



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 10:59 AM JST

PDB ID : 5YSH / pdb_00005ysh
Title : Diol dehydratase - alpha/T172A mutant complexed with AdoCbl, aerobically-prepared crystal
Authors : Shibata, N.
Deposited on : 2017-11-14
Resolution : 1.90 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:

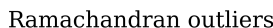
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

i

X-RAY DIFFRACTION

A.

the following graphic. The table shows the number of entries on which the scores are based.

Ramachandran outliers

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.

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Mol	Chain	Length	Quality of chain
2	H	200	
2	K	200	
3	C	137	
3	F	137	
3	I	137	
3	L	137	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	5AD	A	605	-	X	-	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 28331 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 Diol dehydrase alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	551	Total	C	N	O	S	0	4	0
			4218	2632	729	827	30			
1	D	550	Total	C	N	O	S	0	3	0
			4205	2625	725	825	30			
1	G	550	Total	C	N	O	S	0	3	0
			4205	2625	726	824	30			
1	J	551	Total	C	N	O	S	0	2	0
			4207	2625	727	825	30			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	172	ALA	THR	engineered mutation	UNP Q59470
D	172	ALA	THR	engineered mutation	UNP Q59470
G	172	ALA	THR	engineered mutation	UNP Q59470
J	172	ALA	THR	engineered mutation	UNP Q59470

- Molecule 2 is a protein called Diol dehydrase beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	177	Total	C	N	O	S	0	2	0
			1364	863	246	253	2			
2	E	176	Total	C	N	O	S	0	2	0
			1363	862	245	254	2			
2	H	180	Total	C	N	O	S	0	1	0
			1377	871	249	255	2			
2	K	167	Total	C	N	O	S	0	0	0
			1280	810	230	238	2			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	25	MET	-	expression tag	UNP Q59471
B	26	SER	-	expression tag	UNP Q59471
B	27	SER	-	expression tag	UNP Q59471
B	28	HIS	-	expression tag	UNP Q59471
B	29	HIS	-	expression tag	UNP Q59471
B	30	HIS	-	expression tag	UNP Q59471
B	31	HIS	-	expression tag	UNP Q59471
B	32	HIS	-	expression tag	UNP Q59471
B	33	HIS	-	expression tag	UNP Q59471
B	34	SER	-	expression tag	UNP Q59471
B	35	ALA	-	expression tag	UNP Q59471
B	36	ALA	-	expression tag	UNP Q59471
B	37	LEU	-	expression tag	UNP Q59471
B	38	GLU	-	expression tag	UNP Q59471
B	39	VAL	-	expression tag	UNP Q59471
B	40	LEU	-	expression tag	UNP Q59471
B	41	PHE	-	expression tag	UNP Q59471
B	42	GLN	-	expression tag	UNP Q59471
B	43	GLY	-	expression tag	UNP Q59471
B	44	PRO	-	expression tag	UNP Q59471
B	45	GLY	-	expression tag	UNP Q59471
E	25	MET	-	expression tag	UNP Q59471
E	26	SER	-	expression tag	UNP Q59471
E	27	SER	-	expression tag	UNP Q59471
E	28	HIS	-	expression tag	UNP Q59471
E	29	HIS	-	expression tag	UNP Q59471
E	30	HIS	-	expression tag	UNP Q59471
E	31	HIS	-	expression tag	UNP Q59471
E	32	HIS	-	expression tag	UNP Q59471
E	33	HIS	-	expression tag	UNP Q59471
E	34	SER	-	expression tag	UNP Q59471
E	35	ALA	-	expression tag	UNP Q59471
E	36	ALA	-	expression tag	UNP Q59471
E	37	LEU	-	expression tag	UNP Q59471
E	38	GLU	-	expression tag	UNP Q59471
E	39	VAL	-	expression tag	UNP Q59471
E	40	LEU	-	expression tag	UNP Q59471
E	41	PHE	-	expression tag	UNP Q59471
E	42	GLN	-	expression tag	UNP Q59471
E	43	GLY	-	expression tag	UNP Q59471
E	44	PRO	-	expression tag	UNP Q59471
E	45	GLY	-	expression tag	UNP Q59471
H	25	MET	-	expression tag	UNP Q59471

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Chain	Residue	Modelled	Actual	Comment	Reference
H	26	SER	-	expression tag	UNP Q59471
H	27	SER	-	expression tag	UNP Q59471
H	28	HIS	-	expression tag	UNP Q59471
H	29	HIS	-	expression tag	UNP Q59471
H	30	HIS	-	expression tag	UNP Q59471
H	31	HIS	-	expression tag	UNP Q59471
H	32	HIS	-	expression tag	UNP Q59471
H	33	HIS	-	expression tag	UNP Q59471
H	34	SER	-	expression tag	UNP Q59471
H	35	ALA	-	expression tag	UNP Q59471
H	36	ALA	-	expression tag	UNP Q59471
H	37	LEU	-	expression tag	UNP Q59471
H	38	GLU	-	expression tag	UNP Q59471
H	39	VAL	-	expression tag	UNP Q59471
H	40	LEU	-	expression tag	UNP Q59471
H	41	PHE	-	expression tag	UNP Q59471
H	42	GLN	-	expression tag	UNP Q59471
H	43	GLY	-	expression tag	UNP Q59471
H	44	PRO	-	expression tag	UNP Q59471
H	45	GLY	-	expression tag	UNP Q59471
K	25	MET	-	expression tag	UNP Q59471
K	26	SER	-	expression tag	UNP Q59471
K	27	SER	-	expression tag	UNP Q59471
K	28	HIS	-	expression tag	UNP Q59471
K	29	HIS	-	expression tag	UNP Q59471
K	30	HIS	-	expression tag	UNP Q59471
K	31	HIS	-	expression tag	UNP Q59471
K	32	HIS	-	expression tag	UNP Q59471
K	33	HIS	-	expression tag	UNP Q59471
K	34	SER	-	expression tag	UNP Q59471
K	35	ALA	-	expression tag	UNP Q59471
K	36	ALA	-	expression tag	UNP Q59471
K	37	LEU	-	expression tag	UNP Q59471
K	38	GLU	-	expression tag	UNP Q59471
K	39	VAL	-	expression tag	UNP Q59471
K	40	LEU	-	expression tag	UNP Q59471
K	41	PHE	-	expression tag	UNP Q59471
K	42	GLN	-	expression tag	UNP Q59471
K	43	GLY	-	expression tag	UNP Q59471
K	44	PRO	-	expression tag	UNP Q59471
K	45	GLY	-	expression tag	UNP Q59471

- Molecule 3 is a protein called Diol dehydrase gamma subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	136	Total	C	N	O	S	0	2	0
			1098	686	194	214	4			
3	F	136	Total	C	N	O	S	0	1	0
			1095	683	195	213	4			
3	I	136	Total	C	N	O	S	0	1	0
			1092	682	194	212	4			
3	L	136	Total	C	N	O	S	0	0	0
			1087	678	194	212	3			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	37	MET	-	expression tag	UNP Q59472
F	37	MET	-	expression tag	UNP Q59472
I	37	MET	-	expression tag	UNP Q59472
L	37	MET	-	expression tag	UNP Q59472

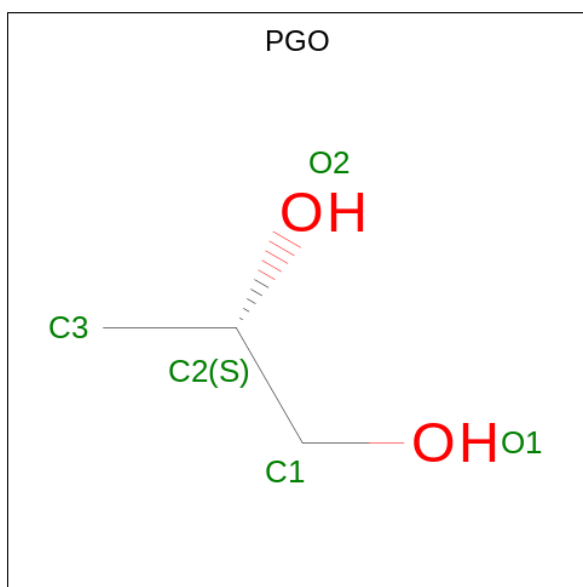
- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		
4	D	1	Total	Ca	0	0
			1	1		
4	G	1	Total	Ca	0	0
			1	1		
4	J	1	Total	Ca	0	0
			1	1		

- Molecule 5 is POTASSIUM ION (CCD ID: K) (formula: K).

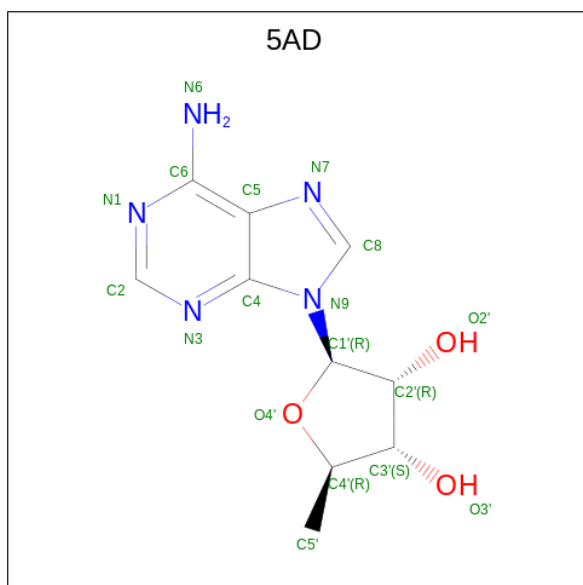
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	K	0	0
			2	2		
5	D	2	Total	K	0	0
			2	2		
5	G	2	Total	K	0	0
			2	2		
5	J	2	Total	K	0	0
			2	2		

- Molecule 6 is S-1,2-PROPANEDIOL (CCD ID: PGO) (formula: C₃H₈O₂).



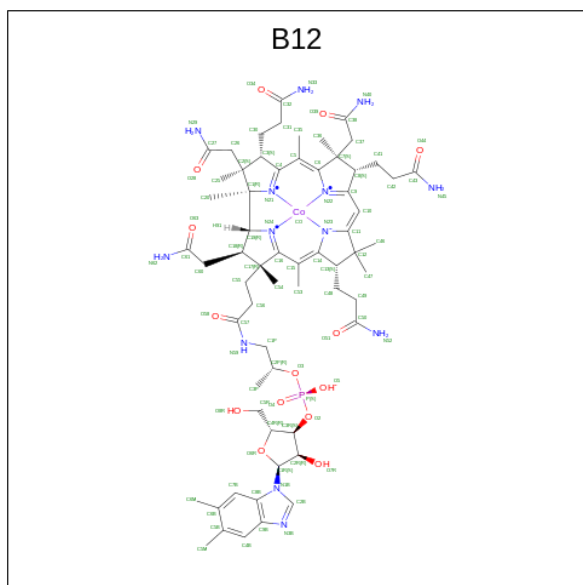
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			5	3	2		
6	D	1	Total	C	O	0	0
			5	3	2		
6	G	1	Total	C	O	0	0
			5	3	2		
6	J	1	Total	C	O	0	0
			5	3	2		

- Molecule 7 is 5'-DEOXYADENOSINE (CCD ID: 5AD) (formula: $C_{10}H_{13}N_5O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C N 11 6 5	0	0
7	D	1	Total C N 11 6 5	0	0
7	G	1	Total C N 11 6 5	0	0
7	J	1	Total C N 11 6 5	0	0

- Molecule 8 is COBALAMIN (CCD ID: B12) (formula: $C_{62}H_{89}CoN_{13}O_{14}P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C Co N O P 91 62 1 13 14 1	0	0
8	E	1	Total C Co N O P 91 62 1 13 14 1	0	0
8	H	1	Total C Co N O P 91 62 1 13 14 1	0	0
8	K	1	Total C Co N O P 91 62 1 13 14 1	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	253	Total O 253 253	0	0
9	B	24	Total O 24 24	0	0

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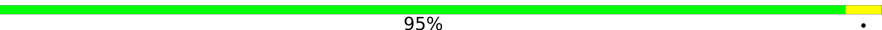
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	C	41	Total 41	O 41	0	0
9	D	388	Total 388	O 388	0	0
9	E	56	Total 56	O 56	0	0
9	F	102	Total 102	O 102	0	0
9	G	208	Total 208	O 208	0	0
9	H	34	Total 34	O 34	0	0
9	I	28	Total 28	O 28	0	0
9	J	151	Total 151	O 151	0	0
9	K	10	Total 10	O 10	0	0
9	L	5	Total 5	O 5	0	0

3 Residue-property plots

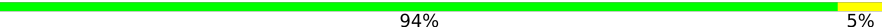
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

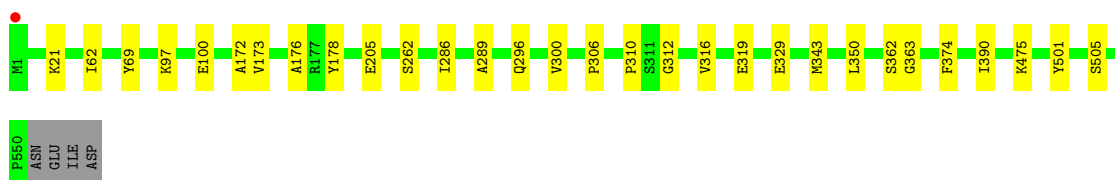
- Molecule 1: Diol dehydrase alpha subunit

Chain A:  95% ..

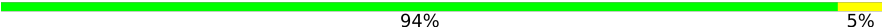


- Molecule 1: Diol dehydrase alpha subunit

Chain D:  94% 5% .



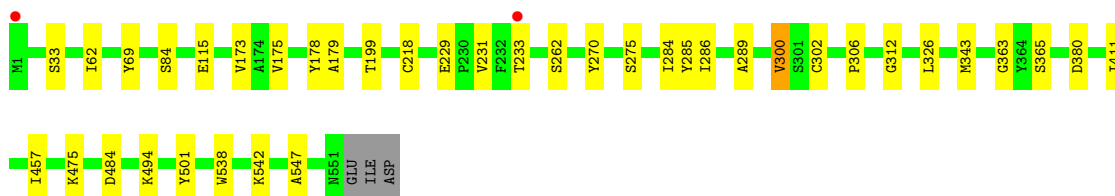
- Molecule 1: Diol dehydrase alpha subunit

Chain G:  94% 5% .

