



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 01:43 pm BST

PDB ID : 1EEX  
Title : CRYSTAL STRUCTURE OF THE DIOL DEHYDRATASE-ADENINYLPENTYLCOBALAMIN COMPLEX FROM KLEBSIELLA OXYTOCA  
Authors : Shibata, N.; Masuda, J.; Toraya, T.; Morimoto, Y.; Yasuoka, N.  
Deposited on : 2000-02-04  
Resolution : 1.70 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

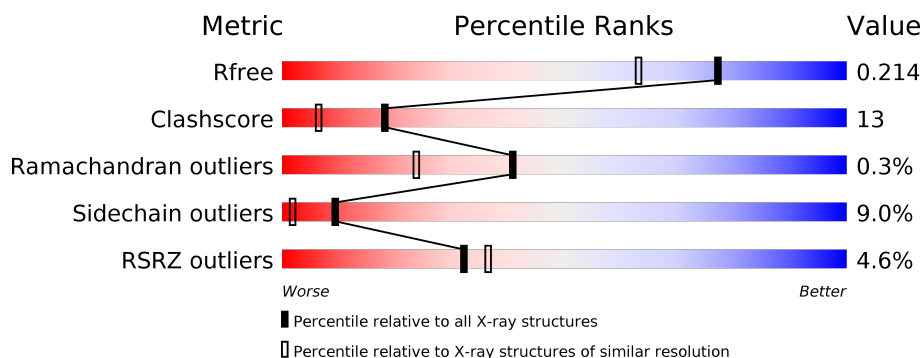
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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

Mol	Chain	Length	Quality of chain
1	A	554	<div> <div>83%</div> <div>14%</div> <div>••</div> </div>
1	L	554	<div> <div>3%</div> <div>77%</div> <div>18%</div> <div>••</div> </div>
2	B	224	<div> <div>65%</div> <div>12%</div> <div>•</div> <div>21%</div> </div>
2	E	224	<div> <div>21%</div> <div>39%</div> <div>32%</div> <div>8%</div> <div>21%</div> </div>
3	G	173	<div> <div>%</div> <div>62%</div> <div>12%</div> <div>••</div> <div>21%</div> </div>
3	M	173	<div> <div>9%</div> <div>51%</div> <div>19%</div> <div>9%</div> <div>21%</div> </div>

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
5	COY	A	601	X	-	-	-
5	COY	L	601	X	-	-	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 15494 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 PROPANEDIOL DEHYDRATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	551	Total	C	N	O	S	0	4	0
			4217	2629	731	828	29			
1	L	551	Total	C	N	O	S	0	7	0
			4225	2632	734	830	29			

- Molecule 2 is a protein called PROPANEDIOL DEHYDRATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	178	Total	C	N	O	S	0	4	0
			1378	871	249	256	2			
2	E	178	Total	C	N	O	S	0	1	0
			1363	863	245	253	2			

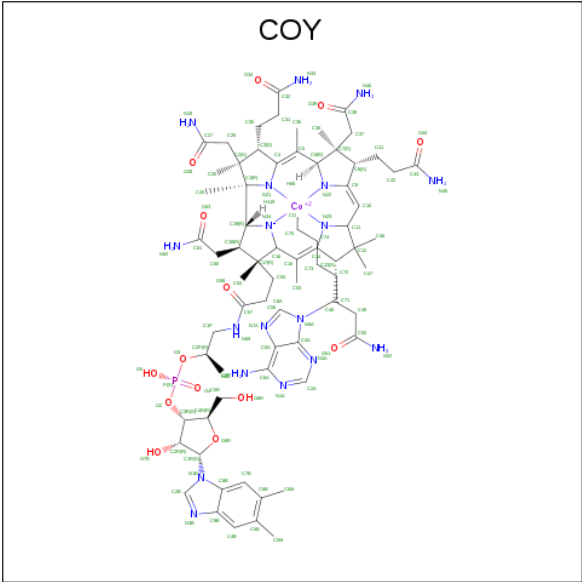
- Molecule 3 is a protein called PROPANEDIOL DEHYDRATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	137	Total	C	N	O	S	0	4	0
			1111	691	200	217	3			
3	M	137	Total	C	N	O	S	0	2	0
			1102	686	196	217	3			

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

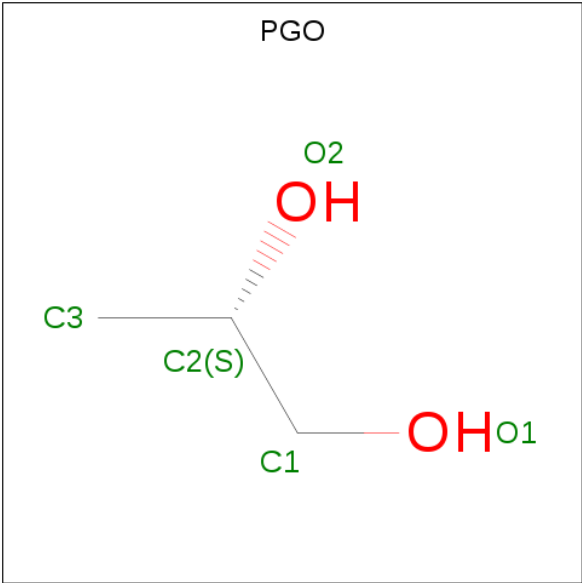
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	K	0	0
			2	2		
4	L	2	Total	K	0	0
			2	2		

- Molecule 5 is CO-(ADENIN-9-YL-PENTYL)-COBALAMIN (three-letter code: COY) (formula: C<sub>72</sub>H<sub>106</sub>CoN<sub>18</sub>O<sub>14</sub>P).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	Co	N	O	P	0	0
			106	72	1	18	14	1		
5	L	1	Total	C	Co	N	O	P	0	0
			106	72	1	18	14	1		

- Molecule 6 is S-1,2-PROPANEDIOL (three-letter code: PGO) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>2</sub>).



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

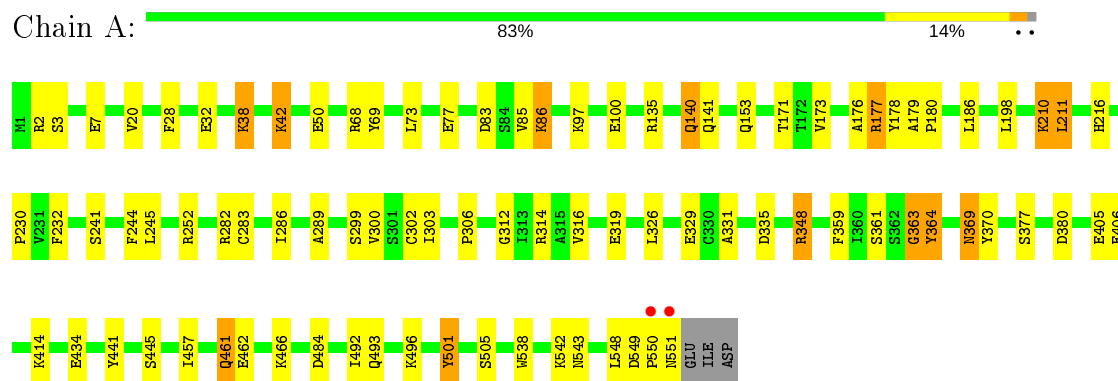
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	688	Total 688	O 688	0	0
7	B	218	Total 218	O 218	0	0
7	G	205	Total 205	O 205	0	0
7	L	498	Total 498	O 498	0	0
7	E	106	Total 106	O 106	0	0
7	M	157	Total 157	O 157	0	0

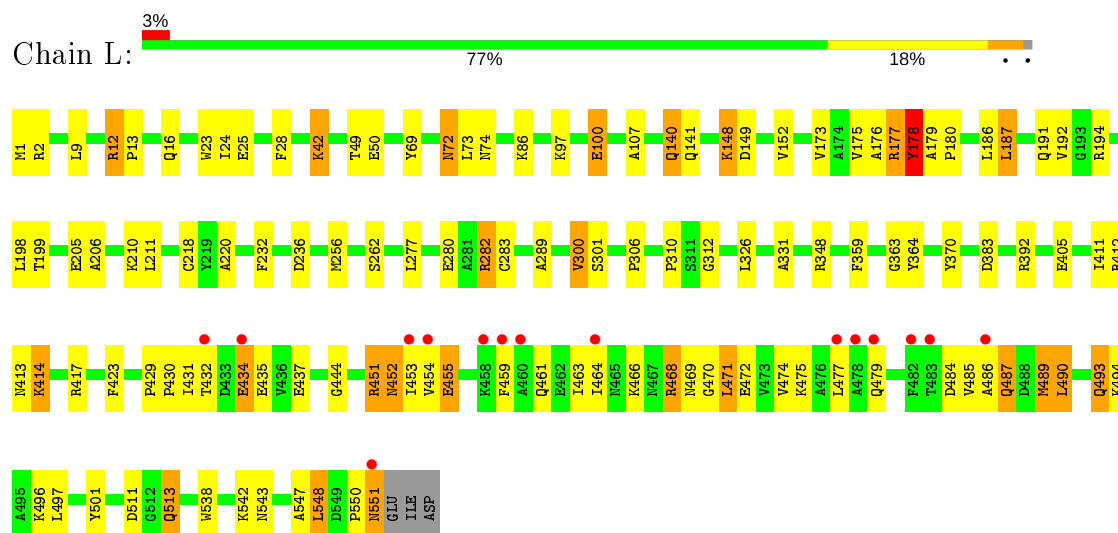
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

