



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:49 AM GMT

PDB ID : 2UWU  
Title : X-RAY HIGH RESOLUTION STRUCTURE OF THE PHOTOSYNTHETIC REACTION CENTER FROM RB. SPHAEROIDES AT PH 6.5 IN THE NEUTRAL STATE, 2ND DATASET  
Authors : Koepke, J.; Diehm, R.; Fritzsche, G.  
Deposited on : 2007-03-23  
Resolution : 2.04 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](mailto: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.

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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 : 1.7 (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

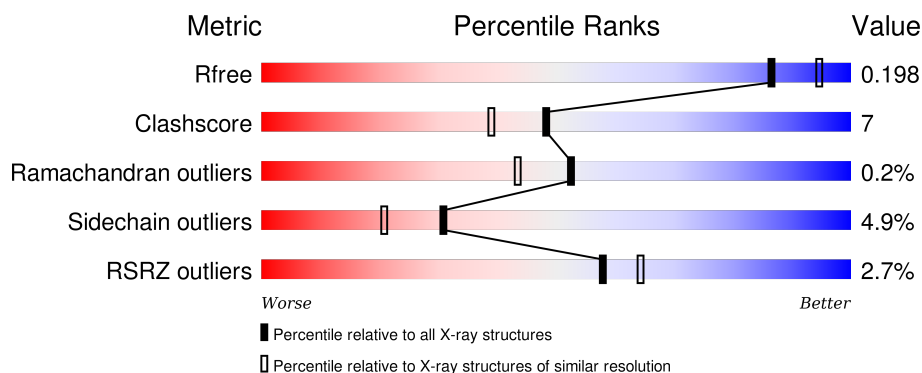
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.04 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	1192 (2.04-2.04)
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)
RSRZ outliers	91569	1194 (2.04-2.04)

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. 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	H	260	<div> <div>2%</div> <div> <div></div> <div>80%</div> <div>12%</div> <div>7%</div> </div> </div>
2	L	281	<div> <div>2%</div> <div> <div></div> <div>88%</div> <div>10%</div> <div></div> </div> </div>
3	M	307	<div> <div>3%</div> <div> <div></div> <div>85%</div> <div>12%</div> <div></div> </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	HTO	L	1290	-	-	-	X
13	SPO	M	1314	-	-	-	X
14	CDL	M	1315	-	-	-	X
4	GOL	H	1251	-	-	X	X
4	GOL	L	1293	-	-	-	X
5	BCL	L	1282	X	-	-	-
5	BCL	L	1288	X	-	-	-
5	BCL	M	1303	X	-	-	-
5	BCL	M	1304	X	-	-	-
6	LDA	L	1283	-	-	-	X
6	LDA	L	1284	-	-	-	X
6	LDA	L	1285	-	-	-	X
6	LDA	M	1305	-	-	-	X
6	LDA	M	1306	-	-	-	X
6	LDA	M	1307	-	-	-	X
6	LDA	M	1308	-	-	-	X
6	LDA	M	1309	-	-	-	X
8	UQ2	L	1287[A]	-	-	-	X
8	UQ2	L	1287[B]	-	-	-	X

## 2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 7785 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 H CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	241	Total	C	N	O	S	0	0	1
			1830	1169	315	337	9			

- Molecule 2 is a protein called REACTION CENTER PROTEIN L CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	281	Total	C	N	O	S	0	0	0
			2232	1507	355	362	8			

- Molecule 3 is a protein called REACTION CENTER PROTEIN M CHAIN.

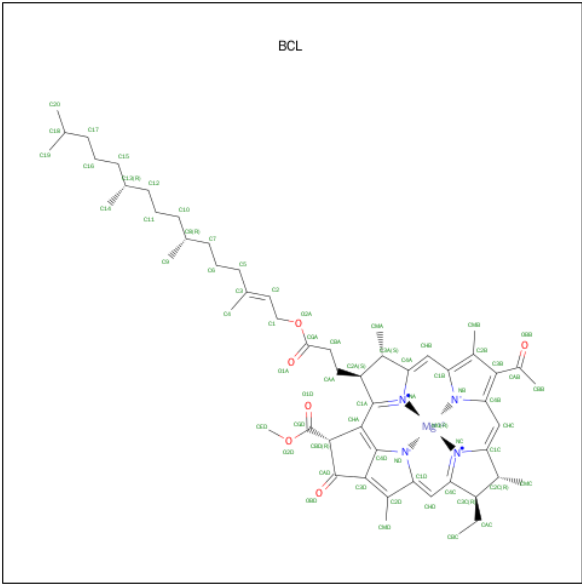
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	303	Total	C	N	O	S	0	0	1
			2409	1607	395	397	10			

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



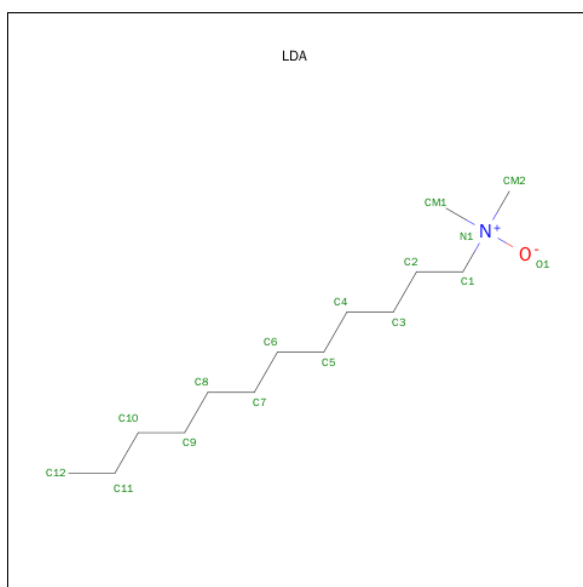
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	L	1	Total	C	O	0	0
			6	3	3		
4	L	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C<sub>55</sub>H<sub>74</sub>MgN<sub>4</sub>O<sub>6</sub>).



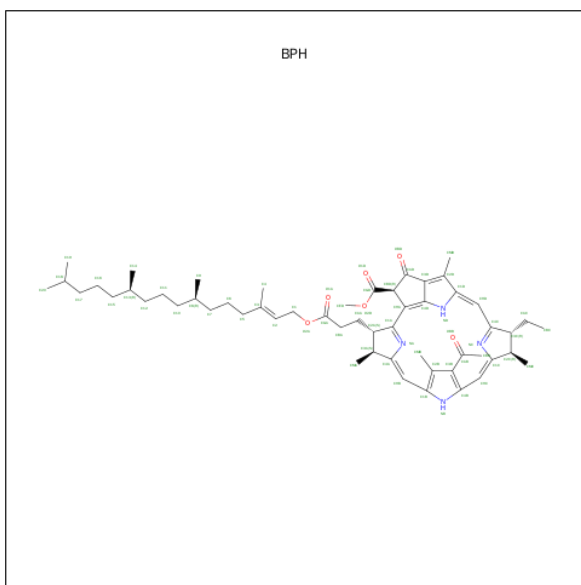
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 6 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: C<sub>14</sub>H<sub>31</sub>NO).



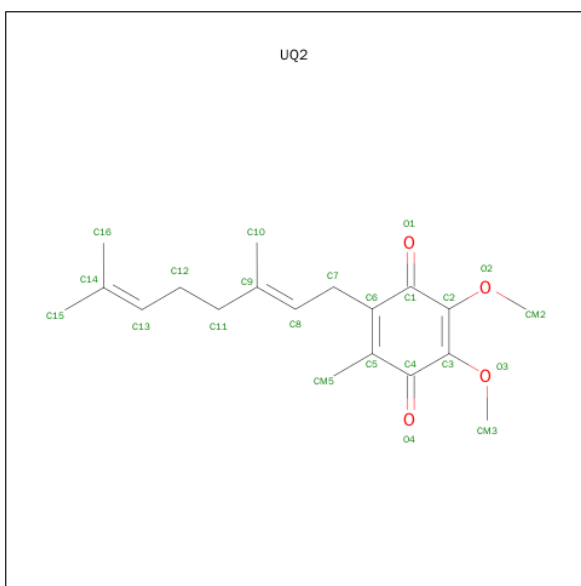
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	L	1	Total	C	N	O	0	0
			16	14	1	1		
6	L	1	Total	C	N	O	0	0
			16	14	1	1		
6	L	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1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

- Molecule 7 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula:  $C_{55}H_{76}N_4O_6$ ).



