



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 11:26 pm BST

PDB ID : 4RAS
Title : Reductive dehalogenase structure suggests a mechanism for B12-dependent dehalogenation
Authors : Quezada, C.P.; Payne, K.A.P.; Leys, D.
Deposited on : 2014-09-11
Resolution : 2.30 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

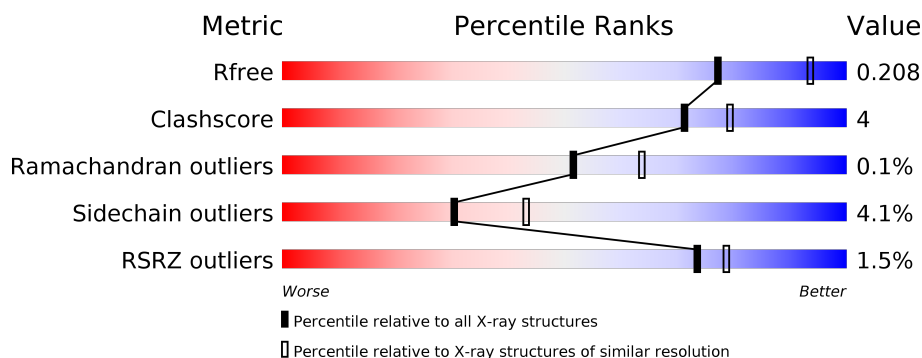
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 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 $\leq 5\%$. 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	704	<div> <div style="width: 90%;"></div> <div style="width: 7%;"></div> <div style="width: 3%;"></div> <div style="width: 2%;"></div> </div> 90% 7% ..
1	B	704	<div> <div style="width: 91%;"></div> <div style="width: 7%;"></div> <div style="width: 3%;"></div> <div style="width: 2%;"></div> </div> 91% 7% ..
1	C	704	<div> <div style="width: 4%;"></div> <div style="width: 90%;"></div> <div style="width: 7%;"></div> <div style="width: 2%;"></div> </div> 4% 90% 7% ..

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16436 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 Oxidoreductase, NAD-binding/iron-sulfur cluster-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	698	Total	C	N	O	S	0	0	0
			5318	3321	972	985	40			
1	B	691	Total	C	N	O	S	0	0	0
			5264	3289	959	976	40			
1	C	692	Total	C	N	O	S	0	0	0
			5246	3281	957	968	40			

There are 18 discrepancies between the modelled and reference sequences:

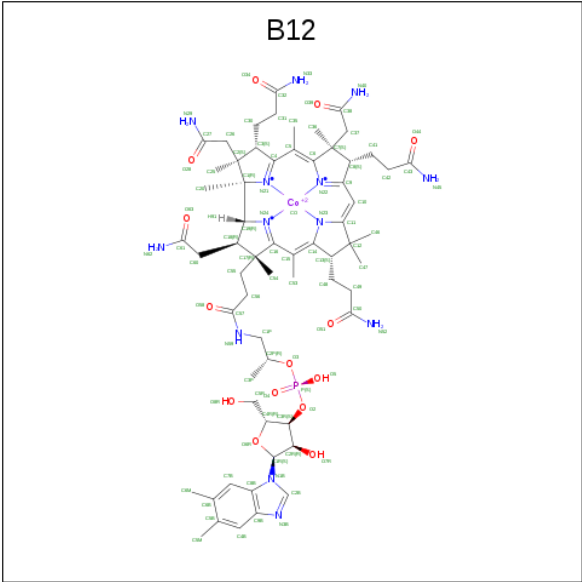
Chain	Residue	Modelled	Actual	Comment	Reference
A	699	HIS	-	EXPRESSION TAG	UNP K2MB66
A	700	HIS	-	EXPRESSION TAG	UNP K2MB66
A	701	HIS	-	EXPRESSION TAG	UNP K2MB66
A	702	HIS	-	EXPRESSION TAG	UNP K2MB66
A	703	HIS	-	EXPRESSION TAG	UNP K2MB66
A	704	HIS	-	EXPRESSION TAG	UNP K2MB66
B	699	HIS	-	EXPRESSION TAG	UNP K2MB66
B	700	HIS	-	EXPRESSION TAG	UNP K2MB66
B	701	HIS	-	EXPRESSION TAG	UNP K2MB66
B	702	HIS	-	EXPRESSION TAG	UNP K2MB66
B	703	HIS	-	EXPRESSION TAG	UNP K2MB66
B	704	HIS	-	EXPRESSION TAG	UNP K2MB66
C	699	HIS	-	EXPRESSION TAG	UNP K2MB66
C	700	HIS	-	EXPRESSION TAG	UNP K2MB66
C	701	HIS	-	EXPRESSION TAG	UNP K2MB66
C	702	HIS	-	EXPRESSION TAG	UNP K2MB66
C	703	HIS	-	EXPRESSION TAG	UNP K2MB66
C	704	HIS	-	EXPRESSION TAG	UNP K2MB66

- Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	C	1	Total	Fe	S	0	0
			8	4	4		
2	C	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 3 is COBALAMIN (three-letter code: B12) (formula: $C_{62}H_{89}CoN_{13}O_{14}P$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		
3	B	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		
3	C	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Cl	0	0
			1	1		
4	A	1	Total	Cl	0	0
			1	1		
4	C	1	Total	Cl	0	0
			1	1		

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Na	0	0
			1	1		
5	A	1	Total	Na	0	0
			1	1		
5	C	1	Total	Na	0	0
			1	1		

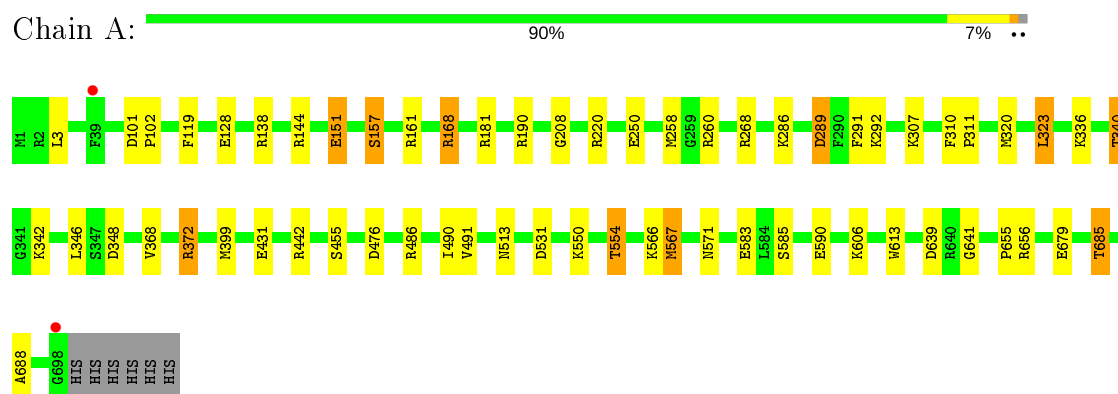
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	148	Total 148	O 148	0	0
6	B	88	Total 88	O 88	0	0
6	C	45	Total 45	O 45	0	0