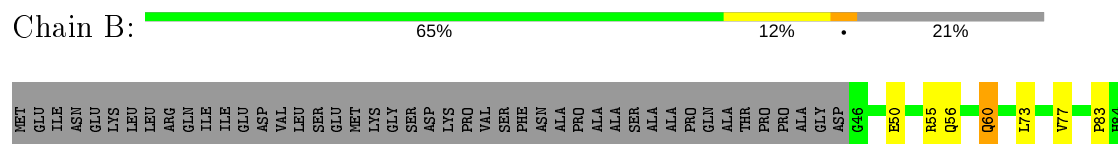
#### • Molecule 1: PROPANEDIOL DEHYDRATASE



#### • Molecule 1: PROPANEDIOL DEHYDRATASE

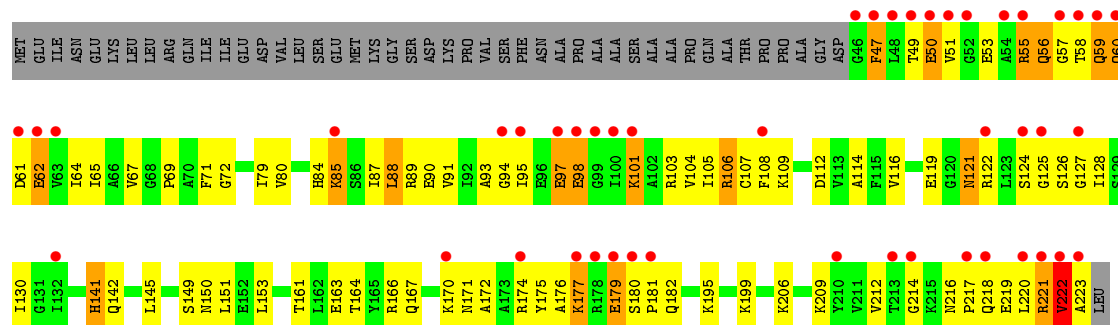


#### • Molecule 2: PROPANEDIOL DEHYDRATASE

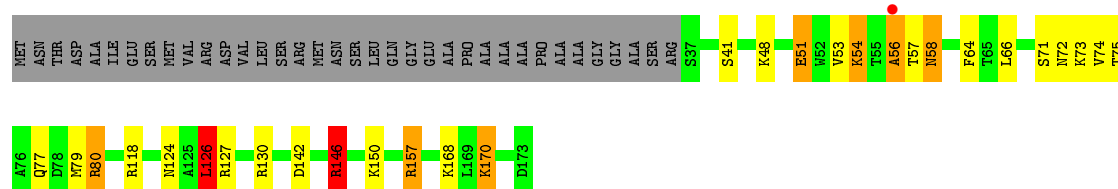




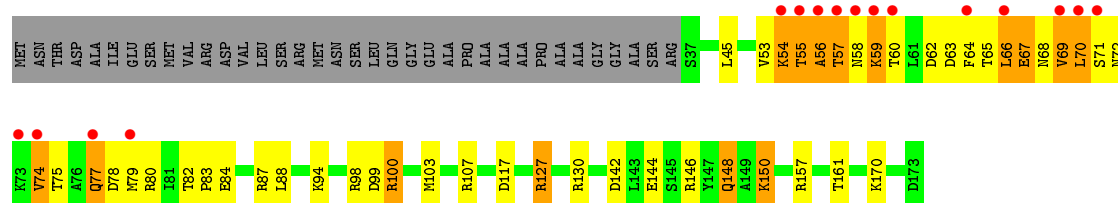
• Molecule 2: PROPANEDIOL DEHYDRATASE



• Molecule 3: PROPANEDIOL DEHYDRATASE



• Molecule 3: PROPANEDIOL DEHYDRATASE





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.38Å 121.40Å 207.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.70 33.54 – 1.69	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-1.70) 85.8 (33.54-1.69)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.48 (at 1.69Å)	Xtriage
Refinement program	SHELXL-97, CNS	Depositor
R, $R_{free}$	0.161 , 0.226 0.162 , 0.214	Depositor DCC
$R_{free}$ test set	8882 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	12.8	Xtriage
Anisotropy	0.483	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 103.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	15494	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: COY, PGO, 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	0.39	0/4308	1.07	15/5832 (0.3%)
1	L	0.39	0/4328	1.17	14/5858 (0.2%)
2	B	0.37	0/1418	1.07	5/1917 (0.3%)
2	E	0.32	0/1389	0.96	1/1879 (0.1%)
3	G	0.38	0/1145	1.24	10/1545 (0.6%)
3	M	0.36	0/1125	1.16	9/1520 (0.6%)
All	All	0.38	0/13713	1.11	54/18551 (0.3%)

There are no bond length outliers.

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	282	ARG	CD-NE-CZ	33.90	171.06	123.60
1	L	282	ARG	NE-CZ-NH1	11.41	126.00	120.30
2	B	122	ARG	CD-NE-CZ	9.69	137.17	123.60
1	A	370	TYR	CB-CG-CD1	9.38	126.63	121.00
1	L	468	ARG	NE-CZ-NH1	9.04	124.82	120.30
2	E	221	ARG	C-N-CA	8.85	143.83	121.70
3	M	127	ARG	NE-CZ-NH1	8.80	124.70	120.30
1	A	314	ARG	NE-CZ-NH1	8.16	124.38	120.30
1	A	364	TYR	CG-CD1-CE1	8.15	127.82	121.30
1	L	12	ARG	NE-CZ-NH1	-8.14	116.23	120.30
1	L	364	TYR	CB-CG-CD1	8.08	125.85	121.00
1	L	468	ARG	NE-CZ-NH2	-7.95	116.33	120.30
1	A	364	TYR	CB-CG-CD1	7.94	125.76	121.00
3	G	80	ARG	CD-NE-CZ	7.82	134.55	123.60
3	G	157	ARG	NE-CZ-NH1	7.60	124.10	120.30
3	M	127	ARG	NE-CZ-NH2	-7.56	116.52	120.30
1	A	282	ARG	NE-CZ-NH1	7.36	123.98	120.30
3	G	80	ARG	NE-CZ-NH1	7.36	123.98	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	127	ARG	CD-NE-CZ	7.34	133.88	123.60
1	L	364	TYR	CG-CD1-CE1	7.06	126.95	121.30
1	L	392	ARG	NE-CZ-NH1	7.06	123.83	120.30
3	G	146[A]	ARG	CD-NE-CZ	7.03	133.44	123.60
3	G	146[B]	ARG	CD-NE-CZ	7.03	133.44	123.60
1	A	501	TYR	CB-CG-CD1	6.86	125.12	121.00
2	B	89	ARG	NE-CZ-NH1	6.81	123.70	120.30
3	G	157	ARG	CD-NE-CZ	6.46	132.64	123.60
3	G	157	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	L	383	ASP	CB-CG-OD1	6.14	123.83	118.30
3	G	80	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	A	252	ARG	NE-CZ-NH2	6.12	123.36	120.30
3	G	126	LEU	CA-CB-CG	6.06	129.24	115.30
1	L	12	ARG	NE-CZ-NH2	5.94	123.27	120.30
1	A	68	ARG	NE-CZ-NH2	-5.93	117.33	120.30
2	B	106	ARG	NE-CZ-NH2	5.73	123.17	120.30
1	L	282	ARG	NE-CZ-NH2	-5.71	117.45	120.30
1	A	484	ASP	CB-CG-OD1	5.70	123.43	118.30
1	L	194	ARG	NE-CZ-NH2	5.65	123.12	120.30
3	M	87	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	A	135	ARG	NE-CZ-NH1	5.53	123.06	120.30
3	M	98	ARG	NE-CZ-NH2	-5.51	117.55	120.30
3	M	56	ALA	C-N-CA	5.49	135.42	121.70
1	A	364	TYR	CD1-CE1-CZ	-5.47	114.88	119.80
1	A	348	ARG	NE-CZ-NH2	-5.46	117.57	120.30
3	M	148	GLN	CA-CB-CG	5.44	125.36	113.40
1	A	380	ASP	CB-CG-OD1	5.43	123.19	118.30
3	M	107	ARG	NE-CZ-NH1	-5.33	117.64	120.30
1	A	244	PHE	CB-CG-CD2	-5.30	117.09	120.80
3	M	100	ARG	CD-NE-CZ	5.28	130.99	123.60
1	A	501	TYR	CB-CG-CD2	-5.25	117.85	121.00
2	B	121	ASN	CA-CB-CG	5.24	124.93	113.40
3	G	127	ARG	NE-CZ-NH1	-5.23	117.69	120.30
1	L	412	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	L	178	TYR	CB-CG-CD2	5.06	124.04	121.00
2	B	122	ARG	NE-CZ-NH1	5.01	122.81	120.30

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	4217	0	4161	70	0
1	L	4225	0	4154	93	0
2	B	1378	0	1432	22	0
2	E	1363	0	1416	100	0
3	G	1111	0	1115	24	0
3	M	1102	0	1105	50	0
4	A	2	0	0	0	0
4	L	2	0	0	0	0
5	A	106	0	100	9	0
5	L	106	0	100	12	0
6	A	5	0	6	0	0
6	L	5	0	6	0	0
7	A	688	0	0	21	0
7	B	218	0	0	3	0
7	E	106	0	0	12	0
7	G	205	0	0	11	0
7	L	498	0	0	13	0
7	M	157	0	0	12	0
All	All	15494	0	13595	366	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 13.

