Full wwPDB X-ray Structure Validation Report (i)

Aug 18, 2026 – 10:56 am BST

PDB ID	:	5M34 / pdb_00005m34
Title	:	Structure of cobinamide-bound BtuF mutant W66Y, the periplasmic vitamin B12 binding protein in E.coli
Authors	:	Mireku, S.A.; Ruetz, M.; Zhou, T.; Korkhov, V.M.; Kraeutler, B.; Locher, K.P.
Deposited on	:	2016-10-14
Resolution	:	1.60 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

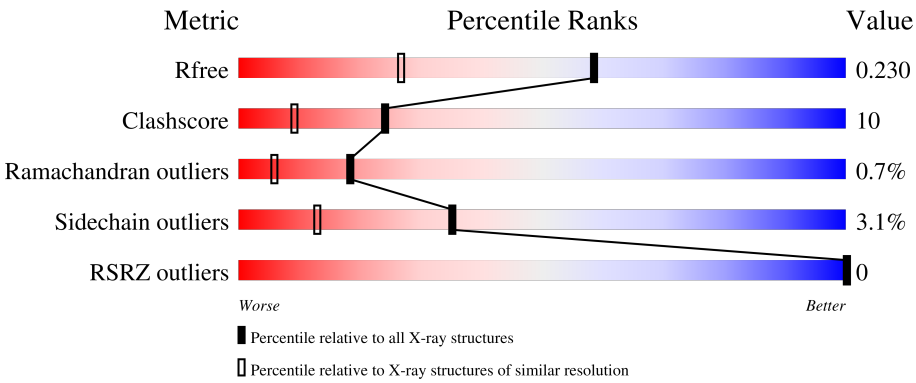
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 1.60 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))
R_{free}	180053	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	289	60% 15% • 21%
1	B	289	57% 20% • 21%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4210 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 Vitamin B12-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	228	1772	1127	308	333	4	0	1	0
1	B	229	1785	1136	312	332	5	0	3	0

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	initiating methionine	UNP P37028
A	-1	LYS	-	expression tag	UNP P37028
A	0	LYS	-	expression tag	UNP P37028
A	1	THR	-	expression tag	UNP P37028
A	2	ALA	-	expression tag	UNP P37028
A	3	ILE	-	expression tag	UNP P37028
A	4	ALA	-	expression tag	UNP P37028
A	5	ILE	-	expression tag	UNP P37028
A	6	ALA	-	expression tag	UNP P37028
A	7	VAL	-	expression tag	UNP P37028
A	8	ALA	-	expression tag	UNP P37028
A	9	LEU	-	expression tag	UNP P37028
A	10	ALA	-	expression tag	UNP P37028
A	11	GLY	-	expression tag	UNP P37028
A	12	PHE	-	expression tag	UNP P37028
A	13	ALA	-	expression tag	UNP P37028
A	14	THR	-	expression tag	UNP P37028
A	15	VAL	-	expression tag	UNP P37028
A	16	ALA	-	expression tag	UNP P37028
A	17	GLN	-	expression tag	UNP P37028
A	18	ALA	-	expression tag	UNP P37028
A	19	ALA	-	expression tag	UNP P37028
A	20	SER	-	expression tag	UNP P37028
A	21	MET	-	expression tag	UNP P37028
A	66	TYR	TRP	engineered mutation	UNP P37028

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Chain	Residue	Modelled	Actual	Comment	Reference
A	267	SER	-	expression tag	UNP P37028
A	268	GLY	-	expression tag	UNP P37028
A	269	SER	-	expression tag	UNP P37028
A	270	LEU	-	expression tag	UNP P37028
A	271	GLU	-	expression tag	UNP P37028
A	272	VAL	-	expression tag	UNP P37028
A	273	LEU	-	expression tag	UNP P37028
A	274	PHE	-	expression tag	UNP P37028
A	275	GLN	-	expression tag	UNP P37028
A	276	GLY	-	expression tag	UNP P37028
A	277	PRO	-	expression tag	UNP P37028
A	278	GLY	-	expression tag	UNP P37028
A	279	GLY	-	expression tag	UNP P37028
A	280	SER	-	expression tag	UNP P37028
A	281	HIS	-	expression tag	UNP P37028
A	282	HIS	-	expression tag	UNP P37028
A	283	HIS	-	expression tag	UNP P37028
A	284	HIS	-	expression tag	UNP P37028
A	285	HIS	-	expression tag	UNP P37028
A	286	HIS	-	expression tag	UNP P37028
B	-2	MET	-	initiating methionine	UNP P37028
B	-1	LYS	-	expression tag	UNP P37028
B	0	LYS	-	expression tag	UNP P37028
B	1	THR	-	expression tag	UNP P37028
B	2	ALA	-	expression tag	UNP P37028
B	3	ILE	-	expression tag	UNP P37028
B	4	ALA	-	expression tag	UNP P37028
B	5	ILE	-	expression tag	UNP P37028
B	6	ALA	-	expression tag	UNP P37028
B	7	VAL	-	expression tag	UNP P37028
B	8	ALA	-	expression tag	UNP P37028
B	9	LEU	-	expression tag	UNP P37028
B	10	ALA	-	expression tag	UNP P37028
B	11	GLY	-	expression tag	UNP P37028
B	12	PHE	-	expression tag	UNP P37028
B	13	ALA	-	expression tag	UNP P37028
B	14	THR	-	expression tag	UNP P37028
B	15	VAL	-	expression tag	UNP P37028
B	16	ALA	-	expression tag	UNP P37028
B	17	GLN	-	expression tag	UNP P37028
B	18	ALA	-	expression tag	UNP P37028
B	19	ALA	-	expression tag	UNP P37028

