



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 01:28 PM GMT

PDB ID : 1P8H  
Title : BACTERIORHODOPSIN M1 INTERMEDIATE PRODUCED AT ROOM TEMPERATURE  
Authors : Lanyi, J.K.  
Deposited on : 2003-05-07  
Resolution : 1.52 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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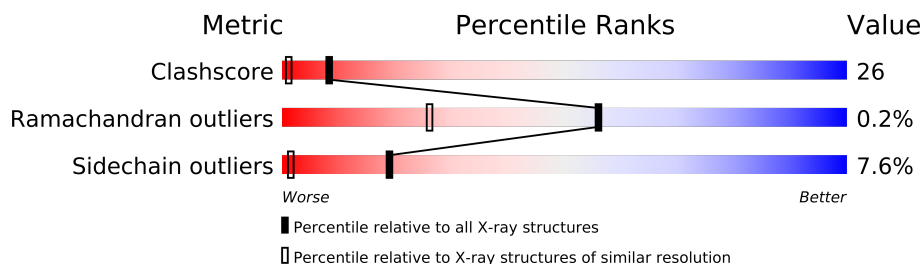
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.52 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	2184 (1.54-1.50)
Ramachandran outliers	78287	2123 (1.54-1.50)
Sidechain outliers	78261	2121 (1.54-1.50)

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  $\geq 3$ , 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	1-A	249	
1	2-A	249	

## 2 Entry composition i

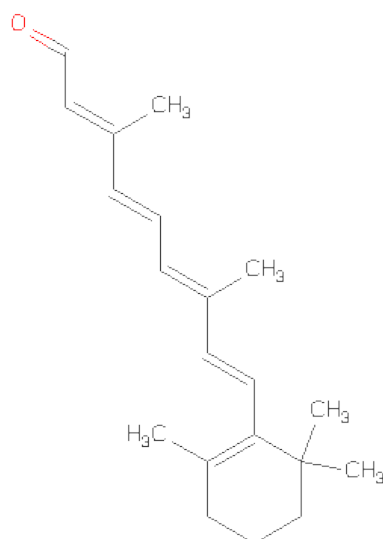
There are 5 unique types of molecules in this entry. The entry contains 4145 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

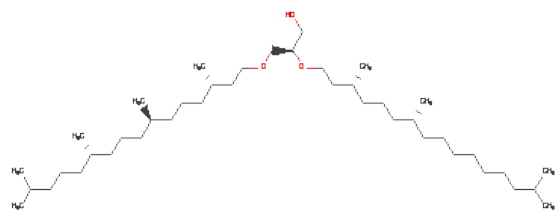
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1-A	222	Total	C	N	O	S	0	0	0
			1720	1159	262	290	9			
1	2-A	222	Total	C	N	O	S	0	0	0
			1719	1159	261	290	9			

- Molecule 2 is RETINAL (three-letter code: RET) (formula: C<sub>20</sub>H<sub>28</sub>O).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	1-A	1	Total	C	0	0
			20	20		
2	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: C<sub>42</sub>H<sub>86</sub>O<sub>3</sub>).



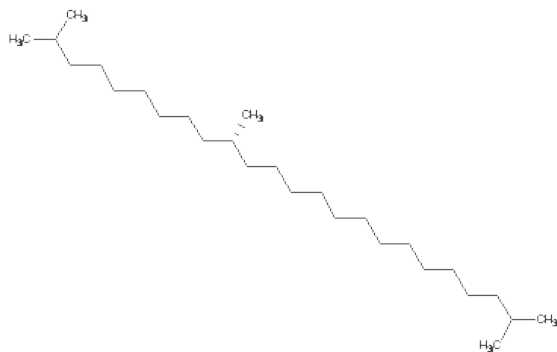
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	1-A	1	Total	C	O	0	0
			32	29	3		
3	1-A	1	Total	C	O	0	0
			40	37	3		
3	1-A	1	Total	C		0	0
			18	18			
3	1-A	1	Total	C		0	0
			16	16			
3	1-A	1	Total	C		0	0
			8	8			
3	1-A	1	Total	C		0	0
			8	8			
3	1-A	1	Total	C	O	0	0
			38	35	3		
3	1-A	1	Total	C		0	0
			18	18			
3	1-A	1	Total	C		0	0
			16	16			
3	1-A	1	Total	C	O	0	0
			40	37	3		
3	1-A	1	Total	C		0	0
			17	17			
3	1-A	1	Total	C		0	0
			18	18			
3	1-A	1	Total	C		0	0
			13	13			
3	2-A	1	Total	C	O	0	0
			32	29	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	2-A	1	Total C O 40 37 3	0	0
3	2-A	1	Total C 18 18	0	0
3	2-A	1	Total C 16 16	0	0
3	2-A	1	Total C 8 8	0	0
3	2-A	1	Total C 8 8	0	0
3	2-A	1	Total C O 38 35 3	0	0
3	2-A	1	Total C 18 18	0	0
3	2-A	1	Total C 16 16	0	0
3	2-A	1	Total C O 40 37 3	0	0
3	2-A	1	Total C 17 17	0	0
3	2-A	1	Total C 18 18	0	0
3	2-A	1	Total C 13 13	0	0

- Molecule 4 is 2,10,23-TRIMETHYL-TETRACOSANE (three-letter code: SQU) (formula:  $C_{27}H_{56}$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	1-A	1	Total C 27 27	0	0
4	2-A	1	Total C 27 27	0	0

- Molecule 5 is water.

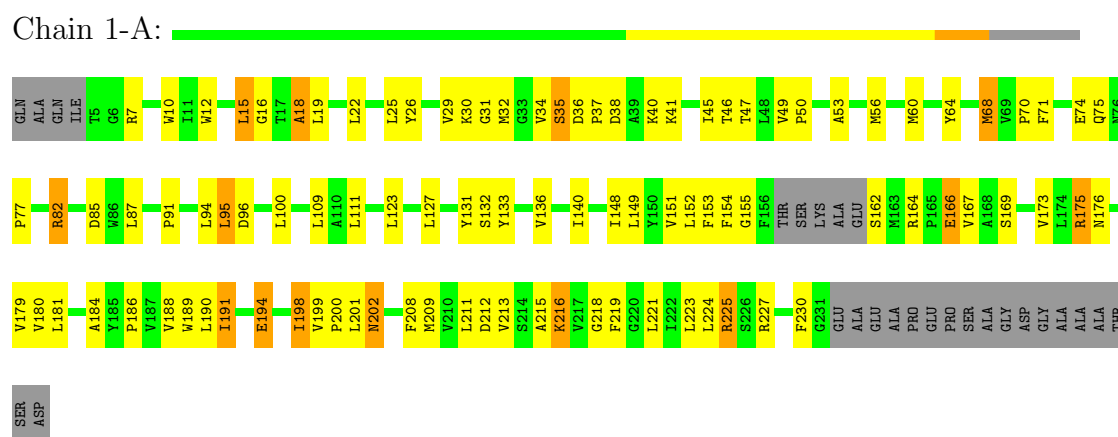
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	1-A	25	Total O 25 25	0	0
5	2-A	23	Total O 23 23	0	0

### 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.

Note EDS was not executed.

