



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 04:46 am GMT

PDB ID : 3EOJ
Title : Fmo protein from Prosthecochloris Aestuarii 2K AT 1.3A Resolution
Authors : Tronrud, D.E.; Wen, J.; Gay, L.; Blankenship, R.E.
Deposited on : 2008-09-27
Resolution : 1.30 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

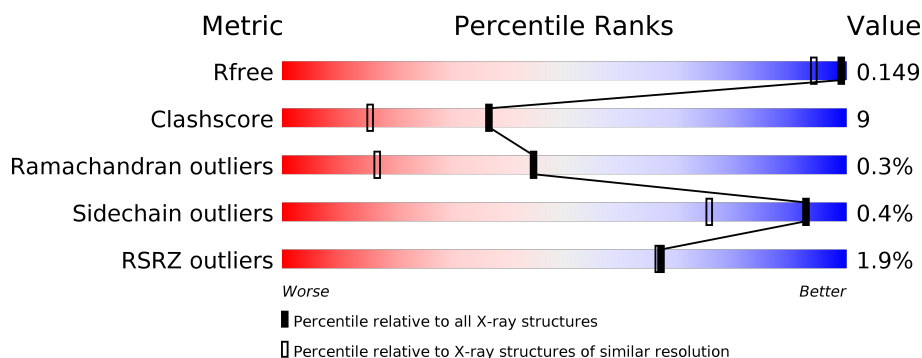
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.30 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}	100719	1131 (1.32-1.28)
Clashscore	112137	1185 (1.32-1.28)
Ramachandran outliers	110173	1138 (1.32-1.28)
Sidechain outliers	110143	1138 (1.32-1.28)
RSRZ outliers	101464	1133 (1.32-1.28)

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	A	366	<div> <div>2%</div> <div>82%</div> <div>15%</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
2	BCL	A	376[C]	-	-	-	X
2	BCL	A	376[D]	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BCL	A	378[B]	-	-	-	X
3	EDO	A	380	-	-	-	X
3	EDO	A	382	-	-	-	X
3	EDO	A	384	-	-	-	X
3	EDO	A	387	-	-	-	X
3	EDO	A	388[A]	-	-	-	X
3	EDO	A	390	-	-	-	X
3	EDO	A	391[A]	-	-	-	X
3	EDO	A	392	-	-	-	X
3	EDO	A	393[B]	-	-	-	X

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 4115 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.

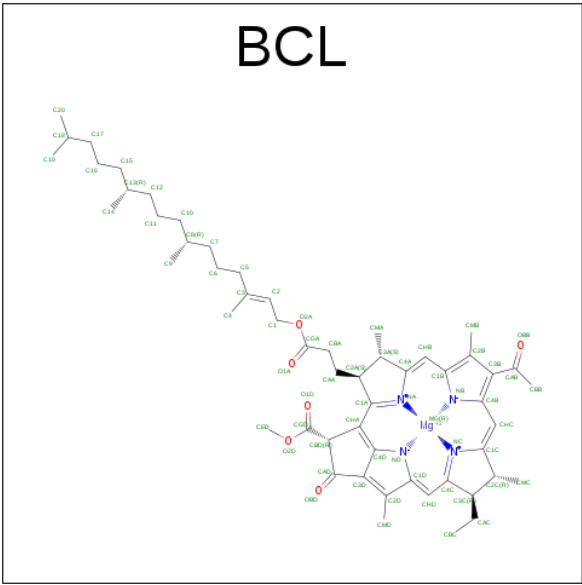
- Molecule 1 is a protein called Bacteriochlorophyll a protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	359	3082	1974	527	573	8	0	60	1

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	117	SER	GLN	SEE REMARK 999	UNP P11741

- Molecule 2 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C₅₅H₇₄MgN₄O₆).



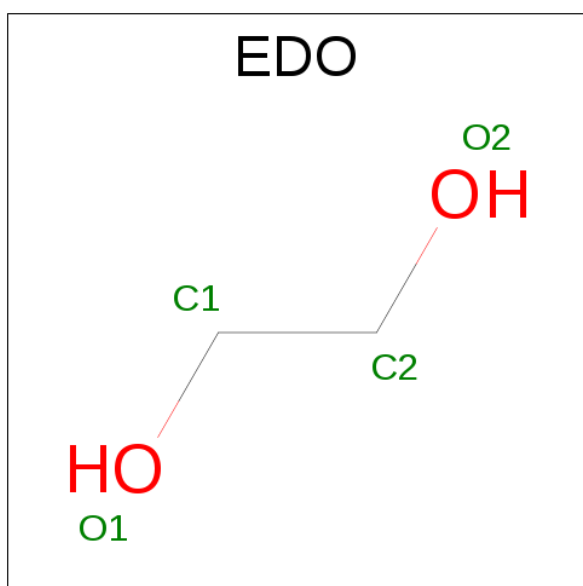
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
2	A	1	71	60	1	4	6	0	1
2	A	1	66	55	1	4	6	0	0
2	A	1	79	68	1	4	6	0	1

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
2	A	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
2	A	1	Total	C	Mg	N	O	0	1
			84	69	1	5	9		
2	A	1	Total	C	Mg	N	O	0	1
			83	71	1	4	7		
2	A	1	Total	C	Mg	N	O	0	1
			47	36	1	4	6		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	1
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		

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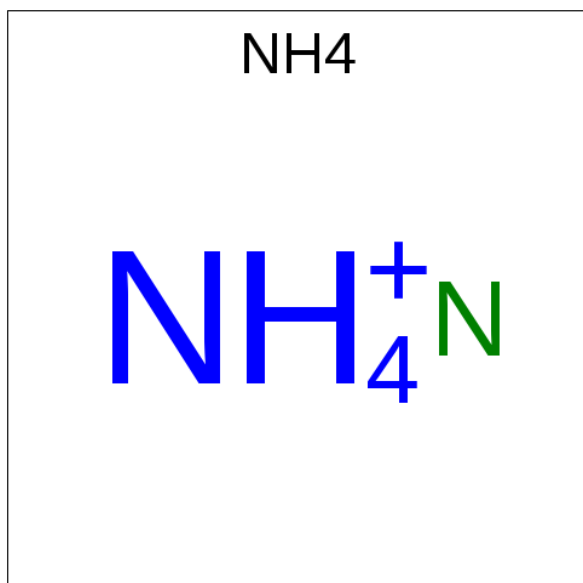
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	1
3	A	1	Total C O 4 2 2	0	1
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	1