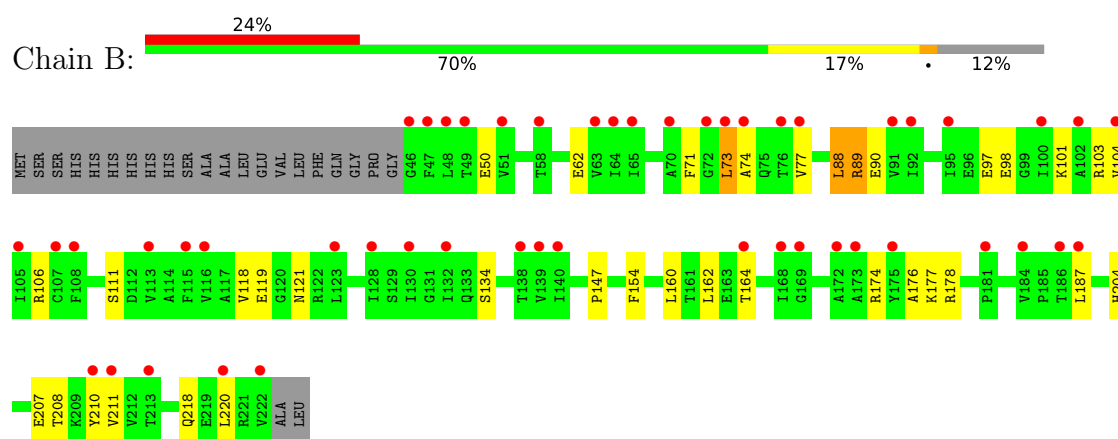


- Molecule 1: Diol dehydrase alpha subunit

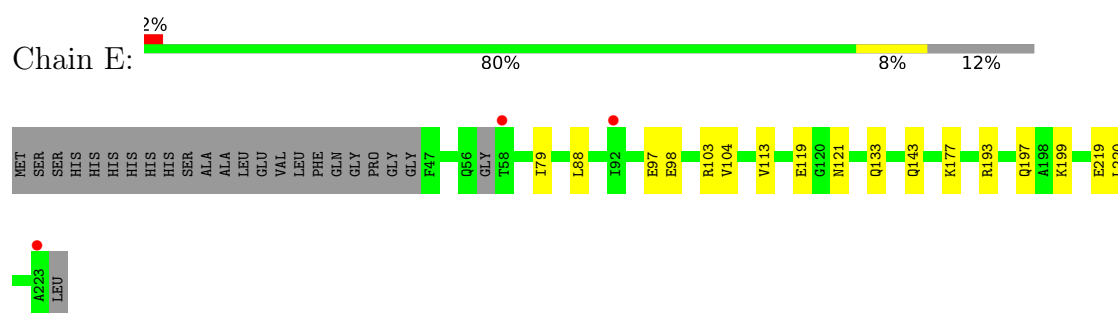
Chain J:  92% 7% .



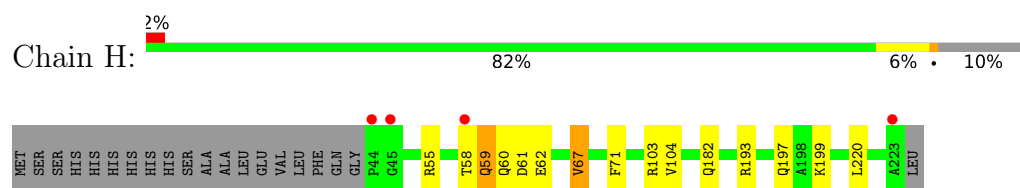
- Molecule 2: Diol dehydrase beta subunit



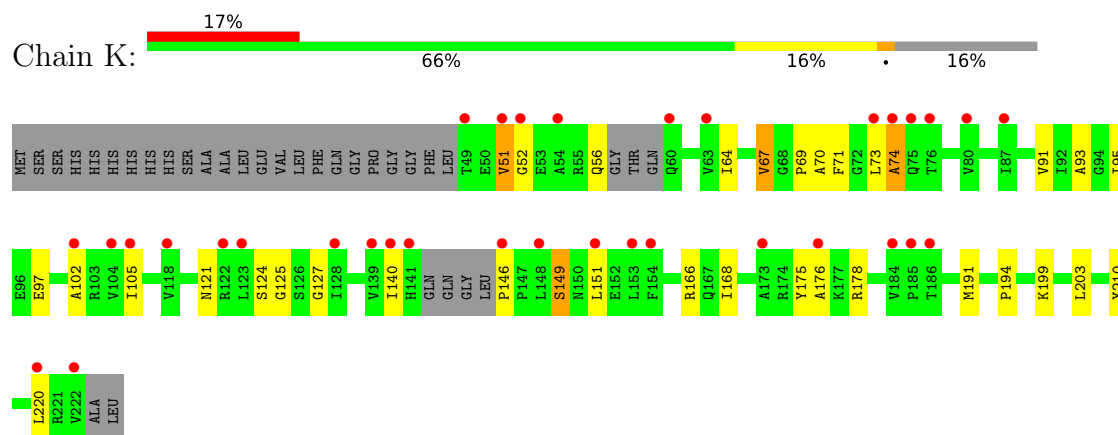
- Molecule 2: Diol dehydrase beta subunit



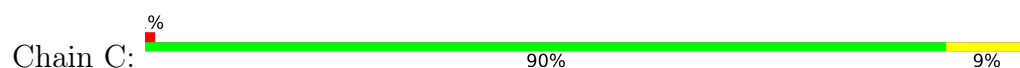
- Molecule 2: Diol dehydrase beta subunit



- Molecule 2: Diol dehydrase beta subunit

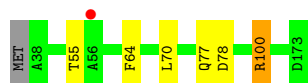
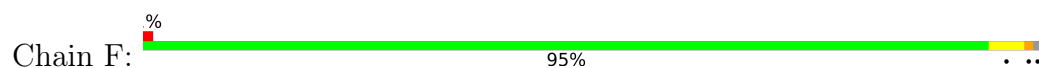


- Molecule 3: Diol dehydrase gamma subunit

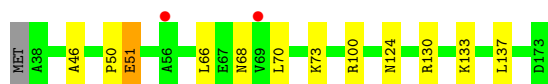
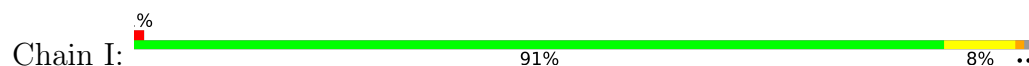




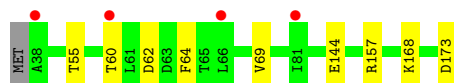
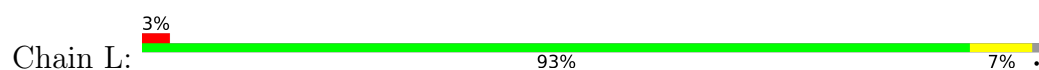
- Molecule 3: Diol dehydrase gamma subunit



- Molecule 3: Diol dehydrase gamma subunit



- Molecule 3: Diol dehydrase gamma subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	70.33Å 110.49Å 115.48Å 92.69° 95.97° 105.44°	Depositor
Resolution (Å)	49.00 – 1.90 49.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.8 (49.00-1.90) 95.4 (49.00-1.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 1.90Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.164 , 0.191 0.164 , 0.192	Depositor DCC
R_{free} test set	2000 reflections (0.77%)	wwPDB-VP
Wilson B-factor (Å ²)	24.2	Xtriage
Anisotropy	0.248	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 43.6	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	0.97	EDS
Total number of atoms	28331	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% 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: CA, B12, PGO, 5AD, K

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	0.38	0/4302	0.56	0/5825
1	D	0.47	0/4286	0.61	0/5803
1	G	0.29	0/4286	0.50	0/5803
1	J	0.26	0/4285	0.47	0/5802
2	B	0.25	0/1392	0.45	0/1883
2	E	0.29	0/1384	0.49	0/1872
2	H	0.23	0/1403	0.43	0/1898
2	K	0.20	0/1299	0.41	0/1755
3	C	0.29	0/1119	0.47	0/1511
3	F	0.37	0/1110	0.56	0/1499
3	I	0.22	0/1110	0.44	0/1499
3	L	0.20	0/1102	0.39	0/1489
All	All	0.33	0/27078	0.51	0/36639

