



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 08:52 PM EDT

PDB ID : 1EGV / pdb_00001egv
Title : CRYSTAL STRUCTURE OF THE DIOL DEHYDRATASE-ADENINYLPENTYLCOBALAMIN COMPLEX FROM KLEBSIELLA OXYTOCA UNDER THE ILLUMINATED CONDITION.
Authors : Masuda, J.; Shibata, N.; Toraya, T.; Morimoto, Y.; Yasuoka, N.
Deposited on : 2000-02-17
Resolution : 1.75 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

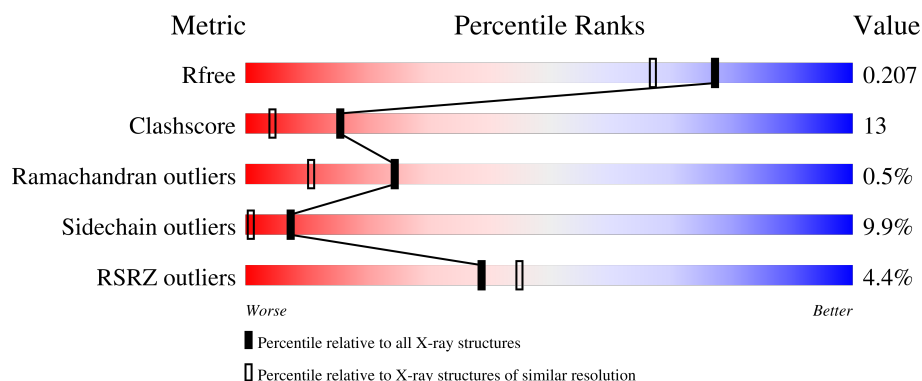
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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

Mol	Chain	Length	Quality of chain
1	A	554	85% 12% ..
1	L	554	3% 75% 19% 5% .
2	B	224	% 61% 15% . 21%
2	E	224	17% 35% 33% 10% . 21%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	G	173	
3	M	173	

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 15471 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			

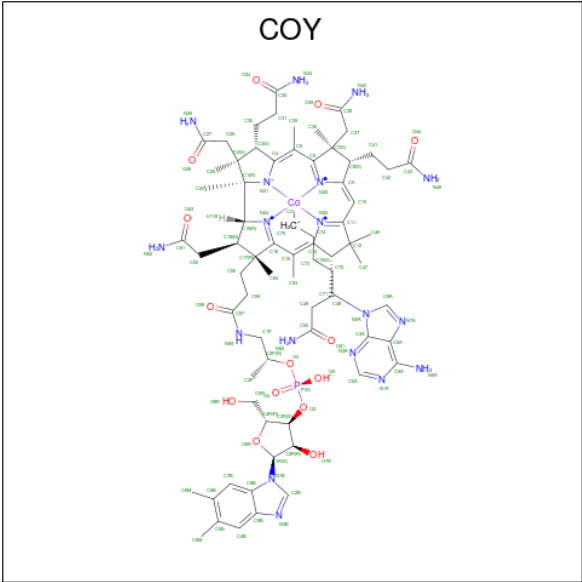
- Molecule 3 is a protein called PROPANEDIOL DEHYDRATASE.

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 (CCD ID: K) (formula: K).

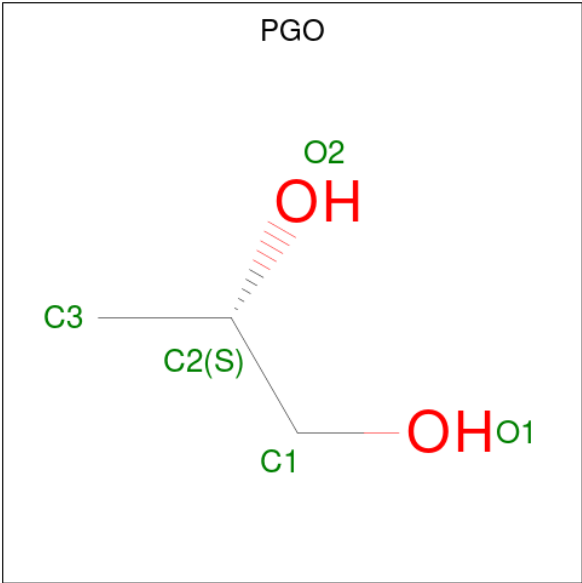
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	K	0	0
			2	2		
4	L	2	Total	K	0	0
			2	2		

- Molecule 5 is CO-(ADENIN-9-YL-PENTYL)-COBALAMIN (CCD ID: COY) (formula: C₇₂H₁₀₃CoN₁₈O₁₄P).