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Na 1 1	0	0

- Molecule 5 is AMMONIUM ION (three-letter code: NH4) (formula: H₄N).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total N 2 2	0	1

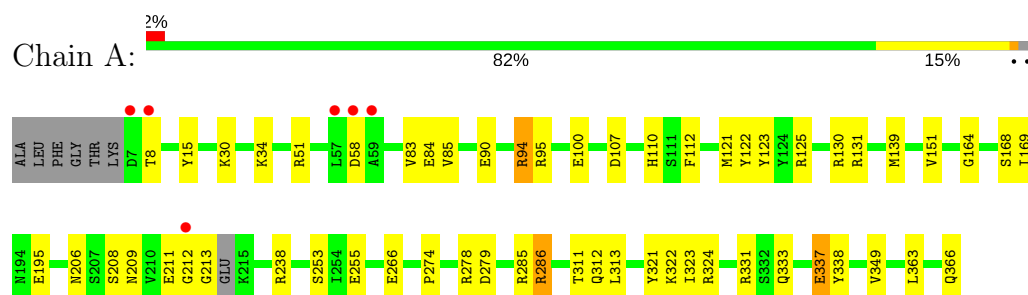
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	406	Total O 408 408	0	50

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: Bacteriochlorophyll a protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	111.24Å 111.24Å 98.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 1.30 48.40 – 1.30	Depositor EDS
% Data completeness (in resolution range)	94.9 (50.00-1.30) 92.4 (48.40-1.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.91 (at 1.30Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.135 , 0.161 0.134 , 0.149	Depositor DCC
R_{free} test set	8438 reflections (5.71%)	DCC
Wilson B-factor (Å ²)	11.5	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 56.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.027 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	4115	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BCL, NH4, EDO, NA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	6.77	4/3302 (0.1%)	1.65	38/4466 (0.9%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	213[A]	GLY	CA-C	271.60	5.86	1.51
1	A	213[B]	GLY	CA-C	271.60	5.86	1.51
1	A	139[A]	MET	SD-CE	33.99	3.68	1.77
1	A	139[B]	MET	SD-CE	33.99	3.68	1.77

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	213[A]	GLY	CA-C-O	-36.76	54.43	120.60
1	A	213[B]	GLY	CA-C-O	-36.76	54.43	120.60
1	A	139[A]	MET	CG-SD-CE	-29.38	53.19	100.20
1	A	139[B]	MET	CG-SD-CE	-29.38	53.19	100.20
1	A	94[A]	ARG	NE-CZ-NH2	15.73	128.16	120.30
1	A	94[B]	ARG	NE-CZ-NH2	15.73	128.16	120.30
1	A	107	ASP	CB-CG-OD1	14.56	131.41	118.30
1	A	131	ARG	NE-CZ-NH1	13.63	127.11	120.30
1	A	130[A]	ARG	CD-NE-CZ	9.47	136.86	123.60
1	A	130[B]	ARG	CD-NE-CZ	9.47	136.86	123.60
1	A	107	ASP	CB-CG-OD2	-8.61	110.55	118.30
1	A	94[A]	ARG	NE-CZ-NH1	-7.99	116.30	120.30
1	A	94[B]	ARG	NE-CZ-NH1	-7.99	116.30	120.30
1	A	123[A]	TYR	CB-CG-CD1	7.92	125.75	121.00
1	A	123[B]	TYR	CB-CG-CD1	7.92	125.75	121.00
1	A	58	ASP	C-N-CA	-6.91	104.42	121.70
1	A	123[A]	TYR	CB-CG-CD2	-6.85	116.89	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	123[B]	TYR	CB-CG-CD2	-6.85	116.89	121.00
1	A	83	VAL	CA-CB-CG2	6.82	121.12	110.90
1	A	279	ASP	CB-CG-OD1	6.82	124.44	118.30
1	A	238	ARG	NE-CZ-NH1	-6.67	116.96	120.30
1	A	286[A]	ARG	NE-CZ-NH1	6.59	123.60	120.30
1	A	286[B]	ARG	NE-CZ-NH1	6.59	123.60	120.30
1	A	366	GLN	CA-CB-CG	6.55	127.82	113.40
1	A	110	HIS	CA-CB-CG	6.17	124.09	113.60
1	A	331[A]	ARG	NE-CZ-NH2	-5.87	117.36	120.30
1	A	331[B]	ARG	NE-CZ-NH2	-5.87	117.36	120.30
1	A	337[A]	GLU	OE1-CD-OE2	5.58	130.00	123.30
1	A	337[B]	GLU	OE1-CD-OE2	5.58	130.00	123.30
1	A	130[A]	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	A	130[B]	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	A	321	TYR	CB-CG-CD2	5.45	124.27	121.00
1	A	95	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	A	130[A]	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	A	130[B]	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	A	212[A]	GLY	C-N-CA	5.15	133.11	122.30
1	A	212[B]	GLY	C-N-CA	5.15	133.11	122.30
1	A	95	ARG	NE-CZ-NH1	5.11	122.86	120.30

There are no chirality outliers.

There are no planarity outliers.

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	A	3082	0	3033	39	0
2	A	562	0	431	20	0
3	A	60	0	89	12	0
4	A	1	0	0	0	0
5	A	2	0	0	1	0
6	A	408	0	0	10	0
All	All	4115	0	3553	59	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 9.

