



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 09:03 PM GMT

PDB ID : 1KGB
Title : structure of ground-state bacteriorhodopsin
Authors : Facciotti, M.T.; Rouhani, S.; Burkard, F.T.; Betancourt, F.M.; Downing, K.H.; Rose, R.B.; McDermott, G.; Glaeser, R.M.
Deposited on : 2001-11-26
Resolution : 1.65 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>

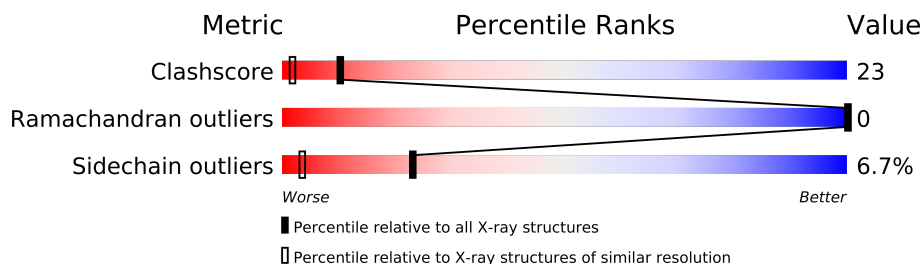
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
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 1.65 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))
Clashscore	79885	1001 (1.66-1.66)
Ramachandran outliers	78287	1581 (1.68-1.64)
Sidechain outliers	78261	1580 (1.68-1.64)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	231	

2 Entry composition i

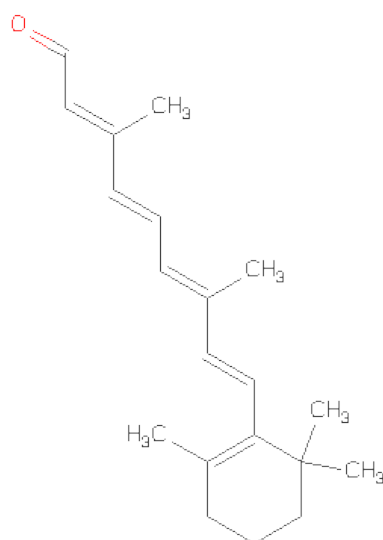
There are 4 unique types of molecules in this entry. The entry contains 2050 atoms, of which 0 are hydrogen and 0 are deuterium.

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 bacteriorhodopsin.

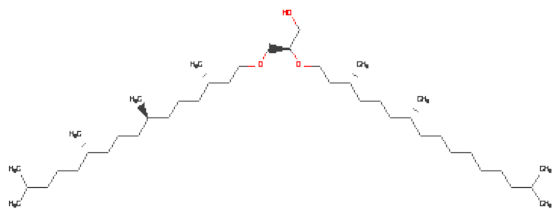
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	222	Total	C	N	O	S	0	0	0
			1720	1159	262	290	9			

- Molecule 2 is RETINAL (three-letter code: RET) (formula: C₂₀H₂₈O).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	C	0	0
			20	20		

- Molecule 3 is 1-[2,6,10,14-TETRAMETHYL-HEXADECAN-16-YL]-2-[2,10,14-TRIMETHYLHEXADECAN-16-YL]GLYCEROL (three-letter code: LI1) (formula: C₄₂H₈₆O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			32	29	3		
3	A	1	Total	C	O	0	0
			41	38	3		
3	A	1	Total	C		0	0
			16	16			
3	A	1	Total	C	O	0	0
			40	37	3		
3	A	1	Total	C		0	0
			17	17			
3	A	1	Total	C		0	0
			18	18			
3	A	1	Total	C		0	0
			18	18			
3	A	1	Total	C		0	0
			13	13			
3	A	1	Total	C		0	0
			16	16			
3	A	1	Total	C		0	0
			8	8			
3	A	1	Total	C		0	0
			8	8			
3	A	1	Total	C	O	0	0
			38	35	3		
3	A	1	Total	C		0	0
			18	18			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	27	Total	O	0	0
			27	27		