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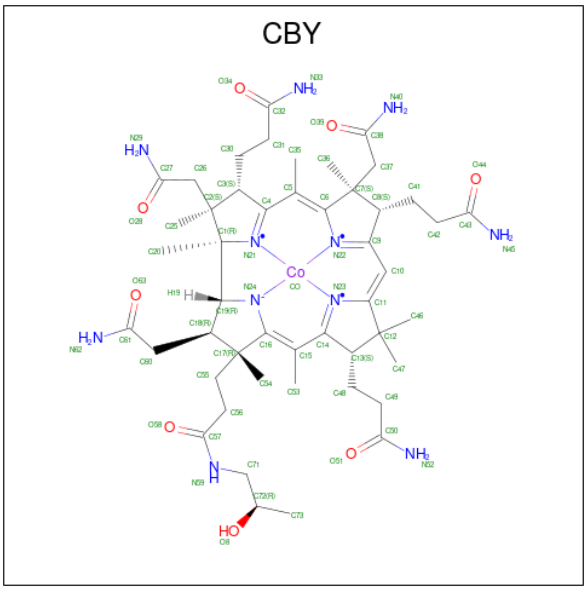
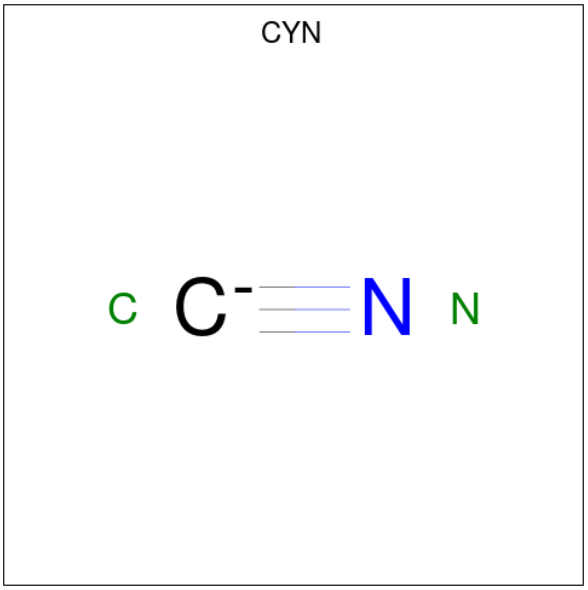
Chain	Residue	Modelled	Actual	Comment	Reference
B	20	SER	-	expression tag	UNP P37028
B	21	MET	-	expression tag	UNP P37028
B	66	TYR	TRP	engineered mutation	UNP P37028
B	267	SER	-	expression tag	UNP P37028
B	268	GLY	-	expression tag	UNP P37028
B	269	SER	-	expression tag	UNP P37028
B	270	LEU	-	expression tag	UNP P37028
B	271	GLU	-	expression tag	UNP P37028
B	272	VAL	-	expression tag	UNP P37028
B	273	LEU	-	expression tag	UNP P37028
B	274	PHE	-	expression tag	UNP P37028
B	275	GLN	-	expression tag	UNP P37028
B	276	GLY	-	expression tag	UNP P37028
B	277	PRO	-	expression tag	UNP P37028
B	278	GLY	-	expression tag	UNP P37028
B	279	GLY	-	expression tag	UNP P37028
B	280	SER	-	expression tag	UNP P37028
B	281	HIS	-	expression tag	UNP P37028
B	282	HIS	-	expression tag	UNP P37028
B	283	HIS	-	expression tag	UNP P37028
B	284	HIS	-	expression tag	UNP P37028
B	285	HIS	-	expression tag	UNP P37028
B	286	HIS	-	expression tag	UNP P37028

- Molecule 2 is COB(II)INAMIDE (CCD ID: CBY) (formula: $C_{48}H_{72}CoN_{11}O_8$).



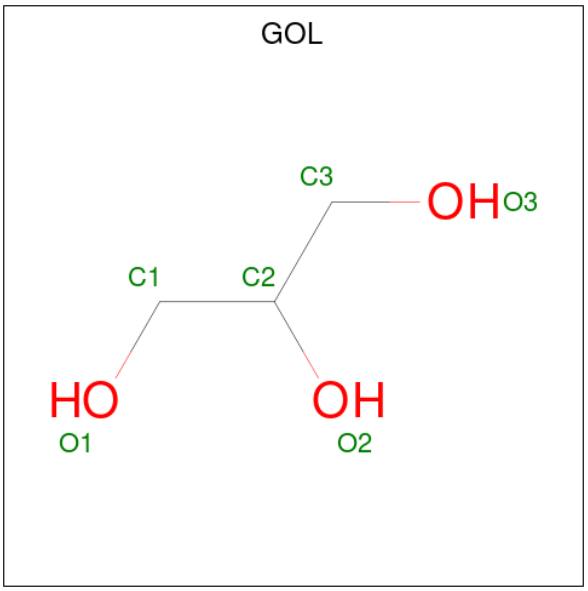
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Co	N	O		
2	A	1	68	48	1	11	8	0	0
			Total	C	Co	N	O		
2	B	1	68	48	1	11	8	0	0

- Molecule 3 is CYANIDE ION (CCD ID: CYN) (formula: CN).



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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is water.

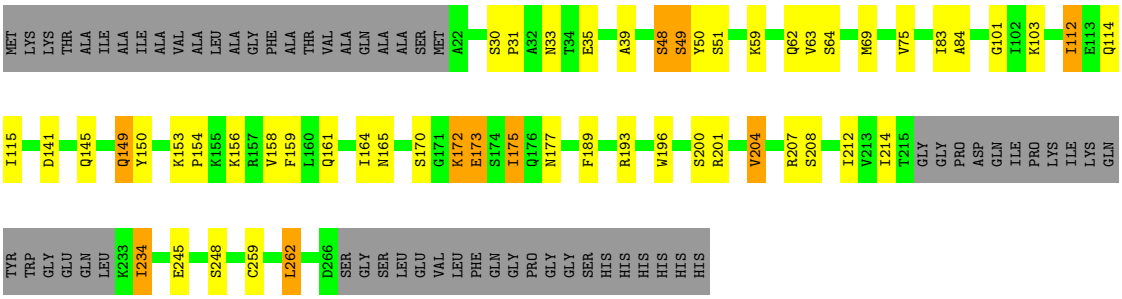
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	240	240	240	0	0
			Total	O		
5	B	259	259	259	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

