0.45	0/1046
6	F	0.29	0/1296	0.48	0/1767
6	J	0.29	0/1296	0.48	0/1767
All	All	0.34	0/30772	0.54	2/41910 (0.0%)

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
2	C	0	1
2	M	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	124	LEU	CA-CB-CG	5.68	128.36	115.30
2	C	124	LEU	CA-CB-CG	5.44	127.81	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	238	VAL	Peptide
2	M	238	VAL	Peptide

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	B	4676	0	0	36	0
1	L	4676	0	0	40	0
2	C	3953	0	0	39	0
2	M	3953	0	0	42	0
3	D	3590	0	0	40	0
3	N	3590	0	0	44	0
4	G	760	0	0	5	0
4	K	760	0	0	5	0
5	A	752	0	0	1	0
5	E	752	0	0	2	0
6	F	1270	0	0	9	0
6	J	1270	0	0	7	0
7	B	34	0	65	5	0
7	C	38	0	73	4	0
7	D	38	0	73	1	0
7	L	34	0	65	12	0
7	M	26	0	50	6	0
7	N	50	0	96	3	0
8	C	36	0	46	3	0
8	M	36	0	46	6	0
9	B	2	0	0	0	0
9	C	2	0	0	0	0
9	D	3	0	0	0	0
9	G	1	0	0	0	0
9	K	1	0	0	0	0
9	L	2	0	0	0	0
9	M	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	N	3	0	0	0	0
All	All	30310	0	514	260	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 8.