#### • Molecule 1: Bacteriorhodopsin



#### • Molecule 1: Bacteriorhodopsin



## 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, $\alpha$ , $\beta$ , $\gamma$	60.91Å 60.91Å 108.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 1.52	Depositor
% Data completeness (in resolution range)	92.1 (25.00-1.52)	Depositor
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	SHELXL-97	Depositor
R, $R_{free}$	0.175 , 0.207	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4145	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	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: SQU, RET, LI1

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	1-A	0.42	0/1767	1.19	7/2413 (0.3%)
1	2-A	0.70	0/1765	1.51	17/2408 (0.7%)
All	All	0.58	0/3532	1.36	24/4821 (0.5%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1-A	216	LYS	CB-CG-CD	12.97	145.31	111.60
1	2-A	175	ARG	NE-CZ-NH1	12.08	126.34	120.30
1	1-A	82	ARG	NE-CZ-NH1	-8.42	116.09	120.30
1	1-A	216	LYS	CA-CB-CG	8.14	131.31	113.40
1	2-A	175	ARG	NE-CZ-NH2	-7.87	116.37	120.30
1	2-A	83	TYR	CG-CD1-CE1	-6.74	115.91	121.30
1	1-A	16	GLY	O-C-N	6.55	133.19	122.70
1	2-A	16	GLY	O-C-N	6.55	133.19	122.70
1	2-A	57	TYR	CB-CG-CD1	-6.53	117.08	121.00
1	2-A	135	PHE	CB-CG-CD1	-6.24	116.43	120.80
1	2-A	88	PHE	CB-CG-CD1	-6.06	116.56	120.80
1	2-A	209	MET	CA-CB-CG	-6.02	103.07	113.30
1	1-A	82	ARG	CD-NE-CZ	-5.79	115.49	123.60
1	2-A	86	TRP	CZ3-CH2-CZ2	-5.74	114.71	121.60
1	2-A	183	SER	O-C-N	-5.64	113.68	122.70
1	1-A	208	PHE	CB-CG-CD2	-5.49	116.95	120.80
1	2-A	57	TYR	CD1-CG-CD2	5.41	123.86	117.90
1	2-A	86	TRP	CH2-CZ2-CE2	5.40	122.80	117.40
1	2-A	83	TYR	CZ-CE2-CD2	-5.25	115.07	119.80
1	2-A	82	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	2-A	219	PHE	CB-CG-CD1	5.06	124.34	120.80
1	1-A	18	ALA	O-C-N	-5.05	114.62	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2-A	18	ALA	O-C-N	-5.05	114.62	122.70
1	2-A	134	ARG	NE-CZ-NH2	-5.05	117.78	120.30

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	1-A	1720	0	1776	100	0
1	2-A	1719	0	1774	54	0
2	1-A	20	0	27	2	0
2	2-A	20	0	27	2	0
3	1-A	282	0	452	55	0
3	2-A	282	0	452	62	0
4	1-A	27	0	53	7	0
4	2-A	27	0	53	7	0
5	1-A	25	0	0	10	0
5	2-A	23	0	0	1	0
All	All	4145	0	4614	229	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 26.

All (229) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:609:LI1:C25	3:A:609:LI1:C26	1.74	1.60
3:A:609:LI1:C26	3:A:609:LI1:C25	1.74	1.60
1:A:164:ARG:HG3	1:A:166:GLU:HG3	1.46	0.97
1:A:19:LEU:C	1:A:20:MET:CA	2.37	0.92
3:A:609:LI1:C25	3:A:609:LI1:C27	2.52	0.88
3:A:609:LI1:C25	3:A:609:LI1:C27	2.52	0.88
3:A:609:LI1:C26	3:A:609:LI1:C23	2.58	0.81
3:A:609:LI1:C26	3:A:609:LI1:C23	2.58	0.81