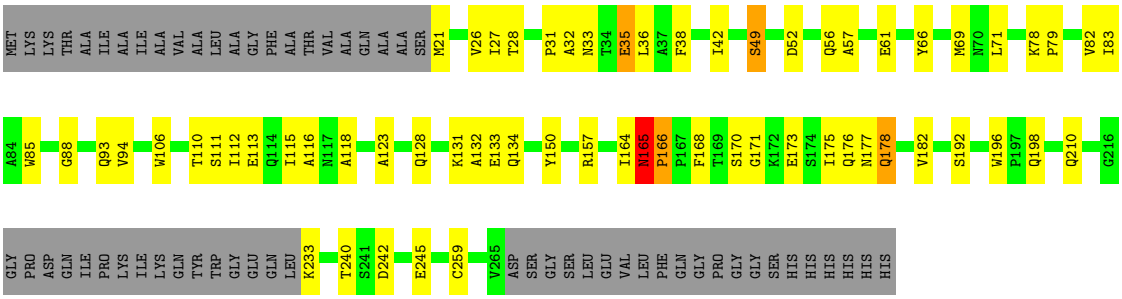
• Molecule 1: Vitamin B12-binding protein

Chain A: 60% 15% • 21%



• Molecule 1: Vitamin B12-binding protein

Chain B: 57% 20% • 21%



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	139.83Å 90.80Å 51.07Å 90.00° 111.25° 90.00°	Depositor
Resolution (Å)	29.48 – 1.60 29.48 – 1.60	Depositor EDS
% Data completeness (in resolution range)	93.2 (29.48-1.60) 93.2 (29.48-1.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.78 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.8.0071, PHENIX 1.10.1-2155	Depositor
R, R_{free}	0.191 , 0.233 0.196 , 0.230	Depositor DCC
R_{free} test set	3678 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	23.3	Xtriage
Anisotropy	0.540	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 37.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.186 for -h-2*l,-k,l	Xtriage
Reported twinning fraction	0.800 for H, K, L 0.200 for H+4/2L, -K, -L	Depositor
Outliers	11 of 73567 reflections (0.015%)	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	4210	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.51% 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, 0.333 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: CYN, CBY, GOL

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	1.68	25/1812 (1.4%)	1.51	15/2470 (0.6%)
1	B	1.63	27/1831 (1.5%)	1.52	19/2493 (0.8%)
All	All	1.65	52/3643 (1.4%)	1.51	34/4963 (0.7%)

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	A	0	1
1	B	0	1
All	All	0	2

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	208	SER	C-O	10.35	1.28	1.23
1	A	208	SER	N-CA	9.19	1.54	1.46
1	B	123	ALA	C-O	-8.99	1.15	1.24
1	B	33	ASN	N-CA	-8.70	1.35	1.46
1	B	106	TRP	N-CA	-8.52	1.35	1.46
1	A	189	PHE	N-CA	8.09	1.55	1.46
1	A	30	SER	N-CA	-7.88	1.37	1.46
1	A	177	ASN	C-O	7.48	1.32	1.24
1	A	49	SER	CA-C	7.46	1.61	1.52
1	B	106	TRP	C-O	7.23	1.32	1.24
1	A	63	VAL	N-CA	7.23	1.53	1.46
1	B	83	ILE	N-CA	-7.08	1.37	1.46
1	A	33	ASN	CA-C	6.85	1.61	1.52
1	A	83	ILE	N-CA	-6.71	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	214	ILE	C-O	-6.70	1.17	1.24
1	A	64	SER	C-O	6.64	1.31	1.23
1	B	26	VAL	C-O	6.62	1.31	1.24
1	B	36	LEU	CA-C	6.52	1.61	1.52
1	A	30	SER	C-N	6.43	1.41	1.34
1	A	31	PRO	C-O	6.40	1.31	1.24
1	B	61	GLU	N-CA	-6.18	1.38	1.46
1	A	115	ILE	CA-C	6.17	1.60	1.52
1	B	78	LYS	C-O	6.17	1.26	1.23
1	A	48	SER	C-O	6.16	1.31	1.23
1	B	35	GLU	CA-CB	-6.15	1.43	1.53
1	B	111	SER	N-CA	5.97	1.53	1.45
1	B	116	ALA	N-CA	-5.92	1.39	1.46
1	B	178	GLN	N-CA	5.87	1.53	1.46
1	B	85	TRP	N-CA	-5.86	1.39	1.46
1	A	59	LYS	CA-C	-5.84	1.44	1.52
1	A	62	GLN	N-CA	5.80	1.53	1.46
1	B	176	GLN	C-O	5.78	1.30	1.24
1	B	28	THR	N-CA	-5.75	1.39	1.46
1	B	83	ILE	C-O	5.62	1.30	1.24
1	A	39	ALA	C-O	-5.55	1.17	1.24
1	A	75	VAL	C-O	-5.55	1.17	1.24
1	A	248	SER	N-CA	-5.54	1.38	1.46
1	B	57	ALA	C-O	5.50	1.30	1.24
1	B	132	ALA	CA-CB	5.47	1.61	1.53
1	A	208	SER	CA-C	5.38	1.57	1.53
1	B	175	ILE	C-O	-5.28	1.17	1.24
1	B	118	ALA	CA-CB	-5.26	1.45	1.53
1	A	83	ILE	CA-CB	5.22	1.60	1.53
1	B	94	VAL	CA-C	5.21	1.59	1.52
1	B	115	ILE	C-O	-5.20	1.18	1.24
1	A	175	ILE	C-O	5.20	1.30	1.24
1	B	52	ASP	N-CA	-5.19	1.39	1.46
1	B	177	ASN	C-O	5.14	1.30	1.24
1	B	35	GLU	N-CA	-5.06	1.40	1.46
1	B	42	ILE	CA-C	5.02	1.58	1.52
1	A	234	ILE	C-O	-5.02	1.18	1.24
1	A	84	ALA	N-CA	-5.01	1.39	1.45

