Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:14 PM GMT

PDB ID	:	4BWI
Title	:	Structure of the phytochrome Cph2 from Synechocystis sp. PCC6803
Authors	:	Anders, K.; Angerer, V.; Widany, G.D.; Mroginski, M.A.; Stetten, D.v.; Essen, L.-O.
Deposited on	:	2013-07-03
Resolution	:	2.60 Å(reported)

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

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

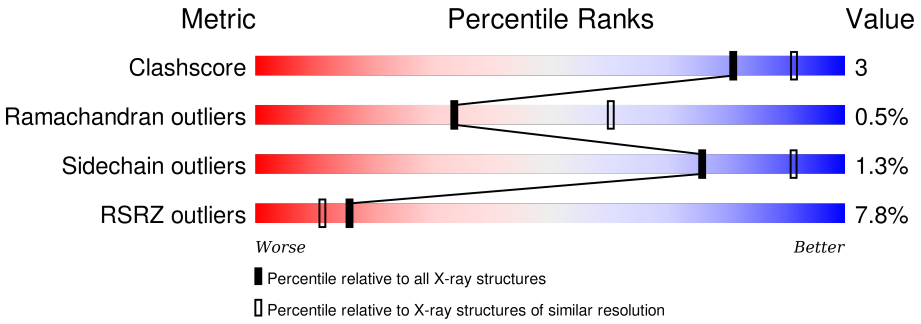
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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 <=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	432	5% 80% 8% 12%
1	B	432	9% 77% 10% 13%

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	GLU	A	1427	-	-	-	X
4	GOL	B	1420	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	FMT	A	1424	-	-	-	X
5	FMT	A	1425	-	-	-	X
5	FMT	B	1423	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 6311 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.

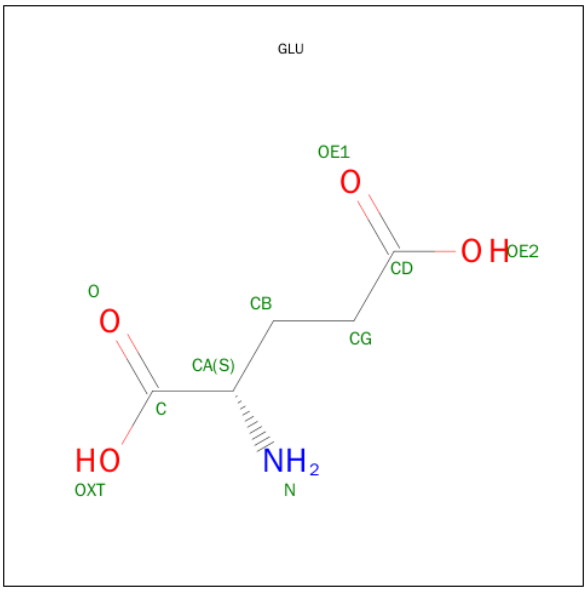
- Molecule 1 is a protein called PHYTOCHROME-LIKE PROTEIN CPH2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	381	Total	C	N	O	S	0	1	0
			3009	1910	540	550	9			
1	B	377	Total	C	N	O	S	0	0	0
			2992	1898	542	544	8			

There are 18 discrepancies between the modelled and reference sequences:

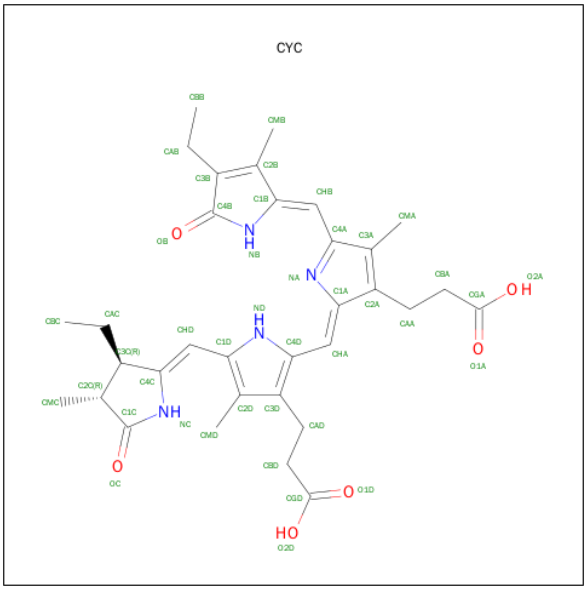
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	EXPRESSION TAG	UNP Q55434
A	425	ALA	-	EXPRESSION TAG	UNP Q55434
A	426	SER	-	EXPRESSION TAG	UNP Q55434
A	427	HIS	-	EXPRESSION TAG	UNP Q55434
A	428	HIS	-	EXPRESSION TAG	UNP Q55434
A	429	HIS	-	EXPRESSION TAG	UNP Q55434
A	430	HIS	-	EXPRESSION TAG	UNP Q55434
A	431	HIS	-	EXPRESSION TAG	UNP Q55434
A	432	HIS	-	EXPRESSION TAG	UNP Q55434
B	1	SER	-	EXPRESSION TAG	UNP Q55434
B	425	ALA	-	EXPRESSION TAG	UNP Q55434
B	426	SER	-	EXPRESSION TAG	UNP Q55434
B	427	HIS	-	EXPRESSION TAG	UNP Q55434
B	428	HIS	-	EXPRESSION TAG	UNP Q55434
B	429	HIS	-	EXPRESSION TAG	UNP Q55434
B	430	HIS	-	EXPRESSION TAG	UNP Q55434
B	431	HIS	-	EXPRESSION TAG	UNP Q55434
B	432	HIS	-	EXPRESSION TAG	UNP Q55434

- Molecule 2 is GLUTAMIC ACID (three-letter code: GLU) (formula: $C_5H_9NO_4$).



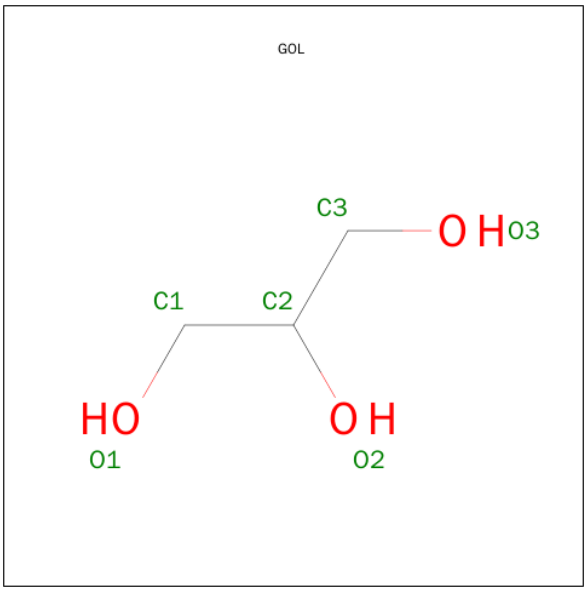
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	5	1	4		

- Molecule 3 is PHYCOCYANOBILIN (three-letter code: CYC) (formula: $C_{33}H_{40}N_4O_6$).



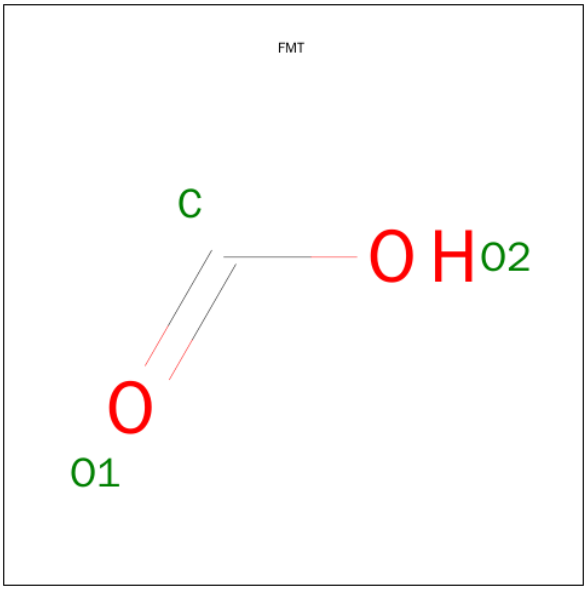
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			43	33	4	6		
3	B	1	Total	C	N	O	0	0
			43	33	4	6		

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0

- Molecule 5 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



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

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

- Molecule 6 is water.

