



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:02 PM GMT

PDB ID : 1RQK
Title : Structure of the reaction centre from Rhodobacter sphaeroides carotenoidless strain R-26.1 reconstituted with 3,4-dihydrospheroidene
Authors : Roszak, A.W.; Hashimoto, H.; Gardiner, A.T.; Cogdell, R.J.; Isaacs, N.W.
Deposited on : 2003-12-05
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

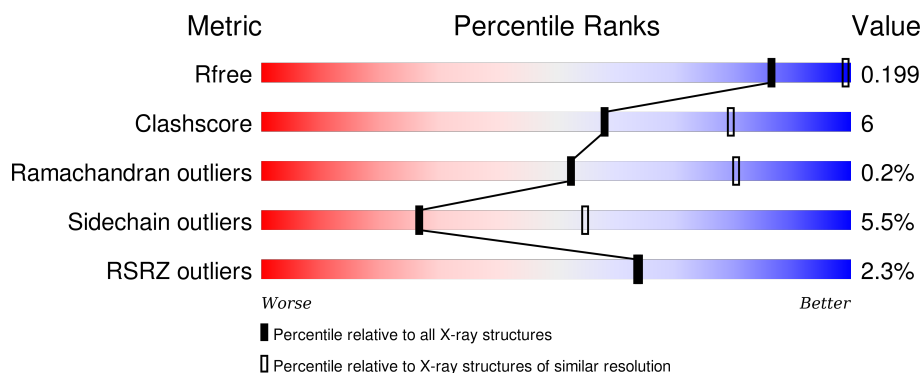
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	L	281	<div> <div></div> <div>86%12%•</div> </div>
2	M	307	<div> <div>2%</div> <div>84%13%••</div> </div>
3	H	260	<div> <div>3%</div> <div>79%12%•7%</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	LDA	L	904	-	-	-	X
10	LDA	L	908	-	-	-	X
10	LDA	M	902	-	-	-	X
10	LDA	M	903	-	-	-	X
10	LDA	M	905	-	-	-	X
10	LDA	M	906	-	-	-	X
7	U10	L	502[A]	-	-	-	X
7	U10	L	502[B]	-	-	-	X
9	CDL	M	800	-	-	-	X

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 7522 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Reaction center protein L chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	281	Total	C	N	O	S	0	5	0
			2249	1518	355	368	8			

- Molecule 2 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	302	Total	C	N	O	S	0	3	0
			2423	1615	400	397	11			

- Molecule 3 is a protein called Reaction center protein H chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	241	Total	C	N	O	S	0	8	0
			1868	1190	324	345	9			

- Molecule 4 is FE (III) ION (three-letter code: FE) (formula: Fe).

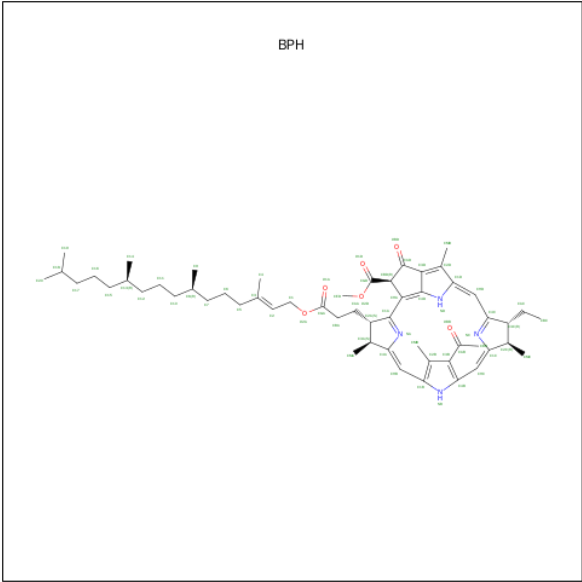
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	M	1	Total	Fe	0	0
			1	1		

- Molecule 5 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C₅₅H₇₄MgN₄O₆).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
5	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
5	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
5	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

- Molecule 6 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: C₅₅H₇₆N₄O₆).



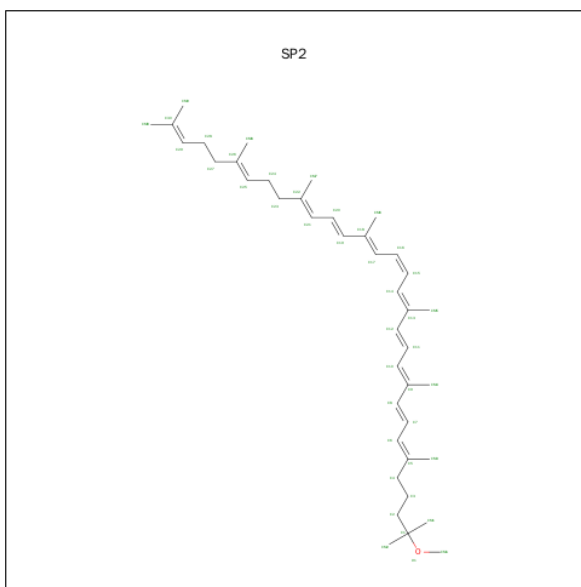
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	M	1	Total	C	N	O	0	0
			65	55	4	6		
6	L	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 7 is UBIQUINONE-10 (three-letter code: U10) (formula: C₅₉H₉₀O₄).



