



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:09 PM UTC

PDB ID : 7XRN / pdb_00007xrn
Title : Ethanolamine ammonia-lyase complexed with AdoMeCbl in the presence of substrate
Authors : Shibata, N.; Toraya, T.
Deposited on : 2022-05-10
Resolution : 2.07 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

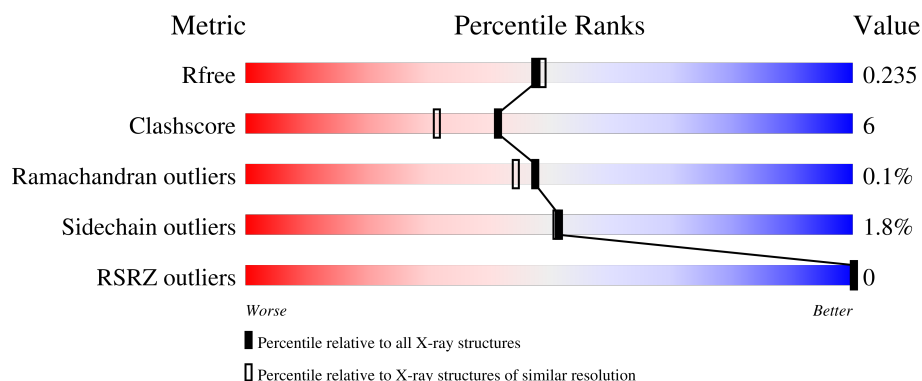
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.07 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	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

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	 89% 10%
1	C	453	 88% 12%
2	B	263	 79% 17% .
2	D	263	 75% 20% . .

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11835 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 large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	453	Total	C	N	O	S	0	2	0
			3475	2177	595	681	22			
1	C	453	Total	C	N	O	S	0	1	0
			3467	2172	593	680	22			

- Molecule 2 is a protein called Ethanolamine ammonia-lyase small subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	252	Total	C	N	O	S	0	2	0
			1930	1205	351	364	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:

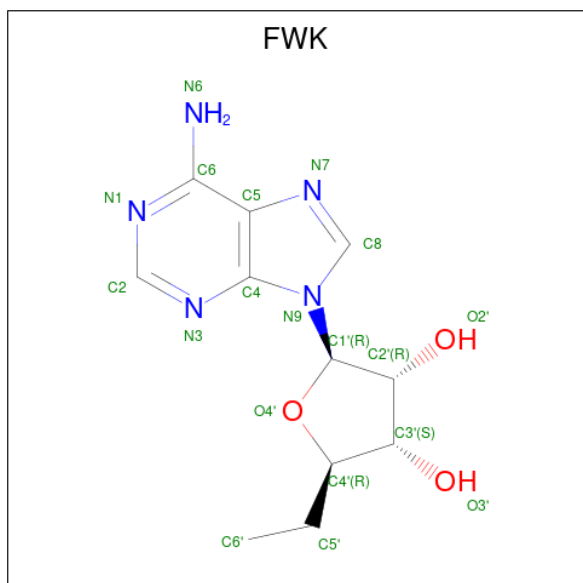
Chain	Residue	Modelled	Actual	Comment	Reference
B	33	MET	-	initiating methionine	UNP P19636
B	34	ASP	-	expression tag	UNP P19636
B	35	GLN	-	expression tag	UNP P19636
B	36	SER	-	expression tag	UNP P19636
B	37	SER	-	expression tag	UNP P19636
B	38	HIS	-	expression tag	UNP P19636
B	39	HIS	-	expression tag	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	-	initiating methionine	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 (2 {R},3 {R},4 {S},5 {R})-2-(6-aminopurin-9-yl)-5-ethyl-oxolane-3,4-diol (CCD ID: FWK) (formula: C₁₁H₁₅N₅O₃).



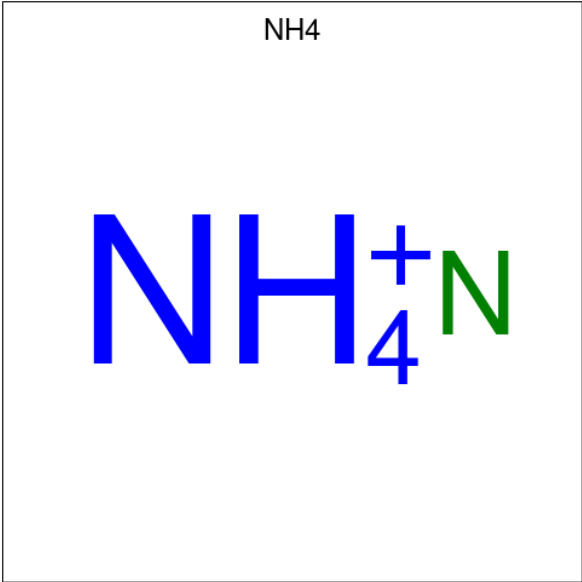
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	1
			36	20	10	6		
3	C	1	Total	C	N	O	0	0
			18	10	5	3		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



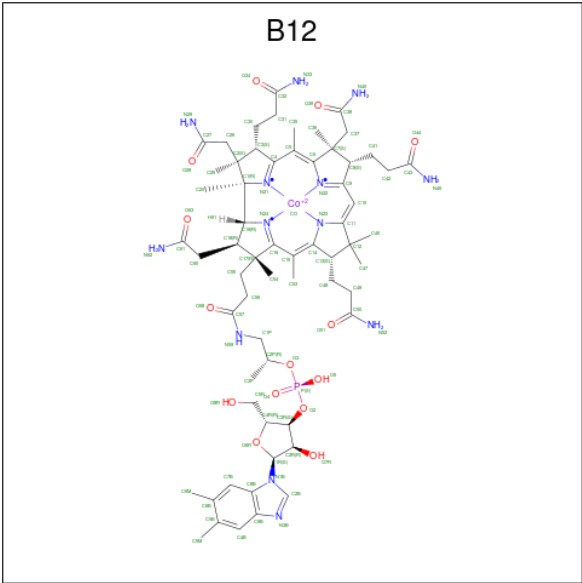
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is AMMONIUM ION (CCD ID: NH4) (formula: H₄N).



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

- Molecule 6 is COBALAMIN (CCD ID: B12) (formula: C₆₂H₈₉CoN₁₃O₁₄P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C Co N O P 95 64 1 14 15 1	0	1
6	D	1	Total C Co N O P 91 62 1 13 14 1	0	0

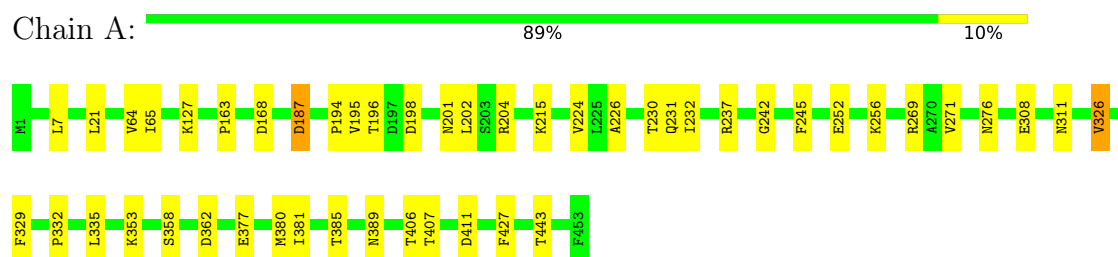
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	294	Total 294	O 294	0	0
7	B	101	Total 101	O 101	0	0
7	C	283	Total 283	O 283	0	0
7	D	91	Total 91	O 91	0	0

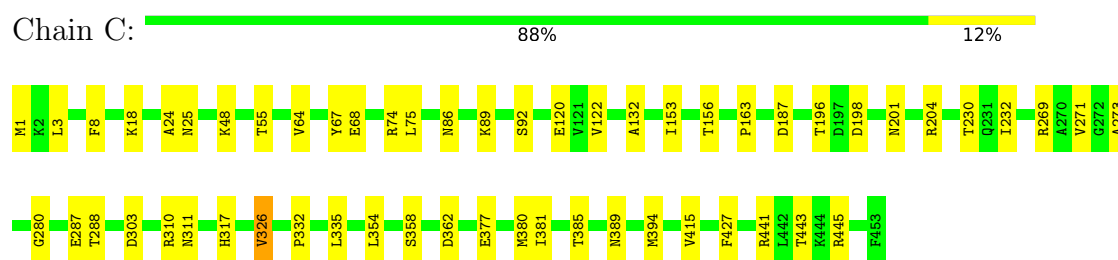
3 Residue-property plots

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.