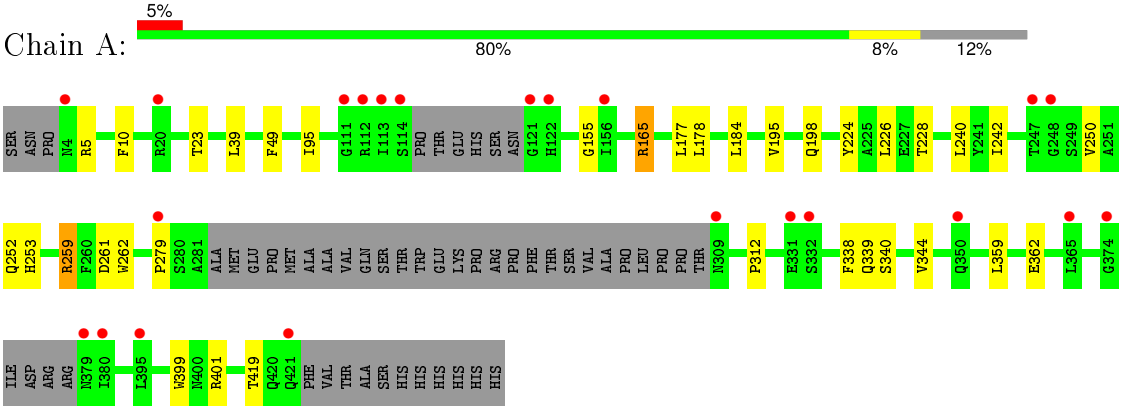
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	89	Total O 89 89	0	0
6	B	92	Total O 92 92	0	0

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.

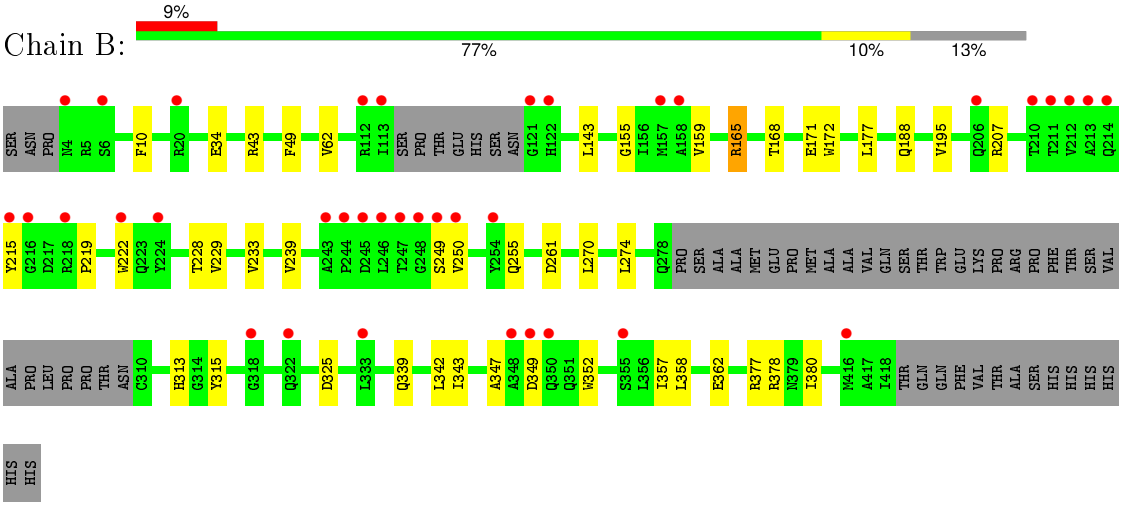
- Molecule 1: PHYTOCHROME-LIKE PROTEIN CPH2

Chain A:



- Molecule 1: PHYTOCHROME-LIKE PROTEIN CPH2

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	77.43Å 88.46Å 84.87Å 90.00° 109.85° 90.00°	Depositor
Resolution (Å)	29.63 – 2.60 29.63 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.4 (29.63-2.60) 98.5 (29.63-2.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.95 (at 2.61Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.200 , 0.253 (Not available) , (Not available)	Depositor DCC
R_{free} test set	NotAvailable	DCC
Wilson B-factor (Å^2)	50.9	Xtriage
Anisotropy	0.526	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 57.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 32779 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6311	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.47% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: CYC, GOL, FMT

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	0.21	0/3078	0.38	0/4181
1	B	0.21	0/3057	0.37	0/4151
All	All	0.21	0/6135	0.38	0/8332

There are no bond length outliers.