All (34) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	38	PHE	N-CA-C	8.71	120.77	111.28
1	B	128	GLN	CA-C-N	8.63	128.77	119.28
1	B	128	GLN	C-N-CA	8.63	128.77	119.28
1	A	30	SER	N-CA-C	-8.46	100.61	108.22
1	B	106	TRP	N-CA-C	-8.17	95.89	109.46
1	B	82	VAL	N-CA-C	6.97	118.17	107.99
1	A	30	SER	O-C-N	6.95	128.03	121.71
1	A	30	SER	CB-CA-C	-6.84	101.19	110.22
1	B	35	GLU	N-CA-C	6.81	118.78	111.36
1	B	32	ALA	O-C-N	-6.60	115.27	122.07
1	A	158	VAL	N-CA-C	6.59	117.97	108.48
1	B	192	SER	N-CA-C	6.50	120.04	110.30
1	A	214	ILE	N-CA-C	6.44	117.13	108.11
1	B	61	GLU	N-CA-C	6.29	119.34	110.23
1	A	30	SER	N-CA-CB	6.23	117.64	111.10
1	A	30	SER	CA-C-O	-5.85	114.70	120.26
1	A	177	ASN	N-CA-C	5.78	117.26	111.07
1	B	28	THR	N-CA-C	5.78	119.24	109.76
1	B	82	VAL	CA-C-N	-5.66	115.52	122.93
1	B	82	VAL	C-N-CA	-5.66	115.52	122.93
1	A	114	GLN	N-CA-C	5.66	118.39	111.82
1	B	49	SER	N-CA-C	-5.59	102.74	110.35
1	A	101	GLY	N-CA-C	-5.55	107.44	115.27
1	B	133	GLU	N-CA-C	-5.43	105.37	111.28
1	B	123	ALA	O-C-N	5.42	126.06	120.70
1	A	35	GLU	CA-C-O	5.38	126.26	120.55
1	B	113	GLU	N-CA-C	-5.37	105.51	111.36
1	B	132	ALA	N-CA-C	5.20	117.35	111.11
1	A	248	SER	O-C-N	5.17	127.26	121.32
1	B	132	ALA	CA-C-N	5.11	127.13	120.28
1	B	132	ALA	C-N-CA	5.11	127.13	120.28
1	A	207	ARG	CA-C-N	-5.08	118.22	123.10
1	A	207	ARG	C-N-CA	-5.08	118.22	123.10
1	A	204	VAL	CB-CA-C	-5.04	105.42	112.02

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	165	ASN	Peptide

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Mol	Chain	Res	Type	Group
1	B	165	ASN	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1772	0	1791	25	0
1	B	1785	0	1818	31	1
2	A	68	0	72	8	0
2	B	68	0	72	11	0
3	A	2	0	0	1	0
3	B	4	0	0	1	0
4	A	6	0	8	0	0
4	B	6	0	8	3	0
5	A	240	0	0	8	2
5	B	259	0	0	17	2
All	All	4210	0	3769	75	4

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 10.

All (75) 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:B:134:GLN:NE2	5:B:401:HOH:O	1.63	1.23
1:A:193:ARG:NH2	5:A:401:HOH:O	1.76	1.16
1:B:56:GLN:HG3	5:B:575:HOH:O	1.43	1.15
1:A:103:LYS:NZ	5:A:402:HOH:O	1.86	0.91
1:A:173:GLU:HG2	5:A:512:HOH:O	1.74	0.88
1:A:149:GLN:O	1:A:149:GLN:HG2	1.77	0.84
1:B:178:GLN:HB2	5:B:564:HOH:O	1.79	0.81
1:B:134:GLN:OE1	5:B:402:HOH:O	2.01	0.78
2:B:302:CBY:H36	2:B:302:CBY:H35A	1.66	0.76
1:B:165:ASN:HB2	1:B:166:PRO:CD	2.18	0.73
1:B:165:ASN:HB2	1:B:166:PRO:HD2	1.74	0.70
1:B:69:MET:HE2	5:B:590:HOH:O	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:GLY:O	5:B:404:HOH:O	2.12	0.68
1:B:210:GLN:OE1	5:B:403:HOH:O	2.12	0.66
1:A:173:GLU:HG3	5:A:594:HOH:O	1.95	0.65
2:A:301:CBY:H36	2:A:301:CBY:C35	2.27	0.65
1:B:240:THR:O	5:B:405:HOH:O	2.14	0.65
1:A:200:SER:O	1:A:204:VAL:HG23	1.96	0.64
1:A:154:PRO:HG2	5:A:479:HOH:O	1.97	0.64
2:A:301:CBY:H36	2:A:301:CBY:H35A	1.81	0.63
2:B:302:CBY:H36	2:B:302:CBY:C35	2.31	0.60
1:B:170:SER:HB2	1:B:196:TRP:CZ3	2.39	0.58
1:A:149:GLN:O	1:A:149:GLN:CG	2.50	0.58
3:B:301:CYN:C	2:B:302:CBY:H20B	2.33	0.58
1:A:170:SER:HB2	1:A:196:TRP:CZ3	2.40	0.56
1:B:131:LYS:CE	5:B:612:HOH:O	2.54	0.56
1:B:131:LYS:HE3	5:B:612:HOH:O	2.05	0.56
1:B:157[A]:ARG:HG2	1:B:157[A]:ARG:HH11	1.71	0.55
1:B:198:GLN:N	5:B:414:HOH:O	2.39	0.55
1:A:141:ASP:O	1:A:145:GLN:HG3	2.07	0.54
1:B:27:ILE:HD12	1:B:79:PRO:HG3	1.90	0.54
1:A:112:ILE:HD12	1:A:175:ILE:HD11	1.88	0.54
1:A:173:GLU:H	1:A:173:GLU:CD	2.16	0.53
1:A:245:GLU:OE1	3:A:302:CYN:N	2.42	0.53
1:A:112:ILE:CD1	1:A:175:ILE:HD11	2.40	0.52
1:B:31:PRO:O	1:B:35:GLU:HG3	2.08	0.52
2:B:302:CBY:H53A	2:B:302:CBY:H55	1.91	0.52
1:B:110:THR:HB	1:B:173:GLU:O	2.09	0.51
1:B:66:TYR:HB2	2:B:302:CBY:N33	2.26	0.51
1:B:49:SER:O	4:B:304:GOL:H11	2.11	0.50
1:B:157[A]:ARG:HG2	1:B:157[A]:ARG:NH1	2.27	0.50
1:B:168:PHE:CE2	5:B:414:HOH:O	2.55	0.50
2:A:301:CBY:H53B	2:A:301:CBY:H54A	1.94	0.49
4:B:304:GOL:H32	5:B:465:HOH:O	2.12	0.48
1:B:150:TYR:CE2	1:B:259:CYS:HB3	2.49	0.48
1:A:172:LYS:HE2	5:A:575:HOH:O	2.14	0.48
2:A:301:CBY:C35	2:A:301:CBY:C36	2.93	0.47
2:B:302:CBY:N33	4:B:304:GOL:O3	2.47	0.47
1:A:149:GLN:NE2	5:A:409:HOH:O	2.40	0.47
2:B:302:CBY:H55	2:B:302:CBY:C53	2.45	0.47
2:B:302:CBY:N29	2:B:302:CBY:H25B	2.29	0.47
1:B:134:GLN:CD	5:B:441:HOH:O	2.59	0.46
1:A:201:ARG:NH1	5:A:414:HOH:O	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:301:CBY:H53A	2:A:301:CBY:H55	1.98	0.45
1:A:173:GLU:CD	1:A:173:GLU:N	2.75	0.45
1:B:69:MET:SD	1:B:71:LEU:HD21	2.56	0.45
2:A:301:CBY:H20	2:A:301:CBY:H30	1.99	0.45
2:B:302:CBY:H20	2:B:302:CBY:H30	1.99	0.45
1:B:165:ASN:CB	1:B:166:PRO:CD	2.93	0.44
1:B:171:GLY:HA3	5:B:534:HOH:O	2.17	0.44
1:A:212:ILE:HG13	1:A:234:ILE:HD11	2.00	0.44
2:B:302:CBY:H35A	2:B:302:CBY:C36	2.42	0.43
2:A:301:CBY:H35A	2:A:301:CBY:C36	2.47	0.43
2:A:301:CBY:H13	2:A:301:CBY:H53	1.90	0.43
2:B:302:CBY:C35	2:B:302:CBY:C36	2.97	0.43
1:A:159:PHE:CE2	1:A:161:GLN:HB2	2.54	0.42
1:A:150:TYR:CZ	1:A:259:CYS:HB3	2.55	0.42
1:A:49:SER:O	1:A:50:TYR:HB2	2.20	0.42
1:A:262:LEU:HD23	1:A:262:LEU:HA	1.90	0.42
1:B:93:GLN:HG2	5:B:406:HOH:O	2.19	0.42
1:B:170:SER:OG	1:B:171:GLY:O	2.39	0.41
1:A:69:MET:HE2	1:A:69:MET:HB3	1.87	0.41
1:B:245:GLU:HB2	5:B:407:HOH:O	2.21	0.41
1:A:48:SER:O	1:A:51:SER:HB2	2.21	0.41