All (366) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:174:ARG:HH11	2:E:179:GLU:HG2	1.24	1.01
1:A:97:LYS:HB2	1:A:100[A]:GLU:HG3	1.53	0.89
1:L:497:LEU:HD21	3:M:79:MET:HA	1.55	0.88
1:L:173:VAL:HG21	1:L:176:ALA:HA	1.55	0.86
2:E:67:VAL:HG13	2:E:71:PHE:HB3	1.56	0.85
3:M:68:ASN:HB3	3:M:74:VAL:HG13	1.60	0.83
1:L:42:LYS:HB2	1:L:50:GLU:HB3	1.61	0.82
3:G:170:LYS:HE2	7:G:298:HOH:O	1.86	0.74
3:G:170:LYS:HG3	7:G:299:HOH:O	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:VAL:HG21	1:A:176:ALA:HA	1.69	0.73
1:L:469:ASN:OD1	1:L:471:LEU:HB2	1.88	0.73
3:M:103:MET:HG3	7:M:261:HOH:O	1.87	0.73
2:E:59:GLN:HG3	2:E:61:ASP:OD1	1.89	0.72
1:L:513:GLN:HG3	7:L:822:HOH:O	1.88	0.72
3:G:51:GLU:O	3:G:54[A]:LYS:HD3	1.90	0.72
1:L:470:GLY:O	1:L:474:VAL:HG23	1.90	0.72
1:A:550:PRO:HG3	1:L:23:TRP:HB2	1.72	0.71
2:B:100:ILE:HD11	2:B:177[B]:LYS:HD3	1.71	0.71
3:M:80:ARG:HD2	7:M:214:HOH:O	1.91	0.71
2:E:174:ARG:HD2	2:E:179:GLU:HG2	1.72	0.70
2:E:195[B]:LYS:HD2	7:E:286:HOH:O	1.91	0.70
1:L:475:LYS:O	1:L:479:GLN:HG2	1.92	0.69
1:A:369:ASN:HD21	1:A:377:SER:H	1.39	0.69
2:B:173:ALA:O	2:B:177[A]:LYS:HG3	1.93	0.69
1:L:413:ASN:ND2	1:L:417:ARG:HE	1.91	0.68
3:M:94:LYS:HD2	3:M:99:ASP:OD2	1.94	0.68
2:E:79:ILE:HG13	2:E:199:LYS:HD3	1.73	0.68
2:E:65:ILE:HB	2:E:104:VAL:HG22	1.76	0.68
3:M:142:ASP:HB3	7:M:314:HOH:O	1.94	0.67
1:A:20:VAL:HG13	1:L:550:PRO:HG3	1.77	0.67
1:L:493:GLN:HB3	7:L:812:HOH:O	1.93	0.67
3:M:75:THR:O	3:M:78:ASP:HB2	1.94	0.67
3:M:69:VAL:HG12	3:M:70:LEU:HD13	1.78	0.66
2:E:177:LYS:O	2:E:177:LYS:HE3	1.96	0.66
2:E:50:GLU:HA	2:E:220:LEU:HD23	1.78	0.66
1:A:38:LYS:HE2	7:A:950:HOH:O	1.97	0.65
2:E:105:ILE:HD12	2:E:217:PRO:HB3	1.79	0.65
2:E:106:ARG:HD2	7:E:253:HOH:O	1.96	0.65
2:E:163:GLU:HG3	7:E:298:HOH:O	1.96	0.65
1:L:432:THR:OG1	1:L:435:GLU:HG3	1.97	0.64
2:E:72:GLY:H	2:E:84:HIS:HD2	1.45	0.64
1:L:493:GLN:O	1:L:496:LYS:HB2	1.98	0.64
2:E:222:VAL:HG22	2:E:223:ALA:H	1.62	0.64
3:G:170:LYS:HE3	7:G:299:HOH:O	1.98	0.62
5:L:601:COY:H301	2:E:153:LEU:HD23	1.82	0.62
5:L:601:COY:H262	5:L:601:COY:H601	1.82	0.61
1:L:97:LYS:HB2	1:L:100[A]:GLU:HG2	1.83	0.61
3:G:75:THR:OG1	3:G:77:GLN:HG2	2.01	0.61
1:L:551:ASN:ND2	1:L:551:ASN:H	1.97	0.60
1:A:493:GLN:HE22	1:A:496:LYS:NZ	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:GLU:HG2	7:A:792:HOH:O	2.00	0.60
1:A:140:GLN:HE22	1:A:361[B]:SER:HB2	1.67	0.59
3:M:54:LYS:HG2	3:M:55:THR:O	2.02	0.59
3:M:144:GLU:OE1	3:M:150:LYS:HE2	2.02	0.59
1:A:177[A]:ARG:NH1	7:A:1277:HOH:O	2.35	0.59
2:E:62:GLU:HB2	2:E:101:LYS:HB2	1.84	0.59
1:A:32:GLU:HB3	7:A:1143:HOH:O	2.03	0.58
1:A:2:ARG:NH1	1:A:2:ARG:HB3	2.19	0.58
3:G:58:ASN:HA	7:G:332:HOH:O	2.03	0.58
3:M:77:GLN:O	3:M:80:ARG:HG2	2.03	0.58
1:L:414:LYS:O	1:L:414:LYS:HG2	2.04	0.58
1:A:434:GLU:HB2	7:A:1141:HOH:O	2.04	0.58
2:E:177:LYS:CG	2:E:179:GLU:HB2	2.34	0.58
3:M:84[B]:GLU:HG3	7:M:223:HOH:O	2.02	0.57
2:E:59:GLN:O	2:E:59:GLN:HG2	2.03	0.57
5:A:601:COY:H492	5:A:601:COY:C2B	2.35	0.57
1:L:431:ILE:HA	1:L:451:ARG:HH21	1.69	0.57
3:M:100:ARG:HD3	3:M:103:MET:CE	2.35	0.57
3:M:55:THR:HG22	7:M:328:HOH:O	2.03	0.57
1:L:205:GLU:HG2	7:L:809:HOH:O	2.04	0.57
1:L:175:VAL:O	1:L:178:TYR:HB2	2.05	0.57
5:A:601:COY:H351	5:A:601:COY:H362	1.86	0.57
2:E:71:PHE:HE1	2:E:88:LEU:HD22	1.68	0.57
2:E:121:ASN:ND2	2:E:122:ARG:HD3	2.20	0.57
3:M:55:THR:HA	7:M:272:HOH:O	2.05	0.56
2:E:89:ARG:HD2	2:E:90:GLU:OE1	2.04	0.56
5:L:601:COY:H552	5:L:601:COY:H531	1.86	0.56
3:M:64:PHE:CE2	3:M:78:ASP:HB3	2.39	0.56
3:G:130:ARG:O	3:G:170:LYS:HE3	2.05	0.56
2:E:206:LYS:HA	7:E:316:HOH:O	2.06	0.56
1:L:547:ALA:HB3	7:L:1022:HOH:O	2.04	0.56
3:M:67:GLU:HG3	3:M:68:ASN:N	2.19	0.56
1:A:42:LYS:HE2	7:A:1186:HOH:O	2.06	0.56
3:M:66:LEU:O	3:M:69:VAL:HG12	2.06	0.56
5:L:601:COY:C2B	5:L:601:COY:H492	2.36	0.55
3:M:57:THR:CG2	3:M:59:LYS:H	2.19	0.55
2:E:59:GLN:O	2:E:125:GLY:HA3	2.05	0.55
1:A:542:LYS:HG2	1:L:310:PRO:CG	2.37	0.55
1:L:477:LEU:HB3	1:L:486:ALA:HB2	1.88	0.55
3:M:54:LYS:HB2	7:M:306:HOH:O	2.06	0.55
2:E:94:GLY:HA2	2:E:97:GLU:OE1	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:121:ASN:ND2	2:B:143:GLN:HA	2.22	0.55
2:E:112:ASP:O	2:E:116:VAL:HG13	2.06	0.55
1:A:140:GLN:HE21	1:A:141:GLN:H	1.53	0.55
2:E:219:GLU:O	2:E:220:LEU:HD23	2.06	0.55
2:E:121:ASN:HD22	2:E:122:ARG:HD3	1.72	0.55
3:M:62:ASP:HA	7:M:330:HOH:O	2.06	0.55
2:E:122:ARG:HG3	7:E:274:HOH:O	2.06	0.55
1:L:431:ILE:HA	1:L:451:ARG:NH2	2.21	0.55
2:B:55:ARG:HG3	7:B:322:HOH:O	2.06	0.54
2:E:50:GLU:HA	2:E:219:GLU:O	2.08	0.54
2:E:161:THR:HB	7:E:302:HOH:O	2.06	0.54
1:L:429:PRO:HD3	1:L:459:PHE:CG	2.42	0.54
1:A:369:ASN:ND2	1:A:377:SER:H	2.04	0.54
2:B:146:PRO:HG2	2:B:149:SER:HB2	1.89	0.54
2:E:69:PRO:HA	2:E:106:ARG:HD3	1.89	0.54
5:A:601:COY:H361	5:A:601:COY:O39	2.06	0.53
2:E:170:LYS:HE2	2:E:171:ASN:OD1	2.08	0.53
2:E:105:ILE:HD12	2:E:217:PRO:CB	2.38	0.53
2:E:49:THR:O	2:E:220:LEU:HA	2.09	0.53
2:E:177:LYS:HG3	2:E:179:GLU:HB2	1.90	0.53
3:M:59:LYS:HB2	3:M:63:ASP:OD1	2.09	0.53
1:A:177[A]:ARG:HG2	1:A:177[A]:ARG:HH11	1.74	0.53
1:L:477:LEU:CB	1:L:486:ALA:HB2	2.39	0.53
2:E:121:ASN:HD22	2:E:122:ARG:N	2.06	0.52
1:L:455:GLU:HG3	7:L:1038:HOH:O	2.08	0.52
5:L:601:COY:H351	5:L:601:COY:H362	1.92	0.52
3:M:157:ARG:HD2	7:M:224:HOH:O	2.08	0.52
3:M:57:THR:HG21	3:M:59:LYS:HD2	1.91	0.52
5:A:601:COY:H601	5:A:601:COY:H262	1.92	0.52