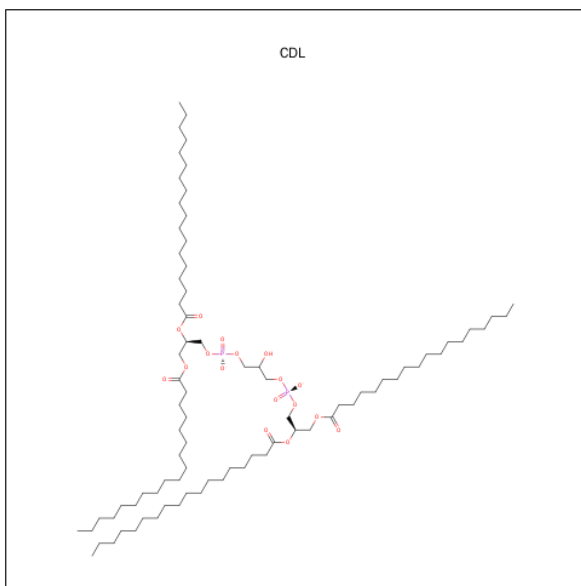
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	M	1	Total	C	O	0	0
			48	44	4		
7	L	1	Total	C	O	0	1
			96	88	8		

- Molecule 8 is 3,4-DIHYDROSPHEROIDENE (three-letter code: SP2) (formula: C₄₁H₆₂O).



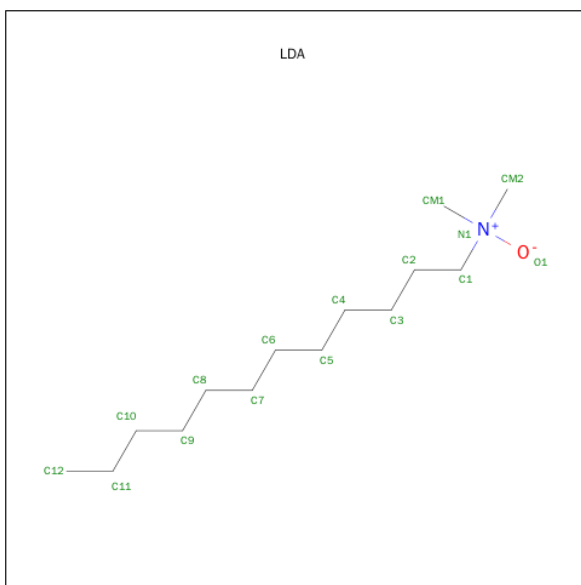
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	M	1	Total	C	O	0	0
			42	41	1		

- Molecule 9 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	M	1	Total	C	O	P	0	0
			81	62	17	2		

- Molecule 10 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	H	1	Total	C	N	O	0	0
			16	14	1	1		
10	M	1	Total	C	N	O	0	0
			16	14	1	1		
10	M	1	Total	C	N	O	0	0
			16	14	1	1		
10	L	1	Total	C	N	O	0	0
			16	14	1	1		
10	M	1	Total	C	N	O	0	0
			16	14	1	1		
10	M	1	Total	C	N	O	0	0
			16	14	1	1		
10	L	1	Total	C	N	O	0	0
			16	14	1	1		

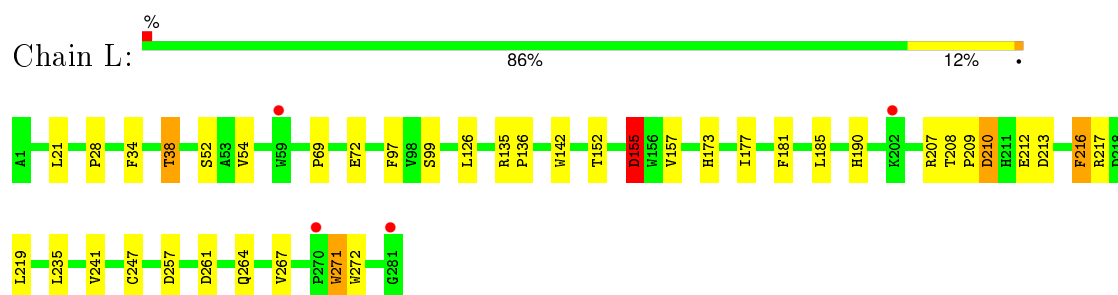
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	H	85	Total	O	0	0
			85	85		
11	L	57	Total	O	0	0
			57	57		
11	M	66	Total	O	0	0
			66	66		

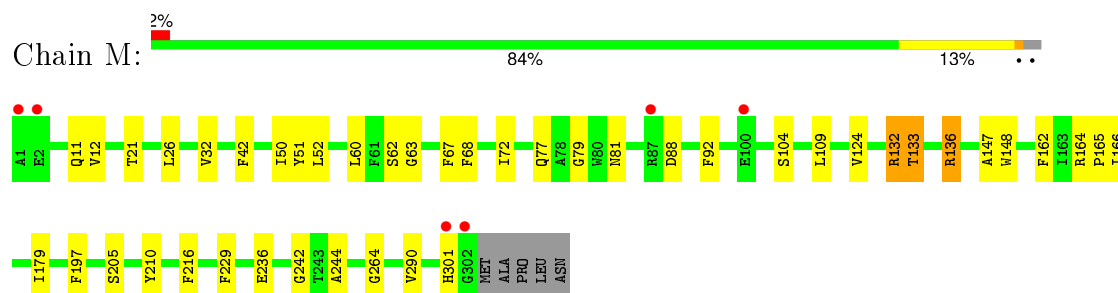
3 Residue-property plots

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.