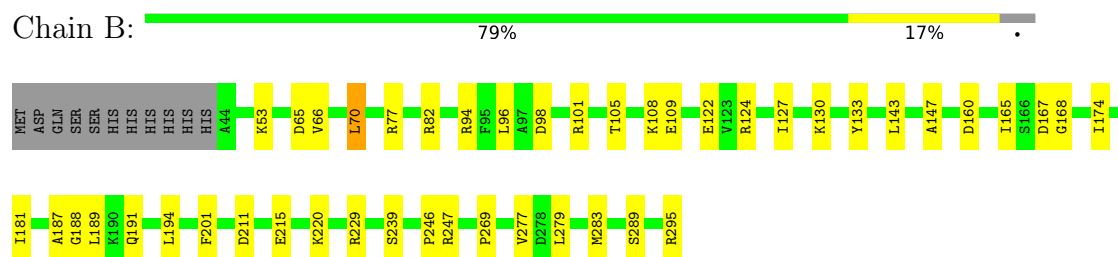
- Molecule 1: Ethanolamine ammonia-lyase large subunit



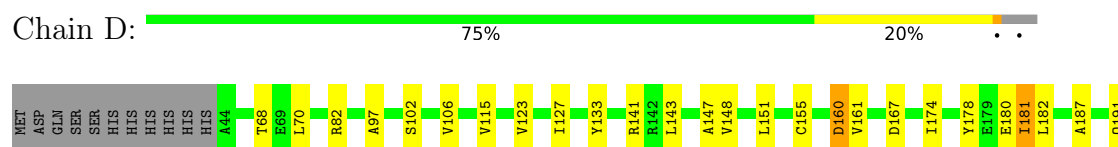
- Molecule 1: Ethanolamine ammonia-lyase large subunit



- Molecule 2: Ethanolamine ammonia-lyase small subunit



- Molecule 2: Ethanolamine ammonia-lyase small subunit





4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	242.38Å 242.38Å 76.59Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.16 – 2.07 48.16 – 2.07	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.16-2.07) 98.6 (48.16-2.07)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.07Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.214 , 0.241 (Not available) , 0.235	Depositor DCC
R_{free} test set	7806 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	27.4	Xtriage
Anisotropy	0.238	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 33.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.18$	Xtriage
Estimated twinning fraction	0.110 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11835	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.13% 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: GOL, FWK, B12, NH4

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	0.08	0/3535	0.25	0/4787
1	C	0.08	0/3524	0.24	0/4772
2	B	0.10	0/1960	0.29	0/2655
2	D	0.09	0/1943	0.26	0/2633
All	All	0.09	0/10962	0.26	0/14847

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	3475	0	3433	32	0
1	C	3467	0	3424	33	0
2	B	1930	0	1990	26	0
2	D	1916	0	1973	38	0
3	A	36	0	0	2	0
3	C	18	0	0	1	0
4	A	12	0	16	0	0
4	B	6	0	8	0	0
4	C	18	0	24	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	B	95	0	8	3	0
6	D	91	0	88	9	0
7	A	294	0	0	3	0
7	B	101	0	0	2	0
7	C	283	0	0	6	0
7	D	91	0	0	1	0
All	All	11835	0	10964	137	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 6.

All (137) 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:160:ASP:HB2	2:B:194:LEU:HD13	1.58	0.85
2:D:180:GLU:HG2	2:D:270:VAL:HG23	1.73	0.69
1:A:237:ARG:NH1	7:A:601:HOH:O	2.26	0.68
1:A:201:ASN:OD1	1:A:204:ARG:NH2	2.27	0.66
2:D:160:ASP:HB2	2:D:194:LEU:HD12	1.80	0.63
1:A:232:ILE:HG23	1:A:271:VAL:HG21	1.82	0.62
1:A:252:GLU:HG2	1:A:256:LYS:HE3	1.84	0.59
1:C:280:GLY:O	7:C:601:HOH:O	2.17	0.58
1:A:21:LEU:O	1:A:127:LYS:NZ	2.37	0.58
1:C:287:GLU:OE1	3:C:501:FWK:O2'	2.22	0.58
1:A:242:GLY:O	1:A:276:ASN:ND2	2.36	0.57
2:D:141:ARG:HG2	2:D:208:LYS:HB2	1.87	0.57
2:B:165:ILE:HD11	2:B:174:ILE:HD12	1.86	0.57
1:C:273:ALA:HA	4:C:503:GOL:H12	1.85	0.57
1:A:269:ARG:NH1	7:A:611:HOH:O	2.37	0.56
2:B:124:ARG:HH11	2:B:124:ARG:HG3	1.69	0.56
2:D:127:ILE:HG21	2:D:133:TYR:HB2	1.87	0.56
2:B:283:MET:HE3	2:B:289:SER:HB3	1.87	0.56
2:B:122:GLU:HG3	2:B:201:PHE:HD2	1.71	0.55
2:D:212:GLN:HA	2:D:248:MET:HE2	1.87	0.55
1:A:215:LYS:NZ	7:A:612:HOH:O	2.37	0.55
1:C:326:VAL:HA	1:C:362:ASP:HB3	1.88	0.55
2:D:211:ASP:HA	2:D:246:PRO:HB2	1.88	0.55
2:D:238:LEU:HB3	2:D:262:ILE:HB	1.87	0.55
1:C:122:VAL:HG13	1:C:354:LEU:HD23	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:441:ARG:NH2	7:C:620:HOH:O	2.40	0.55
2:D:279:LEU:O	2:D:283:MET:HG3	2.07	0.55
1:A:245:PHE:HZ	3:A:501[A]:FWK:O2'	1.90	0.54
2:B:187:ALA:O	2:B:191:GLN:HG3	2.08	0.54
2:D:178:TYR:CZ	2:D:182:LEU:HG	2.42	0.54
6:D:601:B12:H552	6:D:601:B12:H531	1.90	0.53
1:C:288:THR:HB	1:C:311:ASN:HD22	1.73	0.53
2:D:195:LYS:NZ	7:D:704:HOH:O	2.40	0.53
1:A:187:ASP:OD1	1:A:187:ASP:N	2.37	0.53
1:A:196:THR:OG1	1:A:201:ASN:ND2	2.37	0.53
6:D:601:B12:H601	6:D:601:B12:H261	1.91	0.52
4:C:503:GOL:O2	7:C:602:HOH:O	2.19	0.51
1:C:86:ASN:HA	1:C:89:LYS:HD3	1.92	0.51
1:C:232:ILE:HG23	1:C:271:VAL:HG21	1.92	0.51
1:A:231:GLN:NE2	1:A:245:PHE:O	2.42	0.51
1:C:1:MET:HE3	1:C:3:LEU:HD11	1.93	0.51
1:C:269:ARG:NH2	7:C:625:HOH:O	2.43	0.51
2:B:279:LEU:O	2:B:283:MET:HG3	2.11	0.50
2:D:187:ALA:O	2:D:191:GLN:HG3	2.12	0.50
1:C:443:THR:O	2:D:82:ARG:NH2	2.44	0.50
2:B:211:ASP:HA	2:B:246:PRO:HB2	1.94	0.49
1:C:25:ASN:ND2	1:C:303:ASP:OD2	2.45	0.49
6:D:601:B12:C4	6:D:601:B12:H4B	2.42	0.49
1:C:55:THR:HA	1:C:92:SER:HA	1.94	0.49
2:D:187:ALA:HB1	2:D:191:GLN:HE21	1.78	0.49
2:B:143:LEU:HB3	2:B:147:ALA:HB3	1.93	0.49
1:A:202:LEU:HD22	1:A:224:VAL:HG11	1.93	0.49
1:C:445:ARG:NH2	7:C:628:HOH:O	2.45	0.49
2:D:102:SER:OG	2:D:231:GLY:O	2.30	0.49
2:B:77:ARG:NH2	2:B:98:ASP:OD2	2.32	0.49
2:D:155:CYS:SG	2:D:198:THR:OG1	2.70	0.48
2:D:148:VAL:HG13	2:D:216:ILE:HD13	1.94	0.48
2:D:160:ASP:HA	2:D:220:LYS:HB2	1.95	0.48
1:C:377:GLU:HA	1:C:380:MET:SD	2.54	0.48
2:D:283:MET:HE3	2:D:289:SER:HB3	1.96	0.48
2:B:189:LEU:HG	2:B:277:VAL:HG22	1.95	0.47
1:A:326:VAL:HA	1:A:362:ASP:HB3	1.96	0.47
2:D:127:ILE:HD12	2:D:133:TYR:HA	1.96	0.47
1:C:358:SER:OG	1:C:389:ASN:ND2	2.40	0.47
2:D:151:LEU:HB3	2:D:217:LEU:HD21	1.96	0.47
2:D:106:VAL:HG22	2:D:230:PRO:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:160:ASP:HB2	2:D:194:LEU:CD1	2.45	0.47
2:B:127:ILE:HG21	2:B:133:TYR:HB2	1.97	0.46
1:C:75:LEU:HD11	1:C:317:HIS:CG	2.50	0.46
1:A:358:SER:OG	1:A:389:ASN:ND2	2.46	0.46
1:A:406:THR:OG1	1:A:407:THR:N	2.48	0.46
2:B:105:THR:HA	2:B:108:LYS:HG2	1.97	0.46
2:B:130:LYS:NZ	7:B:709:HOH:O	2.39	0.46
2:B:215:GLU:HG2	2:B:247:ARG:HE	1.79	0.45
1:C:24:ALA:O	1:C:48:LYS:NZ	2.41	0.45
1:C:187:ASP:HB3	1:C:427:PHE:CG	2.51	0.45
1:C:198:ASP:OD2	1:C:201:ASN:HB2	2.16	0.45
6:D:601:B12:H2B	6:D:601:B12:H482	1.98	0.45
6:D:601:B12:H351	6:D:601:B12:H372	1.98	0.45
2:D:143:LEU:HB3	2:D:147:ALA:HB3	1.99	0.45
2:B:160:ASP:HA	2:B:220:LYS:HB2	1.98	0.45
2:B:188:GLY:HA2	2:B:191:GLN:HE21	1.82	0.45
1:C:120:GLU:OE2	1:C:310:ARG:NH1	2.46	0.45
1:C:153:ILE:O	1:C:156:THR:OG1	2.31	0.45
2:D:160:ASP:HB3	2:D:220:LYS:HE2	1.99	0.45
2:D:180:GLU:HB3	2:D:269:PRO:HB2	1.98	0.45
6:D:601:B12:H473	6:D:601:B12:H481	1.77	0.45
1:A:237:ARG:HG3	1:A:237:ARG:HH11	1.83	0.44
2:B:130:LYS:HG3	7:B:709:HOH:O	2.17	0.44
1:A:64:VAL:HG23	1:A:65:ILE:HG13	1.98	0.44
1:C:380:MET:HE3	1:C:415:VAL:HG23	1.99	0.44
1:C:394:MET:HE2	1:C:394:MET:HB3	1.83	0.44
2:D:143:LEU:HD12	2:D:212:GLN:HG2	2.00	0.44
1:C:18:LYS:HD3	1:C:64:VAL:HG12	2.01	0.43
1:A:377:GLU:HA	1:A:380:MET:SD	2.58	0.43
2:D:216:ILE:HG22	2:D:217:LEU:HD23	1.98	0.43
2:D:281:LYS:O	2:D:285:GLU:HG3	2.18	0.43
6:D:601:B12:H301	6:D:601:B12:H253	1.67	0.43
2:D:161:VAL:HB	2:D:194:LEU:HD11	2.00	0.43
1:A:353:LYS:HD3	1:A:353:LYS:HA	1.87	0.43
2:B:181:ILE:HB	2:B:269:PRO:HB3	2.01	0.43
1:A:326:VAL:HG12	1:A:329:PHE:HB2	2.00	0.42
2:B:66:VAL:O	2:B:70:LEU:HD22	2.19	0.42
2:D:155:CYS:HG	2:D:198:THR:HG1	1.66	0.42
2:D:228:GLU:HA	6:D:601:B12:H1P2	2.02	0.42
1:A:332:PRO:HA	1:A:335:LEU:O	2.19	0.42
2:B:53:LYS:HG2	2:B:94:ARG:NH1	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:381:ILE:O	1:C:385:THR:HG23	2.19	0.42
2:D:167:ASP:N	2:D:167:ASP:OD1	2.52	0.42
2:D:181:ILE:HB	2:D:269:PRO:HB3	2.02	0.42
1:A:377:GLU:HB3	1:C:132:ALA:HB2	2.01	0.42
1:A:380:MET:SD	1:A:411:ASP:HB3	2.60	0.42
1:A:381:ILE:O	1:A:385:THR:HG23	2.19	0.42
2:B:101:ARG:HD3	1:C:8:PHE:CE2	2.54	0.42
1:C:68:GLU:H	1:C:68:GLU:CD	2.27	0.42
2:D:160:ASP:H	2:D:195:LYS:HB3	1.84	0.42
1:A:308:GLU:O	1:A:311:ASN:HB2	2.20	0.42
2:D:123:VAL:O	2:D:202:VAL:HA	2.19	0.42
2:D:174:ILE:O	2:D:178:TYR:HB2	2.20	0.42
2:B:65:ASP:OD1	2:B:65:ASP:N	2.52	0.41
6:D:601:B12:H562	6:D:601:B12:H18	1.91	0.41
1:A:198:ASP:OD1	1:A:201:ASN:HB2	2.19	0.41
1:A:443:THR:O	2:B:82:ARG:NH2	2.54	0.41
1:A:7:LEU:HD11	2:D:97:ALA:HB1	2.02	0.41
1:A:187:ASP:HB3	1:A:427:PHE:CG	2.56	0.41
1:A:194:PRO:HG3	1:A:226:ALA:HB2	2.02	0.41
2:B:165:ILE:O	2:B:201:PHE:HA	2.21	0.41
1:A:168:ASP:CG	1:A:195:VAL:HG12	2.46	0.41
1:C:332:PRO:HA	1:C:335:LEU:O	2.21	0.41
2:B:167:ASP:OD1	2:B:168:GLY:N	2.54	0.40
1:C:67:TYR:CE2	1:C:74:ARG:HA	2.55	0.40
2:D:143:LEU:HB3	2:D:147:ALA:CB	2.51	0.40
1:C:204:ARG:NH1	7:C:639:HOH:O	2.52	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	453/453 (100%)	432 (95%)	20 (4%)	1 (0%)	43	38
1	C	452/453 (100%)	428 (95%)	23 (5%)	1 (0%)	43	38
2	B	252/263 (96%)	243 (96%)	9 (4%)	0	100	100
2	D	250/263 (95%)	245 (98%)	5 (2%)	0	100	100
All	All	1407/1432 (98%)	1348 (96%)	57 (4%)	2 (0%)	48	44