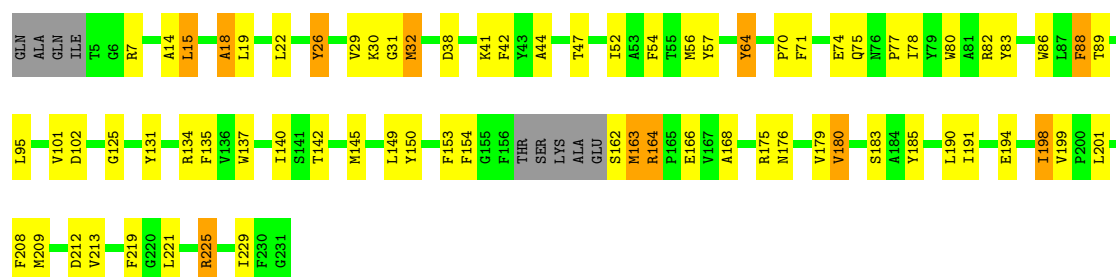
3 Residue-property plots

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.

Note EDS was not executed.

- Molecule 1: bacteriorhodopsin

Chain A: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	60.99Å 60.99Å 109.13Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 1.65	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-1.65)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.130 , 0.188	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2050	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LI1, RET

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	0.88	2/1767 (0.1%)	2.07	72/2413 (3.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	80	TRP	NE1-CE2	-5.12	1.30	1.37
1	A	137	TRP	CG-CD1	-5.03	1.29	1.36