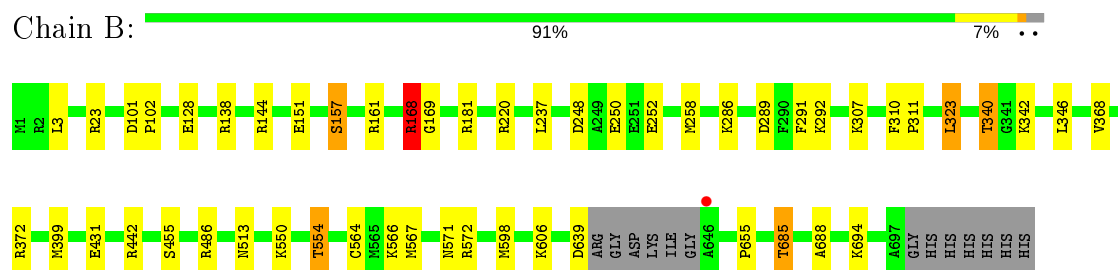
3 Residue-property plots

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.

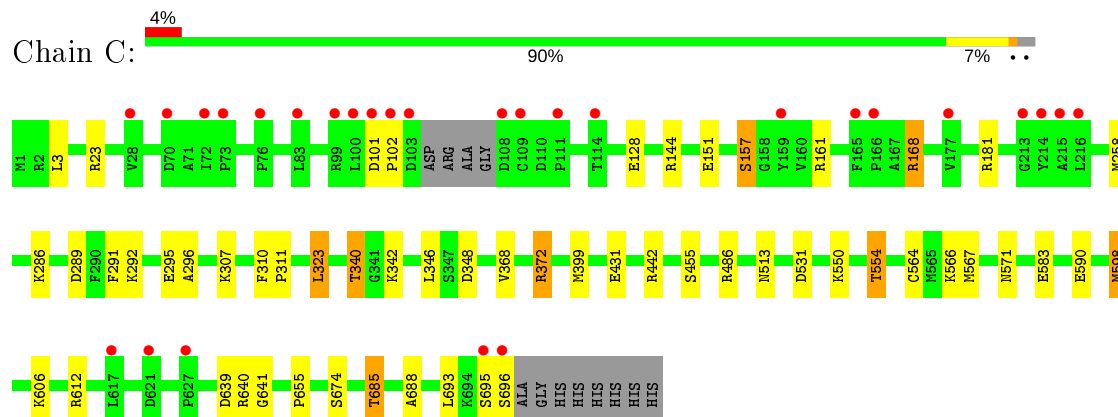
- Molecule 1: Oxidoreductase, NAD-binding/iron-sulfur cluster-binding protein



- Molecule 1: Oxidoreductase, NAD-binding/iron-sulfur cluster-binding protein



- Molecule 1: Oxidoreductase, NAD-binding/iron-sulfur cluster-binding protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	177.34Å 171.51Å 109.02Å 90.00° 98.87° 90.00°	Depositor
Resolution (Å)	76.90 – 2.30 76.90 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.8 (76.90-2.30) 98.7 (76.90-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.181 , 0.207 0.186 , 0.208	Depositor DCC
R_{free} test set	6966 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	45.6	Xtriage
Anisotropy	0.476	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 25.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16436	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% 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: NA, SF4, B12, CL

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	1.07	6/5431 (0.1%)	0.98	14/7350 (0.2%)
1	B	0.91	1/5375 (0.0%)	0.95	11/7275 (0.2%)
1	C	0.82	4/5355 (0.1%)	0.91	9/7247 (0.1%)
All	All	0.94	11/16161 (0.1%)	0.95	34/21872 (0.2%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	157	SER	CB-OG	-8.07	1.31	1.42
1	A	613	TRP	CB-CG	6.65	1.62	1.50
1	A	476	ASP	CB-CG	6.22	1.64	1.51
1	C	583	GLU	CG-CD	6.16	1.61	1.51
1	C	157	SER	CB-OG	-5.77	1.34	1.42
1	A	583	GLU	CG-CD	5.76	1.60	1.51
1	C	590	GLU	CG-CD	5.68	1.60	1.51
1	A	585	SER	CB-OG	5.41	1.49	1.42
1	C	674	SER	CB-OG	-5.22	1.35	1.42
1	A	157	SER	CB-OG	-5.06	1.35	1.42
1	A	590	GLU	CG-CD	5.01	1.59	1.51

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	168	ARG	NE-CZ-NH1	11.88	126.24	120.30
1	B	168	ARG	NE-CZ-NH1	11.74	126.17	120.30
1	C	168	ARG	NE-CZ-NH1	11.02	125.81	120.30
1	B	138	ARG	NE-CZ-NH1	8.04	124.32	120.30
1	A	168	ARG	NE-CZ-NH2	-7.98	116.31	120.30
1	B	168	ARG	NE-CZ-NH2	-7.21	116.69	120.30
1	A	138	ARG	NE-CZ-NH1	7.21	123.90	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	572	ARG	NE-CZ-NH2	-6.77	116.91	120.30
1	C	168	ARG	NE-CZ-NH2	-6.41	117.09	120.30
1	B	168	ARG	CD-NE-CZ	6.38	132.53	123.60
1	C	598	MET	CB-CG-SD	6.29	131.27	112.40
1	A	531	ASP	CB-CG-OD1	6.28	123.95	118.30
1	A	168	ARG	CD-NE-CZ	6.25	132.35	123.60
1	A	168	ARG	CG-CD-NE	6.23	124.89	111.80
1	C	168	ARG	CD-NE-CZ	6.06	132.09	123.60
1	A	567	MET	CG-SD-CE	-5.90	90.77	100.20
1	A	220	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	C	168	ARG	CG-CD-NE	5.79	123.95	111.80
1	B	220	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	C	531	ASP	CB-CG-OD1	5.69	123.42	118.30
1	B	168	ARG	CG-CD-NE	5.69	123.75	111.80
1	B	598	MET	CB-CG-SD	5.60	129.20	112.40
1	A	268	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	C	23	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	A	157	SER	CB-CA-C	-5.36	99.91	110.10
1	C	348	ASP	CB-CG-OD1	5.29	123.06	118.30
1	B	23	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	B	323	LEU	CA-CB-CG	5.21	127.28	115.30
1	A	323	LEU	CB-CG-CD2	5.20	119.84	111.00
1	A	190	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	A	320	MET	CG-SD-CE	5.17	108.47	100.20
1	A	348	ASP	CB-CG-OD1	5.14	122.92	118.30
1	C	323	LEU	CA-CB-CG	5.07	126.96	115.30
1	B	157	SER	CB-CA-C	-5.03	100.55	110.10

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	5318	0	5217	29	0
1	B	5264	0	5160	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	5246	0	5105	27	0
2	A	16	0	0	0	0
2	B	16	0	0	0	0
2	C	16	0	0	0	0
3	A	91	0	88	12	0
3	B	91	0	88	9	0
3	C	91	0	88	12	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
6	A	148	0	0	4	0
6	B	88	0	0	0	0
6	C	45	0	0	0	0
All	All	16436	0	15746	112	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 4.