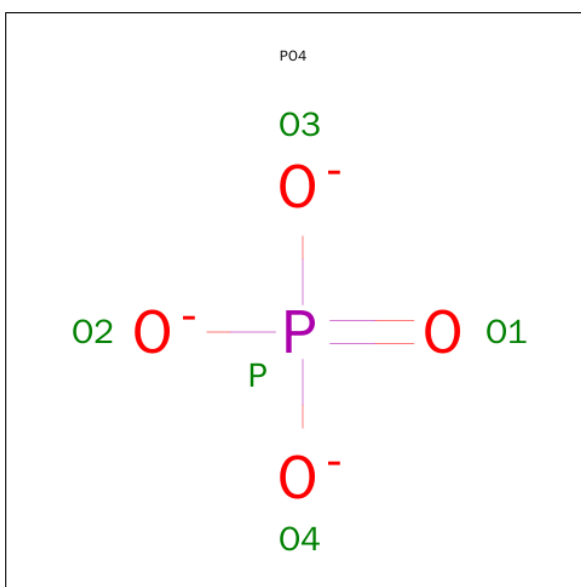
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	L	1	Total	C	N	O	0	0
			65	55	4	6		
7	M	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 8 is UBIQUINONE-2 (three-letter code: UQ2) (formula:  $C_{19}H_{26}O_4$ ).



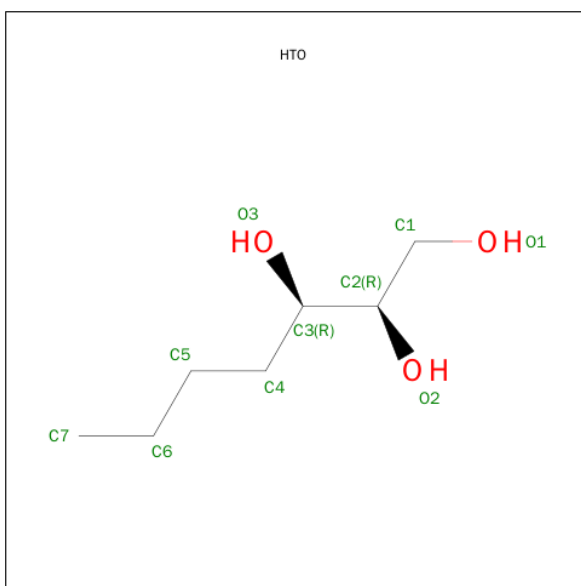
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	L	1	Total	C	O	0	1
			46	38	8		

- Molecule 9 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	L	1	Total	O	P	0	0
			5	4	1		

- Molecule 10 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula:  $C_7H_{16}O_3$ ).



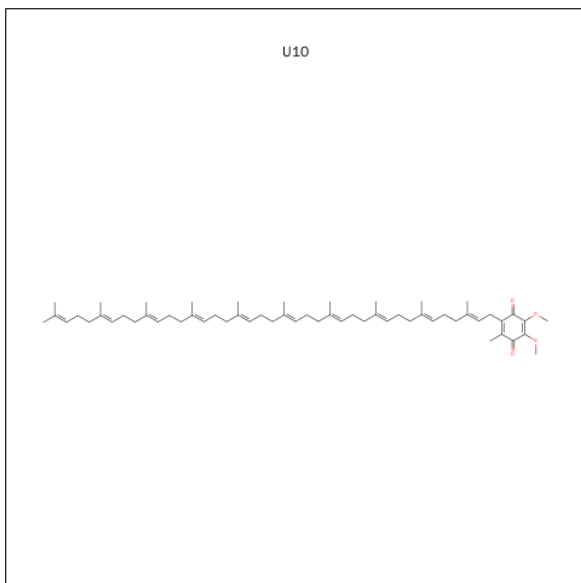
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	L	1	Total	C	O	0	0
			10	7	3		
10	L	1	Total	C	O	0	0
			10	7	3		

- Molecule 11 is FE (III) ION (three-letter code: FE) (formula: Fe).



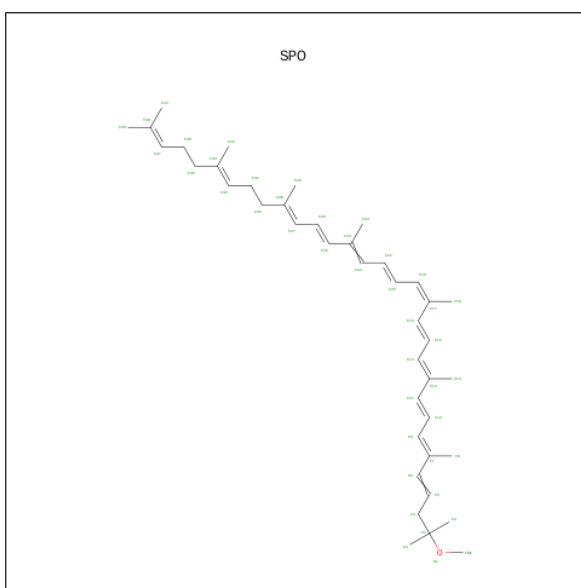
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	M	1	Total	Fe	0	0
			1	1		

- Molecule 12 is UBIQUINONE-10 (three-letter code: U10) (formula:  $C_{59}H_{90}O_4$ ).



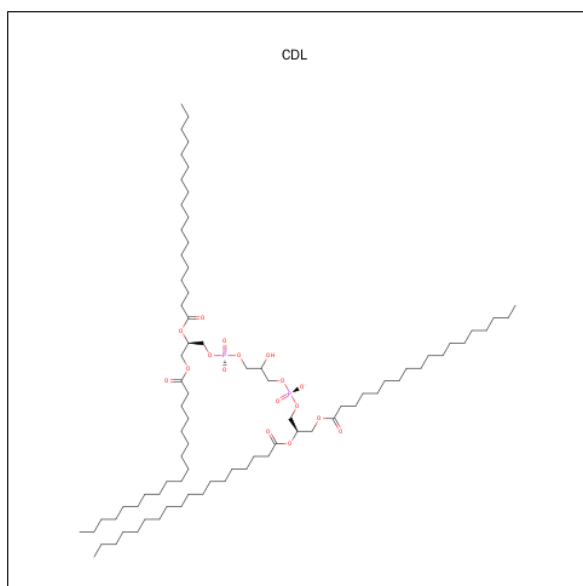
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	M	1	Total	C	O	0	0
			48	44	4		

- Molecule 13 is SPHEROIDENE (three-letter code: SPO) (formula:  $C_{41}H_{60}O$ ).



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

- Molecule 14 is CARDIOLIPIN (three-letter code: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).



