



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 06:28 am GMT

PDB ID : 2J8C
Title : X-RAY HIGH RESOLUTION STRUCTURE OF THE PHOTOSYNTHETIC
REACTION CENTER FROM RB. SPHAEROIDES AT PH 8 IN THE NEU-
TRAL STATE
Authors : Koepke, J.; Diehm, R.; Fritzsche, G.
Deposited on : 2006-10-24
Resolution : 1.87 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

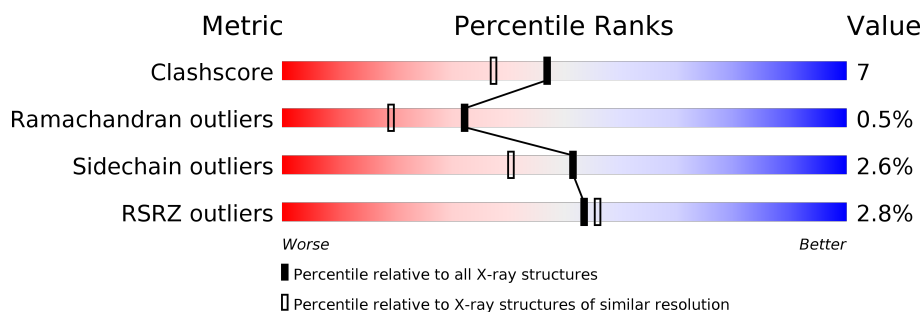
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.87 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	112137	8369 (1.90-1.86)
Ramachandran outliers	110173	8279 (1.90-1.86)
Sidechain outliers	110143	8280 (1.90-1.86)
RSRZ outliers	101464	7571 (1.90-1.86)

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	H	260	 2% 82% 10% • 7%
2	L	281	 2% 92% 7% •
3	M	307	 3% 88% 10% ••

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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	HTO	L	1291	-	-	-	X
12	SPO	M	1310	-	-	-	X
13	CDL	M	1311	-	-	-	X
14	PC1	M	1312	X	-	-	X
15	GGD	M	1313	-	-	-	X
4	GOL	H	1251	-	-	X	X
4	GOL	L	1292	-	-	-	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
7	BPH	M	1308	-	-	-	X
8	U10	L	1287[A]	-	-	-	X
8	U10	L	1287[B]	-	-	-	X

2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 7774 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	5	1
			1850	1183	321	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	2	0
			2239	1513	355	363	8			

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

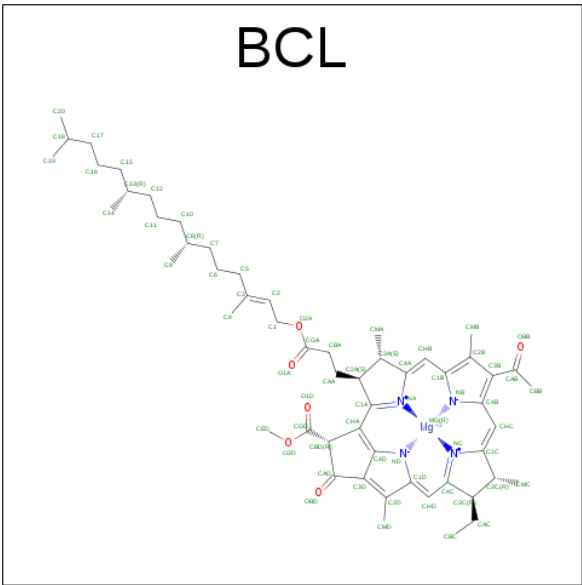
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	303	Total	C	N	O	S	0	1	1
			2411	1607	396	398	10			

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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		
4	L	1	Total	C	O	0	0
			6	3	3		

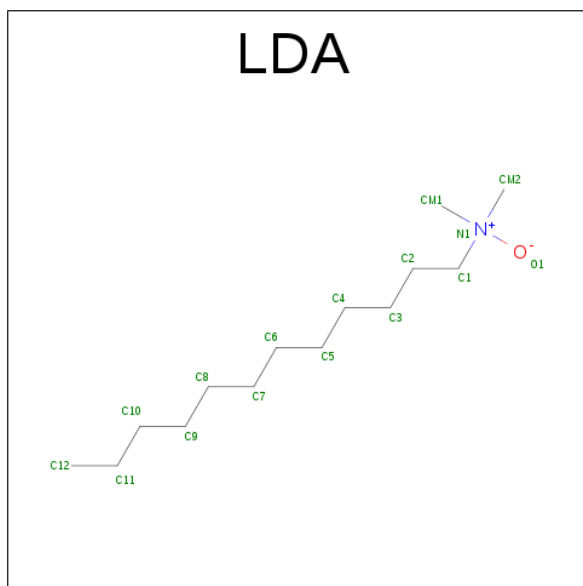
- Molecule 5 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C₅₅H₇₄MgN₄O₆).



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:

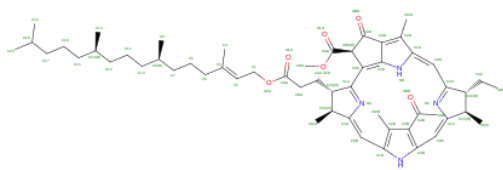
C₁₄H₃₁NO).



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		

- Molecule 7 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: C₅₅H₇₆N₄O₆).

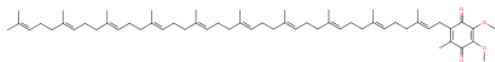
BPH



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		

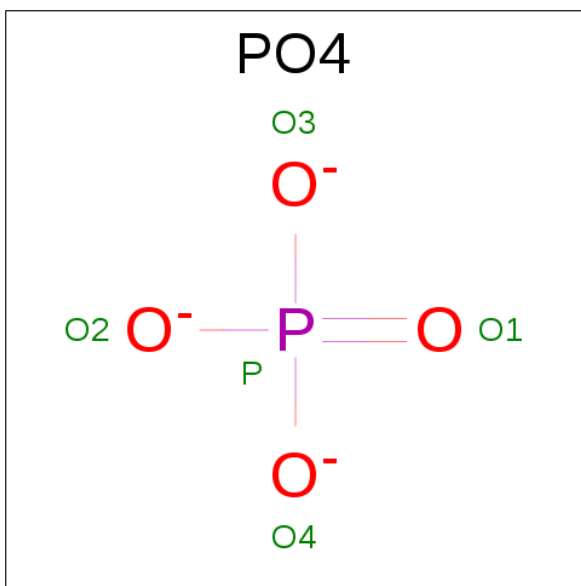
- Molecule 8 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$).

U10



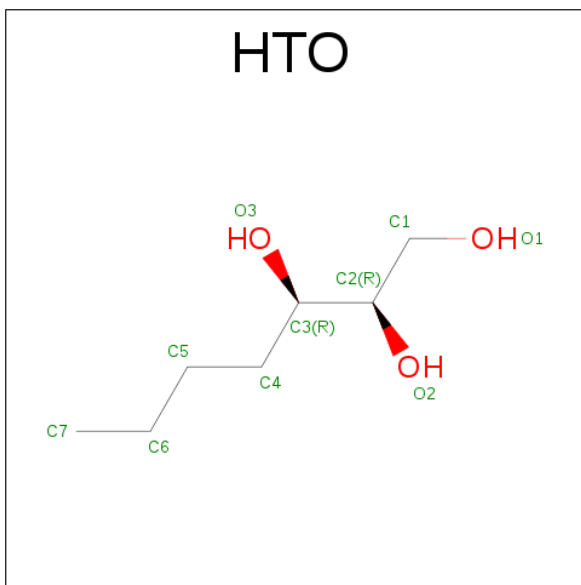
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	L	1	Total	C	O	0	1
			46	38	8		
8	M	1	Total	C	O	0	0
			48	44	4		

- 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: $\text{C}_7\text{H}_{16}\text{O}_3$).

