Full wwPDB X-ray Structure Validation Report ⓘ

Nov 14, 2023 – 02:27 AM JST

PDB ID	:	5YSH
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)

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

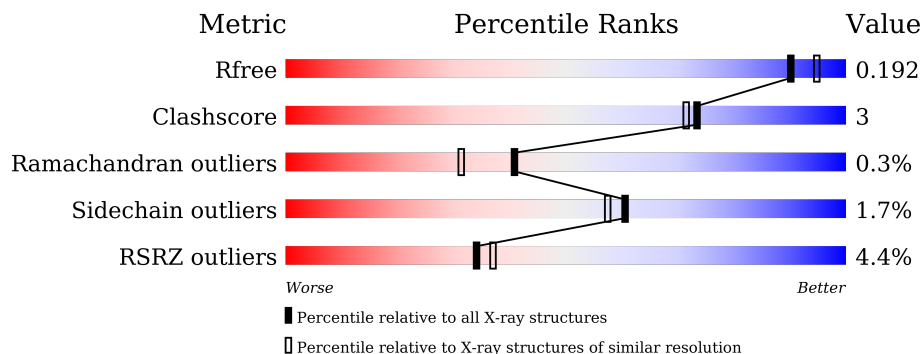|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.90 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	Percentile Ranks	Value
Rfree		0.192
Clashscore		3
Ramachandran outliers		0.3%
Sidechain outliers		1.7%
RSRZ outliers		4.4%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	554	94% 5% •
1	D	554	93% 6% •
1	G	554	.% 94% 5% •
1	J	554	.% 92% 7% •
2	B	200	20% 72% 14% • 12%
2	E	200	2% 78% 10% 12%

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Mol	Chain	Length	Quality of chain
2	H	200	4% / 82% / 7% / 10%
2	K	200	32% / 68% / 14% / 16%
3	C	137	% / 91% / 9%
3	F	137	% / 96%
3	I	137	4% / 88% / 11%
3	L	137	10% / 92% / 7%

2 Entry composition ⓘ

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 (three-letter code: 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 (three-letter code: 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 (three-letter code: PGO) (formula: $C_3H_8O_2$).

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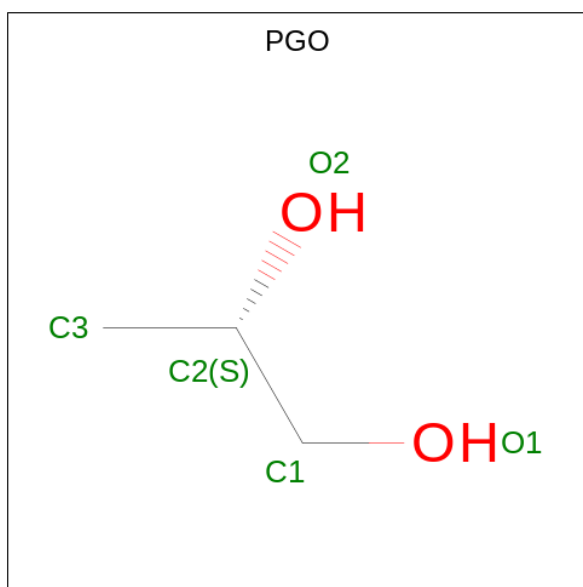
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total 5	C 3	O 2	0	0
6	D	1	Total 5	C 3	O 2	0	0
6	G	1	Total 5	C 3	O 2	0	0
6	J	1	Total 5	C 3	O 2	0	0

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

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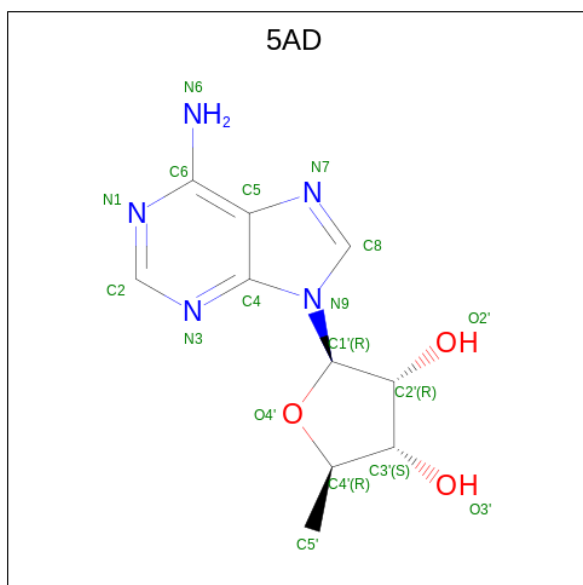
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total 11	C 6	N 5	0	0
7	D	1	Total 11	C 6	N 5	0	0
7	G	1	Total 11	C 6	N 5	0	0
7	J	1	Total 11	C 6	N 5	0	0

• Molecule 8 is COBALAMIN (three-letter code: B12) (formula: $C_{62}H_{89}CoN_{13}O_{14}P$).

B12
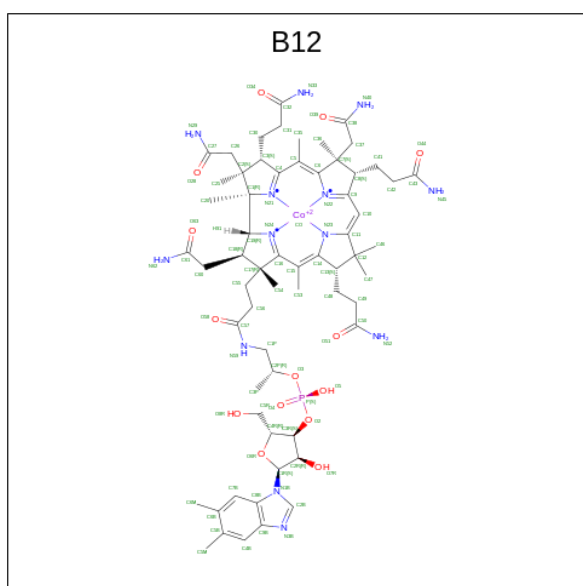
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	B	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0
8	E	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0
8	H	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0
8	K	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0

• Molecule 9 is water.