1:A:177[A]:ARG:HD3	7:A:892:HOH:O	2.11	0.51
2:E:119:GLU:HG2	7:E:276:HOH:O	2.09	0.51
2:E:119:GLU:OE2	2:E:217:PRO:HD3	2.10	0.51
2:E:175:TYR:CD1	2:E:181:PRO:HD2	2.44	0.51
1:L:140:GLN:HE21	1:L:141:GLN:H	1.58	0.51
1:A:466:LYS:HE2	7:A:1051:HOH:O	2.10	0.51
1:L:42:LYS:HB2	1:L:50:GLU:CB	2.36	0.51
2:E:49:THR:O	2:E:51:VAL:HG13	2.10	0.51
1:A:549:ASP:OD2	1:A:551:ASN:OD1	2.29	0.51
2:E:128:ILE:HD12	2:E:175:TYR:HB3	1.92	0.51
2:E:87:ILE:O	2:E:91:VAL:HG23	2.10	0.50
3:M:55:THR:OG1	3:M:59:LYS:O	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:100:ARG:HD3	3:M:103:MET:HE2	1.94	0.50
1:A:316:VAL:O	1:A:319:GLU:HG2	2.11	0.50
3:M:56:ALA:O	3:M:58:ASN:OD1	2.30	0.50
1:L:25:GLU:HB3	7:L:859:HOH:O	2.11	0.50
2:E:90:GLU:O	2:E:166:ARG:HD2	2.12	0.50
3:M:53:VAL:O	3:M:53:VAL:HG12	2.11	0.50
2:E:142:GLN:HB2	2:E:151:LEU:HD11	1.94	0.49
2:E:53:GLU:HA	2:E:218:GLN:NE2	2.27	0.49
1:A:462:GLU:HG3	1:A:466:LYS:HG3	1.95	0.49
2:E:65:ILE:HG21	2:E:88:LEU:HD11	1.94	0.49
1:A:177[A]:ARG:HB3	1:A:457:ILE:HG23	1.94	0.49
1:A:210[A]:LYS:HD2	7:A:1084:HOH:O	2.11	0.49
2:E:72:GLY:H	2:E:84:HIS:CD2	2.27	0.49
2:E:71:PHE:CE1	2:E:88:LEU:HD22	2.47	0.49
1:L:180:PRO:HG3	1:L:464:ILE:HD11	1.94	0.49
1:A:177[B]:ARG:HB3	1:A:457:ILE:HG23	1.94	0.49
2:E:47:PHE:CE1	2:E:85:LYS:HA	2.47	0.49
2:E:94:GLY:O	2:E:97:GLU:OE2	2.30	0.49
2:E:95:ILE:O	2:E:98:GLU:HB2	2.12	0.49
2:E:109:LYS:HG2	2:E:214:GLY:H	1.77	0.49
2:E:177:LYS:HG2	2:E:179:GLU:OE1	2.13	0.48
1:L:538:TRP:O	1:L:542:LYS:HG3	2.13	0.48
5:L:601:COY:H1R	7:E:229:HOH:O	2.12	0.48
2:E:107:CYS:CB	2:E:116:VAL:HB	2.44	0.48
1:L:186:LEU:CD2	1:L:199:THR:HB	2.43	0.48
1:A:177[A]:ARG:NH2	7:A:1202:HOH:O	2.46	0.48
1:A:177[B]:ARG:HG2	1:A:461:GLN:NE2	2.28	0.48
1:A:38:LYS:HD3	7:A:970:HOH:O	2.13	0.48
2:E:93:ALA:O	2:E:97:GLU:OE1	2.31	0.48
1:L:413:ASN:HD21	1:L:417:ARG:HE	1.60	0.48
2:E:64:ILE:HA	2:E:103:ARG:O	2.13	0.48
1:L:179:ALA:HB3	1:L:180:PRO:HD3	1.94	0.48
3:M:65:THR:OG1	3:M:68:ASN:HB2	2.13	0.48
2:E:90:GLU:O	2:E:166:ARG:HA	2.13	0.48
7:L:1093:HOH:O	2:E:195[B]:LYS:HE2	2.13	0.48
1:L:452:ASN:ND2	1:L:455:GLU:H	2.11	0.48
2:E:219:GLU:HG3	2:E:220:LEU:N	2.29	0.48
2:B:204:HIS:HD2	7:B:247:HOH:O	1.97	0.48
2:E:127:GLY:O	2:E:142:GLN:HA	2.14	0.48
1:L:192:VAL:HG13	1:L:414:LYS:HD2	1.95	0.47
1:A:86:LYS:HD3	1:A:86:LYS:HA	1.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:477:LEU:HD13	1:L:485:VAL:HG12	1.96	0.47
1:A:306:PRO:O	1:A:312:GLY:HA3	2.14	0.47
5:A:601:COY:H531	5:A:601:COY:H552	1.96	0.47
1:L:484:ASP:OD2	1:L:485:VAL:HG23	2.15	0.47
3:M:66:LEU:O	3:M:70:LEU:HD13	2.14	0.47
2:E:51:VAL:HG11	2:E:221:ARG:HB2	1.96	0.47
1:A:179:ALA:HB3	1:A:180:PRO:HD3	1.95	0.47
2:E:209:LYS:HG3	7:E:316:HOH:O	2.14	0.47
1:A:2:ARG:HB3	1:A:2:ARG:HH11	1.79	0.47
1:A:331:ALA:HA	1:A:359:PHE:HB2	1.97	0.47
2:E:119:GLU:OE2	2:E:217:PRO:HG3	2.15	0.47
2:E:53:GLU:HG3	2:E:218:GLN:NE2	2.30	0.47
1:L:148:LYS:O	1:L:149:ASP:HB2	2.15	0.47
1:L:175:VAL:HG13	1:L:175:VAL:O	2.15	0.47
2:E:50:GLU:HG3	2:E:50:GLU:O	2.15	0.47
2:E:55:ARG:HA	2:E:55:ARG:HD2	1.44	0.47
3:G:53:VAL:HG13	7:G:326:HOH:O	2.15	0.47
1:L:477:LEU:HD12	1:L:486:ALA:HA	1.97	0.47
3:M:60:THR:HG22	7:M:306:HOH:O	2.14	0.47
3:M:66:LEU:HA	3:M:66:LEU:HD23	1.74	0.47
1:L:152:VAL:HG21	1:L:431:ILE:HG23	1.97	0.46
5:L:601:COY:C6	5:L:601:COY:H4B	2.45	0.46
3:M:60:THR:HB	7:M:221:HOH:O	2.15	0.46
2:B:60:GLN:NE2	7:B:437:HOH:O	2.48	0.46
5:L:601:COY:H202	5:L:601:COY:N3B	2.30	0.46
1:A:210[A]:LYS:HE3	1:A:210[A]:LYS:HB2	1.56	0.46
2:E:60:GLN:HA	2:E:125:GLY:C	2.36	0.46
1:A:153:GLN:HE22	1:A:445:SER:HB3	1.79	0.46
1:L:177[B]:ARG:HG2	1:L:461:GLN:CG	2.46	0.46
1:A:140:GLN:HE21	1:A:141:GLN:N	2.13	0.46
2:B:146:PRO:HG2	2:B:149:SER:CB	2.46	0.46
2:B:157:ALA:HA	2:B:160:LEU:HD22	1.96	0.46
2:B:50:GLU:HG2	2:B:220:LEU:CD2	2.46	0.46
1:L:461:GLN:HA	1:L:461:GLN:NE2	2.31	0.46
5:L:601:COY:HM62	2:E:114:ALA:HB2	1.98	0.46
2:E:60:GLN:HA	2:E:126:SER:HA	1.98	0.46
1:L:463:ILE:HA	1:L:468:ARG:HG3	1.98	0.46
1:A:329:GLU:OE2	1:A:505:SER:HA	2.16	0.45
2:E:103:ARG:HG3	2:E:219:GLU:OE1	2.16	0.45
2:E:98:GLU:OE1	2:E:98:GLU:HA	2.11	0.45
1:L:152:VAL:HG22	1:L:431:ILE:HD13	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:550:PRO:CG	1:L:23:TRP:HB2	2.44	0.45
1:L:469:ASN:O	1:L:472:GLU:HB2	2.16	0.45
2:E:64:ILE:HD12	2:E:124:SER:CA	2.46	0.45
1:L:430:PRO:O	1:L:451:ARG:NH2	2.49	0.45
5:A:601:COY:O28	5:A:601:COY:H3	2.15	0.45
2:B:100:ILE:HD11	2:B:177[B]:LYS:CD	2.42	0.45
1:L:487:GLN:O	1:L:490:LEU:HB2	2.16	0.45
1:A:369:ASN:HD22	1:A:369:ASN:HA	1.59	0.45
2:E:85:LYS:O	2:E:89:ARG:HB2	2.17	0.45
3:M:54:LYS:CG	3:M:58:ASN:HA	2.46	0.45
3:M:59:LYS:HG2	3:M:59:LYS:O	2.17	0.45
2:E:55:ARG:NH1	7:E:311:HOH:O	2.50	0.45
3:G:168:LYS:NZ	7:G:270:HOH:O	2.50	0.45
1:L:148:LYS:HD2	1:L:148:LYS:HA	1.79	0.45
1:L:16:GLN:NE2	7:L:1093:HOH:O	2.49	0.45
1:L:262:SER:HA	7:L:606:HOH:O	2.16	0.45
1:A:2:ARG:NH1	1:L:405:GLU:OE1	2.50	0.45
3:M:117:ASP:OD1	3:M:117:ASP:N	2.50	0.45
3:M:71:SER:O	3:M:72:ASN:HB2	2.17	0.45
1:A:177[B]:ARG:HD2	7:A:1278:HOH:O	2.16	0.45
2:E:108:PHE:O	2:E:212:VAL:N	2.50	0.45
2:E:141:HIS:NE2	2:E:149:SER:O	2.49	0.45
1:A:414:LYS:NZ	7:A:1253:HOH:O	2.50	0.44
2:B:88:LEU:HD12	2:B:88:LEU:HA	1.79	0.44
1:L:490:LEU:HD23	1:L:490:LEU:HA	1.81	0.44
1:A:211:LEU:HD22	1:A:216:HIS:HB2	1.99	0.44
1:A:538:TRP:CE2	1:A:542:LYS:HD2	2.52	0.44
1:L:414:LYS:NZ	7:L:678:HOH:O	2.50	0.44