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	4218	0	4165	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	4205	0	4150	20	0
1	G	4205	0	4152	16	0
1	J	4207	0	4150	24	0
2	B	1364	0	1421	27	0
2	E	1363	0	1411	9	0
2	H	1377	0	1432	9	0
2	K	1280	0	1331	20	0
3	C	1098	0	1111	6	0
3	F	1095	0	1104	6	0
3	I	1092	0	1105	8	0
3	L	1087	0	1096	8	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
4	G	1	0	0	0	0
4	J	1	0	0	0	0
5	A	2	0	0	0	0
5	D	2	0	0	0	0
5	G	2	0	0	0	0
5	J	2	0	0	0	0
6	A	5	0	6	0	0
6	D	5	0	6	0	0
6	G	5	0	6	0	0
6	J	5	0	6	0	0
7	A	11	0	4	1	0
7	D	11	0	4	1	0
7	G	11	0	4	1	0
7	J	11	0	4	2	0
8	B	91	0	88	6	0
8	E	91	0	88	7	0
8	H	91	0	88	8	0
8	K	91	0	88	9	0
9	A	253	0	0	2	0
9	B	24	0	0	1	0
9	C	41	0	0	0	0
9	D	388	0	0	1	0
9	E	56	0	0	1	0
9	F	102	0	0	0	0
9	G	208	0	0	0	0
9	H	34	0	0	0	0
9	I	28	0	0	1	0
9	J	151	0	0	1	0
9	K	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	L	5	0	0	0	0
All	All	28331	0	27020	185	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (185) 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)
8:E:1601:B12:H552	8:E:1601:B12:H531	1.68	0.73
1:A:350:LEU:HD12	1:D:350:LEU:HD12	1.73	0.71
2:H:67:VAL:HG13	2:H:71:PHE:HB3	1.73	0.71
3:C:38:ALA:N	3:C:91:SER:HG	1.87	0.71
3:F:100:ARG:HA	3:F:100:ARG:HE	1.58	0.69
2:H:104:VAL:HG12	2:H:220:LEU:HD12	1.78	0.66
2:B:101:LYS:HE2	2:B:103[B]:ARG:HG3	1.78	0.66
1:A:7:GLU:OE2	9:A:701:HOH:O	2.15	0.65
1:J:231:VAL:HG23	1:J:270:TYR:HB2	1.78	0.65
2:B:50:GLU:HG2	2:B:218:GLN:HB3	1.80	0.63
8:H:1601:B12:H552	8:H:1601:B12:H531	1.80	0.62
2:H:55:ARG:O	2:H:103[B]:ARG:NH2	2.33	0.62
2:B:73:LEU:HD12	2:B:74:ALA:H	1.65	0.62
8:K:1601:B12:H552	8:K:1601:B12:H531	1.80	0.61
8:K:1601:B12:C2B	8:K:1601:B12:H492	2.32	0.60
8:H:1601:B12:H492	8:H:1601:B12:C2B	2.32	0.60
8:E:1601:B12:C2B	8:E:1601:B12:H492	2.31	0.60
8:B:1601:B12:H362	8:B:1601:B12:H351	1.83	0.60
2:K:121:ASN:ND2	2:K:127:GLY:O	2.35	0.60
2:K:95:ILE:HG21	2:K:102:ALA:HB2	1.84	0.59
8:B:1601:B12:C2B	8:B:1601:B12:H492	2.32	0.59
8:B:1601:B12:H552	8:B:1601:B12:H531	1.85	0.59
2:K:199:LYS:HE2	2:K:203:LEU:HD11	1.84	0.59
2:B:164:THR:HG21	2:B:187:LEU:HD11	1.83	0.59
2:K:51:VAL:HG12	2:K:52:GLY:H	1.69	0.58
2:B:90:GLU:HG3	2:B:162:LEU:HB3	1.86	0.57
1:A:2:ARG:HG2	1:A:7:GLU:HG3	1.85	0.57
2:K:97:GLU:HG3	2:K:166:ARG:NH2	2.19	0.57
2:B:176:ALA:O	2:B:178:ARG:NH1	2.38	0.56
8:E:1601:B12:H351	8:E:1601:B12:H362	1.87	0.56
1:A:343[B]:MET:HG2	1:D:390:ILE:HD11	1.87	0.56
2:K:64:ILE:HG12	2:K:105:ILE:HD12	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:93:ALA:O	2:K:97:GLU:HG2	2.06	0.55
1:J:475:LYS:NZ	3:L:69:VAL:O	2.38	0.55
8:E:1601:B12:H531	8:E:1601:B12:C55	2.34	0.54
1:J:229:GLU:O	1:J:233:THR:HG23	2.06	0.54
1:A:284:ILE:HG22	1:A:326:LEU:HD12	1.90	0.53
1:D:172:ALA:HB1	8:E:1601:B12:O28	2.08	0.53
1:G:417:ARG:O	1:G:420[B]:GLN:HG2	2.07	0.53
2:B:174:ARG:HA	2:B:177:LYS:HE3	1.91	0.53
1:A:390:ILE:HD11	1:D:343[B]:MET:HG2	1.92	0.52
1:J:173:VAL:HG11	1:J:179:ALA:HA	1.91	0.52
3:L:55:THR:HG21	3:L:64:PHE:CE2	2.45	0.52
2:K:69:PRO:HB2	2:K:210:TYR:HB2	1.92	0.52
8:K:1601:B12:H262	8:K:1601:B12:H601	1.90	0.52
2:B:118:VAL:HG21	2:B:147:PRO:HA	1.91	0.52
9:A:705:HOH:O	1:D:21:LYS:NZ	2.43	0.51
8:H:1601:B12:H362	8:H:1601:B12:H351	1.92	0.51
1:G:21:LYS:HE3	1:J:547:ALA:HB3	1.93	0.50
1:J:69:TYR:HB2	1:J:289:ALA:HB1	1.93	0.50
2:K:91:VAL:O	2:K:95:ILE:HG12	2.12	0.49
2:B:98:GLU:OE1	2:B:177:LYS:NZ	2.37	0.49
2:K:64:ILE:HD11	2:K:105:ILE:HG13	1.93	0.49
1:J:233:THR:HG21	3:L:168:LYS:NZ	2.27	0.49
2:B:50:GLU:HB3	2:B:218:GLN:HE21	1.77	0.49
3:F:55:THR:HG21	3:F:64:PHE:CZ	2.47	0.49
2:B:71:PHE:HE1	2:B:88:LEU:HD21	1.78	0.49
2:H:193:ARG:HG3	2:H:197:GLN:HB2	1.95	0.48
3:L:55:THR:HG21	3:L:64:PHE:HE2	1.79	0.48
2:B:74:ALA:HB2	2:B:210:TYR:CZ	2.48	0.48
1:A:350:LEU:CD1	1:D:350:LEU:HD12	2.43	0.48
1:D:97:LYS:HB2	1:D:100:GLU:HG3	1.96	0.48
2:B:204:HIS:O	2:B:208:THR:HG23	2.14	0.47
1:A:205:GLU:HG2	9:B:1712:HOH:O	2.14	0.47
3:I:51:GLU:H	3:I:51:GLU:CD	2.22	0.47
3:C:117:ASP:O	3:C:121:GLU:HG3	2.14	0.47
2:B:73:LEU:HD21	2:B:106:ARG:NH1	2.30	0.47
3:C:67:GLU:HG2	3:C:68:ASN:N	2.29	0.47
2:E:121:ASN:OD1	2:E:143[B]:GLN:HA	2.14	0.47
1:G:284:ILE:HG22	1:G:326:LEU:HD12	1.97	0.47
1:J:199:THR:H	1:J:218:CYS:HB2	1.79	0.47
7:G:605:5AD:C4	8:H:1601:B12:H463	2.43	0.47
1:D:475:LYS:HG2	3:F:70:LEU:HD23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:84:SER:OG	1:J:115:GLU:OE2	2.25	0.46
3:L:60:THR:HG22	3:L:62:ASP:H	1.80	0.46
1:G:69:TYR:HB2	1:G:289:ALA:HB1	1.96	0.46
1:J:494:LYS:HE2	3:L:64:PHE:HB2	1.96	0.46
3:L:144:GLU:OE1	3:L:157:ARG:NH2	2.33	0.46
1:A:538:TRP:NE1	1:A:542:LYS:HE2	2.31	0.46
2:B:62:GLU:OE2	2:B:103[A]:ARG:NH2	2.34	0.46
8:H:1601:B12:H531	8:H:1601:B12:C55	2.45	0.46
2:K:70:ALA:HB1	2:K:74:ALA:HB3	1.97	0.46
8:K:1601:B12:H253	8:K:1601:B12:H301	1.75	0.46
1:J:285:TYR:CE1	1:J:326:LEU:HD11	2.51	0.46
8:K:1601:B12:H531	8:K:1601:B12:C55	2.46	0.46
8:B:1601:B12:H531	8:B:1601:B12:C55	2.45	0.46
1:A:69:TYR:HB2	1:A:289:ALA:HB1	1.98	0.45
2:H:58:THR:HG23	2:H:59:GLN:NE2	2.32	0.45
2:K:64:ILE:HG22	2:K:124:SER:HB2	1.98	0.45
8:B:1601:B12:H253	8:B:1601:B12:H301	1.78	0.45
2:H:59:GLN:O	2:H:61:ASP:N	2.46	0.45
1:J:365:SER:HB3	1:J:380:ASP:HA	1.98	0.45
3:I:133:LYS:HE3	3:I:137:LEU:HD11	1.99	0.45
2:K:146:PRO:HB2	2:K:149:SER:HB2	1.97	0.45
2:B:71:PHE:CE1	2:B:88:LEU:HD21	2.52	0.45
2:E:104:VAL:HG12	2:E:220:LEU:HD12	1.99	0.45
1:D:306:PRO:O	1:D:312:GLY:HA3	2.17	0.45
1:G:301:SER:HA	1:G:336:GLN:HG3	1.99	0.45
2:K:56:GLN:NE2	2:K:125:GLY:HA2	2.32	0.45
2:B:134:SER:HB3	2:B:207:GLU:OE2	2.17	0.44
3:I:50:PRO:HD2	3:I:51:GLU:OE2	2.17	0.44
1:J:300:VAL:HB	7:J:605:5AD:N7	2.33	0.44
3:I:124:ASN:O	3:I:130:ARG:HG3	2.17	0.44
2:K:151:LEU:HD13	2:K:175:TYR:CD2	2.52	0.44
3:C:132:THR:OG1	3:C:135:GLU:HG3	2.18	0.44
1:D:172:ALA:HB2	1:D:374:PHE:CZ	2.53	0.44
2:K:67:VAL:HG13	2:K:71:PHE:HB3	1.99	0.44
2:B:89:ARG:HG3	2:B:90:GLU:N	2.33	0.44
1:D:262:SER:HA	9:D:752:HOH:O	2.18	0.44
3:L:173:ASP:OD1	3:L:173:ASP:N	2.42	0.44
1:D:69:TYR:HB2	1:D:289:ALA:HB1	2.00	0.44
1:A:429:PRO:HA	1:A:430:PRO:HD3	1.90	0.43
2:B:104:VAL:HG12	2:B:220:LEU:HD12	1.99	0.43
1:G:346:THR:OG1	1:J:343[B]:MET:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:205:GLU:HG2	9:E:1730:HOH:O	2.18	0.43
8:K:1601:B12:H362	8:K:1601:B12:H351	2.00	0.43
8:K:1601:B12:H401	8:K:1601:B12:H361	1.83	0.43
3:I:100:ARG:NH2	9:I:201:HOH:O	2.27	0.43
1:G:484:ASP:OD1	1:G:484:ASP:N	2.52	0.43
1:A:542:LYS:HD3	1:D:310:PRO:HG2	2.01	0.43
2:B:73:LEU:HD21	2:B:106:ARG:HH12	1.84	0.43
2:H:182:GLN:HE21	2:H:182:GLN:HB2	1.63	0.43
1:J:33:SER:HB3	1:J:275:SER:HB3	2.01	0.43
1:J:175:VAL:HG11	1:J:457:ILE:HD11	2.00	0.43
7:J:605:5AD:C4	8:K:1601:B12:H463	2.49	0.43
2:K:191:MET:C	2:K:194:PRO:HD2	2.43	0.43
1:A:550:PRO:O	1:A:551:ASN:ND2	2.52	0.43
1:J:262:SER:HA	9:J:739:HOH:O	2.19	0.43
1:G:343[B]:MET:HE2	1:G:343[B]:MET:HB2	1.92	0.43
1:G:365:SER:HB3	1:G:380:ASP:HA	2.01	0.43
1:J:538:TRP:O	1:J:542:LYS:HG3	2.19	0.43
8:K:1601:B12:C6	8:K:1601:B12:H4B	2.49	0.43
1:A:306:PRO:O	1:A:312:GLY:HA3	2.18	0.42
1:D:21:LYS:H	1:D:21:LYS:HG2	1.71	0.42
2:E:79:ILE:HG13	2:E:199:LYS:HE3	2.01	0.42
1:J:284:ILE:HG22	1:J:326:LEU:HD12	2.00	0.42
1:J:302:CYS:O	1:J:306:PRO:HD2	2.18	0.42
1:D:296:GLN:HE21	1:D:362:SER:CB	2.31	0.42
1:G:453:ILE:O	1:G:457:ILE:HG12	2.20	0.42
3:I:46:ALA:O	3:I:50:PRO:HG3	2.18	0.42
3:I:66:LEU:O	3:I:70:LEU:HG	2.18	0.42
2:B:118:VAL:HA	2:B:121:ASN:ND2	2.33	0.42
2:B:50:GLU:HG3	2:B:220:LEU:HD23	2.01	0.42
8:E:1601:B12:H301	8:E:1601:B12:H253	1.74	0.42
2:H:67:VAL:HG13	2:H:71:PHE:CB	2.44	0.42
7:A:605:5AD:C4	8:B:1601:B12:H463	2.49	0.42
2:B:154:PHE:HB3	2:B:160:LEU:HD21	2.01	0.42
1:D:173:VAL:HG21	1:D:176:ALA:HA	2.01	0.42
2:H:62:GLU:OE2	2:H:103[B]:ARG:NH1	2.52	0.42
8:H:1601:B12:H363	8:H:1601:B12:H411	1.78	0.42
3:F:55:THR:HG21	3:F:64:PHE:CE2	2.55	0.42
3:F:55:THR:HB	3:F:78:ASP:O	2.20	0.42
1:J:62:ILE:HG23	1:J:286:ILE:HD11	2.02	0.42
2:K:73:LEU:HD23	2:K:73:LEU:HA	1.79	0.42
1:J:306:PRO:O	1:J:312:GLY:HA3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:111:SER:OG	2:B:208:THR:HG22	2.20	0.42
2:B:50:GLU:HG3	2:B:220:LEU:CD2	2.51	0.41
2:B:50:GLU:HB3	2:B:218:GLN:NE2	2.33	0.41
1:D:329:GLU:OE2	1:D:505:SER:HA	2.20	0.41
2:E:193:ARG:HG3	2:E:197:GLN:HB2	2.01	0.41
3:I:68:ASN:OD1	3:I:73:LYS:NZ	2.35	0.41
2:K:140:ILE:HD11	2:K:168:ILE:HG23	2.03	0.41
3:C:64:PHE:CD1	3:C:79:MET:HE2	2.55	0.41
3:F:100:ARG:HE	3:F:100:ARG:CA	2.32	0.41
1:D:62:ILE:HG23	1:D:286:ILE:HD11	2.02	0.41
2:E:98:GLU:HG3	2:E:177:LYS:HE2	2.01	0.41
1:G:20:VAL:HG12	1:G:21:LYS:O	2.20	0.41
2:B:208:THR:O	2:B:211:VAL:HG12	2.21	0.41
3:C:124:ASN:O	3:C:130:ARG:HG3	2.21	0.41
7:D:605:5AD:C4	8:E:1601:B12:H463	2.50	0.41
1:G:306:PRO:O	1:G:312:GLY:HA3	2.21	0.41
1:J:484:ASP:OD1	1:J:484:ASP:N	2.54	0.41
1:D:316:VAL:O	1:D:319:GLU:HG2	2.20	0.41
8:H:1601:B12:H601	8:H:1601:B12:H262	2.02	0.41
2:E:121:ASN:CG	2:E:143[B]:GLN:HA	2.46	0.41
1:G:25:GLU:H	1:G:25:GLU:CD	2.28	0.41
1:G:390:ILE:HD11	1:J:343[B]:MET:HG2	2.03	0.41
8:H:1601:B12:H301	8:H:1601:B12:H253	1.74	0.41
1:A:299:SER:OG	1:A:303:ILE:HA	2.21	0.40
2:E:88:LEU:HD23	2:E:88:LEU:HA	1.85	0.40
2:E:113:VAL:HB	2:E:133:GLN:HG3	2.02	0.40
1:G:395:LYS:HE3	1:G:538:TRP:CE2	2.56	0.40
1:G:177:ARG:HB3	1:G:457:ILE:HG23	2.02	0.40
2:K:176:ALA:C	2:K:178:ARG:H	2.30	0.40
2:E:103:ARG:HD2	2:E:219:GLU:OE2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	553/554 (100%)	533 (96%)	18 (3%)	2 (0%)	30	22
1	D	551/554 (100%)	534 (97%)	15 (3%)	2 (0%)	30	22
1	G	551/554 (100%)	536 (97%)	13 (2%)	2 (0%)	30	22
1	J	551/554 (100%)	533 (97%)	16 (3%)	2 (0%)	30	22
2	B	177/200 (88%)	172 (97%)	5 (3%)	0	100	100
2	E	174/200 (87%)	167 (96%)	7 (4%)	0	100	100
2	H	179/200 (90%)	175 (98%)	3 (2%)	1 (1%)	21	13
2	K	161/200 (80%)	153 (95%)	6 (4%)	2 (1%)	10	4
3	C	136/137 (99%)	134 (98%)	2 (2%)	0	100	100
3	F	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
3	I	135/137 (98%)	133 (98%)	2 (2%)	0	100	100
3	L	134/137 (98%)	130 (97%)	4 (3%)	0	100	100
All	All	3437/3564 (96%)	3332 (97%)	94 (3%)	11 (0%)	36	29

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	60	GLN
2	K	51	VAL
2	K	74	ALA
1	A	300	VAL
1	D	300	VAL
1	G	300	VAL
1	J	300	VAL
1	J	363	GLY
1	D	363	GLY
1	G	363	GLY
1	A	363	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	453/452 (100%)	450 (99%)	3 (1%)	76	78
1	D	451/452 (100%)	449 (100%)	2 (0%)	84	87
1	G	451/452 (100%)	449 (100%)	2 (0%)	84	87
1	J	451/452 (100%)	448 (99%)	3 (1%)	76	78
2	B	148/164 (90%)	142 (96%)	6 (4%)	27	19
2	E	147/164 (90%)	145 (99%)	2 (1%)	59	59
2	H	148/164 (90%)	145 (98%)	3 (2%)	48	46
2	K	139/164 (85%)	136 (98%)	3 (2%)	45	42
3	C	117/116 (101%)	116 (99%)	1 (1%)	70	73
3	F	116/116 (100%)	114 (98%)	2 (2%)	53	52
3	I	116/116 (100%)	115 (99%)	1 (1%)	70	73
3	L	115/116 (99%)	115 (100%)	0	100	100
All	All	2852/2928 (97%)	2824 (99%)	28 (1%)	68	70

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	178	TYR
1	A	501	TYR
1	A	551	ASN
2	B	73	LEU
2	B	77	VAL
2	B	88	LEU
2	B	89	ARG
2	B	97	GLU
2	B	119	GLU
3	C	150	LYS
1	D	178	TYR
1	D	501	TYR
2	E	97	GLU
2	E	119	GLU
3	F	77	GLN
3	F	100	ARG
1	G	178	TYR
1	G	501	TYR
2	H	59	GLN
2	H	67	VAL

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Mol	Chain	Res	Type
2	H	199	LYS
3	I	51	GLU
1	J	178	TYR
1	J	411	ILE
1	J	501	TYR
2	K	67	VAL
2	K	149	SER
2	K	220	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	35	ASN
1	A	388	ASN
1	A	465	ASN
1	A	467	ASN
1	A	543	ASN
1	A	551	ASN
2	B	171	ASN
2	B	218	GLN
1	D	388	ASN
1	D	487	GLN
1	D	513	GLN
2	E	56	GLN
3	F	47	ASN
1	G	95	ASN
1	G	119	HIS
1	G	182	ASN
1	G	513	GLN
2	H	59	GLN
2	H	60	GLN
2	H	150	ASN
2	H	182	GLN
2	H	190	GLN
2	H	216	ASN
3	I	47	ASN
3	I	72	ASN
1	J	45	ASN
1	J	89	ASN
1	J	182	ASN
1	J	479	GLN