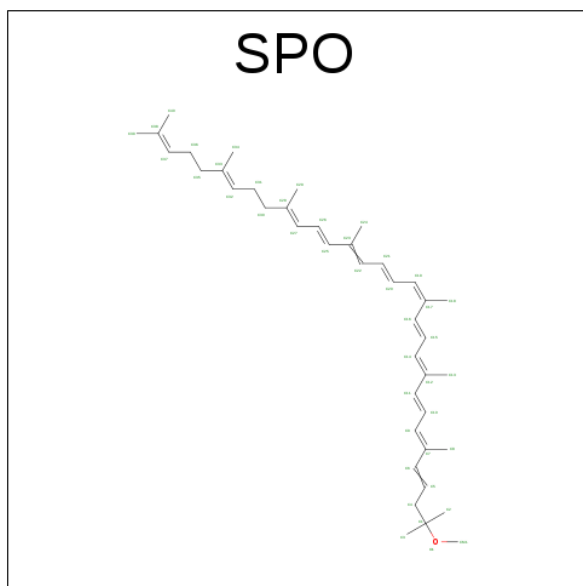


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	L	1	Total	C	O	0	0
			10	7	3		
10	L	1	Total	C	O	0	0
			10	7	3		

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

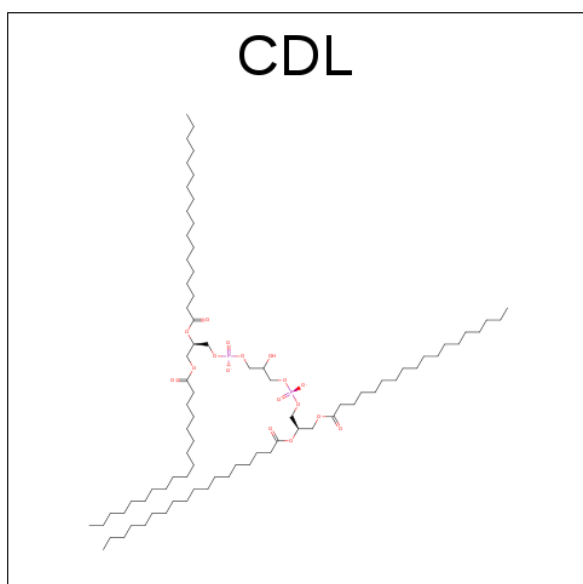
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	M	1	Total	Fe	0	0
			1	1		

- Molecule 12 is SPHEROIDENE (three-letter code: SPO) (formula: C₄₁H₆₀O).



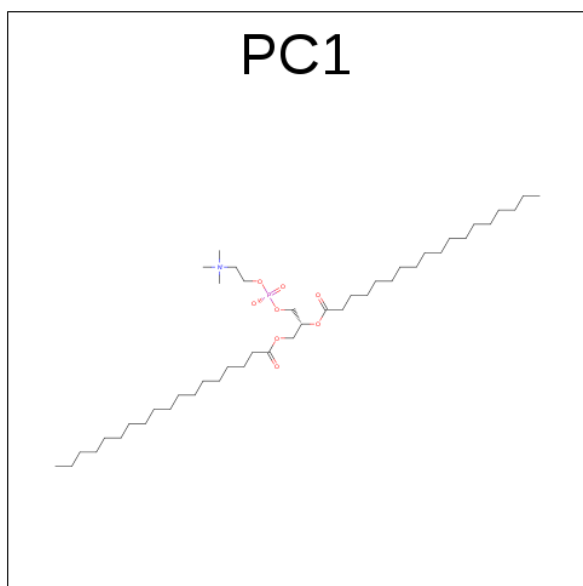
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	M	1	Total	C	O	0	0
			42	41	1		

- Molecule 13 is CARDIOLIPIN (three-letter code: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



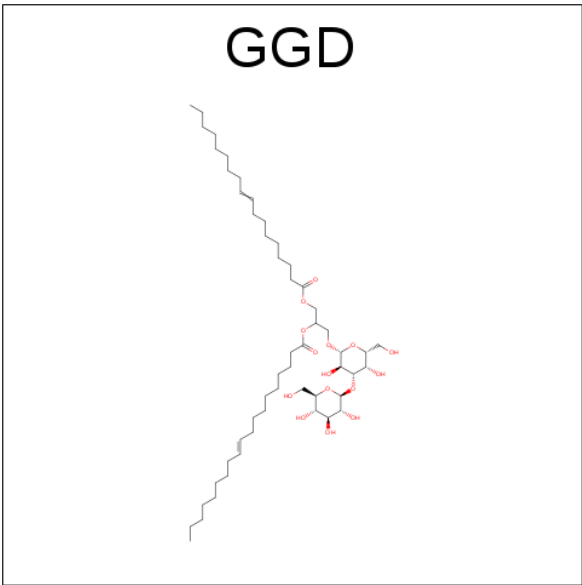
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	M	1	Total	C	O	P	0	0
			81	62	17	2		

- Molecule 14 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	M	1	Total	C	N	O	P	0	0
			43	33	1	8	1		

- Molecule 15 is NONADEC-10-ENOIC ACID 2-[3,4-DIHYDROXY-6-HYDROXYMETHYL-5-(3,4,5-TRIHYDROXY-6-HYDROXYMETHYL-TETRAHYDRO-PYRAN-2-YLOXY)-TETRAHYDRO-PYRAN-2-YLOXY]-1-OCTADEC-9-ENOYLOXYMETHYL-ETHYL ESTER (three-letter code: GGD) (formula: $C_{52}H_{94}O_{15}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	M	1	Total	C	O	0	0
			57	42	15		

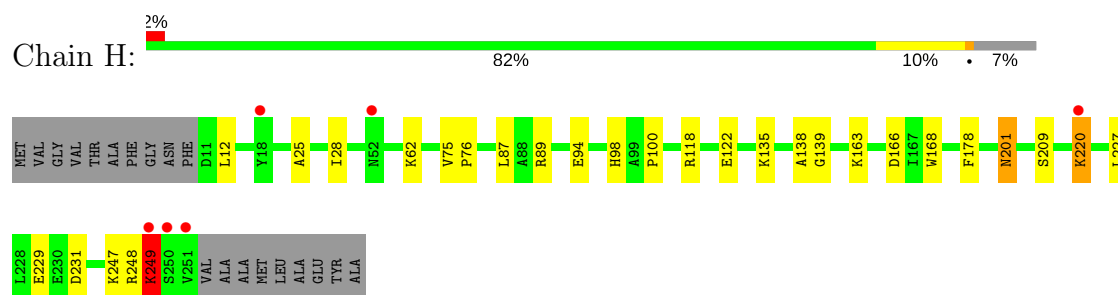
- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	H	172	Total	O	0	0
			172	172		
16	L	116	Total	O	0	0
			116	116		
16	M	127	Total	O	0	0
			127	127		

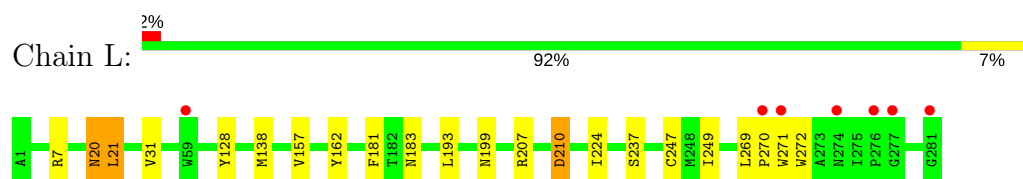
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