All (59) 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:A:208[A]:SER:O	1:A:209[A]:ASN:ND2	1.93	1.01
2:A:375:BCL:H191	2:A:377[E]:BCL:H203	1.53	0.91
1:A:195[B]:GLU:OE2	5:A:2378[B]:NH4:N	2.06	0.88
1:A:337[B]:GLU:HG2	6:A:1100:HOH:O	1.72	0.86
2:A:377[E]:BCL:H151	2:A:377[E]:BCL:H192	1.57	0.85
1:A:208[A]:SER:C	1:A:209[A]:ASN:ND2	2.31	0.84
1:A:285:ARG:HH22	3:A:387:EDO:H11	1.52	0.74
1:A:122:TYR:HB3	1:A:125[C]:ARG:HH11	1.53	0.73
1:A:30[B]:LYS:HG3	6:A:1254:HOH:O	1.92	0.70
1:A:209[B]:ASN:ND2	1:A:211[B]:GLU:HG2	2.06	0.69
1:A:209[B]:ASN:HD22	1:A:211[B]:GLU:HG2	1.56	0.69
1:A:164[B]:GLY:O	1:A:168[B]:SER:N	2.26	0.68
2:A:377[E]:BCL:C15	2:A:377[E]:BCL:H192	2.23	0.68
1:A:285:ARG:HH22	3:A:387:EDO:C1	2.06	0.68
1:A:206[B]:ASN:ND2	6:A:1149:HOH:O	2.22	0.67
2:A:375:BCL:H191	2:A:377[E]:BCL:C20	2.24	0.67
1:A:51[A]:ARG:HG2	1:A:255[A]:GLU:HG2	1.79	0.65
1:A:121[B]:MET:SD	2:A:378[B]:BCL:HED2	2.37	0.64
2:A:375:BCL:HMB1	2:A:375:BCL:HBB2	1.79	0.64
2:A:374:BCL:CBB	2:A:374:BCL:HMB1	2.28	0.63
1:A:169[B]:ILE:HD12	1:A:176:PHE:CD2	2.33	0.63
2:A:372:BCL:HMB1	2:A:372:BCL:HBB3	1.82	0.61
1:A:322[A]:LYS:HD2	6:A:1174:HOH:O	2.03	0.59
1:A:90:GLU:OE1	1:A:94[A]:ARG:HD3	2.02	0.58
1:A:208[A]:SER:C	1:A:209[A]:ASN:HD22	2.02	0.57
1:A:8:THR:O	6:A:1230:HOH:O	2.18	0.56
1:A:169[B]:ILE:HG13	6:A:1191:HOH:O	2.04	0.56
1:A:209[B]:ASN:HD22	1:A:211[B]:GLU:CG	2.18	0.56
2:A:378[B]:BCL:HBB3	2:A:378[B]:BCL:HMB1	1.88	0.56
2:A:372:BCL:HMB1	2:A:372:BCL:CBB	2.37	0.55
1:A:253:SER:OG	3:A:382:EDO:C1	2.55	0.55
1:A:100[B]:GLU:OE2	3:A:385:EDO:O1	2.24	0.54
1:A:286[A]:ARG:HB3	1:A:363:LEU:HD23	1.90	0.54
2:A:378[B]:BCL:HBD	2:A:378[B]:BCL:HAA1	1.90	0.53
3:A:391[A]:EDO:H22	6:A:1121:HOH:O	2.09	0.51
1:A:312[A]:GLN:HG2	1:A:313:LEU:N	2.26	0.49
1:A:34:LYS:HG2	1:A:266[B]:GLU:HG3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:391[A]:EDO:H22	6:A:1136:HOH:O	2.12	0.49
1:A:112:PHE:O	3:A:383[A]:EDO:H21	2.14	0.48
1:A:169[B]:ILE:CG1	6:A:1191:HOH:O	2.61	0.48
1:A:285:ARG:NH2	3:A:387:EDO:H11	2.27	0.46
2:A:374:BCL:HBB2	2:A:374:BCL:HMB1	1.98	0.46
2:A:374:BCL:HBB3	2:A:374:BCL:HMB1	1.97	0.46
1:A:15:TYR:CE1	2:A:374:BCL:H43	2.52	0.44
1:A:311[B]:THR:HG21	1:A:349:VAL:HG21	1.99	0.44
2:A:373[A]:BCL:H203	2:A:373[A]:BCL:H161	1.63	0.44
1:A:278:ARG:CG	3:A:391[A]:EDO:H12	2.49	0.43
1:A:323[A]:ILE:HD12	1:A:338:TYR:CD1	2.54	0.43
1:A:333[B]:GLN:HB3	1:A:338:TYR:CD1	2.54	0.42
3:A:392:EDO:H21	6:A:1141:HOH:O	2.19	0.42
1:A:253:SER:OG	3:A:382:EDO:H12	2.20	0.42
1:A:274:PRO:HG2	2:A:375:BCL:HMB3	2.01	0.41
2:A:374:BCL:C1B	2:A:375:BCL:H42	2.50	0.41
1:A:84:GLU:OE1	3:A:385:EDO:O1	2.38	0.41

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	413/366 (113%)	408 (99%)	3 (1%)	2 (0%)	32 7

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	170[A]	SER
1	A	170[B]	SER

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	A	335/303 (111%)	333 (99%)	2 (1%)	89	64