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:A:701:SQU:H182	4:A:701:SQU:H11	1.64	0.80
4:A:701:SQU:H11	4:A:701:SQU:H182	1.64	0.80
1:A:26:TYR:HD1	3:A:611:LI1:H152	1.47	0.78
1:A:175:ARG:O	1:A:179:VAL:HG23	1.84	0.78
1:A:64:TYR:OH	3:A:607:LI1:H422	1.83	0.77
1:A:221:LEU:O	1:A:225:ARG:HG2	1.85	0.77
1:A:136:VAL:HA	3:A:602:LI1:H552	1.70	0.74
1:A:169:SER:O	1:A:173:VAL:HG23	1.88	0.74
1:A:82:ARG:HG2	5:A:406:HOH:O	1.88	0.74
1:A:223:LEU:HD22	5:A:504:HOH:O	1.87	0.73
1:A:221:LEU:O	1:A:225:ARG:HD3	1.88	0.73
1:A:18:ALA:O	1:A:22:LEU:HD13	1.88	0.71
1:A:37:PRO:O	1:A:40:LYS:HB2	1.90	0.71
1:A:64:TYR:OH	3:A:607:LI1:H422	1.90	0.71
1:A:26:TYR:HD1	3:A:611:LI1:H152	1.56	0.70
3:A:602:LI1:H502	3:A:602:LI1:H222	1.74	0.69
3:A:602:LI1:H502	3:A:602:LI1:H222	1.74	0.69
1:A:56:MET:HE3	3:A:607:LI1:H521	1.74	0.69
1:A:131:TYR:OH	3:A:602:LI1:H13	1.94	0.68
1:A:140:ILE:HG13	3:A:601:LI1:H272	1.76	0.67
1:A:64:TYR:OH	3:A:607:LI1:H32	1.96	0.66
1:A:12:TRP:HB3	1:A:209:MET:HE3	1.79	0.66
1:A:153:PHE:HE2	1:A:179:VAL:HG21	1.62	0.65
1:A:96:ASP:HB3	5:A:504:HOH:O	1.95	0.65
1:A:36:ASP:O	1:A:40:LYS:HG3	1.96	0.65
1:A:131:TYR:OH	3:A:602:LI1:H162	1.96	0.65
1:A:136:VAL:HA	3:A:602:LI1:H552	1.79	0.64
1:A:47:THR:HG21	3:A:612:LI1:H162	1.79	0.64
1:A:31:GLY:O	1:A:34:VAL:HG23	1.98	0.63
3:A:602:LI1:H151	3:A:602:LI1:H412	1.79	0.63
3:A:602:LI1:H412	3:A:602:LI1:H151	1.79	0.63
1:A:64:TYR:OH	3:A:607:LI1:H32	1.99	0.62
1:A:215:ALA:HB1	5:A:501:HOH:O	1.99	0.62
1:A:46:THR:HG23	5:A:502:HOH:O	1.99	0.61
4:A:701:SQU:H182	4:A:701:SQU:C1	2.31	0.61
4:A:701:SQU:C1	4:A:701:SQU:H182	2.31	0.61
4:A:701:SQU:H211	4:A:701:SQU:H13	1.82	0.61
1:A:163:MET:HG3	1:A:168:ALA:HB2	1.82	0.61
4:A:701:SQU:H211	4:A:701:SQU:H13	1.82	0.61
1:A:70:PRO:HG2	1:A:129:LYS:HD3	1.81	0.60
1:A:50:PRO:HA	1:A:53:ALA:HB3	1.82	0.60
1:A:29:VAL:O	1:A:32:MET:HB2	2.01	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:602:LI1:H151	3:A:602:LI1:H12	1.82	0.60
3:A:602:LI1:H12	3:A:602:LI1:H151	1.82	0.60
1:A:180:VAL:HG13	3:A:610:LI1:H591	1.84	0.59
1:A:140:ILE:HG13	3:A:601:LI1:H272	1.84	0.59
1:A:202:ASN:H	1:A:202:ASN:ND2	2.01	0.59
1:A:47:THR:HG21	3:A:612:LI1:H162	1.84	0.58
3:A:610:LI1:C51	3:A:610:LI1:H593	2.33	0.58
3:A:610:LI1:H593	3:A:610:LI1:C51	2.33	0.58
1:A:190:LEU:HD23	3:A:603:LI1:H222	1.86	0.58
1:A:180:VAL:HG13	3:A:610:LI1:H591	1.85	0.57
1:A:153:PHE:CE2	1:A:179:VAL:HG21	2.40	0.57
1:A:148:ILE:O	1:A:152:LEU:HG	2.03	0.57
1:A:149:LEU:O	1:A:152:LEU:HB2	2.05	0.57
1:A:221:LEU:O	1:A:225:ARG:HB2	2.05	0.57
1:A:221:LEU:CD2	4:A:701:SQU:H292	2.34	0.56
3:A:602:LI1:H522	3:A:602:LI1:H592	1.87	0.56
3:A:602:LI1:H592	3:A:602:LI1:H522	1.87	0.56
1:A:212:ASP:O	1:A:216:LYS:HG3	2.06	0.56
1:A:131:TYR:OH	3:A:602:LI1:H13	2.06	0.56
1:A:198:ILE:HD11	3:A:603:LI1:H152	1.86	0.56
1:A:18:ALA:HA	3:A:606:LI1:H211	1.88	0.56
1:A:18:ALA:HA	3:A:606:LI1:H211	1.88	0.56
1:A:87:LEU:HA	5:A:511:HOH:O	2.06	0.55
1:A:153:PHE:CE2	1:A:179:VAL:HG21	2.41	0.55
1:A:47:THR:CG2	3:A:612:LI1:H162	2.37	0.55
1:A:47:THR:CG2	3:A:612:LI1:H162	2.38	0.54
1:A:181:LEU:CD2	1:A:211:LEU:HD23	2.38	0.54
1:A:131:TYR:OH	3:A:602:LI1:H162	2.08	0.54
1:A:18:ALA:HA	3:A:606:LI1:C21	2.38	0.53
1:A:18:ALA:HA	3:A:606:LI1:C21	2.38	0.53
3:A:612:LI1:H143	5:A:512:HOH:O	2.07	0.53
1:A:35:SER:O	1:A:37:PRO:HD3	2.08	0.53
1:A:191:ILE:O	1:A:198:ILE:HB	2.08	0.53
1:A:202:ASN:H	1:A:202:ASN:HD22	1.56	0.53