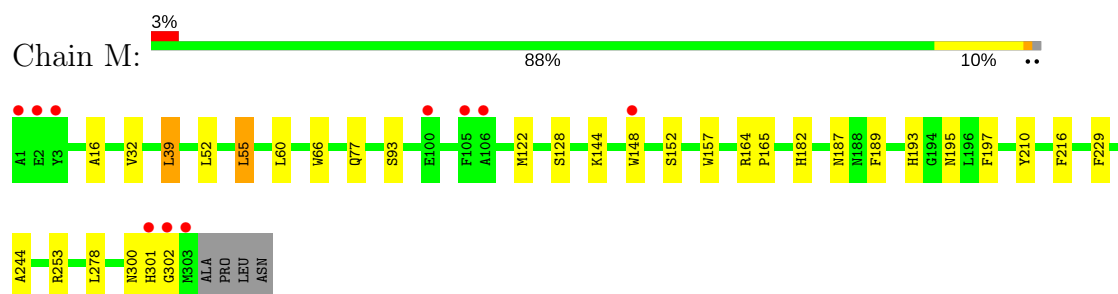
• Molecule 1: REACTION CENTER PROTEIN H CHAIN



• 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, α , β , γ	138.69Å 138.69Å 184.61Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	119.52 – 1.87 29.81 – 1.87	Depositor EDS
% Data completeness (in resolution range)	87.0 (119.52-1.87) 87.0 (29.81-1.87)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 1.87Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.178 , 0.196 0.179 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	23.7	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 70.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7774	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% 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, 0.333 respectively for untwinned datasets, and 0.375, 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, GGD, CDL, BPH, PO4, PC1, HTO, FE, SPO, 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	H	0.63	0/1930	0.70	1/2621 (0.0%)
2	L	0.66	0/2339	0.61	1/3203 (0.0%)
3	M	0.65	0/2508	0.64	0/3424
All	All	0.65	0/6777	0.65	2/9248 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	139	GLY	N-CA-C	-5.27	99.92	113.10
2	L	210	ASP	CB-CG-OD1	5.25	123.03	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	1850	0	1873	29	0
2	L	2239	0	2185	20	0
3	M	2411	0	2319	23	0
4	H	24	0	32	7	0
4	L	18	0	24	2	0
5	L	132	0	147	6	0
5	M	132	0	148	16	0
6	L	48	0	93	0	0
6	M	32	0	62	2	0
7	L	65	0	76	4	0
7	M	65	0	76	12	0
8	L	46	0	46	4	0
8	M	48	0	63	1	0
9	L	5	0	0	0	0
10	L	20	0	32	0	0
11	M	1	0	0	0	0
12	M	42	0	60	4	0
13	M	81	0	90	8	0
14	M	43	0	60	0	0
15	M	57	0	67	2	0
16	H	172	0	0	4	1
16	L	116	0	0	1	0
16	M	127	0	0	1	0
All	All	7774	0	7453	105	1

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 (105) 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)
1:H:248:ARG:HA	1:H:249[A]:LYS:HB2	1.33	1.06
7:M:1308:BPH:HBB3	7:M:1308:BPH:HHC	1.39	1.01
4:H:1251:GOL:H32	16:H:2002:HOH:O	1.67	0.93
7:L:1286:BPH:HBB3	7:L:1286:BPH:HHC	1.58	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:1282:BCL:HHC	5:L:1282:BCL:HBB2	1.59	0.85
1:H:201:ASN:HD22	1:H:201:ASN:H	1.29	0.79
7:L:1286:BPH:HHC	7:L:1286:BPH:CBB	2.13	0.78
1:H:248:ARG:CA	1:H:249[A]:LYS:HB2	2.14	0.77
4:H:1251:GOL:C3	16:H:2002:HOH:O	2.29	0.77
2:L:199:ASN:O	13:M:1311:CDL:HB22	1.85	0.76
3:M:16:ALA:HB1	3:M:32:VAL:HG11	1.68	0.75
1:H:62:LYS:HE3	4:H:1251:GOL:H11	1.70	0.74
2:L:224:ILE:H	8:L:1287[A]:U10:H8	1.55	0.72
3:M:197:PHE:HZ	5:M:1304:BCL:HBB2	1.54	0.72
3:M:197:PHE:CZ	5:M:1304:BCL:HBB2	2.24	0.72
2:L:20:ASN:C	2:L:20:ASN:HD22	1.96	0.69
7:M:1308:BPH:CBB	7:M:1308:BPH:HHC	2.19	0.68
5:M:1303:BCL:HBB2	12:M:1310:SPO:H243	1.75	0.68
1:H:248:ARG:HA	1:H:249[B]:LYS:HB3	1.76	0.68
1:H:248:ARG:HA	1:H:249[B]:LYS:HB2	1.70	0.68
3:M:77:GLN:HE22	3:M:93:SER:H	1.42	0.68
5:L:1282:BCL:HHC	5:L:1282:BCL:CBB	2.24	0.67
8:L:1287[A]:U10:H4M1	16:L:2090:HOH:O	1.93	0.66
5:M:1303:BCL:HBB2	5:M:1303:BCL:HHC	1.77	0.66
2:L:181:PHE:HB3	7:M:1308:BPH:HBB2	1.78	0.66
5:M:1304:BCL:CBB	5:M:1304:BCL:HHC	2.26	0.65
5:M:1303:BCL:HBB3	5:M:1304:BCL:H41	1.77	0.65
5:M:1303:BCL:H71	5:M:1304:BCL:H202	1.78	0.65
5:M:1303:BCL:CBB	12:M:1310:SPO:H243	2.27	0.65
3:M:148:TRP:HE1	13:M:1311:CDL:HB31	1.65	0.61
1:H:62:LYS:CE	4:H:1251:GOL:H11	2.30	0.60
3:M:300:ASN:C	3:M:302:GLY:H	2.03	0.60
7:M:1308:BPH:H5C2	7:M:1308:BPH:H142	1.82	0.60
1:H:98:HIS:CD2	2:L:7:ARG:HH21	2.21	0.58
5:M:1304:BCL:HHC	5:M:1304:BCL:HBB3	1.85	0.57
1:H:98:HIS:HD2	2:L:7:ARG:HH21	1.51	0.57
1:H:201:ASN:H	1:H:201:ASN:ND2	1.99	0.56
1:H:209:SER:OG	1:H:247:LYS:HD3	2.05	0.56
7:L:1286:BPH:HBB2	3:M:210:TYR:HB3	1.88	0.56
2:L:181:PHE:CD2	7:M:1308:BPH:HBB1	2.40	0.56
7:M:1308:BPH:HHD	7:M:1308:BPH:HBC3	1.87	0.56
1:H:220[A]:LYS:HG2	1:H:229:GLU:OE2	2.06	0.55
2:L:128:TYR:HD1	5:L:1282:BCL:HBB1	1.71	0.54
3:M:189:PHE:O	3:M:193:HIS:HD2	1.90	0.54
1:H:201:ASN:HD22	1:H:201:ASN:N	2.00	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:199:ASN:HA	4:L:1292:GOL:H31	1.91	0.52
5:M:1303:BCL:CBB	5:M:1303:BCL:HHC	2.39	0.52
1:H:62:LYS:NZ	4:H:1251:GOL:H11	2.25	0.52
3:M:253:ARG:NH1	15:M:1313:GGD:HC31	2.25	0.52
2:L:181:PHE:HB3	7:M:1308:BPH:CBB	2.39	0.52
7:M:1308:BPH:HBB3	7:M:1308:BPH:CHC	2.26	0.51
1:H:28:ILE:HG22	16:H:2169:HOH:O	2.11	0.51
3:M:144:LYS:H	13:M:1311:CDL:PB2	2.33	0.51
7:L:1286:BPH:CHC	7:L:1286:BPH:HBB3	2.35	0.50
3:M:278:LEU:HD21	13:M:1311:CDL:H782	1.94	0.50
1:H:89:ARG:NH2	1:H:94:GLU:HG2	2.27	0.49
5:M:1304:BCL:HAA2	5:M:1304:BCL:HBD	1.94	0.49
5:L:1288:BCL:HBB3	5:L:1288:BCL:HMB1	1.96	0.47
3:M:39:LEU:HD12	6:M:1306:LDA:H112	1.96	0.47
1:H:62:LYS:HE3	4:H:1251:GOL:C1	2.43	0.47
1:H:118[B]:ARG:HD2	16:M:2106:HOH:O	2.15	0.46
5:L:1288:BCL:HMB1	5:L:1288:BCL:CBB	2.45	0.46
3:M:148:TRP:CD2	13:M:1311:CDL:H522	2.51	0.46
5:L:1282:BCL:H92	15:M:1313:GGD:H401	1.97	0.46
1:H:135:LYS:HE3	1:H:166:ASP:OD2	2.15	0.46
2:L:20:ASN:ND2	2:L:20:ASN:C	2.68	0.46
1:H:25:ALA:HB1	4:H:1252:GOL:H11	1.99	0.45
13:M:1311:CDL:H321	13:M:1311:CDL:H512	1.99	0.45
2:L:138:MET:SD	2:L:249:ILE:HD11	2.56	0.45
3:M:300:ASN:C	3:M:302:GLY:N	2.70	0.45
8:M:1309:U10:O3	8:M:1309:U10:H4M2	2.17	0.44
7:M:1308:BPH:H121	7:M:1308:BPH:H8	1.74	0.44
4:L:1294:GOL:H32	6:M:1305:LDA:HM22	2.00	0.44
13:M:1311:CDL:OA8	13:M:1311:CDL:HB4	2.18	0.44
3:M:229:PHE:HB2	3:M:244:ALA:HB2	2.00	0.44
1:H:248:ARG:CA	1:H:249[B]:LYS:HB2	2.46	0.43
8:L:1287[A]:U10:H1M1	8:L:1287[A]:U10:H71	1.59	0.43
3:M:144:LYS:N	13:M:1311:CDL:OB3	2.44	0.43
5:M:1304:BCL:HHC	5:M:1304:BCL:HBB2	1.98	0.43
2:L:20:ASN:HD22	2:L:21:LEU:N	2.16	0.43
3:M:152:SER:OG	3:M:278:LEU:HG	2.19	0.43
1:H:75:VAL:HA	1:H:76:PRO:C	2.39	0.43
3:M:55:LEU:HD22	3:M:128:SER:HB2	2.01	0.43
2:L:157:VAL:HG11	5:M:1304:BCL:HBB1	2.00	0.43
1:H:87:LEU:HD23	1:H:100:PRO:HA	2.00	0.43
1:H:220[A]:LYS:CG	1:H:229:GLU:OE2	2.67	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:183:ASN:ND2	2:L:237[B]:SER:OG	2.52	0.43
5:M:1304:BCL:H172	7:M:1308:BPH:H9C2	2.00	0.43
7:M:1308:BPH:CBB	7:M:1308:BPH:CHC	2.92	0.42
5:M:1303:BCL:H203	12:M:1310:SPO:H10	2.01	0.42
2:L:269:LEU:HD13	2:L:271[A]:TRP:CZ2	2.55	0.42
2:L:162:TYR:OH	3:M:187:ASN:ND2	2.53	0.42
2:L:270:PRO:HG2	2:L:271[B]:TRP:CD1	2.54	0.42
1:H:168:TRP:HB2	1:H:178:PHE:HB2	2.01	0.41
3:M:60:LEU:HD11	7:M:1308:BPH:H161	2.02	0.41
1:H:122:GLU:HB2	1:H:227:LEU:HD21	2.03	0.41
3:M:157:TRP:CE2	12:M:1310:SPO:H293	2.56	0.41
2:L:193:LEU:HD23	8:L:1287[A]:U10:C2	2.52	0.40
3:M:66:TRP:CD1	3:M:122:MET:HB2	2.56	0.40
1:H:118[B]:ARG:NH2	16:H:2086:HOH:O	2.24	0.40
3:M:164:ARG:HB3	3:M:165:PRO:HD3	2.02	0.40
5:M:1304:BCL:CBB	5:M:1304:BCL:CHC	2.94	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:H:2039:HOH:O	16:H:2039:HOH:O[4_555]	1.66	0.54