All (4) 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)
5:B:656:HOH:O	5:B:659:HOH:O[2_455]	2.01	0.19
1:B:21:MET:SD	1:B:157[A]:ARG:NH1[4_455]	2.06	0.14
5:A:566:HOH:O	5:B:578:HOH:O[4_445]	2.09	0.11
5:A:634:HOH:O	5:A:638:HOH:O[2_454]	2.16	0.04

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	225/289 (78%)	217 (96%)	7 (3%)	1 (0%)	30 14
1	B	228/289 (79%)	219 (96%)	7 (3%)	2 (1%)	14 3
All	All	453/578 (78%)	436 (96%)	14 (3%)	3 (1%)	18 6

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	165	ASN
1	A	149	GLN
1	B	166	PRO

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	192/235 (82%)	185 (96%)	7 (4%)	31 10
1	B	194/235 (83%)	189 (97%)	5 (3%)	40 17
All	All	386/470 (82%)	374 (97%)	12 (3%)	35 13

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	112	ILE
1	A	153	LYS
1	A	156	LYS
1	A	164	ILE
1	A	172	LYS
1	A	173	GLU
1	A	262	LEU
1	B	112	ILE
1	B	164	ILE
1	B	165	ASN
1	B	182	VAL

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Mol	Chain	Res	Type
1	B	233	LYS

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

Mol	Chain	Res	Type
1	A	62	GLN
1	A	134	GLN
1	A	145	GLN
1	B	134	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

7 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	CYN	A	302	-	0,1,1	-	-	-		
2	CBY	B	302	-	65,75,75	1.23	4 (6%)	106,125,125	2.15	23 (21%)
2	CBY	A	301	-	65,75,75	1.35	6 (9%)	106,125,125	2.16	27 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	GOL	A	303	-	5,5,5	0.58	0	5,5,5	0.23	0
3	CYN	B	303	-	0,1,1	-	-	-		
3	CYN	B	301	-	0,1,1	-	-	-		
4	GOL	B	304	-	5,5,5	0.30	0	5,5,5	0.77	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	CBY	B	302	-	-	5/40/191/191	-
2	CBY	A	301	-	-	6/40/191/191	-
4	GOL	A	303	-	-	2/4/4/4	-
4	GOL	B	304	-	-	4/4/4/4	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	CBY	C14-N23	6.97	1.49	1.30
2	B	302	CBY	C14-N23	6.06	1.46	1.30
2	A	301	CBY	C9-N22	3.83	1.40	1.30
2	A	301	CBY	C46-C12	-3.19	1.47	1.54
2	B	302	CBY	C9-N22	3.18	1.38	1.30
2	B	302	CBY	C19-N24	2.59	1.54	1.49
2	A	301	CBY	C41-C8	-2.38	1.49	1.54
2	B	302	CBY	C35-C5	2.32	1.55	1.50
2	A	301	CBY	C43-N45	2.26	1.40	1.32
2	A	301	CBY	C17-C16	2.24	1.59	1.54