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

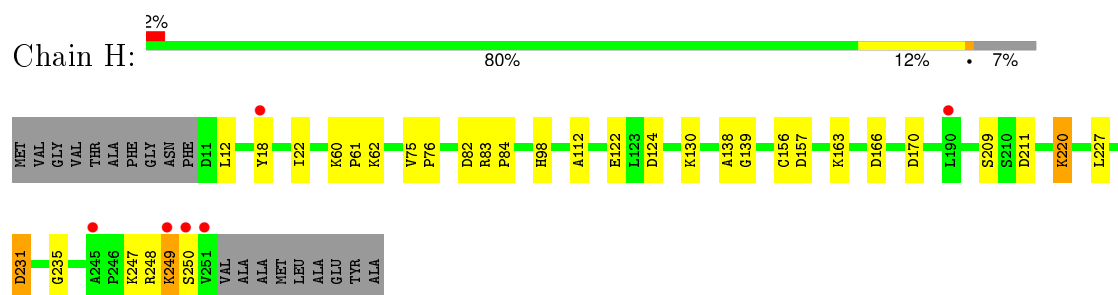
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	H	213	Total	O	0	0
			213	213		
15	L	136	Total	O	0	0
			136	136		
15	M	148	Total	O	0	0
			148	148		

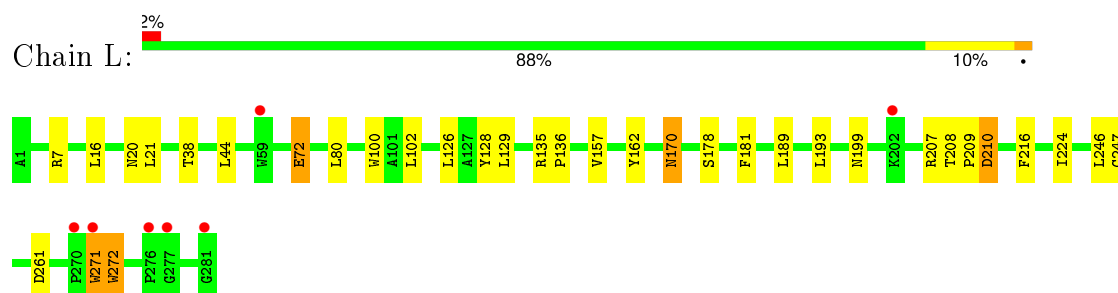
### 3 Residue-property plots [i](#)

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.

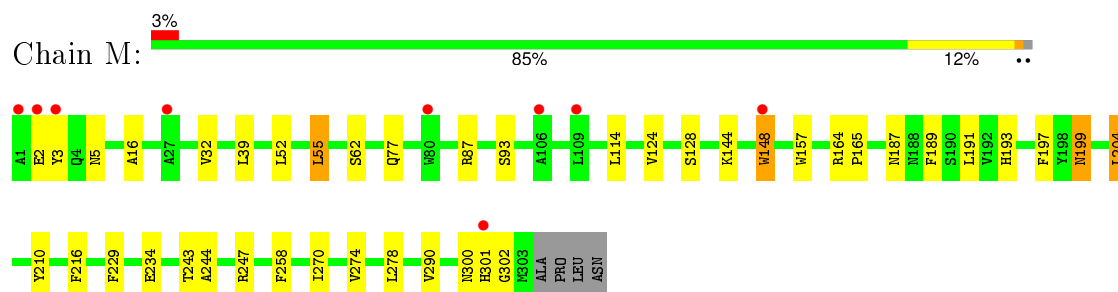
#### • Molecule 1: REACTION CENTER PROTEIN H CHAIN



#### • Molecule 2: REACTION CENTER PROTEIN L CHAIN



#### • Molecule 3: REACTION CENTER PROTEIN M CHAIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	139.45Å 139.45Å 184.39Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	119.52 – 2.04 24.79 – 2.04	Depositor EDS
% Data completeness (in resolution range)	97.2 (119.52-2.04) 88.1 (24.79-2.04)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.22 (at 2.04Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.208 , 0.232 0.199 , 0.198	Depositor DCC
$R_{free}$ test set	2580 reflections (2.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.1	Xtriage
Anisotropy	0.202	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 60.6	EDS
Estimated twinning fraction	0.020 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 128453 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7785	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BCL, GOL, LDA, CDL, BPH, PO4, HTO, FE, SPO, U10, UQ2

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	H	0.74	0/1878	0.82	7/2555 (0.3%)
2	L	0.76	0/2320	0.72	1/3175 (0.0%)
3	M	0.75	0/2501	0.72	2/3415 (0.1%)
All	All	0.75	0/6699	0.75	10/9145 (0.1%)

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
1	H	0	1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	82	ASP	CB-CG-OD2	6.52	124.17	118.30
1	H	231	ASP	CB-CG-OD2	6.31	123.97	118.30
1	H	166	ASP	CB-CG-OD2	6.20	123.88	118.30
1	H	83	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	H	139	GLY	N-CA-C	-5.73	98.78	113.10
3	M	204	LEU	CB-CG-CD1	5.56	120.45	111.00
1	H	157	ASP	CB-CG-OD2	5.40	123.16	118.30
3	M	234	GLU	OE1-CD-OE2	-5.34	116.89	123.30
2	L	261	ASP	CB-CG-OD2	5.24	123.02	118.30
1	H	211	ASP	CB-CG-OD2	5.21	122.99	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	138	ALA	Peptide

## 5.2 Too-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 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	H	1830	0	1836	19	0
2	L	2232	0	2187	25	0
3	M	2409	0	2321	31	0
4	H	24	0	32	5	0
4	L	12	0	16	1	0
5	L	132	0	148	6	0
5	M	132	0	148	17	0
6	L	48	0	93	2	0
6	M	96	0	186	5	0
7	L	65	0	76	7	0
7	M	65	0	76	13	0
8	L	46	0	52	5	0
9	L	5	0	0	0	0
10	L	20	0	32	0	0
11	M	1	0	0	0	0
12	M	48	0	63	0	0
13	M	42	0	60	3	0
14	M	81	0	86	5	0
15	H	213	0	0	5	0
15	L	136	0	0	0	0
15	M	148	0	0	0	0
All	All	7785	0	7412	107	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 7.