1:L:432:THR:OG1	1:L:434:GLU:OE2	2.30	0.44
3:M:64:PHE:HE2	3:M:78:ASP:HB3	1.79	0.44
2:E:55:ARG:NE	2:E:56:GLN:HB2	2.32	0.44
1:L:206:ALA:HB3	7:L:1045:HOH:O	2.18	0.44
2:E:51:VAL:HG23	2:E:51:VAL:O	2.17	0.44
3:G:157:ARG:HD3	7:G:227:HOH:O	2.18	0.44
1:A:405:GLU:OE2	1:L:2[B]:ARG:NH2	2.51	0.44
1:L:477:LEU:CD1	1:L:485:VAL:HG12	2.47	0.44
3:G:142:ASP:OD1	3:G:146[A]:ARG:NH1	2.50	0.44
1:L:468:ARG:HD2	1:L:472:GLU:OE1	2.16	0.44
3:M:130:ARG:O	3:M:170:LYS:HD3	2.17	0.44
1:A:83:ASP:OD2	1:A:85:VAL:N	2.50	0.44
2:E:163:GLU:N	7:E:298:HOH:O	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:58:THR:O	2:E:60:GLN:NE2	2.50	0.44
2:B:113:VAL:HB	2:B:133:GLN:HG3	2.00	0.44
2:E:62:GLU:OE2	2:E:125:GLY:N	2.50	0.44
1:L:452:ASN:HD21	1:L:454:VAL:HB	1.82	0.44
1:L:236:ASP:O	3:M:127:ARG:HD2	2.18	0.44
3:M:54:LYS:HG3	3:M:58:ASN:HA	2.00	0.44
2:E:60:GLN:HA	2:E:125:GLY:O	2.18	0.43
3:G:80:ARG:NH2	7:G:324:HOH:O	2.49	0.43
1:A:283:CYS:HA	1:A:286:ILE:HD12	2.00	0.43
1:A:361[A]:SER:HG	1:A:363:GLY:H	1.66	0.43
1:L:331:ALA:HA	1:L:359:PHE:HB2	2.01	0.43
1:L:69:TYR:HB2	1:L:289:ALA:HB1	1.99	0.43
1:A:97:LYS:HB2	1:A:100[A]:GLU:CG	2.37	0.43
2:E:109:LYS:HG2	2:E:214:GLY:N	2.34	0.43
3:M:66:LEU:HD22	3:M:70:LEU:HD13	2.01	0.43
1:L:12:ARG:HA	1:L:13:PRO:HD3	1.92	0.43
3:M:82:THR:HB	3:M:83:PRO:HD2	2.00	0.43
1:A:177[A]:ARG:NH2	7:A:1193:HOH:O	2.50	0.43
1:A:335:ASP:N	1:A:335:ASP:OD1	2.50	0.43
5:A:601:COY:H531	5:A:601:COY:C55	2.48	0.43
7:A:1153:HOH:O	2:B:204:HIS:HE1	2.02	0.43
3:G:54[B]:LYS:HE3	3:G:58:ASN:ND2	2.34	0.43
1:L:173:VAL:CG2	1:L:176:ALA:HA	2.39	0.43
5:L:601:COY:C2B	5:L:601:COY:H202	2.49	0.43
1:A:20:VAL:HG13	1:L:550:PRO:CG	2.46	0.42
5:L:601:COY:H301	2:E:153:LEU:CD2	2.47	0.42
1:A:461:GLN:NE2	7:A:1145:HOH:O	2.50	0.42
1:L:282:ARG:HD2	7:L:981:HOH:O	2.18	0.42
1:L:72:ASN:HB3	1:L:107:ALA:HA	2.01	0.42
1:L:97:LYS:HB2	1:L:100[A]:GLU:CG	2.48	0.42
3:M:57:THR:HG22	3:M:59:LYS:H	1.83	0.42
1:A:177[A]:ARG:NH1	1:A:177[A]:ARG:HG2	2.34	0.42
2:E:106:ARG:CB	2:E:220:LEU:HD11	2.50	0.42
2:E:56:GLN:HE21	2:E:57:GLY:H	1.67	0.42
3:G:118:ARG:NH2	7:G:259:HOH:O	2.50	0.42
1:L:370:TYR:OH	1:L:444:GLY:HA3	2.19	0.42
1:L:452:ASN:ND2	1:L:454:VAL:HG23	2.34	0.42
1:L:42:LYS:HB3	1:L:49:THR:OG1	2.19	0.42
1:A:140:GLN:HE21	1:A:140:GLN:CA	2.32	0.42
3:G:71:SER:O	3:G:72:ASN:HB2	2.18	0.42
1:L:12:ARG:HH11	1:L:12:ARG:HD3	1.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:489:MET:HG2	7:L:984:HOH:O	2.18	0.42
1:A:69:TYR:HB2	1:A:289:ALA:HB1	2.00	0.42
1:A:86:LYS:HE2	7:A:1095:HOH:O	2.19	0.42
1:L:414:LYS:HZ2	1:L:414:LYS:HG3	1.65	0.42
3:M:57:THR:HG23	3:M:59:LYS:H	1.83	0.42
2:E:97:GLU:O	7:E:304:HOH:O	2.21	0.42
2:E:128:ILE:HG13	2:E:176:ALA:HA	2.01	0.42
2:E:60:GLN:N	2:E:60:GLN:HE21	2.18	0.42
1:L:97:LYS:HE3	1:L:97:LYS:HB2	1.58	0.42
2:B:77:VAL:HG12	2:B:83:PRO:HA	2.01	0.42
1:A:302:CYS:O	1:A:306:PRO:HD2	2.20	0.41
1:L:300:VAL:HG12	1:L:301:SER:N	2.35	0.41
3:M:54:LYS:CD	3:M:58:ASN:HA	2.50	0.41
1:A:299:SER:OG	1:A:303:ILE:HA	2.19	0.41
2:E:161:THR:O	2:E:164:THR:N	2.50	0.41
2:E:55:ARG:CZ	2:E:56:GLN:HB2	2.50	0.41
1:A:441:TYR:CZ	1:L:1:MET:HB3	2.55	0.41
1:L:306:PRO:O	1:L:312:GLY:HA3	2.20	0.41
5:A:601:COY:H4B	5:A:601:COY:C6	2.50	0.41
2:E:216:ASN:HA	2:E:217:PRO:HD3	1.94	0.41
2:E:222:VAL:HG13	2:E:223:ALA:N	2.35	0.41
1:L:429:PRO:HD3	1:L:459:PHE:CD2	2.55	0.41
1:A:493:GLN:HE22	1:A:496:LYS:HZ1	1.68	0.41
1:A:3:SER:O	1:A:7:GLU:HG3	2.21	0.41
1:A:42:LYS:HE3	1:A:42:LYS:HB3	1.88	0.41
2:B:60:GLN:OE1	2:B:60:GLN:N	2.54	0.41
3:M:58:ASN:N	3:M:58:ASN:OD1	2.54	0.41
2:E:105:ILE:HA	2:E:218:GLN:O	2.20	0.41
1:L:187:LEU:O	1:L:191:GLN:HG2	2.19	0.41
3:M:80:ARG:NH2	7:M:270:HOH:O	2.54	0.41
1:A:241:SER:HB3	3:G:126:LEU:HB3	2.02	0.41
2:E:174:ARG:HD2	2:E:179:GLU:CG	2.47	0.41
5:L:601:COY:H411	5:L:601:COY:H363	1.77	0.41
5:A:601:COY:H2P	7:A:1123:HOH:O	2.20	0.41
2:E:130:ILE:HD11	2:E:172:ALA:CB	2.51	0.41
2:E:55:ARG:O	2:E:103:ARG:NH2	2.50	0.41
3:G:57:THR:HA	7:G:333:HOH:O	2.20	0.41
1:L:72:ASN:HB3	1:L:107:ALA:CA	2.50	0.41
1:A:210[B]:LYS:NZ	7:A:846:HOH:O	2.50	0.41
2:E:175:TYR:CE1	2:E:181:PRO:HD2	2.56	0.41
3:G:64:PHE:CE2	3:G:79:MET:HG2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:548:LEU:HD21	7:A:823:HOH:O	2.20	0.41
1:L:177[A]:ARG:HG2	1:L:461:GLN:CG	2.50	0.41
3:G:41:SER:O	3:G:48:LYS:HE2	2.21	0.40
2:B:89:ARG:HD2	2:B:90:GLU:OE1	2.21	0.40
2:E:103:ARG:HD2	2:E:219:GLU:OE2	2.21	0.40
1:L:140:GLN:HE21	1:L:141:GLN:N	2.19	0.40
3:G:56:ALA:HB2	3:G:80:ARG:HB2	2.04	0.40
1:A:171:THR:HB	1:A:186:LEU:HD22	2.04	0.40
1:A:20:VAL:HG22	1:L:548:LEU:HG	2.03	0.40
3:G:58:ASN:HA	3:G:58:ASN:HD22	1.52	0.40
1:L:220:ALA:O	1:L:256:MET:HA	2.21	0.40
1:L:280:GLU:O	1:L:283:CYS:HB2	2.21	0.40
1:L:423:PHE:HD1	1:L:429:PRO:O	2.04	0.40
3:M:146:ARG:O	3:M:146:ARG:HG3	2.21	0.40
1:A:42:LYS:HB2	1:A:50:GLU:HB3	2.04	0.40
7:A:1123:HOH:O	2:B:197:GLN:HG3	2.22	0.40
2:E:49:THR:HG22	2:E:49:THR:O	2.20	0.40
1:L:471:LEU:HA	1:L:471:LEU:HD12	1.88	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%)	536 (97%)	15 (3%)	2 (0%)	34	18
1	L	555/554 (100%)	535 (96%)	18 (3%)	2 (0%)	34	18
2	B	180/224 (80%)	177 (98%)	3 (2%)	0	100	100
2	E	177/224 (79%)	170 (96%)	6 (3%)	1 (1%)	25	11
3	G	139/173 (80%)	135 (97%)	3 (2%)	1 (1%)	22	8
3	M	137/173 (79%)	134 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1741/1902 (92%)	1687 (97%)	48 (3%)	6 (0%)	41	24