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	324[A]	ARG
1	A	324[B]	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 36 ligands modelled in this entry, 1 is monoatomic and 2 are modelled with single atom - leaving 33 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	$\# Z > 2$
2	BCL	A	371[A]	-	55,74,74	1.29	3 (5%)	65,115,115	1.20	9 (13%)
2	BCL	A	371[B]	-	55,74,74	1.27	3 (5%)	65,115,115	1.15	8 (12%)
2	BCL	A	372	6	55,74,74	1.28	2 (3%)	65,115,115	1.16	7 (10%)
2	BCL	A	373[A]	-	55,74,74	1.17	2 (3%)	65,115,115	1.10	6 (9%)
2	BCL	A	373[B]	-	55,74,74	1.17	2 (3%)	65,115,115	1.15	6 (9%)
2	BCL	A	374	1	55,74,74	1.18	2 (3%)	65,115,115	1.07	6 (9%)
2	BCL	A	375	1	55,74,74	1.29	2 (3%)	65,115,115	1.16	8 (12%)
2	BCL	A	376[A]	-	46,61,74	1.61	5 (10%)	51,90,115	1.65	12 (23%)
2	BCL	A	376[B]	-	46,61,74	1.59	5 (10%)	51,90,115	1.62	12 (23%)
2	BCL	A	376[C]	-	48,63,74	2.46	11 (22%)	53,94,115	1.84	14 (26%)
2	BCL	A	376[D]	-	48,63,74	2.40	11 (22%)	53,94,115	1.85	14 (26%)
2	BCL	A	377[A]	-	42,58,74	2.56	6 (14%)	45,89,115	1.40	5 (11%)
2	BCL	A	377[B]	-	42,58,74	2.56	6 (14%)	45,89,115	1.42	6 (13%)
2	BCL	A	377[C]	-	45,63,74	1.28	3 (6%)	50,97,115	1.67	4 (8%)
2	BCL	A	377[D]	-	45,63,74	1.27	3 (6%)	50,97,115	1.67	4 (8%)
2	BCL	A	377[E]	-	46,59,74	2.59	7 (15%)	45,87,115	1.96	7 (15%)
2	BCL	A	377[F]	-	46,59,74	2.59	7 (15%)	45,87,115	2.01	6 (13%)
2	BCL	A	378[B]	1	36,55,74	1.46	2 (5%)	43,92,115	1.67	10 (23%)
3	EDO	A	379	-	3,3,3	0.36	0	2,2,2	0.21	0
3	EDO	A	380	-	3,3,3	0.43	0	2,2,2	0.17	0
3	EDO	A	381	-	3,3,3	0.24	0	2,2,2	1.89	1 (50%)
3	EDO	A	382	-	3,3,3	0.58	0	2,2,2	0.48	0
3	EDO	A	383[A]	-	3,3,3	0.26	0	2,2,2	0.51	0
3	EDO	A	384	-	3,3,3	0.54	0	2,2,2	0.34	0
3	EDO	A	385	-	3,3,3	0.72	0	2,2,2	0.28	0
3	EDO	A	386	-	3,3,3	0.35	0	2,2,2	0.54	0
3	EDO	A	387	-	3,3,3	0.70	0	2,2,2	0.73	0
3	EDO	A	388[A]	-	3,3,3	0.72	0	2,2,2	0.46	0
3	EDO	A	389	-	3,3,3	0.77	0	2,2,2	1.44	0
3	EDO	A	390	-	3,3,3	0.57	0	2,2,2	0.35	0
3	EDO	A	391[A]	-	3,3,3	0.28	0	2,2,2	0.76	0
3	EDO	A	392	-	3,3,3	0.68	0	2,2,2	0.35	0
3	EDO	A	393[B]	-	3,3,3	0.57	0	2,2,2	0.55	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
2	BCL	A	371[A]	-	-	0/37/137/137	0/0/9/9
2	BCL	A	371[B]	-	-	0/37/137/137	0/0/9/9
2	BCL	A	372	6	-	0/37/137/137	0/0/9/9
2	BCL	A	373[A]	-	-	0/37/137/137	0/0/9/9
2	BCL	A	373[B]	-	-	0/37/137/137	0/0/9/9
2	BCL	A	374	1	-	0/37/137/137	0/0/9/9
2	BCL	A	375	1	-	0/37/137/137	0/0/9/9
2	BCL	A	376[A]	-	-	0/33/104/137	0/3/6/9
2	BCL	A	376[B]	-	-	0/33/104/137	0/3/6/9
2	BCL	A	376[C]	-	-	0/35/95/137	0/5/6/9
2	BCL	A	376[D]	-	-	0/35/95/137	0/5/6/9
2	BCL	A	377[A]	-	-	0/28/94/137	0/5/6/9
2	BCL	A	377[B]	-	-	0/28/94/137	0/5/6/9
2	BCL	A	377[C]	-	-	0/32/125/137	0/0/8/9
2	BCL	A	377[D]	-	-	0/32/125/137	0/0/8/9
2	BCL	A	377[E]	-	-	0/38/97/137	0/4/5/9
2	BCL	A	377[F]	-	-	0/38/97/137	0/4/5/9
2	BCL	A	378[B]	1	-	0/15/115/137	0/0/9/9
3	EDO	A	379	-	-	0/1/1/1	0/0/0/0
3	EDO	A	380	-	-	0/1/1/1	0/0/0/0
3	EDO	A	381	-	-	0/1/1/1	0/0/0/0
3	EDO	A	382	-	-	0/1/1/1	0/0/0/0
3	EDO	A	383[A]	-	-	0/1/1/1	0/0/0/0
3	EDO	A	384	-	-	0/1/1/1	0/0/0/0
3	EDO	A	385	-	-	0/1/1/1	0/0/0/0
3	EDO	A	386	-	-	0/1/1/1	0/0/0/0
3	EDO	A	387	-	-	0/1/1/1	0/0/0/0
3	EDO	A	388[A]	-	-	0/1/1/1	0/0/0/0
3	EDO	A	389	-	-	0/1/1/1	0/0/0/0
3	EDO	A	390	-	-	0/1/1/1	0/0/0/0
3	EDO	A	391[A]	-	-	0/1/1/1	0/0/0/0
3	EDO	A	392	-	-	0/1/1/1	0/0/0/0
3	EDO	A	393[B]	-	-	0/1/1/1	0/0/0/0