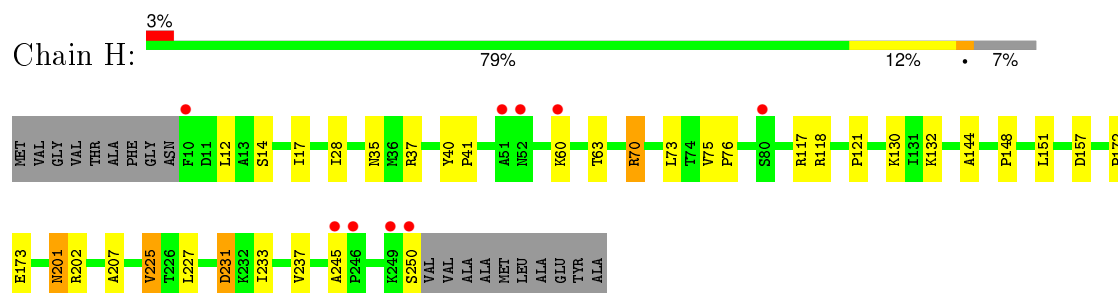
- Molecule 1: Reaction center protein L chain



- Molecule 2: Reaction center protein M chain



- Molecule 3: Reaction center protein H chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	141.72Å 141.72Å 187.18Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.29 – 2.70 15.28 – 2.70	Depositor EDS
% Data completeness (in resolution range)	95.7 (15.29-2.70) 96.4 (15.28-2.70)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.1.9999	Depositor
R, R_{free}	0.162 , 0.194 0.169 , 0.199	Depositor DCC
R_{free} test set	2864 reflections (5.23%)	DCC
Wilson B-factor (Å ²)	49.3	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 83.2	EDS
Estimated twinning fraction	0.014 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 57635 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7522	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BCL, LDA, CDL, BPH, SP2, FE, U10