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

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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.
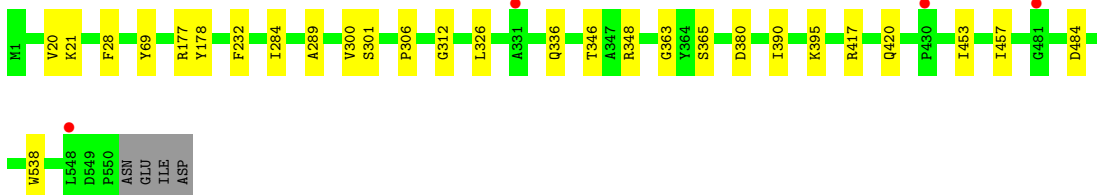
• Molecule 1: Diol dehydrase alpha subunit

Chain A:
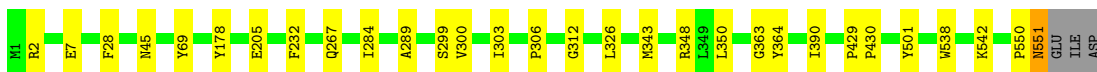
• Molecule 1: Diol dehydrase alpha subunit

Chain D:
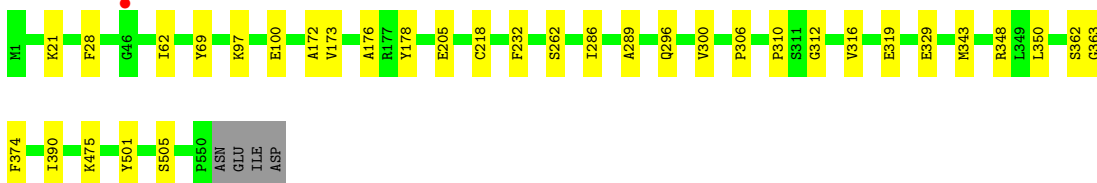
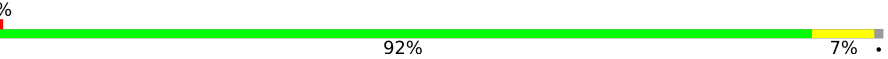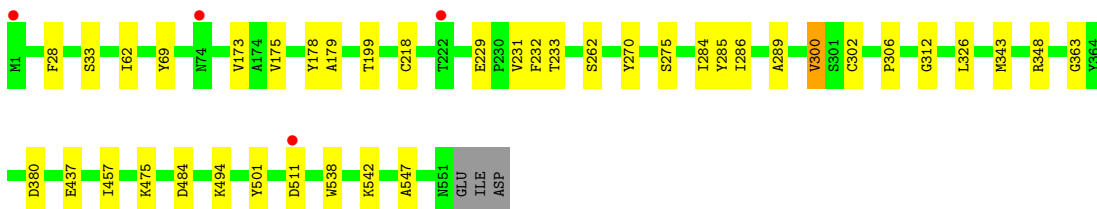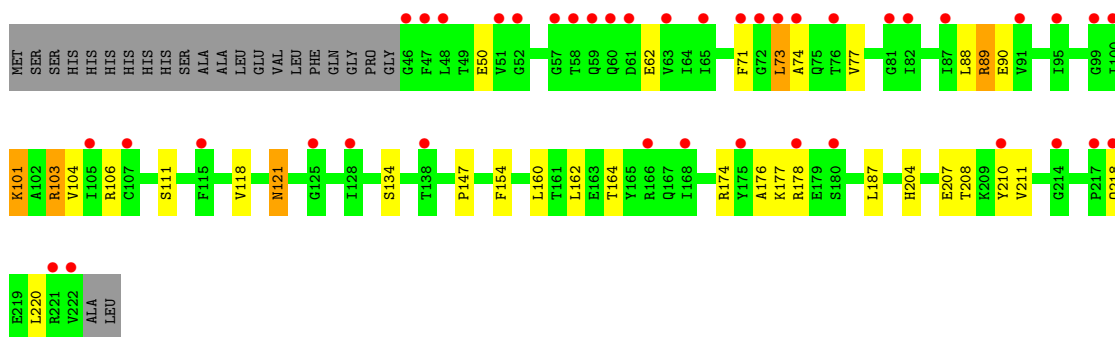• Molecule 1: Diol dehydrase alpha subunit

Chain G:

• Molecule 1: Diol dehydrase alpha subunit

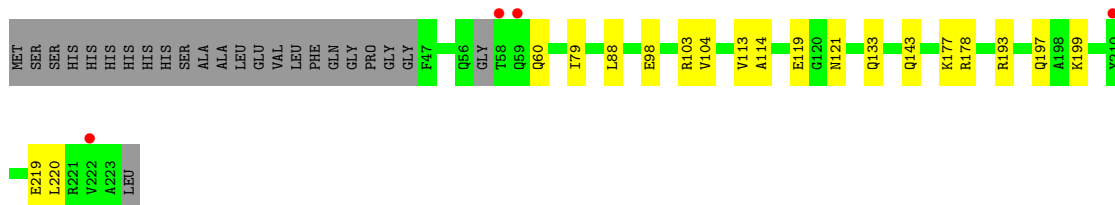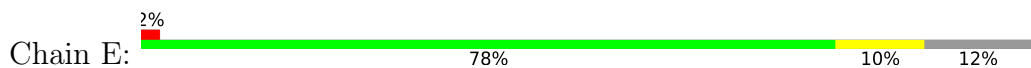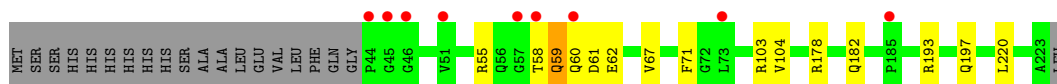Chain J:

• Molecule 2: Diol dehydrase beta subunit

Chain B:

• Molecule 2: Diol dehydrase beta subunit

Chain E:

• Molecule 2: Diol dehydrase beta subunit

Chain H:

• Molecule 2: Diol dehydrase beta subunit

Chain K:

• Molecule 3: Diol dehydrase gamma subunit

Chain C:

MET A38 P50 E67 N68 V69 L70 S91 D117 E121 N124 R130 S131 T132 E135 K150 D173

• Molecule 3: Diol dehydrase gamma subunit

Chain F:

%

96%   • ••

MET A38 T55 A56 F64 L70 D78 R100 D173

• Molecule 3: Diol dehydrase gamma subunit

Chain I:

4%

88%   11%   ••

MET A38 R39 A46 P50 E51 T55 L61 D62 D63 F64 T65 L66 E67 N68 V69 L70 K73 S91 R100 N124 R130 K133 L137 K170 D173

• Molecule 3: Diol dehydrase gamma subunit

Chain L:

10%

92%   7%   •

MET A38 T55 T60 L61 D62 D63 F64 T65 L66 V69 A113 E121 A138 I139 A140 D141 D142 L143 E144 S145 R146 Y147 R157 A160 K168 L169 D172 D173
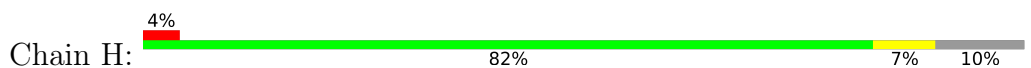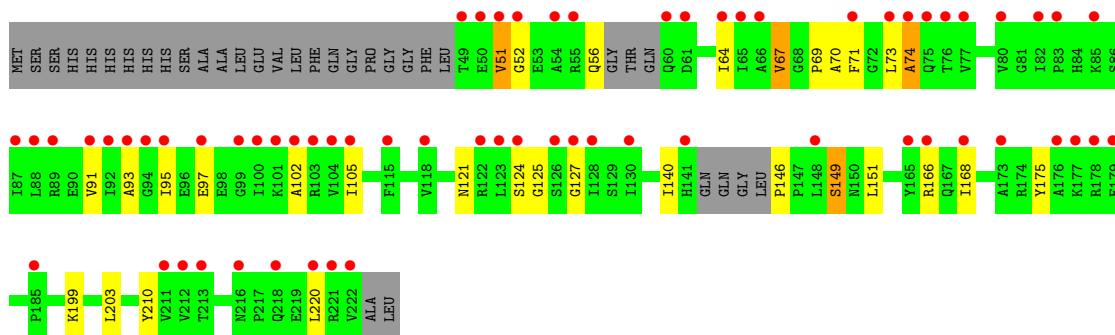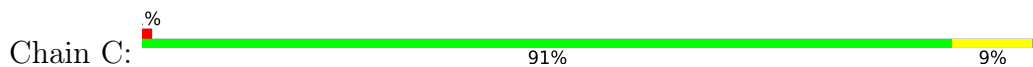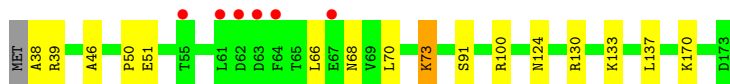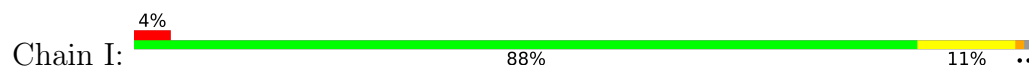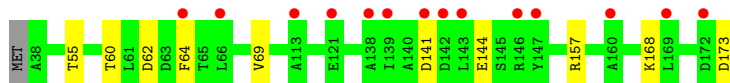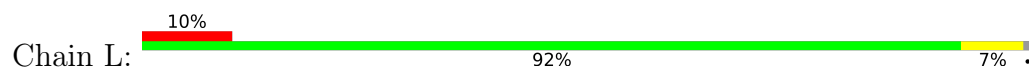
4 Data and refinement statistics ⓘ

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 48.91 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.8 (49.00-1.90) 95.1 (48.91-1.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.25 (at 1.90Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.164 , 0.191 0.163 , 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 , 48.9	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	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.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: B12, CA, PGO, K, 5AD

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	0.43	0/4302	0.60	0/5825
1	D	0.53	1/4286 (0.0%)	0.63	0/5803
1	G	0.36	0/4286	0.54	0/5803
1	J	0.34	0/4285	0.52	0/5802
2	B	0.33	0/1392	0.50	0/1883
2	E	0.35	0/1384	0.54	0/1872
2	H	0.32	0/1403	0.49	0/1898
2	K	0.29	0/1299	0.49	0/1755
3	C	0.37	0/1119	0.52	0/1511
3	F	0.42	0/1110	0.59	0/1499
3	I	0.30	0/1110	0.48	0/1499
3	L	0.29	0/1102	0.45	0/1489
All	All	0.39	1/27078 (0.0%)	0.55	0/36639

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	218	CYS	CB-SG	-8.97	1.67	1.82

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4218	0	4165	15	0
1	D	4205	0	4150	19	0
1	G	4205	0	4152	14	0
1	J	4207	0	4150	23	0
2	B	1364	0	1421	26	0
2	E	1363	0	1411	9	0
2	H	1377	0	1432	9	0
2	K	1280	0	1331	18	0
3	C	1098	0	1111	5	0
3	F	1095	0	1104	6	0
3	I	1092	0	1105	9	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	8	0
8	H	91	0	88	8	0
8	K	91	0	88	9	0
9	A	253	0	0	1	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	178	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 (178) 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
3:C:38:ALA:N	3:C:91:SER:HG	1.86	0.72
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: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
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
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: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: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
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:475:LYS:NZ	3:L:69:VAL:O	2.38	0.46
1:J:494:LYS:HE2	3:L:64:PHE:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:I:38:ALA:N	3:I:91:SER:HG	2.14	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:I:51:GLU:H	3:I:51:GLU:CD	2.22	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
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:114:ALA:HB2	8:E:1601:B12:HM62	2.03	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:E:103:ARG:HD2	2:E:219:GLU:OE2	2.21	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	553/554 (100%)	533 (96%)	18 (3%)	2 (0%)	34	24
1	D	551/554 (100%)	534 (97%)	15 (3%)	2 (0%)	34	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	551/554 (100%)	536 (97%)	13 (2%)	2 (0%)	34	24
1	J	551/554 (100%)	533 (97%)	16 (3%)	2 (0%)	34	24
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%)	25	15
2	K	161/200 (80%)	153 (95%)	6 (4%)	2 (1%)	13	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%)	41	31

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%)	444 (98%)	9 (2%)	55	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	451/452 (100%)	446 (99%)	5 (1%)	73	73
1	G	451/452 (100%)	446 (99%)	5 (1%)	73	73
1	J	451/452 (100%)	444 (98%)	7 (2%)	62	60
2	B	148/164 (90%)	141 (95%)	7 (5%)	26	16
2	E	147/164 (90%)	144 (98%)	3 (2%)	55	51
2	H	148/164 (90%)	146 (99%)	2 (1%)	67	65
2	K	139/164 (85%)	136 (98%)	3 (2%)	52	47
3	C	117/116 (101%)	115 (98%)	2 (2%)	60	57
3	F	116/116 (100%)	115 (99%)	1 (1%)	78	79
3	I	116/116 (100%)	113 (97%)	3 (3%)	46	39
3	L	115/116 (99%)	114 (99%)	1 (1%)	78	79
All	All	2852/2928 (97%)	2804 (98%)	48 (2%)	60	57

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	PHE
1	A	45	ASN
1	A	178	TYR
1	A	232	PHE
1	A	267	GLN
1	A	348	ARG
1	A	364	TYR
1	A	501	TYR
1	A	551	ASN
2	B	73	LEU
2	B	77	VAL
2	B	89	ARG
2	B	101	LYS
2	B	103[A]	ARG
2	B	103[B]	ARG
2	B	121	ASN
3	C	50	PRO
3	C	150	LYS
1	D	28	PHE
1	D	178	TYR
1	D	232	PHE
1	D	348	ARG

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Mol	Chain	Res	Type
1	D	501	TYR
2	E	60	GLN
2	E	119	GLU
2	E	178	ARG
3	F	100	ARG
1	G	28	PHE
1	G	178	TYR
1	G	232	PHE
1	G	348	ARG
1	G	501	TYR
2	H	59	GLN
2	H	178	ARG
3	I	39	ARG
3	I	73	LYS
3	I	170	LYS
1	J	28	PHE
1	J	178	TYR
1	J	232	PHE
1	J	348	ARG
1	J	437	GLU
1	J	501	TYR
1	J	511	ASP
2	K	67	VAL
2	K	149	SER
2	K	220	LEU
3	L	141	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	35	ASN
1	A	74	ASN
1	A	388	ASN
1	A	465	ASN
1	A	543	ASN
1	A	551	ASN
2	B	56	GLN
2	B	150	ASN
2	B	204	HIS
2	B	218	GLN
1	D	15	ASN