All (112) 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)
3:A:803:B12:H362	3:A:803:B12:H351	1.32	1.11
1:C:612:ARG:CA	1:C:612:ARG:CG	2.29	1.11
3:B:803:B12:H351	3:B:803:B12:H362	1.48	0.92
1:A:336:LYS:NZ	6:A:985:HOH:O	2.07	0.86
1:C:295:GLU:CA	1:C:296:ALA:N	2.39	0.85
3:A:803:B12:C36	3:A:803:B12:H351	2.10	0.82
1:C:295:GLU:O	1:C:296:ALA:N	2.15	0.79
1:C:295:GLU:CA	1:C:295:GLU:O	2.31	0.79
1:C:550:LYS:O	1:C:554:THR:HB	1.83	0.79
1:B:550:LYS:O	1:B:554:THR:HB	1.82	0.78
1:B:685:THR:HG22	1:B:688:ALA:H	1.50	0.76
1:A:550:LYS:O	1:A:554:THR:HB	1.86	0.75
1:C:685:THR:HG22	1:C:688:ALA:H	1.52	0.74
1:A:685:THR:HG22	1:A:688:ALA:H	1.53	0.73
3:C:803:B12:H351	3:C:803:B12:H362	1.71	0.72
1:A:340:THR:HG22	1:A:342:LYS:H	1.60	0.66
1:B:248:ASP:O	1:B:252:GLU:HG3	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:803:B12:H531	3:A:803:B12:H552	1.83	0.61
1:C:340:THR:HG22	1:C:342:LYS:H	1.64	0.61
1:B:157:SER:HB3	1:B:161:ARG:NH1	2.16	0.60
1:A:336:LYS:HE2	6:A:1040:HOH:O	2.02	0.60
1:C:340:THR:HG21	1:C:442:ARG:O	2.01	0.60
1:B:340:THR:HG22	1:B:342:LYS:H	1.65	0.59
1:B:566:LYS:HE3	1:B:567:MET:HE2	1.86	0.58
3:A:803:B12:H533	3:A:803:B12:H481	1.85	0.58
3:B:803:B12:H552	3:B:803:B12:H531	1.85	0.57
3:C:803:B12:H531	3:C:803:B12:H552	1.86	0.57
1:B:101:ASP:HB2	1:B:102:PRO:HD2	1.87	0.57
1:C:310:PHE:CD1	1:C:311:PRO:HD3	2.40	0.57
3:C:803:B12:H481	3:C:803:B12:H533	1.87	0.56
1:C:101:ASP:HB2	1:C:102:PRO:HD2	1.88	0.56
1:B:340:THR:HG21	1:B:442:ARG:O	2.04	0.56
1:A:101:ASP:HB2	1:A:102:PRO:HD2	1.88	0.55
1:A:340:THR:HG21	1:A:442:ARG:O	2.07	0.55
1:A:566:LYS:HE3	1:A:567:MET:CE	2.37	0.55
3:B:803:B12:C55	3:B:803:B12:H531	2.36	0.55
3:A:803:B12:H421	3:A:803:B12:C10	2.36	0.54
1:C:566:LYS:HE3	1:C:567:MET:CE	2.38	0.53
3:B:803:B12:H533	3:B:803:B12:H481	1.91	0.53
1:B:310:PHE:CD1	1:B:311:PRO:HD3	2.44	0.53
1:C:157:SER:HB3	1:C:161:ARG:NH1	2.24	0.53
1:A:157:SER:HB3	1:A:161:ARG:NH1	2.25	0.52
1:B:566:LYS:HE3	1:B:567:MET:CE	2.41	0.51
1:B:486:ARG:HD3	1:B:571:ASN:OD1	2.12	0.50
1:A:342:LYS:HE3	6:A:913:HOH:O	2.11	0.50
3:C:803:B12:H601	3:C:803:B12:H252	1.94	0.50
1:A:310:PHE:CD1	1:A:311:PRO:HD3	2.47	0.49
3:A:803:B12:H362	3:A:803:B12:C35	2.23	0.49
1:C:486:ARG:HD3	1:C:571:ASN:OD1	2.13	0.49
3:B:803:B12:H351	3:B:803:B12:C36	2.29	0.49
1:A:566:LYS:HE3	1:A:567:MET:HE2	1.94	0.49
3:C:803:B12:H351	3:C:803:B12:C36	2.43	0.48
3:C:803:B12:H491	3:C:803:B12:H473	1.95	0.48
3:C:803:B12:C48	3:C:803:B12:H533	2.43	0.48
1:C:291:PHE:HB3	1:C:307:LYS:HE2	1.96	0.48
1:C:693:LEU:C	1:C:695:SER:H	2.17	0.48
1:A:486:ARG:HD3	1:A:571:ASN:OD1	2.14	0.48
3:A:803:B12:H533	3:A:803:B12:C48	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:803:B12:H262	3:C:803:B12:H91	1.75	0.47
3:A:803:B12:H1P1	3:A:803:B12:C50	2.45	0.47
1:B:151:GLU:OE1	1:B:431:GLU:OE1	2.34	0.46
3:B:803:B12:C10	3:B:803:B12:H421	2.46	0.46
3:A:803:B12:C55	3:A:803:B12:H531	2.44	0.46
1:B:566:LYS:CD	1:B:567:MET:CE	2.94	0.46
1:B:310:PHE:N	1:B:311:PRO:CD	2.79	0.46
1:B:157:SER:HB3	1:B:161:ARG:HH12	1.80	0.45
1:A:291:PHE:HB3	1:A:307:LYS:HE2	1.97	0.45
3:A:803:B12:H1P1	3:A:803:B12:N52	2.32	0.45
1:C:566:LYS:HE3	1:C:567:MET:HE2	1.97	0.45
1:B:566:LYS:HD3	1:B:567:MET:CE	2.47	0.44
3:A:803:B12:H203	3:A:803:B12:H301	1.97	0.44
1:A:289:ASP:OD1	1:A:289:ASP:C	2.56	0.44
3:C:803:B12:H203	3:C:803:B12:H301	2.00	0.44
1:A:566:LYS:CD	1:A:567:MET:CE	2.96	0.44
1:A:566:LYS:HG2	1:A:567:MET:HE2	1.99	0.44
1:B:291:PHE:HB3	1:B:307:LYS:HE2	1.99	0.43
3:B:803:B12:H533	3:B:803:B12:C48	2.48	0.43
1:C:368:VAL:HG22	1:C:399:MET:HG2	2.00	0.43
1:A:340:THR:HG23	1:A:342:LYS:HG3	2.00	0.43
3:A:803:B12:H1P1	3:A:803:B12:O51	2.19	0.43
1:A:340:THR:CG2	1:A:342:LYS:H	2.27	0.43
1:A:292:LYS:HD2	1:A:292:LYS:HA	1.80	0.42
1:C:566:LYS:CD	1:C:567:MET:CE	2.97	0.42
1:C:566:LYS:HG2	1:C:567:MET:HE2	2.00	0.42
1:A:260:ARG:HD3	6:A:969:HOH:O	2.20	0.42
3:C:803:B12:H301	3:C:803:B12:H253	1.76	0.42
1:A:566:LYS:CE	1:A:567:MET:CE	2.97	0.42
1:B:340:THR:HG23	1:B:342:LYS:HG3	2.01	0.42
3:B:803:B12:O51	3:B:803:B12:H1P1	2.19	0.42
1:C:310:PHE:N	1:C:311:PRO:CD	2.82	0.42
1:A:310:PHE:N	1:A:311:PRO:CD	2.83	0.42
1:B:566:LYS:HG2	1:B:567:MET:HE2	2.02	0.42
1:C:566:LYS:HE3	1:C:567:MET:HE1	2.02	0.42
1:A:490:ILE:HG13	1:A:491:VAL:N	2.34	0.41
1:C:372:ARG:HB3	1:C:372:ARG:HE	1.60	0.41
1:A:151:GLU:OE1	1:A:431:GLU:OE1	2.38	0.41
3:B:803:B12:H601	3:B:803:B12:H262	2.03	0.41
1:C:340:THR:HG23	1:C:342:LYS:HG3	2.03	0.41
1:B:168:ARG:NH1	1:B:169:GLY:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:803:B12:H531	3:C:803:B12:C55	2.44	0.41
1:C:151:GLU:OE1	1:C:431:GLU:OE1	2.39	0.41
1:C:566:LYS:CE	1:C:567:MET:CE	2.99	0.41
3:C:803:B12:H531	3:C:803:B12:H543	2.03	0.41
1:B:368:VAL:HG22	1:B:399:MET:HG2	2.03	0.41
1:C:292:LYS:HA	1:C:292:LYS:HD2	1.81	0.41
1:A:372:ARG:HB3	1:A:372:ARG:HE	1.59	0.41
1:A:119:PHE:CZ	1:A:208:GLY:HA3	2.57	0.40
1:A:368:VAL:HG22	1:A:399:MET:HG2	2.03	0.40
1:B:237:LEU:HD12	1:C:598:MET:HG2	2.03	0.40
1:A:656:ARG:NH1	1:A:679:GLU:OE1	2.53	0.40
1:B:292:LYS:HD2	1:B:292:LYS:HA	1.82	0.40
1:B:566:LYS:CE	1:B:567:MET:CE	2.99	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	696/704 (99%)	676 (97%)	19 (3%)	1 (0%)	51	64
1	B	687/704 (98%)	670 (98%)	17 (2%)	0	100	100
1	C	686/704 (97%)	667 (97%)	18 (3%)	1 (0%)	51	64
All	All	2069/2112 (98%)	2013 (97%)	54 (3%)	2 (0%)	51	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	641	GLY
1	A	641	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	534/552 (97%)	513 (96%)	21 (4%)	32	46
1	B	529/552 (96%)	507 (96%)	22 (4%)	30	42
1	C	519/552 (94%)	497 (96%)	22 (4%)	30	42
All	All	1582/1656 (96%)	1517 (96%)	65 (4%)	30	43