2:A:301:RET:H161	2:A:301:RET:H8	1.90	0.53
1:A:35:SER:O	1:A:40:LYS:HE2	2.09	0.53
1:A:180:VAL:HG21	3:A:610:LI1:C48	2.39	0.52
1:A:133:TYR:HA	1:A:136:VAL:HG23	1.92	0.52
1:A:56:MET:HE1	3:A:607:LI1:H501	1.91	0.52
1:A:140:ILE:CG1	3:A:601:LI1:H272	2.39	0.52
1:A:139:ALA:CB	3:A:602:LI1:H571	2.40	0.51
3:A:610:LI1:H251	3:A:610:LI1:H303	1.92	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:610:LI1:H251	3:A:610:LI1:H303	1.92	0.51
1:A:82:ARG:O	1:A:85:ASP:HB3	2.09	0.51
1:A:68:MET:HB3	1:A:75:GLN:HE22	1.75	0.51
3:A:602:LI1:C52	3:A:602:LI1:H592	2.41	0.51
1:A:44:ALA:HA	3:A:612:LI1:H13	1.93	0.51
1:A:149:LEU:HA	1:A:152:LEU:HB2	1.90	0.51
3:A:602:LI1:H592	3:A:602:LI1:C52	2.41	0.51
1:A:15:LEU:HB3	1:A:209:MET:HE2	1.93	0.51
1:A:68:MET:HB3	1:A:75:GLN:NE2	2.25	0.51
1:A:25:LEU:O	1:A:29:VAL:HG23	2.10	0.51
1:A:19:LEU:O	1:A:20:MET:CA	2.58	0.51
1:A:198:ILE:HD11	3:A:603:LI1:C15	2.41	0.51
1:A:15:LEU:HB3	1:A:209:MET:HE2	1.91	0.51
3:A:602:LI1:H161	3:A:603:LI1:H141	1.92	0.50
1:A:190:LEU:CD2	3:A:603:LI1:H222	2.41	0.50
3:A:602:LI1:H161	3:A:603:LI1:H141	1.92	0.50
1:A:22:LEU:HD11	3:A:611:LI1:C27	2.41	0.50
1:A:29:VAL:HA	1:A:32:MET:SD	2.51	0.50
1:A:149:LEU:HD13	1:A:179:VAL:HG13	1.94	0.50
1:A:70:PRO:HA	1:A:74:GLU:O	2.12	0.50
3:A:610:LI1:H603	3:A:610:LI1:H303	1.95	0.49
3:A:610:LI1:H603	3:A:610:LI1:H303	1.95	0.49
1:A:153:PHE:HE1	3:A:610:LI1:H112	1.76	0.48
1:A:70:PRO:O	1:A:71:PHE:HB3	2.13	0.48
3:A:602:LI1:C15	3:A:602:LI1:H412	2.42	0.48
3:A:602:LI1:H412	3:A:602:LI1:C15	2.42	0.48
1:A:164:ARG:HG3	1:A:167:VAL:HG23	1.96	0.48
1:A:149:LEU:HA	1:A:152:LEU:HG	1.94	0.48
1:A:181:LEU:HD23	1:A:211:LEU:HD23	1.94	0.48
3:A:602:LI1:H2	3:A:602:LI1:H121	1.96	0.48
3:A:602:LI1:H121	3:A:602:LI1:H2	1.96	0.48
3:A:610:LI1:H511	3:A:610:LI1:H551	1.63	0.48
3:A:610:LI1:H551	3:A:610:LI1:H511	1.63	0.48
3:A:602:LI1:C51	3:A:602:LI1:H592	2.44	0.48
1:A:172:LYS:HD3	3:A:610:LI1:H32	1.96	0.48
3:A:602:LI1:H592	3:A:602:LI1:C51	2.44	0.48
1:A:41:LYS:O	1:A:45:ILE:HD12	2.14	0.47
1:A:45:ILE:O	1:A:49:VAL:HG23	2.15	0.47
1:A:209:MET:O	1:A:213:VAL:HG23	2.14	0.47
1:A:151:VAL:HG13	1:A:155:GLY:HA3	1.96	0.47
3:A:601:LI1:H11	3:A:601:LI1:H411	1.35	0.47
3:A:601:LI1:H11	3:A:601:LI1:H411	1.35	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:166:GLU:HG3	1:A:166:GLU:H	1.39	0.47
3:A:610:LI1:C50	3:A:610:LI1:H593	2.46	0.46
1:A:94:LEU:HD22	1:A:111:LEU:HD22	1.96	0.46
3:A:610:LI1:H593	3:A:610:LI1:C50	2.46	0.46
4:A:701:SQU:C26	4:A:701:SQU:H202	2.46	0.46
4:A:701:SQU:C26	4:A:701:SQU:H202	2.46	0.46
1:A:131:TYR:CE2	3:A:602:LI1:H112	2.50	0.46
1:A:47:THR:HG21	3:A:612:LI1:H141	1.98	0.46
1:A:100:LEU:O	1:A:167:VAL:HG11	2.15	0.46
1:A:215:ALA:O	1:A:219:PHE:HB3	2.16	0.46
1:A:190:LEU:CD2	3:A:603:LI1:H222	2.45	0.46
3:A:602:LI1:H502	3:A:602:LI1:C22	2.43	0.46
3:A:602:LI1:H502	3:A:602:LI1:C22	2.43	0.46
1:A:138:TRP:CZ3	3:A:602:LI1:H251	2.51	0.46
3:A:602:LI1:H472	3:A:602:LI1:H512	1.27	0.46
3:A:602:LI1:H512	3:A:602:LI1:H472	1.27	0.46
1:A:221:LEU:HD21	4:A:701:SQU:H292	1.98	0.46
1:A:189:TRP:CE2	1:A:194:GLU:HB3	2.51	0.46
1:A:221:LEU:HD13	4:A:701:SQU:H292	1.97	0.45
1:A:56:MET:HE2	1:A:56:MET:HA	1.98	0.45
1:A:164:ARG:NH2	1:A:230:PHE:O	2.44	0.45
1:A:180:VAL:HA	3:A:610:LI1:C23	2.47	0.45
3:A:610:LI1:H593	3:A:610:LI1:C52	2.47	0.45
1:A:153:PHE:CZ	1:A:175:ARG:HD2	2.51	0.45