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	83	TYR	CB-CG-CD1	-15.91	111.45	121.00
1	A	57	TYR	CB-CG-CD1	-12.35	113.59	121.00
1	A	83	TYR	CG-CD1-CE1	-12.13	111.59	121.30
1	A	82	ARG	NE-CZ-NH2	-11.84	114.38	120.30
1	A	82	ARG	NE-CZ-NH1	-11.38	114.61	120.30
1	A	7	ARG	NE-CZ-NH1	11.23	125.92	120.30
1	A	137	TRP	CE3-CZ3-CH2	-10.89	109.22	121.20
1	A	83	TYR	CB-CG-CD2	10.77	127.46	121.00
1	A	82	ARG	NH1-CZ-NH2	10.55	131.00	119.40
1	A	88	PHE	CB-CG-CD1	-9.88	113.89	120.80
1	A	164	ARG	NE-CZ-NH1	9.32	124.96	120.30
1	A	57	TYR	CD1-CG-CD2	9.08	127.89	117.90
1	A	219	PHE	CB-CG-CD1	8.87	127.01	120.80
1	A	57	TYR	CD1-CE1-CZ	-8.71	111.96	119.80
1	A	137	TRP	CZ3-CH2-CZ2	8.57	131.88	121.60
1	A	137	TRP	CD2-CE2-CZ2	-8.41	112.21	122.30
1	A	82	ARG	CD-NE-CZ	-8.35	111.92	123.60
1	A	57	TYR	CG-CD2-CE2	-8.24	114.71	121.30
1	A	135	PHE	CB-CG-CD1	-8.06	115.16	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	47	THR	CA-C-O	8.04	136.99	120.10
1	A	135	PHE	CB-CG-CD2	7.77	126.24	120.80
1	A	80	TRP	CE3-CZ3-CH2	-7.54	112.91	121.20
1	A	83	TYR	CD1-CE1-CZ	7.48	126.53	119.80
1	A	219	PHE	CZ-CE2-CD2	7.43	129.01	120.10
1	A	175	ARG	NE-CZ-NH2	-7.42	116.59	120.30
1	A	208	PHE	CG-CD1-CE1	-7.42	112.64	120.80
1	A	212	ASP	CB-CG-OD1	-7.25	111.77	118.30
1	A	88	PHE	CG-CD1-CE1	-7.21	112.86	120.80
1	A	175	ARG	NE-CZ-NH1	7.17	123.88	120.30
1	A	83	TYR	CZ-CE2-CD2	-7.13	113.39	119.80
1	A	145	MET	CA-CB-CG	-7.05	101.32	113.30
1	A	137	TRP	CE2-CD2-CG	-6.96	101.73	107.30
1	A	7	ARG	NE-CZ-NH2	-6.83	116.89	120.30
1	A	57	TYR	CE1-CZ-CE2	6.74	130.59	119.80
1	A	18	ALA	O-C-N	-6.54	112.24	122.70
1	A	150	TYR	CB-CG-CD2	6.53	124.92	121.00
1	A	137	TRP	NE1-CE2-CD2	6.46	113.75	107.30
1	A	208	PHE	CD1-CG-CD2	6.38	126.60	118.30
1	A	135	PHE	CG-CD2-CE2	6.36	127.79	120.80
1	A	135	PHE	CZ-CE2-CD2	-6.33	112.50	120.10
1	A	137	TRP	CE2-CD2-CE3	6.28	126.24	118.70
1	A	208	PHE	CZ-CE2-CD2	-6.26	112.59	120.10
1	A	137	TRP	CD1-NE1-CE2	-6.22	103.41	109.00
1	A	88	PHE	CD1-CG-CD2	6.17	126.32	118.30
1	A	208	PHE	CB-CG-CD1	-6.16	116.49	120.80
1	A	185	TYR	CB-CG-CD2	-6.15	117.31	121.00
1	A	164	ARG	CD-NE-CZ	6.04	132.06	123.60
1	A	142	THR	O-C-N	-5.90	113.27	122.70
1	A	83	TYR	CG-CD2-CE2	5.87	125.99	121.30
1	A	219	PHE	CG-CD1-CE1	5.86	127.25	120.80
1	A	134	ARG	O-C-N	-5.79	113.44	122.70
1	A	86	TRP	CG-CD2-CE3	5.78	139.10	133.90
1	A	47	THR	O-C-N	-5.77	113.47	122.70
1	A	80	TRP	CA-C-O	5.68	132.04	120.10
1	A	14	ALA	O-C-N	-5.65	113.66	122.70
1	A	64	TYR	CZ-CE2-CD2	-5.64	114.72	119.80
1	A	80	TRP	CZ3-CH2-CZ2	5.60	128.32	121.60
1	A	208	PHE	CB-CG-CD2	-5.57	116.90	120.80
1	A	213	VAL	O-C-N	-5.50	113.90	122.70
1	A	71	PHE	CB-CG-CD1	5.46	124.62	120.80
1	A	54	PHE	CB-CG-CD1	5.42	124.59	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	180	VAL	O-C-N	-5.38	114.09	122.70
1	A	212	ASP	CB-CG-OD2	5.32	123.09	118.30
1	A	86	TRP	CE2-CD2-CE3	-5.29	112.36	118.70
1	A	64	TYR	CB-CG-CD1	-5.28	117.83	121.00
1	A	209	MET	CG-SD-CE	-5.25	91.81	100.20
1	A	86	TRP	CH2-CZ2-CE2	5.20	122.60	117.40
1	A	26	TYR	O-C-N	-5.19	114.40	122.70
1	A	125	GLY	O-C-N	-5.14	114.48	122.70
1	A	54	PHE	CZ-CE2-CD2	5.10	126.22	120.10
1	A	31	GLY	O-C-N	5.10	130.86	122.70
1	A	183	SER	O-C-N	-5.02	114.67	122.70

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	1720	0	1385	60	0
2	A	20	0	27	1	0
3	A	283	0	457	67	0
4	A	27	0	0	4	0
All	All	2050	0	1869	91	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 23.