All (107) 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)
7:L:1286:BPH:HBB3	7:L:1286:BPH:HHC	1.43	0.96
3:M:197:PHE:HZ	5:M:1304:BCL:HBB2	1.40	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:197:PHE:CZ	5:M:1304:BCL:HBB2	2.13	0.82
5:L:1282:BCL:HHC	5:L:1282:BCL:HBB2	1.62	0.82
1:H:248:ARG:HA	1:H:249:LYS:CB	2.17	0.73
2:L:181:PHE:CD2	7:M:1312:BPH:HBB1	2.23	0.73
7:L:1286:BPH:HHC	7:L:1286:BPH:CBB	2.20	0.71
1:H:248:ARG:HA	1:H:249:LYS:HB3	1.73	0.71
3:M:62:SER:OG	3:M:124:VAL:HG22	1.91	0.71
2:L:181:PHE:HB3	7:M:1312:BPH:HBB2	1.72	0.71
4:H:1251:GOL:C3	15:H:2009:HOH:O	2.41	0.68
7:M:1312:BPH:HHD	7:M:1312:BPH:HBC3	1.76	0.68
5:M:1304:BCL:CBB	5:M:1304:BCL:HHC	2.25	0.67
3:M:144:LYS:N	14:M:1315:CDL:OB3	2.25	0.64
3:M:189:PHE:O	3:M:193:HIS:HD2	1.80	0.64
1:H:62:LYS:HE3	4:H:1251:GOL:H11	1.77	0.64
7:M:1312:BPH:HBB3	7:M:1312:BPH:HHC	1.81	0.63
4:H:1251:GOL:H31	15:H:2009:HOH:O	1.96	0.63
5:M:1304:BCL:HHC	5:M:1304:BCL:HBB3	1.81	0.63
3:M:157:TRP:HB2	5:M:1304:BCL:H71	1.81	0.62
6:L:1284:LDA:H111	6:L:1284:LDA:H62	1.84	0.59
1:H:130:LYS:HE3	1:H:170:ASP:OD2	2.02	0.59
5:M:1303:BCL:CBB	5:M:1303:BCL:HHC	2.33	0.58
7:L:1286:BPH:HBB2	3:M:210:TYR:HB3	1.85	0.58
2:L:181:PHE:HB3	7:M:1312:BPH:CBB	2.34	0.58
5:L:1282:BCL:HHC	5:L:1282:BCL:CBB	2.33	0.58
2:L:199:ASN:HA	4:L:1292:GOL:H31	1.87	0.57
5:M:1303:BCL:HBB2	13:M:1314:SPO:H243	1.86	0.57
5:M:1303:BCL:HBB3	5:M:1304:BCL:H41	1.87	0.56
2:L:170:ASN:C	2:L:170:ASN:HD22	2.09	0.56
2:L:157:VAL:HG11	5:M:1304:BCL:HBB1	1.87	0.56
7:M:1312:BPH:HHC	7:M:1312:BPH:CBB	2.36	0.55
3:M:300:ASN:C	3:M:302:GLY:H	2.10	0.55
6:M:1307:LDA:H81	6:M:1308:LDA:H62	1.89	0.55
7:L:1286:BPH:CHC	7:L:1286:BPH:HBB3	2.27	0.55
2:L:224:ILE:HG22	8:L:1287[B]:UQ2:H8	1.88	0.55
3:M:77:GLN:HE22	3:M:93:SER:H	1.53	0.54
5:M:1303:BCL:CBB	13:M:1314:SPO:H243	2.37	0.54
4:H:1251:GOL:H32	15:H:2009:HOH:O	2.04	0.54
5:L:1282:BCL:H192	7:L:1286:BPH:H7C2	1.89	0.53
7:M:1312:BPH:HBB3	7:M:1312:BPH:CHC	2.39	0.52
5:L:1288:BCL:CBB	5:L:1288:BCL:HMB1	2.39	0.52
2:L:193:LEU:HD23	8:L:1287[B]:UQ2:C4	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:189:PHE:O	3:M:193:HIS:CD2	2.63	0.52
1:H:62:LYS:CE	4:H:1251:GOL:H11	2.40	0.51
15:H:2009:HOH:O	14:M:1315:CDL:HA32	2.10	0.51
1:H:98:HIS:CD2	2:L:7:ARG:HH21	2.29	0.51
2:L:135:ARG:HB3	2:L:136:PRO:HD3	1.93	0.51
2:L:128:TYR:HD1	5:L:1282:BCL:HBB1	1.76	0.50
3:M:197:PHE:HZ	5:M:1304:BCL:CBB	2.17	0.49
2:L:199:ASN:O	14:M:1315:CDL:HB22	2.12	0.49
2:L:272:TRP:CD1	3:M:87:ARG:HG3	2.47	0.49
2:L:208:THR:HB	2:L:209:PRO:HD2	1.95	0.49
7:L:1286:BPH:CHC	7:L:1286:BPH:CBB	2.88	0.49
3:M:55:LEU:HD22	3:M:128:SER:HB2	1.95	0.49
3:M:229:PHE:HB2	3:M:244:ALA:HB2	1.93	0.49
1:H:75:VAL:HA	1:H:76:PRO:C	2.34	0.48
2:L:162:TYR:OH	3:M:187:ASN:ND2	2.46	0.48
5:M:1304:BCL:HAA2	5:M:1304:BCL:HBD	1.94	0.48
2:L:189:LEU:HD23	7:M:1312:BPH:HMD2	1.94	0.48
8:L:1287[B]:UQ2:H71	8:L:1287[B]:UQ2:H5M1	1.69	0.47
5:M:1303:BCL:H102	5:M:1303:BCL:H13	1.65	0.47
3:M:270:ILE:O	3:M:274:VAL:HG13	2.15	0.47
3:M:3:TYR:CZ	3:M:5:ASN:HA	2.50	0.47
1:H:112:ALA:HA	1:H:235:GLY:O	2.15	0.46
1:H:209:SER:OG	1:H:247:LYS:HD2	2.16	0.46
5:M:1303:BCL:HBB2	5:M:1303:BCL:HHC	1.97	0.46
3:M:199:ASN:C	3:M:199:ASN:HD22	2.18	0.46
3:M:258:PHE:HB3	6:M:1307:LDA:H31	1.97	0.46
6:M:1310:LDA:H62	7:M:1312:BPH:H162	1.97	0.46
7:L:1286:BPH:HBB1	3:M:210:TYR:CD2	2.51	0.46
5:L:1288:BCL:HBB3	5:L:1288:BCL:HMB1	1.98	0.46
3:M:148:TRP:HA	3:M:148:TRP:CE3	2.51	0.45
6:M:1305:LDA:H92	6:M:1307:LDA:H121	1.99	0.45
1:H:122:GLU:HB2	1:H:227:LEU:HD21	1.99	0.45
2:L:189:LEU:HB3	8:L:1287[A]:UQ2:H3M3	1.99	0.44
3:M:164:ARG:HB3	3:M:165:PRO:HD3	1.99	0.44
3:M:148:TRP:HA	3:M:148:TRP:HE3	1.83	0.44
1:H:98:HIS:HD2	2:L:7:ARG:HH21	1.66	0.44
3:M:16:ALA:HB1	3:M:32:VAL:HG11	2.01	0.43
8:L:1287[A]:UQ2:H101	8:L:1287[A]:UQ2:H121	1.74	0.43
3:M:278:LEU:HD21	14:M:1315:CDL:H782	2.00	0.43
7:M:1312:BPH:CHD	7:M:1312:BPH:HBC3	2.47	0.42
3:M:300:ASN:C	3:M:302:GLY:N	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:72:GLU:H	2:L:72:GLU:HG3	1.54	0.42
1:H:220:LYS:HE3	15:H:2123:HOH:O	2.19	0.42
7:M:1312:BPH:CBC	7:M:1312:BPH:HHD	2.48	0.42
2:L:178:SER:HB3	6:L:1285:LDA:H62	2.02	0.42
3:M:148:TRP:NE1	14:M:1315:CDL:OB6	2.52	0.42
1:H:124:ASP:HB2	2:L:210:ASP:OD2	2.20	0.42
5:M:1303:BCL:H101	5:M:1304:BCL:H171	2.02	0.42
3:M:187:ASN:HD22	5:M:1304:BCL:CBC	2.32	0.42
7:M:1312:BPH:CHC	7:M:1312:BPH:CBB	2.98	0.42
6:M:1307:LDA:H32	6:M:1308:LDA:H42	2.02	0.42
1:H:248:ARG:CA	1:H:249:LYS:CB	2.94	0.41
1:H:18:TYR:CZ	1:H:22:ILE:HD11	2.55	0.41
2:L:210:ASP:OD1	2:L:210:ASP:N	2.52	0.41
1:H:12:LEU:HD23	3:M:290:VAL:HG21	2.01	0.41
2:L:271:TRP:N	2:L:271:TRP:CD1	2.72	0.41
2:L:189:LEU:CD2	7:M:1312:BPH:HMD2	2.51	0.40
3:M:243:THR:O	3:M:247:ARG:HG3	2.21	0.40
3:M:157:TRP:CE2	13:M:1314:SPO:H293	2.56	0.40
1:H:248:ARG:HA	1:H:249:LYS:HB2	2.00	0.40
5:M:1304:BCL:CBB	5:M:1304:BCL:CHC	2.95	0.40
1:H:156:CYS:SG	1:H:248:ARG:HB2	2.61	0.40
1:H:60:LYS:HA	1:H:61:PRO:HD3	1.94	0.40
2:L:38:THR:HG21	2:L:100:TRP:HE3	1.86	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	239/260 (92%)	236 (99%)	2 (1%)	1 (0%)	39	28
2	L	279/281 (99%)	272 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	M	301/307 (98%)	289 (96%)	11 (4%)	1 (0%)	46	36
All	All	819/848 (97%)	797 (97%)	20 (2%)	2 (0%)	52	43

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	249	LYS
3	M	301	HIS

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	195/208 (94%)	190 (97%)	5 (3%)	54	47
2	L	220/220 (100%)	203 (92%)	17 (8%)	16	7
3	M	236/240 (98%)	226 (96%)	10 (4%)	36	28
All	All	651/668 (98%)	619 (95%)	32 (5%)	31	21

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	84	PRO
1	H	163	LYS
1	H	220	LYS
1	H	231	ASP
1	H	250	SER
2	L	16	LEU
2	L	20	ASN
2	L	21	LEU
2	L	44	LEU
2	L	72	GLU
2	L	80	LEU
2	L	102	LEU
2	L	126	LEU