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	L	0.73	0/2362	0.79	7/3232 (0.2%)
2	M	0.72	0/2530	0.76	1/3452 (0.0%)
3	H	0.80	0/1956	0.89	3/2657 (0.1%)
All	All	0.75	0/6848	0.81	11/9341 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	213	ASP	CB-CG-OD2	8.90	126.31	118.30
3	H	157	ASP	CB-CG-OD2	7.28	124.85	118.30
1	L	210	ASP	CB-CG-OD1	6.75	124.38	118.30
2	M	88	ASP	CB-CG-OD2	6.53	124.18	118.30
1	L	261	ASP	CB-CG-OD2	6.46	124.11	118.30
1	L	155[A]	ASP	CB-CG-OD2	5.69	123.42	118.30
1	L	155[B]	ASP	CB-CG-OD2	5.69	123.42	118.30
1	L	217	ARG	NE-CZ-NH1	5.33	122.97	120.30
3	H	225	VAL	CB-CA-C	-5.24	101.44	111.40
3	H	231	ASP	CB-CG-OD2	5.24	123.02	118.30
1	L	257	ASP	CB-CG-OD2	5.10	122.89	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	2249	0	2205	27	0
2	M	2423	0	2344	30	0
3	H	1868	0	1880	20	0
4	M	1	0	0	0	0
5	L	132	0	148	5	0
5	M	132	0	148	9	0
6	L	65	0	76	5	0
6	M	65	0	76	8	0
7	L	96	0	126	10	0
7	M	48	0	63	0	0
8	M	42	0	62	0	0
9	M	81	0	106	2	0
10	H	16	0	31	1	0
10	L	32	0	62	0	0
10	M	64	0	124	4	0
11	H	85	0	0	2	0
11	L	57	0	0	0	0
11	M	66	0	0	1	0
All	All	7522	0	7451	87	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (87) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:130[A]:LYS:NZ	3:H:173[A]:GLU:OE2	2.04	0.90
6:L:402:BPH:HHC	6:L:402:BPH:HBB3	1.55	0.88
1:L:241:VAL:HG21	6:L:402:BPH:HAC1	1.72	0.71
3:H:117[A]:ARG:NH2	3:H:227:LEU:HD22	2.06	0.71
2:M:51:TYR:O	2:M:132:ARG:NH2	2.24	0.70
2:M:197:PHE:CZ	5:M:502:BCL:HBB2	2.27	0.70
6:M:401:BPH:HHC	6:M:401:BPH:HBB3	1.75	0.68
1:L:34:PHE:O	1:L:38:THR:HG23	1.94	0.67
2:M:179:ILE:HG23	5:M:501:BCL:HED1	1.75	0.67
6:L:402:BPH:HBB2	2:M:210:TYR:HB3	1.76	0.66
1:L:219:LEU:O	2:M:132:ARG:NH1	2.27	0.65
1:L:271:TRP:N	1:L:271:TRP:CD1	2.65	0.64
2:M:197:PHE:HZ	5:M:502:BCL:HBB2	1.63	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:302:BCL:HBB3	5:L:302:BCL:HMB1	1.80	0.62
3:H:132:LYS:NZ	11:H:976:HOH:O	2.30	0.61
5:M:502:BCL:CBB	5:M:502:BCL:HHC	2.31	0.60
1:L:135:ARG:HB3	1:L:136:PRO:HD3	1.84	0.59
5:L:304:BCL:HMB1	5:L:304:BCL:HBB2	1.86	0.58
3:H:37:ARG:NH2	3:H:60:LYS:O	2.36	0.58
1:L:38:THR:HG22	1:L:99:SER:CB	2.35	0.57
2:M:236:GLU:OE2	3:H:118[A]:ARG:NH2	2.34	0.57
3:H:148:PRO:HA	3:H:151:LEU:HD12	1.87	0.56
3:H:14:SER:HA	3:H:17:ILE:HG22	1.88	0.56
3:H:70:ARG:NH2	3:H:121:PRO:O	2.39	0.56
1:L:216:PHE:CD1	7:L:502[B]:U10:H4M2	2.41	0.56
2:M:229:PHE:HB2	2:M:244:ALA:HB2	1.88	0.55
1:L:235[A]:LEU:HD22	2:M:42:PHE:CZ	2.41	0.55
2:M:63:GLY:HA3	6:M:401:BPH:H5C1	1.90	0.54
1:L:216:PHE:CG	7:L:502[B]:U10:H4M2	2.43	0.53
6:M:401:BPH:HBB3	6:M:401:BPH:CHC	2.38	0.53
2:M:21:THR:HG23	2:M:26:LEU:HD21	1.91	0.52
2:M:301:HIS:NE2	11:M:968:HOH:O	2.34	0.52
2:M:242:GLY:CA	3:H:117[A]:ARG:HD3	2.39	0.51
2:M:67:PHE:CD1	6:M:401:BPH:C9	2.93	0.51
2:M:264:GLY:HA3	3:H:35:ASN:OD1	2.11	0.51
1:L:38:THR:HG22	1:L:99:SER:HB3	1.93	0.51
6:L:402:BPH:HHC	6:L:402:BPH:CBB	2.33	0.50
1:L:181:PHE:HB3	6:M:401:BPH:CBB	2.42	0.49
5:L:302:BCL:HMB1	5:L:302:BCL:CBB	2.42	0.49
2:M:67:PHE:CD1	6:M:401:BPH:H9C3	2.47	0.49
1:L:28:PRO:HG3	10:M:903:LDA:HM13	1.94	0.49
2:M:68:PHE:O	2:M:72:ILE:HG12	2.12	0.49
1:L:97:PHE:CE1	5:L:302:BCL:H121	2.48	0.49
1:L:177:ILE:HG12	5:L:302:BCL:HMB3	1.94	0.49
1:L:152:THR:O	1:L:155[B]:ASP:HB2	2.13	0.48
6:L:402:BPH:CHC	6:L:402:BPH:HBB3	2.38	0.48
5:M:501:BCL:HMB1	5:M:501:BCL:CBB	2.43	0.48
3:H:201:ASN:HD22	3:H:201:ASN:H	1.61	0.48
1:L:212:GLU:OE2	7:L:502[A]:U10:C3M	2.62	0.48
3:H:130[B]:LYS:HE3	3:H:172:PRO:HG2	1.96	0.47
1:L:216:PHE:CD2	7:L:502[A]:U10:H102	2.50	0.47
10:M:903:LDA:HM21	10:H:901:LDA:HM22	1.96	0.47
1:L:235[A]:LEU:HD11	7:L:502[A]:U10:H403	1.97	0.47
5:M:502:BCL:HBB3	5:M:502:BCL:HHC	1.95	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:63:THR:HA	3:H:73:LEU:O	2.16	0.46
1:L:157:VAL:HG11	5:M:502:BCL:HBB1	1.97	0.46
2:M:162:PHE:O	2:M:166:ILE:HG12	2.16	0.46
1:L:181:PHE:HB3	6:M:401:BPH:HBB2	1.98	0.46
5:M:501:BCL:HMB1	5:M:501:BCL:HBB2	1.98	0.46
1:L:181:PHE:CD2	6:M:401:BPH:HBB1	2.51	0.45
2:M:77:GLN:NE2	2:M:92:PHE:HB3	2.30	0.45
3:H:207:ALA:HB1	3:H:237:VAL:O	2.17	0.45
2:M:197:PHE:CE1	5:M:502:BCL:HBB2	2.50	0.45
7:L:502[B]:U10:C10	10:M:905:LDA:C12	2.94	0.45
2:M:133:THR:HG21	2:M:147:ALA:HA	1.99	0.45
1:L:69:PRO:HG2	1:L:142:TRP:HB2	1.99	0.44
2:M:136:ARG:NE	2:M:136:ARG:HA	2.33	0.44
3:H:75:VAL:HA	3:H:76:PRO:C	2.38	0.44
7:L:502[B]:U10:H271	7:L:502[B]:U10:H251	1.78	0.43
1:L:264:GLN:HA	1:L:267:VAL:CG1	2.48	0.43
1:L:173:HIS:CE1	1:L:177:ILE:HD11	2.54	0.43
10:M:902:LDA:HM22	11:H:958:HOH:O	2.19	0.43
1:L:190:HIS:HA	7:L:502[A]:U10:O2	2.18	0.43
7:L:502[B]:U10:H1M1	7:L:502[B]:U10:H71	1.87	0.42
2:M:290:VAL:HG21	3:H:12:LEU:HD23	2.00	0.42
3:H:233:ILE:O	3:H:237:VAL:HG13	2.19	0.42
2:M:148:TRP:CE2	9:M:800:CDL:H511	2.54	0.42
1:L:38:THR:HG22	1:L:99:SER:HB2	2.00	0.42
2:M:11:GLN:HB2	3:H:144:ALA:HB3	2.02	0.41
2:M:148:TRP:CD1	9:M:800:CDL:OB6	2.74	0.41
2:M:133:THR:CG2	2:M:147:ALA:HA	2.50	0.41
2:M:164[A]:ARG:HB3	2:M:165:PRO:HD3	2.03	0.41
1:L:208:THR:HB	1:L:209:PRO:HD2	2.03	0.41
3:H:40:TYR:HA	3:H:41:PRO:C	2.40	0.41
7:L:502[A]:U10:H351	7:L:502[A]:U10:H372	1.84	0.40
2:M:242:GLY:HA2	3:H:117[A]:ARG:HD3	2.04	0.40
2:M:164[B]:ARG:HB3	2:M:165:PRO:HD3	2.04	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	L	284/281 (101%)	278 (98%)	6 (2%)	0	100	100
2	M	303/307 (99%)	288 (95%)	14 (5%)	1 (0%)	46	75
3	H	247/260 (95%)	242 (98%)	4 (2%)	1 (0%)	39	69
All	All	834/848 (98%)	808 (97%)	24 (3%)	2 (0%)	52	80