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Mol	Chain	Res	Type
1	J	487	GLN
2	K	75	GLN
2	K	150	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 12 are monoatomic - 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	$\# Z > 2$
6	PGO	D	604	4	3,4,4	0.84	0	1,4,4	1.58	0
6	PGO	J	604	4	3,4,4	0.44	0	1,4,4	0.75	0
8	B12	H	1601	-	93,101,101	1.68	11 (11%)	146,166,166	1.58	23 (15%)
7	5AD	A	605	-	12,12,20	2.07	4 (33%)	17,17,30	2.79	9 (52%)
7	5AD	D	605	-	12,12,20	2.14	5 (41%)	17,17,30	2.68	7 (41%)
6	PGO	A	604	4	3,4,4	0.58	0	1,4,4	0.84	0
8	B12	K	1601	5	93,101,101	1.79	11 (11%)	146,166,166	1.51	21 (14%)
7	5AD	G	605	-	12,12,20	2.06	4 (33%)	17,17,30	2.66	8 (47%)
8	B12	B	1601	-	93,101,101	1.72	9 (9%)	146,166,166	1.53	21 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	B12	E	1601	-	93,101,101	1.63	10 (10%)	146,166,166	1.51	22 (15%)
6	PGO	G	604	4	3,4,4	0.46	0	1,4,4	0.51	0
7	5AD	J	605	-	12,12,20	2.06	4 (33%)	17,17,30	2.50	8 (47%)

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
6	PGO	D	604	4	-	1/2/2/2	-
6	PGO	J	604	4	-	1/2/2/2	-
8	B12	H	1601	-	-	9/56/223/223	0/3/11/11
7	5AD	A	605	-	-	-	0/2/2/3
7	5AD	D	605	-	-	-	0/2/2/3
6	PGO	A	604	4	-	1/2/2/2	-
8	B12	K	1601	5	-	11/56/223/223	0/3/11/11
7	5AD	G	605	-	-	-	0/2/2/3
8	B12	B	1601	-	-	6/56/223/223	0/3/11/11
8	B12	E	1601	-	-	7/56/223/223	0/3/11/11
6	PGO	G	604	4	-	1/2/2/2	-
7	5AD	J	605	-	-	-	0/2/2/3

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	K	1601	B12	C19-N24	-11.43	1.27	1.48
8	B	1601	B12	C19-N24	-10.79	1.28	1.48
8	H	1601	B12	C19-N24	-10.37	1.29	1.48
8	E	1601	B12	C19-N24	-9.70	1.30	1.48
8	E	1601	B12	C8B-C9B	5.84	1.50	1.40
8	K	1601	B12	C8B-C9B	5.41	1.49	1.40
8	B	1601	B12	C8B-C9B	5.40	1.49	1.40
8	H	1601	B12	C8B-C9B	5.28	1.49	1.40
8	H	1601	B12	C14-N23	-4.99	1.28	1.35
7	D	605	5AD	C5-C4	4.95	1.48	1.39
7	J	605	5AD	C5-C4	4.93	1.48	1.39
7	G	605	5AD	C5-C4	4.86	1.48	1.39
7	A	605	5AD	C5-C4	4.86	1.48	1.39
8	K	1601	B12	C14-N23	-4.72	1.29	1.35
8	K	1601	B12	C11-N23	4.49	1.45	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	1601	B12	C14-N23	-4.46	1.29	1.35
8	B	1601	B12	C11-N23	4.29	1.45	1.37
8	E	1601	B12	C14-N23	-4.20	1.29	1.35
8	E	1601	B12	C11-N23	4.07	1.44	1.37
8	H	1601	B12	C11-N23	3.71	1.44	1.37
8	H	1601	B12	C16-C15	-3.60	1.34	1.44
8	B	1601	B12	C6B-C5B	3.57	1.49	1.40
8	B	1601	B12	C16-C15	-3.55	1.34	1.44
8	K	1601	B12	C16-C15	-3.45	1.35	1.44
8	K	1601	B12	C6B-C5B	3.43	1.49	1.40
8	E	1601	B12	C6B-C5B	3.41	1.49	1.40
8	H	1601	B12	C6B-C5B	3.17	1.48	1.40
8	E	1601	B12	C16-C15	-3.13	1.35	1.44
8	B	1601	B12	C14-C15	2.87	1.50	1.38
7	D	605	5AD	C5-C6	2.84	1.49	1.41
8	E	1601	B12	C14-C15	2.82	1.50	1.38
8	K	1601	B12	C14-C15	2.78	1.50	1.38
7	G	605	5AD	C5-C6	2.78	1.48	1.41
8	K	1601	B12	C10-C9	2.76	1.47	1.39
7	A	605	5AD	C5-C6	2.75	1.48	1.41
8	K	1601	B12	C9B-N3B	-2.75	1.34	1.39
8	E	1601	B12	C9B-N3B	-2.73	1.34	1.39
8	E	1601	B12	C10-C9	2.72	1.46	1.39
8	H	1601	B12	C10-C9	2.69	1.46	1.39
8	H	1601	B12	C14-C15	2.69	1.49	1.38
7	D	605	5AD	C8-N7	2.68	1.36	1.31
8	B	1601	B12	C10-C9	2.60	1.46	1.39
7	J	605	5AD	C5-C6	2.57	1.48	1.41
7	J	605	5AD	C8-N7	2.52	1.36	1.31
8	B	1601	B12	C8B-N1B	-2.50	1.34	1.39
7	G	605	5AD	C8-N7	2.42	1.36	1.31
8	H	1601	B12	C9B-N3B	-2.42	1.35	1.39
7	A	605	5AD	C8-N7	2.41	1.36	1.31
8	H	1601	B12	C8B-N1B	-2.31	1.34	1.39
8	E	1601	B12	C8B-N1B	-2.31	1.34	1.39
7	A	605	5AD	C5-N7	-2.28	1.34	1.39
8	K	1601	B12	C8B-N1B	-2.27	1.34	1.39
7	D	605	5AD	C1'-N9	2.27	1.50	1.46
7	J	605	5AD	C5-N7	-2.24	1.34	1.39
7	G	605	5AD	C5-N7	-2.18	1.34	1.39
8	H	1601	B12	C2B-N1B	-2.08	1.33	1.37
8	K	1601	B12	C1-C2	-2.04	1.54	1.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	605	5AD	C5-N7	-2.03	1.35	1.39

All (119) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	605	5AD	C5-C4-N3	-6.79	117.89	126.75
7	D	605	5AD	C5-C4-N3	-6.69	118.02	126.75
7	G	605	5AD	C5-C4-N3	-6.57	118.18	126.75
8	H	1601	B12	C8B-C9B-N3B	-6.53	102.76	109.97
8	B	1601	B12	C8B-C9B-N3B	-6.36	102.95	109.97
8	H	1601	B12	C9B-N3B-C2B	6.21	111.84	104.44
7	J	605	5AD	C5-C4-N3	-5.95	118.99	126.75
8	K	1601	B12	C8B-C9B-N3B	-5.86	103.50	109.97
8	E	1601	B12	C8B-C9B-N3B	-5.84	103.52	109.97
8	B	1601	B12	C9B-N3B-C2B	5.78	111.33	104.44
8	K	1601	B12	C9B-N3B-C2B	5.70	111.24	104.44
8	E	1601	B12	C20-C1-C19	-5.28	104.26	109.36
8	E	1601	B12	C9B-N3B-C2B	5.16	110.59	104.44
8	K	1601	B12	C18-C19-N24	4.88	109.73	102.31
8	B	1601	B12	C18-C19-N24	4.51	109.18	102.31
8	H	1601	B12	C18-C19-N24	4.42	109.03	102.31
8	B	1601	B12	C4B-C9B-N3B	4.26	137.81	130.51
8	H	1601	B12	C13-C14-N23	4.17	114.77	109.10
8	H	1601	B12	C4B-C9B-N3B	4.07	137.50	130.51
8	B	1601	B12	C20-C1-C19	-4.05	105.45	109.36
8	E	1601	B12	C4B-C9B-N3B	4.05	137.46	130.51
8	E	1601	B12	C13-C14-N23	4.03	114.59	109.10
7	A	605	5AD	C2-N3-C4	4.02	121.24	111.75
8	E	1601	B12	C18-C19-N24	4.00	108.40	102.31
8	H	1601	B12	C9-C10-C11	-3.93	120.29	125.97
8	B	1601	B12	C9-C10-C11	-3.90	120.33	125.97
7	D	605	5AD	C2-N3-C4	3.83	120.80	111.75
7	A	605	5AD	C4-C5-N7	-3.78	106.02	110.62
7	G	605	5AD	C2-N3-C4	3.75	120.62	111.75
8	K	1601	B12	C20-C1-C19	-3.72	105.77	109.36
8	E	1601	B12	C9-C10-C11	-3.72	120.59	125.97
7	G	605	5AD	C4-C5-N7	-3.70	106.11	110.62
8	H	1601	B12	C20-C1-C19	-3.70	105.79	109.36
8	K	1601	B12	C4B-C9B-N3B	3.68	136.82	130.51
7	J	605	5AD	C2-N3-C4	3.64	120.34	111.75
7	A	605	5AD	N3-C4-N9	3.63	135.91	126.92
8	K	1601	B12	C48-C13-C14	3.61	117.49	108.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	K	1601	B12	C9-C10-C11	-3.59	120.77	125.97
7	D	605	5AD	C4-C5-N7	-3.57	106.28	110.62
7	D	605	5AD	N3-C4-N9	3.56	135.73	126.92
8	K	1601	B12	C13-C14-N23	3.54	113.92	109.10
7	G	605	5AD	N3-C4-N9	3.48	135.54	126.92
7	A	605	5AD	C5-N7-C8	3.47	108.45	103.51
8	B	1601	B12	C13-C14-N23	3.39	113.71	109.10
7	G	605	5AD	C5-N7-C8	3.37	108.30	103.51
8	B	1601	B12	C48-C13-C14	3.33	116.80	108.49
8	H	1601	B12	C13-C14-C15	-3.29	119.28	124.32
7	J	605	5AD	N3-C4-N9	3.27	135.01	126.92
7	D	605	5AD	C5-N7-C8	3.22	108.09	103.51
8	B	1601	B12	C8B-N1B-C2B	3.22	109.37	106.37
7	J	605	5AD	C4-C5-N7	-3.17	106.76	110.62
8	E	1601	B12	C9B-C8B-N1B	3.16	106.69	105.35
8	H	1601	B12	N1B-C2B-N3B	-3.15	109.60	113.91
8	B	1601	B12	C17-C16-C15	3.13	131.19	126.26
7	J	605	5AD	N3-C2-N1	-3.10	123.75	128.60
8	H	1601	B12	C9B-C8B-N1B	3.03	106.63	105.35
8	B	1601	B12	C17-C16-N24	-3.00	106.52	111.15
8	H	1601	B12	C2P-C1P-N59	-3.00	108.52	112.93
7	A	605	5AD	N3-C2-N1	-3.00	123.92	128.60
8	H	1601	B12	C8B-N1B-C2B	3.00	109.16	106.37
8	K	1601	B12	N1B-C2B-N3B	-2.99	109.83	113.91
8	K	1601	B12	C36-C7-C37	2.97	115.70	110.80
8	B	1601	B12	N1B-C2B-N3B	-2.96	109.86	113.91
8	H	1601	B12	C48-C13-C14	2.96	115.86	108.49
8	K	1601	B12	C17-C16-C15	2.96	130.92	126.26
8	K	1601	B12	C8B-N1B-C2B	2.87	109.05	106.37
8	K	1601	B12	C55-C56-C57	-2.84	105.04	111.23
7	G	605	5AD	N3-C2-N1	-2.83	124.18	128.60
7	D	605	5AD	N3-C2-N1	-2.81	124.21	128.60
8	K	1601	B12	C2P-C1P-N59	-2.79	108.82	112.93
8	E	1601	B12	C2P-C1P-N59	-2.76	108.86	112.93
8	H	1601	B12	C17-C16-N24	-2.75	106.91	111.15
8	B	1601	B12	C13-C14-C15	-2.74	120.13	124.32
8	E	1601	B12	C13-C14-C15	-2.73	120.15	124.32
7	J	605	5AD	C5-N7-C8	2.71	107.36	103.51
8	K	1601	B12	C13-C14-C15	-2.69	120.20	124.32
8	B	1601	B12	C9B-C8B-N1B	2.69	106.49	105.35
8	E	1601	B12	C17-C16-C15	2.66	130.45	126.26
8	H	1601	B12	C17-C16-C15	2.62	130.38	126.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	1601	B12	C53-C15-C16	2.55	124.77	120.38
8	E	1601	B12	C30-C3-C2	-2.50	113.80	119.09
8	K	1601	B12	C30-C3-C2	-2.49	113.81	119.09
8	E	1601	B12	C19-C1-N21	2.48	104.71	102.16
8	H	1601	B12	C12-C11-C10	2.47	126.58	123.37
8	K	1601	B12	C9B-C8B-N1B	2.46	106.39	105.35
8	B	1601	B12	C30-C3-C4	2.45	115.32	109.63
8	K	1601	B12	C17-C16-N24	-2.44	107.39	111.15
8	B	1601	B12	C19-C1-N21	2.44	104.66	102.16
8	H	1601	B12	C1-C19-N24	2.42	108.96	106.24
8	H	1601	B12	C55-C56-C57	-2.41	105.98	111.23
8	E	1601	B12	C2-C1-C19	2.36	122.33	118.60
7	A	605	5AD	N9-C8-N7	-2.34	110.84	114.26
8	K	1601	B12	C20-C1-N21	2.28	114.00	110.27
8	H	1601	B12	C36-C7-C37	2.27	114.55	110.80
8	H	1601	B12	C30-C3-C2	-2.25	114.32	119.09
8	K	1601	B12	C53-C15-C16	2.24	124.24	120.38
8	E	1601	B12	C12-C11-C10	2.22	126.26	123.37
7	G	605	5AD	N9-C8-N7	-2.22	111.02	114.26
8	H	1601	B12	O3-C2P-C1P	2.19	111.28	106.92
8	H	1601	B12	C8-C9-C10	-2.18	118.62	123.32
7	D	605	5AD	N9-C8-N7	-2.17	111.09	114.26
8	E	1601	B12	N1B-C2B-N3B	-2.17	110.95	113.91
8	B	1601	B12	C1-C19-N24	2.15	108.66	106.24
8	B	1601	B12	C30-C3-C2	-2.11	114.63	119.09
8	B	1601	B12	C53-C15-C16	2.09	123.98	120.38
8	E	1601	B12	C1-C19-N24	2.09	108.59	106.24
8	E	1601	B12	C53-C15-C14	-2.08	114.23	118.43
7	A	605	5AD	C6-C5-N7	2.07	135.88	132.02
7	J	605	5AD	N6-C6-N1	2.06	122.87	118.35
8	K	1601	B12	C8-C9-C10	-2.06	118.88	123.32
8	B	1601	B12	C2P-C1P-N59	-2.05	109.91	112.93
8	E	1601	B12	C26-C2-C1	2.05	113.20	110.01
7	G	605	5AD	C6-C5-N7	2.05	135.83	132.02
7	A	605	5AD	N6-C6-N1	2.04	122.81	118.35
7	J	605	5AD	C2-N1-C6	2.03	122.26	118.77
8	E	1601	B12	C8B-N1B-C2B	2.02	108.25	106.37
8	E	1601	B12	O3-C2P-C1P	2.01	110.92	106.92
8	E	1601	B12	C48-C13-C14	2.00	113.48	108.49
8	B	1601	B12	C1R-N1B-C2B	-2.00	122.62	127.14

There are no chirality outliers.