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Mol	Chain	Res	Type
2	L	129	LEU
2	L	170	ASN
2	L	207	ARG
2	L	210	ASP
2	L	216	PHE
2	L	246	LEU
2	L	247	CYS
2	L	271	TRP
2	L	272	TRP
3	M	2	GLU
3	M	39	LEU
3	M	52	LEU
3	M	55	LEU
3	M	114	LEU
3	M	148	TRP
3	M	191	LEU
3	M	199	ASN
3	M	204	LEU
3	M	216	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	98	HIS
1	H	141	HIS
2	L	20	ASN
2	L	159	ASN
2	L	170	ASN
2	L	183	ASN
2	L	264	GLN
3	M	77	GLN
3	M	187	ASN
3	M	193	HIS
3	M	199	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules 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 ⓘ

Of 30 ligands modelled in this entry, 1 is monoatomic - leaving 29 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$
4	GOL	H	1251	-	5,5,5	0.57	0	5,5,5	1.08	0
4	GOL	H	1252	-	5,5,5	0.37	0	5,5,5	0.36	0
4	GOL	H	1253	-	5,5,5	0.37	0	5,5,5	0.17	0
4	GOL	H	1254	-	5,5,5	0.31	0	5,5,5	0.33	0
5	BCL	L	1282	2	53,74,74	2.01	6 (11%)	57,115,115	1.92	12 (21%)
6	LDA	L	1283	-	15,15,15	3.74	1 (6%)	16,17,17	0.76	0
6	LDA	L	1284	-	15,15,15	3.73	1 (6%)	16,17,17	0.63	0
6	LDA	L	1285	-	15,15,15	3.78	2 (13%)	16,17,17	0.55	0
7	BPH	L	1286	-	64,70,70	2.82	17 (26%)	73,101,101	1.87	15 (20%)
8	UQ2	L	1287[A]	-	23,23,23	2.75	7 (30%)	28,31,31	1.22	3 (10%)
8	UQ2	L	1287[B]	-	23,23,23	2.66	8 (34%)	28,31,31	1.66	7 (25%)
5	BCL	L	1288	2	53,74,74	2.05	5 (9%)	57,115,115	1.87	14 (24%)
9	PO4	L	1289	-	4,4,4	0.44	0	6,6,6	0.29	0
10	HTO	L	1290	-	9,9,9	0.38	0	8,10,10	0.59	0
10	HTO	L	1291	-	9,9,9	0.32	0	8,10,10	0.94	0
4	GOL	L	1292	-	5,5,5	0.32	0	5,5,5	0.80	0
4	GOL	L	1293	-	5,5,5	0.32	0	5,5,5	0.37	0
5	BCL	M	1303	3	53,74,74	2.06	5 (9%)	57,115,115	1.84	9 (15%)
5	BCL	M	1304	3	53,74,74	2.09	4 (7%)	57,115,115	1.90	13 (22%)
6	LDA	M	1305	-	15,15,15	3.55	2 (13%)	16,17,17	1.18	2 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	LDA	M	1306	-	15,15,15	3.76	2 (13%)	16,17,17	0.58	0
6	LDA	M	1307	-	15,15,15	3.44	2 (13%)	16,17,17	0.93	0
6	LDA	M	1308	-	15,15,15	3.77	2 (13%)	16,17,17	0.59	0
6	LDA	M	1309	-	15,15,15	3.80	2 (13%)	16,17,17	0.89	1 (6%)
6	LDA	M	1310	-	15,15,15	3.76	2 (13%)	16,17,17	0.69	0
7	BPH	M	1312	-	64,70,70	2.90	19 (29%)	73,101,101	1.75	12 (16%)
12	U10	M	1313	-	48,48,63	2.99	11 (22%)	58,61,79	1.76	12 (20%)
13	SPO	M	1314	-	40,41,41	3.97	12 (30%)	45,50,50	2.25	19 (42%)
14	CDL	M	1315	-	80,80,99	1.96	16 (20%)	82,92,111	2.85	13 (15%)

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
4	GOL	H	1251	-	-	0/4/4/4	0/0/0/0
4	GOL	H	1252	-	-	0/4/4/4	0/0/0/0
4	GOL	H	1253	-	-	0/4/4/4	0/0/0/0
4	GOL	H	1254	-	-	0/4/4/4	0/0/0/0
5	BCL	L	1282	2	2/2/21/25	0/37/137/137	0/0/9/9
6	LDA	L	1283	-	-	0/13/13/13	0/0/0/0
6	LDA	L	1284	-	-	0/13/13/13	0/0/0/0
6	LDA	L	1285	-	-	0/13/13/13	0/0/0/0
7	BPH	L	1286	-	-	0/54/105/105	0/1/6/6
8	UQ2	L	1287[A]	-	-	0/15/39/39	0/1/1/1
8	UQ2	L	1287[B]	-	-	0/15/39/39	0/1/1/1
5	BCL	L	1288	2	2/2/21/25	0/37/137/137	0/0/9/9
9	PO4	L	1289	-	-	0/0/0/0	0/0/0/0
10	HTO	L	1290	-	-	0/10/10/10	0/0/0/0
10	HTO	L	1291	-	-	0/10/10/10	0/0/0/0
4	GOL	L	1292	-	-	0/4/4/4	0/0/0/0
4	GOL	L	1293	-	-	0/4/4/4	0/0/0/0
5	BCL	M	1303	3	2/2/21/25	0/37/137/137	0/0/9/9
5	BCL	M	1304	3	2/2/21/25	0/37/137/137	0/0/9/9
6	LDA	M	1305	-	-	0/13/13/13	0/0/0/0
6	LDA	M	1306	-	-	0/13/13/13	0/0/0/0
6	LDA	M	1307	-	-	0/13/13/13	0/0/0/0
6	LDA	M	1308	-	-	0/13/13/13	0/0/0/0
6	LDA	M	1309	-	-	0/13/13/13	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	LDA	M	1310	-	-	0/13/13/13	0/0/0/0
7	BPH	M	1312	-	-	0/54/105/105	0/1/6/6
12	U10	M	1313	-	-	0/45/69/87	0/1/1/1
13	SPO	M	1314	-	-	0/47/47/47	0/0/0/0
14	CDL	M	1315	-	-	0/91/91/110	0/0/0/0