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	163	PRO
1	C	163	PRO

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	372/370 (100%)	369 (99%)	3 (1%)	73	77
1	C	371/370 (100%)	368 (99%)	3 (1%)	73	77
2	B	208/217 (96%)	202 (97%)	6 (3%)	37	33
2	D	206/217 (95%)	197 (96%)	9 (4%)	25	19
All	All	1157/1174 (99%)	1136 (98%)	21 (2%)	51	51

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	187	ASP
1	A	230	THR
1	A	326	VAL
2	B	70	LEU
2	B	96	LEU
2	B	109	GLU
2	B	229	ARG
2	B	239	SER
2	B	295	ARG

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Mol	Chain	Res	Type
1	C	196	THR
1	C	230	THR
1	C	326	VAL
2	D	68	THR
2	D	70	LEU
2	D	115	VAL
2	D	160	ASP
2	D	181	ILE
2	D	229	ARG
2	D	236	GLU
2	D	239	SER
2	D	271	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	ASN
1	A	276	ASN
2	B	154	GLN
2	B	191	GLN
2	B	261	ASN
2	B	264	GLN
1	C	10	ASN
1	C	13	GLN
1	C	87	GLN
1	C	201	ASN
2	D	60	ASN
2	D	177	ASN
2	D	191	GLN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 2 are modelled with single atom - leaving 12 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	FWK	A	501[B]	-	20,20,21	1.57	4 (20%)	28,30,31	2.26	11 (39%)
6	B12	B	601[B]	-	94,101,101	1.44	12 (12%)	149,166,166	1.42	24 (16%)
4	GOL	A	502	-	5,5,5	0.94	0	5,5,5	1.06	0
4	GOL	C	502	-	5,5,5	0.94	0	5,5,5	1.09	0
3	FWK	A	501[A]	-	20,20,21	1.58	4 (20%)	28,30,31	2.60	11 (39%)
3	FWK	C	501	-	20,20,21	1.60	4 (20%)	28,30,31	2.44	8 (28%)
4	GOL	C	504	-	5,5,5	0.95	0	5,5,5	1.07	0
6	B12	B	601[A]	-	94,101,101	1.44	12 (12%)	149,166,166	1.41	24 (16%)
4	GOL	A	503	-	5,5,5	0.92	0	5,5,5	1.06	0
4	GOL	C	503	-	5,5,5	0.98	0	5,5,5	1.08	0
4	GOL	B	602	-	5,5,5	0.93	0	5,5,5	1.09	0
6	B12	D	601	-	94,101,101	1.44	13 (13%)	149,166,166	1.40	23 (15%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FWK	A	501[B]	-	-	0/4/20/22	0/3/3/3
6	B12	B	601[B]	-	-	16/56/223/223	0/3/11/11
4	GOL	A	502	-	-	2/4/4/4	-
4	GOL	C	502	-	-	2/4/4/4	-
3	FWK	A	501[A]	-	-	2/4/20/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FWK	C	501	-	-	2/4/20/22	0/3/3/3
4	GOL	C	504	-	-	2/4/4/4	-
6	B12	B	601[A]	-	-	16/56/223/223	0/3/11/11
4	GOL	A	503	-	-	2/4/4/4	-
4	GOL	C	503	-	-	4/4/4/4	-
4	GOL	B	602	-	-	0/4/4/4	-
6	B12	D	601	-	-	16/56/223/223	0/3/11/11

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	601[A]	B12	C8B-C9B	5.36	1.49	1.40
6	B	601[B]	B12	C8B-C9B	5.36	1.49	1.40
6	D	601	B12	C8B-C9B	5.33	1.49	1.40
6	B	601[A]	B12	C14-N23	-5.13	1.28	1.35
6	B	601[B]	B12	C14-N23	-5.13	1.28	1.35
6	D	601	B12	C14-N23	-5.04	1.28	1.35
3	C	501	FWK	C5-C4	4.94	1.47	1.39
3	A	501[A]	FWK	C5-C4	4.78	1.47	1.39
3	A	501[B]	FWK	C5-C4	4.66	1.47	1.39
6	D	601	B12	C11-N23	4.18	1.44	1.36
6	B	601[A]	B12	C11-N23	4.10	1.44	1.36
6	B	601[B]	B12	C11-N23	4.10	1.44	1.36
6	B	601[A]	B12	C16-C15	-3.81	1.33	1.44
6	B	601[B]	B12	C16-C15	-3.81	1.33	1.44
6	D	601	B12	C16-C15	-3.80	1.33	1.44
6	D	601	B12	C19-N24	-3.68	1.44	1.49
6	B	601[A]	B12	C19-N24	-3.66	1.44	1.49
6	B	601[B]	B12	C19-N24	-3.66	1.44	1.49
6	B	601[A]	B12	C6B-C5B	3.48	1.49	1.40
6	B	601[B]	B12	C6B-C5B	3.48	1.49	1.40
6	D	601	B12	C6B-C5B	3.44	1.49	1.40
6	B	601[A]	B12	C9B-N3B	-3.23	1.33	1.39
6	B	601[B]	B12	C9B-N3B	-3.23	1.33	1.39
6	D	601	B12	C9B-N3B	-3.19	1.33	1.39
3	A	501[A]	FWK	C5-C6	2.86	1.49	1.41
3	C	501	FWK	C5-C6	2.72	1.48	1.41
6	B	601[A]	B12	C14-C15	2.72	1.50	1.38
6	B	601[B]	B12	C14-C15	2.72	1.50	1.38
3	A	501[B]	FWK	C5-C6	2.72	1.48	1.41
6	D	601	B12	C14-C15	2.71	1.50	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	601[A]	B12	C8B-N1B	-2.54	1.34	1.39
6	B	601[B]	B12	C8B-N1B	-2.54	1.34	1.39
6	D	601	B12	C8B-N1B	-2.53	1.34	1.39
6	D	601	B12	C10-C9	2.49	1.46	1.39
6	B	601[A]	B12	C10-C9	2.44	1.46	1.39
6	B	601[B]	B12	C10-C9	2.44	1.46	1.39
3	A	501[B]	FWK	C8-N7	2.37	1.36	1.31
3	C	501	FWK	C5-N7	-2.35	1.34	1.39
3	A	501[A]	FWK	C8-N7	2.34	1.36	1.31
6	D	601	B12	CO-N22	-2.23	1.85	1.96
3	A	501[B]	FWK	C5-N7	-2.19	1.35	1.39
6	D	601	B12	C1-C19	-2.18	1.50	1.55
6	B	601[A]	B12	CO-N22	-2.18	1.86	1.96
6	B	601[B]	B12	CO-N22	-2.18	1.86	1.96
3	C	501	FWK	C8-N7	2.18	1.35	1.31
6	D	601	B12	C1-C2	-2.09	1.54	1.58
3	A	501[A]	FWK	C5-N7	-2.08	1.35	1.39
6	B	601[A]	B12	C1-C19	-2.01	1.50	1.55
6	B	601[B]	B12	C1-C19	-2.01	1.50	1.55