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Mol	Chain	Res	Type
1	D	388	ASN
1	D	513	GLN
2	H	59	GLN
2	H	60	GLN
2	H	182	GLN
3	I	72	ASN
1	J	45	ASN
1	J	182	ASN
1	J	467	ASN
1	J	479	GLN
2	K	121	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\#|Z| > 2$
8	B12	H	1601	-	90,101,101	1.65	8 (8%)	137,166,166	1.33	19 (13%)
6	PGO	J	604	4	3,4,4	0.44	0	1,4,4	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
7	5AD	D	605	-	10,12,20	1.43	2 (20%)	8,17,30	1.79	2 (25%)
6	PGO	D	604	4	3,4,4	0.84	0	1,4,4	1.58	0
7	5AD	G	605	-	10,12,20	1.33	1 (10%)	8,17,30	1.84	2 (25%)
6	PGO	A	604	4	3,4,4	0.58	0	1,4,4	0.84	0
7	5AD	J	605	-	10,12,20	1.30	1 (10%)	8,17,30	1.86	4 (50%)
6	PGO	G	604	4	3,4,4	0.46	0	1,4,4	0.51	0
8	B12	K	1601	5	90,101,101	1.76	9 (10%)	137,166,166	1.31	17 (12%)
8	B12	E	1601	-	90,101,101	1.58	8 (8%)	137,166,166	1.35	19 (13%)
7	5AD	A	605	-	10,12,20	1.35	1 (10%)	8,17,30	1.90	3 (37%)
8	B12	B	1601	-	90,101,101	1.69	8 (8%)	137,166,166	1.29	16 (11%)

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
8	B12	H	1601	-	-	9/52/223/223	0/3/11/11
6	PGO	J	604	4	-	1/2/2/2	-
7	5AD	D	605	-	-	-	0/2/2/3
6	PGO	D	604	4	-	1/2/2/2	-
7	5AD	G	605	-	-	-	0/2/2/3
6	PGO	A	604	4	-	1/2/2/2	-
8	B12	K	1601	5	-	11/52/223/223	0/3/11/11
6	PGO	G	604	4	-	1/2/2/2	-
7	5AD	J	605	-	-	-	0/2/2/3
8	B12	E	1601	-	-	7/52/223/223	0/3/11/11
7	5AD	A	605	-	-	-	0/2/2/3
8	B12	B	1601	-	-	6/52/223/223	0/3/11/11

All (38) 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	H	1601	B12	C14-N23	-4.99	1.28	1.35
8	E	1601	B12	C8B-C9B	4.74	1.50	1.40
8	K	1601	B12	C14-N23	-4.72	1.29	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	K	1601	B12	C11-N23	4.49	1.45	1.37
8	B	1601	B12	C14-N23	-4.46	1.29	1.35
8	K	1601	B12	C8B-C9B	4.38	1.49	1.40
8	B	1601	B12	C8B-C9B	4.37	1.49	1.40
8	B	1601	B12	C11-N23	4.29	1.45	1.37
8	H	1601	B12	C8B-C9B	4.28	1.49	1.40
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
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	D	605	5AD	C5-C4	2.77	1.48	1.40
8	K	1601	B12	C10-C9	2.76	1.47	1.39
7	J	605	5AD	C5-C4	2.75	1.48	1.40
8	E	1601	B12	C10-C9	2.72	1.46	1.39
7	G	605	5AD	C5-C4	2.71	1.48	1.40
7	A	605	5AD	C5-C4	2.70	1.48	1.40
8	H	1601	B12	C10-C9	2.69	1.46	1.39
8	H	1601	B12	C14-C15	2.69	1.49	1.38
8	B	1601	B12	C10-C9	2.60	1.46	1.39
7	D	605	5AD	C2-N3	2.14	1.35	1.32
8	K	1601	B12	C1-C2	-2.04	1.54	1.58

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	E	1601	B12	C20-C1-C19	-5.28	104.26	109.36
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	H	1601	B12	C13-C14-N23	4.17	114.77	109.10
8	B	1601	B12	C20-C1-C19	-4.05	105.45	109.36
8	E	1601	B12	C13-C14-N23	4.03	114.59	109.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
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
8	H	1601	B12	C20-C1-C19	-3.70	105.79	109.36
8	K	1601	B12	C48-C13-C14	3.61	117.49	108.49
8	K	1601	B12	C9-C10-C11	-3.59	120.77	125.97
8	K	1601	B12	C13-C14-N23	3.54	113.92	109.10
8	B	1601	B12	C13-C14-N23	3.39	113.71	109.10
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	A	605	5AD	C4-C5-N7	-3.24	106.02	109.40
7	G	605	5AD	C4-C5-N7	-3.16	106.11	109.40
7	J	605	5AD	N3-C2-N1	-3.15	123.75	128.68
8	B	1601	B12	C17-C16-C15	3.13	131.19	126.26
7	A	605	5AD	N3-C2-N1	-3.05	123.92	128.68
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	D	605	5AD	C4-C5-N7	-3.00	106.28	109.40
8	K	1601	B12	C36-C7-C37	2.97	115.70	110.80
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
7	G	605	5AD	N3-C2-N1	-2.88	124.18	128.68
7	D	605	5AD	N3-C2-N1	-2.86	124.21	128.68
8	K	1601	B12	C55-C56-C57	-2.84	105.04	111.23
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
8	K	1601	B12	C13-C14-C15	-2.69	120.20	124.32
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
8	B	1601	B12	C4B-C9B-N3B	2.59	137.81	130.88
8	H	1601	B12	C53-C15-C16	2.55	124.77	120.38
7	J	605	5AD	C4-C5-N7	-2.53	106.76	109.40
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	C4B-C9B-N3B	2.47	137.50	130.88
8	H	1601	B12	C12-C11-C10	2.47	126.58	123.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	E	1601	B12	C4B-C9B-N3B	2.46	137.46	130.88
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	H	1601	B12	C8B-C9B-N3B	-2.40	102.76	107.83
8	E	1601	B12	C2-C1-C19	2.36	122.33	118.60
8	B	1601	B12	C8B-C9B-N3B	-2.32	102.95	107.83
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
8	K	1601	B12	C4B-C9B-N3B	2.22	136.82	130.88
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
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	J	605	5AD	N6-C6-N1	2.07	122.87	118.57
8	K	1601	B12	C8-C9-C10	-2.06	118.88	123.32
8	K	1601	B12	C8B-C9B-N3B	-2.06	103.50	107.83
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	J	605	5AD	C2-N1-C6	2.05	122.26	118.75
8	E	1601	B12	C8B-C9B-N3B	-2.04	103.52	107.83
7	A	605	5AD	N6-C6-N1	2.04	122.81	118.57
8	E	1601	B12	C4B-C9B-C8B	-2.03	119.02	121.10
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

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

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Mol	Chain	Res	Type	Atoms
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 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	H	1601	B12	8	0
7	D	605	5AD	1	0
7	G	605	5AD	1	0
7	J	605	5AD	2	0