All (126) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	1309	LDA	O1-N1	-14.47	1.25	1.39
6	M	1306	LDA	O1-N1	-14.31	1.25	1.39
6	L	1285	LDA	O1-N1	-14.30	1.26	1.39
6	M	1308	LDA	O1-N1	-14.30	1.26	1.39
6	M	1310	LDA	O1-N1	-14.29	1.26	1.39
6	L	1283	LDA	O1-N1	-14.28	1.26	1.39
6	L	1284	LDA	O1-N1	-14.22	1.26	1.39
6	M	1305	LDA	O1-N1	-13.29	1.26	1.39
6	M	1307	LDA	O1-N1	-13.01	1.27	1.39
14	M	1315	CDL	C11-CA5	-7.47	1.28	1.50
8	L	1287[B]	UQ2	O2-C2	-5.23	1.23	1.37
8	L	1287[A]	UQ2	O2-C2	-4.71	1.24	1.37
14	M	1315	CDL	C32-C31	-4.62	1.34	1.52
14	M	1315	CDL	C19-C18	-4.35	1.26	1.51
14	M	1315	CDL	C17-C16	-4.32	1.26	1.51
8	L	1287[A]	UQ2	O3-C3	-4.32	1.25	1.37
14	M	1315	CDL	C16-C15	-4.32	1.26	1.51
14	M	1315	CDL	C20-C19	-4.32	1.26	1.51
8	L	1287[B]	UQ2	O3-C3	-4.06	1.26	1.37
7	M	1312	BPH	C3D-CAD	-3.70	1.39	1.46
12	M	1313	U10	O3-C3	-3.70	1.27	1.37
12	M	1313	U10	O4-C4	-3.36	1.28	1.37
7	L	1286	BPH	C3D-CAD	-3.31	1.40	1.46
14	M	1315	CDL	C34-C33	-3.22	1.32	1.51
8	L	1287[A]	UQ2	C3-C4	-3.21	1.39	1.48
5	L	1288	BCL	O2D-CGD	-3.21	1.24	1.33
8	L	1287[B]	UQ2	C3-C4	-3.16	1.39	1.48
7	L	1286	BPH	C3D-C4D	-2.97	1.37	1.41
12	M	1313	U10	C4-C5	-2.96	1.40	1.48
14	M	1315	CDL	C79-C78	-2.94	1.34	1.51
14	M	1315	CDL	C37-C36	-2.94	1.34	1.51
14	M	1315	CDL	C80-C79	-2.91	1.34	1.51
7	M	1312	BPH	C3D-C4D	-2.91	1.37	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	M	1315	CDL	C22-C21	-2.88	1.34	1.51
7	L	1286	BPH	O2D-CGD	-2.87	1.25	1.33
7	M	1312	BPH	O2A-CGA	-2.82	1.24	1.33
8	L	1287[A]	UQ2	C2-C1	-2.71	1.41	1.48
6	M	1307	LDA	C1-N1	-2.66	1.46	1.51
6	L	1285	LDA	C1-N1	-2.62	1.46	1.51
5	M	1304	BCL	O2D-CGD	-2.54	1.26	1.33
7	L	1286	BPH	CBB-CAB	-2.54	1.44	1.50
7	M	1312	BPH	O2D-CGD	-2.52	1.26	1.33
5	M	1303	BCL	O2D-CGD	-2.44	1.26	1.33
8	L	1287[B]	UQ2	C6-C1	-2.43	1.39	1.46
14	M	1315	CDL	C33-C32	-2.41	1.37	1.51
5	L	1288	BCL	C3D-CAD	-2.41	1.39	1.45
6	M	1308	LDA	C1-N1	-2.36	1.47	1.51
5	L	1282	BCL	O2A-CGA	-2.36	1.26	1.33
8	L	1287[B]	UQ2	C2-C1	-2.32	1.42	1.48
7	M	1312	BPH	C1B-C2B	-2.30	1.40	1.45
7	L	1286	BPH	O2A-CGA	-2.26	1.26	1.33
6	M	1310	LDA	C1-N1	-2.26	1.47	1.51
5	L	1282	BCL	C3D-CAD	-2.20	1.39	1.45
5	L	1282	BCL	O2D-CGD	-2.15	1.27	1.33
5	M	1303	BCL	O2A-CGA	-2.15	1.26	1.33
6	M	1309	LDA	C1-N1	-2.13	1.47	1.51
6	M	1305	LDA	CM1-N1	-2.06	1.46	1.49
6	M	1306	LDA	C1-N1	-2.06	1.47	1.51
7	M	1312	BPH	CBB-CAB	-2.00	1.45	1.50
8	L	1287[B]	UQ2	C6-C5	2.02	1.40	1.35
7	L	1286	BPH	C1D-CHD	2.23	1.48	1.40
7	M	1312	BPH	CHA-C1A	2.25	1.42	1.37
8	L	1287[A]	UQ2	C6-C5	2.67	1.41	1.35
12	M	1313	U10	C6-C1	2.82	1.41	1.35
7	M	1312	BPH	C1D-CHD	2.97	1.51	1.40
7	L	1286	BPH	C3D-C2D	3.04	1.47	1.40
7	L	1286	BPH	CHB-C4A	3.18	1.46	1.40
7	L	1286	BPH	CHD-C4C	3.35	1.46	1.38
7	M	1312	BPH	C3D-C2D	3.47	1.48	1.40
5	L	1282	BCL	C2-C3	3.54	1.39	1.33
13	M	1314	SPO	C21-C20	3.61	1.45	1.35
7	M	1312	BPH	CHC-C4B	3.63	1.49	1.40
5	M	1304	BCL	C2-C3	3.69	1.40	1.33
7	M	1312	BPH	CHD-C4C	3.77	1.47	1.38
5	M	1303	BCL	C2-C3	3.85	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	1286	BPH	CHC-C4B	3.97	1.50	1.40
7	M	1312	BPH	CHB-C4A	4.07	1.48	1.40
5	L	1288	BCL	C2-C3	4.07	1.41	1.33
13	M	1314	SPO	C15-C16	4.17	1.45	1.34
13	M	1314	SPO	C26-C25	4.22	1.45	1.34
14	M	1315	CDL	OB8-CB7	4.38	1.46	1.33
14	M	1315	CDL	OA6-CA5	4.44	1.47	1.34
13	M	1314	SPO	C10-C11	4.45	1.46	1.34
14	M	1315	CDL	OB6-CB5	4.45	1.47	1.34
14	M	1315	CDL	OA8-CA7	4.81	1.47	1.33
13	M	1314	SPO	C6-C5	4.90	1.45	1.31
8	L	1287[A]	UQ2	C13-C14	5.07	1.47	1.32
12	M	1313	U10	C38-C39	5.16	1.48	1.32
5	L	1282	BCL	O1A-CGA	5.17	1.38	1.22
7	L	1286	BPH	CHC-C1C	5.22	1.46	1.36
8	L	1287[B]	UQ2	C13-C14	5.27	1.48	1.32
7	M	1312	BPH	CHB-C1B	5.49	1.49	1.38
13	M	1314	SPO	C37-C38	5.52	1.49	1.32
5	M	1304	BCL	O1A-CGA	5.52	1.39	1.22
7	M	1312	BPH	CHC-C1C	5.57	1.47	1.36
5	M	1303	BCL	O1A-CGA	5.63	1.39	1.22
7	L	1286	BPH	CHB-C1B	5.77	1.49	1.38
7	M	1312	BPH	O1A-CGA	5.79	1.39	1.22
7	L	1286	BPH	O1A-CGA	6.26	1.41	1.22
5	L	1288	BCL	O1A-CGA	6.50	1.42	1.22
12	M	1313	U10	C18-C19	6.82	1.46	1.33
7	L	1286	BPH	O1D-CGD	6.86	1.38	1.21
12	M	1313	U10	C23-C24	7.09	1.46	1.33
7	M	1312	BPH	O1D-CGD	7.19	1.39	1.21
12	M	1313	U10	C28-C29	7.28	1.47	1.33
12	M	1313	U10	C8-C9	7.34	1.47	1.33
12	M	1313	U10	C13-C14	7.58	1.47	1.33
8	L	1287[B]	UQ2	C8-C9	7.65	1.48	1.33
7	M	1312	BPH	C2-C3	7.71	1.48	1.33
13	M	1314	SPO	C32-C33	7.73	1.48	1.33
7	L	1286	BPH	C2-C3	7.79	1.48	1.33
13	M	1314	SPO	C22-C23	8.13	1.46	1.35
13	M	1314	SPO	C14-C12	8.16	1.46	1.35
8	L	1287[A]	UQ2	C8-C9	8.16	1.49	1.33
7	M	1312	BPH	OB8-CAB	8.33	1.41	1.23
13	M	1314	SPO	C19-C17	8.39	1.46	1.35
12	M	1313	U10	C33-C34	8.67	1.50	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	1314	SPO	C9-C7	9.19	1.47	1.35
7	L	1286	BPH	OBD-CAD	9.57	1.37	1.22
7	L	1286	BPH	OBB-CAB	9.84	1.44	1.23
5	L	1288	BCL	OBD-CAD	10.91	1.39	1.22
7	M	1312	BPH	OBD-CAD	11.32	1.39	1.22
5	L	1282	BCL	OBD-CAD	11.57	1.40	1.22
5	M	1303	BCL	OBD-CAD	11.57	1.40	1.22
5	M	1304	BCL	OBD-CAD	12.07	1.40	1.22
13	M	1314	SPO	C27-C28	12.27	1.47	1.34