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	79	GLY
3	H	245	ALA

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	225/220 (102%)	208 (92%)	17 (8%)	16	37
2	M	239/240 (100%)	224 (94%)	15 (6%)	22	48
3	H	203/208 (98%)	196 (97%)	7 (3%)	44	75
All	All	667/668 (100%)	628 (94%)	39 (6%)	27	52

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	21	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	38	THR
1	L	52	SER
1	L	54	VAL
1	L	72[A]	GLU
1	L	72[B]	GLU
1	L	126[A]	LEU
1	L	126[B]	LEU
1	L	155[A]	ASP
1	L	155[B]	ASP
1	L	185	LEU
1	L	207	ARG
1	L	210	ASP
1	L	216	PHE
1	L	247	CYS
1	L	271	TRP
1	L	272	TRP
2	M	12	VAL
2	M	32	VAL
2	M	50	ILE
2	M	52	LEU
2	M	60	LEU
2	M	62	SER
2	M	81	ASN
2	M	104	SER
2	M	109	LEU
2	M	124	VAL
2	M	132	ARG
2	M	133	THR
2	M	136	ARG
2	M	205	SER
2	M	216	PHE
3	H	28	ILE
3	H	70	ARG
3	H	201	ASN
3	H	202	ARG
3	H	225	VAL
3	H	231	ASP
3	H	250	SER

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

Mol	Chain	Res	Type
2	M	44	ASN
2	M	77	GLN
2	M	299	GLN
3	H	201	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 1 is monoatomic - leaving 18 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
10	LDA	H	901	-	15,15,15	4.04	2 (13%)	16,17,17	0.85	0
5	BCL	L	302	1	53,74,74	0.72	0	57,115,115	1.41	11 (19%)
5	BCL	L	304	1	53,74,74	0.81	0	57,115,115	1.59	10 (17%)
6	BPH	L	402	-	64,70,70	0.62	0	73,101,101	1.42	9 (12%)
7	U10	L	502[A]	-	48,48,63	1.12	3 (6%)	58,61,79	1.40	10 (17%)
7	U10	L	502[B]	-	48,48,63	1.01	3 (6%)	58,61,79	1.59	8 (13%)
10	LDA	L	904	-	15,15,15	4.08	2 (13%)	16,17,17	1.02	2 (12%)
10	LDA	L	908	-	15,15,15	3.31	1 (6%)	16,17,17	0.61	0
6	BPH	M	401	-	64,70,70	0.73	0	73,101,101	1.31	9 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	BCL	M	501	2	53,74,74	0.68	0	57,115,115	1.62	12 (21%)
5	BCL	M	502	2	53,74,74	0.76	1 (1%)	57,115,115	1.37	6 (10%)
7	U10	M	503	-	48,48,63	1.10	3 (6%)	58,61,79	1.44	9 (15%)
8	SP2	M	600	-	40,41,41	1.18	4 (10%)	47,50,50	1.71	13 (27%)
9	CDL	M	800	-	80,80,99	1.11	4 (5%)	82,92,111	1.18	8 (9%)
10	LDA	M	902	-	15,15,15	3.53	1 (6%)	16,17,17	1.33	2 (12%)
10	LDA	M	903	-	15,15,15	3.49	1 (6%)	16,17,17	0.69	0
10	LDA	M	905	-	15,15,15	3.52	2 (13%)	16,17,17	0.97	1 (6%)
10	LDA	M	906	-	15,15,15	3.44	1 (6%)	16,17,17	0.70	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	LDA	H	901	-	-	0/13/13/13	0/0/0/0
5	BCL	L	302	1	-	0/37/137/137	0/0/9/9
5	BCL	L	304	1	-	0/37/137/137	0/0/9/9
6	BPH	L	402	-	-	0/54/105/105	0/1/6/6
7	U10	L	502[A]	-	-	0/45/69/87	0/1/1/1
7	U10	L	502[B]	-	-	0/45/69/87	0/1/1/1
10	LDA	L	904	-	-	0/13/13/13	0/0/0/0
10	LDA	L	908	-	-	0/13/13/13	0/0/0/0
6	BPH	M	401	-	-	0/54/105/105	0/1/6/6
5	BCL	M	501	2	-	0/37/137/137	0/0/9/9
5	BCL	M	502	2	-	0/37/137/137	0/0/9/9
7	U10	M	503	-	-	0/45/69/87	0/1/1/1
8	SP2	M	600	-	-	0/47/47/47	0/0/0/0
9	CDL	M	800	-	-	0/91/91/110	0/0/0/0
10	LDA	M	902	-	-	0/13/13/13	0/0/0/0
10	LDA	M	903	-	-	0/13/13/13	0/0/0/0
10	LDA	M	905	-	-	0/13/13/13	0/0/0/0
10	LDA	M	906	-	-	0/13/13/13	0/0/0/0