There are no bond angle outliers.

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	3009	0	2929	21	0
1	B	2992	0	2941	26	0
2	A	10	0	5	0	0
3	A	43	0	37	1	0
3	B	43	0	37	0	0
4	A	6	0	8	1	0
4	B	6	0	8	0	0
5	A	9	0	3	0	0
5	B	12	0	4	0	0
6	A	89	0	0	1	0
6	B	92	0	0	1	0
All	All	6311	0	5972	40	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 3.

All (40) 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:5:ARG:NH1	1:B:34:GLU:OE1	2.34	0.60
1:B:219:PRO:HA	1:B:222:TRP:HD1	1.67	0.60
1:A:259:ARG:HH22	1:A:338:PHE:HE2	1.50	0.59
1:A:177:LEU:HD11	1:B:195:VAL:HG22	1.86	0.57
1:B:339:GLN:HG3	1:B:362:GLU:HB2	1.87	0.56
1:B:347:ALA:HB2	1:B:352:TRP:HD1	1.74	0.52
1:B:255:GLN:HE22	1:B:261:ASP:HA	1.75	0.51
1:A:401:ARG:NH1	6:A:2086:HOH:O	2.43	0.51
1:B:239:VAL:HB	1:B:357:ILE:HB	1.93	0.50
1:A:253:HIS:NE2	1:A:261:ASP:OD1	2.45	0.50
1:A:95:ILE:HD12	3:A:1422:CYC:HBA1	1.92	0.50
1:B:49:PHE:CD2	1:B:155:GLY:HA2	2.47	0.49
1:A:339:GLN:HG3	1:A:362:GLU:HB2	1.93	0.49
1:A:39:LEU:O	1:A:165:ARG:NH2	2.47	0.48
1:A:224:TYR:O	1:A:228:THR:OG1	2.28	0.47
1:B:219:PRO:HA	1:B:222:TRP:CD1	2.48	0.46
1:B:377:ARG:HH21	1:B:380:ILE:HG21	1.80	0.46
1:A:312:PRO:HB3	1:A:344:VAL:HG22	1.97	0.46
1:A:178:LEU:HD11	1:B:10:PHE:HZ	1.82	0.44
1:A:10:PHE:HE1	1:B:34:GLU:HB3	1.82	0.44
1:A:242:ILE:HB	1:A:252:GLN:HB2	1.99	0.44
1:B:168:THR:O	1:B:172:TRP:HD1	2.00	0.44
1:B:274:LEU:HB3	1:B:343:ILE:HD13	2.00	0.44
1:A:195:VAL:HG22	1:B:177:LEU:HD11	2.00	0.43
1:B:43:ARG:HG3	1:B:62:VAL:HB	2.00	0.43
1:A:184:LEU:HD11	1:B:188:GLN:HG3	2.01	0.42
1:A:49:PHE:CD2	1:A:155:GLY:HA2	2.55	0.42
1:B:342:LEU:HB3	1:B:358:LEU:HB2	2.01	0.42
1:A:184:LEU:HD21	1:B:188:GLN:HG2	2.02	0.42
1:B:313:HIS:HD2	1:B:315:TYR:CZ	2.37	0.42
1:B:229:VAL:O	1:B:233:VAL:HG23	2.20	0.42
1:B:143:LEU:HB3	1:B:159:VAL:HB	2.01	0.42
1:A:224:TYR:CE2	4:A:1423:GOL:H11	2.54	0.41
1:A:262:TRP:CH2	1:A:359:LEU:HD21	2.55	0.41
1:A:340:SER:HG	1:A:399:TRP:HE1	1.66	0.41
1:B:165:ARG:NH1	1:B:171:GLU:OE1	2.51	0.41
1:B:270:LEU:HA	1:B:325:ASP:OD2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:207:ARG:HG2	1:B:228:THR:HG21	2.03	0.41
1:B:378:ARG:NH2	6:B:2084:HOH:O	2.53	0.40
1:A:226:LEU:HD13	1:A:240:LEU:HB2	2.03	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	A	374/432 (87%)	353 (94%)	19 (5%)	2 (0%)	34	60
1	B	371/432 (86%)	357 (96%)	12 (3%)	2 (0%)	34	60
All	All	745/864 (86%)	710 (95%)	31 (4%)	4 (0%)	34	60