All (101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501[A]	FWK	C5-C4-N3	-6.86	117.27	126.72
3	C	501	FWK	C5-C4-N3	-6.80	117.35	126.72
3	A	501[B]	FWK	C5-C4-N3	-5.75	118.80	126.72
3	A	501[A]	FWK	N3-C4-N9	5.66	136.79	127.17
6	B	601[A]	B12	C8B-C9B-N3B	-5.60	103.95	110.00
6	B	601[B]	B12	C8B-C9B-N3B	-5.60	103.95	110.00
6	D	601	B12	C8B-C9B-N3B	-5.58	103.96	110.00
3	C	501	FWK	N3-C4-N9	5.48	136.49	127.17
6	D	601	B12	C9B-N3B-C2B	5.16	110.73	104.40
3	A	501[A]	FWK	C5'-C4'-C3'	-5.06	110.39	115.70
6	B	601[A]	B12	C9B-N3B-C2B	4.98	110.51	104.40
6	B	601[B]	B12	C9B-N3B-C2B	4.98	110.51	104.40
3	A	501[B]	FWK	N3-C4-N9	4.61	135.00	127.17
3	C	501	FWK	C5'-C4'-C3'	-4.47	111.00	115.70
6	B	601[A]	B12	C9B-C8B-N1B	4.44	107.27	105.30
6	B	601[B]	B12	C9B-C8B-N1B	4.44	107.27	105.30
3	A	501[A]	FWK	C2-N3-C4	4.37	122.50	111.83
6	D	601	B12	C9B-C8B-N1B	4.00	107.08	105.30
3	C	501	FWK	C2-N3-C4	3.97	121.53	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501[B]	FWK	C2-N3-C4	3.69	120.85	111.83
6	B	601[A]	B12	C17-C16-C15	3.52	131.82	126.26
6	B	601[B]	B12	C17-C16-C15	3.52	131.82	126.26
6	D	601	B12	C17-C16-C15	3.50	131.80	126.26
3	A	501[A]	FWK	N1-C2-N3	-3.46	123.34	128.58
3	A	501[B]	FWK	C4-C5-N7	-3.42	106.67	110.58
3	A	501[B]	FWK	C5'-C4'-C3'	-3.37	112.16	115.70
6	B	601[A]	B12	C9-C10-C11	-3.35	121.18	125.97
6	B	601[B]	B12	C9-C10-C11	-3.35	121.18	125.97
6	D	601	B12	C9-C10-C11	-3.33	121.22	125.97
3	C	501	FWK	C4-C5-N7	-3.31	106.80	110.58
3	A	501[B]	FWK	N1-C2-N3	-3.27	123.64	128.58
6	B	601[A]	B12	C13-C14-N23	3.24	113.48	109.09
6	B	601[B]	B12	C13-C14-N23	3.24	113.48	109.09
3	A	501[A]	FWK	C4-C5-N7	-3.24	106.88	110.58
6	D	601	B12	C13-C14-N23	3.22	113.46	109.09
6	D	601	B12	C2P-C1P-N59	-3.20	108.22	112.92
6	B	601[A]	B12	C2P-C1P-N59	-3.13	108.32	112.92
6	B	601[B]	B12	C2P-C1P-N59	-3.13	108.32	112.92
6	D	601	B12	C4B-C9B-N3B	3.12	135.75	130.51
6	B	601[A]	B12	C4B-C9B-N3B	3.07	135.68	130.51
6	B	601[B]	B12	C4B-C9B-N3B	3.07	135.68	130.51
3	C	501	FWK	N1-C2-N3	-3.02	124.02	128.58
6	B	601[B]	B12	C26-C2-C3	2.82	112.34	107.42
6	B	601[A]	B12	C26-C2-C3	2.82	112.33	107.42
3	A	501[B]	FWK	C4-N9-C8	2.81	108.68	105.74
6	D	601	B12	N1B-C2B-N3B	-2.79	109.97	113.94
6	D	601	B12	C13-C14-C15	-2.77	120.10	124.32
6	D	601	B12	C20-C1-N21	2.67	114.67	110.26
6	B	601[A]	B12	C30-C3-C2	-2.58	113.31	119.00
6	B	601[B]	B12	C30-C3-C2	-2.58	113.31	119.00
6	B	601[A]	B12	C13-C14-C15	-2.58	120.40	124.32
6	B	601[B]	B12	C13-C14-C15	-2.58	120.40	124.32
3	A	501[A]	FWK	O4'-C1'-N9	2.58	113.03	108.09
3	A	501[B]	FWK	C5-N7-C8	2.52	107.42	103.45
6	B	601[A]	B12	N1B-C2B-N3B	-2.51	110.37	113.94
6	B	601[B]	B12	N1B-C2B-N3B	-2.51	110.37	113.94
6	D	601	B12	C30-C3-C2	-2.50	113.48	119.00
3	A	501[A]	FWK	C3'-C2'-C1'	2.50	106.19	101.46
3	A	501[A]	FWK	C4-N9-C8	2.48	108.35	105.74
3	A	501[A]	FWK	C5-N7-C8	2.48	107.35	103.45
6	B	601[A]	B12	C7-C8-C9	2.47	104.02	100.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	601[B]	B12	C7-C8-C9	2.47	104.02	100.89
3	C	501	FWK	C5-N7-C8	2.46	107.31	103.45
3	C	501	FWK	C3'-C2'-C1'	2.43	106.06	101.46
6	B	601[A]	B12	C41-C8-C9	2.43	115.42	111.19
6	B	601[B]	B12	C41-C8-C9	2.43	115.42	111.19
6	D	601	B12	C19-N24-C16	2.41	109.92	107.29
6	D	601	B12	C17-C16-N24	-2.39	107.52	111.17
6	D	601	B12	C54-C17-C18	-2.38	109.58	112.99
6	B	601[A]	B12	C19-N24-C16	2.36	109.88	107.29
6	B	601[B]	B12	C19-N24-C16	2.36	109.88	107.29
6	B	601[A]	B12	C8-C9-N22	2.36	115.43	110.77
6	B	601[B]	B12	C8-C9-N22	2.36	115.43	110.77
6	B	601[A]	B12	C17-C16-N24	-2.35	107.58	111.17
6	B	601[B]	B12	C17-C16-N24	-2.35	107.58	111.17
6	D	601	B12	C7-C8-C9	2.34	103.86	100.89
6	B	601[A]	B12	C54-C17-C18	-2.33	109.65	112.99
6	B	601[B]	B12	C54-C17-C18	-2.33	109.65	112.99
6	D	601	B12	C8-C9-N22	2.32	115.35	110.77
6	B	601[A]	B12	C20-C1-N21	2.31	114.07	110.26
6	B	601[B]	B12	C20-C1-N21	2.31	114.07	110.26
6	D	601	B12	C41-C8-C9	2.26	115.12	111.19
6	D	601	B12	C53-C15-C16	2.23	124.14	120.36
6	B	601[A]	B12	C53-C15-C16	2.22	124.13	120.36
6	B	601[B]	B12	C53-C15-C16	2.22	124.13	120.36
6	B	601[A]	B12	C18-C17-C16	2.20	103.34	100.69
6	B	601[B]	B12	C18-C17-C16	2.20	103.34	100.69
6	D	601	B12	C8B-N1B-C2B	2.19	108.25	106.26
6	B	601[A]	B12	C3R-C2R-C1R	2.18	104.68	99.89
6	B	601[B]	B12	C3R-C2R-C1R	2.18	104.68	99.89
3	A	501[B]	FWK	C2'-C1'-N9	-2.17	107.90	113.30
6	D	601	B12	C18-C17-C16	2.15	103.28	100.69
6	D	601	B12	C3R-C2R-C1R	2.11	104.54	99.89
3	A	501[A]	FWK	C6-C5-N7	2.11	136.16	132.09
3	A	501[B]	FWK	C6-C5-N7	2.10	136.14	132.09
6	B	601[A]	B12	C8-C9-C10	-2.09	118.89	123.33
6	B	601[B]	B12	C8-C9-C10	-2.09	118.89	123.33
3	A	501[B]	FWK	N9-C8-N7	-2.06	111.02	113.94
6	D	601	B12	C8-C9-C10	-2.05	118.96	123.33
6	B	601[A]	B12	C60-C18-C17	-2.04	110.25	115.82
6	B	601[B]	B12	C60-C18-C17	-2.04	110.25	115.82

There are no chirality outliers.