All (132) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	1303	BCL	CMB-C2B-C1B	-7.07	116.67	128.36
13	M	1314	SPO	C4-C5-C6	-6.15	115.92	124.67
5	M	1304	BCL	CMB-C2B-C1B	-5.89	118.62	128.36
5	L	1288	BCL	CMB-C2B-C1B	-5.34	119.53	128.36
7	L	1286	BPH	O1D-CGD-CBD	-5.14	117.26	124.62
13	M	1314	SPO	C15-C14-C12	-4.72	120.38	127.20
7	L	1286	BPH	OBD-CAD-CBD	-4.68	118.88	125.94
7	M	1312	BPH	CHC-C4B-NB	-4.55	116.25	124.91
5	L	1282	BCL	O1D-CGD-CBD	-4.50	118.17	124.62
5	M	1303	BCL	O1D-CGD-CBD	-4.33	118.42	124.62
5	L	1282	BCL	CMB-C2B-C1B	-4.32	121.21	128.36
13	M	1314	SPO	C20-C19-C17	-4.07	121.32	127.20
13	M	1314	SPO	C10-C9-C7	-4.01	121.40	127.20
5	L	1288	BCL	C1D-CHD-C4C	-3.89	120.12	126.07
7	M	1312	BPH	O1D-CGD-CBD	-3.84	119.12	124.62
7	M	1312	BPH	OBD-CAD-CBD	-3.77	120.26	125.94
5	L	1288	BCL	O2D-CGD-O1D	-3.44	116.69	123.79
5	L	1288	BCL	OBD-CAD-CBD	-3.36	120.87	125.94
5	M	1304	BCL	C16-C15-C13	-3.30	104.54	115.49
12	M	1313	U10	C30-C29-C28	-3.23	117.16	123.50
13	M	1314	SPO	C21-C22-C23	-3.22	122.54	127.20
8	L	1287[B]	UQ2	O1-C1-C6	-3.18	115.70	121.68
12	M	1313	U10	C22-C23-C24	-3.18	120.85	127.76
7	L	1286	BPH	C1B-NB-C4B	-3.06	100.46	106.51
7	L	1286	BPH	CBB-CAB-C3B	-3.04	113.77	120.52
5	M	1303	BCL	OBD-CAD-CBD	-2.92	121.53	125.94
12	M	1313	U10	C27-C28-C29	-2.88	121.51	127.76
8	L	1287[B]	UQ2	CM5-C5-C6	-2.84	118.02	124.10
5	L	1282	BCL	C1D-CHD-C4C	-2.84	121.74	126.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	1288	BCL	CHD-C4C-NC	-2.82	121.78	125.06
13	M	1314	SPO	C20-C21-C22	-2.79	117.22	123.39
6	M	1305	LDA	O1-N1-CM2	-2.75	105.38	109.05
5	L	1288	BCL	C3C-C4C-CHD	-2.73	117.24	123.33
7	M	1312	BPH	OBD-CAD-C3D	-2.68	122.88	128.35
5	L	1282	BCL	OBD-CAD-CBD	-2.63	121.97	125.94
7	L	1286	BPH	OBD-CAD-C3D	-2.60	123.05	128.35
12	M	1313	U10	C12-C13-C14	-2.60	122.11	127.76
5	M	1304	BCL	OBD-CAD-CBD	-2.53	122.12	125.94
7	L	1286	BPH	C1C-NC-C4C	-2.48	107.90	110.44
8	L	1287[B]	UQ2	C7-C8-C9	-2.47	122.51	126.70
13	M	1314	SPO	C14-C15-C16	-2.42	115.76	123.13
5	M	1304	BCL	C1D-CHD-C4C	-2.36	122.47	126.07
5	M	1304	BCL	O2D-CGD-O1D	-2.31	119.01	123.79
5	L	1288	BCL	O2A-CGA-O1A	-2.31	117.53	123.49
13	M	1314	SPO	C16-C17-C19	-2.30	115.27	118.98
12	M	1313	U10	O5-C5-C4	-2.27	115.88	120.79
13	M	1314	SPO	C27-C26-C25	-2.23	116.34	123.13
7	M	1312	BPH	CAA-C2A-C1A	-2.22	107.01	112.86
13	M	1314	SPO	C31-C32-C33	-2.22	122.94	127.76
5	L	1282	BCL	O2D-CGD-O1D	-2.20	119.25	123.79
5	L	1282	BCL	CAA-C2A-C1A	-2.20	104.72	112.47
5	M	1303	BCL	C1D-CHD-C4C	-2.19	122.72	126.07
6	M	1309	LDA	O1-N1-CM1	-2.18	106.15	109.05
12	M	1313	U10	C26-C27-C28	-2.17	106.00	111.69
7	M	1312	BPH	O2D-CGD-O1D	-2.17	119.31	123.79
13	M	1314	SPO	C25-C23-C22	-2.15	115.53	118.98
14	M	1315	CDL	CA4-OA6-CA5	-2.14	112.75	117.89
5	M	1304	BCL	C3C-C4C-CHD	-2.14	118.56	123.33
7	L	1286	BPH	O2A-CGA-O1A	-2.14	117.97	123.49
5	L	1282	BCL	CAA-C2A-C3A	-2.13	107.08	113.22
5	M	1303	BCL	O2A-CGA-O1A	-2.11	118.04	123.49
5	M	1304	BCL	O2A-CGA-O1A	-2.10	118.08	123.49
5	L	1288	BCL	CMA-C3A-C2A	-2.07	105.19	114.35
5	L	1288	BCL	CMD-C2D-C3D	-2.04	121.09	125.09
13	M	1314	SPO	C9-C10-C11	-2.02	116.97	123.13
8	L	1287[A]	UQ2	O2-C2-C3	-2.02	115.43	124.17
7	M	1312	BPH	CHB-C1B-NB	-2.02	120.89	124.66
5	L	1282	BCL	C5-C3-C2	-2.02	117.23	121.05
8	L	1287[B]	UQ2	C16-C14-C15	2.01	119.58	114.64
8	L	1287[A]	UQ2	C16-C14-C15	2.03	119.64	114.64
8	L	1287[B]	UQ2	CM2-O2-C2	2.05	123.89	116.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	1314	SPO	C40-C38-C39	2.06	119.70	114.64
13	M	1314	SPO	C24-C23-C25	2.11	121.62	118.10
13	M	1314	SPO	C18-C17-C16	2.12	121.62	118.10
14	M	1315	CDL	CA6-OA8-CA7	2.26	123.16	116.85
5	L	1288	BCL	CED-O2D-CGD	2.30	121.38	115.99
7	M	1312	BPH	O2A-CGA-CBA	2.35	119.05	111.90
7	L	1286	BPH	O2A-CGA-CBA	2.42	119.29	111.90
7	L	1286	BPH	CMB-C2B-C1B	2.43	129.01	125.06
5	M	1303	BCL	CED-O2D-CGD	2.43	121.70	115.99
12	M	1313	U10	C35-C34-C36	2.49	119.21	115.41
5	L	1288	BCL	C14-C13-C12	2.51	120.73	111.08
7	L	1286	BPH	C2D-C1D-ND	2.54	114.44	110.29
5	M	1304	BCL	CHD-C4C-NC	2.54	128.01	125.06
7	L	1286	BPH	OBB-CAB-C3B	2.55	125.24	120.31
13	M	1314	SPO	C8-C7-C6	2.55	122.35	118.10
13	M	1314	SPO	C34-C33-C35	2.62	119.41	115.41
5	L	1282	BCL	CMB-C2B-C3B	2.63	130.22	125.09
14	M	1315	CDL	OB8-CB7-C71	2.90	120.74	111.90
5	L	1288	BCL	O2A-CGA-CBA	2.92	120.80	111.90
8	L	1287[A]	UQ2	C10-C9-C11	2.94	119.89	115.41
7	M	1312	BPH	C2B-C1B-NB	2.98	114.19	109.73
12	M	1313	U10	C25-C24-C26	3.02	120.02	115.41
13	M	1314	SPO	C13-C12-C11	3.08	123.22	118.10
7	M	1312	BPH	CED-O2D-CGD	3.12	123.31	115.99
8	L	1287[B]	UQ2	CM3-O3-C3	3.16	127.84	116.61
12	M	1313	U10	C20-C19-C21	3.17	120.25	115.41
5	M	1304	BCL	CMB-C2B-C3B	3.18	131.30	125.09
5	L	1288	BCL	CMB-C2B-C3B	3.22	131.39	125.09
14	M	1315	CDL	OA8-CA7-C31	3.27	121.85	111.90
5	M	1303	BCL	O2A-CGA-CBA	3.30	121.96	111.90
12	M	1313	U10	C15-C14-C16	3.33	120.49	115.41
5	L	1282	BCL	O2A-CGA-CBA	3.33	122.06	111.90
5	M	1304	BCL	CED-O2D-CGD	3.39	123.94	115.99
6	M	1305	LDA	O1-N1-C1	3.47	114.18	110.27
5	M	1304	BCL	OBB-CAB-C3B	3.53	125.59	120.00
5	L	1282	BCL	C4-C3-C5	3.54	120.81	115.41
12	M	1313	U10	C10-C9-C11	3.69	121.05	115.41
8	L	1287[B]	UQ2	C10-C9-C11	3.74	121.12	115.41
13	M	1314	SPO	C29-C28-C30	4.02	121.55	115.41
5	M	1304	BCL	O2A-CGA-CBA	4.02	124.16	111.90
7	L	1286	BPH	C2B-C1B-NB	4.20	116.03	109.73
5	M	1303	BCL	CMB-C2B-C3B	4.28	133.45	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	M	1315	CDL	OB6-CB5-C51	4.35	120.97	111.53
7	L	1286	BPH	CED-O2D-CGD	4.38	126.26	115.99
7	M	1312	BPH	C3C-C4C-NC	4.56	112.50	107.93
7	L	1286	BPH	C3C-C4C-NC	4.57	112.51	107.93
14	M	1315	CDL	OA6-CA5-C11	4.66	121.66	111.53
14	M	1315	CDL	C34-C33-C32	5.16	141.20	114.53
14	M	1315	CDL	C13-C12-C11	5.32	132.79	113.29
12	M	1313	U10	C30-C29-C31	5.55	123.88	115.41
5	M	1304	BCL	O2D-CGD-CBD	5.72	119.14	111.30
5	M	1303	BCL	O2D-CGD-CBD	5.85	119.33	111.30
5	L	1288	BCL	O2D-CGD-CBD	6.21	119.82	111.30
14	M	1315	CDL	C12-C11-CA5	6.54	139.31	113.59
7	L	1286	BPH	O2D-CGD-CBD	7.13	121.08	111.30
7	M	1312	BPH	O2D-CGD-CBD	7.48	121.56	111.30
14	M	1315	CDL	C33-C32-C31	7.60	141.18	113.29
5	L	1282	BCL	O2D-CGD-CBD	8.22	122.58	111.30
14	M	1315	CDL	C35-C34-C33	9.78	165.03	114.53
14	M	1315	CDL	C17-C16-C15	11.03	171.48	114.53
14	M	1315	CDL	C20-C19-C18	12.63	179.75	114.53