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	L	904	LDA	O1-N1	-15.43	1.24	1.39
10	H	901	LDA	O1-N1	-15.39	1.24	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	M	902	LDA	O1-N1	-13.44	1.26	1.39
10	M	905	LDA	O1-N1	-13.41	1.26	1.39
10	M	903	LDA	O1-N1	-13.38	1.26	1.39
10	M	906	LDA	O1-N1	-13.18	1.27	1.39
10	L	908	LDA	O1-N1	-12.71	1.27	1.39
10	H	901	LDA	C1-N1	-2.40	1.47	1.51
10	L	904	LDA	C1-N1	-2.27	1.47	1.51
5	M	502	BCL	CBA-CGA	-2.18	1.44	1.50
10	M	905	LDA	C1-N1	-2.17	1.47	1.51
8	M	600	SP2	C15-C14	2.00	1.50	1.43
7	M	503	U10	C33-C34	2.01	1.36	1.33
7	L	502[B]	U10	C33-C34	2.03	1.36	1.33
8	M	600	SP2	C25-C26	2.08	1.37	1.33
7	L	502[A]	U10	C23-C24	2.15	1.37	1.33
7	L	502[A]	U10	O4-C4	2.53	1.43	1.37
8	M	600	SP2	C6-C5	2.61	1.37	1.34
7	M	503	U10	O4-C4	2.81	1.44	1.37
7	L	502[B]	U10	O4-C4	3.43	1.46	1.37
7	L	502[A]	U10	O3-C3	3.45	1.46	1.37
7	L	502[B]	U10	O3-C3	3.46	1.46	1.37
7	M	503	U10	O3-C3	3.70	1.46	1.37
9	M	800	CDL	OA6-CA5	3.95	1.46	1.34
9	M	800	CDL	OB8-CB7	4.30	1.46	1.33
9	M	800	CDL	OA8-CA7	4.45	1.46	1.33
9	M	800	CDL	OB6-CB5	4.60	1.48	1.34
8	M	600	SP2	C16-C17	4.75	1.58	1.43

