



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 07:36 AM UTC

PDB ID : 3AO0 / pdb_00003ao0
Title : Crystal structure of ethanolamine ammonia-lyase from Escherichia coli complexed with CN-CBL and (S)-2-amino-1-propanol
Authors : Shibata, N.
Deposited on : 2010-09-16
Resolution : 2.25 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
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	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

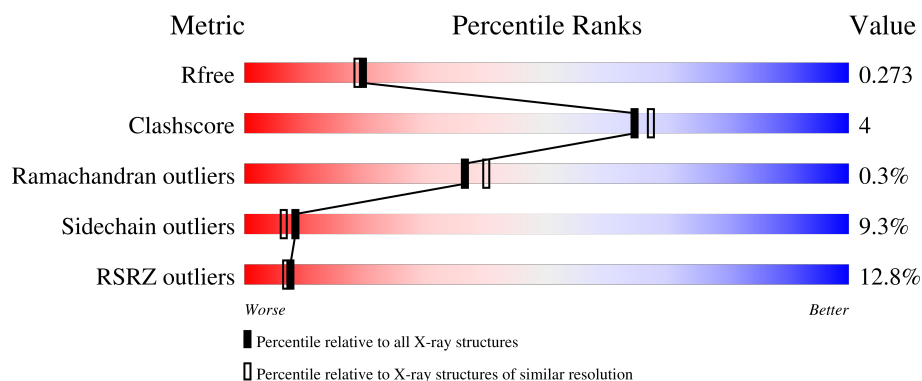
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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 $\leq 5\%$. 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	453	
1	C	453	
2	B	263	
2	D	263	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11550 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 Ethanolamine ammonia-lyase heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	453	Total	C	N	O	S	0	0	0
			3464	2170	593	679	22			
1	C	453	Total	C	N	O	S	0	1	0
			3469	2173	594	680	22			

- Molecule 2 is a protein called Ethanolamine ammonia-lyase light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	252	Total	C	N	O	S	0	0	0
			1916	1197	347	362	10			
2	D	252	Total	C	N	O	S	0	0	0
			1916	1197	347	362	10			

There are 22 discrepancies between the modelled and reference sequences:

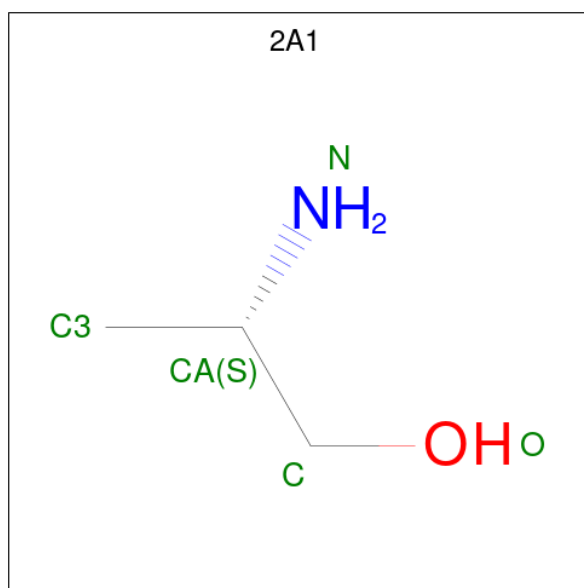
Chain	Residue	Modelled	Actual	Comment	Reference
B	33	MET	-	expression tag	UNP P19636
B	34	ASP	-	expression tag	UNP P19636
B	35	GLN	-	expression tag	UNP P19636
B	36	SER	-	expression tag	UNP P19636
B	37	SER	-	expression tag	UNP P19636
B	38	HIS	-	expression tag	UNP P19636
B	39	HIS	-	expression tag	UNP P19636
B	40	HIS	-	expression tag	UNP P19636
B	41	HIS	-	expression tag	UNP P19636
B	42	HIS	-	expression tag	UNP P19636
B	43	HIS	-	expression tag	UNP P19636
D	33	MET	-	expression tag	UNP P19636
D	34	ASP	-	expression tag	UNP P19636
D	35	GLN	-	expression tag	UNP P19636
D	36	SER	-	expression tag	UNP P19636
D	37	SER	-	expression tag	UNP P19636

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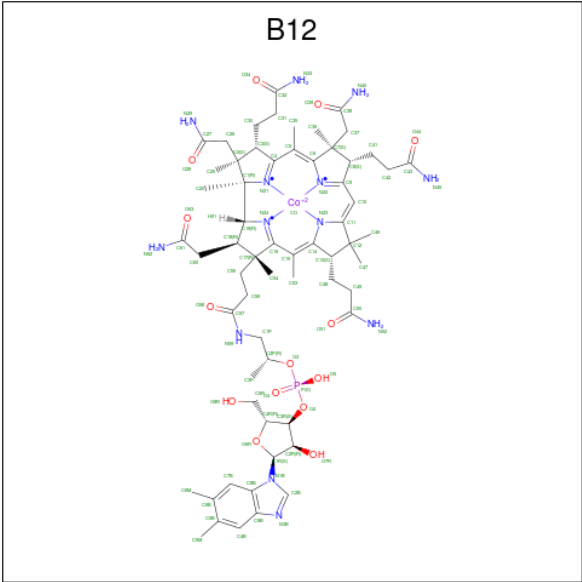
Chain	Residue	Modelled	Actual	Comment	Reference
D	38	HIS	-	expression tag	UNP P19636
D	39	HIS	-	expression tag	UNP P19636
D	40	HIS	-	expression tag	UNP P19636
D	41	HIS	-	expression tag	UNP P19636
D	42	HIS	-	expression tag	UNP P19636
D	43	HIS	-	expression tag	UNP P19636

- Molecule 3 is (2S)-2-aminopropan-1-ol (CCD ID: 2A1) (formula: C_3H_9NO).



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

- Molecule 4 is COBALAMIN (CCD ID: B12) (formula: $C_{62}H_{89}CoN_{13}O_{14}P$).