All (82) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	377[A]	BCL	C2D-C3D	-11.81	1.40	1.56
2	A	377[B]	BCL	C2D-C3D	-11.81	1.40	1.56
2	A	377[E]	BCL	C2D-C3D	-11.81	1.40	1.56
2	A	377[F]	BCL	C2D-C3D	-11.81	1.40	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	376[C]	BCL	C2D-C3D	-10.93	1.41	1.56
2	A	376[D]	BCL	C2D-C3D	-10.30	1.42	1.56
2	A	377[E]	BCL	C4B-NB	-7.70	1.37	1.47
2	A	377[F]	BCL	C4B-NB	-7.70	1.37	1.47
2	A	376[C]	BCL	C3D-CAD	-5.49	1.43	1.52
2	A	376[D]	BCL	C3D-CAD	-5.35	1.43	1.52
2	A	377[A]	BCL	C3D-CAD	-5.04	1.44	1.52
2	A	377[B]	BCL	C3D-CAD	-5.04	1.44	1.52
2	A	377[E]	BCL	C3D-CAD	-5.04	1.44	1.52
2	A	377[F]	BCL	C3D-CAD	-5.04	1.44	1.52
2	A	377[A]	BCL	C2D-C1D	-4.81	1.43	1.51
2	A	377[B]	BCL	C2D-C1D	-4.81	1.43	1.51
2	A	377[E]	BCL	C2D-C1D	-4.81	1.43	1.51
2	A	377[F]	BCL	C2D-C1D	-4.81	1.43	1.51
2	A	376[D]	BCL	CHC-C4B	-4.50	1.40	1.49
2	A	376[C]	BCL	CHC-C4B	-4.50	1.40	1.49
2	A	376[D]	BCL	C2D-C1D	-4.49	1.44	1.51
2	A	376[C]	BCL	C2D-C1D	-4.49	1.44	1.51
2	A	377[A]	BCL	CHC-C4B	-4.09	1.41	1.49
2	A	377[B]	BCL	CHC-C4B	-4.09	1.41	1.49
2	A	377[C]	BCL	C2B-C1B	-3.16	1.44	1.52
2	A	377[E]	BCL	C2B-C1B	-3.16	1.44	1.52
2	A	377[D]	BCL	C2B-C1B	-3.16	1.44	1.52
2	A	377[F]	BCL	C2B-C1B	-3.16	1.44	1.52
2	A	376[D]	BCL	O1A-CGA	-2.85	1.14	1.22
2	A	376[A]	BCL	O1A-CGA	-2.85	1.14	1.22
2	A	376[B]	BCL	O1A-CGA	-2.85	1.14	1.22
2	A	376[C]	BCL	O1A-CGA	-2.85	1.14	1.22
2	A	376[D]	BCL	CBD-CGD	-2.61	1.47	1.53
2	A	376[C]	BCL	CBD-CGD	-2.54	1.47	1.53
2	A	376[D]	BCL	C2-C3	-2.29	1.27	1.33
2	A	376[A]	BCL	C2-C3	-2.29	1.27	1.33
2	A	376[B]	BCL	C2-C3	-2.29	1.27	1.33
2	A	376[C]	BCL	C2-C3	-2.29	1.27	1.33
2	A	377[C]	BCL	C4B-CHC	-2.15	1.41	1.48
2	A	377[D]	BCL	C4B-CHC	-2.15	1.41	1.48
2	A	376[D]	BCL	C3B-C4B	2.12	1.46	1.40
2	A	376[C]	BCL	C3B-C4B	2.12	1.46	1.40
2	A	371[A]	BCL	C3C-C4C	2.32	1.54	1.51
2	A	371[B]	BCL	C3C-C4C	2.32	1.54	1.51
2	A	376[D]	BCL	C5-C3	3.08	1.58	1.51
2	A	376[A]	BCL	C5-C3	3.08	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	376[B]	BCL	C5-C3	3.08	1.58	1.51
2	A	376[C]	BCL	C5-C3	3.08	1.58	1.51
2	A	377[E]	BCL	MG-NA	3.24	2.17	2.05
2	A	377[F]	BCL	MG-NA	3.24	2.17	2.05
2	A	374	BCL	CHB-C4A	4.33	1.39	1.33
2	A	376[D]	BCL	CHD-C1D	4.33	1.42	1.33
2	A	376[C]	BCL	CHD-C1D	4.33	1.42	1.33
2	A	372	BCL	CHB-C4A	4.41	1.39	1.33
2	A	378[B]	BCL	CHB-C4A	4.42	1.39	1.33
2	A	377[A]	BCL	CHD-C1D	4.61	1.43	1.33
2	A	377[B]	BCL	CHD-C1D	4.61	1.43	1.33
2	A	377[E]	BCL	CHD-C1D	4.61	1.43	1.33
2	A	377[F]	BCL	CHD-C1D	4.61	1.43	1.33
2	A	373[A]	BCL	CHB-C4A	4.63	1.39	1.33
2	A	373[B]	BCL	CHB-C4A	4.63	1.39	1.33
2	A	373[A]	BCL	CHC-C1C	4.96	1.39	1.33
2	A	373[B]	BCL	CHC-C1C	4.96	1.39	1.33
2	A	371[A]	BCL	CHB-C4A	5.25	1.40	1.33
2	A	371[B]	BCL	CHB-C4A	5.25	1.40	1.33
2	A	376[D]	BCL	CHB-C4A	5.26	1.40	1.33
2	A	376[A]	BCL	CHB-C4A	5.26	1.40	1.33
2	A	376[B]	BCL	CHB-C4A	5.26	1.40	1.33
2	A	376[C]	BCL	CHB-C4A	5.26	1.40	1.33
2	A	375	BCL	CHB-C4A	5.28	1.40	1.33
2	A	371[A]	BCL	CHC-C1C	5.32	1.40	1.33
2	A	371[B]	BCL	CHC-C1C	5.32	1.40	1.33
2	A	378[B]	BCL	CHC-C1C	5.53	1.40	1.33
2	A	375	BCL	CHC-C1C	5.72	1.40	1.33
2	A	377[A]	BCL	CHB-C4A	5.87	1.41	1.33
2	A	377[B]	BCL	CHB-C4A	5.87	1.41	1.33
2	A	372	BCL	CHC-C1C	6.01	1.41	1.33
2	A	377[D]	BCL	CHC-C1C	6.27	1.40	1.33
2	A	377[C]	BCL	CHC-C1C	6.28	1.40	1.33
2	A	374	BCL	CHC-C1C	6.34	1.41	1.33
2	A	376[B]	BCL	CHC-C1C	6.38	1.41	1.33
2	A	376[A]	BCL	CHC-C1C	6.53	1.41	1.33