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	H	245/260 (94%)	241 (98%)	2 (1%)	2 (1%)	22	10
2	L	281/281 (100%)	275 (98%)	5 (2%)	1 (0%)	38	25
3	M	302/307 (98%)	293 (97%)	7 (2%)	2 (1%)	25	12
All	All	828/848 (98%)	809 (98%)	14 (2%)	5 (1%)	32	15

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	249[A]	LYS
1	H	249[B]	LYS
3	M	301	HIS
3	M	195	ASN
2	L	31	VAL

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	H	200/208 (96%)	190 (95%)	10 (5%)	28	15
2	L	221/220 (100%)	215 (97%)	6 (3%)	50	39
3	M	237/240 (99%)	232 (98%)	5 (2%)	59	50
All	All	658/668 (98%)	637 (97%)	21 (3%)	51	31

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	12	LEU
1	H	163[A]	LYS
1	H	163[B]	LYS
1	H	201	ASN
1	H	220[A]	LYS
1	H	220[B]	LYS
1	H	220[C]	LYS
1	H	231	ASP
1	H	249[A]	LYS
1	H	249[B]	LYS
2	L	20	ASN
2	L	21	LEU
2	L	207	ARG
2	L	210	ASP
2	L	247	CYS
2	L	272	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	M	39	LEU
3	M	52	LEU
3	M	55	LEU
3	M	182	HIS
3	M	216	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	98	HIS
1	H	201	ASN
2	L	20	ASN
2	L	159	ASN
2	L	183	ASN
2	L	264	GLN
3	M	4	GLN
3	M	77	GLN
3	M	187	ASN
3	M	193	HIS

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 29 ligands modelled in this entry, 1 is monoatomic - leaving 28 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	0.45	0	5,5,5	0.80	0
4	GOL	H	1252	-	5,5,5	0.41	0	5,5,5	0.36	0
4	GOL	H	1253	-	5,5,5	0.34	0	5,5,5	0.16	0
4	GOL	H	1254	-	5,5,5	0.35	0	5,5,5	0.24	0
5	BCL	L	1282	2	55,74,74	2.16	8 (14%)	65,115,115	2.06	18 (27%)
6	LDA	L	1283	-	13,15,15	2.36	1 (7%)	14,17,17	0.46	0
6	LDA	L	1284	-	13,15,15	2.36	1 (7%)	14,17,17	0.46	0
6	LDA	L	1285	-	13,15,15	2.42	1 (7%)	14,17,17	0.60	0
7	BPH	L	1286	-	65,70,70	2.67	18 (27%)	75,101,101	1.74	16 (21%)
8	U10	L	1287[A]	-	23,23,63	2.41	7 (30%)	28,31,79	1.83	9 (32%)
8	U10	L	1287[B]	-	23,23,63	2.61	7 (30%)	28,31,79	1.21	1 (3%)
5	BCL	L	1288	2	55,74,74	2.11	8 (14%)	65,115,115	1.99	17 (26%)
9	PO4	L	1289	-	4,4,4	0.87	0	6,6,6	0.67	0
10	HTO	L	1290	-	9,9,9	0.28	0	9,10,10	0.82	0
10	HTO	L	1291	-	9,9,9	0.32	0	9,10,10	0.90	1 (11%)
4	GOL	L	1292	-	5,5,5	0.43	0	5,5,5	0.84	0
4	GOL	L	1293	-	5,5,5	0.39	0	5,5,5	0.26	0
4	GOL	L	1294	-	5,5,5	0.33	0	5,5,5	0.19	0
5	BCL	M	1303	3	55,74,74	2.17	9 (16%)	65,115,115	1.80	9 (13%)
5	BCL	M	1304	3	55,74,74	2.18	8 (14%)	65,115,115	1.93	14 (21%)
6	LDA	M	1305	-	13,15,15	2.33	1 (7%)	14,17,17	0.50	0
6	LDA	M	1306	-	13,15,15	2.36	2 (15%)	14,17,17	0.56	0
7	BPH	M	1308	-	65,70,70	2.77	18 (27%)	75,101,101	1.87	13 (17%)
8	U10	M	1309	-	48,48,63	2.43	11 (22%)	58,61,79	1.52	10 (17%)
12	SPO	M	1310	-	40,41,41	3.77	12 (30%)	49,50,50	2.31	20 (40%)
13	CDL	M	1311	-	79,79,99	1.87	16 (20%)	80,90,111	2.75	14 (17%)
14	PC1	M	1312	-	42,42,53	1.72	8 (19%)	47,50,61	1.36	6 (12%)
15	GGD	M	1313	-	58,58,68	2.19	12 (20%)	72,72,82	1.86	20 (27%)