All (91) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:149:LEU:HD22	1:A:179:VAL:HG22	1.38	1.02
1:A:154:PHE:HZ	3:A:609:LI1:H152	1.44	0.83
1:A:198:ILE:HG22	1:A:199:VAL:HG23	1.64	0.80
3:A:601:LI1:H302	3:A:608:LI1:H303	1.63	0.79
1:A:88:PHE:HB2	4:A:515:HOH:O	1.83	0.78

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:26:TYR:HD1	3:A:611:LI1:H152	1.47	0.78
1:A:89:THR:HG23	4:A:515:HOH:O	1.84	0.77
1:A:18:ALA:HA	3:A:606:LI1:H211	1.69	0.74
1:A:52:ILE:HG21	4:A:515:HOH:O	1.88	0.74
1:A:131:TYR:OH	3:A:602:LI1:H162	1.88	0.73
1:A:18:ALA:O	1:A:22:LEU:HD13	1.88	0.72
1:A:64:TYR:OH	3:A:607:LI1:H32	1.90	0.71
1:A:164:ARG:HE	1:A:166:GLU:HG3	1.55	0.70
3:A:602:LI1:H151	3:A:602:LI1:H443	1.74	0.70
1:A:29:VAL:O	1:A:32:MET:HB2	1.93	0.69
1:A:153:PHE:HE2	1:A:179:VAL:HG21	1.58	0.67
1:A:140:ILE:HG13	3:A:601:LI1:H272	1.75	0.67
1:A:190:LEU:HD23	3:A:603:LI1:H222	1.77	0.66
3:A:602:LI1:H593	3:A:608:LI1:H302	1.78	0.64
1:A:153:PHE:CE2	1:A:179:VAL:HG21	2.33	0.64
1:A:180:VAL:HG21	3:A:610:LI1:H521	1.79	0.63
3:A:610:LI1:H411	3:A:610:LI1:H122	1.80	0.63
1:A:26:TYR:CE1	3:A:611:LI1:H121	2.34	0.63
1:A:164:ARG:HG3	1:A:166:GLU:HG3	1.81	0.63
1:A:26:TYR:CD1	3:A:611:LI1:H152	2.33	0.61
1:A:131:TYR:OH	3:A:602:LI1:H13	2.04	0.58
3:A:610:LI1:H593	3:A:610:LI1:H303	1.85	0.57
1:A:140:ILE:CG1	3:A:601:LI1:H272	2.35	0.57
3:A:609:LI1:C28	3:A:603:LI1:H293	2.36	0.56
1:A:131:TYR:CE2	3:A:602:LI1:H13	2.41	0.56
3:A:602:LI1:H161	3:A:603:LI1:H141	1.88	0.56
1:A:221:LEU:O	1:A:225:ARG:HG2	2.05	0.56
3:A:610:LI1:H122	3:A:610:LI1:C41	2.36	0.55
1:A:154:PHE:CZ	3:A:609:LI1:H152	2.33	0.54
1:A:131:TYR:CE2	3:A:602:LI1:H112	2.43	0.54
1:A:153:PHE:HE1	3:A:610:LI1:H112	1.72	0.53
1:A:180:VAL:HG11	3:A:610:LI1:H551	1.91	0.53
1:A:164:ARG:HE	1:A:166:GLU:CG	2.22	0.53
3:A:610:LI1:H272	3:A:610:LI1:H58	1.90	0.52
3:A:602:LI1:C15	3:A:602:LI1:H443	2.40	0.52
1:A:176:ASN:OD1	3:A:610:LI1:H121	2.09	0.52
1:A:180:VAL:CG2	3:A:610:LI1:H521	2.41	0.51
1:A:131:TYR:HE2	3:A:602:LI1:H112	1.75	0.50
1:A:164:ARG:CG	1:A:166:GLU:HG3	2.41	0.50
2:A:301:RET:H171	2:A:301:RET:H8	1.93	0.50
3:A:602:LI1:C44	3:A:602:LI1:H172	2.43	0.49