All (37) torsion outliers are listed below:

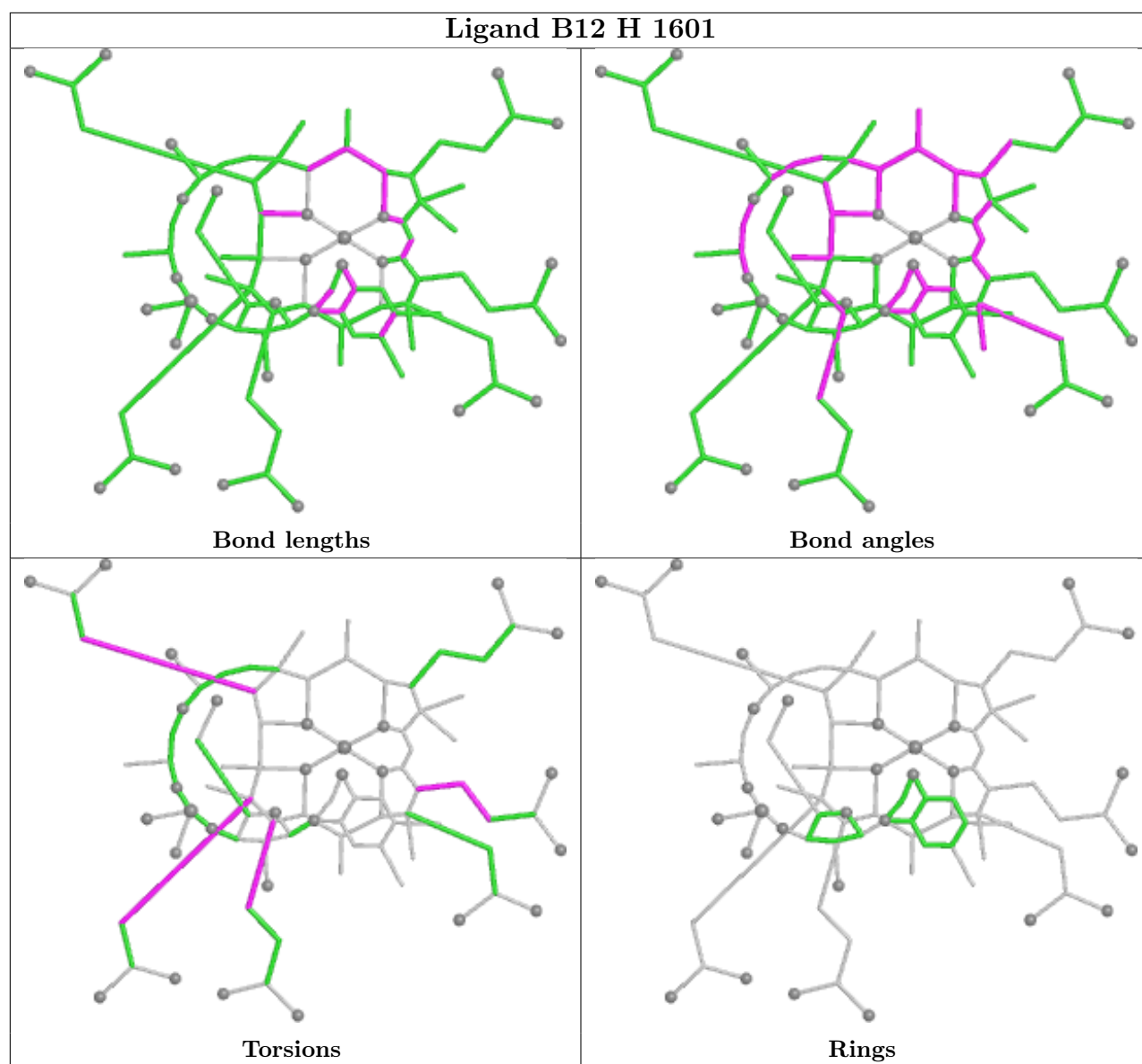
Mol	Chain	Res	Type	Atoms
8	K	1601	B12	C7-C37-C38-O39
8	K	1601	B12	C7-C37-C38-N40
8	K	1601	B12	C2-C3-C30-C31
8	E	1601	B12	C1-C2-C26-C27
8	E	1601	B12	C25-C2-C26-C27
8	E	1601	B12	C3-C2-C26-C27
8	H	1601	B12	C1-C2-C26-C27
8	H	1601	B12	C3-C2-C26-C27
8	H	1601	B12	C2-C3-C30-C31
8	K	1601	B12	C4-C3-C30-C31
8	H	1601	B12	C25-C2-C26-C27
8	K	1601	B12	C1-C2-C26-C27
8	K	1601	B12	C25-C2-C26-C27
6	D	604	PGO	O1-C1-C2-O2
6	G	604	PGO	O1-C1-C2-O2
8	H	1601	B12	C42-C41-C8-C9
8	K	1601	B12	C42-C41-C8-C9
8	H	1601	B12	C4-C3-C30-C31
8	B	1601	B12	C1-C2-C26-C27
8	K	1601	B12	C3-C2-C26-C27
8	B	1601	B12	C42-C41-C8-C9
8	E	1601	B12	C42-C41-C8-C9
8	B	1601	B12	C3-C2-C26-C27
8	B	1601	B12	C17-C18-C60-C61
8	E	1601	B12	C17-C18-C60-C61
8	K	1601	B12	C17-C18-C60-C61
8	K	1601	B12	C19-C18-C60-C61
8	E	1601	B12	C12-C13-C48-C49
6	A	604	PGO	O1-C1-C2-O2
8	B	1601	B12	C25-C2-C26-C27
8	B	1601	B12	C19-C18-C60-C61
8	E	1601	B12	C19-C18-C60-C61
8	H	1601	B12	C19-C18-C60-C61
8	K	1601	B12	C8-C41-C42-C43
8	H	1601	B12	C8-C41-C42-C43
6	J	604	PGO	O1-C1-C2-O2
8	H	1601	B12	C17-C18-C60-C61

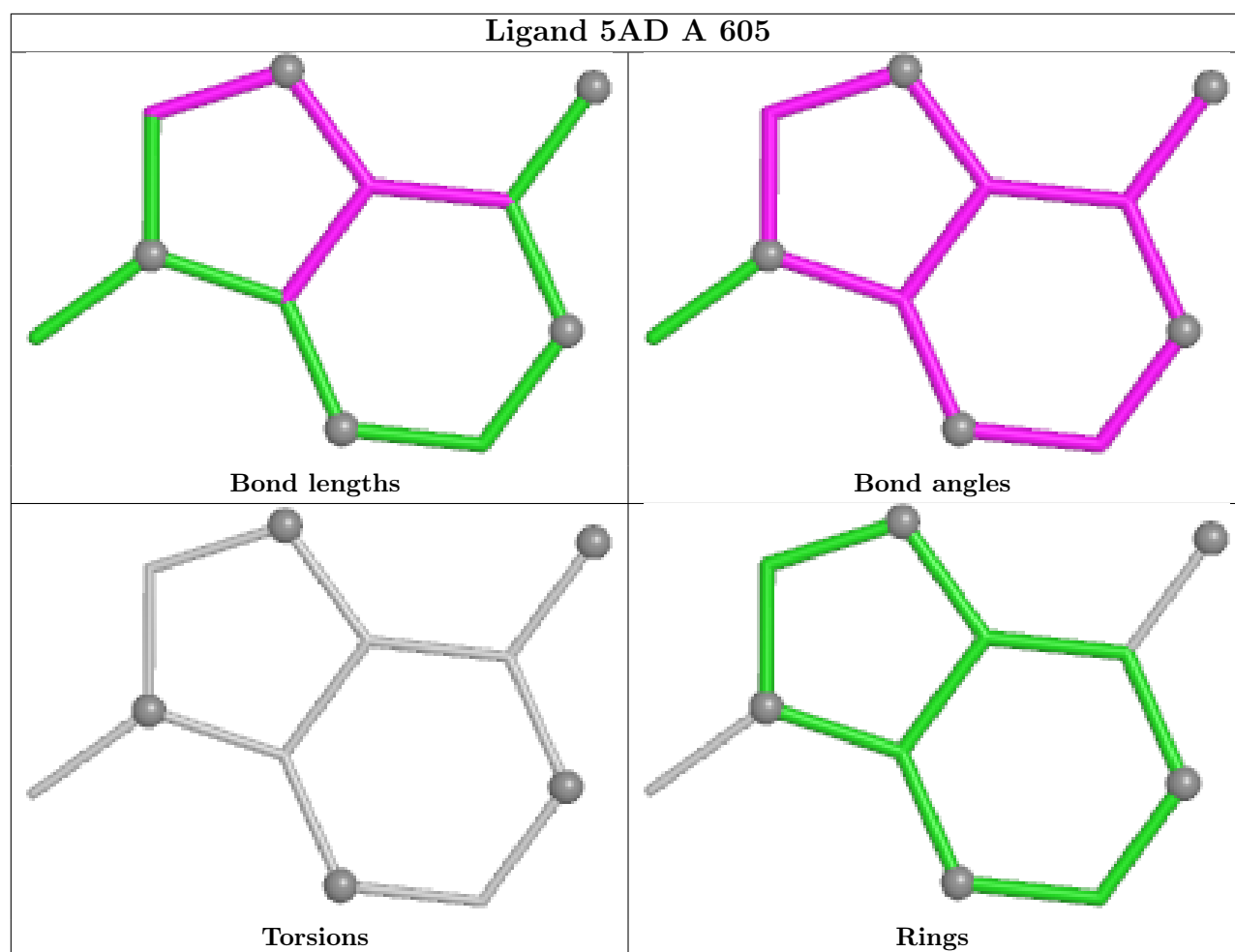
There are no ring outliers.

8 monomers are involved in 31 short contacts:

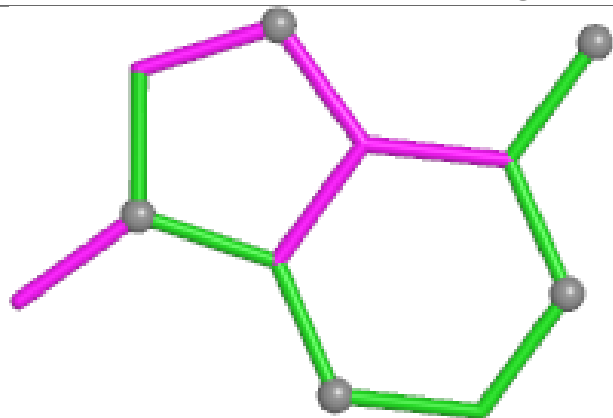
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	H	1601	B12	8	0
7	A	605	5AD	1	0
7	D	605	5AD	1	0
8	K	1601	B12	9	0
7	G	605	5AD	1	0
8	B	1601	B12	6	0
8	E	1601	B12	7	0
7	J	605	5AD	2	0

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.