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	U10	L	1287[A]	-	-	0/15/39/87	0/1/1/1
8	U10	L	1287[B]	-	-	0/15/39/87	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
4	GOL	L	1294	-	-	0/4/4/4	0/0/0/0
5	BCL	M	1303	3	2/2/21/25	1/37/137/137	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
7	BPH	M	1308	-	-	0/54/105/105	0/1/6/6
8	U10	M	1309	-	-	0/45/69/87	0/1/1/1
12	SPO	M	1310	-	-	0/47/47/47	0/0/0/0
13	CDL	M	1311	-	-	0/88/88/110	0/0/0/0
14	PC1	M	1312	-	1/1/5/5	0/46/46/57	0/0/0/0
15	GGD	M	1313	-	-	0/47/87/97	0/2/2/2

All (148) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	1285	LDA	O1-N1	-8.44	1.25	1.42
6	L	1284	LDA	O1-N1	-8.26	1.25	1.42
6	L	1283	LDA	O1-N1	-8.22	1.26	1.42
6	M	1306	LDA	O1-N1	-8.21	1.26	1.42
6	M	1305	LDA	O1-N1	-8.12	1.26	1.42
13	M	1311	CDL	C11-CA5	-7.04	1.30	1.50
15	M	1313	GGD	C14-CC5	-5.73	1.34	1.50
15	M	1313	GGD	CC3-CC4	-5.55	1.35	1.50
15	M	1313	GGD	C31-CC7	-5.51	1.34	1.50
14	M	1312	PC1	C22-C21	-5.45	1.34	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	M	1313	GGD	CC6-CC4	-5.35	1.35	1.50
8	L	1287[B]	U10	O3-C3	-5.13	1.24	1.36
8	L	1287[B]	U10	O4-C4	-5.12	1.24	1.36
15	M	1313	GGD	C15-C14	-5.00	1.33	1.52
8	L	1287[A]	U10	O4-C4	-4.91	1.24	1.36
15	M	1313	GGD	C36-C37	-4.89	1.33	1.52
15	M	1313	GGD	C20-C21	-4.77	1.34	1.52
13	M	1311	CDL	C12-C11	-4.46	1.35	1.52
13	M	1311	CDL	C20-C19	-4.26	1.27	1.51
8	L	1287[A]	U10	O3-C3	-4.10	1.26	1.36
7	L	1286	BPH	C3D-C4D	-3.96	1.36	1.41
13	M	1311	CDL	C13-C12	-3.90	1.29	1.51
7	M	1308	BPH	C3D-CAD	-3.71	1.38	1.47
13	M	1311	CDL	C17-C16	-3.58	1.31	1.51
8	M	1309	U10	O3-C3	-3.51	1.28	1.36
8	M	1309	U10	O4-C4	-3.50	1.28	1.36
7	L	1286	BPH	C3D-CAD	-3.49	1.39	1.47
7	M	1308	BPH	C3D-C4D	-3.34	1.37	1.41
15	M	1313	GGD	C20-C19	-3.12	1.33	1.51
13	M	1311	CDL	C32-C31	-3.12	1.40	1.52
8	L	1287[B]	U10	C3-C2	-3.11	1.40	1.48
8	L	1287[B]	U10	C4-C5	-3.05	1.40	1.48
14	M	1312	PC1	C39-C38	-3.05	1.34	1.51
5	L	1288	BCL	O2D-CGD	-3.01	1.25	1.33
13	M	1311	CDL	C34-C33	-2.98	1.25	1.49
13	M	1311	CDL	C79-C78	-2.97	1.34	1.51
13	M	1311	CDL	C80-C79	-2.95	1.34	1.51
13	M	1311	CDL	C22-C21	-2.93	1.34	1.51
5	M	1303	BCL	O2D-CGD	-2.93	1.25	1.33
8	M	1309	U10	C4-C5	-2.85	1.40	1.48
5	L	1282	BCL	O2D-CGD	-2.81	1.26	1.33
7	M	1308	BPH	O2D-CGD	-2.78	1.26	1.33
8	L	1287[A]	U10	C4-C5	-2.78	1.41	1.48
13	M	1311	CDL	C19-C18	-2.75	1.35	1.51
8	L	1287[A]	U10	C3-C2	-2.74	1.41	1.48
7	L	1286	BPH	O2D-CGD	-2.72	1.26	1.33
7	L	1286	BPH	C1B-C2B	-2.69	1.40	1.45
7	M	1308	BPH	O2A-CGA	-2.63	1.25	1.33
7	L	1286	BPH	CBB-CAB	-2.60	1.44	1.50
5	L	1288	BCL	C3D-CAD	-2.60	1.38	1.46
14	M	1312	PC1	C12-N	-2.60	1.42	1.51
7	M	1308	BPH	C1B-C2B	-2.57	1.40	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	1311	CDL	C16-C15	-2.54	1.37	1.51
14	M	1312	PC1	C3A-C39	-2.48	1.34	1.51
5	M	1304	BCL	O2A-CGA	-2.31	1.26	1.33
7	L	1286	BPH	O2A-CGA	-2.27	1.26	1.33
7	M	1308	BPH	CBB-CAB	-2.25	1.45	1.50
5	L	1288	BCL	O2A-CGA	-2.22	1.26	1.33
5	L	1282	BCL	O2A-CGA	-2.21	1.26	1.33
5	L	1282	BCL	C3D-CAD	-2.20	1.39	1.46
5	M	1304	BCL	C3D-CAD	-2.10	1.40	1.46
5	M	1303	BCL	C3D-CAD	-2.08	1.40	1.46
5	M	1303	BCL	O2A-CGA	-2.03	1.27	1.33
6	M	1306	LDA	C1-N1	-2.01	1.46	1.51
8	L	1287[A]	U10	C6-C5	-2.00	1.40	1.46
7	L	1286	BPH	C1D-CHD	2.06	1.48	1.40
5	M	1303	BCL	CHD-C4C	2.22	1.47	1.41
7	M	1308	BPH	C1D-CHD	2.23	1.48	1.40
5	M	1304	BCL	OBb-CAB	2.45	1.30	1.22
5	L	1282	BCL	C2-C3	2.56	1.39	1.33
7	L	1286	BPH	CHB-C4A	2.64	1.46	1.40
7	M	1308	BPH	CHB-C4A	2.65	1.46	1.40
14	M	1312	PC1	C37-C36	2.66	1.66	1.51
7	M	1308	BPH	CHD-C4C	2.68	1.45	1.38
8	L	1287[B]	U10	C6-C1	2.70	1.41	1.35
5	L	1288	BCL	C2-C3	2.76	1.39	1.33
5	M	1304	BCL	C2-C3	2.80	1.40	1.33
5	M	1303	BCL	C2-C3	2.89	1.40	1.33
14	M	1312	PC1	C36-C35	2.97	1.68	1.51
15	M	1313	GGD	C22-C23	3.12	1.53	1.29
7	L	1286	BPH	CHD-C4C	3.12	1.46	1.38
12	M	1310	SPO	C21-C20	3.32	1.44	1.35
8	M	1309	U10	C6-C1	3.52	1.43	1.35
15	M	1313	GGD	C39-C38	3.58	1.51	1.31
7	L	1286	BPH	C3D-C2D	3.71	1.47	1.39
12	M	1310	SPO	C15-C16	3.84	1.44	1.34
12	M	1310	SPO	C10-C11	3.87	1.44	1.34
7	M	1308	BPH	C3D-C2D	3.88	1.48	1.39
7	L	1286	BPH	CHC-C4B	3.98	1.50	1.40
7	M	1308	BPH	CHC-C4B	4.05	1.50	1.40
15	M	1313	GGD	OC8-CC7	4.06	1.45	1.33
12	M	1310	SPO	C26-C25	4.19	1.45	1.34
15	M	1313	GGD	OC6-CC5	4.24	1.46	1.34
14	M	1312	PC1	O21-C21	4.27	1.46	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	1311	CDL	OA6-CA5	4.32	1.46	1.34
13	M	1311	CDL	OB8-CB7	4.35	1.46	1.33
5	L	1288	BCL	CHB-C4A	4.57	1.39	1.33
14	M	1312	PC1	O31-C31	4.59	1.46	1.33
5	L	1282	BCL	CHC-C1C	4.64	1.39	1.33
13	M	1311	CDL	OA8-CA7	4.66	1.47	1.33
13	M	1311	CDL	OB6-CB5	4.67	1.47	1.34
5	M	1303	BCL	CHC-C1C	4.84	1.39	1.33
7	L	1286	BPH	CHC-C1C	4.91	1.46	1.36
8	M	1309	U10	C38-C39	4.94	1.46	1.32
12	M	1310	SPO	C6-C5	4.97	1.45	1.31
5	L	1282	BCL	O1A-CGA	4.98	1.37	1.22
5	M	1304	BCL	CHB-C4A	5.06	1.40	1.33
8	M	1309	U10	C8-C9	5.10	1.45	1.33
7	L	1286	BPH	CHB-C1B	5.11	1.48	1.38
8	M	1309	U10	C23-C24	5.11	1.45	1.33
8	L	1287[B]	U10	C13-C14	5.16	1.47	1.32
7	M	1308	BPH	CHC-C1C	5.19	1.46	1.36
8	L	1287[A]	U10	C13-C14	5.23	1.47	1.32
8	M	1309	U10	C18-C19	5.25	1.46	1.33
7	M	1308	BPH	CHB-C1B	5.39	1.49	1.38
7	L	1286	BPH	C2-C3	5.47	1.46	1.33
5	L	1288	BCL	O1A-CGA	5.50	1.39	1.22
7	M	1308	BPH	O1A-CGA	5.61	1.39	1.22
5	L	1282	BCL	CHB-C4A	5.66	1.40	1.33
5	M	1304	BCL	O1A-CGA	5.73	1.39	1.22
7	L	1286	BPH	O1A-CGA	5.73	1.39	1.22
5	M	1303	BCL	CHB-C4A	5.74	1.40	1.33
7	M	1308	BPH	C2-C3	5.80	1.47	1.33
12	M	1310	SPO	C37-C38	5.82	1.49	1.32
5	M	1304	BCL	CHC-C1C	5.83	1.40	1.33
8	L	1287[A]	U10	C8-C9	5.83	1.47	1.33
8	M	1309	U10	C13-C14	5.86	1.47	1.33
5	M	1303	BCL	O1A-CGA	5.88	1.40	1.22
12	M	1310	SPO	C32-C33	5.98	1.47	1.33
8	L	1287[B]	U10	C8-C9	6.10	1.48	1.33
8	M	1309	U10	C28-C29	6.20	1.48	1.33
5	L	1288	BCL	CHC-C1C	6.23	1.41	1.33
8	M	1309	U10	C33-C34	6.27	1.48	1.33
7	M	1308	BPH	O1D-CGD	6.51	1.37	1.21
7	L	1286	BPH	O1D-CGD	6.79	1.38	1.21
12	M	1310	SPO	C14-C12	7.55	1.45	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	M	1310	SPO	C22-C23	7.95	1.46	1.35
12	M	1310	SPO	C19-C17	8.20	1.46	1.35
12	M	1310	SPO	C9-C7	8.22	1.46	1.35
7	M	1308	BPH	OBB-CAB	8.79	1.42	1.23
7	L	1286	BPH	OBB-CAB	8.97	1.42	1.23
7	L	1286	BPH	OBD-CAD	9.98	1.36	1.22
5	L	1288	BCL	OBD-CAD	10.30	1.37	1.22
5	M	1303	BCL	OBD-CAD	10.62	1.37	1.22
5	M	1304	BCL	OBD-CAD	10.93	1.38	1.22
5	L	1282	BCL	OBD-CAD	11.07	1.38	1.22
7	M	1308	BPH	OBD-CAD	11.40	1.38	1.22
12	M	1310	SPO	C27-C28	12.42	1.47	1.34