All (260) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:19:ALA:O	7:L:615:LFA:H22	1.68	0.93
7:B:615:LFA:H21	7:C:513:LFA:H12	1.50	0.91
1:B:19:ALA:O	7:B:615:LFA:H22	1.74	0.87
2:M:387:LEU:CD2	7:M:512:LFA:H22	2.08	0.84
1:B:404:ALA:O	1:B:408:ALA:CB	2.27	0.83
1:L:404:ALA:O	1:L:408:ALA:CB	2.28	0.80
1:B:168:MET:CE	8:C:510:CA7:HALA	2.14	0.76
2:C:387:LEU:CD2	7:C:513:LFA:H22	2.20	0.71
7:B:615:LFA:C2	7:C:513:LFA:H12	2.21	0.69
2:M:435:TYR:CD1	2:M:436:SER:N	2.60	0.69
7:L:615:LFA:H21	7:M:512:LFA:H12	1.74	0.68
2:C:435:TYR:CD1	2:C:436:SER:N	2.62	0.67
2:C:228:PHE:O	2:C:231:PHE:N	2.29	0.66
2:M:228:PHE:O	2:M:231:PHE:N	2.29	0.65
7:L:615:LFA:C2	7:M:512:LFA:H12	2.27	0.65
1:L:200:MET:O	1:L:204:ALA:CB	2.46	0.64
1:B:487:HIS:ND1	1:B:488:GLY:N	2.46	0.64
1:L:487:HIS:ND1	1:L:488:GLY:N	2.45	0.64
2:M:434:VAL:CG2	8:M:510:CA7:HAM	2.28	0.63
2:M:232:ALA:CB	7:M:511:LFA:H12	2.29	0.63
1:B:200:MET:O	1:B:204:ALA:CB	2.46	0.63
1:B:22:ARG:NH1	7:B:615:LFA:H31	2.15	0.62
3:N:70:ASP:OD1	3:N:256:ARG:NH2	2.34	0.61
1:B:22:ARG:CG	7:B:615:LFA:H13	2.31	0.60
3:N:364:GLY:C	3:N:366:PHE:N	2.56	0.59
1:L:340:PHE:CE2	7:L:616:LFA:H31	2.37	0.59
3:D:70:ASP:OD1	3:D:256:ARG:NH2	2.35	0.59
3:N:95:LEU:O	3:N:98:TYR:N	2.36	0.58
3:D:101:ASN:ND2	6:F:160:ARG:NH2	2.51	0.58
3:D:95:LEU:O	3:D:98:TYR:N	2.37	0.57
2:M:262:ILE:O	2:M:265:LYS:N	2.38	0.57
3:D:364:GLY:C	3:D:366:PHE:N	2.58	0.56
3:N:101:ASN:ND2	6:J:160:ARG:NH2	2.53	0.56
2:C:262:ILE:O	2:C:265:LYS:N	2.39	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:232:ALA:CB	7:C:511:LFA:H12	2.36	0.56
3:N:349:SER:CB	3:N:350:PRO:CD	2.84	0.56
4:G:62:TYR:C	4:G:62:TYR:CD2	2.79	0.56
4:G:24:ILE:O	6:F:87:TRP:NE1	2.39	0.56
1:L:22:ARG:NH1	7:L:615:LFA:H31	2.22	0.55
1:L:428:TYR:CD1	1:L:429:THR:N	2.75	0.55
3:D:349:SER:CB	3:D:350:PRO:CD	2.85	0.55
1:L:22:ARG:CG	7:L:615:LFA:H13	2.37	0.55
1:B:479:LEU:N	1:B:480:PRO:CD	2.70	0.54
1:B:598:MET:SD	3:D:216:PHE:CD1	3.01	0.54
1:L:479:LEU:N	1:L:480:PRO:CD	2.70	0.54
1:L:257:THR:O	1:L:260:THR:OG1	2.25	0.54
4:K:24:ILE:O	6:J:87:TRP:NE1	2.40	0.54
1:B:592:ARG:NH1	6:F:87:TRP:CZ2	2.76	0.54
1:B:257:THR:O	1:B:260:THR:OG1	2.26	0.54
1:B:428:TYR:CD1	1:B:429:THR:N	2.76	0.54
2:C:319:SER:OG	2:C:348:HIS:CE1	2.61	0.53
3:N:309:LEU:CD2	3:N:329:TYR:CD2	2.92	0.53
2:C:244:LEU:CD1	2:C:248:HIS:CE1	2.91	0.53
2:M:319:SER:OG	2:M:348:HIS:CE1	2.61	0.53
3:D:309:LEU:CD2	3:D:329:TYR:CD2	2.90	0.53
1:B:478:VAL:O	1:B:479:LEU:CB	2.57	0.53
1:L:478:VAL:O	1:L:479:LEU:CB	2.57	0.53
2:M:244:LEU:CD1	2:M:248:HIS:CE1	2.92	0.53
1:L:598:MET:SD	3:N:216:PHE:CD1	3.01	0.53
1:L:553:PHE:CE2	8:M:510:CA7:HAJ	2.44	0.53
4:K:62:TYR:C	4:K:62:TYR:CD2	2.82	0.53
1:L:340:PHE:CZ	7:L:616:LFA:H31	2.44	0.53
2:C:441:HIS:ND1	2:C:445:PHE:CD2	2.77	0.52
4:K:25:ARG:NH2	6:J:22:HIS:O	2.42	0.52
4:G:25:ARG:NH2	6:F:22:HIS:O	2.42	0.52
2:M:441:HIS:ND1	2:M:445:PHE:CD2	2.78	0.52
3:N:180:GLN:OE1	3:N:181:SER:OG	2.28	0.52
3:N:364:GLY:O	3:N:366:PHE:N	2.43	0.52
3:N:471:PRO:O	3:N:472:GLN:C	2.48	0.52
3:D:216:PHE:CD2	3:D:216:PHE:C	2.84	0.51
3:D:471:PRO:O	3:D:472:GLN:C	2.48	0.51
2:M:332:THR:O	2:M:334:SER:N	2.43	0.51
5:A:68:PHE:CE1	5:A:126:THR:C	2.84	0.51
3:D:392:PHE:CD2	3:D:392:PHE:C	2.81	0.51
5:E:68:PHE:CE1	5:E:126:THR:C	2.84	0.50
3:N:283:PHE:CD1	3:N:283:PHE:N	2.79	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:N:216:PHE:C	3:N:216:PHE:CD2	2.84	0.50
3:D:283:PHE:CD1	3:D:283:PHE:N	2.79	0.50
3:N:392:PHE:CD2	3:N:392:PHE:C	2.82	0.50
3:D:180:GLN:OE1	3:D:181:SER:OG	2.29	0.49
3:D:211:ILE:O	3:D:212:VAL:C	2.50	0.49
2:C:228:PHE:O	2:C:229:ILE:C	2.50	0.49
2:M:228:PHE:O	2:M:229:ILE:C	2.51	0.49
3:N:158:LYS:NZ	3:N:229:ASP:OD2	2.46	0.49
3:D:364:GLY:O	3:D:366:PHE:N	2.46	0.49
2:C:375:GLY:O	2:C:377:LEU:N	2.46	0.48
3:D:72:PHE:CD1	3:D:256:ARG:NH1	2.81	0.48
2:C:287:ALA:N	2:C:288:PRO:CD	2.77	0.47
2:C:332:THR:O	2:C:334:SER:N	2.47	0.47
1:L:366:GLY:O	1:L:367:GLY:C	2.52	0.47
2:M:287:ALA:N	2:M:288:PRO:CD	2.77	0.47