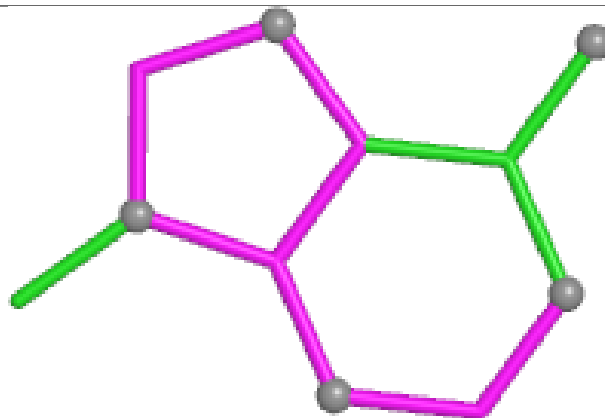




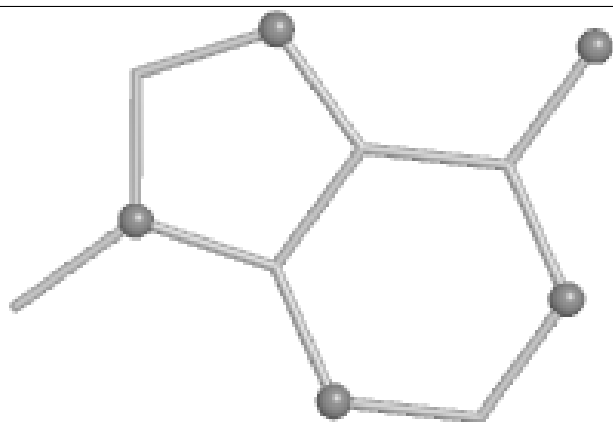
Ligand 5AD D 605



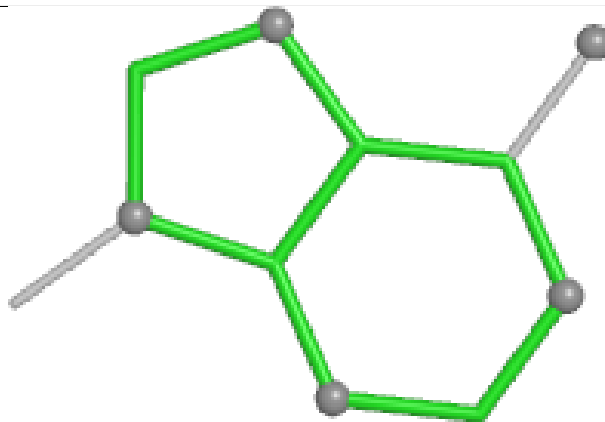
Bond lengths



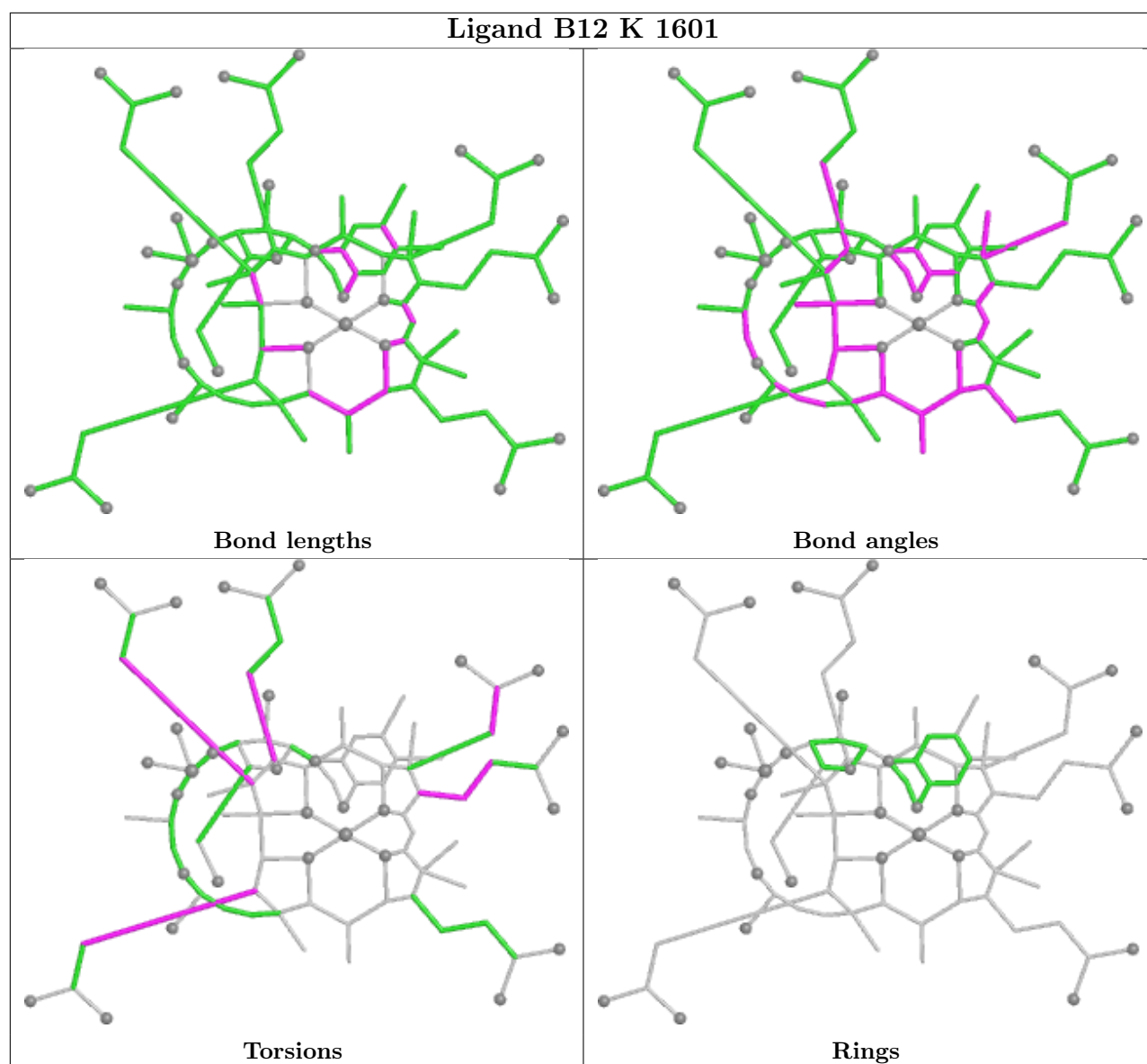
Bond angles

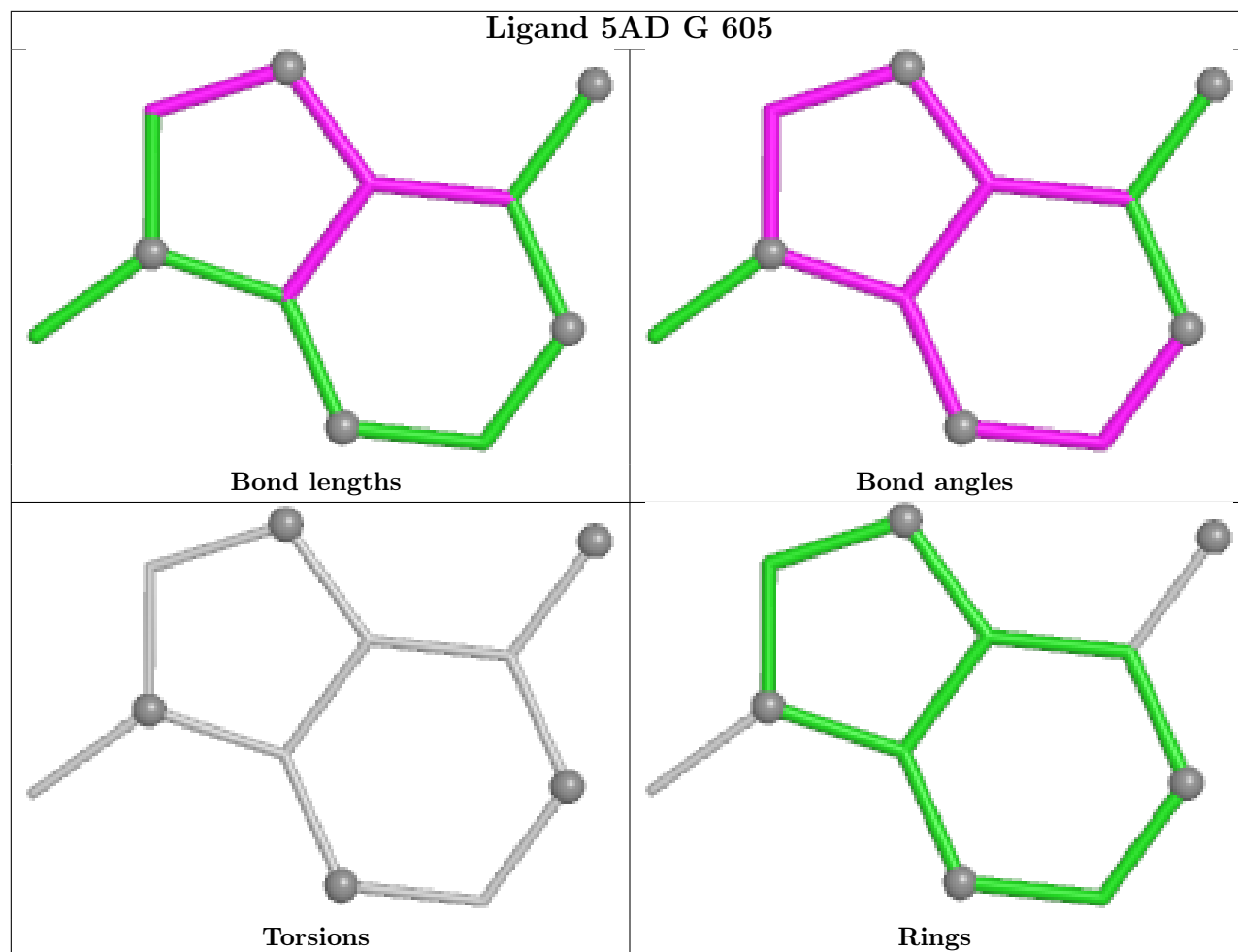


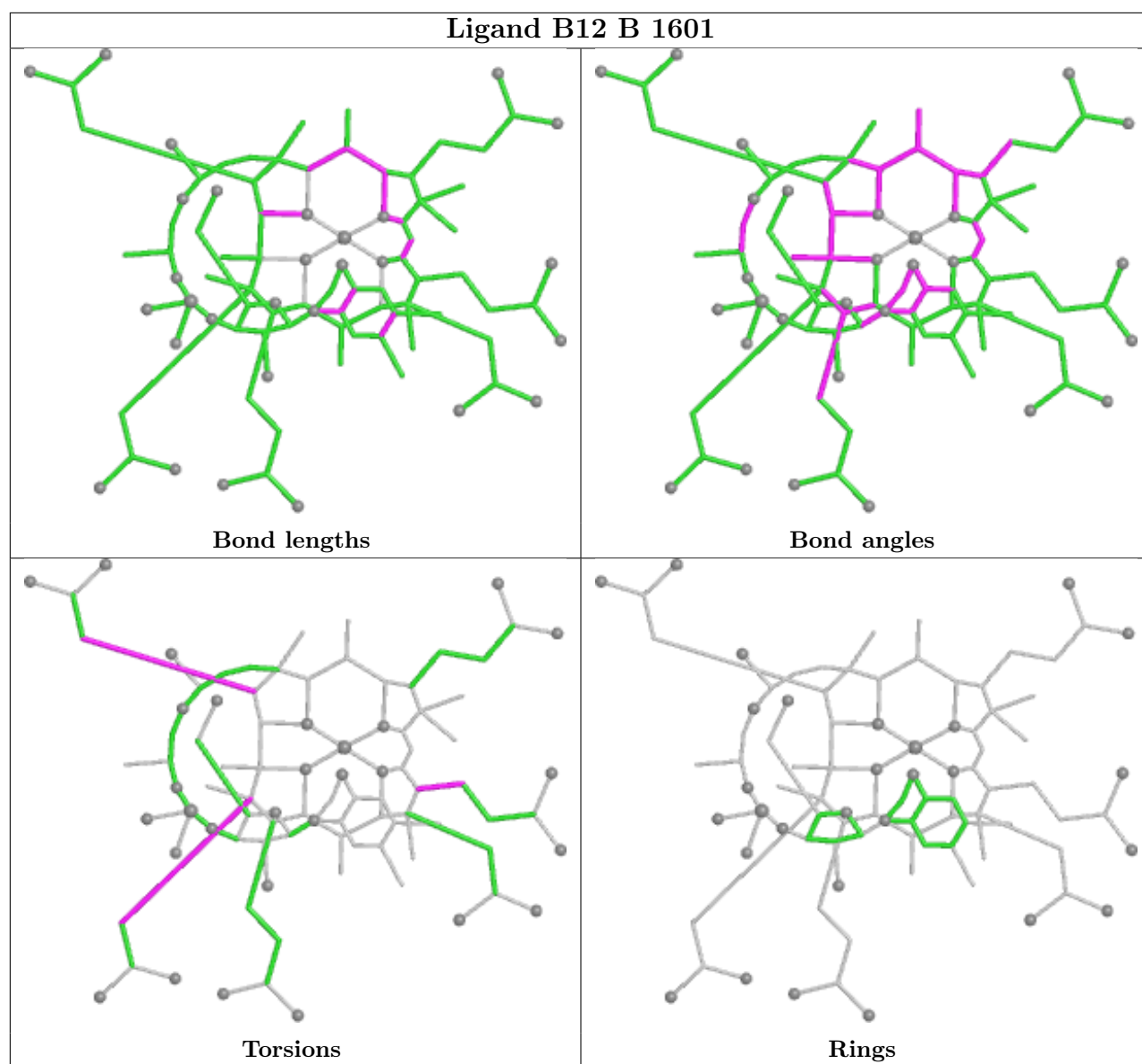
Torsions

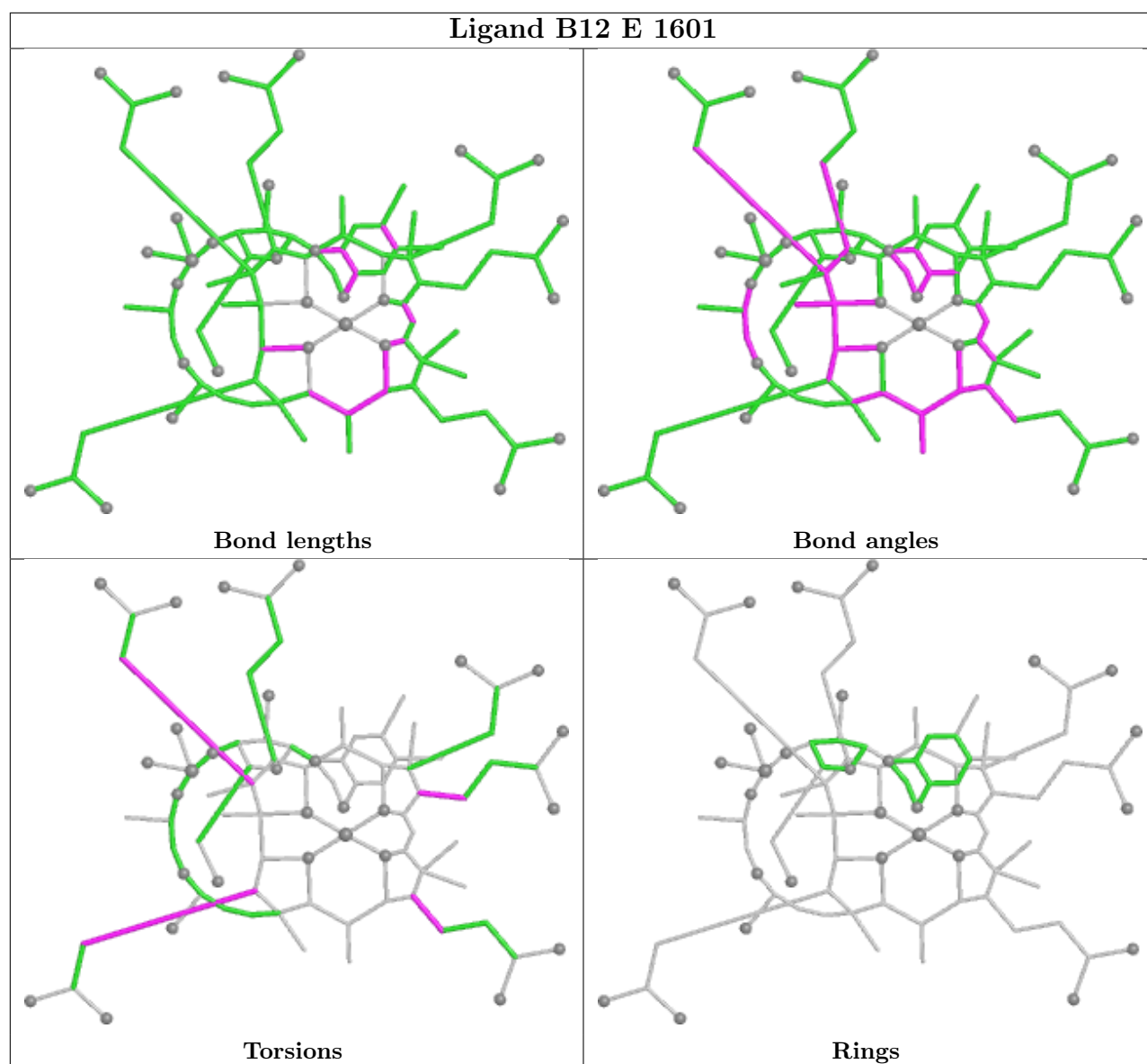


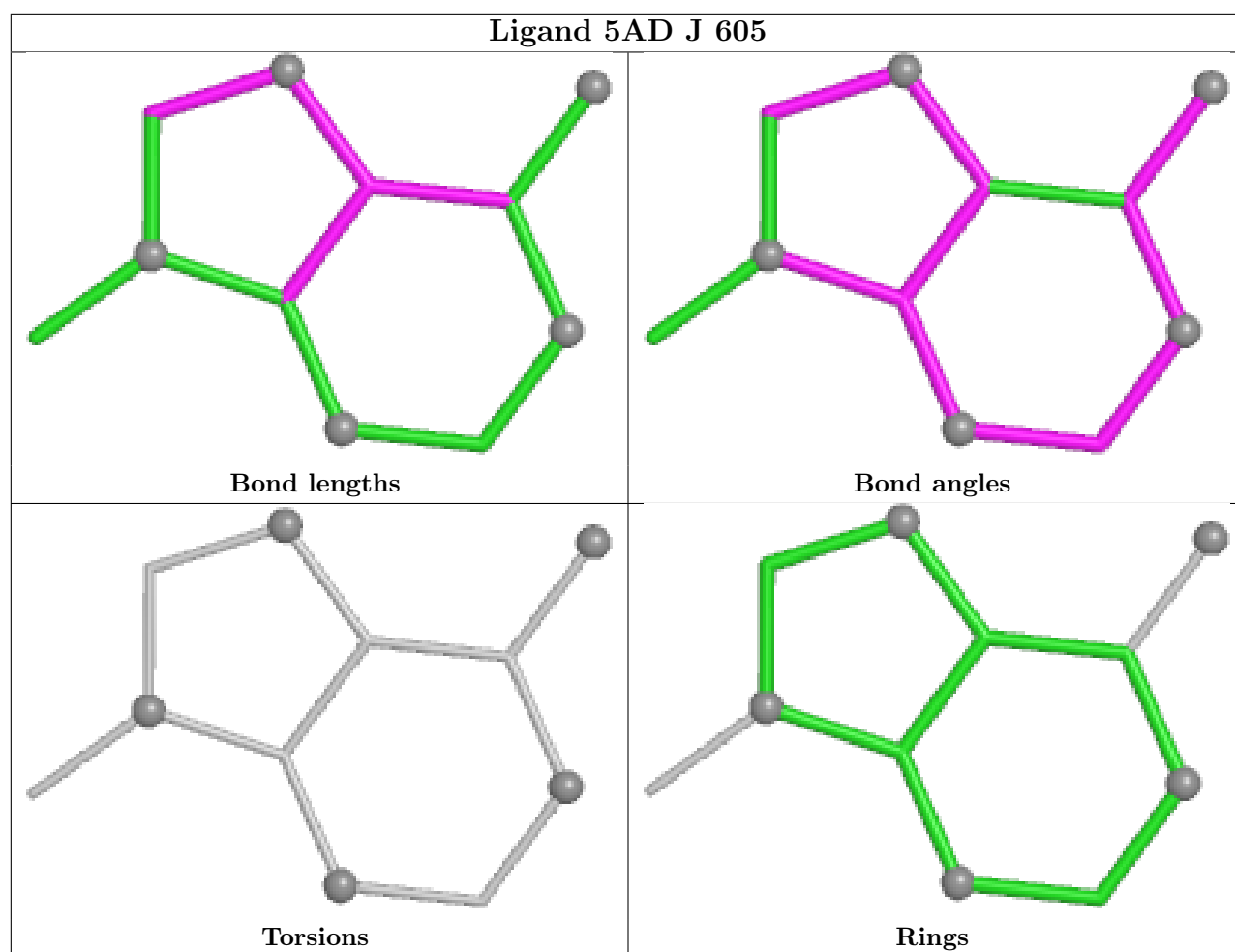
Rings











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	551/554 (99%)	-0.43	0 100 100	11, 31, 55, 90	4 (0%)
1	D	550/554 (99%)	-0.72	1 (0%) 91 92	8, 21, 44, 89	4 (0%)
1	G	550/554 (99%)	-0.21	1 (0%) 91 92	17, 36, 66, 91	3 (0%)
1	J	551/554 (99%)	0.07	2 (0%) 88 90	21, 47, 72, 91	3 (0%)
2	B	177/200 (88%)	1.52	49 (27%) 1 1	35, 73, 98, 111	2 (1%)
2	E	176/200 (88%)	0.31	3 (1%) 69 72	24, 48, 71, 112	2 (1%)
2	H	180/200 (90%)	0.40	4 (2%) 62 66	34, 57, 86, 136	1 (0%)
2	K	167/200 (83%)	1.41	34 (20%) 3 2	55, 94, 119, 131	0
3	C	136/137 (99%)	0.09	1 (0%) 84 86	25, 45, 66, 78	3 (2%)
3	F	136/137 (99%)	-0.35	1 (0%) 84 86	14, 33, 51, 66	1 (0%)
3	I	136/137 (99%)	0.31	2 (1%) 72 75	27, 54, 83, 100	2 (1%)
3	L	136/137 (99%)	0.89	4 (2%) 53 57	53, 74, 97, 110	0
All	All	3446/3564 (96%)	0.01	102 (2%) 52 56	8, 41, 89, 136	25 (0%)

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	44	PRO	3.7
2	B	123	LEU	3.7
2	B	222	VAL	3.6
2	B	47	PHE	3.6
2	H	45	GLY	3.6
2	B	46	GLY	3.5
2	B	51	VAL	3.5
2	K	220	LEU	3.4
2	K	141	HIS	3.4
2	B	128	ILE	3.3
3	L	38	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
2	K	146	PRO	3.2
2	B	105	ILE	3.2
2	K	105	ILE	3.2
2	K	222	VAL	3.2
2	B	65	ILE	3.2
2	B	92	ILE	3.2
2	H	223	ALA	3.2
2	B	116	VAL	3.2
2	H	58	THR	3.1
2	B	115	PHE	3.1
2	K	186	THR	3.1
2	E	58	THR	3.1
2	B	73	LEU	3.1
2	B	91	VAL	3.0
3	C	56	ALA	2.9
2	B	63	VAL	2.9
2	B	213	THR	2.8
2	K	51	VAL	2.8
2	B	48	LEU	2.8
2	B	107	CYS	2.8
2	B	220	LEU	2.7
2	K	140	ILE	2.7
3	F	56	ALA	2.7
2	B	168	ILE	2.7
1	J	1	MET	2.6
2	B	58	THR	2.6
2	B	49	THR	2.6
2	B	164	THR	2.6
2	K	153	LEU	2.6
2	B	77	VAL	2.6
2	B	108	PHE	2.5
2	B	184	VAL	2.5
2	B	210	TYR	2.5
2	B	70	ALA	2.5
2	K	176	ALA	2.5
2	K	49	THR	2.5
2	K	154	PHE	2.4
2	K	87	ILE	2.4
2	K	128	ILE	2.4
2	B	172	ALA	2.4
2	K	123	LEU	2.4
2	B	130	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
2	K	102	ALA	2.4
2	K	173	ALA	2.4
2	K	148	LEU	2.4
3	L	60	THR	2.4