3:A:610:LI1:H593	3:A:610:LI1:C52	2.47	0.45
1:A:164:ARG:NH2	1:A:166:GLU:OE1	2.50	0.45
1:A:111:LEU:HD23	1:A:148:ILE:HG23	1.99	0.45
1:A:143:ALA:HB2	3:A:608:LI1:H272	1.98	0.45
1:A:221:LEU:HD22	4:A:701:SQU:H292	1.98	0.44
1:A:26:TYR:CD1	3:A:611:LI1:H152	2.45	0.44
3:A:605:LI1:H171	3:A:605:LI1:H211	1.54	0.44
1:A:184:ALA:O	1:A:188:VAL:HG23	2.17	0.44
3:A:605:LI1:H211	3:A:605:LI1:H171	1.54	0.44
1:A:140:ILE:CG1	3:A:601:LI1:H272	2.44	0.44
1:A:199:VAL:HA	1:A:200:PRO:HD3	1.89	0.44
3:A:610:LI1:C30	3:A:610:LI1:H251	2.48	0.44
3:A:610:LI1:C30	3:A:610:LI1:H251	2.48	0.44
1:A:123:LEU:HD11	1:A:127:LEU:HD11	1.99	0.44
1:A:9:GLU:HB3	1:A:202:ASN:HA	2.00	0.44
1:A:202:ASN:ND2	5:A:415:HOH:O	2.51	0.44
2:A:301:RET:H7	2:A:301:RET:H181	1.43	0.44
1:A:96:ASP:O	1:A:100:LEU:HB2	2.18	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:216:LYS:NZ	5:A:402:HOH:O	2.50	0.44
1:A:198:ILE:HG22	1:A:199:VAL:N	2.32	0.44
1:A:70:PRO:CG	1:A:129:LYS:HD3	2.45	0.44
1:A:176:ASN:ND2	3:A:610:LI1:O2	2.50	0.44
1:A:194:GLU:N	1:A:194:GLU:OE2	2.50	0.43
2:A:301:RET:H7	2:A:301:RET:H181	1.80	0.43
1:A:15:LEU:HD22	1:A:19:LEU:CD1	2.47	0.43
3:A:610:LI1:C60	3:A:610:LI1:H303	2.48	0.43
3:A:610:LI1:C60	3:A:610:LI1:H303	2.48	0.43
1:A:15:LEU:HD22	1:A:19:LEU:CD1	2.47	0.43
1:A:60:MET:HE2	5:A:401:HOH:O	2.18	0.43
1:A:191:ILE:HG22	1:A:198:ILE:HD12	1.99	0.43
1:A:56:MET:HE1	3:A:607:LI1:H501	2.00	0.43
1:A:91:PRO:O	1:A:95:LEU:HB2	2.19	0.42
1:A:164:ARG:NH2	1:A:230:PHE:O	2.48	0.42
1:A:91:PRO:O	1:A:95:LEU:N	2.50	0.42
1:A:180:VAL:HG21	3:A:610:LI1:C48	2.49	0.42
1:A:221:LEU:HD11	4:A:701:SQU:H271	2.02	0.42
1:A:35:SER:C	1:A:40:LYS:HE2	2.40	0.42
3:A:610:LI1:H522	3:A:610:LI1:H593	2.02	0.42
3:A:610:LI1:H593	3:A:610:LI1:H522	2.02	0.42
1:A:12:TRP:O	1:A:209:MET:HE2	2.20	0.42
1:A:7:ARG:O	1:A:10:TRP:HD1	2.03	0.42
1:A:7:ARG:O	1:A:10:TRP:HD1	2.03	0.42
3:A:610:LI1:H472	3:A:610:LI1:H172	2.02	0.42
3:A:604:LI1:H211	3:A:604:LI1:H172	1.66	0.42
3:A:610:LI1:H472	3:A:610:LI1:H172	2.02	0.42
1:A:56:MET:CE	3:A:607:LI1:H501	2.50	0.42
3:A:604:LI1:H172	3:A:604:LI1:H211	1.66	0.42
1:A:30:LYS:NZ	1:A:224:LEU:O	2.50	0.42
1:A:190:LEU:HD23	3:A:603:LI1:H222	2.02	0.41
1:A:149:LEU:HD23	1:A:152:LEU:HD12	2.01	0.41
1:A:77:PRO:HG2	1:A:201:LEU:HD22	2.01	0.41
1:A:56:MET:HE2	1:A:56:MET:HA	2.03	0.41
1:A:164:ARG:HG2	1:A:164:ARG:H	1.50	0.41
2:A:301:RET:H8	2:A:301:RET:H171	2.02	0.41
1:A:78:ILE:HD12	1:A:194:GLU:HG3	2.02	0.41
1:A:218:GLY:CA	4:A:701:SQU:H152	2.50	0.41
1:A:82:ARG:NH1	5:A:406:HOH:O	2.49	0.41
3:A:610:LI1:C59	3:A:610:LI1:H502	2.50	0.41
1:A:176:ASN:ND2	3:A:610:LI1:O2	2.54	0.41
3:A:610:LI1:C59	3:A:610:LI1:H502	2.50	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:136:VAL:HA	3:A:602:LI1:C55	2.47	0.41
1:A:139:ALA:HB2	3:A:602:LI1:H571	2.02	0.41
3:A:610:LI1:H502	3:A:610:LI1:H593	2.03	0.41
3:A:610:LI1:H593	3:A:610:LI1:H502	2.03	0.41
1:A:201:LEU:O	1:A:201:LEU:HD12	2.21	0.41
1:A:24:THR:CG2	3:A:612:LI1:H303	2.51	0.41
3:A:610:LI1:H172	3:A:610:LI1:H461	2.02	0.40
1:A:169:SER:O	1:A:173:VAL:HG23	2.22	0.40
3:A:610:LI1:H172	3:A:610:LI1:H461	2.02	0.40
3:A:602:LI1:H412	3:A:602:LI1:H12	1.83	0.40
3:A:602:LI1:H412	3:A:602:LI1:H12	1.83	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	1-A	218/249 (88%)	208 (95%)	9 (4%)	1 (0%)	38	11
1	2-A	216/249 (87%)	214 (99%)	2 (1%)	0	100	100
All	All	434/498 (87%)	422 (97%)	11 (2%)	1 (0%)	56	26