All (168) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	1303	BCL	CMB-C2B-C1B	-6.86	117.92	128.46
5	L	1288	BCL	CMB-C2B-C1B	-6.64	118.26	128.46
5	L	1282	BCL	CMB-C2B-C1B	-6.39	118.64	128.46
12	M	1310	SPO	C20-C19-C17	-6.36	118.23	127.31
5	M	1304	BCL	CMB-C2B-C1B	-6.28	118.81	128.46
12	M	1310	SPO	C21-C22-C23	-5.54	119.40	127.31
7	M	1308	BPH	O1D-CGD-CBD	-5.43	114.84	124.60
12	M	1310	SPO	C4-C5-C6	-4.78	117.71	124.57
5	M	1303	BCL	OBD-CAD-CBD	-4.73	118.80	125.94
5	L	1288	BCL	OBD-CAD-CBD	-4.58	119.02	125.94
12	M	1310	SPO	C10-C9-C7	-4.58	120.77	127.31
5	L	1282	BCL	OBD-CAD-CBD	-4.35	119.37	125.94
5	L	1282	BCL	O1D-CGD-CBD	-4.22	117.02	124.60
5	L	1288	BCL	CMA-C3A-C4A	-4.20	100.49	111.77
5	M	1303	BCL	O1D-CGD-CBD	-4.02	117.37	124.60
5	M	1304	BCL	C16-C15-C13	-4.01	102.58	115.73
7	L	1286	BPH	C1C-NC-C4C	-3.98	106.96	110.54
7	M	1308	BPH	CAC-C3C-C2C	-3.81	104.66	114.24
13	M	1311	CDL	CA4-OA6-CA5	-3.68	109.18	117.88
7	L	1286	BPH	O1D-CGD-CBD	-3.54	118.25	124.60
12	M	1310	SPO	C15-C14-C12	-3.54	122.26	127.31
5	L	1288	BCL	C4B-CHC-C1C	-3.44	123.31	130.12
5	L	1282	BCL	CMA-C3A-C4A	-3.41	102.60	111.77
8	L	1287[A]	U10	C7-C8-C9	-3.33	121.14	126.71
8	L	1287[A]	U10	C1M-C1-C6	-3.29	117.52	124.20
5	M	1304	BCL	C1D-CHD-C4C	-3.27	121.04	125.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	M	1310	SPO	C5-C6-C7	-3.24	121.00	125.89
7	M	1308	BPH	C1C-NC-C4C	-3.21	107.65	110.54
12	M	1310	SPO	C14-C15-C16	-3.18	113.48	123.23
7	L	1286	BPH	C1-C2-C3	-3.12	120.20	125.96
5	L	1288	BCL	C3C-C4C-CHD	-3.08	116.86	123.34
8	L	1287[A]	U10	O5-C5-C6	-3.08	116.15	121.82
5	M	1304	BCL	OBD-CAD-CBD	-3.07	121.31	125.94
12	M	1310	SPO	C27-C26-C25	-3.02	113.98	123.23
7	M	1308	BPH	CBA-CAA-C2A	-2.87	105.20	113.80
7	L	1286	BPH	CMA-C3A-C4A	-2.72	104.20	112.37
12	M	1310	SPO	C10-C11-C12	-2.69	118.85	126.42
8	M	1309	U10	C17-C18-C19	-2.69	120.93	127.68
8	M	1309	U10	C27-C28-C29	-2.68	120.95	127.68
13	M	1311	CDL	OA6-CA5-OA7	-2.67	117.01	123.68
14	M	1312	PC1	O31-C31-O32	-2.65	116.96	123.55
5	M	1304	BCL	CBB-CAB-C3B	-2.64	112.70	120.39
5	L	1288	BCL	CAA-C2A-C3A	-2.64	105.58	112.81
7	M	1308	BPH	CBB-CAB-C3B	-2.60	114.95	120.52
5	M	1304	BCL	O1D-CGD-CBD	-2.60	119.94	124.60
7	L	1286	BPH	CBA-CAA-C2A	-2.60	106.03	113.80
5	L	1282	BCL	C4B-CHC-C1C	-2.53	125.11	130.12
5	L	1288	BCL	CAA-C2A-C1A	-2.46	103.92	111.97
15	M	1313	GGD	CB4-CB3-CB2	-2.46	106.50	110.84
5	L	1282	BCL	CAA-C2A-C3A	-2.45	106.10	112.81
8	M	1309	U10	C22-C23-C24	-2.40	121.65	127.68
7	M	1308	BPH	C1B-NB-C4B	-2.39	101.80	106.52
15	M	1313	GGD	CB3-CB4-CB5	-2.38	106.02	110.22
7	L	1286	BPH	O2A-CGA-O1A	-2.38	117.64	123.55
5	L	1282	BCL	C1D-CHD-C4C	-2.37	122.39	125.92
12	M	1310	SPO	C9-C10-C11	-2.37	115.97	123.23
5	L	1282	BCL	C5-C3-C2	-2.37	116.26	121.10
5	M	1304	BCL	C7-C6-C5	-2.35	106.58	113.11
12	M	1310	SPO	C20-C21-C22	-2.32	118.51	123.46
15	M	1313	GGD	C21-C22-C23	-2.32	112.17	131.33
7	L	1286	BPH	CBB-CAB-C3B	-2.32	115.56	120.52
13	M	1311	CDL	OA8-CA7-OA9	-2.31	117.80	123.55
5	L	1288	BCL	O2A-CGA-O1A	-2.30	117.84	123.55
13	M	1311	CDL	OB8-CB7-OB9	-2.30	117.85	123.55
8	L	1287[A]	U10	C7-C6-C1	-2.29	118.97	123.47
7	L	1286	BPH	C1B-NB-C4B	-2.25	102.06	106.52
7	L	1286	BPH	C3B-C2B-C1B	-2.25	102.48	105.82
14	M	1312	PC1	C26-C25-C24	-2.20	103.12	114.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	L	1291	HTO	C5-C4-C3	-2.18	110.55	114.22
15	M	1313	GGD	OC6-CC5-OC7	-2.18	118.25	123.68
5	L	1282	BCL	C1-C2-C3	-2.18	121.95	125.96
12	M	1310	SPO	C6-C7-C9	-2.17	115.62	118.94
12	M	1310	SPO	C21-C20-C19	-2.15	118.88	123.46
7	M	1308	BPH	OBD-CAD-CBD	-2.15	122.69	125.94
12	M	1310	SPO	C2-C1-C4	-2.12	107.28	110.90
8	M	1309	U10	C12-C13-C14	-2.09	122.43	127.68
12	M	1310	SPO	C1-C4-C5	-2.09	107.48	112.87
5	L	1282	BCL	CHA-C1A-NA	-2.08	121.34	126.18
5	L	1282	BCL	CAA-C2A-C1A	-2.07	105.18	111.97
15	M	1313	GGD	C37-C38-C39	-2.06	109.75	124.81
12	M	1310	SPO	C25-C23-C22	-2.05	115.79	118.94
15	M	1313	GGD	OC8-CC7-OC9	-2.04	118.49	123.55
15	M	1313	GGD	C16-C15-C14	2.02	120.63	113.24