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

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

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

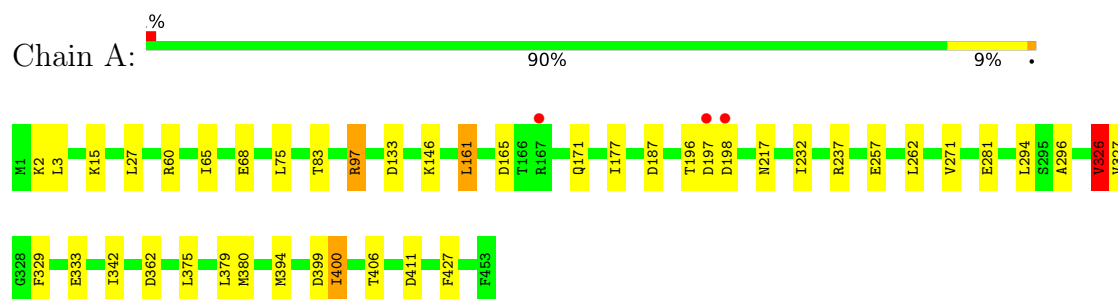
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	246	Total	O	0	0
			246	246		
6	B	63	Total	O	0	0
			63	63		
6	C	229	Total	O	0	0
			229	229		
6	D	54	Total	O	0	0
			54	54		

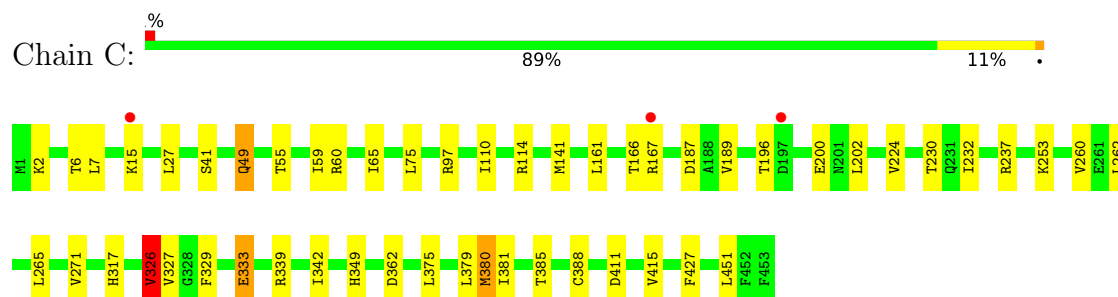
3 Residue-property plots

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.

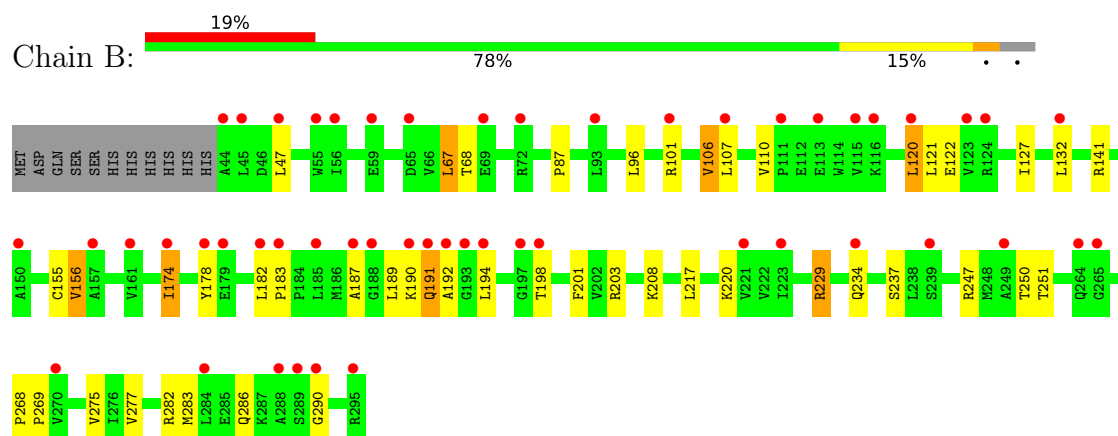
- Molecule 1: Ethanolamine ammonia-lyase heavy chain



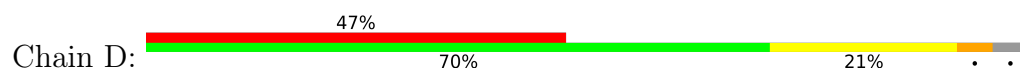
- Molecule 1: Ethanolamine ammonia-lyase heavy chain

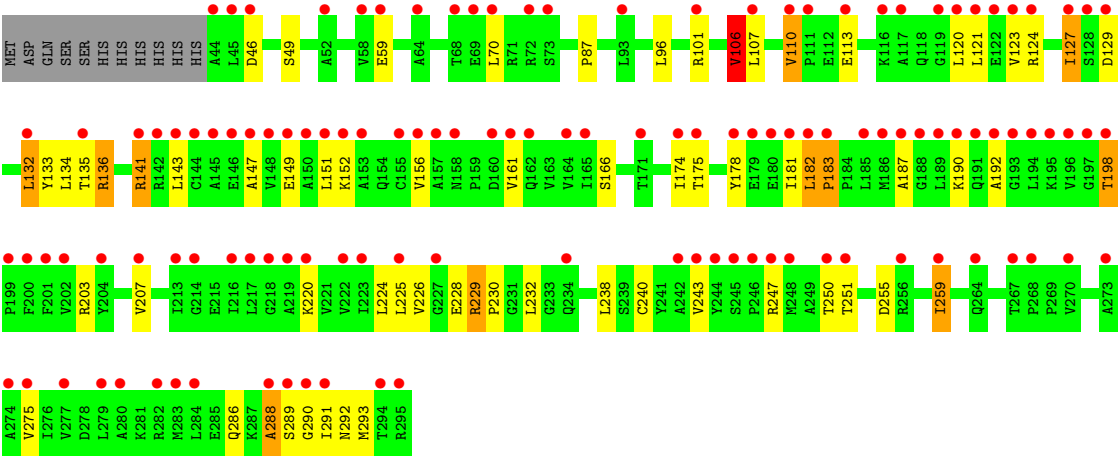


- Molecule 2: Ethanolamine ammonia-lyase light chain



- Molecule 2: Ethanolamine ammonia-lyase light chain





4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	243.85Å 243.85Å 76.81Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.00 – 2.25 48.00 – 2.25	Depositor EDS
% Data completeness (in resolution range)	98.5 (48.00-2.25) 98.4 (48.00-2.25)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.235 , 0.257 0.246 , 0.273	Depositor DCC
R_{free} test set	6112 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	25.7	Xtriage
Anisotropy	0.191	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 35.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.055 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	11550	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.06% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 2A1, NA, B12

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	0.79	1/3518 (0.0%)	0.66	0/4764
1	C	0.79	2/3526 (0.1%)	0.66	0/4775
2	B	0.85	3/1943 (0.2%)	0.67	0/2633
2	D	0.85	2/1943 (0.1%)	0.66	0/2633
All	All	0.81	8/10930 (0.1%)	0.66	0/14805

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	3
1	C	0	2
2	B	0	2
2	D	0	3
All	All	0	10

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	183	PRO	CA-C	7.56	1.59	1.52
2	B	183	PRO	CA-C	6.95	1.58	1.52
1	C	189	VAL	CA-CB	6.57	1.60	1.55
2	B	156	VAL	CA-CB	6.08	1.61	1.54
1	A	327	VAL	CA-CB	5.80	1.61	1.54
2	B	106	VAL	CA-CB	5.38	1.61	1.54
1	C	327	VAL	CA-CB	5.26	1.60	1.54
2	D	106	VAL	CA-CB	5.25	1.61	1.54

There are no bond angle outliers.