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	M	1304	BCL	C8
5	M	1304	BCL	C13
5	L	1288	BCL	C8
5	L	1288	BCL	C13
5	L	1282	BCL	C8
5	L	1282	BCL	C13
5	M	1303	BCL	C8
5	M	1303	BCL	C13

There are no torsion outliers.

There are no ring outliers.

18 monomers are involved in 65 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	1251	GOL	5	0
5	L	1282	BCL	4	0
6	L	1284	LDA	1	0
6	L	1285	LDA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	L	1286	BPH	7	0
8	L	1287[A]	UQ2	2	0
8	L	1287[B]	UQ2	3	0
5	L	1288	BCL	2	0
4	L	1292	GOL	1	0
5	M	1303	BCL	7	0
5	M	1304	BCL	12	0
6	M	1305	LDA	1	0
6	M	1307	LDA	4	0
6	M	1308	LDA	2	0
6	M	1310	LDA	1	0
7	M	1312	BPH	13	0
13	M	1314	SPO	3	0
14	M	1315	CDL	5	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	H	241/260 (92%)	-0.34	6 (2%) 61 67	29, 37, 49, 79	0
2	L	281/281 (100%)	-0.35	7 (2%) 61 67	27, 36, 58, 66	0
3	M	303/307 (98%)	-0.37	9 (2%) 54 61	26, 40, 60, 72	0
All	All	825/848 (97%)	-0.36	22 (2%) 58 64	26, 37, 58, 79	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	251	VAL	10.5
3	M	1	ALA	9.0
1	H	250	SER	5.4
2	L	59	TRP	5.1
2	L	271	TRP	4.0
3	M	2	GLU	3.9
1	H	18	TYR	3.7
2	L	281	GLY	3.6
3	M	106	ALA	3.2
2	L	270	PRO	3.1
1	H	249	LYS	3.0
2	L	202	LYS	2.9
3	M	301	HIS	2.8
2	L	277	GLY	2.8
3	M	3	TYR	2.8
2	L	276	PRO	2.5
3	M	109	LEU	2.5
3	M	27	ALA	2.4
1	H	245	ALA	2.3
3	M	80	TRP	2.2
3	M	148	TRP	2.1
1	H	190	LEU	2.1

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
6	LDA	L	1284	16/16	0.27	0.38	18.36	71,83,95,95	0
10	HTO	L	1290	10/10	0.64	0.42	16.20	85,88,88,88	0
6	LDA	L	1285	16/16	0.37	0.31	12.94	101,105,111,111	0
6	LDA	M	1308	16/16	0.35	0.35	11.54	97,100,104,105	0
4	GOL	H	1251	6/6	0.78	0.26	9.69	47,59,62,62	0
6	LDA	L	1283	16/16	-0.12	0.40	9.24	80,99,109,110	0
6	LDA	M	1305	16/16	0.74	0.25	8.27	41,67,76,76	0
6	LDA	M	1309	16/16	0.55	0.23	5.88	96,98,104,104	0
8	UQ2	L	1287[A]	23/23	0.84	0.27	4.65	27,36,51,51	23
8	UQ2	L	1287[B]	23/23	0.84	0.27	4.51	28,36,52,53	23
14	CDL	M	1315	81/100	0.63	0.37	4.41	64,97,111,113	0
4	GOL	L	1293	6/6	0.63	0.23	4.39	98,99,99,99	0
13	SPO	M	1314	42/42	0.80	0.20	3.78	38,49,68,71	0
6	LDA	M	1306	16/16	0.70	0.23	3.32	66,71,83,83	0
6	LDA	M	1307	16/16	0.76	0.19	3.21	58,60,64,65	0
12	U10	M	1313	48/63	0.92	0.12	1.09	26,42,67,69	0
4	GOL	L	1292	6/6	0.82	0.19	1.09	49,56,57,60	0
7	BPH	M	1312	65/65	0.93	0.11	0.99	29,37,93,95	0
5	BCL	M	1303	66/66	0.95	0.12	0.94	26,33,79,81	0
5	BCL	L	1282	66/66	0.97	0.11	0.72	25,30,57,59	0
5	BCL	L	1288	66/66	0.97	0.10	0.66	25,31,48,55	0
5	BCL	M	1304	66/66	0.97	0.10	0.66	26,30,54,62	0
7	BPH	L	1286	65/65	0.96	0.08	-0.16	22,29,41,42	0
9	PO4	L	1289	5/5	0.98	0.12	-0.41	62,63,64,64	0
11	FE	M	1311	1/1	0.99	0.03	-1.89	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
10	HTO	L	1291	10/10	0.35	0.52	-	111,114,114,115	0
4	GOL	H	1253	6/6	0.49	0.34	-	113,114,114,114	0
4	GOL	H	1252	6/6	0.84	0.24	-	74,75,75,77	0
6	LDA	M	1310	16/16	0.11	0.38	-	90,96,104,104	0
4	GOL	H	1254	6/6	0.35	0.31	-	104,104,105,105	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.