3:D:293:ASN:O	3:D:294:ILE:C	2.53	0.47
1:B:85:SER:OG	1:B:268:ARG:NH1	2.48	0.47
1:B:366:GLY:O	1:B:367:GLY:C	2.52	0.47
3:N:211:ILE:O	3:N:212:VAL:C	2.50	0.47
1:L:139:MET:O	1:L:142:GLY:N	2.47	0.47
1:B:484:GLU:N	1:B:484:GLU:CD	2.67	0.47
3:D:145:TYR:CD1	6:F:157:HIS:NE2	2.83	0.47
3:D:158:LYS:NZ	3:D:229:ASP:OD2	2.47	0.47
1:B:139:MET:O	1:B:142:GLY:N	2.48	0.47
3:D:178:TYR:C	3:D:178:TYR:CD2	2.89	0.47
3:N:293:ASN:O	3:N:294:ILE:C	2.52	0.47
1:L:223:LEU:O	1:L:224:GLY:C	2.53	0.47
1:L:592:ARG:NH1	6:J:87:TRP:CZ2	2.83	0.46
2:C:451:GLN:OE1	2:C:452:ILE:N	2.48	0.46
2:M:137:PHE:CE1	3:N:396:PHE:CE1	3.03	0.46
1:B:223:LEU:O	1:B:224:GLY:C	2.52	0.46
3:D:426:LEU:O	3:D:427:ARG:C	2.54	0.46
3:N:178:TYR:C	3:N:178:TYR:CD2	2.88	0.46
1:L:484:GLU:CD	1:L:484:GLU:N	2.69	0.46
2:M:451:GLN:OE1	2:M:452:ILE:N	2.48	0.46
3:N:426:LEU:O	3:N:427:ARG:C	2.54	0.46
3:D:106:TYR:N	3:D:106:TYR:CD1	2.84	0.46
1:B:202:GLU:O	1:B:205:PRO:CD	2.64	0.46
2:M:375:GLY:O	2:M:377:LEU:N	2.48	0.46
2:C:237:VAL:CG1	2:C:238:VAL:N	2.79	0.45
3:N:106:TYR:N	3:N:106:TYR:CD1	2.84	0.45
3:D:364:GLY:O	3:D:432:LEU:O	2.34	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:466:PHE:CD2	1:L:466:PHE:C	2.90	0.45
1:L:85:SER:OG	1:L:268:ARG:NH1	2.49	0.45
3:D:403:VAL:O	3:D:406:HIS:N	2.50	0.45
3:N:424:TYR:CE1	3:N:425:TYR:CE2	3.05	0.45
7:L:615:LFA:H32	2:M:386:ALA:CB	2.47	0.45
1:B:466:PHE:CD2	1:B:466:PHE:C	2.91	0.45
2:M:237:VAL:CG1	2:M:238:VAL:N	2.80	0.45
1:L:202:GLU:O	1:L:205:PRO:CD	2.64	0.45
4:K:61:MET:O	4:K:64:LEU:N	2.50	0.45
1:B:588:ASN:O	1:B:590:TYR:N	2.50	0.45
1:L:67:TRP:O	1:L:67:TRP:CD1	2.70	0.44
2:C:447:LYS:O	2:C:449:LYS:N	2.50	0.44
2:M:235:MET:O	2:M:264:LEU:CD2	2.65	0.44
2:C:235:MET:O	2:C:264:LEU:CD2	2.66	0.44
3:N:364:GLY:O	3:N:432:LEU:O	2.35	0.44
2:C:375:GLY:O	2:C:376:GLY:C	2.56	0.44
3:D:424:TYR:CE1	3:D:425:TYR:CE2	3.05	0.44
2:M:197:TYR:O	2:M:201:GLY:N	2.51	0.44
2:C:137:PHE:CE1	3:D:396:PHE:CE1	3.05	0.44
1:L:549:PHE:CE1	7:L:614:LFA:H81	2.53	0.44
2:M:447:LYS:O	2:M:449:LYS:N	2.50	0.44
1:L:168:MET:CE	8:M:510:CA7:HAL	2.47	0.44
3:D:364:GLY:CA	3:D:367:TRP:CD1	3.01	0.44
1:B:67:TRP:O	1:B:67:TRP:CD1	2.71	0.44
2:M:365:ARG:NH2	2:M:464:GLU:OE1	2.51	0.44
1:B:296:PHE:CD1	1:B:535:TRP:CH2	3.06	0.44
3:N:159:TYR:O	3:N:163:SER:CB	2.66	0.44
2:M:8:LEU:O	2:M:11:PHE:N	2.50	0.43
1:L:182:ALA:O	1:L:185:LEU:N	2.51	0.43
2:C:404:PHE:O	2:C:405:VAL:C	2.56	0.43
2:M:11:PHE:CZ	2:M:145:MET:SD	3.11	0.43
6:F:50:PHE:O	6:F:54:LEU:CB	2.66	0.43
3:N:49:LEU:O	3:N:52:LEU:N	2.51	0.43
2:C:365:ARG:NH2	2:C:464:GLU:OE1	2.51	0.43
6:J:50:PHE:O	6:J:54:LEU:CB	2.67	0.43
1:L:296:PHE:CD1	1:L:535:TRP:CH2	3.06	0.43
1:L:168:MET:CE	8:M:510:CA7:CAL	2.95	0.43
1:L:588:ASN:O	1:L:590:TYR:N	2.51	0.43
2:C:366:ILE:O	2:C:367:HIS:C	2.56	0.43
2:M:366:ILE:O	2:M:367:HIS:C	2.57	0.43
1:L:553:PHE:CD2	8:M:510:CA7:HASA	2.53	0.43
2:M:445:PHE:O	8:M:510:CA7:H4	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:N:76:TYR:CE2	3:N:252:GLY:CA	3.01	0.43
3:D:381:LEU:O	3:D:382:SER:C	2.57	0.43
3:D:49:LEU:O	3:D:52:LEU:N	2.51	0.43
3:D:159:TYR:O	3:D:163:SER:CB	2.66	0.43
2:C:197:TYR:O	2:C:201:GLY:N	2.51	0.43
3:D:46:ASN:ND2	7:D:486:LFA:H111	2.33	0.43
3:N:364:GLY:CA	3:N:367:TRP:CD1	3.02	0.43
3:D:145:TYR:CE1	6:F:157:HIS:CE1	3.07	0.43
3:D:146:ALA:O	3:D:148:ARG:N	2.52	0.43
3:N:145:TYR:CD1	6:J:157:HIS:NE2	2.86	0.43
3:N:386:ILE:O	3:N:389:THR:OG1	2.36	0.43
1:B:400:ASP:O	1:B:401:GLU:C	2.57	0.43
7:L:615:LFA:H21	7:M:512:LFA:H32	2.01	0.43
2:C:177:TYR:CD1	2:C:243:TRP:CD1	3.07	0.43
3:N:408:TRP:CZ2	7:N:486:LFA:H62	2.54	0.43
2:C:144:GLU:CD	2:C:179:GLN:NE2	2.72	0.43
2:C:148:VAL:CB	2:C:149:PRO:CD	2.96	0.43
4:G:61:MET:O	4:G:64:LEU:N	2.52	0.43
3:D:386:ILE:O	3:D:389:THR:OG1	2.37	0.43
3:N:146:ALA:O	3:N:148:ARG:N	2.52	0.43
2:C:127:VAL:O	2:C:130:VAL:N	2.52	0.43
1:L:396:PHE:CE2	1:L:400:ASP:OD2	2.72	0.42
2:C:338:TYR:CD1	2:C:338:TYR:N	2.87	0.42
2:M:426:THR:O	2:M:429:LEU:CB	2.67	0.42