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	128	GLU
1	A	144	ARG
1	A	151	GLU
1	A	168	ARG
1	A	181	ARG
1	A	250	GLU
1	A	258	MET
1	A	286	LYS
1	A	289	ASP
1	A	323	LEU
1	A	340	THR
1	A	346	LEU
1	A	372	ARG
1	A	455	SER
1	A	513	ASN
1	A	554	THR
1	A	606	LYS
1	A	639	ASP
1	A	655	PRO
1	A	685	THR
1	B	3	LEU
1	B	128	GLU
1	B	144	ARG
1	B	168	ARG
1	B	181	ARG

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Mol	Chain	Res	Type
1	B	250	GLU
1	B	258	MET
1	B	286	LYS
1	B	289	ASP
1	B	323	LEU
1	B	340	THR
1	B	346	LEU
1	B	372	ARG
1	B	455	SER
1	B	513	ASN
1	B	554	THR
1	B	564	CYS
1	B	606	LYS
1	B	639	ASP
1	B	655	PRO
1	B	685	THR
1	B	694	LYS
1	C	3	LEU
1	C	128	GLU
1	C	144	ARG
1	C	168	ARG
1	C	181	ARG
1	C	258	MET
1	C	286	LYS
1	C	289	ASP
1	C	323	LEU
1	C	340	THR
1	C	346	LEU
1	C	372	ARG
1	C	455	SER
1	C	513	ASN
1	C	554	THR
1	C	564	CYS
1	C	606	LYS
1	C	639	ASP
1	C	640	ARG
1	C	655	PRO
1	C	685	THR
1	C	696	SER

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

Mol	Chain	Res	Type
1	A	525	ASN
1	B	11	ASN
1	B	603	GLN
1	C	525	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 15 ligands modelled in this entry, 6 are monoatomic - leaving 9 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	$\# Z > 2$
3	B12	A	803	-	80,101,101	1.18	4 (5%)	101,166,166	1.73	16 (15%)
2	SF4	B	801	1	0,12,12	0.00	-	-		
3	B12	B	803	-	80,101,101	1.36	6 (7%)	101,166,166	1.77	14 (13%)
2	SF4	C	801	1	0,12,12	0.00	-	-		
2	SF4	B	802	1	0,12,12	0.00	-	-		
2	SF4	A	802	1	0,12,12	0.00	-	-		
2	SF4	C	802	1	0,12,12	0.00	-	-		
3	B12	C	803	-	80,101,101	0.83	2 (2%)	101,166,166	1.83	20 (19%)
2	SF4	A	801	1	0,12,12	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
2	SF4	B	801	1	-	-	0/6/5/5
3	B12	B	803	-	-	12/51/223/223	0/3/11/11
3	B12	C	803	-	-	12/51/223/223	0/3/11/11
2	SF4	B	802	1	-	-	0/6/5/5
2	SF4	A	802	1	-	-	0/6/5/5
2	SF4	A	801	1	-	-	0/6/5/5
2	SF4	C	802	1	-	-	0/6/5/5
2	SF4	C	801	1	-	-	0/6/5/5
3	B12	A	803	-	-	9/51/223/223	0/3/11/11