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	279	PRO
1	B	349	ASP
1	A	250	VAL
1	B	249	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	310/375 (83%)	305 (98%)	5 (2%)	70 89
1	B	311/375 (83%)	308 (99%)	3 (1%)	82 94
All	All	621/750 (83%)	613 (99%)	8 (1%)	76 91

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	THR
1	A	165	ARG
1	A	198	GLN
1	A	259	ARG
1	A	419	THR
1	B	165	ARG
1	B	215	TYR
1	B	250	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	74	HIS
1	B	190	GLN
1	B	201	GLN
1	B	255	GLN
1	B	313	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)

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	CYC	A	1422	1	35,46,46	3.67	17 (48%)	47,67,67	3.87	19 (40%)
4	GOL	A	1423	-	5,5,5	0.33	0	5,5,5	0.23	0
5	FMT	A	1424	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	A	1425	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	A	1426	-	0,2,2	0.00	-	0,1,1	0.00	-
2	GLU	A	1427	-	3,9,9	0.35	0	2,11,11	0.07	0
3	CYC	B	1419	1	35,46,46	3.70	17 (48%)	47,67,67	3.85	20 (42%)
4	GOL	B	1420	-	5,5,5	0.33	0	5,5,5	0.20	0
5	FMT	B	1421	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	B	1422	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	B	1423	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	B	1424	-	0,2,2	0.00	-	0,1,1	0.00	-

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
3	CYC	A	1422	1	-	2/21/74/74	0/4/4/4
4	GOL	A	1423	-	-	0/4/4/4	0/0/0/0
5	FMT	A	1424	-	-	0/0/0/0	0/0/0/0
5	FMT	A	1425	-	-	0/0/0/0	0/0/0/0
5	FMT	A	1426	-	-	0/0/0/0	0/0/0/0
2	GLU	A	1427	-	-	0/3/9/9	0/0/0/0
3	CYC	B	1419	1	-	2/21/74/74	0/4/4/4
4	GOL	B	1420	-	-	0/4/4/4	0/0/0/0
5	FMT	B	1421	-	-	0/0/0/0	0/0/0/0
5	FMT	B	1422	-	-	0/0/0/0	0/0/0/0
5	FMT	B	1423	-	-	0/0/0/0	0/0/0/0
5	FMT	B	1424	-	-	0/0/0/0	0/0/0/0

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1419	CYC	CAC-C3C	-4.08	1.45	1.54
3	A	1422	CYC	CAC-C3C	-4.02	1.45	1.54
3	B	1419	CYC	OB-C4B	-2.51	1.18	1.23
3	A	1422	CYC	OB-C4B	-2.47	1.18	1.23
3	B	1419	CYC	C1A-C2A	-2.31	1.41	1.45
3	A	1422	CYC	C1A-C2A	-2.26	1.41	1.45
3	A	1422	CYC	C4C-NC	2.09	1.42	1.37
3	B	1419	CYC	C4C-NC	2.10	1.42	1.37
3	A	1422	CYC	C2C-C3C	2.36	1.61	1.54
3	B	1419	CYC	C2C-C3C	2.51	1.62	1.54
3	B	1419	CYC	CAD-C3D	2.67	1.56	1.52
3	A	1422	CYC	CAD-C3D	2.89	1.57	1.52
3	B	1419	CYC	CMB-C2B	3.06	1.57	1.50
3	A	1422	CYC	CMB-C2B	3.10	1.57	1.50
3	A	1422	CYC	C1B-C2B	3.21	1.51	1.45
3	B	1419	CYC	C1B-C2B	3.22	1.51	1.45
3	B	1419	CYC	C1C-NC	3.75	1.42	1.37
3	A	1422	CYC	C1C-NC	3.99	1.42	1.37
3	B	1419	CYC	C4D-CHA	4.15	1.56	1.40
3	A	1422	CYC	C4D-CHA	4.16	1.56	1.40
3	B	1419	CYC	C1D-CHD	4.41	1.57	1.40
3	A	1422	CYC	C1D-CHD	4.43	1.57	1.40
3	A	1422	CYC	CHB-C4A	4.49	1.51	1.40
3	B	1419	CYC	CHB-C4A	4.53	1.51	1.40
3	B	1419	CYC	C4A-NA	4.94	1.48	1.37
3	B	1419	CYC	C2A-C3A	4.97	1.47	1.36
3	A	1422	CYC	C4A-NA	5.03	1.48	1.37
3	A	1422	CYC	C4A-C3A	5.04	1.56	1.45
3	B	1419	CYC	C4A-C3A	5.11	1.56	1.45
3	A	1422	CYC	C2A-C3A	5.13	1.47	1.36
3	A	1422	CYC	C3B-C2B	9.55	1.57	1.36
3	B	1419	CYC	C3B-C2B	9.69	1.57	1.36
3	A	1422	CYC	CHA-C1A	12.16	1.45	1.35
3	B	1419	CYC	CHA-C1A	12.45	1.46	1.35