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 (CCD ID: PGO) (formula: C₃H₈O₂).



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		

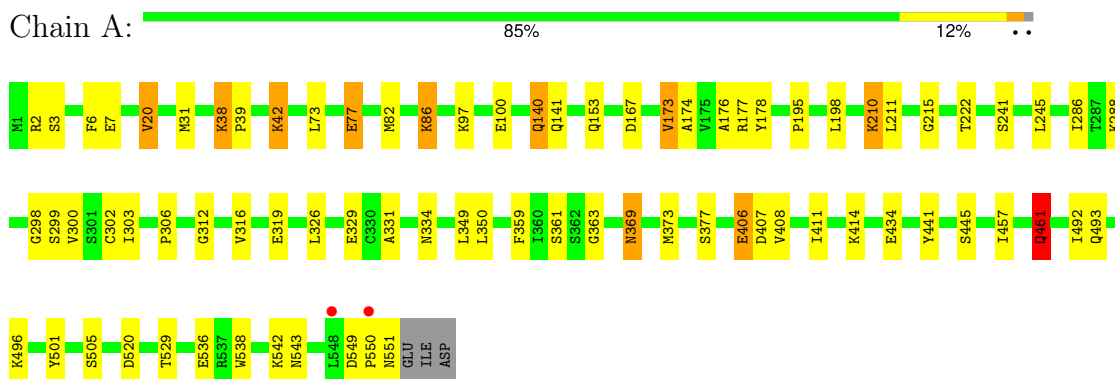
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	675	Total 675	O 675	0	0
7	B	215	Total 215	O 215	0	0
7	G	204	Total 204	O 204	0	0
7	L	498	Total 498	O 498	0	0
7	E	106	Total 106	O 106	0	0
7	M	151	Total 151	O 151	0	0

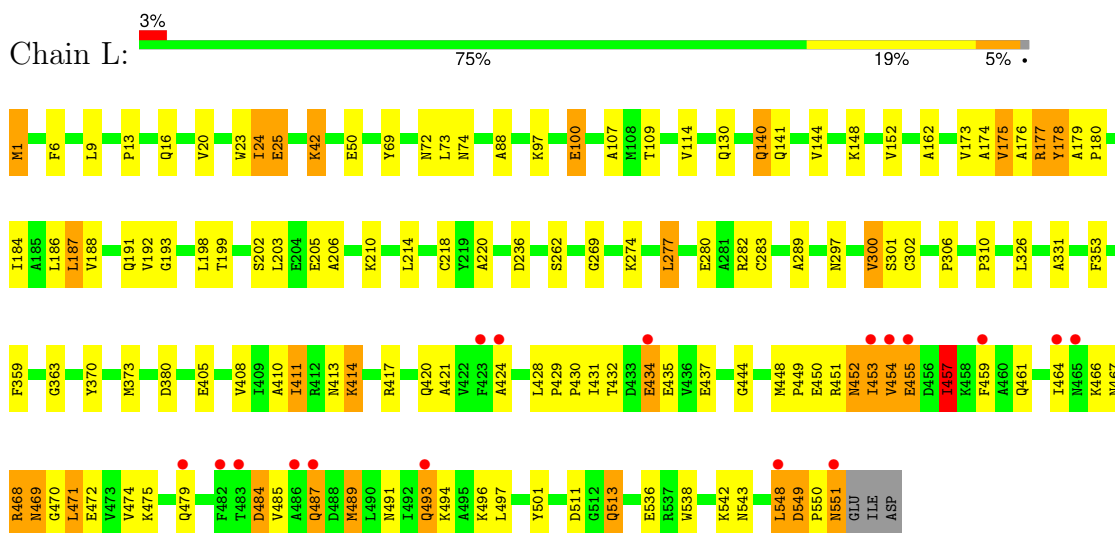
3 Residue-property plots

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.