1:A:30:LYS:HE3	1:A:225:ARG:HD3	1.95	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:176:ASN:ND2	3:A:610:LI1:H412	2.28	0.48
3:A:610:LI1:H251	3:A:610:LI1:H562	1.96	0.48
1:A:56:MET:CE	3:A:607:LI1:H512	2.44	0.48
3:A:612:LI1:H143	4:A:512:HOH:O	2.13	0.48
1:A:180:VAL:HG13	3:A:610:LI1:H562	1.96	0.47
1:A:26:TYR:CD1	3:A:611:LI1:H121	2.48	0.47
3:A:610:LI1:C59	3:A:610:LI1:H303	2.44	0.47
3:A:608:LI1:H162	3:A:608:LI1:H193	1.71	0.47
3:A:603:LI1:H262	3:A:603:LI1:H303	1.50	0.47
3:A:610:LI1:C46	3:A:610:LI1:H152	2.45	0.46
1:A:164:ARG:NE	1:A:166:GLU:HG3	2.27	0.46
1:A:198:ILE:HD11	3:A:603:LI1:H151	1.97	0.46
3:A:602:LI1:H443	3:A:602:LI1:H172	1.97	0.46
3:A:602:LI1:H422	3:A:602:LI1:H2	1.43	0.46
3:A:607:LI1:H12	3:A:607:LI1:H122	1.59	0.46
1:A:154:PHE:CE1	3:A:609:LI1:H121	2.50	0.46
1:A:153:PHE:CE1	3:A:610:LI1:H112	2.51	0.45
1:A:22:LEU:HD11	3:A:611:LI1:C27	2.47	0.45
3:A:601:LI1:H191	3:A:601:LI1:H211	1.71	0.45
3:A:608:LI1:H262	3:A:608:LI1:H292	1.35	0.45
1:A:131:TYR:CZ	3:A:602:LI1:H13	2.53	0.44
1:A:190:LEU:CD2	3:A:603:LI1:H222	2.47	0.44
3:A:611:LI1:H262	3:A:611:LI1:H241	1.65	0.44
3:A:602:LI1:H593	3:A:608:LI1:C30	2.47	0.43
3:A:601:LI1:H152	3:A:601:LI1:O1	2.00	0.43
1:A:190:LEU:HD21	3:A:603:LI1:H202	2.00	0.43
1:A:70:PRO:HG2	1:A:70:PRO:O	2.19	0.43
1:A:154:PHE:CZ	3:A:609:LI1:H121	2.53	0.43
1:A:163:MET:HG3	1:A:168:ALA:HB2	1.99	0.43
1:A:190:LEU:CD2	3:A:603:LI1:H202	2.49	0.43
1:A:78:ILE:HD12	1:A:194:GLU:HG3	2.01	0.43
1:A:198:ILE:HD11	3:A:603:LI1:C15	2.49	0.42
1:A:42:PHE:CD2	1:A:229:ILE:HB	2.53	0.42
3:A:613:LI1:H191	3:A:613:LI1:H211	1.72	0.42
1:A:176:ASN:CG	3:A:610:LI1:H412	2.40	0.42
1:A:44:ALA:HA	3:A:612:LI1:H13	2.01	0.42
1:A:77:PRO:HG2	1:A:201:LEU:HD22	2.02	0.42
1:A:56:MET:HE3	3:A:607:LI1:H512	2.01	0.42
1:A:101:VAL:O	1:A:102:ASP:HB3	2.20	0.41
3:A:602:LI1:H262	3:A:602:LI1:H241	1.78	0.41
3:A:607:LI1:H462	3:A:607:LI1:H441	1.48	0.41
3:A:613:LI1:H202	3:A:613:LI1:H162	1.53	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:15:LEU:HD22	1:A:19:LEU:CD1	2.51	0.40
3:A:610:LI1:H292	3:A:610:LI1:H261	1.65	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	218/231 (94%)	212 (97%)	6 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	178/185 (96%)	166 (93%)	12 (7%)	23	3