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-A	198	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	1-A	178/195 (91%)	160 (90%)	18 (10%)	11	0
1	2-A	177/195 (91%)	168 (95%)	9 (5%)	33	5
All	All	355/390 (91%)	328 (92%)	27 (8%)	19	1

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	15	LEU
1	1-A	35	SER
1	1-A	38	ASP
1	1-A	68	MET
1	1-A	74	GLU
1	1-A	95	LEU
1	1-A	109	LEU
1	1-A	132	SER
1	1-A	154	PHE
1	1-A	162	SER
1	1-A	166	GLU
1	1-A	175	ARG
1	1-A	186	PRO
1	1-A	191	ILE
1	1-A	194	GLU
1	1-A	202	ASN
1	1-A	225	ARG
1	1-A	227	ARG
1	2-A	15	LEU
1	2-A	38	ASP
1	2-A	74	GLU
1	2-A	95	LEU
1	2-A	162	SER
1	2-A	163	MET
1	2-A	164	ARG
1	2-A	166	GLU
1	2-A	202	ASN

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

Mol	Chain	Res	Type
1	1-A	76	ASN
1	1-A	202	ASN
1	2-A	105	GLN

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Mol	Chain	Res	Type
1	2-A	202	ASN

### 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 ⓘ

30 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	1-A	301	1	19,20,21	0.86	0	26,27,28	5.61	13 (50%)
3	LI1	1-A	601	-	30,31,44	1.51	3 (10%)	26,33,51	1.83	4 (15%)
3	LI1	1-A	602	-	39,39,44	1.32	3 (7%)	39,43,51	1.95	6 (15%)
3	LI1	1-A	603	-	17,17,44	1.52	1 (5%)	13,18,51	2.04	2 (15%)
3	LI1	1-A	604	-	15,15,44	1.86	2 (13%)	7,14,51	1.24	1 (14%)
3	LI1	1-A	605	-	6,7,44	1.28	1 (16%)	3,6,51	1.26	0
3	LI1	1-A	606	-	6,7,44	1.19	1 (16%)	3,6,51	1.00	0
3	LI1	1-A	607	-	36,37,44	1.43	3 (8%)	28,38,51	1.44	4 (14%)
3	LI1	1-A	608	-	17,17,44	1.53	1 (5%)	14,18,51	2.42	3 (21%)
3	LI1	1-A	609	-	15,15,44	1.97	2 (13%)	7,14,51	1.30	1 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	LI1	1-A	610	-	39,39,44	1.39	3 (7%)	31,41,51	1.73	3 (9%)
3	LI1	1-A	611	-	16,16,44	1.67	2 (12%)	17,18,51	3.01	7 (41%)
3	LI1	1-A	612	-	17,17,44	1.63	2 (11%)	13,18,51	2.02	2 (15%)
3	LI1	1-A	613	-	12,12,44	1.00	1 (8%)	9,12,51	1.64	3 (33%)
4	SQU	1-A	701	-	26,26,26	1.27	4 (15%)	28,28,28	1.76	10 (35%)
2	RET	2-A	301	1	19,20,21	1.00	2 (10%)	26,27,28	2.01	10 (38%)
3	LI1	2-A	601	-	30,31,44	1.51	3 (10%)	26,33,51	1.83	4 (15%)
3	LI1	2-A	602	-	39,39,44	1.32	3 (7%)	39,43,51	1.95	6 (15%)
3	LI1	2-A	603	-	17,17,44	1.52	1 (5%)	13,18,51	2.04	2 (15%)
3	LI1	2-A	604	-	15,15,44	1.86	2 (13%)	7,14,51	1.24	1 (14%)
3	LI1	2-A	605	-	6,7,44	1.28	1 (16%)	3,6,51	1.26	0
3	LI1	2-A	606	-	6,7,44	1.19	1 (16%)	3,6,51	1.00	0
3	LI1	2-A	607	-	36,37,44	1.43	3 (8%)	28,38,51	1.44	4 (14%)
3	LI1	2-A	608	-	17,17,44	1.53	1 (5%)	14,18,51	2.42	3 (21%)
3	LI1	2-A	609	-	15,15,44	1.97	2 (13%)	7,14,51	1.30	1 (14%)
3	LI1	2-A	610	-	39,39,44	1.39	3 (7%)	31,41,51	1.73	3 (9%)
3	LI1	2-A	611	-	16,16,44	1.67	2 (12%)	17,18,51	3.01	7 (41%)
3	LI1	2-A	612	-	17,17,44	1.63	2 (11%)	13,18,51	2.02	2 (15%)
3	LI1	2-A	613	-	12,12,44	1.00	1 (8%)	9,12,51	1.64	3 (33%)
4	SQU	2-A	701	-	26,26,26	1.27	4 (15%)	28,28,28	1.76	10 (35%)

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	1-A	301	1	-	0/13/30/31	0/1/1/1
3	LI1	1-A	601	-	2/2/3/8	0/31/32/49	0/0/0/0
3	LI1	1-A	602	-	-	0/42/42/49	0/0/0/0
3	LI1	1-A	603	-	-	0/16/16/49	0/0/0/0
3	LI1	1-A	604	-	-	0/12/13/49	0/0/0/0
3	LI1	1-A	605	-	-	1/5/5/49	0/0/0/0
3	LI1	1-A	606	-	-	0/5/5/49	0/0/0/0
3	LI1	1-A	607	-	-	0/37/38/49	0/0/0/0
3	LI1	1-A	608	-	-	0/16/16/49	0/0/0/0
3	LI1	1-A	609	-	-	0/12/13/49	0/0/0/0
3	LI1	1-A	610	-	-	0/39/39/49	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LI1	1-A	611	-	2/2/3/8	0/17/17/49	0/0/0/0
3	LI1	1-A	612	-	-	0/16/16/49	0/0/0/0
3	LI1	1-A	613	-	1/1/1/8	0/10/11/49	0/0/0/0
4	SQU	1-A	701	-	-	0/25/25/25	0/0/0/0
2	RET	2-A	301	1	-	0/13/30/31	0/1/1/1
3	LI1	2-A	601	-	2/2/3/8	0/31/32/49	0/0/0/0
3	LI1	2-A	602	-	-	0/42/42/49	0/0/0/0
3	LI1	2-A	603	-	-	0/16/16/49	0/0/0/0
3	LI1	2-A	604	-	-	0/12/13/49	0/0/0/0
3	LI1	2-A	605	-	-	1/5/5/49	0/0/0/0
3	LI1	2-A	606	-	-	0/5/5/49	0/0/0/0
3	LI1	2-A	607	-	-	0/37/38/49	0/0/0/0
3	LI1	2-A	608	-	-	0/16/16/49	0/0/0/0
3	LI1	2-A	609	-	-	0/12/13/49	0/0/0/0
3	LI1	2-A	610	-	-	0/39/39/49	0/0/0/0
3	LI1	2-A	611	-	2/2/3/8	0/17/17/49	0/0/0/0
3	LI1	2-A	612	-	-	0/16/16/49	0/0/0/0
3	LI1	2-A	613	-	1/1/1/8	0/10/11/49	0/0/0/0
4	SQU	2-A	701	-	-	0/25/25/25	0/0/0/0