3:D:294:ILE:CG2	3:D:295:LYS:N	2.82	0.42
2:C:8:LEU:O	2:C:11:PHE:N	2.52	0.42
1:B:182:ALA:O	1:B:185:LEU:N	2.52	0.42
2:M:404:PHE:O	2:M:405:VAL:C	2.57	0.42
1:B:396:PHE:CE2	1:B:400:ASP:OD2	2.73	0.42
2:C:426:THR:O	2:C:429:LEU:CB	2.68	0.42
3:N:42:VAL:CG2	7:N:487:LFA:H72	2.49	0.42
6:F:137:TYR:O	6:F:138:VAL:C	2.57	0.42
3:N:430:VAL:O	3:N:433:TYR:N	2.53	0.42
3:N:381:LEU:O	3:N:382:SER:C	2.57	0.42
1:L:202:GLU:C	1:L:204:ALA:N	2.73	0.42
2:M:375:GLY:O	2:M:376:GLY:C	2.56	0.42
2:M:8:LEU:O	2:M:9:ILE:C	2.58	0.42
2:C:11:PHE:CZ	2:C:145:MET:SD	3.13	0.42
2:C:124:LEU:O	2:C:127:VAL:CG1	2.67	0.42
3:D:430:VAL:O	3:D:433:TYR:N	2.53	0.42
3:D:76:TYR:CE2	3:D:252:GLY:CA	3.03	0.42
3:N:62:ASP:OD1	2:C:451:GLN:OE1	2.38	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:M:148:VAL:CB	2:M:149:PRO:CD	2.97	0.42
2:M:318:THR:CG2	2:M:319:SER:N	2.82	0.42
2:M:295:VAL:CG2	2:M:296:ILE:N	2.83	0.42
3:N:91:ALA:CB	3:N:105:PHE:CE2	3.03	0.42
1:B:583:LEU:O	1:B:585:LEU:N	2.53	0.42
3:N:403:VAL:O	3:N:406:HIS:N	2.52	0.42
3:N:72:PHE:CD1	3:N:256:ARG:NH1	2.87	0.42
3:N:228:PRO:O	3:N:229:ASP:C	2.58	0.42
4:G:50:GLY:O	4:G:53:TRP:O	2.38	0.42
1:L:512:TRP:O	1:L:514:GLY:N	2.53	0.42
1:L:175:ARG:O	1:L:178:ASP:N	2.53	0.42
2:C:248:HIS:CD2	2:C:256:SER:OG	2.73	0.41
2:M:248:HIS:CD2	2:M:256:SER:OG	2.73	0.41
2:M:333:GLY:O	2:M:334:SER:C	2.58	0.41
1:L:70:VAL:CG1	1:L:71:GLY:N	2.83	0.41
1:L:594:TYR:N	1:L:594:TYR:CD2	2.88	0.41
2:M:124:LEU:O	2:M:127:VAL:CG1	2.68	0.41
3:D:421:GLY:O	3:D:422:LEU:C	2.58	0.41
2:M:151:TYR:C	2:M:151:TYR:CD2	2.93	0.41
2:C:151:TYR:C	2:C:151:TYR:CD2	2.93	0.41
1:B:70:VAL:CG1	1:B:71:GLY:N	2.83	0.41
1:B:592:ARG:CZ	6:F:87:TRP:CZ2	3.03	0.41
3:N:392:PHE:O	3:N:395:LYS:N	2.53	0.41
1:B:512:TRP:O	1:B:514:GLY:N	2.52	0.41
1:L:400:ASP:O	1:L:401:GLU:C	2.57	0.41
2:M:225:LEU:O	2:M:226:GLY:C	2.59	0.41
2:C:318:THR:CG2	2:C:319:SER:N	2.83	0.41
2:C:145:MET:O	2:C:149:PRO:CD	2.68	0.41
6:J:137:TYR:O	6:J:138:VAL:C	2.58	0.41
8:C:510:CA7:HAJA	8:C:510:CA7:HALA	1.86	0.41
1:B:583:LEU:C	1:B:585:LEU:N	2.73	0.41
3:N:469:VAL:CG1	3:N:469:VAL:O	2.68	0.41
3:N:481:ALA:CB	7:N:488:LFA:H72	2.51	0.41
1:B:202:GLU:C	1:B:204:ALA:N	2.74	0.41
2:C:8:LEU:O	2:C:9:ILE:C	2.59	0.41
3:D:393:ILE:N	3:D:393:ILE:CD1	2.83	0.41
3:D:32:ARG:NH1	3:D:101:ASN:CB	2.84	0.41
1:L:583:LEU:C	1:L:585:LEU:N	2.74	0.41
1:B:65:TRP:CD1	1:B:66:THR:N	2.89	0.41
1:B:594:TYR:N	1:B:594:TYR:CD2	2.89	0.41
3:N:421:GLY:O	3:N:422:LEU:C	2.58	0.41
1:L:148:LEU:CD2	7:L:615:LFA:H122	2.51	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:M:283:SER:O	2:M:286:PHE:N	2.54	0.41
3:N:393:ILE:CD1	3:N:393:ILE:N	2.84	0.41
2:M:338:TYR:N	2:M:338:TYR:CD1	2.89	0.40
2:M:144:GLU:CD	2:M:179:GLN:NE2	2.74	0.40
2:C:445:PHE:O	8:C:510:CA7:H4	2.22	0.40
3:N:410:LEU:N	3:N:410:LEU:CD2	2.85	0.40
7:L:615:LFA:C1	7:M:512:LFA:H12	2.50	0.40
2:M:127:VAL:O	2:M:130:VAL:N	2.54	0.40
3:D:417:GLY:O	3:D:418:SER:C	2.59	0.40
5:E:108:PHE:C	5:E:108:PHE:CD2	2.95	0.40
1:L:583:LEU:O	1:L:585:LEU:N	2.54	0.40
1:B:175:ARG:O	1:B:178:ASP:N	2.55	0.40
2:C:225:LEU:O	2:C:226:GLY:C	2.58	0.40
2:M:145:MET:O	2:M:149:PRO:CD	2.70	0.40
1:B:282:LEU:O	1:B:283:VAL:C	2.60	0.40
4:K:50:GLY:O	4:K:53:TRP:O	2.39	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	B	610/613 (100%)	515 (84%)	85 (14%)	10 (2%)	14	56
1	L	610/613 (100%)	514 (84%)	86 (14%)	10 (2%)	14	56
2	C	502/509 (99%)	412 (82%)	77 (15%)	13 (3%)	8	39
2	M	502/509 (99%)	408 (81%)	80 (16%)	14 (3%)	8	37
3	D	467/485 (96%)	359 (77%)	90 (19%)	18 (4%)	5	26
3	N	467/485 (96%)	358 (77%)	90 (19%)	19 (4%)	4	24
4	G	98/100 (98%)	87 (89%)	10 (10%)	1 (1%)	22	70
4	K	98/100 (98%)	87 (89%)	9 (9%)	2 (2%)	11	48
5	A	91/147 (62%)	82 (90%)	9 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	91/147 (62%)	82 (90%)	9 (10%)	0	100	100
6	F	166/184 (90%)	140 (84%)	23 (14%)	3 (2%)	13	53
6	J	166/184 (90%)	140 (84%)	23 (14%)	3 (2%)	13	53
All	All	3868/4076 (95%)	3184 (82%)	591 (15%)	93 (2%)	9	42