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	237	ARG	Peptide
1	A	326	VAL	Peptide
1	A	400	ILE	Peptide
2	B	120	LEU	Peptide
2	B	191	GLN	Peptide
1	C	237	ARG	Peptide
1	C	326	VAL	Peptide
2	D	120	LEU	Peptide
2	D	192	ALA	Peptide
2	D	288	ALA	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3464	0	3419	16	0
1	C	3469	0	3425	14	0
2	B	1916	0	1973	20	0
2	D	1916	0	1973	21	0
3	A	5	0	0	0	0
3	C	5	0	0	0	0
4	B	91	0	88	9	0
4	D	91	0	88	11	0
5	C	1	0	0	0	0
6	A	246	0	0	0	0
6	B	63	0	0	0	0
6	C	229	0	0	0	0
6	D	54	0	0	0	0
All	All	11550	0	10966	86	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 (86) 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)
2:B:229:ARG:HH21	2:B:229:ARG:HG2	1.01	1.17
2:B:229:ARG:HG2	2:B:229:ARG:NH2	1.79	0.87
4:D:601:B12:H552	4:D:601:B12:H531	1.58	0.85
4:B:601:B12:H362	4:B:601:B12:H351	1.58	0.84
1:C:329:PHE:O	2:D:229:ARG:NH2	2.11	0.82
4:B:601:B12:H552	4:B:601:B12:H531	1.62	0.82
4:D:601:B12:H362	4:D:601:B12:H351	1.66	0.78
1:A:257:GLU:HG3	1:A:296:ALA:HB1	1.70	0.73
1:A:394:MET:HE1	1:A:399:ASP:HB2	1.69	0.72
1:A:394:MET:HE2	1:A:406:THR:HG22	1.73	0.70
2:B:110:VAL:O	2:B:203:ARG:NH2	2.27	0.67
1:A:97:ARG:NH2	2:D:87:PRO:O	2.28	0.67
2:D:110:VAL:O	2:D:203:ARG:NH2	2.30	0.63
2:B:229:ARG:HH21	2:B:229:ARG:CG	1.92	0.62
4:B:601:B12:H482	4:B:601:B12:H2B	1.82	0.61
1:C:202:LEU:HD22	1:C:224:VAL:HG11	1.83	0.59
4:D:601:B12:H601	4:D:601:B12:H262	1.83	0.59
4:B:601:B12:H362	4:B:601:B12:C35	2.33	0.57
1:A:394:MET:HE2	1:A:406:THR:CG2	2.35	0.55
2:B:234:GLN:HE22	2:B:237:SER:HB2	1.72	0.55
4:D:601:B12:H533	4:D:601:B12:H492	1.88	0.54
2:D:129:ASP:HB2	2:D:132:LEU:HB2	1.89	0.54
2:B:122:GLU:HG3	2:B:201:PHE:HD1	1.73	0.54
2:B:87:PRO:O	1:C:97:ARG:NH2	2.39	0.54
4:B:601:B12:H601	4:B:601:B12:H262	1.89	0.54
1:C:349:HIS:CE1	1:C:388:CYS:HA	2.43	0.53
2:D:174:ILE:O	2:D:178:TYR:HB2	2.09	0.53
4:D:601:B12:H552	4:D:601:B12:C53	2.35	0.52
2:B:141:ARG:HG2	2:B:208:LYS:HB2	1.93	0.51
1:A:394:MET:CE	1:A:406:THR:HG22	2.41	0.51
4:D:601:B12:H362	4:D:601:B12:C35	2.38	0.51
2:B:187:ALA:O	2:B:191:GLN:HB3	2.11	0.51
2:D:106:VAL:HG12	2:D:230:PRO:HG2	1.92	0.51
2:B:247:ARG:HB3	2:B:250:THR:HB	1.94	0.50
1:A:187:ASP:HB3	1:A:427:PHE:CG	2.47	0.49
1:C:75:LEU:HD21	1:C:317:HIS:HB2	1.95	0.49
2:B:247:ARG:O	2:B:251:THR:HG22	2.13	0.48
1:A:380:MET:SD	1:A:411:ASP:HB3	2.53	0.47
2:D:247:ARG:HB3	2:D:250:THR:HB	1.96	0.47
2:D:225:LEU:HB3	2:D:238:LEU:HD21	1.95	0.47
2:B:174:ILE:O	2:B:178:TYR:HB2	2.15	0.47
2:D:240:CYS:HB3	2:D:259:ILE:HG23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:ILE:HA	1:A:379:LEU:HD13	1.98	0.46
1:A:187:ASP:OD1	1:A:187:ASP:N	2.46	0.46
2:D:182:LEU:HB3	2:D:183:PRO:CD	2.45	0.46
1:C:342:ILE:HA	1:C:379:LEU:HD13	1.98	0.46
4:B:601:B12:H552	4:B:601:B12:C53	2.39	0.46
1:C:333:GLU:H	1:C:333:GLU:HG3	1.60	0.46
2:D:156:VAL:HG22	2:D:198:THR:HG22	1.98	0.46
4:D:601:B12:H541	4:D:601:B12:H602	1.79	0.46
1:C:380:MET:SD	1:C:411:ASP:HB3	2.56	0.45
1:A:161:LEU:HD21	1:A:177:ILE:HA	1.97	0.45
2:D:127:ILE:HG21	2:D:133:TYR:HB2	1.98	0.45
2:D:135:THR:HG23	2:D:136:ARG:HG2	1.97	0.45
4:B:601:B12:H261	4:B:601:B12:H91	1.92	0.44
2:B:155:CYS:HA	2:B:198:THR:HG21	2.00	0.44
4:B:601:B12:H521	4:B:601:B12:H481	1.44	0.44
2:D:255:ASP:O	2:D:289:SER:HB3	2.17	0.44
2:B:282:ARG:O	2:B:286:GLN:HG2	2.17	0.44
2:B:189:LEU:HG	2:B:277:VAL:HG22	1.99	0.44
1:C:187:ASP:HB3	1:C:427:PHE:CG	2.52	0.44
1:A:165:ASP:HA	1:A:400:ILE:HD11	2.00	0.44
4:D:601:B12:H472	4:D:601:B12:H10	1.79	0.43
4:B:601:B12:H481	4:B:601:B12:H473	1.51	0.43
2:D:143:LEU:HB3	2:D:147:ALA:HB3	2.00	0.43
1:A:326:VAL:HG12	1:A:329:PHE:HB2	2.00	0.43
2:D:228:GLU:HA	4:D:601:B12:H1P2	2.00	0.43
2:D:247:ARG:O	2:D:251:THR:HG22	2.17	0.43
1:C:326:VAL:HA	1:C:362:ASP:HB3	2.00	0.43
1:C:110:ILE:HD13	1:C:141:MET:HG2	1.99	0.43
1:A:326:VAL:HA	1:A:362:ASP:HB3	2.01	0.43
2:B:120:LEU:HD13	2:B:201:PHE:HB2	2.01	0.43
2:B:67:LEU:HD12	2:B:67:LEU:HA	1.86	0.43
2:D:46:ASP:HB3	2:D:49:SER:HB3	1.99	0.42
1:A:97:ARG:NH1	1:A:133:ASP:OD2	2.50	0.42
2:B:155:CYS:HA	2:B:198:THR:CG2	2.49	0.42
2:D:166:SER:HB3	2:D:226:VAL:HG23	2.02	0.41
1:C:232:ILE:HG23	1:C:271:VAL:HG21	2.01	0.41
2:D:141:ARG:HE	2:D:141:ARG:HB3	1.50	0.41
4:D:601:B12:H562	4:D:601:B12:H18	1.91	0.41
2:B:268:PRO:HA	2:B:269:PRO:HD3	1.88	0.41
2:D:286:GLN:HG3	2:D:288:ALA:HB3	2.03	0.41
1:A:232:ILE:HG23	1:A:271:VAL:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:601:B12:H261	4:D:601:B12:H91	1.96	0.40
1:C:381:ILE:O	1:C:385:THR:HG23	2.21	0.40
2:B:47:LEU:HD11	1:C:49:GLN:HG3	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	451/453 (100%)	432 (96%)	19 (4%)	0	100	100
1	C	452/453 (100%)	431 (95%)	21 (5%)	0	100	100
2	B	250/263 (95%)	237 (95%)	11 (4%)	2 (1%)	16	14
2	D	250/263 (95%)	239 (96%)	9 (4%)	2 (1%)	16	14
All	All	1403/1432 (98%)	1339 (95%)	60 (4%)	4 (0%)	36	40