All (145) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	376[D]	BCL	C11-C10-C8	-5.71	97.00	115.73
2	A	376[A]	BCL	C11-C10-C8	-5.71	97.00	115.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	376[B]	BCL	C11-C10-C8	-5.71	97.00	115.73
2	A	376[C]	BCL	C11-C10-C8	-5.71	97.00	115.73
2	A	378[B]	BCL	CMB-C2B-C1B	-4.58	121.42	128.46
2	A	371[A]	BCL	CHA-C1A-NA	-3.45	118.17	126.18
2	A	371[B]	BCL	CHA-C1A-NA	-3.45	118.17	126.18
2	A	375	BCL	C4-C3-C5	-3.34	109.49	115.29
2	A	376[D]	BCL	C4-C3-C5	-3.26	109.63	115.29
2	A	376[A]	BCL	C4-C3-C5	-3.26	109.63	115.29
2	A	376[B]	BCL	C4-C3-C5	-3.26	109.63	115.29
2	A	376[C]	BCL	C4-C3-C5	-3.26	109.63	115.29
2	A	378[B]	BCL	OBD-CAD-CBD	-3.26	121.02	125.94
2	A	376[D]	BCL	O2A-CGA-O1A	-3.16	115.71	123.55
2	A	376[A]	BCL	O2A-CGA-O1A	-3.16	115.71	123.55
2	A	376[B]	BCL	O2A-CGA-O1A	-3.16	115.71	123.55
2	A	376[C]	BCL	O2A-CGA-O1A	-3.16	115.71	123.55
2	A	372	BCL	CMB-C2B-C1B	-3.15	123.62	128.46
2	A	374	BCL	OBD-CAD-CBD	-3.12	121.23	125.94
2	A	373[A]	BCL	CHA-C1A-NA	-3.10	118.97	126.18
2	A	373[B]	BCL	CHA-C1A-NA	-3.10	118.97	126.18
2	A	377[A]	BCL	CMB-C2B-C1B	-3.10	123.70	128.46
2	A	377[B]	BCL	CMB-C2B-C1B	-3.10	123.70	128.46
2	A	374	BCL	CMB-C2B-C1B	-3.09	123.71	128.46
2	A	375	BCL	CMB-C2B-C1B	-3.04	123.79	128.46
2	A	371[A]	BCL	C1-C2-C3	-2.98	120.47	125.96
2	A	371[B]	BCL	C1-C2-C3	-2.98	120.47	125.96
2	A	375	BCL	OBD-CAD-CBD	-2.68	121.89	125.94
2	A	376[D]	BCL	CMB-C2B-C1B	-2.65	124.40	128.46
2	A	376[A]	BCL	CMB-C2B-C1B	-2.65	124.40	128.46
2	A	376[B]	BCL	CMB-C2B-C1B	-2.65	124.40	128.46
2	A	376[C]	BCL	CMB-C2B-C1B	-2.65	124.40	128.46
2	A	373[A]	BCL	OBD-CAD-CBD	-2.61	122.00	125.94
2	A	373[B]	BCL	OBD-CAD-CBD	-2.61	122.00	125.94
2	A	371[A]	BCL	OBD-CAD-CBD	-2.58	122.04	125.94
2	A	371[B]	BCL	OBD-CAD-CBD	-2.58	122.04	125.94
2	A	371[A]	BCL	CMB-C2B-C1B	-2.54	124.56	128.46
2	A	371[B]	BCL	CMB-C2B-C1B	-2.54	124.56	128.46
2	A	375	BCL	O2A-CGA-O1A	-2.51	117.32	123.55
2	A	375	BCL	CHA-C1A-NA	-2.50	120.38	126.18
2	A	372	BCL	OBD-CAD-CBD	-2.49	122.18	125.94
2	A	376[C]	BCL	O2D-CGD-O1D	-2.46	118.86	123.82
2	A	377[E]	BCL	C16-C17-C18	-2.46	104.21	115.96
2	A	372	BCL	C1-C2-C3	-2.45	121.44	125.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	378[B]	BCL	O2A-CGA-O1A	-2.40	115.17	123.12
2	A	376[D]	BCL	C11-C12-C13	-2.40	107.86	115.73
2	A	376[A]	BCL	C11-C12-C13	-2.40	107.86	115.73
2	A	376[B]	BCL	C11-C12-C13	-2.40	107.86	115.73
2	A	376[C]	BCL	C11-C12-C13	-2.40	107.86	115.73
2	A	376[D]	BCL	C14-C13-C15	-2.38	102.67	111.36
2	A	376[A]	BCL	C14-C13-C15	-2.38	102.67	111.36
2	A	376[B]	BCL	C14-C13-C15	-2.38	102.67	111.36
2	A	376[C]	BCL	C14-C13-C15	-2.38	102.67	111.36
2	A	372	BCL	CHA-C1A-NA	-2.38	120.66	126.18
2	A	377[A]	BCL	O2A-CGA-O1A	-2.31	117.81	123.55
2	A	377[C]	BCL	O2A-CGA-O1A	-2.31	117.81	123.55
2	A	377[B]	BCL	O2A-CGA-O1A	-2.31	117.81	123.55
2	A	377[E]	BCL	O2A-CGA-O1A	-2.31	117.81	123.55
2	A	377[D]	BCL	O2A-CGA-O1A	-2.31	117.81	123.55
2	A	377[F]	BCL	O2A-CGA-O1A	-2.31	117.81	123.55
2	A	376[D]	BCL	C15-C13-C12	-2.28	101.16	112.10
2	A	376[A]	BCL	C15-C13-C12	-2.28	101.16	112.10
2	A	376[B]	BCL	C15-C13-C12	-2.28	101.16	112.10
2	A	376[C]	BCL	C15-C13-C12	-2.28	101.16	112.10