All (93) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	392	VAL
1	L	479	LEU
2	M	239	PRO
3	N	294	ILE
3	N	434	LEU
1	B	392	VAL
1	B	479	LEU
2	C	239	PRO
3	D	294	ILE
3	D	434	LEU
1	L	367	GLY
2	M	228	PHE
2	M	333	GLY
2	M	376	GLY
2	M	397	GLY
3	N	349	SER
1	B	367	GLY
2	C	228	PHE
2	C	229	ILE
2	C	333	GLY
2	C	397	GLY
3	D	349	SER
2	M	106	TRP
2	M	229	ILE
2	M	452	ILE
3	N	100	ASP
3	N	105	PHE
3	N	151	ARG
3	N	334	LEU
6	J	123	PRO
2	C	106	TRP
2	C	376	GLY
2	C	448	ALA

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Mol	Chain	Res	Type
2	C	452	ILE
3	D	100	ASP
3	D	105	PHE
3	D	151	ARG
3	D	334	LEU
6	F	123	PRO
1	L	112	GLY
1	L	373	PRO
2	M	448	ALA
2	M	491	SER
3	N	34	HIS
3	N	147	PHE
3	N	322	SER
3	N	363	ARG
3	N	396	PHE
4	K	88	GLN
1	B	112	GLY
1	B	373	PRO
3	D	147	PHE
3	D	295	LYS
3	D	322	SER
3	D	396	PHE
4	G	88	GLN
1	L	400	ASP
2	M	372	ARG
2	M	465	LEU
3	N	212	VAL
3	N	295	LYS
1	B	400	ASP
2	C	463	ARG
2	C	491	SER
3	D	34	HIS
3	D	212	VAL
2	M	463	ARG
3	N	423	TYR
4	K	74	SER
2	C	465	LEU
3	D	423	TYR
1	L	71	GLY
2	M	405	VAL
3	N	275	ILE
3	N	393	ILE