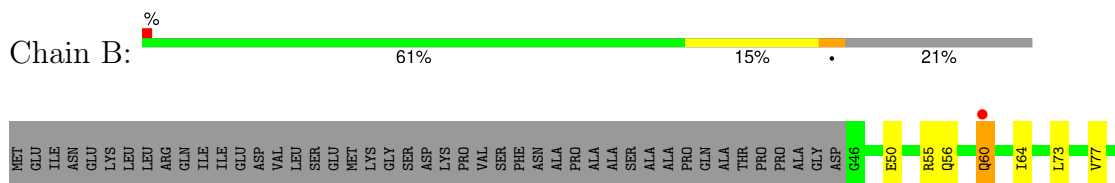
• Molecule 1: PROPANEDIOL DEHYDRATASE

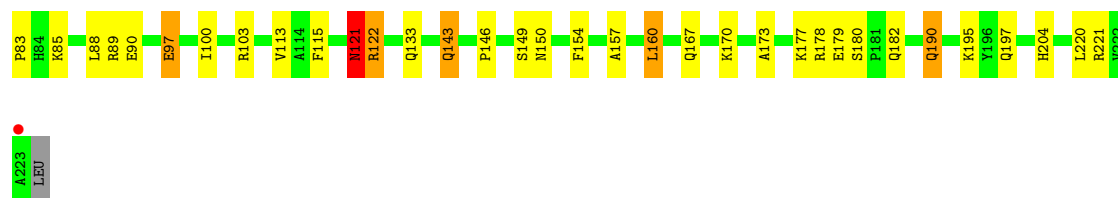


• Molecule 1: PROPANEDIOL DEHYDRATASE

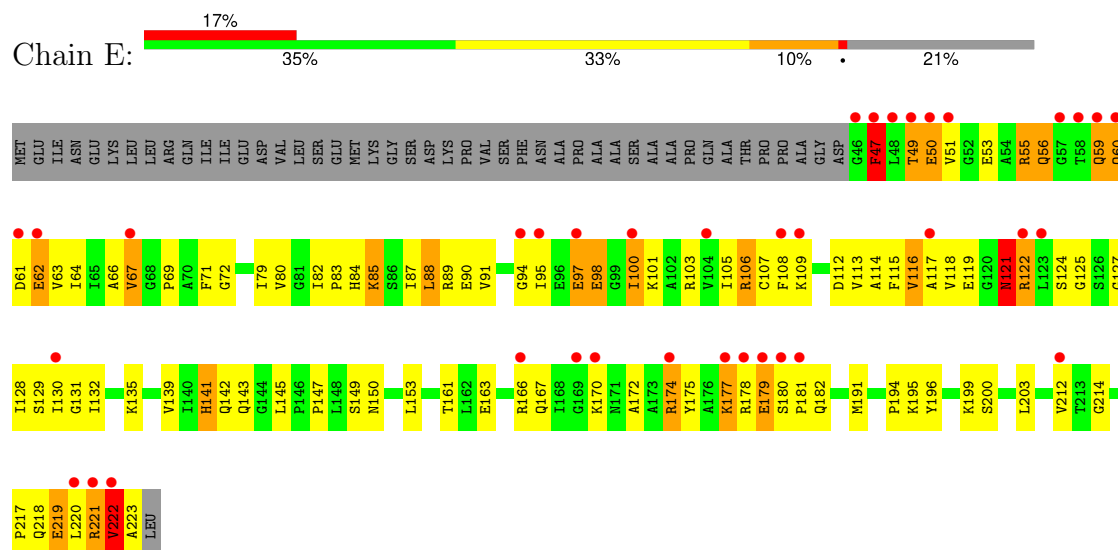


• Molecule 2: PROPANEDIOL DEHYDRATASE

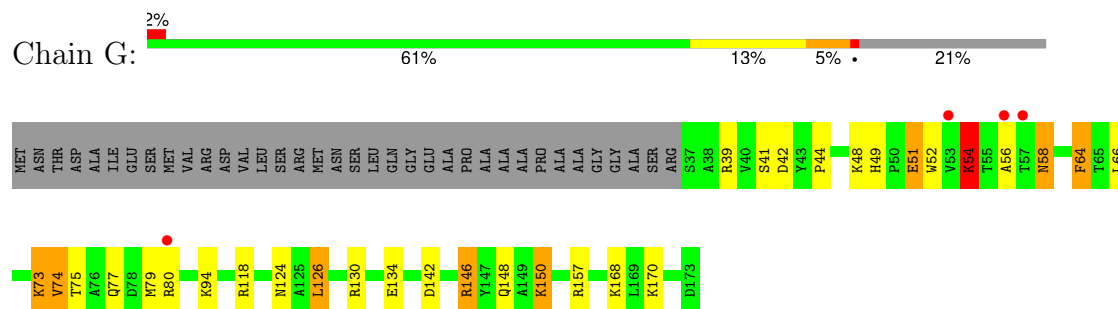




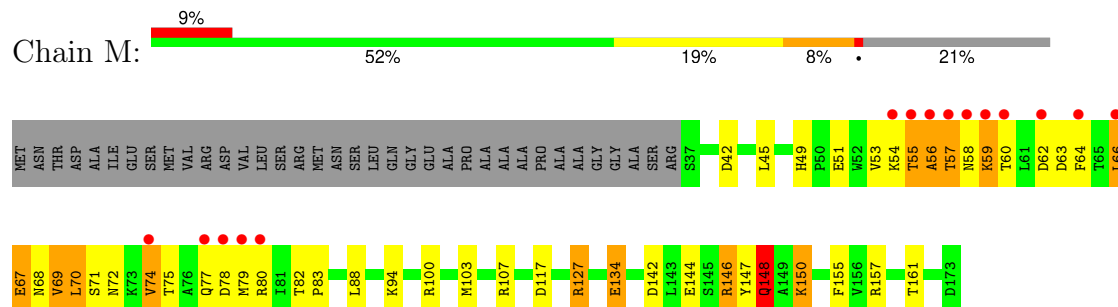
● Molecule 2: PROPANEDIOL DEHYDRATASE



● 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, α , β , γ	73.38Å 121.40Å 207.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.75 30.00 – 1.75	Depositor EDS
% Data completeness (in resolution range)	80.0 (30.00-1.75) 80.3 (30.00-1.75)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.78 (at 1.74Å)	Xtriage
Refinement program	SHELXL-97, CNS	Depositor
R, R_{free}	0.152 , 0.214 0.152 , 0.207	Depositor DCC
R_{free} test set	7562 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	13.8	Xtriage
Anisotropy	0.566	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 107.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15471	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: COY, K, PGO

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	0.44	0/4308	1.30	14/5832 (0.2%)
1	L	0.44	0/4328	1.39	24/5858 (0.4%)
2	B	0.43	0/1418	1.42	9/1917 (0.5%)
2	E	0.40	0/1389	1.42	13/1879 (0.7%)
3	G	0.44	0/1145	1.38	6/1545 (0.4%)
3	M	0.40	0/1125	1.35	5/1520 (0.3%)
All	All	0.43	0/13713	1.37	71/18551 (0.4%)

There are no bond length outliers.