15	M	1313	GGD	CA3-CA4-CA5	2.03	114.02	109.67
8	L	1287[A]	U10	O3-C3-C2	2.03	122.90	116.60
15	M	1313	GGD	C19-C20-C21	2.03	121.55	113.74
5	M	1304	BCL	C9-C8-C10	2.06	118.88	111.36
5	L	1288	BCL	C14-C13-C12	2.06	118.88	111.36
14	M	1312	PC1	C23-C22-C21	2.08	121.18	113.58
5	L	1288	BCL	C11-C12-C13	2.12	122.68	115.73
5	M	1303	BCL	C3D-CAD-CBD	2.15	110.64	107.60
8	M	1309	U10	C35-C34-C36	2.16	119.03	115.29
5	L	1282	BCL	C1-O2A-CGA	2.19	122.03	116.77
8	L	1287[A]	U10	C16-C14-C15	2.22	119.79	114.60
5	M	1303	BCL	C2A-C3A-C4A	2.24	105.49	101.87
8	L	1287[A]	U10	C7-C6-C5	2.26	121.36	118.47
12	M	1310	SPO	C29-C28-C30	2.28	119.25	115.29
15	M	1313	GGD	CB1-OB5-CB5	2.33	118.10	113.72
12	M	1310	SPO	C8-C7-C6	2.33	121.81	118.10
5	M	1304	BCL	CHD-C4C-NC	2.33	127.66	125.08
5	L	1282	BCL	CED-O2D-CGD	2.33	121.44	115.97
14	M	1312	PC1	C11-C12-N	2.42	124.07	115.86
8	M	1309	U10	C30-C29-C31	2.43	119.50	115.29
8	M	1309	U10	C41-C39-C40	2.43	120.27	114.60
7	L	1286	BPH	C4A-NA-C1A	2.43	110.13	108.16
5	L	1288	BCL	C14-C13-C15	2.43	120.24	111.36
5	L	1288	BCL	C9-C8-C7	2.48	120.40	111.36
5	L	1288	BCL	C1-O2A-CGA	2.52	122.83	116.77
15	M	1313	GGD	CA1-OA5-CA5	2.60	118.61	113.72
7	M	1308	BPH	C1-O2A-CGA	2.65	123.12	116.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	1282	BCL	OBB-CAB-C3B	2.65	125.00	119.95
8	L	1287[B]	U10	C10-C9-C11	2.65	119.89	115.29
12	M	1310	SPO	C24-C23-C25	2.71	122.42	118.10
15	M	1313	GGD	OC8-CC7-C31	2.75	119.92	111.90
8	L	1287[A]	U10	C10-C9-C11	2.78	120.11	115.29
7	L	1286	BPH	CED-O2D-CGD	2.80	122.55	115.97
5	L	1288	BCL	C4-C3-C5	2.81	120.16	115.29
13	M	1311	CDL	OB8-CB7-C71	2.85	120.18	111.90
12	M	1310	SPO	C34-C33-C35	2.87	120.28	115.29
7	L	1286	BPH	O2A-CGA-CBA	2.96	120.50	111.90
5	M	1303	BCL	O2A-CGA-CBA	2.98	120.57	111.90
7	M	1308	BPH	CED-O2D-CGD	3.15	123.35	115.97
13	M	1311	CDL	OA8-CA7-C31	3.15	121.07	111.90
15	M	1313	GGD	OC6-CC4-CC3	3.18	120.00	108.44
7	L	1286	BPH	C4D-C3D-CAD	3.18	109.60	107.78
5	M	1304	BCL	CED-O2D-CGD	3.24	123.58	115.97
8	M	1309	U10	C15-C14-C16	3.28	120.98	115.29
15	M	1313	GGD	CC6-CC4-CC3	3.28	119.26	111.86
8	L	1287[A]	U10	C3M-O3-C3	3.38	128.51	116.44
15	M	1313	GGD	OC6-CC4-CC6	3.38	120.74	108.44
5	L	1288	BCL	O2D-CGD-CBD	3.42	117.42	111.30
15	M	1313	GGD	CC3-OA1-CA1	3.45	120.83	113.76
7	M	1308	BPH	C4D-C3D-CAD	3.47	109.76	107.78
5	L	1282	BCL	CMB-C2B-C3B	3.50	131.39	124.89
14	M	1312	PC1	O31-C31-C32	3.57	122.29	111.90
5	M	1303	BCL	C1-O2A-CGA	3.60	125.41	116.77
8	M	1309	U10	C10-C9-C11	3.60	121.54	115.29
5	L	1282	BCL	C4-C3-C5	3.64	121.60	115.29
5	M	1304	BCL	OBB-CAB-C3B	3.64	126.88	119.95
5	M	1304	BCL	O2A-CGA-CBA	3.65	122.52	111.90
5	L	1288	BCL	O2A-CGA-CBA	3.70	122.66	111.90
7	L	1286	BPH	C2B-C1B-NB	3.71	115.32	109.82
5	L	1282	BCL	O2A-CGA-CBA	3.75	122.81	111.90
7	M	1308	BPH	C2B-C1B-NB	3.76	115.39	109.82
5	M	1304	BCL	CMB-C2B-C3B	3.78	131.90	124.89
15	M	1313	GGD	OB1-CA3-CA2	3.92	116.62	107.19
8	M	1309	U10	C25-C24-C26	4.05	122.32	115.29
13	M	1311	CDL	OB6-CB5-C51	4.08	120.03	111.55
13	M	1311	CDL	C33-C32-C31	4.21	133.09	113.42
5	M	1303	BCL	CMB-C2B-C3B	4.29	132.86	124.89
5	L	1288	BCL	CMB-C2B-C3B	4.31	132.88	124.89
15	M	1313	GGD	OA1-CC3-CC4	4.37	121.39	110.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	M	1312	PC1	O21-C21-C22	4.53	120.97	111.55
5	M	1304	BCL	O2D-CGD-CBD	4.71	119.71	111.30
13	M	1311	CDL	C34-C33-C32	4.72	150.27	113.42
15	M	1313	GGD	OC6-CC5-C14	4.79	121.50	111.55
13	M	1311	CDL	OA6-CA5-C11	5.00	121.94	111.55
5	M	1303	BCL	O2D-CGD-CBD	5.05	120.33	111.30
7	L	1286	BPH	C3C-C4C-NC	5.07	112.75	107.97
15	M	1313	GGD	OC8-CC6-CC4	5.07	121.40	108.66
7	L	1286	BPH	O2D-CGD-CBD	5.59	121.29	111.30
5	L	1282	BCL	O2D-CGD-CBD	5.99	122.01	111.30
7	M	1308	BPH	C3C-C4C-NC	6.15	113.77	107.97
7	M	1308	BPH	O2D-CGD-CBD	7.09	123.98	111.30
13	M	1311	CDL	C12-C11-CA5	7.53	141.08	113.58
13	M	1311	CDL	C20-C19-C18	9.26	162.17	114.45
13	M	1311	CDL	C17-C16-C15	11.52	173.84	114.45
13	M	1311	CDL	C13-C12-C11	12.70	159.78	113.24