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Mol	Chain	Res	Type
3	N	475	ILE
1	B	71	GLY
1	B	109	GLY
1	B	589	GLY
3	D	275	ILE
3	D	475	ILE
1	L	109	GLY
1	L	589	GLY
3	N	211	ILE
2	C	405	VAL
3	D	211	ILE
6	F	138	VAL
1	L	304	ILE
6	J	138	VAL
3	D	393	ILE
6	J	63	ILE
1	B	304	ILE
6	F	63	ILE

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	B	485/486 (100%)	475 (98%)	10 (2%)	66	94
1	L	485/486 (100%)	474 (98%)	11 (2%)	63	93
2	C	413/418 (99%)	391 (95%)	22 (5%)	32	74
2	M	413/418 (99%)	391 (95%)	22 (5%)	32	74
3	D	377/385 (98%)	362 (96%)	15 (4%)	42	84
3	N	377/385 (98%)	362 (96%)	15 (4%)	42	84
4	G	79/79 (100%)	78 (99%)	1 (1%)	80	96
4	K	79/79 (100%)	77 (98%)	2 (2%)	60	92
5	A	73/119 (61%)	72 (99%)	1 (1%)	78	96
5	E	73/119 (61%)	72 (99%)	1 (1%)	78	96
6	F	132/146 (90%)	127 (96%)	5 (4%)	44	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	J	132/146 (90%)	127 (96%)	5 (4%)	44 85
All	All	3118/3266 (96%)	3008 (96%)	110 (4%)	48 87

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	126	SER
1	L	163	ASN
1	L	254	HIS
1	L	264	TYR
1	L	266	ILE
1	L	368	LEU
1	L	391	LEU
1	L	409	ASN
1	L	487	HIS
1	L	534	TRP
1	L	546	ASP
2	M	74	ARG
2	M	84	ASP
2	M	104	CYS
2	M	134	ILE
2	M	179	GLN
2	M	187	ILE
2	M	197	TYR
2	M	216	SER
2	M	224	MET
2	M	235	MET
2	M	238	VAL
2	M	240	LEU
2	M	256	SER
2	M	269	TYR
2	M	271	LEU
2	M	303	TRP
2	M	318	THR
2	M	384	LEU
2	M	435	TYR
2	M	475	LEU
2	M	485	ILE
2	M	497	GLN
3	N	51	SER
3	N	101	ASN
3	N	102	LYS

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Mol	Chain	Res	Type
3	N	123	ASN
3	N	134	LEU
3	N	178	TYR
3	N	189	LEU
3	N	207	PHE
3	N	214	LEU
3	N	222	PRO
3	N	306	LEU
3	N	352	ARG
3	N	365	LEU
3	N	372	LEU
3	N	410	LEU
4	K	46	PHE
4	K	47	VAL
5	A	29	LEU
6	J	8	CYS
6	J	71	VAL
6	J	81	ILE
6	J	132	THR
6	J	156	PHE
1	B	100	HIS
1	B	163	ASN
1	B	254	HIS
1	B	266	ILE
1	B	368	LEU
1	B	391	LEU
1	B	409	ASN
1	B	487	HIS
1	B	534	TRP
1	B	546	ASP
2	C	36	MET
2	C	74	ARG
2	C	84	ASP
2	C	104	CYS
2	C	134	ILE
2	C	179	GLN
2	C	187	ILE
2	C	197	TYR
2	C	216	SER
2	C	224	MET
2	C	235	MET
2	C	238	VAL