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1-A	609	LI1	C26-C25	6.04	1.74	1.52
3	2-A	609	LI1	C26-C25	6.04	1.74	1.52
3	1-A	612	LI1	C26-C25	5.91	1.74	1.52
3	2-A	612	LI1	C26-C25	5.91	1.74	1.52
3	2-A	611	LI1	C25-C26	5.90	1.74	1.53
3	1-A	611	LI1	C25-C26	5.90	1.74	1.53
3	1-A	604	LI1	C26-C25	5.89	1.74	1.52
3	2-A	604	LI1	C26-C25	5.89	1.74	1.52
3	2-A	602	LI1	C25-C26	5.88	1.74	1.53
3	1-A	602	LI1	C25-C26	5.88	1.74	1.53
3	1-A	601	LI1	C26-C25	5.85	1.74	1.52
3	2-A	601	LI1	C26-C25	5.85	1.74	1.52
3	2-A	607	LI1	C26-C25	5.83	1.74	1.52
3	1-A	607	LI1	C26-C25	5.83	1.74	1.52
3	1-A	608	LI1	C26-C25	5.80	1.73	1.52
3	2-A	608	LI1	C26-C25	5.80	1.73	1.52
3	1-A	610	LI1	C26-C25	5.78	1.73	1.52
3	2-A	610	LI1	C26-C25	5.78	1.73	1.52
3	1-A	603	LI1	C26-C25	5.78	1.73	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2-A	603	LI1	C26-C25	5.78	1.73	1.52
3	1-A	609	LI1	C30-C28	3.59	1.55	1.49
3	2-A	609	LI1	C30-C28	3.59	1.55	1.49
4	2-A	701	SQU	C14-C12	-3.17	1.35	1.52
4	1-A	701	SQU	C14-C12	-3.17	1.35	1.52
3	1-A	610	LI1	O3-C3	2.99	1.55	1.42
3	2-A	610	LI1	O3-C3	2.99	1.55	1.42
3	2-A	602	LI1	O3-C3	2.97	1.55	1.42
3	1-A	602	LI1	O3-C3	2.97	1.55	1.42
3	1-A	601	LI1	O3-C3	2.90	1.55	1.42
3	2-A	601	LI1	O3-C3	2.90	1.55	1.42
3	2-A	607	LI1	O3-C3	2.82	1.54	1.42
3	1-A	607	LI1	O3-C3	2.82	1.54	1.42
4	2-A	701	SQU	C23-C22	-2.80	1.34	1.51
4	1-A	701	SQU	C23-C22	-2.80	1.34	1.51
3	2-A	607	LI1	C60-C58	2.75	1.54	1.49
3	1-A	607	LI1	C60-C58	2.75	1.54	1.49
3	1-A	604	LI1	C29-C28	2.72	1.54	1.49
3	2-A	604	LI1	C29-C28	2.72	1.54	1.49
3	2-A	611	LI1	C27-C26	-2.70	1.54	1.55
3	1-A	611	LI1	C27-C26	-2.70	1.54	1.55
3	1-A	605	LI1	C22-C21	-2.68	1.54	1.55
3	2-A	605	LI1	C22-C21	-2.68	1.54	1.55
4	2-A	701	SQU	C18-C17	-2.68	1.35	1.51
4	1-A	701	SQU	C18-C17	-2.68	1.35	1.51
2	2-A	301	RET	C2-C3	-2.64	1.45	1.52
4	2-A	701	SQU	C9-C7	-2.60	1.35	1.51
4	1-A	701	SQU	C9-C7	-2.60	1.35	1.51
3	2-A	606	LI1	C22-C21	-2.49	1.54	1.55
3	1-A	606	LI1	C22-C21	-2.49	1.54	1.55
3	1-A	610	LI1	C12-C11	2.28	1.55	1.51
3	2-A	610	LI1	C12-C11	2.28	1.55	1.51
3	1-A	613	LI1	C24-C23	2.26	1.53	1.49
3	2-A	613	LI1	C24-C23	2.26	1.53	1.49
3	1-A	612	LI1	C11-C12	-2.15	1.54	1.55
3	2-A	612	LI1	C11-C12	-2.15	1.54	1.55
3	1-A	601	LI1	C12-C11	2.11	1.54	1.51
3	2-A	601	LI1	C12-C11	2.11	1.54	1.51
3	2-A	602	LI1	C27-C26	-2.08	1.54	1.55
3	1-A	602	LI1	C27-C26	-2.08	1.54	1.55
2	2-A	301	RET	C17-C1	2.01	1.58	1.53