All (9) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	M	1304	BCL	C8
5	M	1304	BCL	C13
5	L	1282	BCL	C8
5	L	1282	BCL	C13
5	M	1303	BCL	C8
5	M	1303	BCL	C13
14	M	1312	PC1	C2
5	L	1288	BCL	C8
5	L	1288	BCL	C13

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	M	1303	BCL	C1-C2-C3-C4

There are no ring outliers.

17 monomers are involved in 62 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	1251	GOL	6	0
4	H	1252	GOL	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	1282	BCL	4	0
7	L	1286	BPH	4	0
8	L	1287[A]	U10	4	0
5	L	1288	BCL	2	0
4	L	1292	GOL	1	0
4	L	1294	GOL	1	0
5	M	1303	BCL	7	0
5	M	1304	BCL	11	0
6	M	1305	LDA	1	0
6	M	1306	LDA	1	0
7	M	1308	BPH	12	0
8	M	1309	U10	1	0
12	M	1310	SPO	4	0
13	M	1311	CDL	8	0
15	M	1313	GGD	2	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, 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	H	241/260 (92%)	-0.33	6 (2%) 58 60	17, 24, 33, 61	3 (1%)
2	L	281/281 (100%)	-0.49	7 (2%) 58 60	16, 21, 37, 50	0
3	M	303/307 (98%)	-0.24	10 (3%) 47 49	14, 25, 42, 56	6 (1%)
All	All	825/848 (97%)	-0.35	23 (2%) 53 56	14, 23, 41, 61	9 (1%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	251	VAL	9.8
1	H	250	SER	8.3
3	M	1	ALA	5.5
3	M	301	HIS	5.3
2	L	281	GLY	4.7
3	M	3	TYR	4.5
3	M	2	GLU	4.2
2	L	59	TRP	4.1
2	L	271[A]	TRP	4.1
2	L	277	GLY	3.9
1	H	249[A]	LYS	3.9
3	M	106	ALA	3.3
2	L	276	PRO	3.3
1	H	220[A]	LYS	3.1
2	L	270	PRO	3.0
3	M	100	GLU	2.9
3	M	303	MET	2.9
1	H	18	TYR	2.7
3	M	148	TRP	2.7
1	H	52	ASN	2.6
3	M	302	GLY	2.5
3	M	105	PHE	2.4
2	L	274	ASN	2.4

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
6	LDA	L	1285	16/16	0.56	0.34	26.73	72,76,80,81	0
10	HTO	L	1291	10/10	0.35	0.56	16.49	78,80,81,82	0
6	LDA	L	1284	16/16	0.43	0.34	13.93	72,73,77,77	0
10	HTO	L	1290	10/10	0.72	0.28	11.67	60,62,63,64	0
4	GOL	H	1251	6/6	0.79	0.27	10.50	32,46,47,49	0
8	U10	L	1287[B]	23/63	0.70	0.34	10.42	34,42,44,44	23
8	U10	L	1287[A]	23/63	0.70	0.34	9.84	24,40,48,49	23
14	PC1	M	1312	43/54	0.33	0.36	9.57	66,82,95,96	0
13	CDL	M	1311	81/100	0.71	0.38	8.93	42,69,83,83	0
6	LDA	M	1305	16/16	0.80	0.20	6.94	31,45,51,51	0
6	LDA	L	1283	16/16	0.56	0.30	6.22	41,64,73,74	0
15	GGD	M	1313	57/67	0.43	0.36	5.63	47,73,90,90	0
6	LDA	M	1306	16/16	0.79	0.23	4.97	54,58,63,64	0
4	GOL	L	1292	6/6	0.64	0.21	4.92	29,42,44,45	0
12	SPO	M	1310	42/42	0.88	0.15	2.07	21,26,48,51	0
7	BPH	M	1308	65/65	0.94	0.12	2.04	17,22,69,71	0
4	GOL	L	1293	6/6	0.93	0.15	2.01	66,68,68,69	0
5	BCL	M	1303	66/66	0.96	0.12	1.79	16,21,58,58	0
5	BCL	L	1282	66/66	0.97	0.11	1.40	13,18,41,43	0
5	BCL	L	1288	66/66	0.97	0.10	1.36	14,17,31,37	0
5	BCL	M	1304	66/66	0.96	0.11	1.25	12,19,38,46	0
8	U10	M	1309	48/63	0.92	0.13	1.20	15,25,45,48	0
7	BPH	L	1286	65/65	0.98	0.08	0.82	10,16,26,28	0
9	PO4	L	1289	5/5	0.99	0.13	0.43	33,35,36,36	0
11	FE	M	1307	1/1	1.00	0.04	-2.79	15,15,15,15	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	GOL	H	1253	6/6	0.59	0.28	-	65,66,67,68	0
4	GOL	H	1254	6/6	0.79	0.19	-	63,64,64,65	0
4	GOL	H	1252	6/6	0.80	0.26	-	63,63,63,64	0
4	GOL	L	1294	6/6	0.60	0.18	-	80,81,81,81	0

6.5 Other polymers [i](#)

There are no such residues in this entry.