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Mol	Chain	Res	Type
2	C	240	LEU
2	C	256	SER
2	C	269	TYR
2	C	271	LEU
2	C	303	TRP
2	C	318	THR
2	C	384	LEU
2	C	435	TYR
2	C	475	LEU
2	C	485	ILE
3	D	51	SER
3	D	101	ASN
3	D	102	LYS
3	D	123	ASN
3	D	134	LEU
3	D	178	TYR
3	D	189	LEU
3	D	207	PHE
3	D	214	LEU
3	D	222	PRO
3	D	306	LEU
3	D	352	ARG
3	D	365	LEU
3	D	372	LEU
3	D	410	LEU
4	G	46	PHE
5	E	29	LEU
6	F	8	CYS
6	F	71	VAL
6	F	81	ILE
6	F	132	THR
6	F	156	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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 ⓘ

20 ligands are modelled in this entry.

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	$\# Z > 2$
7	LFA	B	614	-	11,11,19	0.67	0	10,10,18	0.67	0
7	LFA	B	615	-	13,13,19	0.52	0	12,12,18	0.73	0
7	LFA	B	616	-	7,7,19	1.46	1 (14%)	6,6,18	0.46	0
8	CA7	C	510	-	38,38,38	0.87	3 (7%)	51,51,51	1.60	7 (13%)
7	LFA	C	511	-	13,13,19	0.66	0	12,12,18	0.79	0
7	LFA	C	512	-	11,11,19	0.61	0	10,10,18	0.78	0
7	LFA	C	513	-	11,11,19	1.32	1 (9%)	10,10,18	0.87	0
7	LFA	D	486	-	13,13,19	0.96	1 (7%)	12,12,18	0.64	0
7	LFA	D	487	-	11,11,19	0.90	1 (9%)	10,10,18	0.72	0
7	LFA	D	488	-	11,11,19	1.93	1 (9%)	10,10,18	0.99	0
7	LFA	L	614	-	11,11,19	0.48	0	10,10,18	0.60	0
7	LFA	L	615	-	13,13,19	0.62	0	12,12,18	0.65	0
7	LFA	L	616	-	7,7,19	1.38	1 (14%)	6,6,18	0.51	0
8	CA7	M	510	-	38,38,38	0.94	1 (2%)	51,51,51	1.79	10 (19%)
7	LFA	M	511	-	13,13,19	0.58	0	12,12,18	0.71	0
7	LFA	M	512	-	11,11,19	1.50	1 (9%)	10,10,18	0.89	0
7	LFA	N	486	-	11,11,19	0.70	0	10,10,18	0.78	0
7	LFA	N	487	-	13,13,19	0.81	1 (7%)	12,12,18	0.63	0
7	LFA	N	488	-	11,11,19	0.82	1 (9%)	10,10,18	0.75	0
7	LFA	N	489	-	11,11,19	2.11	1 (9%)	10,10,18	1.07	1 (10%)

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
7	LFA	B	614	-	-	0/9/9/17	0/0/0/0
7	LFA	B	615	-	-	0/11/11/17	0/0/0/0
7	LFA	B	616	-	-	0/5/5/17	0/0/0/0
8	CA7	C	510	-	-	0/19/67/67	0/3/3/3
7	LFA	C	511	-	-	0/11/11/17	0/0/0/0
7	LFA	C	512	-	-	0/9/9/17	0/0/0/0
7	LFA	C	513	-	-	0/9/9/17	0/0/0/0
7	LFA	D	486	-	-	0/11/11/17	0/0/0/0
7	LFA	D	487	-	-	0/9/9/17	0/0/0/0
7	LFA	D	488	-	-	0/9/9/17	0/0/0/0
7	LFA	L	614	-	-	0/9/9/17	0/0/0/0
7	LFA	L	615	-	-	0/11/11/17	0/0/0/0
7	LFA	L	616	-	-	0/5/5/17	0/0/0/0
8	CA7	M	510	-	-	0/19/67/67	0/3/3/3
7	LFA	M	511	-	-	0/11/11/17	0/0/0/0
7	LFA	M	512	-	-	0/9/9/17	0/0/0/0
7	LFA	N	486	-	-	0/9/9/17	0/0/0/0
7	LFA	N	487	-	-	0/11/11/17	0/0/0/0
7	LFA	N	488	-	-	0/9/9/17	0/0/0/0
7	LFA	N	489	-	-	0/9/9/17	0/0/0/0

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	N	489	LFA	C12-C11	-6.90	1.52	1.55
7	D	488	LFA	C12-C11	-6.28	1.52	1.55
7	M	512	LFA	C12-C11	-4.86	1.53	1.55
7	C	513	LFA	C12-C11	-4.24	1.53	1.55
7	B	616	LFA	C8-C7	-3.62	1.53	1.55
7	L	616	LFA	C8-C7	-3.45	1.53	1.55
8	M	510	CA7	OAX-CBH	3.30	1.46	1.40
7	D	486	LFA	C14-C13	-3.16	1.53	1.55
7	D	487	LFA	C12-C11	-2.64	1.54	1.55
7	N	487	LFA	C14-C13	-2.63	1.54	1.55
8	C	510	CA7	CAT-CAZ	2.39	1.58	1.52
7	N	488	LFA	C12-C11	-2.33	1.54	1.55
8	C	510	CA7	OAX-CBH	2.22	1.44	1.40
8	C	510	CA7	O5-C1	2.04	1.47	1.41