2	A	377[B]	BCL	C4B-C3B-CAB	-2.27	122.92	127.41
2	A	377[C]	BCL	CHA-C1A-NA	-2.22	121.03	126.18
2	A	377[D]	BCL	CHA-C1A-NA	-2.22	121.03	126.18
2	A	378[B]	BCL	CHD-C4C-NC	-2.19	122.64	125.08
2	A	371[A]	BCL	C16-C15-C13	-2.17	108.60	115.73
2	A	376[D]	BCL	C6-C7-C8	-2.08	108.90	115.73
2	A	376[A]	BCL	C6-C7-C8	-2.08	108.90	115.73
2	A	376[B]	BCL	C6-C7-C8	-2.08	108.90	115.73
2	A	376[C]	BCL	C6-C7-C8	-2.08	108.90	115.73
2	A	378[B]	BCL	OBB-CAB-CBB	-2.08	115.42	120.16
2	A	377[E]	BCL	C16-C15-C13	-2.04	109.04	115.73
2	A	371[A]	BCL	CBA-CAA-C2A	2.03	119.88	113.80
2	A	371[B]	BCL	CBA-CAA-C2A	2.03	119.88	113.80
2	A	372	BCL	OBB-CAB-C3B	2.05	123.86	119.95
2	A	375	BCL	CMD-C2D-C3D	2.06	128.72	124.89
2	A	378[B]	BCL	C2A-C3A-C4A	2.08	105.22	101.87
2	A	376[D]	BCL	C1-O2A-CGA	2.08	121.77	116.77
2	A	376[A]	BCL	C1-O2A-CGA	2.08	121.77	116.77
2	A	376[B]	BCL	C1-O2A-CGA	2.08	121.77	116.77
2	A	376[C]	BCL	C1-O2A-CGA	2.08	121.77	116.77
2	A	374	BCL	C2A-C1A-CHA	2.13	127.70	123.92
2	A	371[A]	BCL	CAA-C2A-C1A	2.18	119.12	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	371[B]	BCL	CAA-C2A-C1A	2.18	119.12	111.97
2	A	378[B]	BCL	O2A-CGA-CBA	2.19	121.38	112.33
2	A	373[A]	BCL	C6-C5-C3	2.26	117.79	112.66
2	A	373[B]	BCL	C6-C5-C3	2.26	117.79	112.66
2	A	376[D]	BCL	OBD-CAD-C3D	2.28	132.76	127.42
2	A	373[A]	BCL	C11-C10-C8	2.28	123.22	115.73
2	A	374	BCL	C4A-NA-C1A	2.31	109.32	106.45
2	A	373[A]	BCL	C2A-C1A-CHA	2.32	128.04	123.92
2	A	373[B]	BCL	C2A-C1A-CHA	2.32	128.04	123.92
2	A	377[C]	BCL	O2D-CGD-CBD	2.33	115.45	111.30
2	A	377[D]	BCL	O2D-CGD-CBD	2.33	115.45	111.30
2	A	376[D]	BCL	C5-C3-C2	2.33	125.87	121.10
2	A	376[A]	BCL	C5-C3-C2	2.33	125.87	121.10
2	A	376[B]	BCL	C5-C3-C2	2.33	125.87	121.10
2	A	376[C]	BCL	C5-C3-C2	2.33	125.87	121.10
2	A	371[A]	BCL	CMB-C2B-C3B	2.34	129.23	124.89
2	A	371[B]	BCL	CMB-C2B-C3B	2.34	129.23	124.89
2	A	375	BCL	C4-C3-C2	2.34	129.94	123.69
2	A	377[E]	BCL	CHC-C4B-NB	2.36	120.59	113.89
2	A	377[F]	BCL	CHC-C4B-NB	2.36	120.59	113.89
2	A	375	BCL	CMB-C2B-C3B	2.36	129.27	124.89
2	A	377[A]	BCL	O2D-CGD-CBD	2.40	115.45	111.30
2	A	377[B]	BCL	O2D-CGD-CBD	2.40	115.45	111.30
2	A	377[E]	BCL	O2D-CGD-CBD	2.40	115.45	111.30
2	A	377[F]	BCL	O2D-CGD-CBD	2.40	115.45	111.30
2	A	378[B]	BCL	CMD-C2D-C3D	2.46	129.45	124.89
2	A	371[A]	BCL	C2A-C1A-CHA	2.58	128.49	123.92
2	A	371[B]	BCL	C2A-C1A-CHA	2.58	128.49	123.92
2	A	376[D]	BCL	C14-C13-C12	2.59	120.80	111.36
2	A	376[A]	BCL	C14-C13-C12	2.59	120.80	111.36
2	A	376[B]	BCL	C14-C13-C12	2.59	120.80	111.36
2	A	376[C]	BCL	C14-C13-C12	2.59	120.80	111.36
2	A	372	BCL	CMD-C2D-C3D	2.59	129.70	124.89
3	A	381	EDO	O1-C1-C2	2.63	130.91	112.08
2	A	373[A]	BCL	CMD-C2D-C3D	2.63	129.77	124.89
2	A	373[B]	BCL	CMD-C2D-C3D	2.63	129.77	124.89
2	A	378[B]	BCL	C4A-NA-C1A	2.68	109.77	106.45
2	A	376[D]	BCL	CMB-C2B-C3B	2.70	129.90	124.89
2	A	376[A]	BCL	CMB-C2B-C3B	2.70	129.90	124.89
2	A	376[B]	BCL	CMB-C2B-C3B	2.70	129.90	124.89
2	A	376[C]	BCL	CMB-C2B-C3B	2.70	129.90	124.89
2	A	374	BCL	CMB-C2B-C3B	2.82	130.13	124.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	377[A]	BCL	CMB-C2B-C3B	2.86	130.19	124.89
2	A	377[B]	BCL	CMB-C2B-C3B	2.94	130.35	124.89
2	A	372	BCL	CMB-C2B-C3B	3.08	130.62	124.89