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1422	CYC	C4B-C3B-C2B	-11.49	101.49	108.05
3	B	1419	CYC	C4B-C3B-C2B	-11.18	101.67	108.05
3	B	1419	CYC	C1B-C2B-C3B	-5.99	101.42	107.81
3	B	1419	CYC	OC-C1C-C2C	-5.85	121.52	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1422	CYC	OC-C1C-C2C	-5.80	121.56	126.25
3	A	1422	CYC	C1B-C2B-C3B	-5.72	101.71	107.81
3	A	1422	CYC	OB-C4B-C3B	-4.85	122.28	128.09
3	B	1419	CYC	OB-C4B-C3B	-4.65	122.52	128.09
3	A	1422	CYC	CHA-C1A-NA	-3.63	122.18	128.67
3	B	1419	CYC	CHA-C1A-NA	-3.55	122.32	128.67
3	B	1419	CYC	C1B-CHB-C4A	-3.16	119.89	128.06
3	A	1422	CYC	C1B-NB-C4B	-3.14	106.13	110.73
3	B	1419	CYC	C1B-NB-C4B	-2.94	106.44	110.73
3	A	1422	CYC	CHB-C1B-C2B	-2.78	121.11	126.89
3	B	1419	CYC	OC-C1C-NC	-2.29	122.06	124.83
3	A	1422	CYC	C3C-C2C-C1C	-2.29	101.50	103.41
3	A	1422	CYC	OC-C1C-NC	-2.25	122.10	124.83
3	B	1419	CYC	C3C-C2C-C1C	-2.10	101.65	103.41
3	B	1419	CYC	CHB-C1B-C2B	-2.03	122.67	126.89
3	A	1422	CYC	CMA-C3A-C4A	2.02	128.35	125.06
3	B	1419	CYC	CAD-CBD-CGD	2.17	116.73	112.75
3	B	1419	CYC	CMA-C3A-C4A	2.35	128.88	125.06
3	A	1422	CYC	CBD-CAD-C3D	2.38	116.80	112.53
3	B	1419	CYC	CBD-CAD-C3D	2.68	117.33	112.53
3	A	1422	CYC	CAD-CBD-CGD	2.87	118.01	112.75
3	A	1422	CYC	CMB-C2B-C1B	3.77	129.22	124.20
3	B	1419	CYC	CMB-C2B-C1B	4.04	129.57	124.20
3	B	1419	CYC	C2A-C1A-NA	4.34	116.59	109.86
3	A	1422	CYC	C2A-C1A-NA	4.43	116.74	109.86
3	B	1419	CYC	C2B-C1B-NB	5.69	115.25	107.00
3	A	1422	CYC	C2B-C1B-NB	5.71	115.28	107.00
3	A	1422	CYC	C3C-C4C-NC	8.20	116.15	107.93
3	A	1422	CYC	C2C-C1C-NC	8.41	116.33	108.30
3	B	1419	CYC	C2C-C1C-NC	8.50	116.42	108.30
3	B	1419	CYC	CAB-C3B-C4B	8.69	129.10	121.51
3	B	1419	CYC	C3C-C4C-NC	9.00	116.95	107.93
3	B	1419	CYC	C3B-C4B-NB	9.34	115.23	106.74
3	A	1422	CYC	C3B-C4B-NB	9.52	115.39	106.74
3	A	1422	CYC	CAB-C3B-C4B	9.59	129.88	121.51