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	192	ALA
2	D	290	GLY
2	D	187	ALA
2	B	290	GLY

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	370/370 (100%)	347 (94%)	23 (6%)	16	16
1	C	371/370 (100%)	342 (92%)	29 (8%)	11	10
2	B	206/217 (95%)	187 (91%)	19 (9%)	8	6
2	D	206/217 (95%)	170 (82%)	36 (18%)	2	0
All	All	1153/1174 (98%)	1046 (91%)	107 (9%)	8	6

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	3	LEU
1	A	15	LYS
1	A	27	LEU
1	A	60	ARG
1	A	65	ILE
1	A	68	GLU
1	A	75	LEU
1	A	83	THR
1	A	97	ARG
1	A	146	LYS
1	A	161	LEU
1	A	171	GLN
1	A	196	THR
1	A	197	ASP
1	A	198	ASP
1	A	217	ASN
1	A	262	LEU
1	A	281	GLU
1	A	294	LEU
1	A	326	VAL
1	A	333	GLU
1	A	375	LEU
2	B	67	LEU
2	B	68	THR
2	B	96	LEU
2	B	101	ARG
2	B	106	VAL
2	B	107	LEU
2	B	121	LEU
2	B	127	ILE

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Mol	Chain	Res	Type
2	B	132	LEU
2	B	156	VAL
2	B	174	ILE
2	B	182	LEU
2	B	190	LYS
2	B	194	LEU
2	B	217	LEU
2	B	220	LYS
2	B	229	ARG
2	B	275	VAL
2	B	283	MET
1	C	2	LYS
1	C	6	THR
1	C	7	LEU
1	C	15	LYS
1	C	27	LEU
1	C	41	SER
1	C	49	GLN
1	C	55	THR
1	C	59	ILE
1	C	60	ARG
1	C	65	ILE
1	C	114	ARG
1	C	161	LEU
1	C	166	THR
1	C	167	ARG
1	C	196	THR
1	C	200	GLU
1	C	230	THR
1	C	253	LYS
1	C	260	VAL
1	C	262	LEU
1	C	265	LEU
1	C	326	VAL
1	C	333	GLU
1	C	339	ARG
1	C	375	LEU
1	C	380	MET
1	C	415	VAL
1	C	451	LEU
2	D	59	GLU
2	D	70	LEU

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Mol	Chain	Res	Type
2	D	96	LEU
2	D	101	ARG
2	D	106	VAL
2	D	107	LEU
2	D	110	VAL
2	D	113	GLU
2	D	121	LEU
2	D	123	VAL
2	D	124	ARG
2	D	127	ILE
2	D	132	LEU
2	D	134	LEU
2	D	136	ARG
2	D	141	ARG
2	D	149	GLU
2	D	151	LEU
2	D	152	LYS
2	D	161	VAL
2	D	175	THR
2	D	181	ILE
2	D	182	LEU
2	D	190	LYS
2	D	198	THR
2	D	207	VAL
2	D	220	LYS
2	D	224	LEU
2	D	229	ARG
2	D	232	LEU
2	D	243	VAL
2	D	259	ILE
2	D	275	VAL
2	D	291	ILE
2	D	292	ASN
2	D	293	MET

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

Mol	Chain	Res	Type
1	A	90	ASN
2	B	131	ASN
2	B	177	ASN
2	B	234	GLN

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Mol	Chain	Res	Type
1	C	10	ASN
1	C	86	ASN
1	C	217	ASN
1	C	276	ASN
1	C	349	HIS
2	D	292	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	B12	D	601	-	94,101,101	1.52	12 (12%)	149,166,166	1.31	19 (12%)
4	B12	B	601	-	94,101,101	1.61	16 (17%)	149,166,166	1.26	16 (10%)
3	2A1	C	602	-	4,4,4	0.80	0	1,4,4	0.17	0
3	2A1	A	602	-	4,4,4	0.78	0	1,4,4	0.18	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
4	B12	D	601	-	-	21/56/223/223	0/3/11/11
4	B12	B	601	-	-	20/56/223/223	0/3/11/11
3	2A1	C	602	-	-	0/2/2/2	-
3	2A1	A	602	-	-	2/2/2/2	-