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
1	A	32	MET
1	A	38	ASP
1	A	41	LYS
1	A	74	GLU
1	A	75	GLN
1	A	95	LEU
1	A	162	SER

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Mol	Chain	Res	Type
1	A	163	MET
1	A	191	ILE
1	A	198	ILE
1	A	225	ARG

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

Mol	Chain	Res	Type
1	A	105	GLN

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 ⓘ

14 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$
2	RET	A	301	1	19,20,21	1.41	3 (15%)	26,27,28	2.52	11 (42%)
3	LI1	A	601	-	30,31,44	1.10	3 (10%)	26,33,51	1.53	8 (30%)
3	LI1	A	602	-	40,40,44	0.91	2 (5%)	43,45,51	1.29	5 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	LI1	A	603	-	17,17,44	0.87	1 (5%)	13,18,51	1.59	2 (15%)
3	LI1	A	604	-	15,15,44	1.20	1 (6%)	7,14,51	1.11	0
3	LI1	A	605	-	6,7,44	0.91	0	3,6,51	1.95	1 (33%)
3	LI1	A	606	-	6,7,44	0.86	0	3,6,51	1.94	2 (66%)
3	LI1	A	607	-	36,37,44	0.94	1 (2%)	28,38,51	1.46	3 (10%)
3	LI1	A	608	-	17,17,44	0.66	0	14,18,51	1.74	4 (28%)
3	LI1	A	609	-	15,15,44	1.17	1 (6%)	7,14,51	0.92	0
3	LI1	A	610	-	39,39,44	0.95	1 (2%)	31,41,51	1.22	3 (9%)
3	LI1	A	611	-	16,16,44	0.68	1 (6%)	17,18,51	1.58	4 (23%)
3	LI1	A	612	-	17,17,44	1.00	1 (5%)	13,18,51	1.41	2 (15%)
3	LI1	A	613	-	12,12,44	1.11	1 (8%)	9,12,51	2.30	3 (33%)

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
2	RET	A	301	1	-	0/13/30/31	0/1/1/1
3	LI1	A	601	-	2/2/3/8	1/31/32/49	0/0/0/0
3	LI1	A	602	-	-	0/44/44/49	0/0/0/0
3	LI1	A	603	-	-	0/16/16/49	0/0/0/0
3	LI1	A	604	-	-	0/12/13/49	0/0/0/0
3	LI1	A	605	-	-	0/5/5/49	0/0/0/0
3	LI1	A	606	-	-	0/5/5/49	0/0/0/0
3	LI1	A	607	-	-	0/37/38/49	0/0/0/0
3	LI1	A	608	-	-	0/16/16/49	0/0/0/0
3	LI1	A	609	-	-	0/12/13/49	0/0/0/0
3	LI1	A	610	-	-	0/39/39/49	0/0/0/0
3	LI1	A	611	-	1/1/3/8	0/17/17/49	0/0/0/0
3	LI1	A	612	-	-	0/16/16/49	0/0/0/0
3	LI1	A	613	-	1/1/1/8	0/10/11/49	0/0/0/0

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	LI1	C27-C26	-3.25	1.53	1.55
2	A	301	RET	C20-C13	-3.24	1.45	1.51
3	A	609	LI1	C30-C28	3.18	1.54	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	604	LI1	C29-C28	3.14	1.54	1.49
3	A	612	LI1	C11-C12	-3.04	1.53	1.55
3	A	601	LI1	O3-C3	2.87	1.54	1.42
3	A	610	LI1	O3-C3	2.77	1.54	1.42
3	A	602	LI1	O3-C3	2.70	1.54	1.42
3	A	607	LI1	O3-C3	2.64	1.53	1.42
3	A	613	LI1	C24-C23	2.58	1.53	1.49
3	A	601	LI1	C12-C11	2.30	1.55	1.51
3	A	603	LI1	C11-C12	-2.19	1.54	1.55
2	A	301	RET	C17-C1	2.18	1.58	1.53
3	A	611	LI1	C27-C26	-2.12	1.54	1.55
3	A	601	LI1	C42-C41	2.04	1.54	1.51
2	A	301	RET	C5-C6	2.03	1.37	1.34