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1419	CYC	C1B-CHB-C4A-C3A
3	A	1422	CYC	C1B-CHB-C4A-C3A

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Mol	Chain	Res	Type	Atoms
3	B	1419	CYC	C1B-CHB-C4A-NA
3	A	1422	CYC	C1B-CHB-C4A-NA

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1422	CYC	1	0
4	A	1423	GOL	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	381/432 (88%)	0.05	22 (5%) 26 20	27, 53, 113, 153	0
1	B	377/432 (87%)	0.36	37 (9%) 10 6	22, 70, 143, 196	0
All	All	758/864 (87%)	0.20	59 (7%) 16 11	22, 59, 130, 196	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	213	ALA	8.0
1	A	247	THR	6.1
1	B	249	SER	5.6
1	B	246	LEU	5.3
1	A	332	SER	5.3
1	B	4	ASN	5.2
1	B	247	THR	5.1
1	A	421	GLN	5.1
1	B	349	ASP	5.1
1	A	374	GLY	4.7
1	B	214	GLN	4.6
1	A	111	GLY	4.6
1	A	113	ILE	4.4
1	A	122	HIS	4.3
1	A	121	GLY	4.3
1	B	211	THR	4.2
1	B	216	GLY	4.2
1	B	245	ASP	4.2
1	B	121	GLY	4.0
1	B	250	VAL	4.0
1	A	114	SER	3.9
1	A	365	LEU	3.8
1	A	380	ILE	3.8
1	A	331	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	350	GLN	3.6
1	B	215	TYR	3.6
1	B	416	MET	3.5
1	B	350	GLN	3.4
1	B	318	GLY	3.3
1	A	379	ASN	3.3
1	A	112	ARG	3.2
1	B	243	ALA	3.1
1	B	122	HIS	3.1
1	B	158	ALA	3.0
1	B	248	GLY	3.0
1	A	20	ARG	3.0
1	B	244	PRO	3.0
1	A	4	ASN	2.9
1	B	322	GLN	2.8
1	B	348	ALA	2.8
1	A	309	ASN	2.8
1	B	20	ARG	2.7
1	B	112	ARG	2.7
1	A	248	GLY	2.7
1	B	222	TRP	2.6
1	B	212	VAL	2.6
1	A	156	ILE	2.5
1	B	355	SER	2.4
1	A	395	LEU	2.4
1	B	206	GLN	2.4
1	B	254	TYR	2.4
1	B	210	THR	2.3
1	B	224	TYR	2.3
1	B	333	LEU	2.3
1	A	279	PRO	2.2
1	B	157	MET	2.2
1	B	113	ILE	2.1
1	B	218	ARG	2.1
1	B	6	SER	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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
5	FMT	A	1425	3/3	0.79	0.57	16.35	70,70,71,72	0
5	FMT	B	1423	3/3	0.83	0.31	15.49	52,52,62,67	0
5	FMT	A	1424	3/3	0.79	0.43	7.21	83,83,87,88	0
2	GLU	A	1427	10/10	0.68	0.37	3.60	79,87,90,91	0
4	GOL	B	1420	6/6	0.86	0.23	2.08	44,50,61,61	0
4	GOL	A	1423	6/6	0.91	0.20	1.07	58,63,78,82	0
3	CYC	B	1419	43/43	0.96	0.20	0.41	18,31,53,60	0
3	CYC	A	1422	43/43	0.91	0.22	0.17	26,40,54,66	0
5	FMT	B	1422	3/3	0.78	0.30	-	81,81,85,85	0
5	FMT	B	1424	3/3	0.48	0.25	-	103,103,105,106	0
5	FMT	A	1426	3/3	0.60	0.37	-	86,86,88,88	0
5	FMT	B	1421	3/3	0.49	0.20	-	75,75,80,83	0

6.5 Other polymers (i)

There are no such residues in this entry.