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	222	VAL
3	G	56	ALA
1	A	300	VAL
1	L	300	VAL
1	L	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	454/453 (100%)	429 (94%)	25 (6%)	21	7
1	L	456/453 (101%)	413 (91%)	43 (9%)	8	1
2	B	150/183 (82%)	133 (89%)	17 (11%)	6	1
2	E	147/183 (80%)	123 (84%)	24 (16%)	2	0
3	G	120/141 (85%)	106 (88%)	14 (12%)	5	1
3	M	118/141 (84%)	103 (87%)	15 (13%)	4	1
All	All	1445/1554 (93%)	1307 (90%)	138 (10%)	9	1

All (138) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	PHE
1	A	38	LYS
1	A	42	LYS
1	A	73	LEU
1	A	86	LYS
1	A	140	GLN

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Mol	Chain	Res	Type
1	A	177[A]	ARG
1	A	177[B]	ARG
1	A	178	TYR
1	A	198	LEU
1	A	210[A]	LYS
1	A	210[B]	LYS
1	A	211	LEU
1	A	230	PRO
1	A	232	PHE
1	A	245	LEU
1	A	326	LEU
1	A	348	ARG
1	A	364	TYR
1	A	369	ASN
1	A	406	GLU
1	A	461	GLN
1	A	492	ILE
1	A	501	TYR
1	A	543	ASN
2	B	56	GLN
2	B	60	GLN
2	B	73	LEU
2	B	85	LYS
2	B	121	ASN
2	B	122	ARG
2	B	150	ASN
2	B	160	LEU
2	B	177[A]	LYS
2	B	177[B]	LYS
2	B	178	ARG
2	B	180	SER
2	B	190[A]	GLN
2	B	190[B]	GLN
2	B	195	LYS
2	B	221[A]	ARG
2	B	221[B]	ARG
3	G	51	GLU
3	G	54[A]	LYS
3	G	54[B]	LYS
3	G	58	ASN
3	G	66	LEU
3	G	73	LYS

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Mol	Chain	Res	Type
3	G	74	VAL
3	G	124[A]	ASN
3	G	124[B]	ASN
3	G	126	LEU
3	G	146[A]	ARG
3	G	146[B]	ARG
3	G	150	LYS
3	G	170	LYS
1	L	9	LEU
1	L	24	ILE
1	L	28	PHE
1	L	42	LYS
1	L	72	ASN
1	L	73	LEU
1	L	74	ASN
1	L	100[A]	GLU
1	L	100[B]	GLU
1	L	140	GLN
1	L	148	LYS
1	L	177[A]	ARG
1	L	177[B]	ARG
1	L	178	TYR
1	L	187	LEU
1	L	198	LEU
1	L	210	LYS
1	L	211	LEU
1	L	218	CYS
1	L	232	PHE
1	L	277	LEU
1	L	326	LEU
1	L	348	ARG
1	L	411	ILE
1	L	414	LYS
1	L	434	GLU
1	L	451	ARG
1	L	452	ASN
1	L	453	ILE
1	L	455	GLU
1	L	466	LYS
1	L	471	LEU
1	L	487	GLN
1	L	489	MET

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Mol	Chain	Res	Type
1	L	490	LEU
1	L	493	GLN
1	L	494	LYS
1	L	501	TYR
1	L	511	ASP
1	L	513	GLN
1	L	543	ASN
1	L	548	LEU
1	L	551	ASN
2	E	47	PHE
2	E	50	GLU
2	E	55	ARG
2	E	56	GLN
2	E	59	GLN
2	E	60	GLN
2	E	62	GLU
2	E	80	VAL
2	E	85	LYS
2	E	88	LEU
2	E	97	GLU
2	E	98	GLU
2	E	101	LYS
2	E	106	ARG
2	E	121	ASN
2	E	141	HIS
2	E	145	LEU
2	E	150	ASN
2	E	167	GLN
2	E	177	LYS
2	E	179	GLU
2	E	180	SER
2	E	182	GLN
2	E	222	VAL
3	M	45	LEU
3	M	54	LYS
3	M	55	THR
3	M	57	THR
3	M	59	LYS
3	M	66	LEU
3	M	67	GLU
3	M	69	VAL
3	M	70	LEU

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Mol	Chain	Res	Type
3	M	74	VAL
3	M	77	GLN
3	M	88	LEU
3	M	148	GLN
3	M	150	LYS
3	M	161	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	A	74	ASN
1	A	140	GLN
1	A	153	GLN
1	A	369	ASN
1	A	388	ASN
1	A	461	GLN
1	A	465	ASN
1	A	467	ASN
1	A	479	GLN
1	A	493	GLN
2	B	59	GLN
2	B	121	ASN
2	B	142	GLN
2	B	204	HIS
3	G	47	ASN
3	G	58	ASN
1	L	35	ASN
1	L	72	ASN
1	L	140	GLN
1	L	267	GLN
1	L	413	ASN
1	L	452	ASN
1	L	465	ASN
1	L	467	ASN
1	L	479	GLN
1	L	487	GLN
1	L	493	GLN
1	L	534	GLN
1	L	551	ASN
2	E	56	GLN
2	E	60	GLN

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Mol	Chain	Res	Type
2	E	84	HIS
2	E	121	ASN
2	E	143	GLN
2	E	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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	COY	L	601	-	93,118,118	1.06	4 (4%)	121,192,192	1.28	9 (7%)
6	PGO	A	602	4	3,4,4	0.53	0	1,4,4	0.21	0
6	PGO	L	602	4	3,4,4	0.57	0	1,4,4	0.24	0
5	COY	A	601	-	93,118,118	1.05	2 (2%)	121,192,192	1.29	12 (9%)

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	L	602	4	-	0/2/2/2	-
6	PGO	A	602	4	-	0/2/2/2	-
5	COY	L	601	-	2/2/36/38	10/57/241/241	0/5/13/13
5	COY	A	601	-	3/3/36/38	9/57/241/241	0/5/13/13

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	601	COY	C11-C10	-5.42	1.37	1.50
5	L	601	COY	C11-C10	-5.19	1.38	1.50
5	L	601	COY	O58-C57	2.55	1.28	1.23
5	A	601	COY	O58-C57	2.37	1.28	1.23
5	L	601	COY	C17-C18	2.12	1.59	1.55
5	L	601	COY	C8A-N7A	-2.09	1.31	1.34

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	601	COY	C53-C15-C14	-5.61	114.74	124.25
5	A	601	COY	C35-C5-C4	-5.59	114.77	124.25
5	L	601	COY	C35-C5-C4	-5.45	115.00	124.25
5	A	601	COY	C53-C15-C14	-4.82	116.08	124.25
5	A	601	COY	C55-C17-C16	4.09	123.21	112.16
5	L	601	COY	C55-C17-C16	3.44	121.46	112.16
5	A	601	COY	O58-C57-C56	-3.21	116.14	122.02
5	L	601	COY	C56-C57-N59	3.14	121.71	116.42
5	L	601	COY	O58-C57-C56	-2.77	116.96	122.02
5	A	601	COY	C47-C12-C13	2.72	121.40	111.72
5	A	601	COY	C36-C7-C6	2.63	118.18	111.28
5	L	601	COY	C47-C12-C13	2.44	120.41	111.72
5	A	601	COY	C54-C17-C16	-2.42	104.93	111.28
5	L	601	COY	C11-N23-C14	-2.35	108.07	111.89
5	A	601	COY	C56-C57-N59	2.27	120.25	116.42
5	A	601	COY	C46-C12-C11	-2.17	105.48	111.53
5	A	601	COY	C18-C19-N24	2.16	105.43	101.94
5	L	601	COY	C54-C17-C18	-2.07	107.85	111.71
5	A	601	COY	C60-C18-C17	2.05	118.02	114.44
5	A	601	COY	C5A-C6A-N6A	2.03	123.44	120.35
5	L	601	COY	C4B-C9B-C8B	-2.02	119.03	121.10