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	803	B12	P-O3	-6.85	1.42	1.60
3	B	803	B12	P-O3	-6.83	1.42	1.60
3	B	803	B12	C26-C2	-4.99	1.43	1.55
3	B	803	B12	C11-C10	-4.38	1.33	1.40
3	C	803	B12	P-O3	-4.00	1.50	1.60
3	B	803	B12	O3-C2P	-2.90	1.37	1.45
3	B	803	B12	P-O2	2.76	1.67	1.60
3	C	803	B12	C1P-C2P	2.35	1.57	1.51
3	A	803	B12	O3-C2P	-2.30	1.39	1.45
3	A	803	B12	C1P-C2P	2.27	1.57	1.51
3	A	803	B12	C4B-C9B	-2.07	1.38	1.41
3	B	803	B12	C37-C38	2.05	1.58	1.51

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	803	B12	O3-C2P-C1P	-10.68	85.61	106.92
3	B	803	B12	O3-C2P-C1P	-7.96	91.03	106.92
3	C	803	B12	C2P-C1P-N59	-7.77	101.47	112.93
3	B	803	B12	C56-C55-C17	7.51	130.04	115.50
3	B	803	B12	C2P-C1P-N59	-5.90	104.24	112.93
3	C	803	B12	C55-C56-C57	-4.61	101.16	111.23
3	C	803	B12	C30-C3-C2	-4.47	109.65	119.13
3	C	803	B12	C56-C55-C17	4.45	124.11	115.50
3	C	803	B12	C55-C17-C16	4.21	123.95	109.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	803	B12	C56-C57-N59	4.14	123.40	116.42
3	A	803	B12	C56-C55-C17	3.70	122.66	115.50
3	C	803	B12	C19-C1-N21	3.63	105.88	102.16
3	B	803	B12	C56-C57-N59	3.48	122.29	116.42
3	C	803	B12	C5-C6-N22	-3.45	118.52	124.81
3	C	803	B12	C60-C18-C19	-3.45	105.66	114.62
3	C	803	B12	O3-C2P-C1P	-3.41	100.10	106.92
3	C	803	B12	O5-P-O3	-3.37	93.47	106.78
3	C	803	B12	C13-C14-C15	-3.26	119.86	131.68
3	B	803	B12	C19-C1-N21	3.26	105.50	102.16
3	A	803	B12	C19-C1-N21	3.22	105.46	102.16
3	B	803	B12	C54-C17-C55	3.12	114.42	109.26
3	B	803	B12	O58-C57-N59	-3.11	117.14	123.01
3	A	803	B12	C30-C3-C2	-3.07	112.62	119.13
3	A	803	B12	O5-P-O4	2.97	126.93	112.24
3	B	803	B12	C36-C7-C8	-2.78	107.10	112.11
3	A	803	B12	C13-C14-C15	-2.71	121.86	131.68
3	C	803	B12	C12-C11-C10	-2.70	120.07	124.64
3	B	803	B12	C13-C14-C15	-2.69	121.91	131.68
3	A	803	B12	C55-C56-C57	-2.68	105.39	111.23
3	C	803	B12	O58-C57-N59	-2.66	118.00	123.01
3	C	803	B12	O3-P-O4	2.62	119.30	109.47
3	A	803	B12	O58-C57-N59	-2.61	118.09	123.01
3	B	803	B12	C36-C7-C37	2.58	115.23	110.83
3	A	803	B12	C36-C7-C8	-2.56	107.49	112.11
3	A	803	B12	C56-C57-N59	2.49	120.61	116.42
3	A	803	B12	C36-C7-C37	2.43	114.97	110.83
3	A	803	B12	C3-C4-C5	-2.37	123.10	131.68
3	B	803	B12	C1-C19-N24	-2.36	103.58	106.24
3	A	803	B12	O2-P-O4	2.36	118.30	109.47
3	B	803	B12	C16-C15-C14	-2.29	120.69	124.27
3	A	803	B12	C6-C5-C4	-2.29	120.70	124.27
3	C	803	B12	C9-C10-C11	-2.27	122.99	130.91
3	C	803	B12	C26-C2-C3	-2.24	103.35	107.47
3	C	803	B12	C26-C2-C1	2.24	113.50	110.02
3	A	803	B12	C1-C19-N24	-2.18	103.79	106.24
3	A	803	B12	C25-C2-C1	-2.14	110.63	113.80
3	B	803	B12	O5-P-O3	-2.07	98.61	106.78
3	C	803	B12	C36-C7-C8	-2.05	108.41	112.11
3	C	803	B12	C2-C1-C19	-2.05	115.37	118.60
3	B	803	B12	C4B-C9B-C8B	-2.01	119.04	121.10

There are no chirality outliers.

All (33) torsion outliers are listed below:

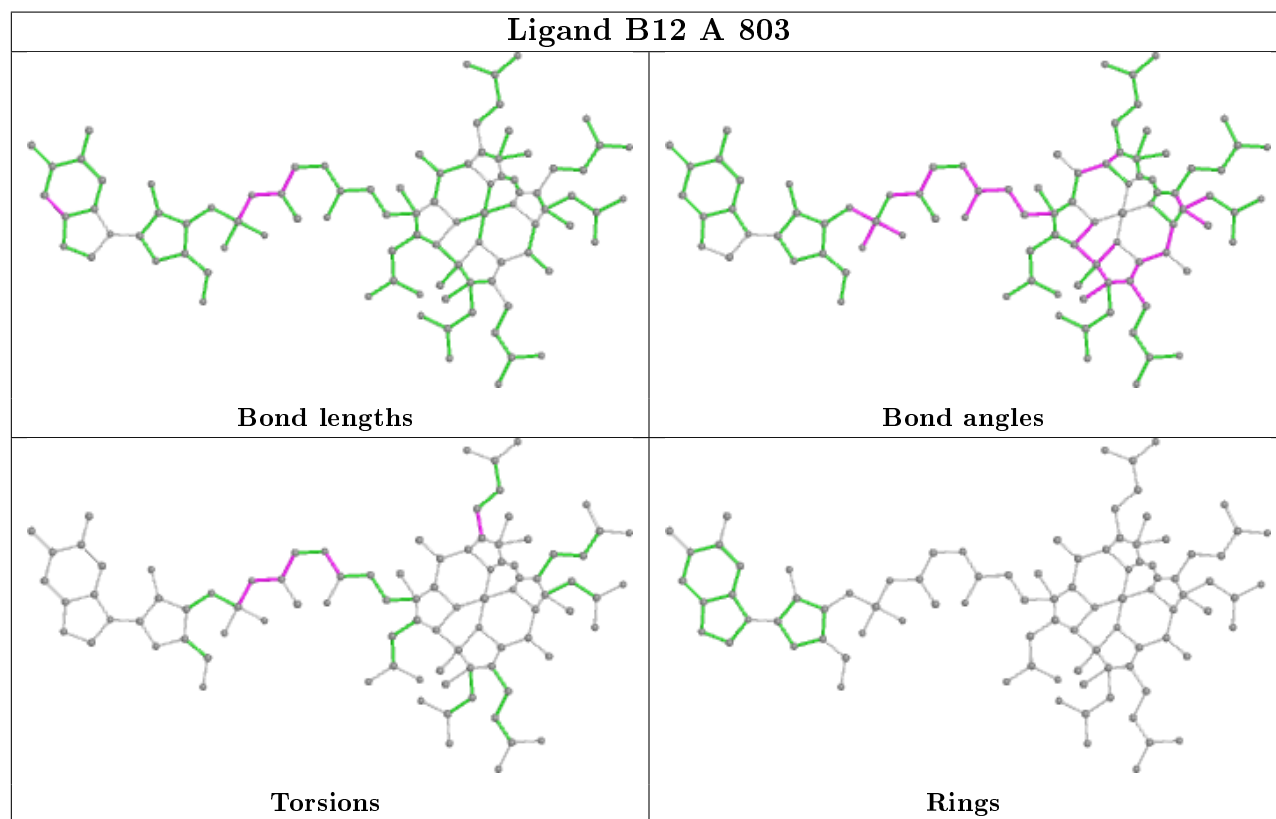
Mol	Chain	Res	Type	Atoms
3	A	803	B12	C56-C57-N59-C1P
3	A	803	B12	O58-C57-N59-C1P
3	A	803	B12	N59-C1P-C2P-C3P
3	A	803	B12	N59-C1P-C2P-O3
3	A	803	B12	C1P-C2P-O3-P
3	B	803	B12	C56-C57-N59-C1P
3	B	803	B12	O58-C57-N59-C1P
3	B	803	B12	N59-C1P-C2P-C3P
3	B	803	B12	N59-C1P-C2P-O3
3	B	803	B12	C1P-C2P-O3-P
3	B	803	B12	C3P-C2P-O3-P
3	C	803	B12	C56-C57-N59-C1P
3	C	803	B12	O58-C57-N59-C1P
3	C	803	B12	N59-C1P-C2P-C3P
3	C	803	B12	N59-C1P-C2P-O3
3	C	803	B12	C1P-C2P-O3-P
3	C	803	B12	C3P-C2P-O3-P
3	A	803	B12	C2P-O3-P-O2
3	B	803	B12	C38-C37-C7-C36
3	A	803	B12	C3P-C2P-O3-P
3	B	803	B12	C2P-O3-P-O2
3	C	803	B12	C2P-O3-P-O2
3	B	803	B12	C54-C17-C55-C56
3	A	803	B12	C14-C13-C48-C49
3	B	803	B12	C14-C13-C48-C49
3	C	803	B12	C4-C3-C30-C31
3	C	803	B12	C14-C13-C48-C49
3	A	803	B12	C2P-O3-P-O5
3	C	803	B12	C38-C37-C7-C36
3	C	803	B12	C2-C3-C30-C31
3	C	803	B12	C2P-C1P-N59-C57
3	B	803	B12	C16-C17-C55-C56
3	B	803	B12	C18-C17-C55-C56