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	282	ARG	CD-NE-CZ	28.54	164.35	124.40
2	B	121	ASN	CA-CB-CG	13.46	126.06	112.60
2	E	121	ASN	CA-CB-CG	11.00	123.60	112.60
2	E	221	ARG	CA-C-N	9.82	139.66	121.97
2	E	221	ARG	C-N-CA	9.82	139.66	121.97
3	G	73	LYS	CA-C-O	8.27	129.44	120.10
2	B	154	PHE	CA-CB-CG	-8.07	105.73	113.80
2	B	122	ARG	CD-NE-CZ	7.83	135.36	124.40
1	L	469	ASN	CA-C-N	7.68	129.80	120.13
1	L	469	ASN	C-N-CA	7.68	129.80	120.13
2	B	179	GLU	CA-C-N	-6.97	114.05	123.46
2	B	179	GLU	C-N-CA	-6.97	114.05	123.46
1	L	549	ASP	CA-C-N	6.62	126.87	119.32
1	L	549	ASP	C-N-CA	6.62	126.87	119.32
2	E	63	VAL	CA-C-N	-6.55	113.54	122.91
2	E	63	VAL	C-N-CA	-6.55	113.54	122.91
1	A	520	ASP	CA-C-N	6.37	130.07	120.77
1	A	520	ASP	C-N-CA	6.37	130.07	120.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	115	PHE	CA-CB-CG	-6.31	107.49	113.80
3	G	54[A]	LYS	CA-C-O	-6.25	112.59	120.28
3	G	54[B]	LYS	CA-C-O	-6.25	112.59	120.28
1	L	6	PHE	CA-CB-CG	-6.04	107.76	113.80
2	B	143	GLN	CA-C-N	-5.98	116.96	123.30
2	B	143	GLN	C-N-CA	-5.98	116.96	123.30
3	M	56	ALA	CA-C-N	5.98	131.60	121.14
3	M	56	ALA	C-N-CA	5.98	131.60	121.14
1	A	195	PRO	CA-C-N	-5.92	117.02	123.30
1	A	195	PRO	C-N-CA	-5.92	117.02	123.30
1	L	109	THR	CA-C-O	-5.92	114.25	120.88
1	L	175	VAL	CA-C-N	5.91	128.47	120.38
1	L	175	VAL	C-N-CA	5.91	128.47	120.38
3	G	64	PHE	CA-CB-CG	-5.89	107.91	113.80
1	A	167	ASP	CA-CB-CG	-5.88	106.72	112.60
1	L	448	MET	O-C-N	5.74	127.05	121.66
1	A	6	PHE	CA-CB-CG	-5.69	108.11	113.80
2	E	131	GLY	CA-C-O	-5.68	116.18	121.18
1	L	353	PHE	CA-CB-CG	5.64	119.44	113.80
1	L	380	ASP	CA-CB-CG	5.64	118.24	112.60
1	L	220	ALA	CA-C-O	-5.59	114.57	121.06
2	E	135	LYS	CA-C-N	-5.53	116.88	123.08
2	E	135	LYS	C-N-CA	-5.53	116.88	123.08
1	A	461	GLN	CA-C-O	5.53	126.41	120.55
1	L	457	ILE	CA-C-N	5.39	127.45	120.44
1	L	457	ILE	C-N-CA	5.39	127.45	120.44
1	A	31	MET	CA-C-O	-5.38	115.68	121.38
3	G	74	VAL	N-CA-CB	-5.35	102.67	111.44
1	L	282	ARG	NE-CZ-NH1	5.33	126.83	121.50
1	L	410	ALA	CA-C-O	5.31	126.40	120.82
1	A	298	GLY	CA-C-N	5.28	131.62	121.54
1	A	298	GLY	C-N-CA	5.28	131.62	121.54
1	L	484	ASP	CA-CB-CG	5.27	117.87	112.60
1	L	144	VAL	O-C-N	5.24	127.54	122.30
1	L	428	LEU	O-C-N	5.24	128.15	121.34
2	E	115	PHE	CA-C-N	-5.23	111.73	120.30
2	E	115	PHE	C-N-CA	-5.23	111.73	120.30
3	M	148	GLN	CA-CB-CG	5.20	124.51	114.10
1	A	286	ILE	CA-C-O	5.19	126.35	120.95
2	B	121	ASN	OD1-CG-ND2	-5.17	117.43	122.60
1	L	297	ASN	CA-CB-CG	5.15	117.75	112.60
3	G	49	HIS	CA-CB-CG	5.12	118.92	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	269	GLY	CA-C-N	-5.12	114.42	122.76
1	L	269	GLY	C-N-CA	-5.12	114.42	122.76
1	L	88	ALA	CA-C-O	5.10	125.95	120.55
3	M	155	PHE	CA-CB-CG	5.09	118.89	113.80
2	E	147	PRO	CA-C-N	-5.08	114.55	122.73
2	E	147	PRO	C-N-CA	-5.08	114.55	122.73
1	A	77	GLU	CA-C-O	5.06	125.78	120.42
3	M	42	ASP	CA-CB-CG	-5.04	107.56	112.60
2	E	47	PHE	CA-CB-CG	5.01	118.81	113.80
1	A	288	LYS	CA-C-N	5.00	126.98	120.28
1	A	288	LYS	C-N-CA	5.00	126.98	120.28