2	A	374	BCL	CMD-C2D-C3D	3.24	130.90	124.89
2	A	373[B]	BCL	C17-C16-C15	3.65	130.92	113.25
2	A	378[B]	BCL	CBA-CAA-C2A	3.87	125.37	113.80
2	A	377[F]	BCL	C16-C15-C13	4.34	129.98	115.73
2	A	376[D]	BCL	CMD-C2D-C1D	5.25	125.69	112.08
2	A	376[C]	BCL	CMD-C2D-C1D	5.25	125.69	112.08
2	A	377[A]	BCL	CMD-C2D-C1D	5.89	127.37	112.08
2	A	377[B]	BCL	CMD-C2D-C1D	5.89	127.37	112.08
2	A	377[E]	BCL	CMD-C2D-C1D	5.89	127.37	112.08
2	A	377[F]	BCL	CMD-C2D-C1D	5.89	127.37	112.08
2	A	377[C]	BCL	CMB-C2B-C1B	9.46	123.70	113.17
2	A	377[E]	BCL	CMB-C2B-C1B	9.46	123.70	113.17
2	A	377[D]	BCL	CMB-C2B-C1B	9.46	123.70	113.17
2	A	377[F]	BCL	CMB-C2B-C1B	9.46	123.70	113.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	372	BCL	2	0
2	A	373[A]	BCL	1	0
2	A	374	BCL	5	0
2	A	375	BCL	5	0
2	A	377[A]	BCL	1	0
2	A	377[B]	BCL	2	0
2	A	377[E]	BCL	4	0
2	A	378[B]	BCL	3	0
3	A	382	EDO	2	0
3	A	383[A]	EDO	1	0
3	A	385	EDO	2	0
3	A	387	EDO	3	0
3	A	391[A]	EDO	3	0
3	A	392	EDO	1	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	A	359/366 (98%)	-0.21	7 (1%) 67 66	8, 14, 26, 48	14 (3%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	8	THR	5.1
1	A	59	ALA	4.5
1	A	212[A]	GLY	3.0
1	A	58	ASP	2.7
1	A	57	LEU	2.4
1	A	7	ASP	2.3
1	A	193	ILE	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, 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(\AA^2)	Q<0.9
3	EDO	A	391[A]	4/4	0.66	0.31	20.02	29,29,39,39	4
3	EDO	A	388[A]	4/4	0.90	0.25	8.77	17,19,21,22	4
3	EDO	A	382	4/4	0.48	0.22	6.94	64,72,72,77	0
3	EDO	A	380	4/4	0.86	0.20	6.15	34,35,38,60	0
2	BCL	A	376[C]	58/66	0.97	0.07	4.86	9,12,27,29	10
3	EDO	A	387	4/4	0.81	0.18	4.31	23,27,33,45	0
3	EDO	A	392	4/4	0.71	0.32	3.77	39,41,44,55	0
3	EDO	A	384	4/4	0.83	0.21	3.25	25,27,38,47	0
2	BCL	A	378[B]	47/66	0.93	0.16	3.12	13,19,26,33	47
3	EDO	A	390	4/4	0.94	0.15	3.11	19,20,30,32	0
3	EDO	A	393[B]	4/4	0.89	0.17	2.05	24,27,28,32	4
3	EDO	A	385	4/4	0.86	0.14	1.57	34,35,37,42	0
2	BCL	A	376[D]	58/66	0.97	0.07	1.29	9,12,27,29	10
2	BCL	A	376[A]	56/66	0.97	0.07	1.29	8,12,27,29	8
3	EDO	A	386	4/4	0.94	0.10	0.96	25,27,32,39	0
3	EDO	A	383[A]	4/4	0.88	0.12	0.83	20,25,28,30	4
2	BCL	A	373[B]	66/66	0.99	0.07	0.71	8,10,17,19	13
2	BCL	A	373[A]	66/66	0.99	0.07	0.71	8,10,16,17	13
3	EDO	A	389	4/4	0.98	0.12	0.69	15,17,28,29	0
2	BCL	A	374	66/66	0.98	0.06	0.36	8,11,14,18	0
2	BCL	A	377[F]	55/66	0.98	0.10	0.09	7,9,25,31	6
2	BCL	A	377[A]	53/66	0.98	0.10	0.09	7,9,14,14	4
2	BCL	A	377[B]	53/66	0.98	0.10	0.09	7,9,14,14	4
2	BCL	A	377[E]	55/66	0.98	0.10	0.09	7,9,25,27	6
2	BCL	A	377[C]	56/66	0.98	0.10	0.09	7,9,14,14	7
2	BCL	A	377[D]	56/66	0.98	0.10	0.09	7,9,14,14	7
2	BCL	A	376[B]	56/66	0.97	0.07	-0.06	8,12,27,29	8
2	BCL	A	375	66/66	0.98	0.06	-0.23	9,12,22,30	0
2	BCL	A	372	66/66	0.98	0.06	-0.24	9,11,18,21	0
2	BCL	A	371[A]	66/66	0.98	0.05	-0.45	10,12,16,19	5
2	BCL	A	371[B]	66/66	0.98	0.05	-0.45	10,12,15,19	5
3	EDO	A	381	4/4	0.97	0.10	-0.83	13,19,20,25	0
5	NH4	A	2378[B]	1/1	0.88	0.91	-	6,6,6,6	1
3	EDO	A	379	4/4	0.93	0.11	-	28,41,43,50	0
4	NA	A	1232	1/1	0.99	0.29	-	27,27,27,27	0
5	NH4	A	2378[A]	1/1	0.88	0.91	-	27,27,27,27	1

6.5 Other polymers ⓘ

There are no such residues in this entry.