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

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

Ligand B12 H 1601

Bond lengths

Bond angles

Torsions

Rings

Ligand 5AD D 605

Bond lengths

Bond angles

Torsions

Rings

Ligand 5AD G 605

Bond lengths

Bond angles

Torsions

Rings

Ligand 5AD J 605

Bond lengths

Bond angles

Torsions

Rings

Ligand B12 K 1601

Bond lengths

Bond angles

Torsions

Rings

Ligand B12 E 1601

Bond lengths

Bond angles

Torsions

Rings

Ligand 5AD A 605

Bond lengths

Bond angles

Torsions

Rings

Ligand B12 B 1601

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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(Å²)	Q<0.9
1	A	551/554 (99%)	-0.37	0	100	100	12, 31, 55, 90	0
1	D	550/554 (99%)	-0.31	1 (0%)	95	95	11, 21, 44, 89	1 (0%)
1	G	550/554 (99%)	-0.18	4 (0%)	87	88	22, 36, 66, 91	0
1	J	551/554 (99%)	-0.05	4 (0%)	87	88	25, 47, 72, 91	1 (0%)
2	B	177/200 (88%)	1.22	41 (23%)	0	0	35, 73, 98, 111	0
2	E	176/200 (88%)	0.02	4 (2%)	60	63	24, 48, 71, 112	0
2	H	180/200 (90%)	0.44	9 (5%)	28	32	34, 58, 86, 136	0
2	K	167/200 (83%)	1.77	65 (38%)	0	0	55, 94, 119, 131	0
3	C	136/137 (99%)	-0.14	1 (0%)	87	88	28, 45, 66, 78	1 (0%)
3	F	136/137 (99%)	-0.49	1 (0%)	87	88	17, 33, 51, 66	0
3	I	136/137 (99%)	0.07	6 (4%)	34	37	36, 54, 83, 100	1 (0%)
3	L	136/137 (99%)	0.70	14 (10%)	6	7	53, 74, 97, 110	0
All	All	3446/3564 (96%)	0.03	150 (4%)	34	37	11, 41, 89, 136	4 (0%)

All (150) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	44	PRO	23.4
2	H	45	GLY	11.7
2	K	122	ARG	6.9
2	K	105	ILE	6.5
2	K	220	LEU	6.3
2	B	222	VAL	6.3
2	K	176	ALA	5.6
2	K	102	ALA	5.2
2	B	48	LEU	5.1
2	B	60	GLN	5.0
2	H	46	GLY	4.9