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	301	CBY	C11-N23-C14	-10.48	102.34	106.31
2	B	302	CBY	C19-C1-N21	8.90	112.97	101.67
2	B	302	CBY	C11-N23-C14	-8.16	103.22	106.31
2	A	301	CBY	C20-C1-N21	-7.40	98.13	110.27
2	B	302	CBY	C20-C1-N21	-7.13	98.57	110.27
2	A	301	CBY	C19-C1-N21	5.57	108.75	101.67
2	B	302	CBY	C12-C11-C10	5.42	128.49	123.54
2	B	302	CBY	C7-C6-C5	-5.09	120.06	128.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	302	CBY	C36-C7-C37	4.67	118.50	110.80
2	B	302	CBY	C2-C1-N21	4.39	107.89	101.77
2	A	301	CBY	C56-C57-N59	4.13	123.38	116.42
2	A	301	CBY	C25-C2-C1	-3.88	107.93	113.78
2	B	302	CBY	C20-C1-C2	-3.82	106.90	113.28
2	A	301	CBY	C2-C1-N21	3.71	106.94	101.77
2	A	301	CBY	C17-C16-C15	3.47	132.00	126.73
2	A	301	CBY	C47-C12-C46	3.42	115.14	109.35
2	A	301	CBY	C5-C4-N21	-3.36	118.73	124.19
2	B	302	CBY	C18-C17-C16	3.35	105.69	100.33
2	B	302	CBY	C12-C13-C14	-3.32	97.46	101.86
2	A	301	CBY	C48-C13-C14	3.28	117.25	109.63
2	A	301	CBY	C3-C4-C5	3.22	129.24	123.81
2	A	301	CBY	C7-C6-C5	-3.21	123.02	128.07
2	A	301	CBY	C48-C13-C12	-3.10	107.94	116.63
2	B	302	CBY	C5-C6-N22	3.01	128.47	123.88
2	B	302	CBY	C17-C16-C15	2.99	131.26	126.73
2	A	301	CBY	C20-C1-C2	-2.84	108.54	113.28
2	B	302	CBY	C3-C4-C5	2.80	128.53	123.81
2	A	301	CBY	C13-C12-C11	2.79	104.71	100.90
2	B	302	CBY	C2-C26-C27	-2.75	107.50	115.22
2	A	301	CBY	O58-C57-N59	-2.73	117.86	123.01
2	A	301	CBY	C36-C7-C8	2.69	117.05	112.08
2	B	302	CBY	C15-C14-N23	-2.65	121.42	126.68
2	B	302	CBY	C7-C8-C9	2.63	104.27	100.90
2	B	302	CBY	C17-C16-N24	-2.60	106.50	110.87
2	B	302	CBY	C5-C4-N21	-2.48	120.17	124.19
2	B	302	CBY	C55-C56-C57	2.48	116.64	111.23
2	A	301	CBY	C12-C13-C14	-2.47	98.59	101.86
2	A	301	CBY	C35-C5-C4	-2.42	111.85	116.79
2	A	301	CBY	C30-C3-C2	-2.42	113.98	119.09
2	B	302	CBY	C47-C12-C11	-2.32	102.25	110.29
2	A	301	CBY	C16-C15-C14	2.31	124.47	121.30
2	B	302	CBY	C13-C14-N23	2.29	114.32	109.39
2	A	301	CBY	C71-N59-C57	2.28	127.64	122.69
2	A	301	CBY	C7-C8-C9	2.20	103.71	100.90
2	A	301	CBY	C15-C16-N24	-2.19	120.16	122.38
2	A	301	CBY	C9-C10-C11	-2.18	122.67	125.88
2	A	301	CBY	C55-C17-C18	2.11	115.23	111.15
2	B	302	CBY	C37-C7-C8	-2.10	102.76	108.39
2	B	302	CBY	C26-C2-C3	2.06	111.05	107.41
2	A	301	CBY	C17-C16-N24	-2.01	107.49	110.87

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	CBY	N59-C71-C72-C73
2	A	301	CBY	N59-C71-C72-O8
2	B	302	CBY	N59-C71-C72-O8
4	A	303	GOL	C1-C2-C3-O3
4	B	304	GOL	O1-C1-C2-O2
4	B	304	GOL	O1-C1-C2-C3
2	A	301	CBY	C56-C57-N59-C71
2	A	301	CBY	O58-C57-N59-C71
4	B	304	GOL	C1-C2-C3-O3
4	A	303	GOL	O2-C2-C3-O3
4	B	304	GOL	O2-C2-C3-O3
2	B	302	CBY	C48-C49-C50-O51
2	B	302	CBY	C48-C49-C50-N52
2	A	301	CBY	C48-C49-C50-O51
2	B	302	CBY	N59-C71-C72-C73
2	A	301	CBY	C48-C49-C50-N52
2	B	302	CBY	C14-C13-C48-C49

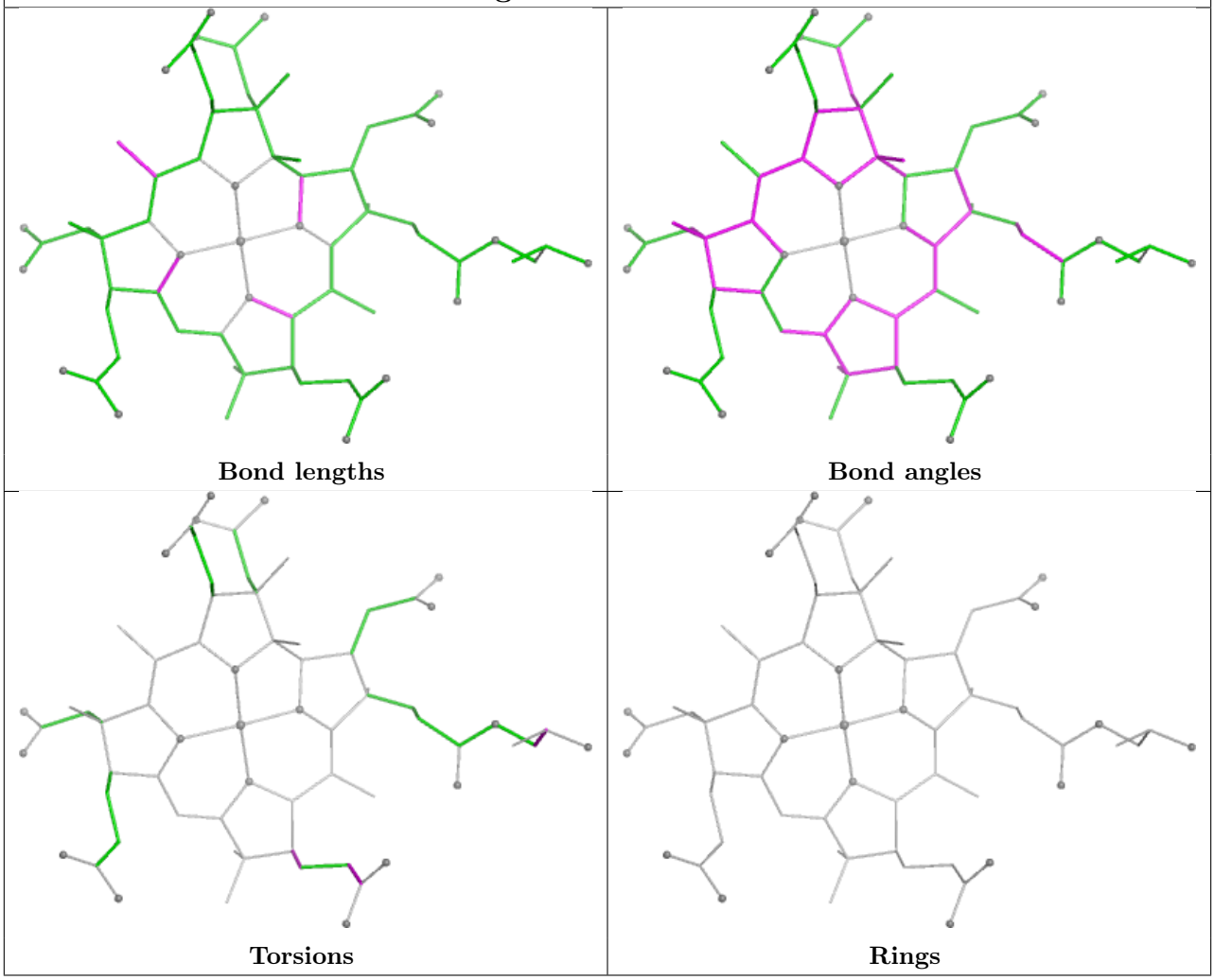
There are no ring outliers.