All (64) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	503	GOL	C1-C2-C3-O3
4	A	503	GOL	O2-C2-C3-O3
4	C	502	GOL	O1-C1-C2-C3
4	C	504	GOL	C1-C2-C3-O3
4	C	504	GOL	O2-C2-C3-O3
6	B	601[A]	B12	C1-C2-C26-C27
6	B	601[A]	B12	C25-C2-C26-C27
6	B	601[A]	B12	C3-C2-C26-C27
6	B	601[A]	B12	C42-C41-C8-C9
6	B	601[B]	B12	C1-C2-C26-C27
6	B	601[B]	B12	C25-C2-C26-C27
6	B	601[B]	B12	C3-C2-C26-C27
6	B	601[B]	B12	C42-C41-C8-C9
6	D	601	B12	C1-C2-C26-C27
6	D	601	B12	C25-C2-C26-C27
6	D	601	B12	C3-C2-C26-C27
6	D	601	B12	C42-C41-C8-C9
6	D	601	B12	C3R-O2-P-O4
6	D	601	B12	C13-C48-C49-C50
6	B	601[A]	B12	C4-C3-C30-C31
6	B	601[B]	B12	C4-C3-C30-C31
6	B	601[A]	B12	C13-C48-C49-C50
6	B	601[B]	B12	C13-C48-C49-C50
4	A	502	GOL	O1-C1-C2-O2
6	B	601[A]	B12	C2-C3-C30-C31
6	B	601[B]	B12	C2-C3-C30-C31
6	B	601[A]	B12	C16-C17-C55-C56
6	B	601[B]	B12	C16-C17-C55-C56
6	D	601	B12	C16-C17-C55-C56
6	D	601	B12	C4-C3-C30-C31
4	A	502	GOL	O1-C1-C2-C3
4	C	503	GOL	O1-C1-C2-C3
4	C	503	GOL	C1-C2-C3-O3
6	B	601[A]	B12	O6R-C1R-N1B-C8B
6	B	601[B]	B12	O6R-C1R-N1B-C8B
4	C	502	GOL	O1-C1-C2-O2
4	C	503	GOL	O1-C1-C2-O2
6	D	601	B12	C2-C3-C30-C31
6	B	601[A]	B12	C18-C17-C55-C56
6	B	601[B]	B12	C18-C17-C55-C56
3	C	501	FWK	C2'-C1'-N9-C4
6	B	601[A]	B12	C2R-C1R-N1B-C8B

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Mol	Chain	Res	Type	Atoms
6	B	601[B]	B12	C2R-C1R-N1B-C8B
6	D	601	B12	O6R-C1R-N1B-C8B
6	D	601	B12	C18-C17-C55-C56
6	D	601	B12	C2R-C1R-N1B-C8B
6	B	601[A]	B12	C2P-O3-P-O5
6	B	601[B]	B12	C2P-O3-P-O5
3	C	501	FWK	C2'-C1'-N9-C8
6	D	601	B12	C18-C60-C61-O63
4	C	503	GOL	O2-C2-C3-O3
3	A	501[A]	FWK	C2'-C1'-N9-C8
6	D	601	B12	C38-C37-C7-C36
3	A	501[A]	FWK	C2'-C1'-N9-C4
6	D	601	B12	C18-C60-C61-N62
6	B	601[A]	B12	C38-C37-C7-C36
6	B	601[B]	B12	C38-C37-C7-C36
6	B	601[A]	B12	C2P-O3-P-O4
6	B	601[A]	B12	C3R-O2-P-O4
6	B	601[A]	B12	C3R-O2-P-O5
6	B	601[B]	B12	C2P-O3-P-O4
6	B	601[B]	B12	C3R-O2-P-O4
6	B	601[B]	B12	C3R-O2-P-O5
6	D	601	B12	C38-C37-C7-C8

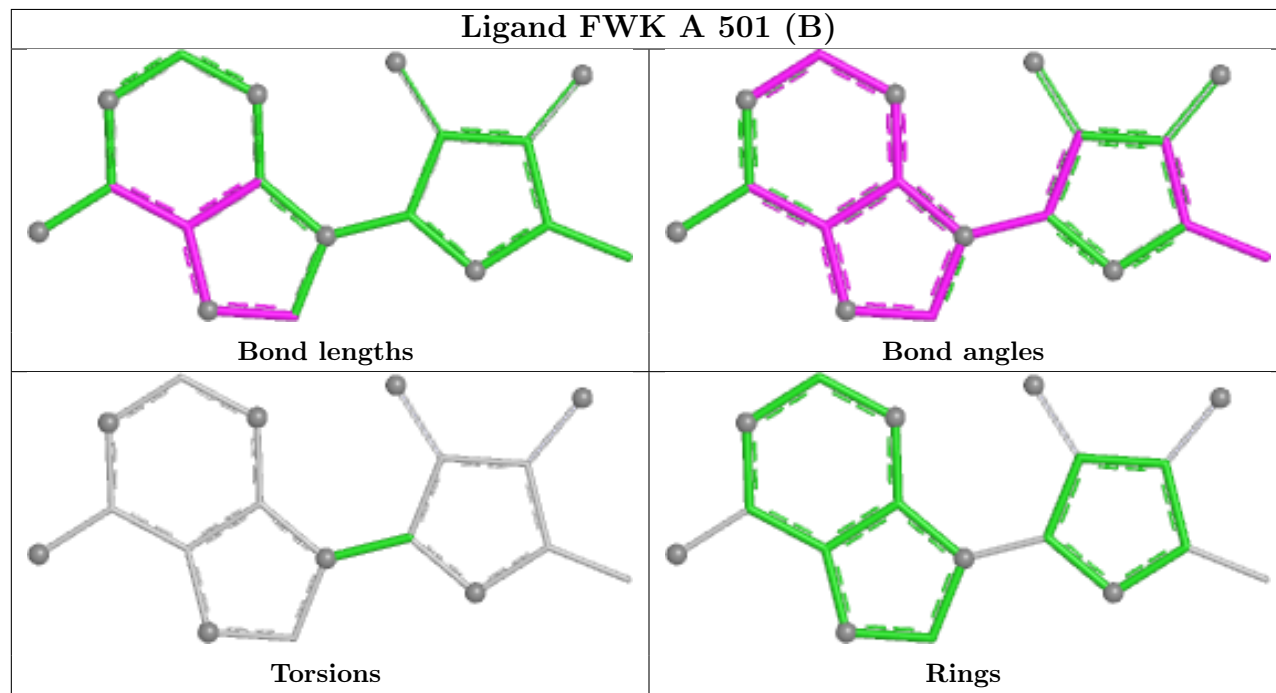
There are no ring outliers.

7 monomers are involved in 17 short contacts:

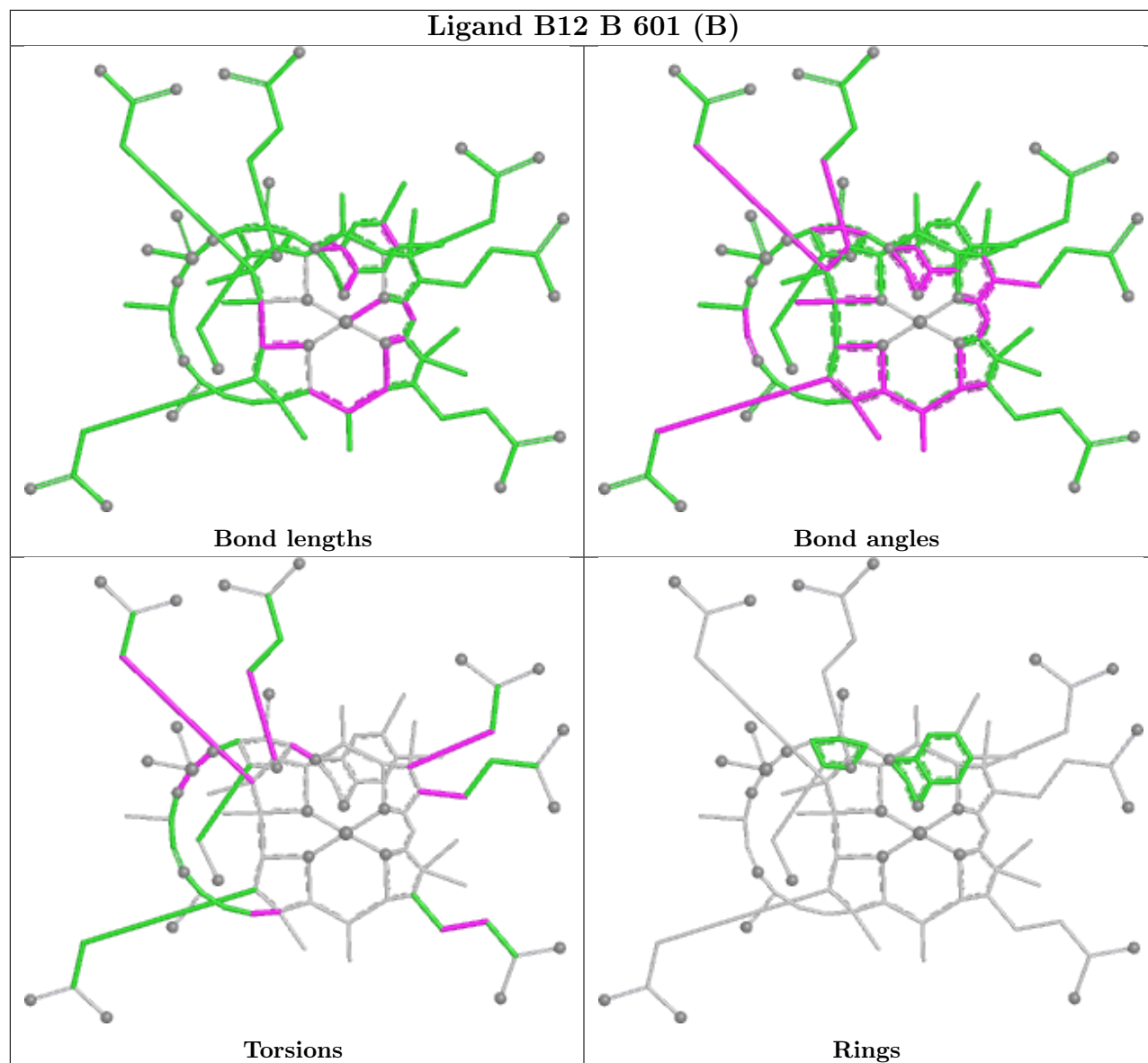
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501[B]	FWK	1	0
6	B	601[B]	B12	2	0
3	A	501[A]	FWK	1	0
3	C	501	FWK	1	0
6	B	601[A]	B12	1	0
4	C	503	GOL	2	0
6	D	601	B12	9	0