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	601	B12	C19-N24	-8.06	1.39	1.49
4	D	601	B12	C19-N24	-7.83	1.39	1.49
4	B	601	B12	C14-N23	4.20	1.40	1.35
4	D	601	B12	C8B-C9B	4.00	1.46	1.40
4	D	601	B12	C46-C12	-3.90	1.46	1.54
4	B	601	B12	C9-N22	3.75	1.39	1.30
4	D	601	B12	C6B-C5B	3.72	1.49	1.40
4	B	601	B12	C8B-C9B	3.68	1.46	1.40
4	B	601	B12	C6B-C5B	3.64	1.49	1.40
4	B	601	B12	C47-C12	-3.64	1.46	1.54
4	B	601	B12	C46-C12	-3.61	1.46	1.54
4	D	601	B12	C12-C11	-3.52	1.46	1.52
4	D	601	B12	C9-N22	3.17	1.38	1.30
4	B	601	B12	C9B-N3B	-3.14	1.33	1.39
4	D	601	B12	C9B-N3B	-3.11	1.34	1.39
4	B	601	B12	C2B-N3B	3.08	1.37	1.31
4	D	601	B12	C2B-N3B	3.04	1.37	1.31
4	D	601	B12	C8B-N1B	-2.77	1.33	1.39
4	B	601	B12	C16-C15	-2.52	1.37	1.44
4	B	601	B12	C11-N23	2.48	1.41	1.36
4	B	601	B12	C8B-N1B	-2.47	1.34	1.39
4	D	601	B12	C10-C11	-2.44	1.30	1.37
4	D	601	B12	C17-C18	2.42	1.59	1.54
4	B	601	B12	C17-C18	2.33	1.59	1.54
4	B	601	B12	C12-C11	-2.28	1.48	1.52
4	D	601	B12	C14-C15	2.26	1.48	1.38
4	B	601	B12	C14-C15	2.21	1.48	1.38
4	B	601	B12	C10-C11	-2.16	1.31	1.37

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	601	B12	C19-N24-C16	4.85	112.59	107.29
4	B	601	B12	C19-N24-C16	4.62	112.34	107.29
4	D	601	B12	C9B-C8B-N1B	4.08	107.11	105.30
4	B	601	B12	C9B-C8B-N1B	3.99	107.08	105.30
4	D	601	B12	C18-C19-N24	3.73	107.93	102.33
4	B	601	B12	C18-C19-N24	3.60	107.73	102.33
4	B	601	B12	C1-C19-N24	3.52	110.17	106.25
4	D	601	B12	C47-C12-C46	3.24	114.77	109.41
4	D	601	B12	C54-C17-C18	-3.12	108.51	112.99
4	B	601	B12	C9B-N3B-C2B	3.12	108.22	104.40
4	D	601	B12	C9B-N3B-C2B	3.08	108.18	104.40
4	D	601	B12	C8B-C9B-N3B	-2.96	106.80	110.00
4	B	601	B12	C8B-C9B-N3B	-2.90	106.86	110.00
4	D	601	B12	N1B-C2B-N3B	-2.88	109.85	113.94
4	B	601	B12	N1B-C2B-N3B	-2.88	109.85	113.94
4	D	601	B12	C12-C11-C10	-2.69	119.93	123.40
4	B	601	B12	C30-C3-C2	-2.58	113.31	119.00
4	D	601	B12	C15-C14-N23	-2.57	123.16	126.26
4	B	601	B12	C54-C17-C18	-2.55	109.32	112.99
4	B	601	B12	C7-C6-C5	-2.54	124.11	128.07
4	D	601	B12	C30-C3-C2	-2.47	113.56	119.00
4	D	601	B12	C7-C6-C5	-2.42	124.29	128.07
4	D	601	B12	C1-C19-N24	2.30	108.81	106.25
4	D	601	B12	C25-C2-C1	-2.30	110.32	113.75
4	B	601	B12	C7-C8-C9	2.25	103.74	100.89
4	D	601	B12	C19-C1-N21	2.24	104.45	102.14
4	D	601	B12	C20-C1-C19	-2.20	107.24	109.35
4	B	601	B12	C19-C1-N21	2.18	104.39	102.14
4	D	601	B12	C48-C13-C12	-2.14	110.39	116.52
4	B	601	B12	C9-C10-C11	-2.11	122.95	125.97
4	D	601	B12	C9-N22-C6	2.11	107.82	105.28
4	B	601	B12	C47-C12-C46	2.09	112.86	109.41
4	B	601	B12	C25-C2-C1	-2.07	110.66	113.75
4	D	601	B12	C3R-C2R-C1R	2.06	104.41	99.89
4	B	601	B12	C9-N22-C6	2.04	107.73	105.28

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	2A1	O-C-CA-N
4	B	601	B12	C38-C37-C7-C6
4	B	601	B12	C38-C37-C7-C36