2	B	139	VAL	2.4
2	B	76	THR	2.3
2	B	64	ILE	2.3
2	B	104	VAL	2.3
2	K	104	VAL	2.3
2	K	151	LEU	2.3
2	B	72	GLY	2.3
2	K	60	GLN	2.3
2	B	175	TYR	2.3
2	B	181	PRO	2.3
2	K	122	ARG	2.3
2	K	118	VAL	2.3
2	B	186	THR	2.3
3	L	66	LEU	2.3
2	B	173	ALA	2.2
2	K	185	PRO	2.2
1	G	430	PRO	2.2
2	K	74	ALA	2.2
2	K	139	VAL	2.2
2	K	52	GLY	2.2
2	E	223	ALA	2.2
2	B	132	ILE	2.2
3	L	81	ILE	2.2
2	B	211	VAL	2.2
2	K	63	VAL	2.2
2	K	80	VAL	2.2
2	B	138	THR	2.2
2	K	76	THR	2.2
2	K	75	GLN	2.1
1	J	233	THR	2.1
2	K	184	VAL	2.1
2	B	169	GLY	2.1
2	B	187	LEU	2.1
2	B	74	ALA	2.1
2	B	102	ALA	2.1
3	I	56	ALA	2.1
2	B	140	ILE	2.1
2	B	113	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
3	I	69	VAL	2.1
1	D	1	MET	2.1
2	B	95	ILE	2.1
2	K	73	LEU	2.1
2	K	54	ALA	2.1
2	E	92	ILE	2.0
2	B	100	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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($\text{\AA}^2$)	Q<0.9
7	5AD	J	605	11/18	0.76	0.16	60,64,72,79	0
7	5AD	G	605	11/18	0.78	0.13	36,46,54,59	0
6	PGO	J	604	5/5	0.84	0.20	35,53,61,64	0
7	5AD	A	605	11/18	0.84	0.11	36,37,50,60	0
7	5AD	D	605	11/18	0.85	0.11	25,35,48,52	0
6	PGO	G	604	5/5	0.87	0.15	30,33,49,53	0
6	PGO	A	604	5/5	0.92	0.12	24,25,43,48	0
6	PGO	D	604	5/5	0.93	0.13	18,19,35,42	0
5	K	J	602	1/1	0.95	0.08	34,34,34,34	0
5	K	J	603	1/1	0.95	0.08	54,54,54,54	0
8	B12	K	1601	91/91	0.95	0.11	61,70,75,79	0
8	B12	B	1601	91/91	0.96	0.08	34,42,50,57	0
8	B12	H	1601	91/91	0.97	0.07	29,36,45,55	0
5	K	G	603	1/1	0.97	0.07	36,36,36,36	0
8	B12	E	1601	91/91	0.98	0.06	18,26,34,36	0
4	CA	G	601	1/1	0.98	0.07	26,26,26,26	0

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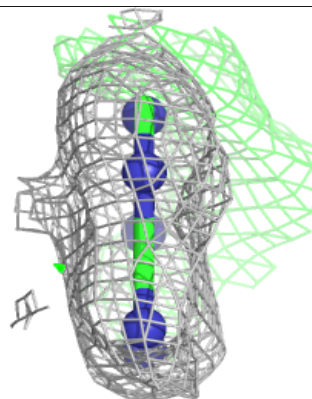
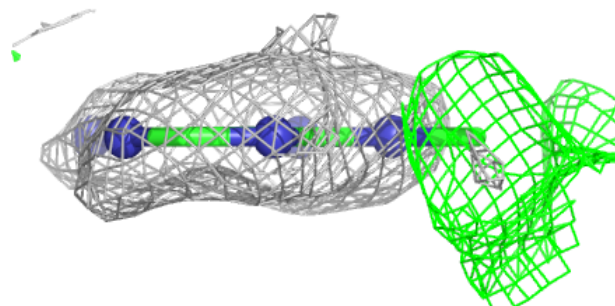
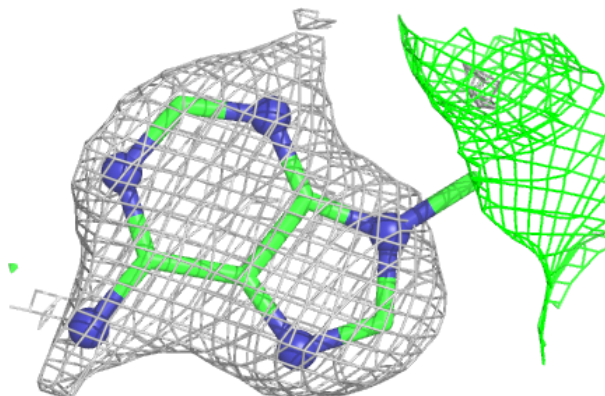
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CA	J	601	1/1	0.98	0.06	32,32,32,32	0
4	CA	D	601	1/1	0.99	0.13	6,6,6,6	0
5	K	A	602	1/1	0.99	0.02	27,27,27,27	0
5	K	A	603	1/1	0.99	0.05	35,35,35,35	0
5	K	D	602	1/1	0.99	0.02	22,22,22,22	0
5	K	D	603	1/1	0.99	0.07	27,27,27,27	0
5	K	G	602	1/1	0.99	0.04	30,30,30,30	0
4	CA	A	601	1/1	0.99	0.03	20,20,20,20	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.

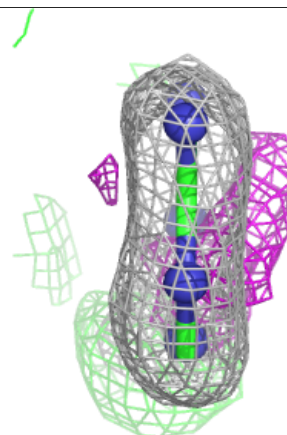
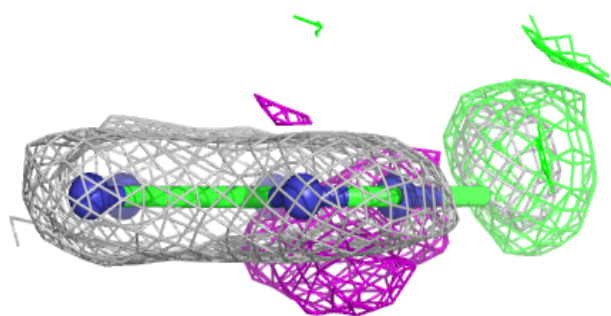
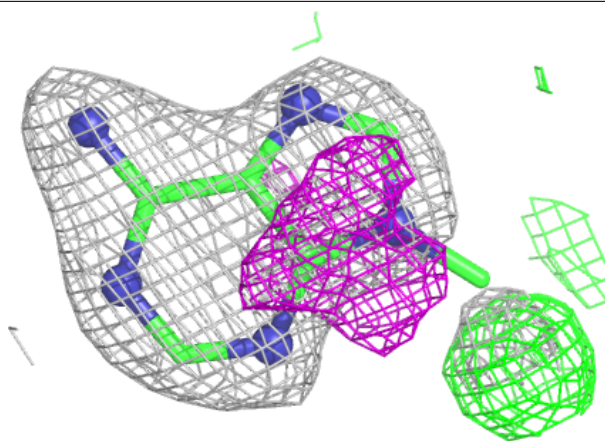
Electron density around 5AD J 605:

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



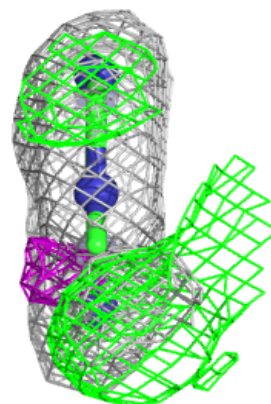
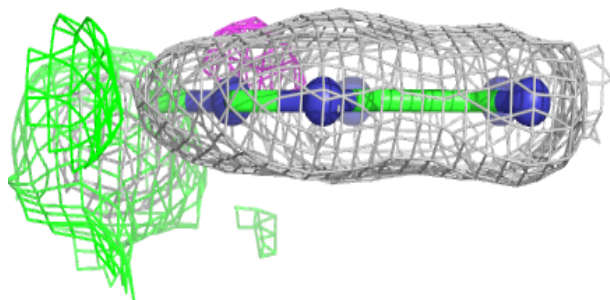
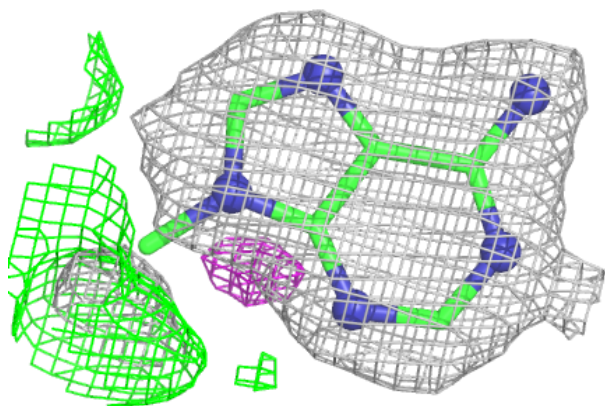
Electron density around 5AD G 605:

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



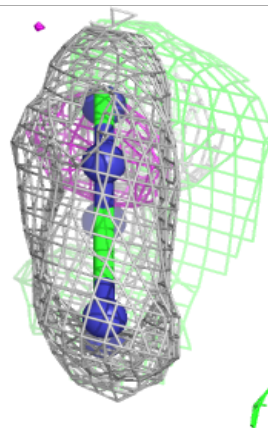
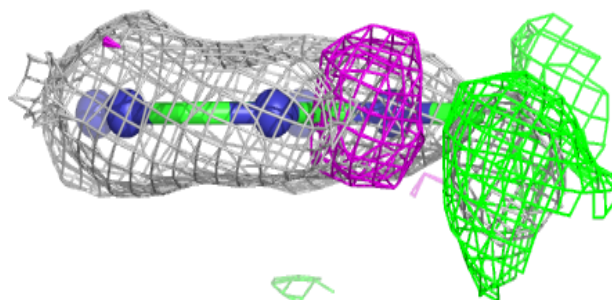
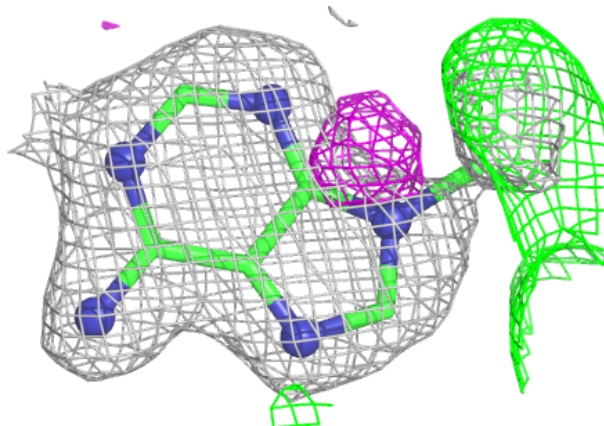
Electron density around 5AD A 605:

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



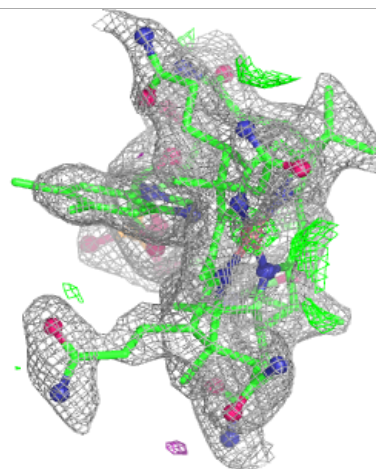
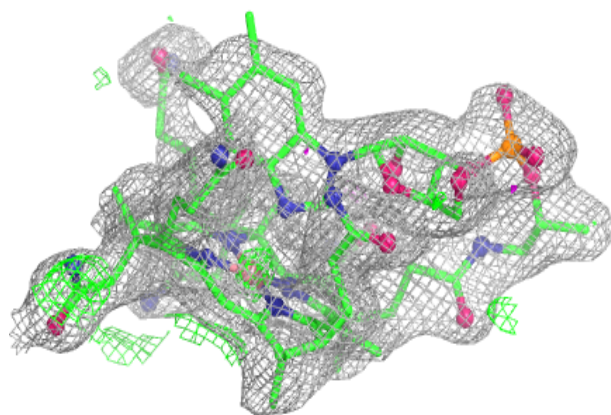
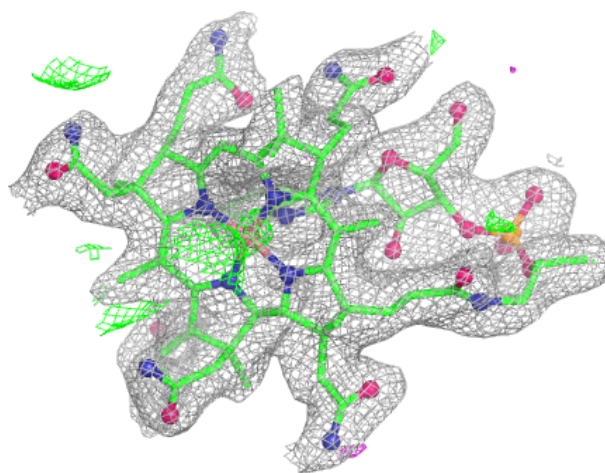
Electron density around 5AD D 605:

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



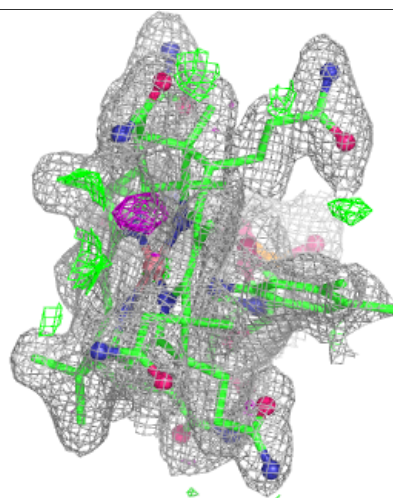
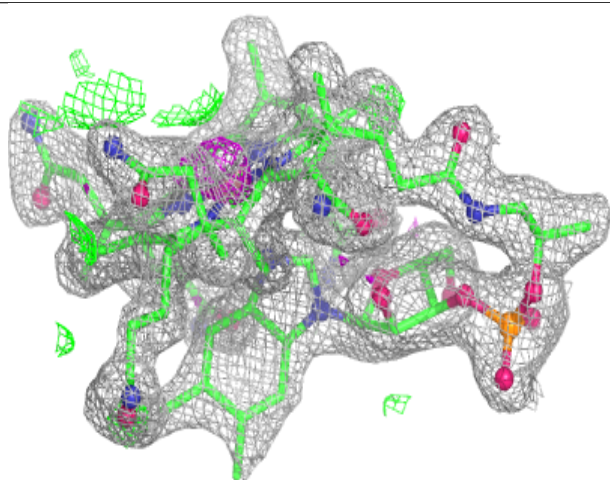
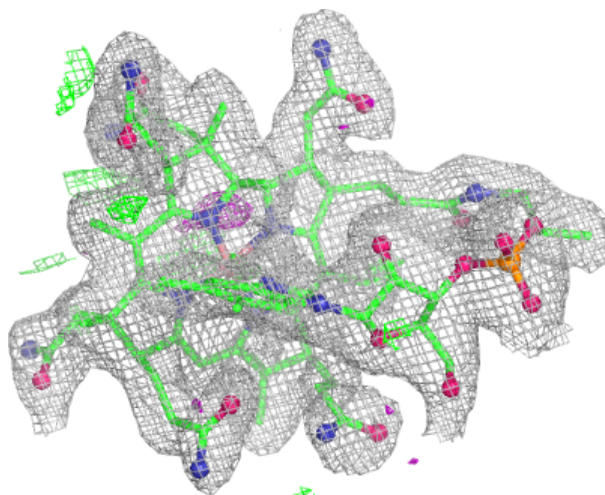
Electron density around B12 K 1601:

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



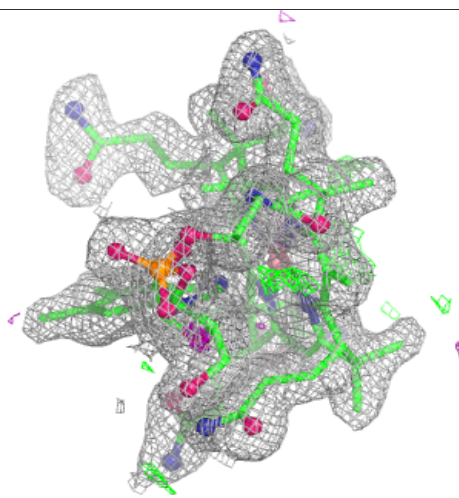
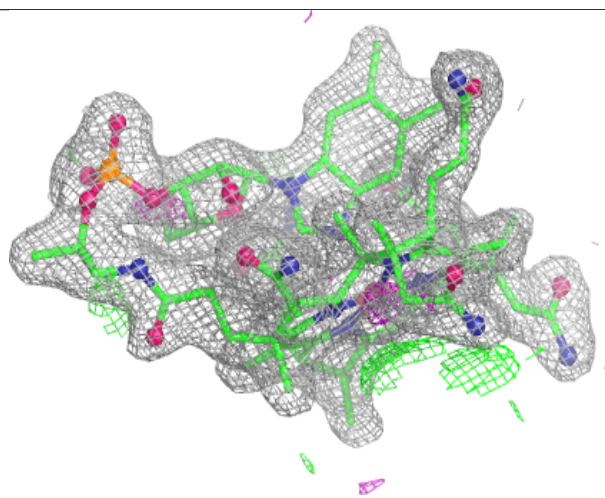
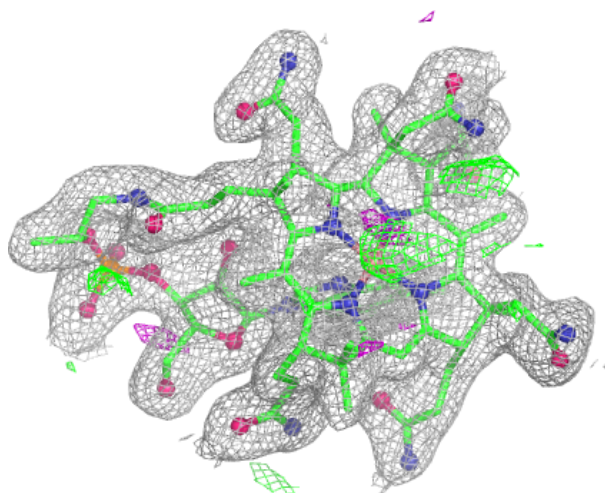
Electron density around B12 B 1601:

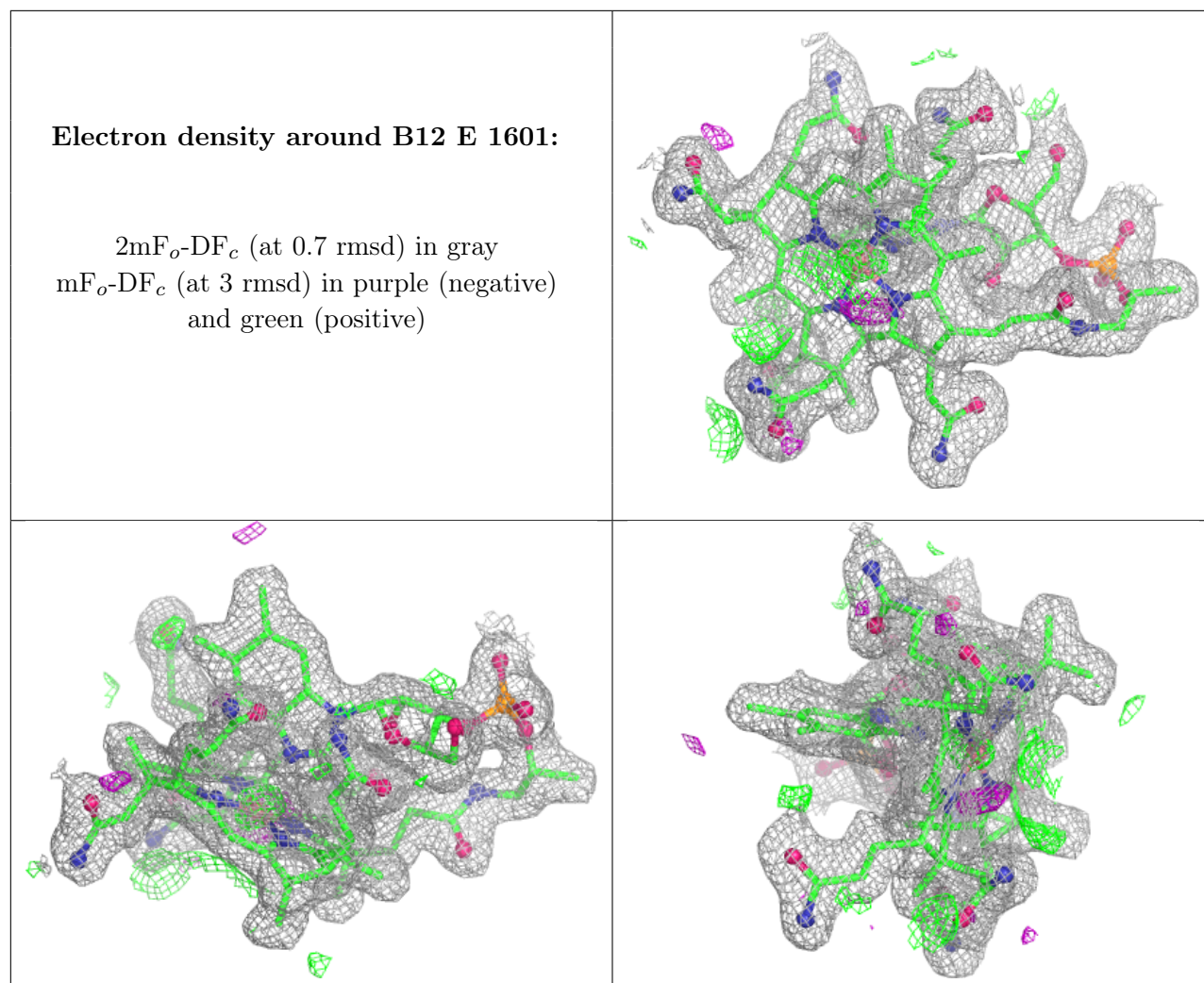
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around B12 H 1601:

$2mF_o-DF_c$ (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.