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

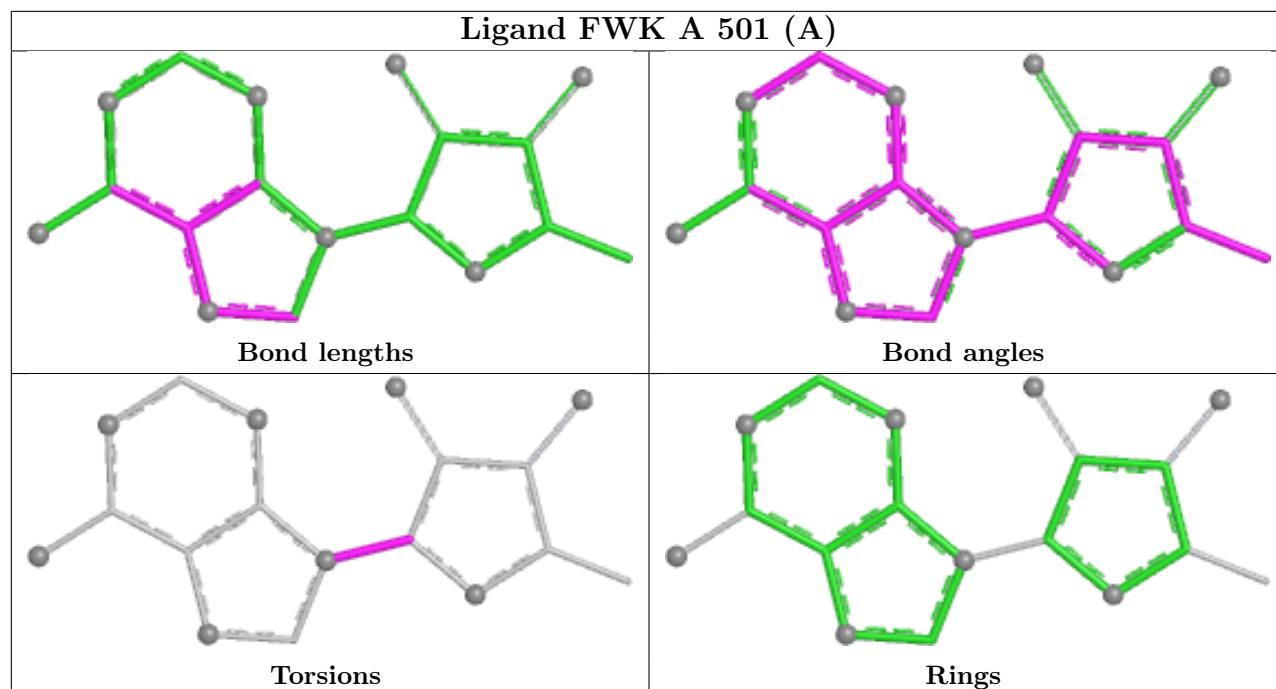
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



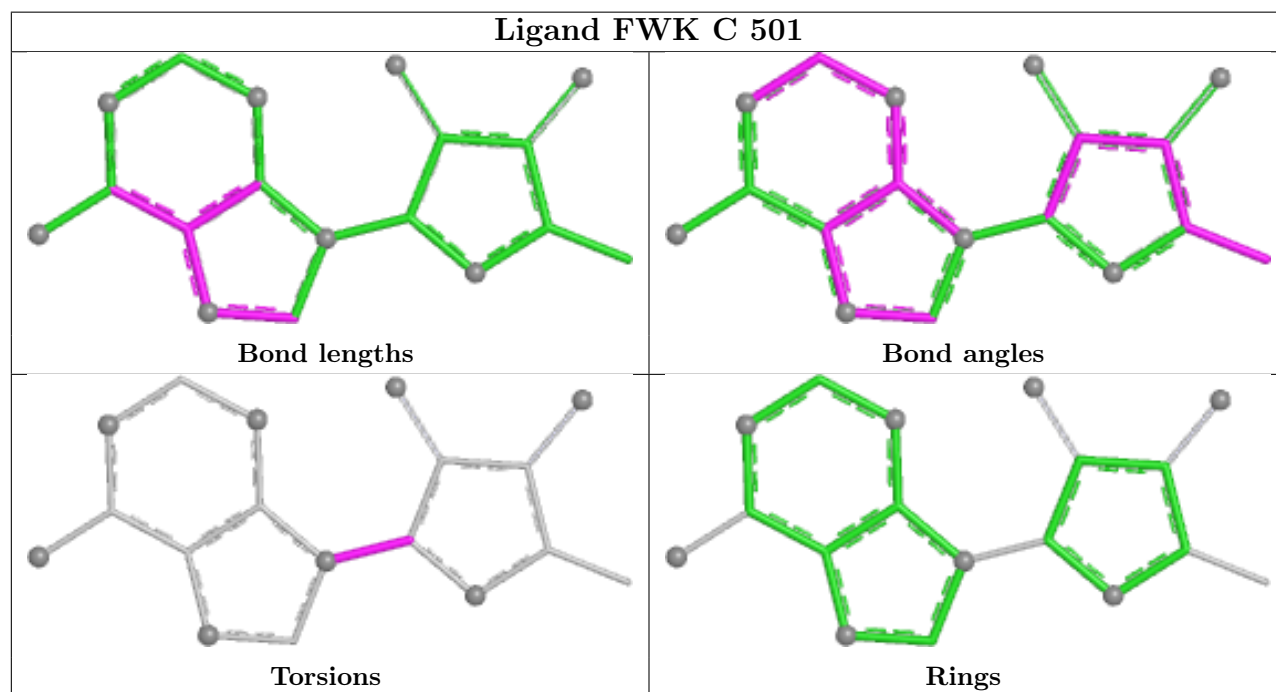
Ligand B12 B 601 (B)



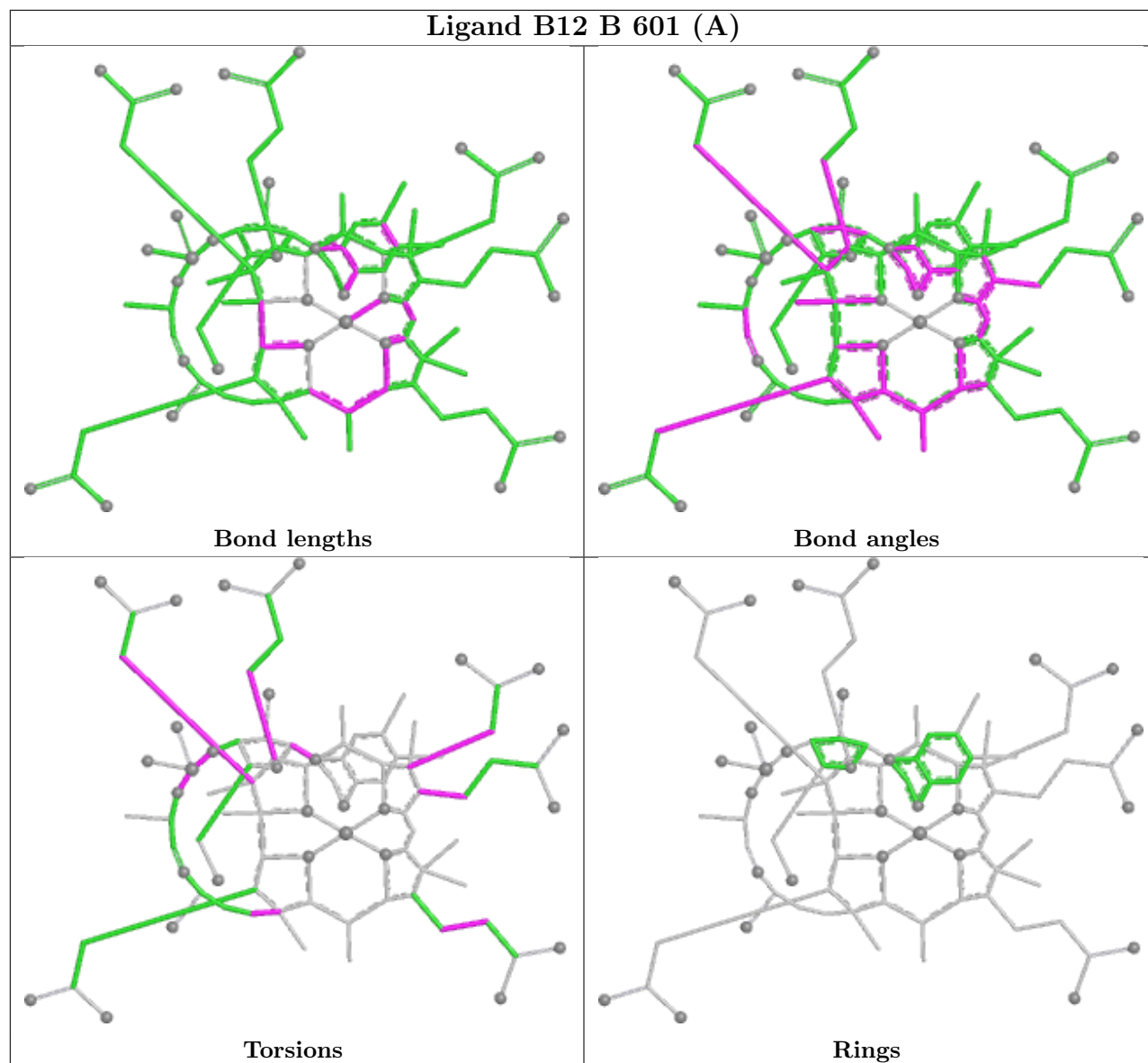
Ligand FWK A 501 (A)