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	501	BCL	CMB-C2B-C1B	-5.24	119.69	128.36
7	M	503	U10	C26-C27-C28	-4.42	100.12	111.69
5	L	304	BCL	CAC-C3C-C2C	-4.27	103.39	114.13
7	M	503	U10	C32-C33-C34	-3.79	119.52	127.76
5	M	502	BCL	O2D-CGD-O1D	-3.55	116.45	123.79
8	M	600	SP2	C15-C14-C13	-3.54	122.08	127.20
10	M	902	LDA	CM2-N1-CM1	-3.47	104.92	108.83
5	L	304	BCL	O1D-CGD-CBD	-3.41	119.74	124.62
10	M	902	LDA	O1-N1-C1	-3.32	106.53	110.27
5	M	501	BCL	C6-C5-C3	-3.23	105.39	112.48
5	L	304	BCL	CMB-C2B-C1B	-3.22	123.03	128.36
5	L	302	BCL	CAC-C3C-C4C	-3.21	105.46	112.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	502[B]	U10	C35-C34-C33	-3.18	117.26	123.50
6	L	402	BPH	C2B-C1B-NB	-3.12	105.04	109.73
8	M	600	SP2	CM4-C9-C10	-3.08	118.36	122.90
8	M	600	SP2	C16-C17-C18	-3.04	122.80	127.20
10	L	904	LDA	O1-N1-CM2	-2.98	105.07	109.05
5	M	502	BCL	CAC-C3C-C4C	-2.93	106.09	112.58
7	L	502[A]	U10	O2-C2-C3	-2.92	114.46	120.79
7	L	502[A]	U10	C17-C18-C19	-2.91	121.43	127.76
5	L	302	BCL	CAA-C2A-C3A	-2.91	104.84	113.22
7	M	503	U10	C31-C29-C28	-2.90	115.54	121.05
5	L	302	BCL	CMB-C2B-C1B	-2.83	123.67	128.36
6	M	401	BPH	CAA-C2A-C3A	-2.83	105.08	113.22
5	M	502	BCL	CHA-C1A-NA	-2.80	119.16	126.06
7	L	502[B]	U10	C31-C29-C28	-2.80	115.73	121.05
6	M	401	BPH	C2B-C1B-NB	-2.79	105.55	109.73
6	L	402	BPH	C3B-C4B-NB	-2.75	104.13	109.98
5	L	304	BCL	CAC-C3C-C4C	-2.75	106.49	112.58
5	L	302	BCL	CHA-C1A-NA	-2.72	119.36	126.06
5	M	502	BCL	OB B-CAB-CBB	-2.63	113.84	120.13
7	M	503	U10	C22-C23-C24	-2.62	122.06	127.76
5	M	501	BCL	CHA-C1A-NA	-2.61	119.64	126.06
5	L	302	BCL	C11-C12-C13	-2.58	106.93	115.49
6	L	402	BPH	OBD-CAD-CBD	-2.57	122.05	125.94
10	M	905	LDA	O1-N1-C1	-2.54	107.41	110.27
7	L	502[A]	U10	C35-C34-C33	-2.54	118.52	123.50
5	L	304	BCL	CAA-C2A-C3A	-2.51	105.99	113.22
9	M	800	CDL	OA6-CA5-OA7	-2.50	116.96	123.67
6	M	401	BPH	C3B-C4B-NB	-2.45	104.78	109.98
5	L	302	BCL	C17-C16-C15	-2.44	100.88	112.99
9	M	800	CDL	OA8-CA7-OA9	-2.42	117.26	123.49
5	M	501	BCL	C11-C12-C13	-2.39	107.55	115.49
5	L	302	BCL	C5-C3-C2	-2.36	116.57	121.05
7	L	502[B]	U10	C22-C23-C24	-2.34	122.67	127.76
5	L	302	BCL	OBD-CAD-CBD	-2.33	122.43	125.94
5	L	304	BCL	C5-C3-C2	-2.32	116.64	121.05
5	M	501	BCL	OB B-CAB-CBB	-2.32	114.56	120.13
7	L	502[A]	U10	C22-C23-C24	-2.30	122.77	127.76
7	M	503	U10	C35-C34-C33	-2.28	119.03	123.50
6	L	402	BPH	C1C-NC-C4C	-2.27	108.11	110.44
8	M	600	SP2	C4-C5-C6	-2.27	115.90	122.35
5	L	304	BCL	CAA-C2A-C1A	-2.23	104.59	112.47
8	M	600	SP2	C19-C18-C17	-2.22	115.40	118.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	M	800	CDL	CB6-CB4-CB3	-2.21	106.91	112.07
8	M	600	SP2	C11-C10-C9	-2.18	124.05	127.20
8	M	600	SP2	C10-C11-C12	-2.13	116.64	123.13
5	L	302	BCL	O2A-CGA-O1A	-2.13	118.00	123.49
7	L	502[A]	U10	C15-C14-C13	-2.11	119.36	123.50
8	M	600	SP2	C21-C20-C19	-2.11	116.70	123.13
6	L	402	BPH	O2D-CGD-O1D	-2.10	119.45	123.79
6	M	401	BPH	CMA-C3A-C2A	-2.07	105.19	114.35
10	L	904	LDA	O1-N1-CM1	-2.07	106.29	109.05
7	L	502[B]	U10	C16-C14-C13	-2.03	117.20	121.05
7	L	502[A]	U10	C1-C6-C5	-2.02	117.81	120.12
7	M	503	U10	C4M-O4-C4	2.06	123.94	116.61
7	L	502[A]	U10	C3M-O3-C3	2.08	124.00	116.61
6	M	401	BPH	CMD-C2D-C3D	2.11	129.21	125.09
9	M	800	CDL	OB8-CB7-C71	2.12	118.35	111.90
7	M	503	U10	C15-C14-C16	2.18	118.73	115.41
8	M	600	SP2	CM8-C26-C27	2.28	118.90	115.41
7	L	502[A]	U10	C30-C29-C31	2.35	118.99	115.41
5	L	304	BCL	C2C-C3C-C4C	2.39	105.55	101.50
5	M	501	BCL	CAA-CBA-CGA	2.42	120.42	113.32
5	L	302	BCL	OBB-CAB-C3B	2.43	123.85	120.00
7	M	503	U10	C35-C34-C36	2.47	119.17	115.41
5	M	501	BCL	C5-C3-C2	2.47	125.74	121.05
7	L	502[A]	U10	C36-C34-C33	2.57	125.93	121.05
6	M	401	BPH	O2D-CGD-CBD	2.61	114.88	111.30
8	M	600	SP2	C3-C4-C5	2.64	118.29	112.48
8	M	600	SP2	CM4-C9-C8	2.71	122.61	118.10
5	M	501	BCL	OBB-CAB-C3B	2.72	124.31	120.00
5	M	501	BCL	C1D-CHD-C4C	2.73	130.24	126.07
6	M	401	BPH	C1B-NB-C4B	2.83	112.11	106.51
5	L	302	BCL	C4-C3-C5	2.83	119.74	115.41
9	M	800	CDL	CB6-OB8-CB7	2.85	124.83	116.85
5	L	304	BCL	OBB-CAB-C3B	2.86	124.54	120.00
5	M	501	BCL	O2D-CGD-CBD	2.90	115.27	111.30
6	M	401	BPH	CHC-C4B-NB	2.97	130.57	124.91
6	L	402	BPH	O2D-CGD-CBD	2.99	115.39	111.30
7	L	502[A]	U10	C25-C24-C26	2.99	119.98	115.41
5	M	501	BCL	C2C-C3C-C4C	3.00	106.59	101.50
5	M	502	BCL	OBB-CAB-C3B	3.09	124.90	120.00
9	M	800	CDL	OA8-CA7-C31	3.20	121.66	111.90
5	M	501	BCL	CMB-C2B-C3B	3.32	131.58	125.09
8	M	600	SP2	CM7-C22-C23	3.39	120.58	115.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	502[B]	U10	C25-C24-C26	3.42	120.63	115.41
6	L	402	BPH	C1B-NB-C4B	3.57	113.56	106.51
7	L	502[B]	U10	C15-C14-C16	3.68	121.03	115.41
7	L	502[B]	U10	C30-C29-C31	3.79	121.20	115.41
6	L	402	BPH	CAC-C3C-C4C	3.81	122.46	112.67
6	M	401	BPH	C3C-C4C-NC	3.85	111.79	107.93
5	L	304	BCL	O2D-CGD-CBD	3.90	116.65	111.30
9	M	800	CDL	OA6-CA5-C11	4.08	120.39	111.53
7	M	503	U10	C30-C29-C31	4.14	121.73	115.41
8	M	600	SP2	CM3-C5-C4	4.29	121.95	115.41
7	L	502[B]	U10	C20-C19-C21	4.53	122.33	115.41
6	L	402	BPH	C3C-C4C-NC	4.59	112.53	107.93
9	M	800	CDL	OB6-CB5-C51	4.73	121.80	111.53
5	M	502	BCL	O2D-CGD-CBD	4.96	118.10	111.30