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	L	601	COY	C16
5	L	601	COY	C11
5	A	601	COY	C6
5	A	601	COY	C16
5	A	601	COY	C11

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	L	601	COY	C72-C71-N9A-C8A
5	L	601	COY	C72-C71-N9A-C4A
5	A	601	COY	C72-C71-N9A-C8A
5	A	601	COY	C72-C71-N9A-C4A
5	A	601	COY	C12-C13-C48-C49
5	L	601	COY	C38-C37-C7-C6
5	A	601	COY	C38-C37-C7-C6
5	L	601	COY	C71-C72-C73-C74
5	L	601	COY	C30-C31-C32-O34
5	L	601	COY	C30-C31-C32-N33
5	A	601	COY	C30-C31-C32-O34
5	L	601	COY	C12-C13-C48-C49
5	L	601	COY	C8-C41-C42-C43
5	A	601	COY	C30-C31-C32-N33
5	A	601	COY	C42-C41-C8-C9
5	A	601	COY	C19-C18-C60-C61
5	L	601	COY	C42-C41-C8-C9
5	L	601	COY	C19-C18-C60-C61
5	A	601	COY	C17-C18-C60-C61

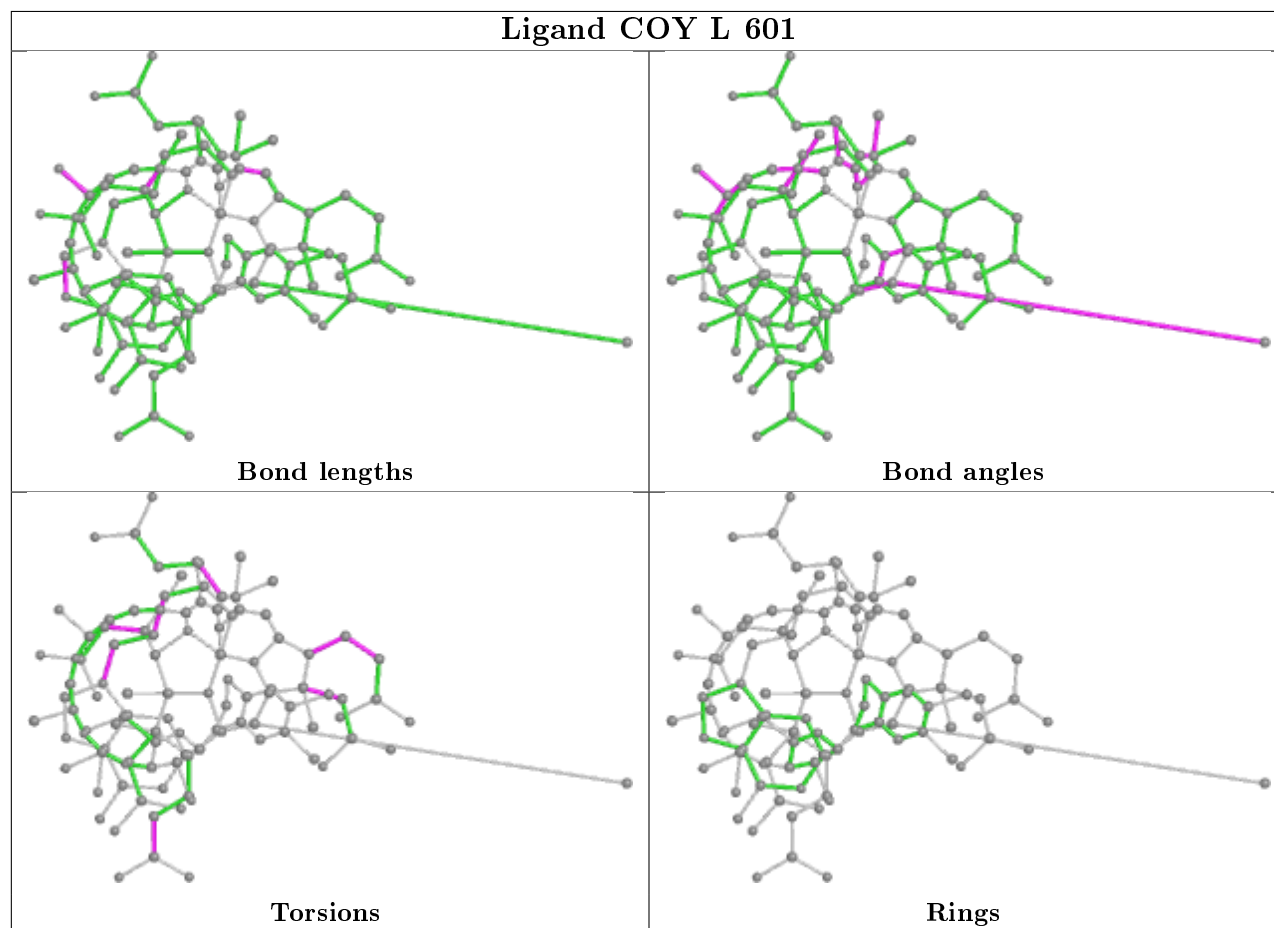
There are no ring outliers.

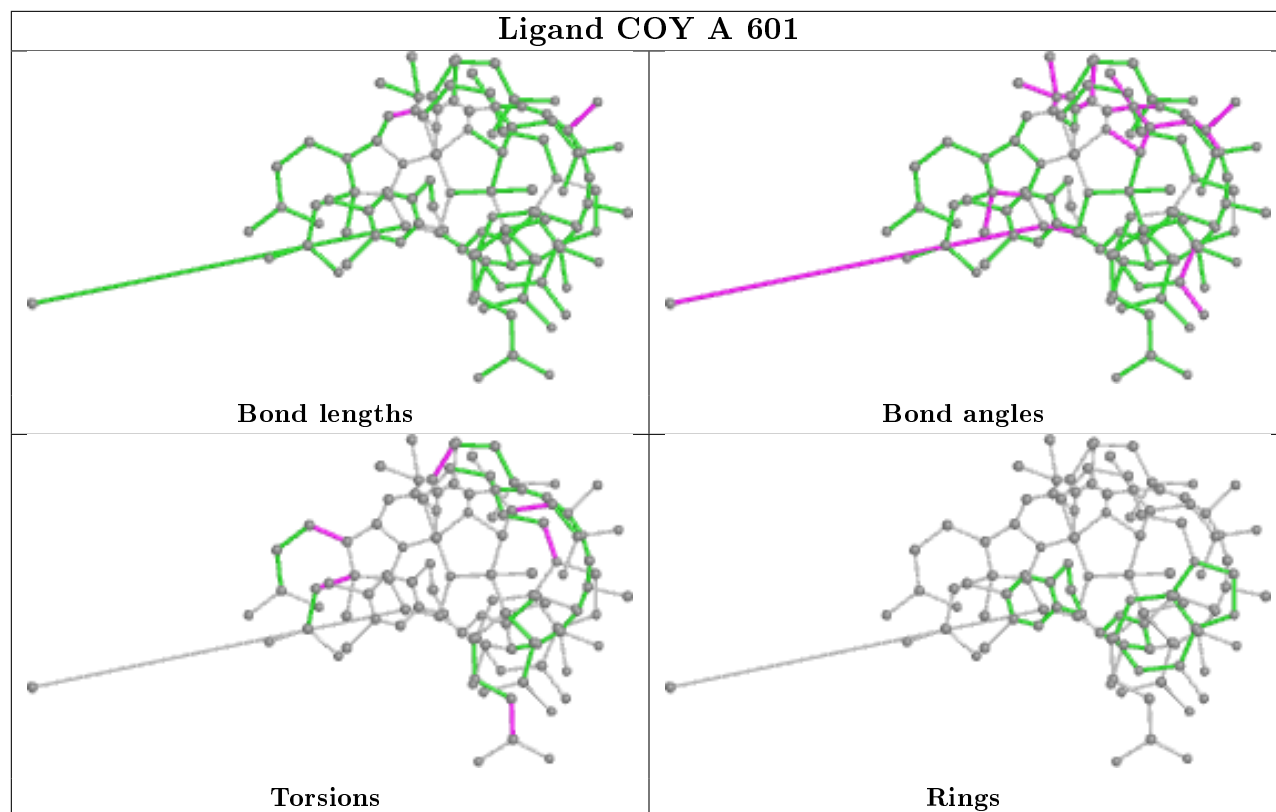
2 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	601	COY	12	0
5	A	601	COY	9	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

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





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	551/554 (99%)	-0.44	2 (0%) 92 93	8, 12, 27, 74	0
1	L	551/554 (99%)	-0.17	15 (2%) 54 58	9, 16, 43, 71	1 (0%)
2	B	178/224 (79%)	-0.22	0 100 100	11, 19, 37, 59	0
2	E	178/224 (79%)	1.41	46 (25%) 0 0	16, 37, 86, 112	0
3	G	137/173 (79%)	-0.30	1 (0%) 87 90	11, 17, 37, 55	0
3	M	137/173 (79%)	0.27	16 (11%) 4 5	13, 21, 61, 97	0
All	All	1732/1902 (91%)	-0.07	80 (4%) 32 36	8, 16, 48, 112	1 (0%)