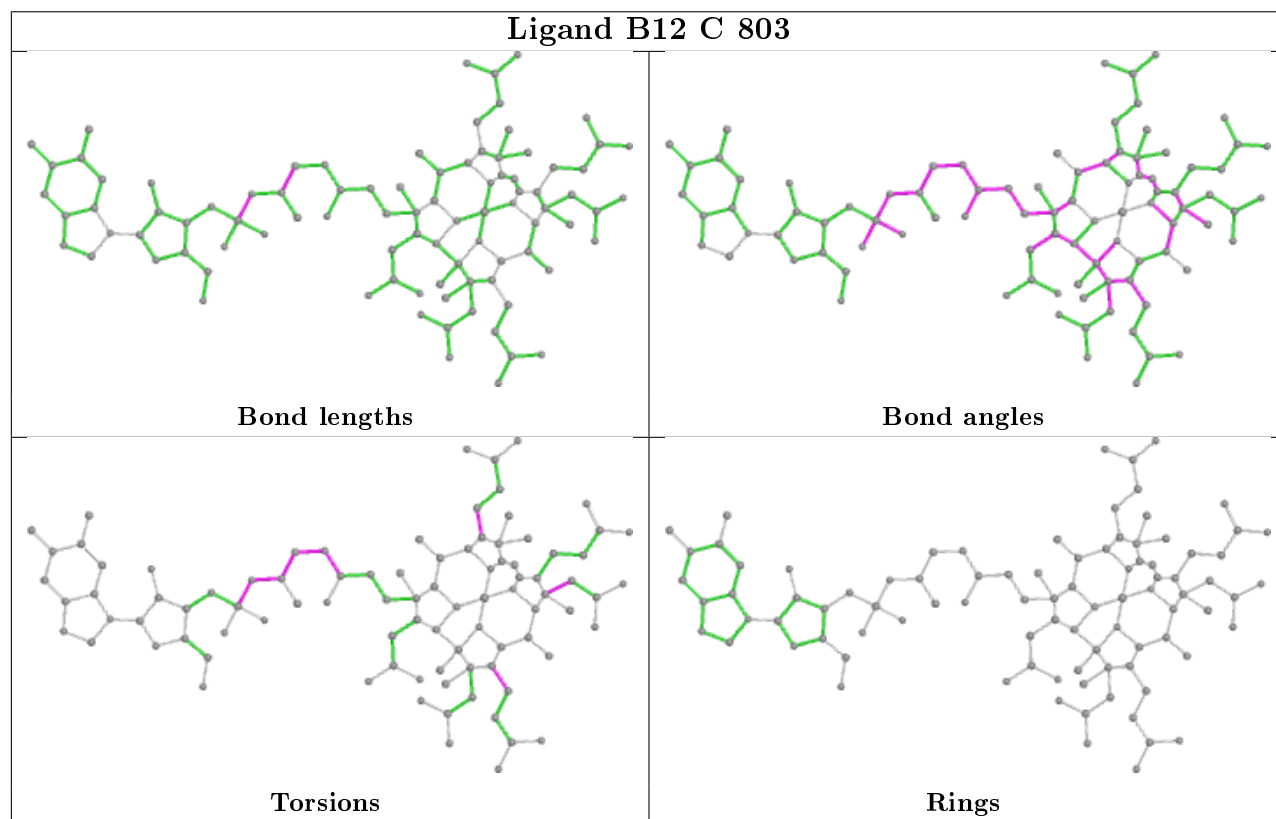
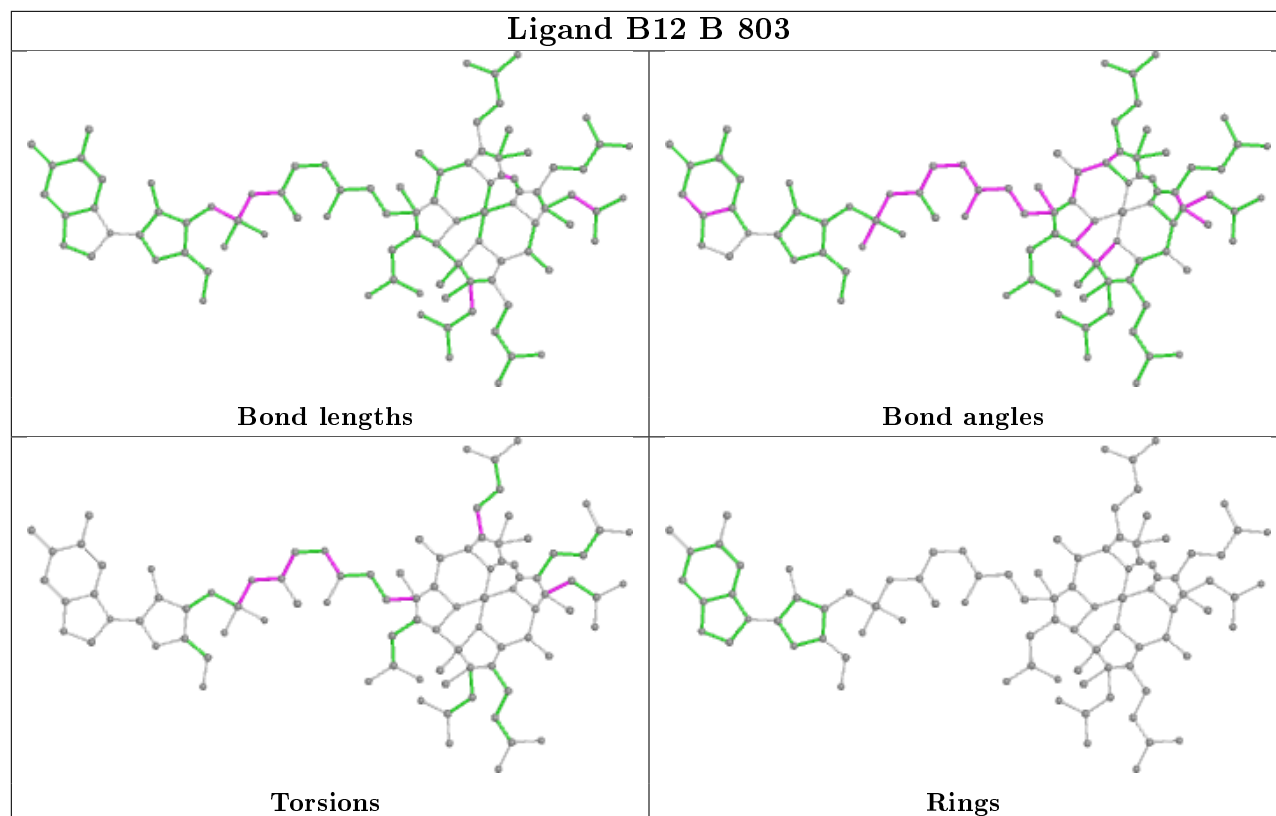
There are no ring outliers.

3 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	803	B12	12	0
3	B	803	B12	9	0
3	C	803	B12	12	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 than 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.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	698/704 (99%)	-0.20	2 (0%) 94 96	30, 41, 64, 103	0
1	B	691/704 (98%)	-0.12	1 (0%) 95 97	36, 48, 72, 109	0
1	C	692/704 (98%)	0.10	28 (4%) 38 45	43, 63, 90, 129	0
All	All	2081/2112 (98%)	-0.07	31 (1%) 73 79	30, 51, 82, 129	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	695	SER	4.8
1	B	646	ALA	4.6
1	C	103	ASP	4.5
1	C	100	LEU	4.2
1	C	102	PRO	3.7
1	C	109	CYS	3.3
1	C	696	SER	3.3
1	C	214	TYR	3.2
1	C	114	THR	3.1
1	C	28	VAL	3.1
1	C	108	ASP	2.9
1	C	216	LEU	2.9
1	C	101	ASP	2.8
1	C	165	PHE	2.8
1	C	159	TYR	2.7
1	C	99	ARG	2.6
1	C	617	LEU	2.5
1	C	621	ASP	2.5
1	C	76	PRO	2.5
1	C	73	PRO	2.4
1	C	627	PRO	2.4
1	C	111	PRO	2.3
1	C	177	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	215	ALA	2.3
1	C	83	LEU	2.3
1	C	72	ILE	2.3
1	A	698	GLY	2.2
1	C	166	PRO	2.1
1	C	70	ASP	2.1
1	A	39	PHE	2.1
1	C	213	GLY	2.1