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	60	0
1	L	4225	0	4154	100	0
2	B	1378	0	1432	20	0
2	E	1363	0	1417	100	0
3	G	1111	0	1115	26	0
3	M	1102	0	1105	52	0
4	A	2	0	0	0	0
4	L	2	0	0	0	0
5	A	106	0	100	11	0
5	L	106	0	100	11	0
6	A	5	0	6	0	0
6	L	5	0	6	0	0
7	A	675	0	0	18	0
7	B	215	0	0	2	0
7	E	106	0	0	6	0
7	G	204	0	0	10	0
7	L	498	0	0	11	0
7	M	151	0	0	12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	15471	0	13596	364	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 (364) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:100:ILE:HD11	2:B:177[B]:LYS:HD3	1.51	0.92
1:A:97:LYS:HB2	1:A:100[A]:GLU:HG3	1.53	0.90
1:L:497:LEU:HD21	3:M:79:MET:HA	1.53	0.89
3:M:68:ASN:HB3	3:M:74:VAL:HG13	1.55	0.86
1:L:173:VAL:HG21	1:L:176:ALA:HA	1.57	0.86
2:E:67:VAL:HG13	2:E:71:PHE:HB3	1.58	0.83
2:E:55:ARG:HE	2:E:56:GLN:HB2	1.41	0.83
2:E:174:ARG:HH11	2:E:179:GLU:HG2	1.48	0.78
1:L:42:LYS:HB2	1:L:50:GLU:HB3	1.66	0.78
3:M:69:VAL:HG12	3:M:70:LEU:HD13	1.66	0.77
2:E:55:ARG:HE	2:E:56:GLN:H	1.33	0.77
3:M:54:LYS:HE2	3:M:58:ASN:O	1.86	0.76
3:M:80:ARG:HD2	7:M:214:HOH:O	1.86	0.75
3:M:103:MET:HG3	7:M:258:HOH:O	1.87	0.74
2:E:121:ASN:ND2	2:E:122:ARG:HD3	2.01	0.74
1:L:469:ASN:OD1	1:L:471:LEU:HB2	1.87	0.73
2:E:174:ARG:HD2	2:E:179:GLU:HG2	1.70	0.73
3:M:142:ASP:HB3	7:M:309:HOH:O	1.87	0.73
1:L:413:ASN:ND2	1:L:417:ARG:HE	1.87	0.73
1:L:455:GLU:HG3	7:L:1041:HOH:O	1.89	0.72
1:L:475:LYS:O	1:L:479:GLN:HG2	1.90	0.72
3:M:55:THR:OG1	3:M:57:THR:HG22	1.89	0.72
1:A:369:ASN:HD21	1:A:377:SER:H	1.35	0.72
2:E:195[B]:LYS:HD2	7:E:288:HOH:O	1.91	0.71
3:M:59:LYS:HB2	3:M:63:ASP:OD1	1.90	0.71
1:L:192:VAL:HG13	1:L:414:LYS:HD2	1.72	0.70
1:A:173:VAL:HG21	1:A:176:ALA:HA	1.74	0.70
2:B:55:ARG:HG3	7:B:325:HOH:O	1.91	0.70
3:M:75:THR:O	3:M:78:ASP:HB2	1.93	0.69
3:G:58:ASN:HA	7:G:332:HOH:O	1.93	0.69
3:M:54:LYS:HB2	7:M:301:HOH:O	1.90	0.69
2:E:121:ASN:HD22	2:E:122:ARG:HD3	1.59	0.68
2:B:97:GLU:OE2	2:B:170:LYS:HD2	1.94	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:493:GLN:O	1:L:496:LYS:HB2	1.92	0.68
1:A:550:PRO:HG3	1:L:23:TRP:HB2	1.77	0.67
2:E:222:VAL:HG22	2:E:223:ALA:H	1.60	0.66
1:L:513:GLN:HG3	7:L:825:HOH:O	1.96	0.64
2:E:50:GLU:HA	2:E:220:LEU:HD23	1.79	0.64
3:G:148:GLN:O	3:G:150:LYS:HE3	1.96	0.64
2:E:122:ARG:NH1	7:E:320:HOH:O	2.31	0.64
2:E:55:ARG:NE	2:E:56:GLN:H	1.95	0.64
2:E:49:THR:O	2:E:220:LEU:HA	1.98	0.63
1:L:551:ASN:ND2	1:L:551:ASN:H	1.97	0.63
1:L:97:LYS:HB2	1:L:100[A]:GLU:HG2	1.79	0.62
2:E:94:GLY:HA2	2:E:97:GLU:OE1	1.98	0.62
2:B:173:ALA:O	2:B:177[A]:LYS:HG3	2.00	0.61