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	RET	C20-C13-C12	5.04	126.25	118.09
2	A	301	RET	C19-C9-C8	4.80	125.85	118.09
3	A	613	LI1	C16-C17-C18	-4.27	102.83	115.14
2	A	301	RET	C11-C10-C9	-4.06	121.44	127.29
3	A	603	LI1	C15-C16-C17	-3.87	107.01	114.68
2	A	301	RET	C2-C1-C6	3.78	116.73	110.44
3	A	602	LI1	C26-C25-C23	-3.65	107.68	115.42
3	A	607	LI1	O1-C11-C12	3.57	117.23	109.22
3	A	608	LI1	C20-C21-C22	-3.47	107.80	114.68
2	A	301	RET	C10-C11-C12	-3.47	111.54	123.24
3	A	613	LI1	C21-C20-C18	-3.46	105.17	115.14
2	A	301	RET	C11-C12-C13	-3.31	116.93	126.38
3	A	610	LI1	C27-C26-C25	-3.30	108.14	114.68
2	A	301	RET	C8-C9-C10	-3.29	113.91	118.97
3	A	608	LI1	C17-C16-C15	-3.14	108.47	114.68
2	A	301	RET	C14-C13-C12	-3.10	108.84	119.62
3	A	611	LI1	C16-C17-C18	-3.08	106.28	115.14
3	A	612	LI1	C27-C26-C25	-3.06	108.62	114.68
3	A	611	LI1	C26-C25-C23	-3.00	109.05	115.42
3	A	603	LI1	C27-C26-C25	-2.97	108.81	114.68
3	A	612	LI1	C15-C16-C17	-2.95	108.83	114.68
3	A	613	LI1	C17-C16-C15	-2.94	108.86	114.68
2	A	301	RET	C4-C5-C6	-2.81	119.10	122.84
3	A	610	LI1	O2-C41-C42	2.79	112.94	107.52
3	A	607	LI1	C45-C46-C47	-2.77	109.20	114.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	607	LI1	C46-C45-C43	-2.75	107.22	115.14
3	A	605	LI1	C22-C21-C20	-2.73	108.32	114.46
3	A	601	LI1	C16-C17-C18	-2.66	107.48	115.14
3	A	602	LI1	C15-C16-C17	-2.65	109.44	114.68
3	A	611	LI1	C27-C26-C25	-2.60	108.61	114.46
3	A	601	LI1	O3-C3-C2	-2.58	105.61	111.90
3	A	606	LI1	C22-C21-C20	-2.54	108.76	114.46
2	A	301	RET	C1-C6-C7	2.47	122.53	115.69
2	A	301	RET	C17-C1-C6	2.44	114.37	110.33
3	A	601	LI1	C21-C20-C18	-2.41	108.20	115.14
3	A	608	LI1	C27-C26-C25	-2.35	110.03	114.68
3	A	602	LI1	O3-C3-C2	-2.33	106.21	111.90
3	A	601	LI1	C20-C21-C22	-2.31	110.11	114.68
3	A	601	LI1	C27-C26-C25	-2.26	110.20	114.68
3	A	601	LI1	C17-C16-C15	-2.26	110.21	114.68
3	A	610	LI1	O3-C3-C2	-2.25	106.41	111.90
3	A	601	LI1	O1-C11-C12	2.23	114.24	109.22
3	A	601	LI1	C50-C48-C47	-2.22	107.08	127.24
3	A	611	LI1	C21-C20-C18	-2.19	108.82	115.14
3	A	602	LI1	C46-C45-C43	-2.16	108.92	115.14
3	A	608	LI1	C16-C17-C18	-2.12	109.03	115.14
3	A	602	LI1	C46-C47-C48	-2.01	109.34	115.14
3	A	606	LI1	C15-C16-C17	-2.01	107.75	113.69

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	611	LI1	C13
3	A	601	LI1	C2
3	A	601	LI1	C18
3	A	613	LI1	C18

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	LI1	C15-C13-C12-C11

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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.