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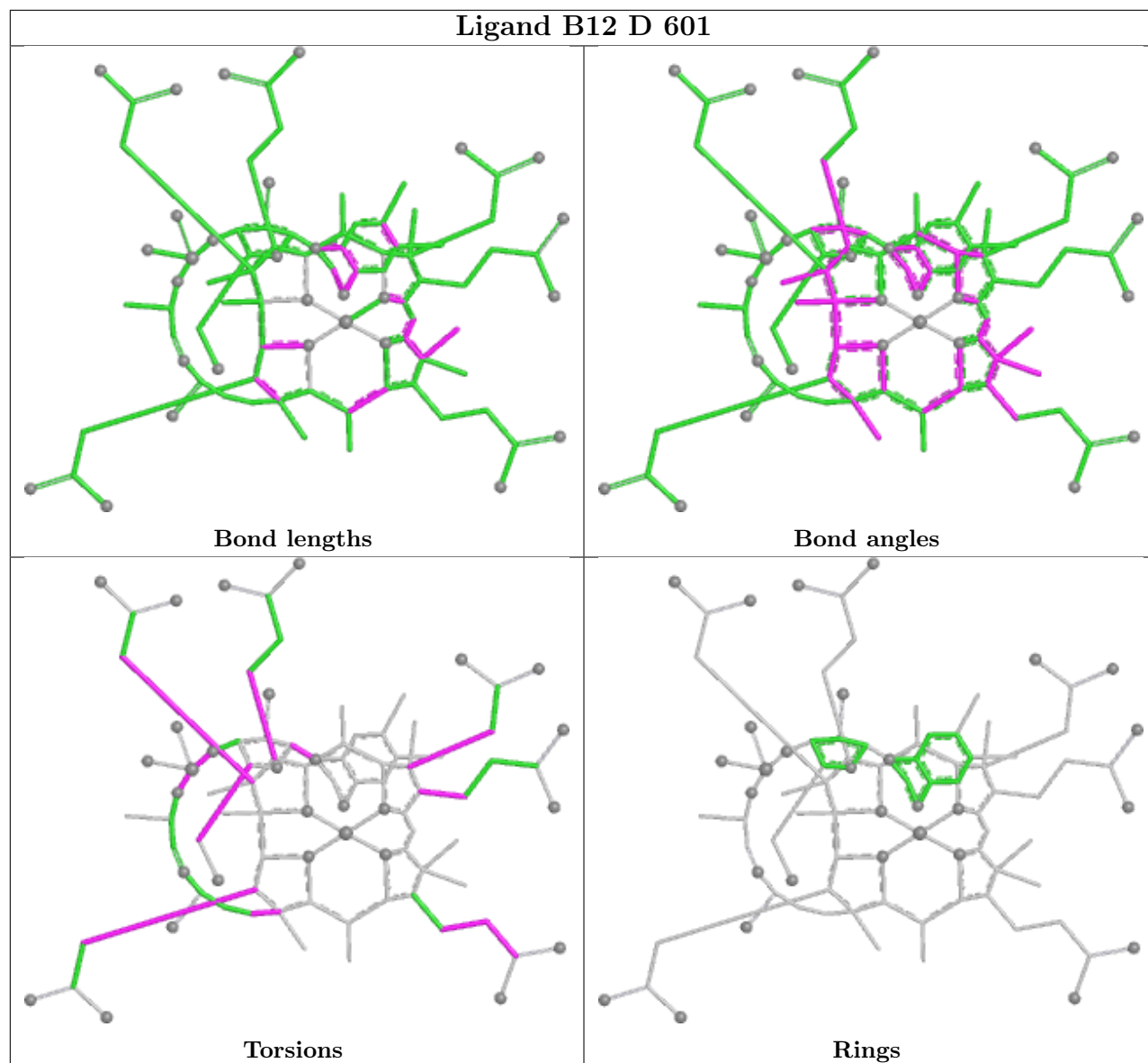
Mol	Chain	Res	Type	Atoms
4	B	601	B12	C38-C37-C7-C8
4	B	601	B12	C42-C41-C8-C9
4	B	601	B12	C14-C13-C48-C49
4	B	601	B12	C2R-C1R-N1B-C8B
4	B	601	B12	O6R-C1R-N1B-C8B
4	D	601	B12	C38-C37-C7-C6
4	D	601	B12	C38-C37-C7-C36
4	D	601	B12	C38-C37-C7-C8
4	D	601	B12	C42-C41-C8-C9
4	D	601	B12	C2P-O3-P-O5
4	D	601	B12	O6R-C4R-C5R-O8R
4	D	601	B12	C3R-C4R-C5R-O8R
4	B	601	B12	O6R-C4R-C5R-O8R
4	B	601	B12	C3R-C4R-C5R-O8R
4	B	601	B12	C13-C48-C49-C50
4	D	601	B12	C18-C17-C55-C56
4	B	601	B12	C12-C13-C48-C49
4	B	601	B12	C16-C17-C55-C56
4	D	601	B12	C16-C17-C55-C56
4	D	601	B12	C2R-C1R-N1B-C8B
4	D	601	B12	O6R-C1R-N1B-C8B
4	B	601	B12	C2-C3-C30-C31
4	D	601	B12	C2-C3-C30-C31
4	D	601	B12	C13-C48-C49-C50
4	B	601	B12	C18-C17-C55-C56
4	B	601	B12	C4-C3-C30-C31
4	D	601	B12	C4-C3-C30-C31
4	D	601	B12	C48-C49-C50-O51
4	D	601	B12	C48-C49-C50-N52
4	D	601	B12	C2P-O3-P-O4
3	A	602	2A1	O-C-CA-C3
4	B	601	B12	N59-C1P-C2P-O3
4	B	601	B12	C48-C49-C50-N52
4	D	601	B12	C17-C18-C60-C61
4	D	601	B12	C19-C18-C60-C61
4	B	601	B12	C2P-O3-P-O4
4	D	601	B12	C3R-O2-P-O5
4	B	601	B12	C25-C2-C26-C27
4	D	601	B12	C25-C2-C26-C27
4	B	601	B12	C48-C49-C50-O51

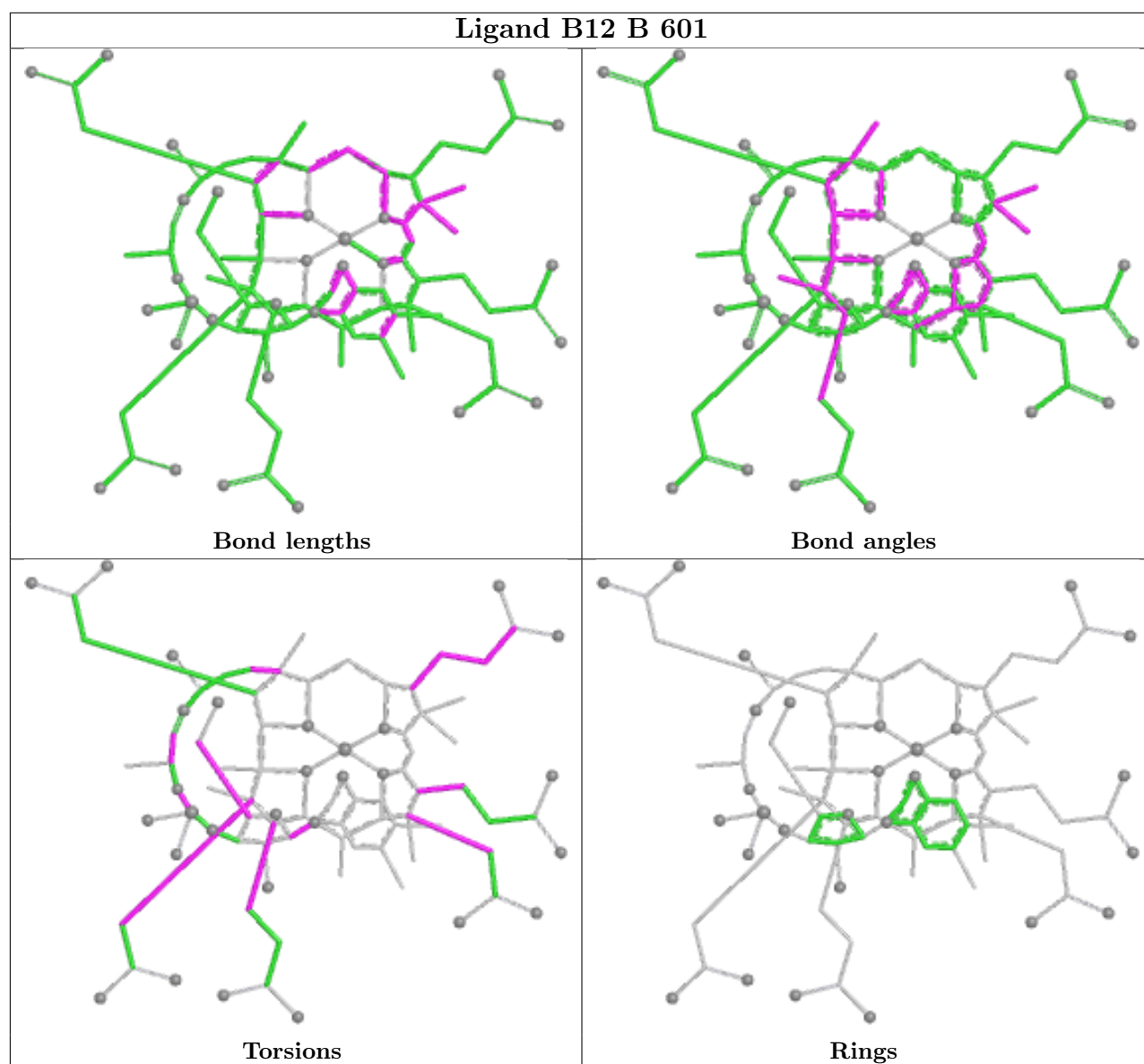
There are no ring outliers.