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	51	VAL	10.3
3	M	57	THR	7.5
3	M	58	ASN	7.5
2	E	48	LEU	6.5
2	E	46	GLY	6.3
2	E	61	ASP	6.0
1	L	454	VAL	5.8
2	E	58	THR	5.8
2	E	47	PHE	5.8
3	M	55	THR	5.7
2	E	179	GLU	5.5
2	E	222	VAL	4.9
3	M	56	ALA	4.7
2	E	49	THR	4.4
2	E	221	ARG	4.3
3	M	66	LEU	4.3
2	E	50	GLU	4.3
2	E	60	GLN	4.2
2	E	95	ILE	4.2

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Mol	Chain	Res	Type	RSRZ
2	E	59	GLN	4.1
2	E	100	ILE	4.1
2	E	177	LYS	4.0
3	G	56	ALA	4.0
2	E	218	GLN	3.9
1	L	458	LYS	3.7
1	L	551	ASN	3.7
3	M	70	LEU	3.7
2	E	178	ARG	3.6
1	L	483	THR	3.6
1	L	479	GLN	3.4
2	E	62	GLU	3.4
2	E	220	LEU	3.4
2	E	94	GLY	3.3
2	E	97	GLU	3.3
2	E	99	GLY	3.3
2	E	223	ALA	3.3
1	L	482	PHE	3.3
1	L	453	ILE	3.3
2	E	180	SER	3.2
3	M	77	GLN	3.2
3	M	74	VAL	3.1
3	M	73	LYS	3.0
1	L	464	ILE	3.0
3	M	60	THR	2.9
2	E	174	ARG	2.9
2	E	181	PRO	2.9
3	M	64	PHE	2.9
1	L	459	PHE	2.8
2	E	170	LYS	2.7
2	E	132	ILE	2.6
2	E	210	TYR	2.6
2	E	122	ARG	2.6
2	E	98	GLU	2.6
2	E	52	GLY	2.6
2	E	214	GLY	2.5
2	E	54	ALA	2.5
3	M	59	LYS	2.5
2	E	213	THR	2.5
2	E	57	GLY	2.5
1	A	550	PRO	2.5
1	A	551	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	L	460	ALA	2.4
2	E	85	LYS	2.4
3	M	79	MET	2.4
1	L	434	GLU	2.4
2	E	127	GLY	2.4
2	E	217	PRO	2.4
3	M	69	VAL	2.4
1	L	432	THR	2.3
2	E	125	GLY	2.3
3	M	54	LYS	2.3
2	E	101	LYS	2.2
3	M	71	SER	2.2
1	L	478	ALA	2.2
1	L	477	LEU	2.1
2	E	124	SER	2.1
2	E	108	PHE	2.1
2	E	63	VAL	2.0
2	E	55	ARG	2.0
1	L	486	ALA	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 carbohydrates 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	COY	L	601	106/106	0.97	0.09	11,19,31,57	0
6	PGO	L	602	5/5	0.97	0.08	11,13,17,20	0
6	PGO	A	602	5/5	0.97	0.11	9,10,11,19	0
5	COY	A	601	106/106	0.98	0.08	6,12,16,31	0

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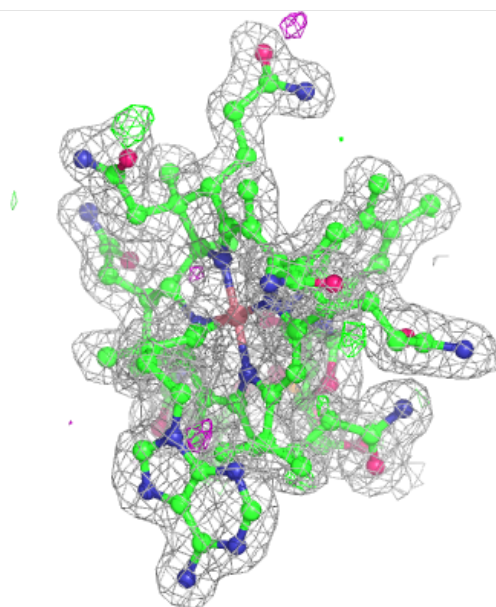
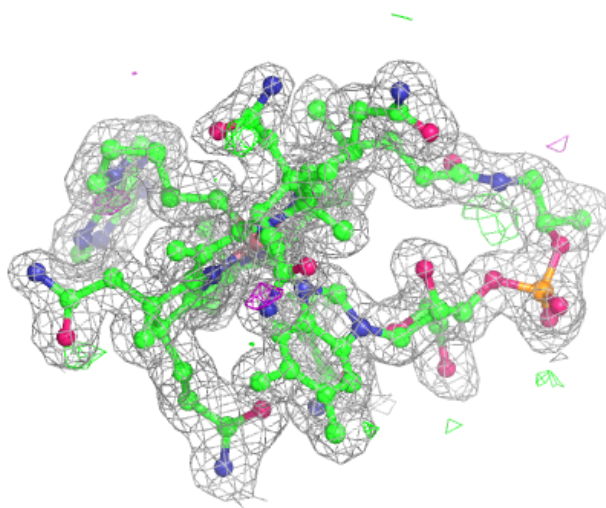
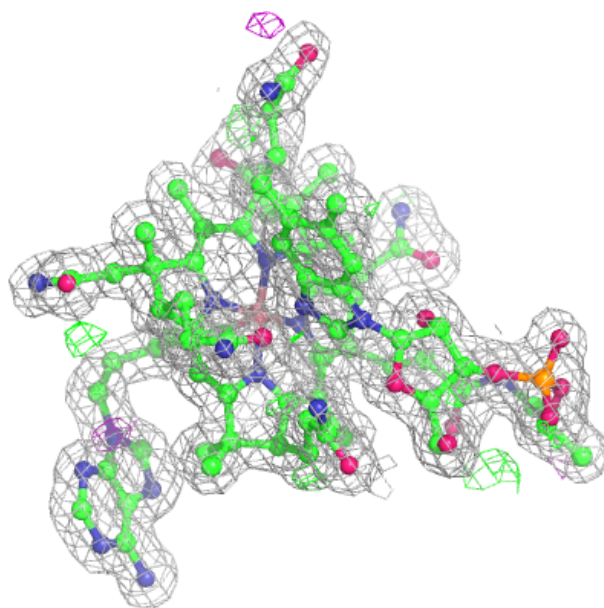
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	K	A	603	1/1	1.00	0.05	9,9,9,9	0
4	K	L	603	1/1	1.00	0.05	12,12,12,12	0
4	K	L	604	1/1	1.00	0.05	14,14,14,14	0
4	K	A	604	1/1	1.00	0.08	12,12,12,12	0

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.

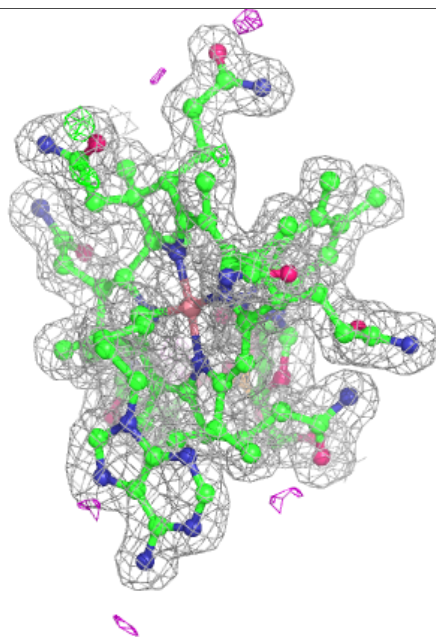
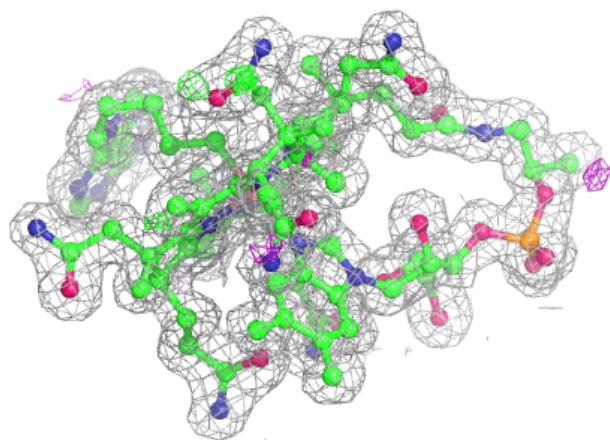
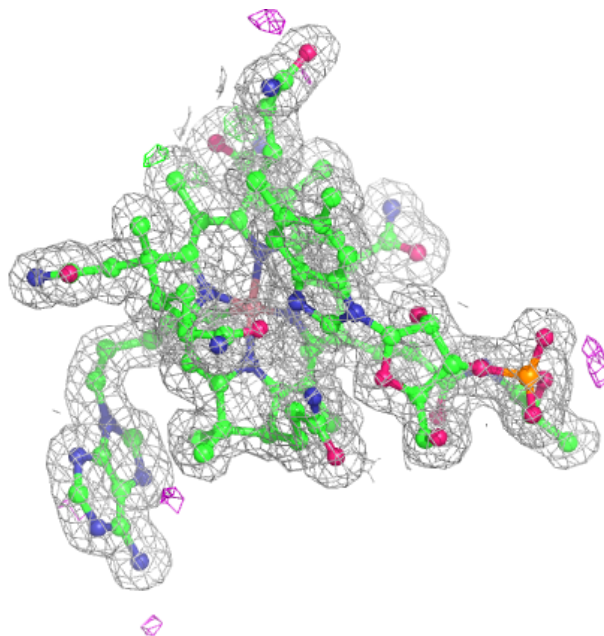
#### Electron density around COY L 601:

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around COY A 601:**

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



## 6.5 Other polymers ⓘ

There are no such residues in this entry.