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

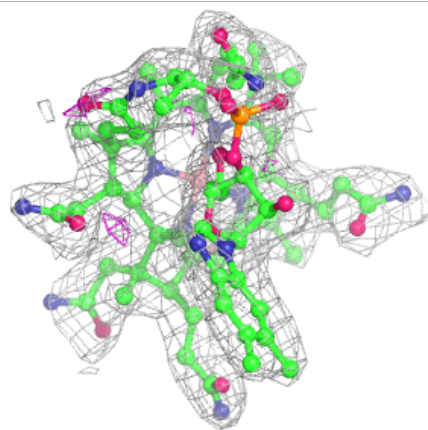
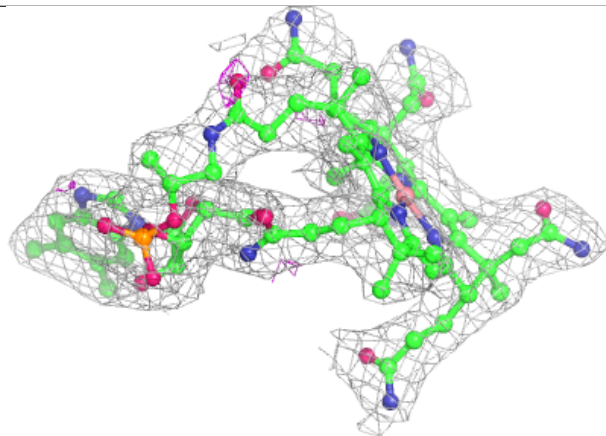
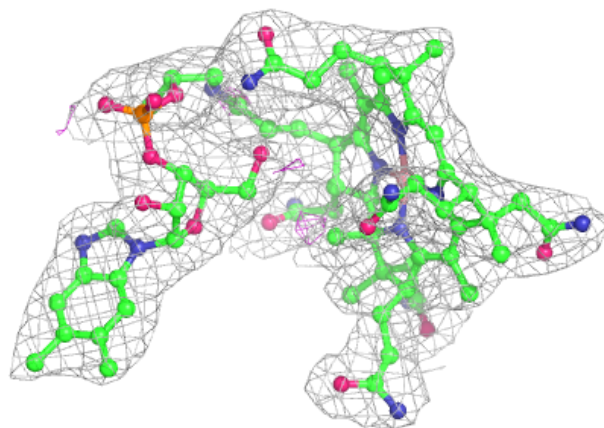
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	CL	B	804	1/1	0.91	0.24	63,63,63,63	0
5	NA	A	805	1/1	0.94	0.16	33,33,33,33	0
4	CL	A	804	1/1	0.96	0.15	54,54,54,54	0
3	B12	C	803	91/91	0.97	0.13	44,47,56,60	0
5	NA	B	805	1/1	0.97	0.18	38,38,38,38	0
5	NA	C	805	1/1	0.97	0.23	42,42,42,42	0
3	B12	B	803	91/91	0.98	0.14	31,36,42,47	0
2	SF4	C	801	8/8	0.98	0.10	38,40,41,41	0
3	B12	A	803	91/91	0.98	0.13	27,31,37,40	0
2	SF4	C	802	8/8	0.99	0.09	45,47,48,49	0
2	SF4	B	801	8/8	0.99	0.12	36,38,38,39	0
2	SF4	A	801	8/8	0.99	0.12	27,28,28,29	0
2	SF4	B	802	8/8	0.99	0.10	37,38,39,41	0
4	CL	C	804	1/1	0.99	0.11	62,62,62,62	0
2	SF4	A	802	8/8	0.99	0.11	28,31,32,34	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.

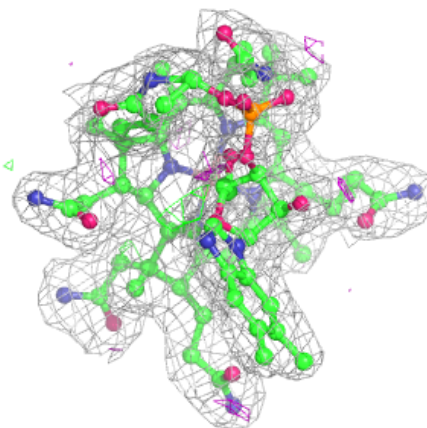
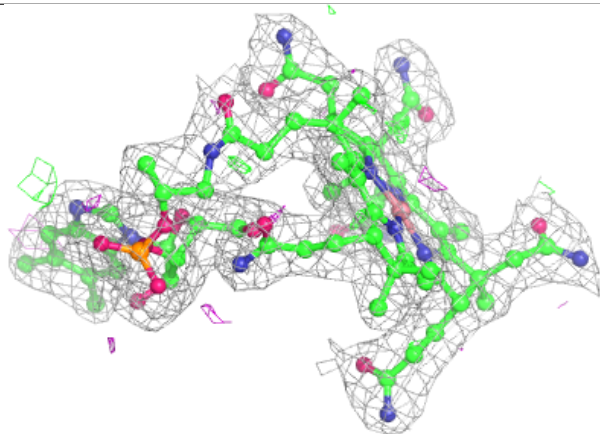
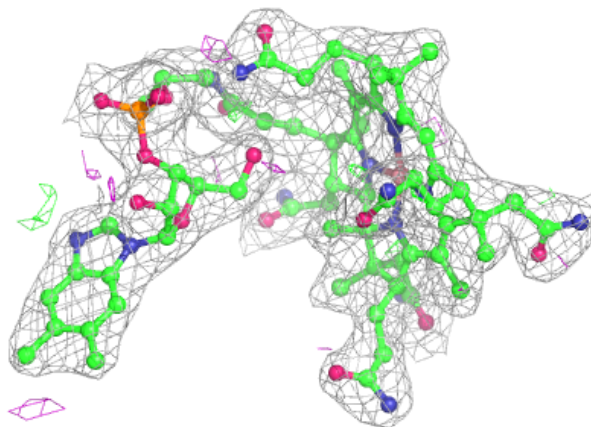
Electron density around B12 C 803:

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



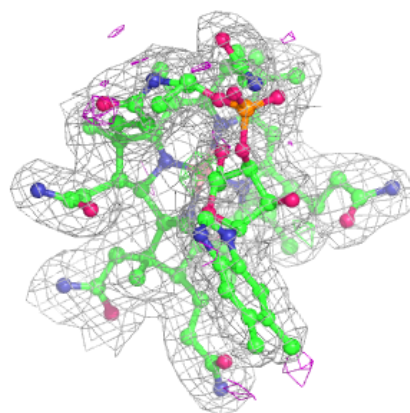
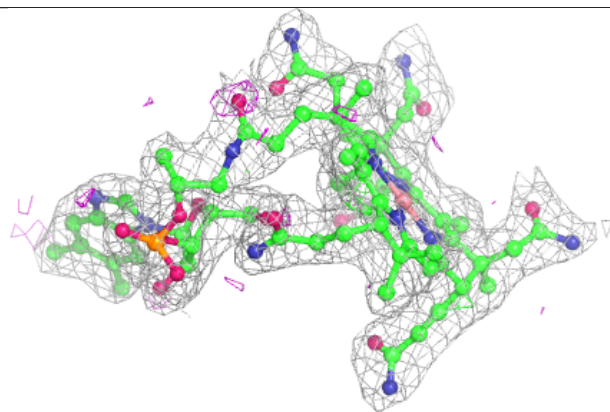
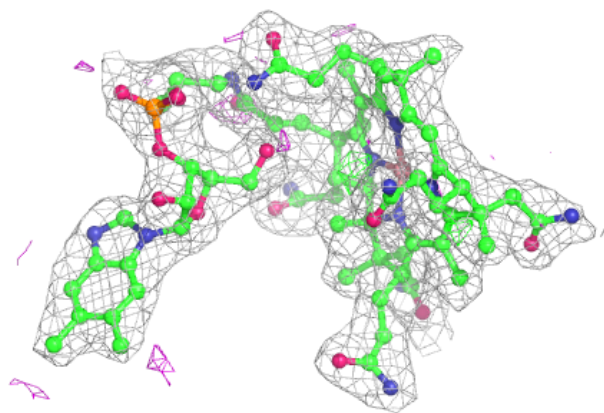
Electron density around B12 B 803:

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



Electron density around B12 A 803:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.