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	510	CA7	CAR-CBB-CBJ	-6.23	95.72	113.25
8	C	510	CA7	OAV-CBH-CBF	-5.22	99.61	110.31
8	M	510	CA7	OAV-CBB-CAR	-4.54	95.19	106.34
8	C	510	CA7	O5-C5-C6	4.04	116.27	106.34
8	C	510	CA7	O1-CBJ-CBG	3.92	117.22	107.16
8	M	510	CA7	OAX-CBH-CBF	3.58	112.73	108.18
8	M	510	CA7	O5-C5-C6	3.55	115.07	106.34
8	C	510	CA7	C6-C5-C4	-3.00	105.75	113.00
7	N	489	LFA	C12-C11-C10	-2.52	108.80	114.46
8	C	510	CA7	OAX-CBH-CBF	-2.44	105.07	108.18
8	M	510	CA7	OAV-CBB-CBJ	2.43	114.77	109.70
8	C	510	CA7	OAG-CBG-CBF	-2.14	105.54	110.35
8	C	510	CA7	O1-CBJ-CBB	2.14	114.90	109.33
8	M	510	CA7	C1-C2-C3	2.14	114.16	110.00
8	M	510	CA7	O1-CBJ-CBG	2.13	112.64	107.16
8	M	510	CA7	OAG-CBG-CBF	-2.08	105.69	110.35
8	M	510	CA7	O1-CBJ-CBB	2.05	114.66	109.33
8	M	510	CA7	CAP-OAX-CBH	2.04	117.63	113.96

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	B	612/613 (99%)	-0.46	1 (0%) 93 54	35, 81, 131, 196	0
1	L	612/613 (99%)	-0.45	0 100 100	35, 83, 131, 196	0
2	C	504/509 (99%)	-0.56	0 100 100	16, 56, 107, 181	0
2	M	504/509 (99%)	-0.57	0 100 100	14, 56, 107, 184	0
3	D	473/485 (97%)	-0.54	0 100 100	17, 58, 113, 201	0
3	N	473/485 (97%)	-0.56	0 100 100	15, 57, 111, 202	0
4	G	100/100 (100%)	-0.44	0 100 100	43, 80, 127, 166	0
4	K	100/100 (100%)	-0.37	0 100 100	39, 79, 127, 166	0
5	A	95/147 (64%)	-0.36	0 100 100	53, 93, 152, 178	0
5	E	95/147 (64%)	-0.19	0 100 100	57, 94, 153, 179	0
6	F	168/184 (91%)	-0.27	2 (1%) 75 20	49, 98, 165, 192	0
6	J	168/184 (91%)	-0.27	2 (1%) 75 20	51, 96, 160, 186	0
All	All	3904/4076 (95%)	-0.48	5 (0%) 93 63	14, 72, 133, 202	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	J	1	MET	2.7
1	B	212	ASN	2.6
6	F	1	MET	2.4
6	J	2	GLU	2.2
6	F	85	ARG	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
7	LFA	L	614	12/20	0.20	7.16	23,66,140,147	0
7	LFA	N	488	12/20	0.25	4.05	22,50,94,102	0
7	LFA	D	488	12/20	0.22	3.69	19,78,116,133	0
7	LFA	D	487	12/20	0.24	3.65	13,44,101,112	0
7	LFA	C	513	12/20	0.38	2.75	56,96,117,119	0
7	LFA	C	512	12/20	0.19	2.46	24,60,65,69	0
7	LFA	B	616	8/20	0.26	1.94	24,73,104,123	0
7	LFA	C	511	14/20	0.22	1.68	11,46,79,83	0
7	LFA	N	486	12/20	0.18	1.67	23,40,69,85	0
7	LFA	M	512	12/20	0.33	1.60	47,75,111,115	0
7	LFA	M	511	14/20	0.18	1.45	7,54,73,82	0
7	LFA	B	614	12/20	0.17	1.41	14,66,119,129	0
7	LFA	N	487	14/20	0.20	0.95	19,75,100,101	0
7	LFA	D	486	14/20	0.23	0.95	27,63,118,118	0
8	CA7	M	510	36/36	0.16	0.87	12,97,165,215	0
7	LFA	N	489	12/20	0.16	0.67	6,75,116,122	0
7	LFA	L	616	8/20	0.22	0.66	52,61,96,118	0
7	LFA	B	615	14/20	0.19	0.59	23,50,100,103	0
8	CA7	C	510	36/36	0.13	0.53	20,82,148,192	0
7	LFA	L	615	14/20	0.19	0.45	25,65,116,119	0

6.5 Other polymers ⓘ

There are no such residues in this entry.