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	H	901	LDA	1	0
5	L	302	BCL	4	0
5	L	304	BCL	1	0
6	L	402	BPH	5	0
7	L	502[A]	U10	5	0
7	L	502[B]	U10	5	0
6	M	401	BPH	8	0
5	M	501	BCL	3	0
5	M	502	BCL	6	0
9	M	800	CDL	2	0
10	M	902	LDA	1	0
10	M	903	LDA	2	0
10	M	905	LDA	1	0

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	L	281/281 (100%)	-0.68	4 (1%) 78 77	38, 47, 61, 67	0
2	M	302/307 (98%)	-0.60	6 (1%) 68 69	41, 48, 59, 85	0
3	H	241/260 (92%)	-0.47	9 (3%) 45 45	39, 46, 60, 94	0
All	All	824/848 (97%)	-0.59	19 (2%) 64 64	38, 47, 60, 94	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	250	SER	5.7
2	M	1	ALA	5.6
3	H	249	LYS	4.4
2	M	302	GLY	4.0
2	M	301	HIS	3.9
2	M	2	GLU	3.7
3	H	245	ALA	3.6
3	H	10	PHE	3.4
3	H	246	PRO	3.4
1	L	202	LYS	3.0
2	M	100	GLU	2.8
1	L	281	GLY	2.7
3	H	52	ASN	2.6
3	H	60	LYS	2.5
2	M	87	ARG	2.3
3	H	80	SER	2.3
1	L	59	TRP	2.2
1	L	270	PRO	2.2
3	H	51	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
10	LDA	L	908	16/16	0.62	0.33	10.63	57,61,77,78	16
7	U10	L	502[A]	48/63	0.74	0.36	8.88	61,69,71,72	48
7	U10	L	502[B]	48/63	0.74	0.36	7.45	52,61,74,74	48
10	LDA	M	905	16/16	0.67	0.34	6.81	52,56,60,61	16
10	LDA	L	904	16/16	0.69	0.38	6.53	52,55,57,57	16
10	LDA	M	906	16/16	0.44	0.40	5.46	53,56,63,63	16
10	LDA	M	903	16/16	0.67	0.31	4.21	52,57,64,65	16
10	LDA	M	902	16/16	0.85	0.21	3.42	61,62,68,69	16
9	CDL	M	800	81/100	0.76	0.30	2.37	47,60,68,71	81
6	BPH	M	401	65/65	0.93	0.14	1.68	47,51,100,102	0
8	SP2	M	600	42/42	0.87	0.21	1.66	52,61,83,84	0
5	BCL	M	501	66/66	0.93	0.14	1.52	42,48,101,103	0
7	U10	M	503	48/63	0.93	0.16	1.37	44,56,82,83	0
5	BCL	M	502	66/66	0.96	0.13	0.65	40,43,68,78	0
10	LDA	H	901	16/16	0.94	0.14	0.46	60,64,71,72	16
5	BCL	L	302	66/66	0.96	0.12	0.30	35,43,60,65	0
6	BPH	L	402	65/65	0.97	0.11	0.10	39,46,54,55	0
5	BCL	L	304	66/66	0.97	0.10	-0.60	36,44,62,65	0
4	FE	M	500	1/1	1.00	0.04	-1.70	49,49,49,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.