2 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	601	B12	11	0
4	B	601	B12	9	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	453/453 (100%)	-0.15	3 (0%) 84 85	16, 29, 46, 57	0
1	C	453/453 (100%)	-0.09	3 (0%) 84 85	12, 29, 50, 64	1 (0%)
2	B	252/263 (95%)	1.32	51 (20%) 3 2	38, 70, 99, 117	0
2	D	252/263 (95%)	2.10	124 (49%) 0 0	36, 87, 139, 154	0
All	All	1410/1432 (98%)	0.53	181 (12%) 7 7	12, 38, 108, 154	1 (0%)

All (181) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	194	LEU	8.0
2	D	192	ALA	7.1
2	D	44	ALA	6.7
2	D	153	ALA	5.9
2	D	161	VAL	5.4
2	D	190	LYS	5.3
2	B	289	SER	5.0
2	B	44	ALA	4.9
2	D	289	SER	4.9
2	D	223	ILE	4.8
2	D	145	ALA	4.7
2	D	119	GLY	4.5
2	B	191	GLN	4.4
2	D	116	LYS	4.3
2	D	196	VAL	4.2
2	D	187	ALA	4.2
2	D	216	ILE	4.1
2	D	69	GLU	4.1
2	D	107	LEU	4.0
2	D	156	VAL	4.0
2	B	107	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
2	D	123	VAL	3.9
2	D	152	LYS	3.8
2	B	288	ALA	3.8
1	A	197	ASP	3.8
2	B	179	GLU	3.8
2	D	295	ARG	3.8
2	D	250	THR	3.7
2	D	59	GLU	3.7
2	D	158	ASN	3.7
2	D	270	VAL	3.7
2	D	291	ILE	3.6
2	D	191	GLN	3.6
2	B	190	LYS	3.6
2	B	192	ALA	3.6
2	D	175	THR	3.6
2	D	148	VAL	3.6
2	D	110	VAL	3.5
2	D	267	THR	3.5
2	D	174	ILE	3.5
2	D	193	GLY	3.5
2	B	116	LYS	3.4
2	D	290	GLY	3.4
2	B	234	GLN	3.4
2	D	121	LEU	3.3
2	B	270	VAL	3.3
2	D	183	PRO	3.3
2	D	277	VAL	3.3
2	D	45	LEU	3.2
2	D	251	THR	3.2
2	D	275	VAL	3.2
2	D	288	ALA	3.2
2	B	55	TRP	3.2
2	D	248	MET	3.2
2	D	214	GLY	3.1
2	D	234	GLN	3.1
2	D	213	ILE	3.1
2	D	124	ARG	3.1
2	D	162	GLN	3.1
2	D	144	CYS	3.0
2	D	164	VAL	3.0
2	D	200	PHE	3.0
2	D	132	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
2	D	151	LEU	3.0
2	D	225	LEU	2.9
2	D	160	ASP	2.9
2	D	246	PRO	2.9
2	D	294	THR	2.9
2	B	113	GLU	2.9
2	D	129	ASP	2.9
2	D	227	GLY	2.9
2	D	150	ALA	2.9
2	D	149	GLU	2.9
2	D	178	TYR	2.8
2	B	182	LEU	2.8
2	B	193	GLY	2.8
2	B	295	ARG	2.8
2	D	243	VAL	2.8
2	D	182	LEU	2.8
2	D	273	ALA	2.8
1	A	167	ARG	2.8
2	B	120	LEU	2.7
2	D	274	ALA	2.7
2	D	111	PRO	2.7
2	B	45	LEU	2.7
2	B	47	LEU	2.7
2	B	59	GLU	2.7
2	D	146	GLU	2.7
2	D	157	ALA	2.6
2	D	280	ALA	2.6
2	B	239	SER	2.6
2	D	64	ALA	2.6
2	D	147	ALA	2.6
2	B	72	ARG	2.6
2	D	198	THR	2.6
2	D	218	GLY	2.6
2	D	199	PRO	2.6
2	D	72	ARG	2.6
2	B	111	PRO	2.6
2	B	115	VAL	2.6
2	D	244	TYR	2.6
2	D	142	ARG	2.6
1	C	197	ASP	2.6
2	B	194	LEU	2.5
2	B	101	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	188	GLY	2.5
2	B	290	GLY	2.5
2	D	181	ILE	2.5
2	D	219	ALA	2.5
2	D	222	VAL	2.5
2	D	120	LEU	2.5
2	D	68	THR	2.4
2	D	141	ARG	2.4
2	D	101	ARG	2.4
2	D	127	ILE	2.4
2	B	178	TYR	2.4
2	B	157	ALA	2.4
2	D	220	LYS	2.4
2	B	132	LEU	2.4
2	D	188	GLY	2.4
1	C	15	LYS	2.4
2	B	198	THR	2.4
2	B	223	ILE	2.4
2	D	201	PHE	2.4
2	D	207	VAL	2.4
2	D	283	MET	2.4
2	D	185	LEU	2.4
2	D	264	GLN	2.4
2	D	179	GLU	2.4
2	B	249	ALA	2.3
2	D	117	ALA	2.3
2	B	161	VAL	2.3
2	D	165	ILE	2.3
2	D	70	LEU	2.3
2	D	217	LEU	2.3
2	B	187	ALA	2.3
2	B	124	ARG	2.3
2	B	264	GLN	2.3
2	D	189	LEU	2.2
2	D	202	VAL	2.3
2	B	197	GLY	2.2
2	D	259	ILE	2.2
2	B	185	LEU	2.2
2	B	221	VAL	2.2
2	D	58	VAL	2.2
2	D	279	LEU	2.2
2	D	155	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	197	GLY	2.2
2	D	122	GLU	2.2
2	D	242	ALA	2.2
1	A	198	ASP	2.2
2	D	46	ASP	2.2
2	D	186	MET	2.2
2	D	52	ALA	2.2
2	D	245	SER	2.2
2	B	93	LEU	2.2
2	D	268	PRO	2.2
2	D	113	GLU	2.2
2	D	171	THR	2.2
1	C	167	ARG	2.1
2	D	204	TYR	2.1
2	D	282	ARG	2.1
2	D	93	LEU	2.1
2	B	265	GLY	2.1
2	B	150	ALA	2.1
2	D	284	LEU	2.1
2	B	123	VAL	2.1
2	B	174	ILE	2.1
2	D	143	LEU	2.1
2	D	247	ARG	2.1
2	D	128	SER	2.1
2	D	195	LYS	2.1
2	B	183	PRO	2.1
2	D	73	SER	2.0
2	D	135	THR	2.0
2	D	256	ARG	2.0
2	B	69	GLU	2.0
2	D	180	GLU	2.0
2	B	65	ASP	2.0
2	B	284	LEU	2.0
2	B	56	ILE	2.0

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 oligosaccharides in this entry.