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Mol	Chain	Res	Type	RSRZ
2	K	103	ARG	4.8
2	B	47	PHE	4.7
2	H	58	THR	4.7
2	K	92	ILE	4.5
2	K	76	THR	4.5
2	K	123	LEU	4.4
2	K	51	VAL	4.3
2	K	95	ILE	4.2
3	L	66	LEU	4.2
2	K	222	VAL	4.2
3	L	138	ALA	4.2
2	K	165	TYR	4.1
2	K	73	LEU	4.0
2	E	59	GLN	4.0
2	K	74	ALA	4.0
2	K	97	GLU	4.0
2	B	58	THR	4.0
2	K	61	ASP	3.9
2	B	46	GLY	3.9
2	K	85	LYS	3.9
2	K	178	ARG	3.8
2	K	99	GLY	3.8
2	B	59	GLN	3.8
2	K	173	ALA	3.7
2	K	212	VAL	3.7
2	K	75	GLN	3.7
3	L	64	PHE	3.6
2	K	87	ILE	3.6
2	K	126	SER	3.6
2	K	101	LYS	3.6
2	H	57	GLY	3.6
2	K	50	GLU	3.6
2	B	214	GLY	3.5
2	K	130	ILE	3.4
2	K	52	GLY	3.4
2	B	73	LEU	3.4
2	K	55	ARG	3.3
2	K	185	PRO	3.3
2	B	52	GLY	3.2
1	G	430	PRO	3.2
3	L	139	ILE	3.2
2	K	91	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	168	ILE	3.1
2	B	221	ARG	3.0
2	K	88	LEU	3.0
2	B	99	GLY	3.0
2	B	72	GLY	2.9
2	B	217	PRO	2.9
3	I	55	THR	2.9
2	K	89	ARG	2.9
3	L	113	ALA	2.8
2	K	211	VAL	2.8
2	K	218	GLN	2.8
2	K	148	LEU	2.8
2	K	124	SER	2.8
2	B	82	ILE	2.8
2	K	93	ALA	2.8
2	B	115	PHE	2.8
2	E	222	VAL	2.8
1	J	74	ASN	2.8
2	K	66	ALA	2.8
2	K	168	ILE	2.8
2	K	213	THR	2.7
2	K	128	ILE	2.7
2	K	118	VAL	2.7
2	H	51	VAL	2.7
2	K	77	VAL	2.7
2	K	49	THR	2.7
2	K	221	ARG	2.7
2	K	216	ASN	2.7
3	I	62	ASP	2.7
3	L	141	ASP	2.6
3	L	147	TYR	2.6
2	H	60	GLN	2.6
1	G	548	LEU	2.6
3	L	160	ALA	2.6
2	B	166	ARG	2.6
2	K	80	VAL	2.6
2	B	61	ASP	2.5
2	E	58	THR	2.5
2	K	100	ILE	2.5
3	F	56	ALA	2.5
3	L	172	ASP	2.5
3	I	64	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	175	TYR	2.5
3	I	61	LEU	2.5
3	L	143	LEU	2.5
2	K	141	HIS	2.5
2	K	166	ARG	2.5
2	B	95	ILE	2.5
2	B	51	VAL	2.5
2	K	60	GLN	2.5
2	B	210	TYR	2.5
2	K	83	PRO	2.4
2	B	91	VAL	2.4
2	B	81	GLY	2.4