2:E:174:ARG:HB3	2:E:181:PRO:HD3	1.82	0.61
3:M:62:ASP:HA	7:M:324:HOH:O	1.99	0.61
2:E:62:GLU:HB2	2:E:101:LYS:HB2	1.81	0.61
1:A:2:ARG:HB3	1:A:2:ARG:NH1	2.16	0.61
2:E:55:ARG:NE	2:E:56:GLN:HB2	2.13	0.61
2:E:55:ARG:HH21	2:E:56:GLN:HB2	1.66	0.60
1:L:538:TRP:O	1:L:542:LYS:HG3	2.02	0.60
1:L:431:ILE:HA	1:L:451:ARG:NH2	2.17	0.59
5:L:601:COY:H262	5:L:601:COY:H601	1.84	0.59
3:M:55:THR:HG22	7:M:322:HOH:O	2.01	0.59
2:E:105:ILE:HD12	2:E:217:PRO:HB3	1.83	0.59
2:E:177:LYS:HE3	2:E:177:LYS:O	2.01	0.59
2:E:219:GLU:HG3	2:E:220:LEU:N	2.17	0.59
2:E:59:GLN:O	2:E:125:GLY:HA3	2.02	0.59
1:A:140:GLN:HE21	1:A:141:GLN:H	1.49	0.59
5:A:601:COY:C2B	5:A:601:COY:H492	2.33	0.59
5:L:601:COY:H301	2:E:153:LEU:HD23	1.85	0.59
1:A:536:GLU:HG2	7:A:1271:HOH:O	2.03	0.58
2:E:177:LYS:HG2	2:E:179:GLU:OE1	2.02	0.58
3:M:67:GLU:HG3	3:M:68:ASN:N	2.19	0.58
1:L:414:LYS:O	1:L:414:LYS:HG2	2.02	0.58
1:L:493:GLN:HB3	7:L:815:HOH:O	2.03	0.57
1:L:431:ILE:HA	1:L:451:ARG:HH21	1.67	0.57
1:L:484:ASP:OD2	1:L:485:VAL:HG23	2.04	0.57
3:M:100:ARG:HD3	3:M:103:MET:CE	2.34	0.57
3:G:130:ARG:O	3:G:170:LYS:HE3	2.04	0.57
5:A:601:COY:H362	5:A:601:COY:H351	1.85	0.57
2:E:98:GLU:OE1	2:E:98:GLU:HA	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210[A]:LYS:HD2	7:A:1075:HOH:O	2.05	0.57
2:E:59:GLN:H	2:E:59:GLN:NE2	2.03	0.57
1:L:413:ASN:HD21	1:L:417:ARG:HE	1.52	0.56
1:A:20:VAL:HG22	1:L:548:LEU:HG	1.86	0.56
1:L:42:LYS:HB2	1:L:50:GLU:CB	2.33	0.56
5:L:601:COY:H552	5:L:601:COY:H531	1.86	0.56
1:A:177[B]:ARG:HD2	7:A:1266:HOH:O	2.06	0.56
1:A:441:TYR:CD2	1:L:1:MET:HG2	2.40	0.56
3:G:54[B]:LYS:HG2	7:G:332:HOH:O	2.05	0.56
1:L:408:VAL:O	1:L:411:ILE:HG22	2.06	0.56
2:E:55:ARG:HE	2:E:56:GLN:N	2.01	0.56
2:E:72:GLY:H	2:E:84:HIS:HD2	1.53	0.56
1:A:369:ASN:ND2	1:A:377:SER:H	2.03	0.55
5:L:601:COY:C2B	5:L:601:COY:H492	2.36	0.55
2:E:161:THR:HB	7:E:305:HOH:O	2.05	0.55
2:B:146:PRO:HG2	2:B:149:SER:HB2	1.88	0.55
2:E:79:ILE:HG13	2:E:199:LYS:HD3	1.88	0.55
3:M:55:THR:HA	7:M:268:HOH:O	2.06	0.55
2:E:66:ALA:HB1	2:E:107:CYS:SG	2.47	0.55
1:L:421:ALA:O	1:L:424:ALA:HB3	2.07	0.55
1:L:214:LEU:HD21	1:L:467:ASN:HA	1.87	0.54
2:E:71:PHE:HE1	2:E:88:LEU:HD22	1.72	0.54
2:E:87:ILE:O	2:E:91:VAL:HG23	2.07	0.54
1:L:25:GLU:HB3	7:L:862:HOH:O	2.06	0.54
1:A:542:LYS:HG2	1:L:310:PRO:CG	2.37	0.54
2:E:49:THR:HG22	2:E:51:VAL:HG13	1.88	0.54
2:E:174:ARG:NH1	2:E:179:GLU:HG2	2.20	0.54
2:B:89:ARG:HD2	2:B:90:GLU:OE1	2.07	0.54
1:A:38:LYS:HD3	7:A:962:HOH:O	2.08	0.53
2:E:175:TYR:CD1	2:E:181:PRO:HD2	2.43	0.53
3:M:146:ARG:HD2	3:M:147:TYR:CZ	2.43	0.53