All (115) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1-A	301	RET	C20-C13-C12	19.03	148.86	118.09
2	1-A	301	RET	C20-C13-C14	-11.76	86.95	122.17
2	1-A	301	RET	C19-C9-C10	-8.04	111.50	122.92
3	2-A	611	LI1	C24-C23-C25	7.86	139.86	111.02
3	1-A	611	LI1	C24-C23-C25	7.86	139.86	111.02
2	1-A	301	RET	C11-C12-C13	-7.78	104.19	126.38
3	1-A	608	LI1	C27-C26-C25	-7.52	99.79	114.68
3	2-A	608	LI1	C27-C26-C25	-7.52	99.79	114.68
3	1-A	610	LI1	C27-C26-C25	-7.40	100.02	114.68
3	2-A	610	LI1	C27-C26-C25	-7.40	100.02	114.68
2	1-A	301	RET	C7-C6-C5	-6.92	105.02	121.57
3	1-A	603	LI1	C27-C26-C25	-6.81	101.20	114.68
3	2-A	603	LI1	C27-C26-C25	-6.81	101.20	114.68
3	1-A	612	LI1	C27-C26-C25	-6.59	101.62	114.68
3	2-A	612	LI1	C27-C26-C25	-6.59	101.62	114.68
3	1-A	601	LI1	C27-C26-C25	-6.52	101.77	114.68
3	2-A	601	LI1	C27-C26-C25	-6.52	101.77	114.68
3	2-A	611	LI1	C27-C26-C25	-6.30	100.31	114.46
3	1-A	611	LI1	C27-C26-C25	-6.30	100.31	114.46
3	2-A	602	LI1	C27-C26-C25	-6.15	100.64	114.46
3	1-A	602	LI1	C27-C26-C25	-6.15	100.64	114.46
2	1-A	301	RET	C8-C9-C10	6.05	128.27	118.97
2	1-A	301	RET	C1-C6-C7	5.69	131.46	115.69
2	2-A	301	RET	C11-C10-C9	-5.54	119.32	127.29
3	2-A	602	LI1	C26-C25-C23	-5.51	103.74	115.42
3	1-A	602	LI1	C26-C25-C23	-5.51	103.74	115.42
3	2-A	602	LI1	C24-C23-C25	-5.49	90.86	111.02
3	1-A	602	LI1	C24-C23-C25	-5.49	90.86	111.02
3	2-A	611	LI1	C26-C25-C23	-5.28	104.23	115.42
3	1-A	611	LI1	C26-C25-C23	-5.28	104.23	115.42
2	1-A	301	RET	C7-C8-C9	5.18	133.97	126.22
4	2-A	701	SQU	C15-C14-C12	4.62	128.45	115.14
4	1-A	701	SQU	C15-C14-C12	4.62	128.45	115.14
3	2-A	607	LI1	C27-C26-C25	-4.31	100.98	113.69
3	1-A	607	LI1	C27-C26-C25	-4.31	100.98	113.69
2	2-A	301	RET	C8-C9-C10	-3.73	113.23	118.97
2	1-A	301	RET	C8-C7-C6	-3.65	116.53	127.32
3	1-A	610	LI1	O3-C3-C2	-3.34	103.76	111.90
3	2-A	610	LI1	O3-C3-C2	-3.34	103.76	111.90
3	1-A	608	LI1	C20-C21-C22	-3.32	108.11	114.68
3	2-A	608	LI1	C20-C21-C22	-3.32	108.11	114.68
3	1-A	610	LI1	O2-C41-C42	3.22	113.78	107.52
3	2-A	610	LI1	O2-C41-C42	3.22	113.78	107.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2-A	602	LI1	O3-C3-C2	-3.11	104.30	111.90
3	1-A	602	LI1	O3-C3-C2	-3.11	104.30	111.90
3	1-A	601	LI1	O3-C3-C2	-3.10	104.33	111.90
3	2-A	601	LI1	O3-C3-C2	-3.10	104.33	111.90
2	1-A	301	RET	C10-C11-C12	-3.03	113.00	123.24
3	2-A	607	LI1	C46-C45-C43	-3.00	106.51	115.14
3	1-A	607	LI1	C46-C45-C43	-3.00	106.51	115.14
4	2-A	701	SQU	C10-C9-C7	2.95	130.57	114.61
4	1-A	701	SQU	C10-C9-C7	2.95	130.57	114.61
3	1-A	613	LI1	C20-C21-C22	-2.83	109.08	114.68
3	2-A	613	LI1	C20-C21-C22	-2.83	109.08	114.68
3	1-A	601	LI1	C17-C16-C15	-2.76	109.22	114.68
3	2-A	601	LI1	C17-C16-C15	-2.76	109.22	114.68
3	1-A	613	LI1	C17-C16-C15	-2.74	109.25	114.68
3	2-A	613	LI1	C17-C16-C15	-2.74	109.25	114.68
3	1-A	601	LI1	O2-C41-C42	2.67	112.71	107.52
3	2-A	601	LI1	O2-C41-C42	2.67	112.71	107.52
2	1-A	301	RET	C2-C1-C6	2.65	114.84	110.44
2	2-A	301	RET	C10-C11-C12	-2.64	114.32	123.24
4	2-A	701	SQU	C26-C27-C28	2.62	128.99	115.69
4	1-A	701	SQU	C26-C27-C28	2.62	128.99	115.69
3	2-A	607	LI1	C45-C46-C47	-2.59	109.55	114.68
3	1-A	607	LI1	C45-C46-C47	-2.59	109.55	114.68
3	1-A	608	LI1	C17-C16-C15	-2.58	109.58	114.68
3	2-A	608	LI1	C17-C16-C15	-2.58	109.58	114.68
3	1-A	609	LI1	C27-C26-C25	-2.58	100.36	113.86
3	2-A	609	LI1	C27-C26-C25	-2.58	100.36	113.86
2	2-A	301	RET	C20-C13-C12	2.54	122.20	118.09
4	2-A	701	SQU	C25-C23-C22	2.54	128.34	114.61
4	1-A	701	SQU	C25-C23-C22	2.54	128.34	114.61
3	2-A	611	LI1	C21-C22-C23	-2.53	107.86	115.14
3	1-A	611	LI1	C21-C22-C23	-2.53	107.86	115.14
3	2-A	611	LI1	C21-C20-C18	-2.52	107.89	115.14
3	1-A	611	LI1	C21-C20-C18	-2.52	107.89	115.14
3	1-A	604	LI1	C27-C26-C25	-2.50	100.76	113.86
3	2-A	604	LI1	C27-C26-C25	-2.50	100.76	113.86
4	2-A	701	SQU	C5-C4-C2	2.48	128.26	115.69
4	1-A	701	SQU	C5-C4-C2	2.48	128.26	115.69
3	1-A	612	LI1	C15-C16-C17	-2.43	109.88	114.68
3	2-A	612	LI1	C15-C16-C17	-2.43	109.88	114.68
3	2-A	607	LI1	O3-C3-C2	-2.41	106.03	111.90
3	1-A	607	LI1	O3-C3-C2	-2.41	106.03	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2-A	301	RET	C1-C6-C7	2.40	122.35	115.69
3	2-A	602	LI1	C45-C46-C47	-2.38	109.97	114.68
3	1-A	602	LI1	C45-C46-C47	-2.38	109.97	114.68
3	2-A	602	LI1	C46-C45-C43	-2.37	108.30	115.14
3	1-A	602	LI1	C46-C45-C43	-2.37	108.30	115.14
3	2-A	611	LI1	C16-C17-C18	-2.37	108.31	115.14
3	1-A	611	LI1	C16-C17-C18	-2.37	108.31	115.14
4	2-A	701	SQU	C23-C22-C21	2.35	127.34	114.61
4	1-A	701	SQU	C23-C22-C21	2.35	127.34	114.61
4	2-A	701	SQU	C18-C17-C16	2.32	127.17	114.61
4	1-A	701	SQU	C18-C17-C16	2.32	127.17	114.61
2	1-A	301	RET	C4-C5-C6	-2.26	119.83	122.84
2	1-A	301	RET	C3-C4-C5	-2.25	110.33	113.74
2	2-A	301	RET	C14-C13-C12	-2.23	111.88	119.62
4	2-A	701	SQU	C9-C7-C6	2.21	126.58	114.61
4	1-A	701	SQU	C9-C7-C6	2.21	126.58	114.61
4	2-A	701	SQU	C14-C12-C11	2.21	123.31	111.92
4	1-A	701	SQU	C14-C12-C11	2.21	123.31	111.92
2	2-A	301	RET	C18-C5-C4	-2.16	109.38	113.34
3	1-A	613	LI1	C21-C20-C18	-2.13	109.00	115.14
3	2-A	613	LI1	C21-C20-C18	-2.13	109.00	115.14
2	2-A	301	RET	C19-C9-C8	2.13	121.53	118.09
4	2-A	701	SQU	C20-C18-C17	2.10	126.00	114.61
4	1-A	701	SQU	C20-C18-C17	2.10	126.00	114.61
3	2-A	611	LI1	C16-C15-C13	-2.09	109.11	115.14
3	1-A	611	LI1	C16-C15-C13	-2.09	109.11	115.14
3	1-A	603	LI1	C15-C16-C17	-2.08	110.57	114.68
3	2-A	603	LI1	C15-C16-C17	-2.08	110.57	114.68
2	2-A	301	RET	C18-C5-C6	2.06	126.84	124.51
2	2-A	301	RET	C2-C1-C6	2.05	113.84	110.44

All (10) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	1-A	613	LI1	C18
3	1-A	601	LI1	C2
3	1-A	601	LI1	C18
3	2-A	611	LI1	C13
3	2-A	611	LI1	C23
3	1-A	611	LI1	C13
3	1-A	611	LI1	C23
3	2-A	613	LI1	C18

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Mol	Chain	Res	Type	Atom
3	2-A	601	LI1	C2
3	2-A	601	LI1	C18

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	1-A	605	LI1	C17-C18-C20-C21
3	2-A	605	LI1	C17-C18-C20-C21

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.