2	B	128	ILE	2.4
2	K	177	LYS	2.4
1	J	511	ASP	2.4
2	K	71	PHE	2.4
2	B	107	CYS	2.4
2	B	105	ILE	2.4
2	K	65	ILE	2.4
2	B	57	GLY	2.3
2	B	218	GLN	2.3
2	K	115	PHE	2.3
2	H	185	PRO	2.3
2	K	104	VAL	2.3
2	B	76	THR	2.3
1	G	481	GLY	2.3
2	B	125	GLY	2.3
2	K	64	ILE	2.3
2	B	71	PHE	2.2
2	B	74	ALA	2.2
2	K	179	GLU	2.2
2	B	63	VAL	2.2
2	B	87	ILE	2.2
2	B	100	ILE	2.2
3	L	169	LEU	2.2
3	I	67	GLU	2.2
2	B	65	ILE	2.2
3	L	121	GLU	2.1
2	B	180	SER	2.1
1	J	1	MET	2.1
3	I	63	ASP	2.1
2	H	73	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
2	E	210	TYR	2.1
2	K	127	GLY	2.1
1	D	46	GLY	2.1
1	G	331	ALA	2.1
3	L	142	ASP	2.1
2	K	94	GLY	2.1
1	J	222	THR	2.1
2	K	54	ALA	2.1
2	K	82	ILE	2.1
2	B	178	ARG	2.0
2	B	138	THR	2.0
3	L	146	ARG	2.0
3	C	70	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	5AD	J	605	11/18	0.83	0.18	60,64,72,79	0
6	PGO	J	604	5/5	0.87	0.34	35,53,61,64	0
7	5AD	G	605	11/18	0.90	0.14	36,46,54,59	0
7	5AD	D	605	11/18	0.94	0.12	25,35,48,52	0
6	PGO	G	604	5/5	0.94	0.25	30,33,49,53	0
6	PGO	A	604	5/5	0.94	0.22	24,25,43,48	0
8	B12	K	1601	91/91	0.94	0.18	61,70,75,79	0
6	PGO	D	604	5/5	0.95	0.28	18,19,35,42	0
7	5AD	A	605	11/18	0.95	0.12	36,37,50,60	0
8	B12	B	1601	91/91	0.96	0.13	34,42,50,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	K	J	602	1/1	0.96	0.08	34,34,34,34	0
4	CA	J	601	1/1	0.97	0.09	32,32,32,32	0
8	B12	E	1601	91/91	0.97	0.10	18,26,34,36	0
8	B12	H	1601	91/91	0.97	0.11	29,36,45,55	0
5	K	J	603	1/1	0.97	0.08	54,54,54,54	0
5	K	G	603	1/1	0.98	0.08	36,36,36,36	0
5	K	G	602	1/1	0.99	0.11	30,30,30,30	0
4	CA	D	601	1/1	0.99	0.04	6,6,6,6	0
4	CA	G	601	1/1	0.99	0.04	26,26,26,26	0
4	CA	A	601	1/1	0.99	0.07	20,20,20,20	0
5	K	A	602	1/1	0.99	0.12	27,27,27,27	0