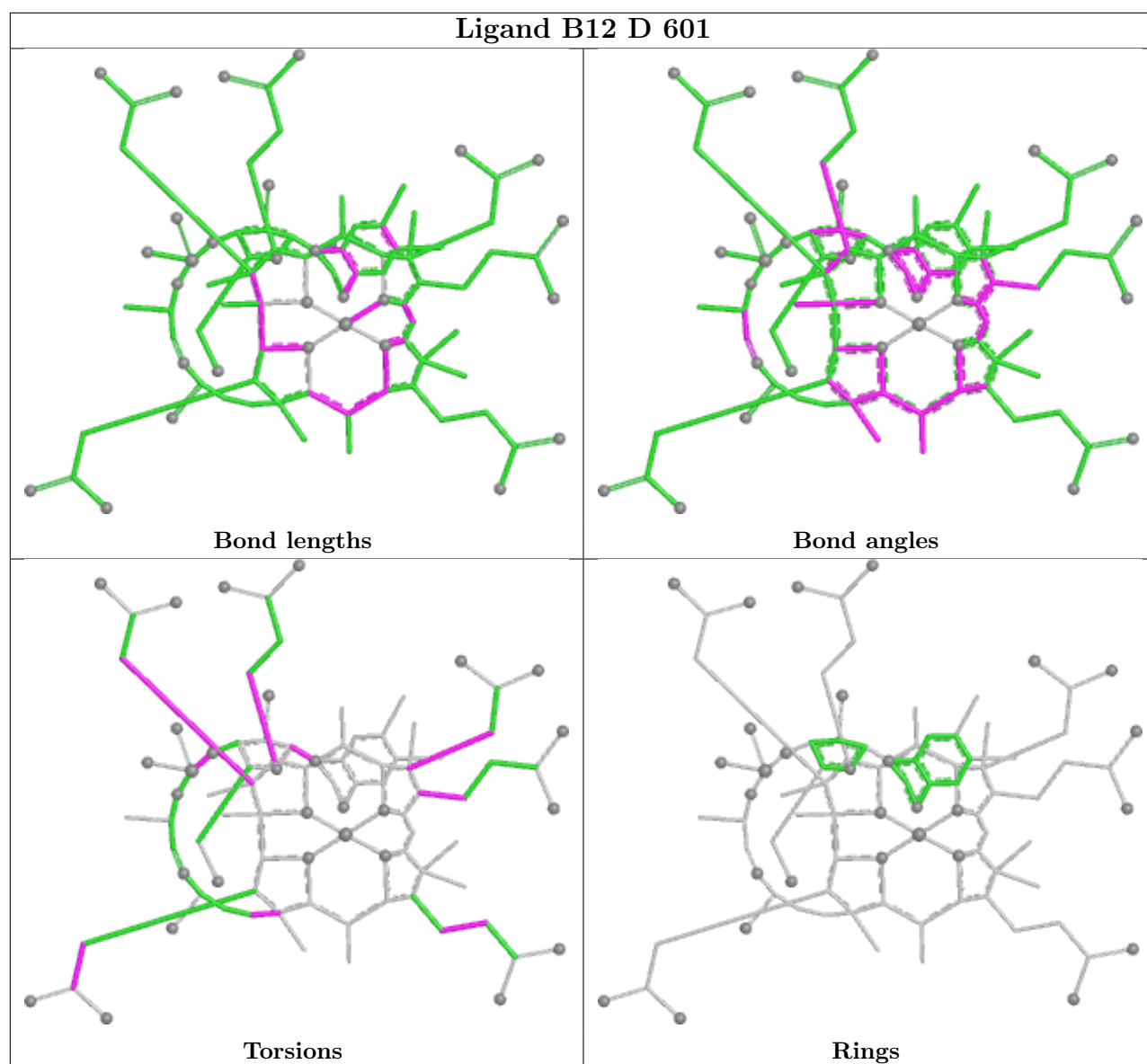


Ligand FWK C 501



Ligand B12 B 601 (A)





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	453/453 (100%)	-1.31	0 100 100	17, 27, 39, 51	2 (0%)
1	C	453/453 (100%)	-1.28	0 100 100	16, 28, 44, 67	1 (0%)
2	B	252/263 (95%)	-0.81	0 100 100	22, 45, 59, 81	2 (0%)
2	D	252/263 (95%)	-0.68	0 100 100	20, 50, 72, 96	0
All	All	1410/1432 (98%)	-1.10	0 100 100	16, 33, 60, 96	5 (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
4	GOL	A	502	6/6	0.98	0.06	38,45,48,56	0
4	GOL	A	503	6/6	0.98	0.07	33,34,41,49	0
4	GOL	C	502	6/6	0.98	0.05	30,33,37,38	0
3	FWK	A	501[A]	18/19	0.99	0.05	28,31,32,33	18

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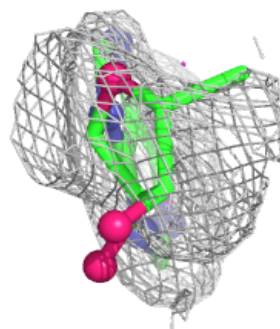
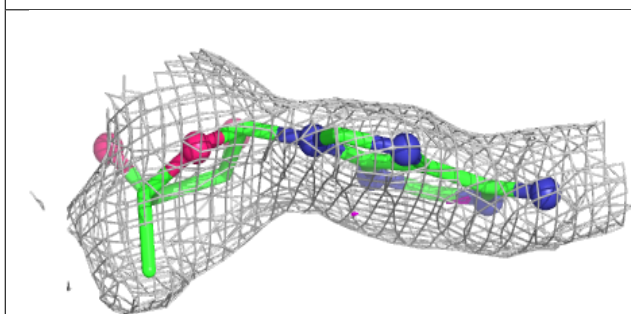
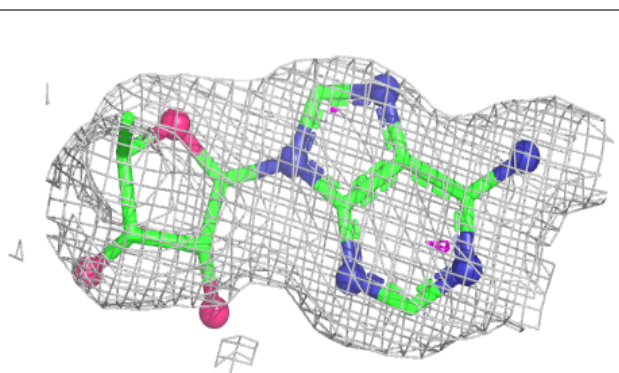
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	FWK	A	501[B]	18/19	0.99	0.05	28,31,32,34	18
4	GOL	B	602	6/6	0.99	0.06	35,40,44,45	0
3	FWK	C	501	18/19	0.99	0.05	34,35,42,49	0
4	GOL	C	503	6/6	0.99	0.05	23,29,38,40	0
4	GOL	C	504	6/6	0.99	0.07	23,29,31,31	0
5	NH4	C	505	1/1	0.99	0.08	26,26,26,26	0
6	B12	B	601[A]	91/91	0.99	0.04	28,33,40,45	4
6	B12	B	601[B]	91/91	0.99	0.04	28,33,40,45	4
6	B12	D	601	91/91	0.99	0.04	33,35,41,45	0
5	NH4	A	504	1/1	1.00	0.04	21,21,21,21	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.

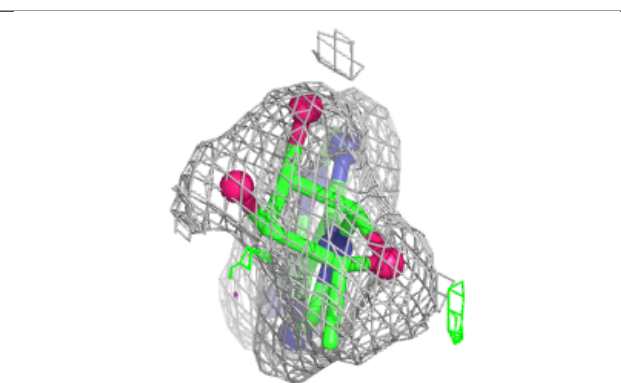
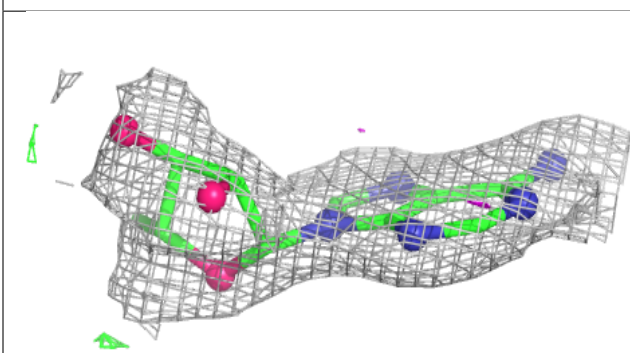
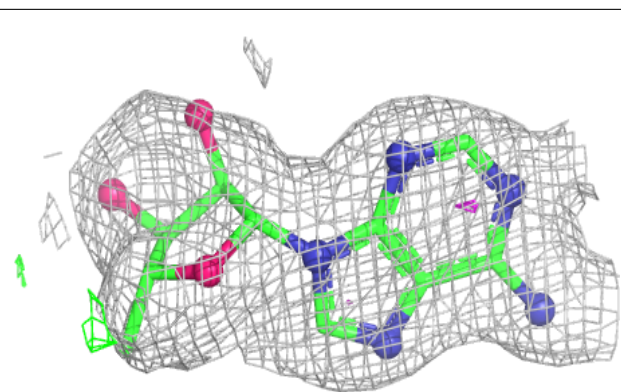
Electron density around FWK A 501 (A):