6.4 Ligands

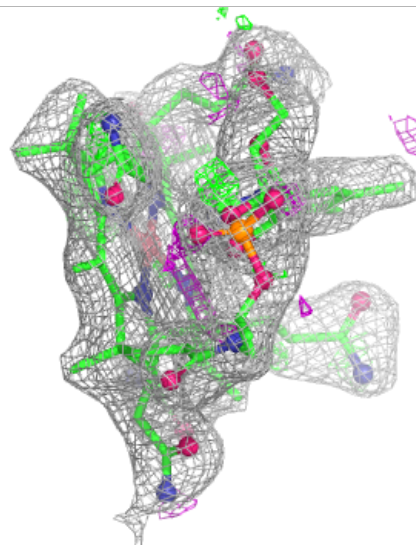
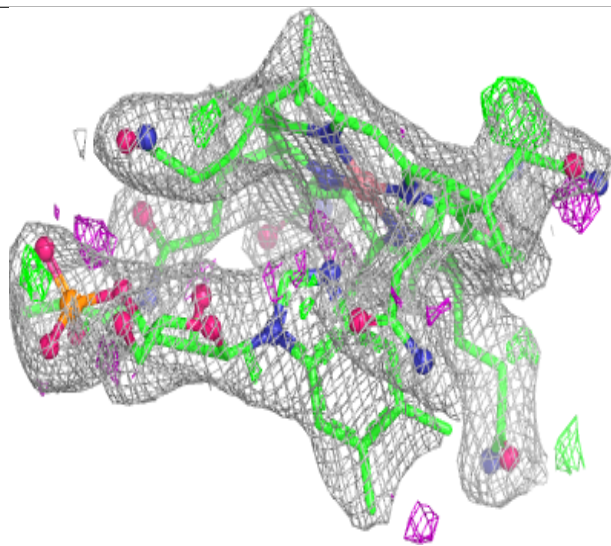
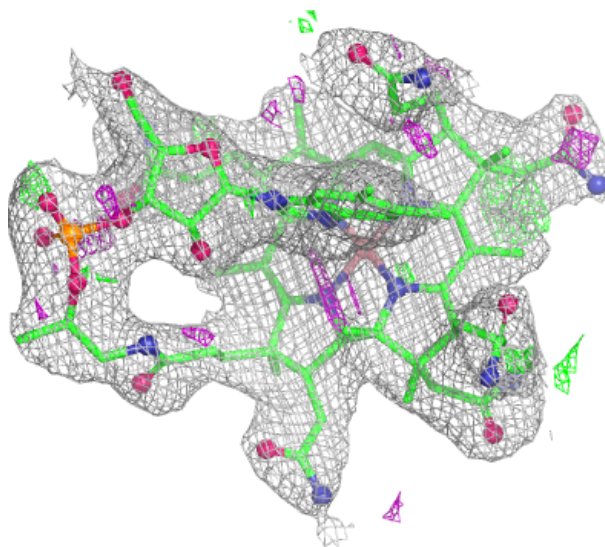
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NA	C	454	1/1	0.92	0.52	66,66,66,66	0
4	B12	D	601	91/91	0.93	0.13	35,45,58,60	0
3	2A1	A	602	5/5	0.94	0.11	31,31,36,36	0
4	B12	B	601	91/91	0.95	0.12	28,38,47,51	0
3	2A1	C	602	5/5	0.96	0.09	23,29,31,31	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.

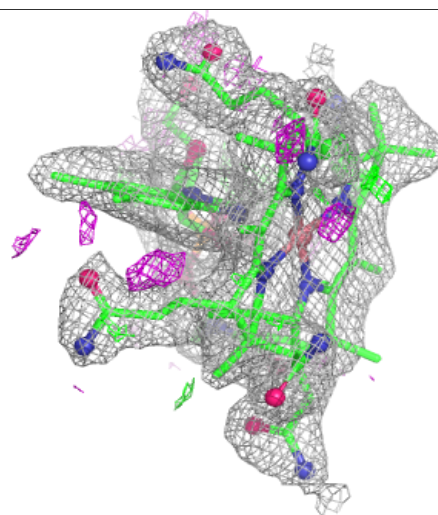
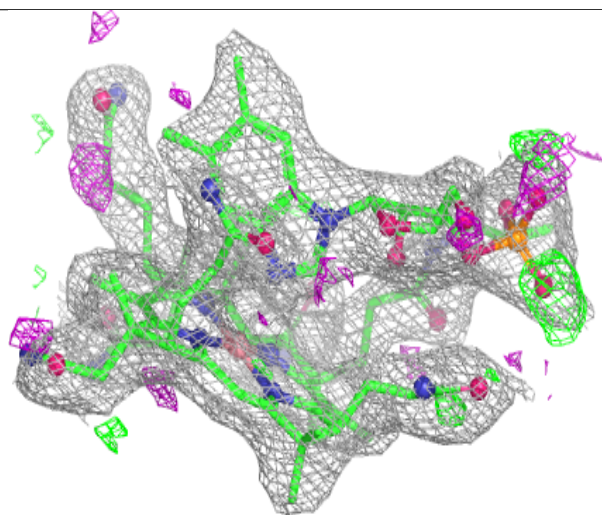
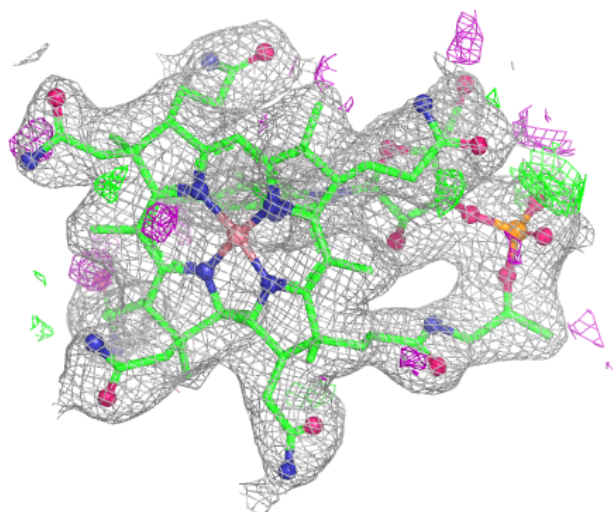
Electron density around B12 D 601:

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



Electron density around B12 B 601:

$2mF_o-DF_c$ (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.