5	K	A	603	1/1	0.99	0.07	35,35,35,35	0
5	K	D	602	1/1	0.99	0.12	22,22,22,22	0
5	K	D	603	1/1	0.99	0.21	27,27,27,27	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
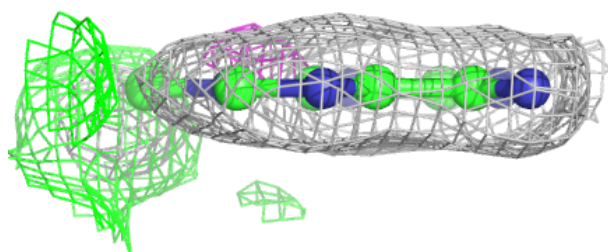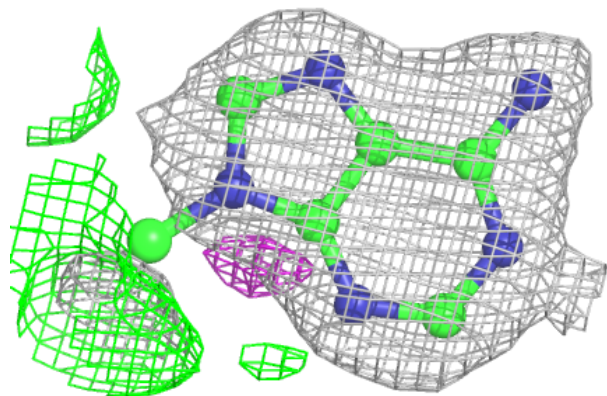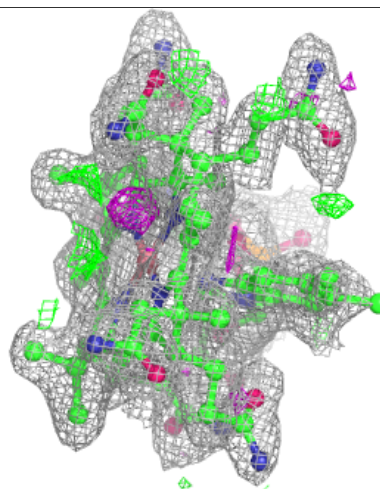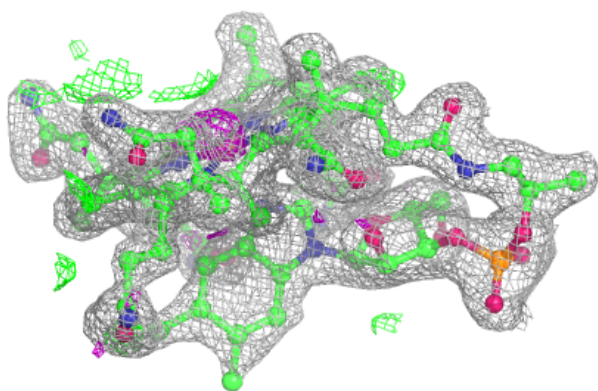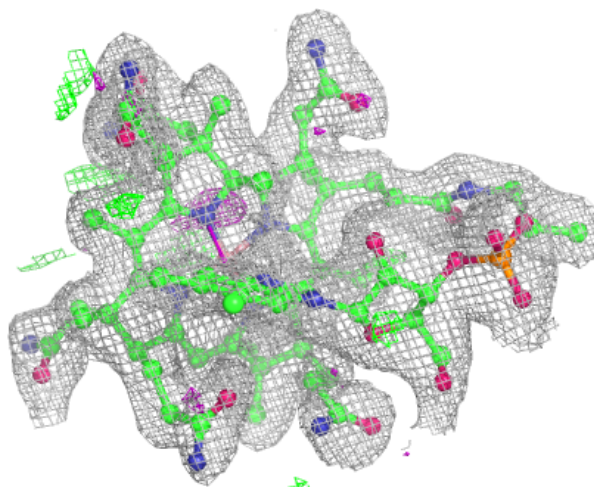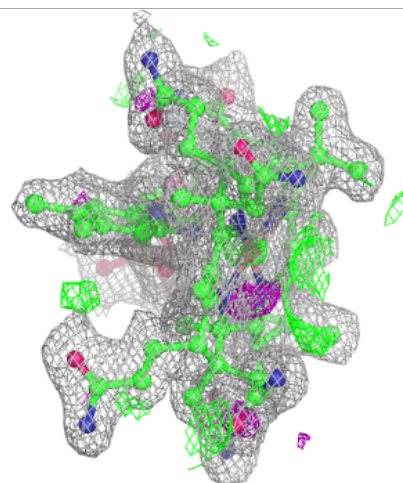mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)
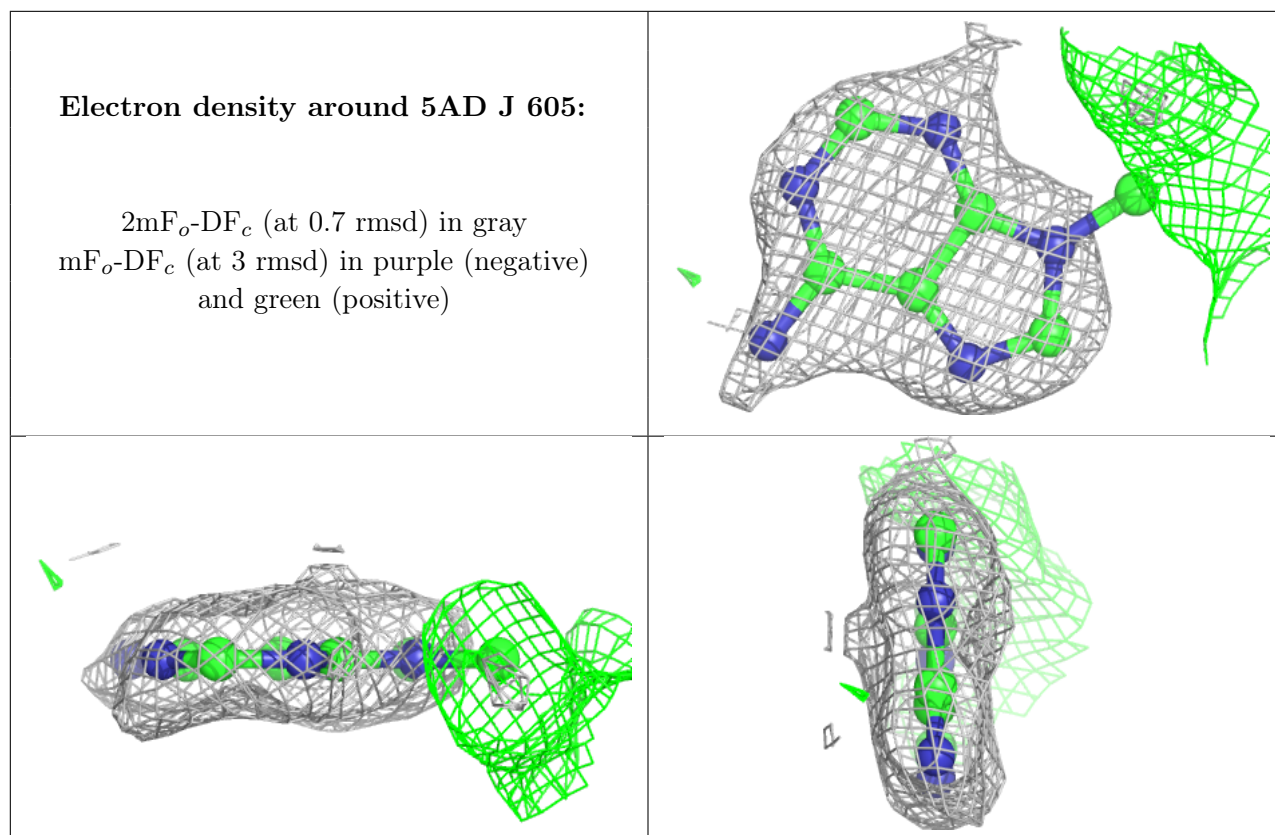
Electron density around 5AD G 605:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
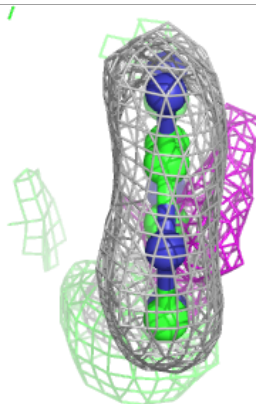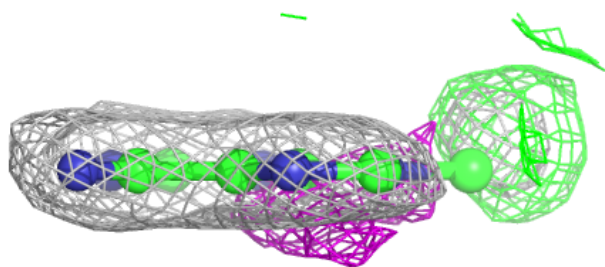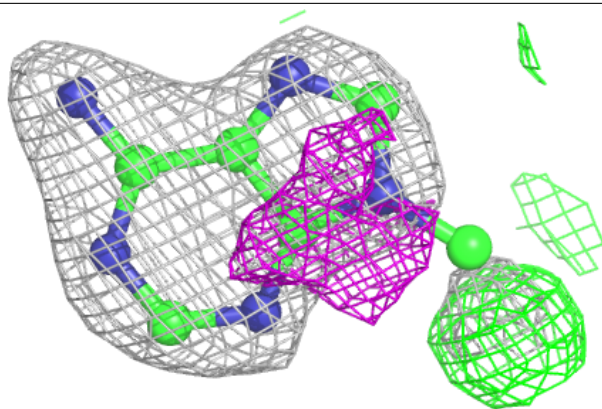
Electron density around 5AD D 605:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
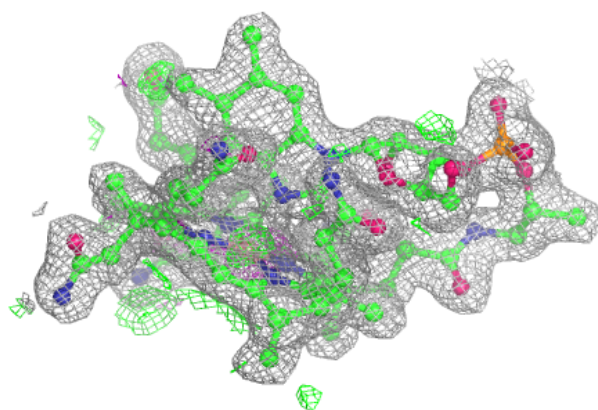mF_o-DF_c (at 3 rmsd) in purple (negative)
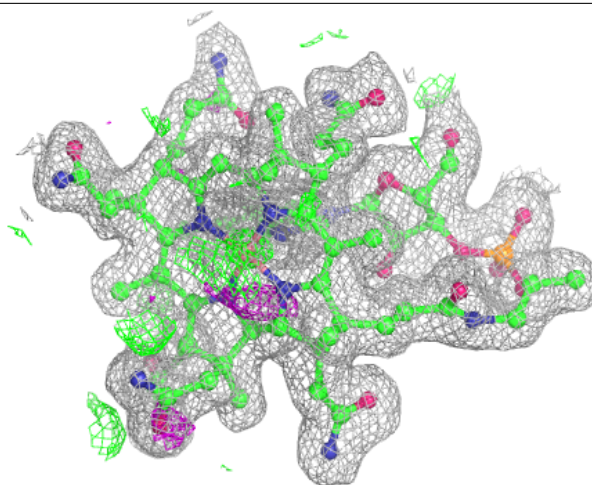and green (positive)
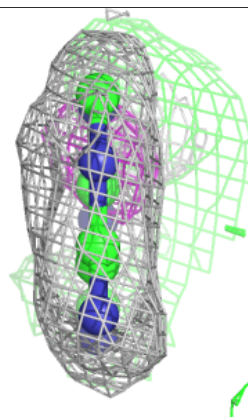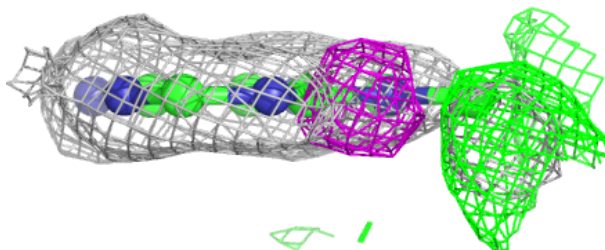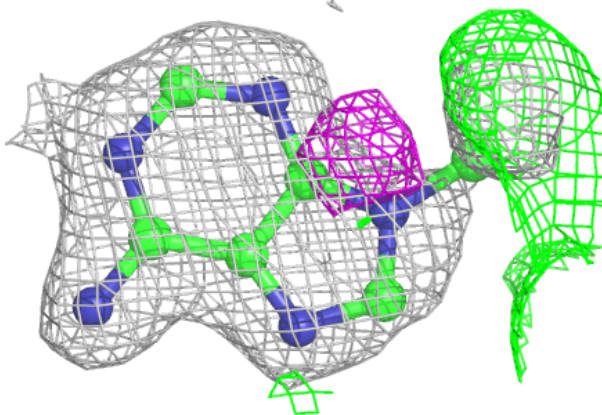
Electron density around B12 K 1601:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
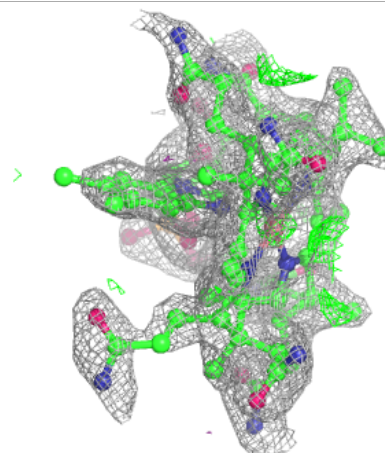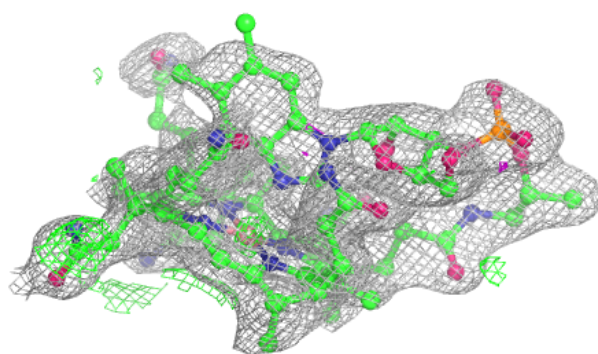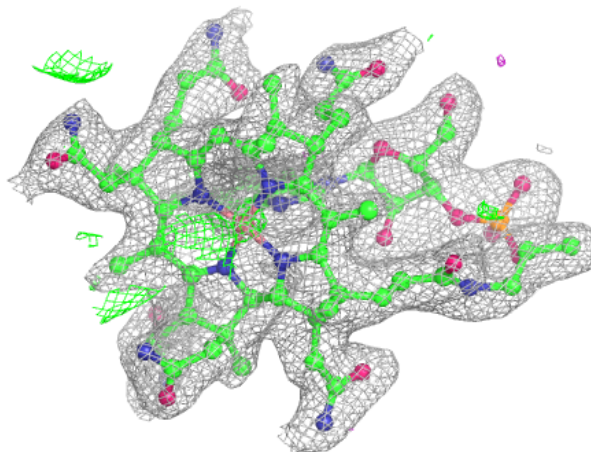
Electron density around 5AD A 605:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
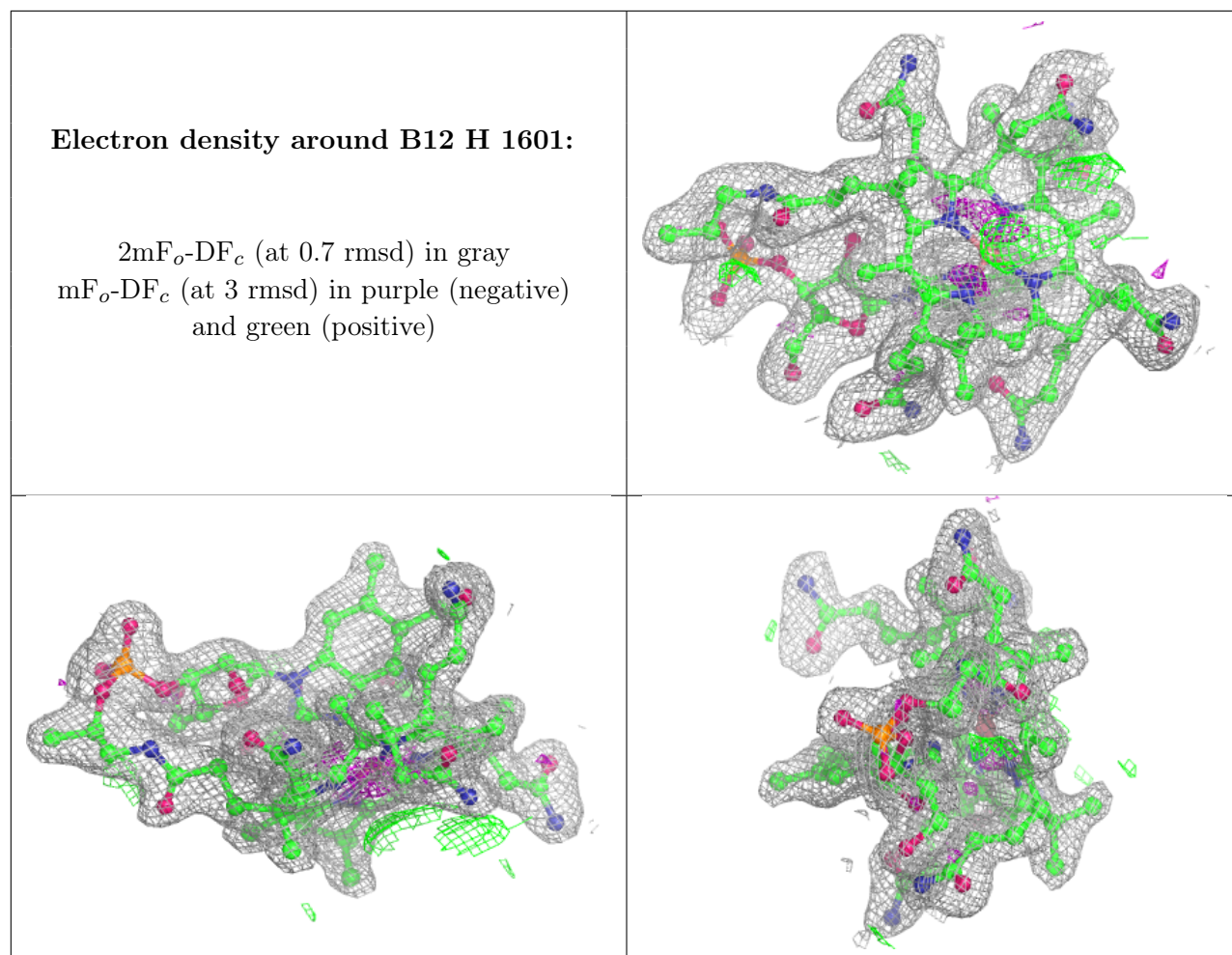and green (positive)
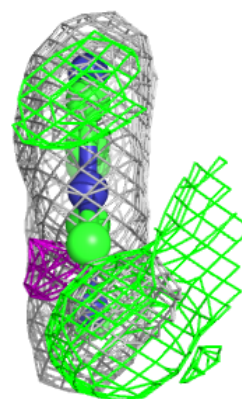
Electron density around B12 B 1601:

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

Electron density around B12 E 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.