5 monomers are involved in 22 short contacts:

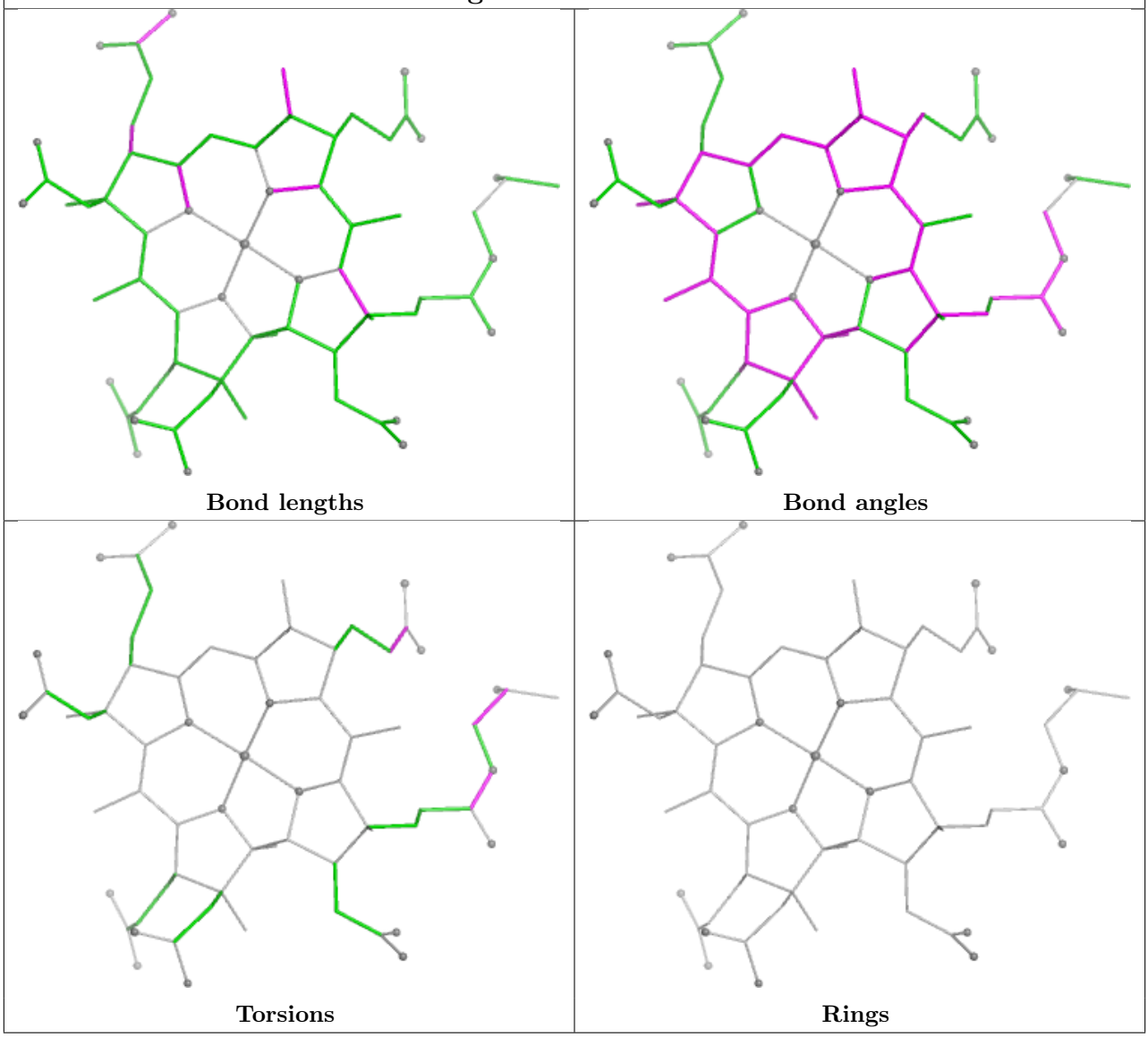
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	302	CYN	1	0
2	B	302	CBY	11	0
2	A	301	CBY	8	0
3	B	301	CYN	1	0
4	B	304	GOL	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand CBY B 302



Ligand CBY A 301



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	228/289 (78%)	-1.00	0	100	100	15, 29, 58, 82	1 (0%)
1	B	229/289 (79%)	-0.97	0	100	100	18, 30, 56, 87	3 (1%)
All	All	457/578 (79%)	-0.98	0	100	100	15, 29, 58, 87	4 (0%)

There are no RSRZ outliers to report.

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 oligosaccharides in this entry.