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

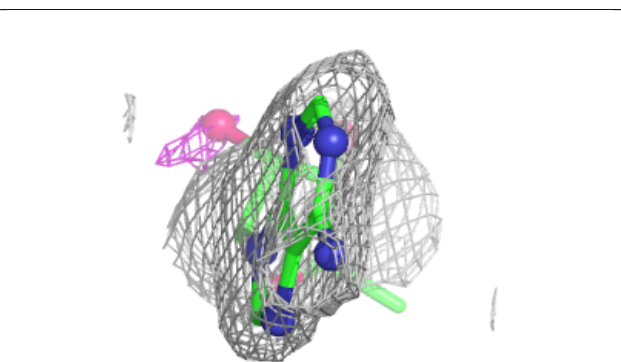
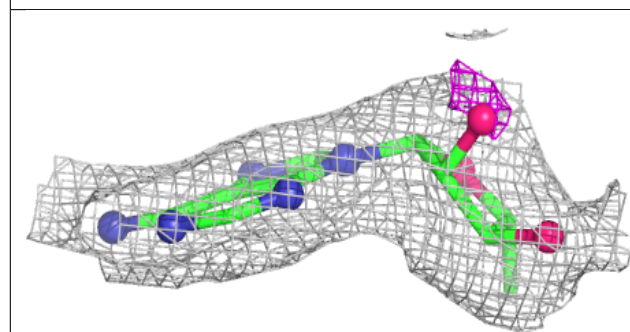
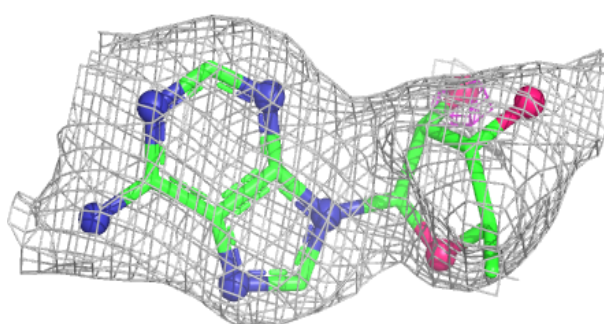


Electron density around FWK A 501 (B):

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

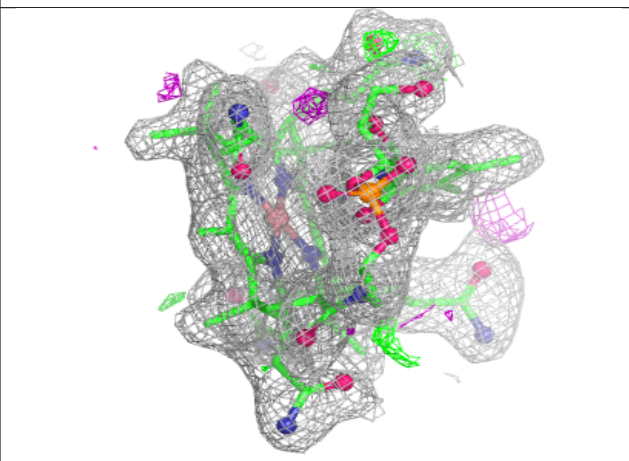
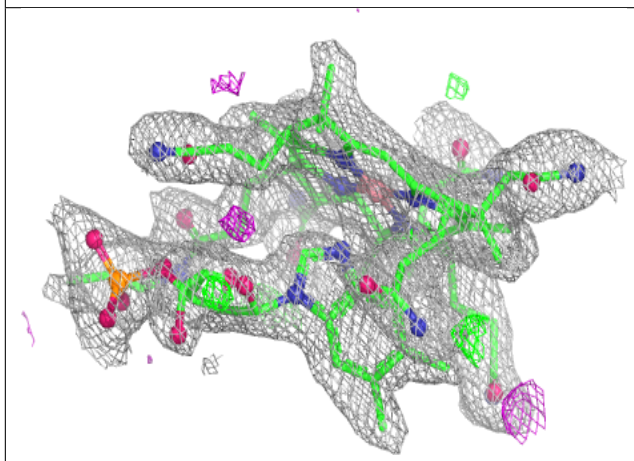
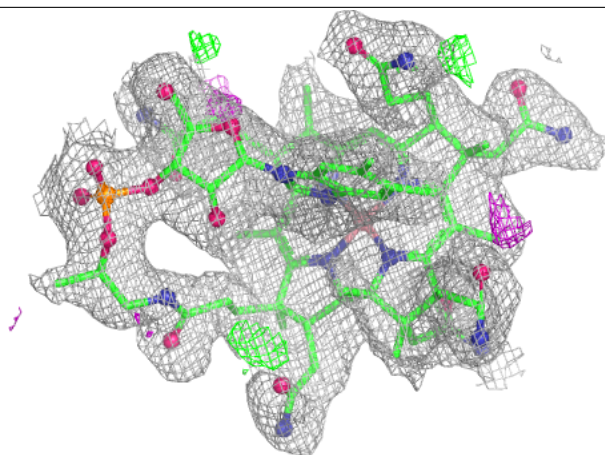
**Electron density around FWK C 501:**

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



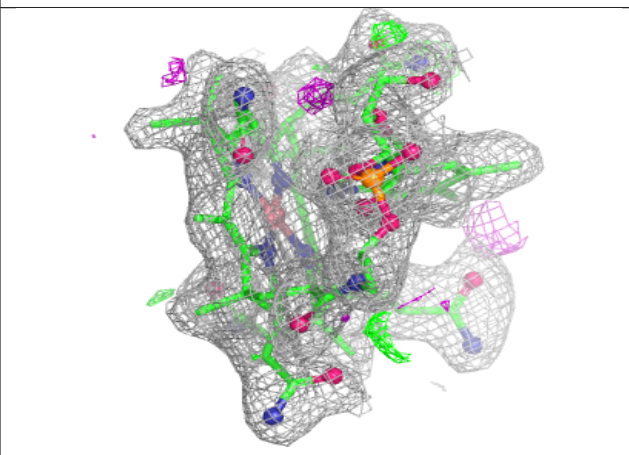
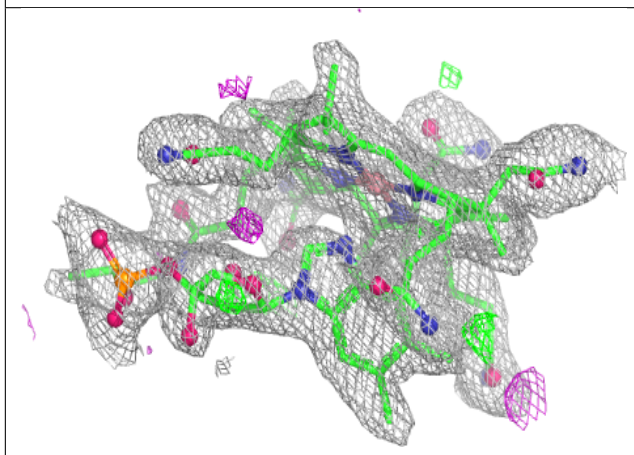
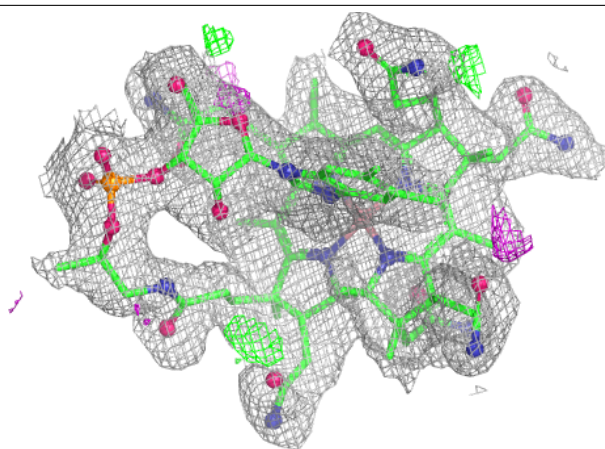
Electron density around B12 B 601 (A):

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



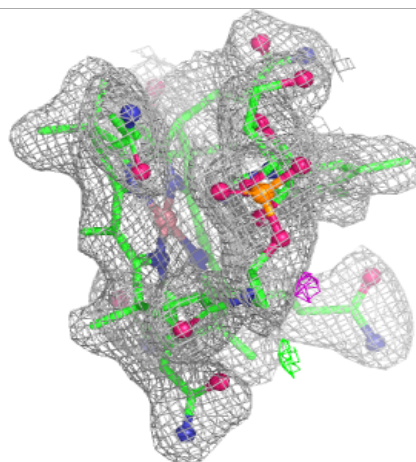
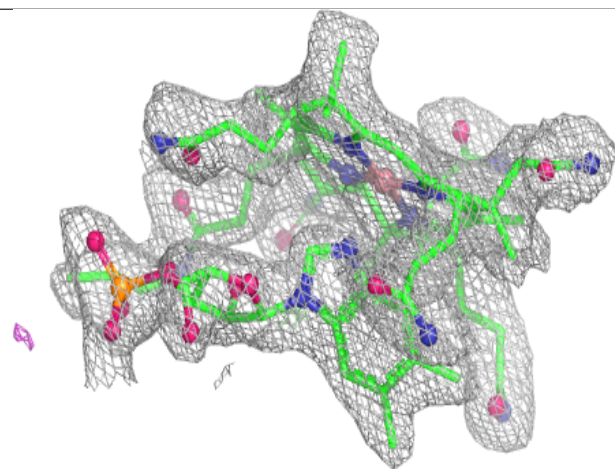
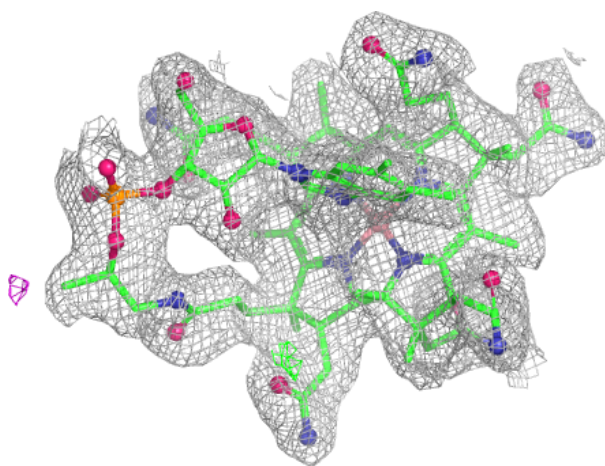
Electron density around B12 B 601 (B):

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



Electron density around B12 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.