6.4 Ligands (i)

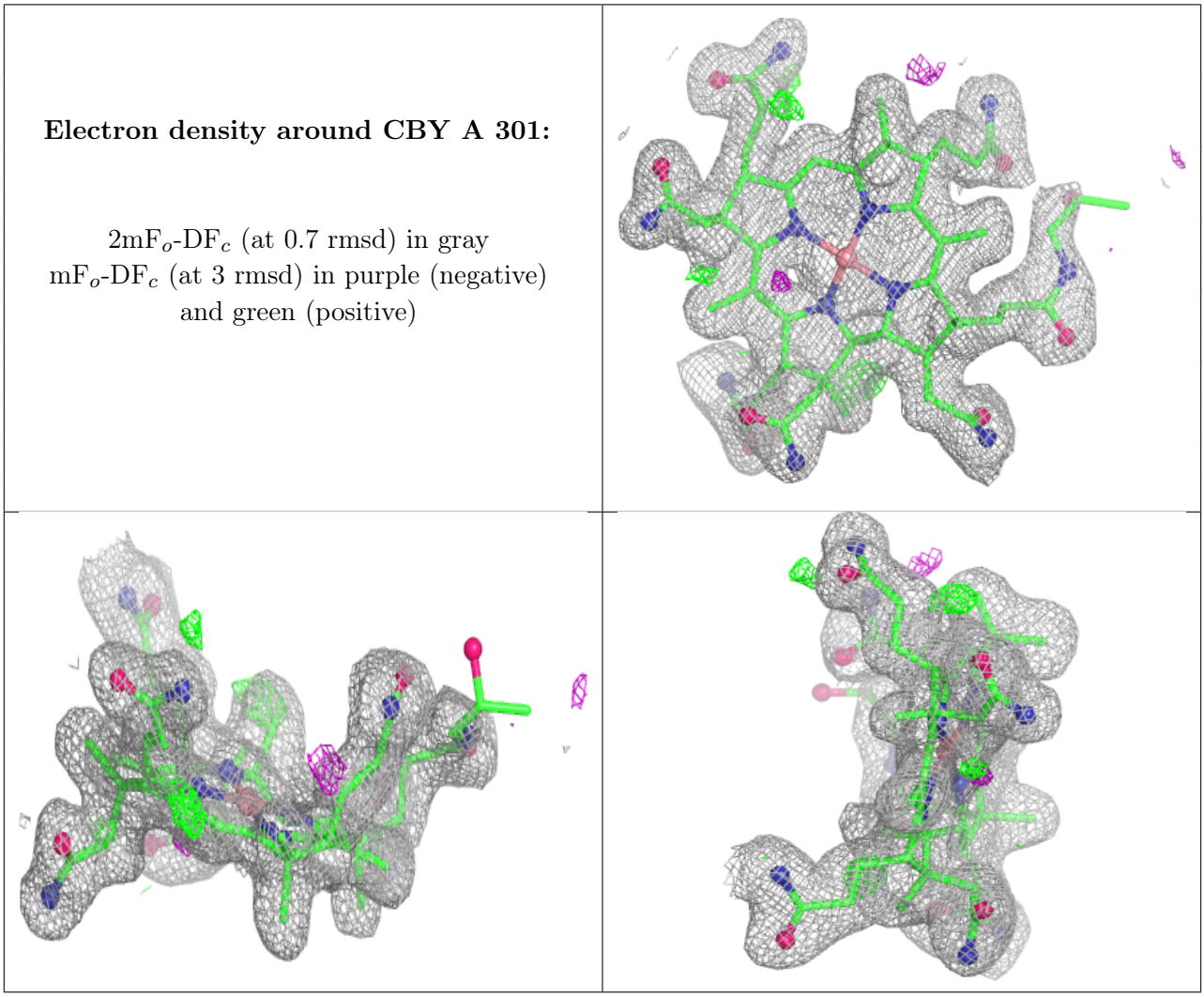
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

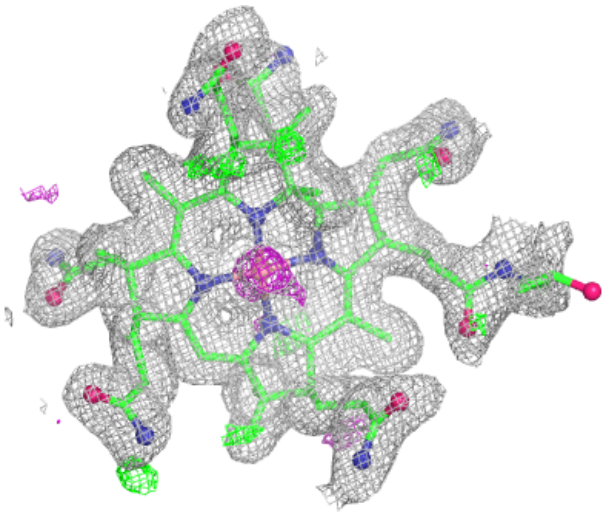
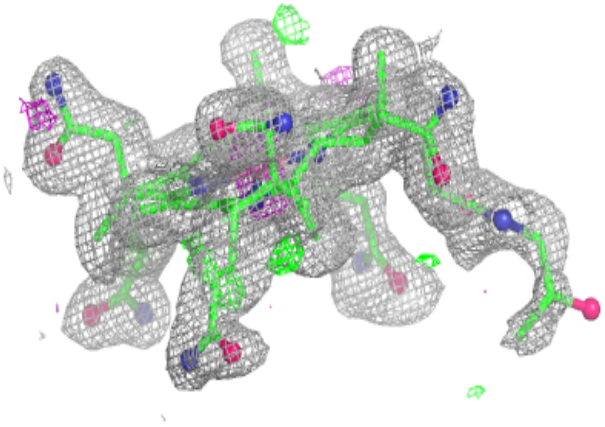
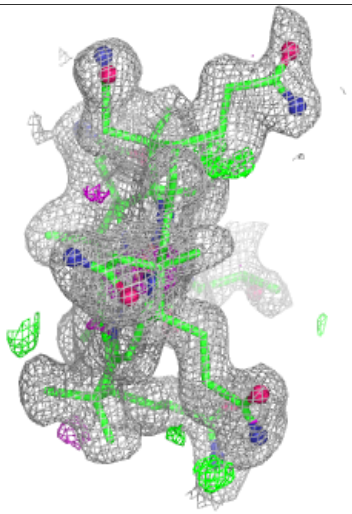
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CYN	A	302	2/2	0.97	0.06	28,28,28,36	0
3	CYN	B	301	2/2	0.97	0.06	21,21,21,29	0
4	GOL	A	303	6/6	0.98	0.05	47,51,56,58	0
4	GOL	B	304	6/6	0.98	0.08	58,61,68,70	0
3	CYN	B	303	2/2	0.99	0.06	18,18,18,38	0
2	CBY	A	301	68/68	0.99	0.04	17,27,48,73	0
2	CBY	B	302	68/68	0.99	0.05	21,30,59,83	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around CBY A 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CBY B 302: 2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)	
	

6.5 Other polymers (i)

There are no such residues in this entry.