1:L:152:VAL:HG22	1:L:431:ILE:HD13	1.90	0.53
2:E:106:ARG:HG2	2:E:108:PHE:CZ	2.44	0.53
2:E:59:GLN:HG3	2:E:61:ASP:OD1	2.08	0.53
3:M:54:LYS:HD3	3:M:58:ASN:HA	1.91	0.53
1:A:177[A]:ARG:HB3	1:A:457:ILE:HG23	1.91	0.52
1:A:177[B]:ARG:HB3	1:A:457:ILE:HG23	1.91	0.52
5:L:601:COY:H362	5:L:601:COY:H351	1.92	0.52
2:B:121:ASN:ND2	2:B:143:GLN:HA	2.25	0.52
1:A:241:SER:HB3	3:G:126:LEU:HB3	1.90	0.52
3:M:66:LEU:O	3:M:70:LEU:HD13	2.08	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:128:ILE:HD12	2:E:175:TYR:HB3	1.91	0.52
1:A:493:GLN:HE22	1:A:496:LYS:NZ	2.08	0.52
1:A:42:LYS:HE2	7:A:1174:HOH:O	2.10	0.51
1:L:175:VAL:O	1:L:178:TYR:HB2	2.10	0.51
2:E:177:LYS:CG	2:E:179:GLU:HB2	2.40	0.51
1:A:38:LYS:HG2	7:A:962:HOH:O	2.11	0.51
1:A:434:GLU:HB2	7:A:1131:HOH:O	2.10	0.51
1:L:453:ILE:HG23	1:L:457:ILE:HD12	1.93	0.51
2:E:119:GLU:OE2	2:E:217:PRO:HD3	2.10	0.51
1:A:529:THR:HB	7:A:1022:HOH:O	2.09	0.51
2:E:109:LYS:HG2	2:E:214:GLY:H	1.76	0.51
1:L:429:PRO:HG2	1:L:455:GLU:O	2.10	0.51
3:M:53:VAL:HG12	3:M:53:VAL:O	2.10	0.51
3:G:51:GLU:O	3:G:54[A]:LYS:HD3	2.09	0.51
2:E:50:GLU:O	2:E:50:GLU:HG3	2.09	0.51
1:A:140:GLN:HE21	1:A:141:GLN:N	2.08	0.51
1:A:549:ASP:OD2	1:A:551:ASN:OD1	2.29	0.51
1:L:205:GLU:HG2	7:L:812:HOH:O	2.11	0.50
2:E:107:CYS:CB	2:E:116:VAL:HB	2.41	0.50
2:E:219:GLU:O	2:E:220:LEU:HD23	2.10	0.50
2:E:106:ARG:HB2	2:E:220:LEU:HD11	1.94	0.50
3:M:56:ALA:O	3:M:58:ASN:OD1	2.30	0.50
1:A:77:GLU:HG2	7:A:786:HOH:O	2.10	0.50
5:A:601:COY:O39	5:A:601:COY:H361	2.11	0.50
2:B:113:VAL:HB	2:B:133:GLN:HG3	1.94	0.50
2:E:101:LYS:HD2	2:E:101:LYS:N	2.26	0.50
2:E:105:ILE:HD12	2:E:217:PRO:CB	2.41	0.50
3:M:144:GLU:OE1	3:M:150:LYS:HE2	2.11	0.50
1:L:187:LEU:O	1:L:191:GLN:HG2	2.12	0.49
2:B:146:PRO:HG2	2:B:149:SER:CB	2.43	0.49
3:M:64:PHE:CE2	3:M:78:ASP:HB3	2.47	0.49
1:L:236:ASP:O	3:M:127:ARG:HD2	2.12	0.49
2:E:64:ILE:HD12	2:E:124:SER:HA	1.93	0.49
3:M:69:VAL:HG12	3:M:70:LEU:CD1	2.40	0.49
1:A:316:VAL:O	1:A:319:GLU:HG2	2.12	0.49
1:L:206:ALA:HB3	7:L:1048:HOH:O	2.12	0.49
2:E:64:ILE:HD12	2:E:124:SER:CA	2.43	0.49
1:A:177[B]:ARG:HG2	1:A:461:GLN:NE2	2.28	0.49
7:L:1093:HOH:O	2:E:195[B]:LYS:HE2	2.13	0.49
3:M:60:THR:HG22	7:M:301:HOH:O	2.12	0.49
1:A:2:ARG:HB3	1:A:2:ARG:HH11	1.76	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:66:LEU:HD22	3:M:70:LEU:CD1	2.43	0.49
5:L:601:COY:H1R	7:E:229:HOH:O	2.13	0.49
3:M:49:HIS:HA	3:M:51:GLU:OE2	2.13	0.49
3:M:55:THR:CB	3:M:57:THR:HG22	2.43	0.49
2:E:62:GLU:CD	2:E:125:GLY:H	2.21	0.48
2:E:64:ILE:HA	2:E:103:ARG:O	2.13	0.48
1:A:153:GLN:HE22	1:A:445:SER:HB3	1.77	0.48
2:E:50:GLU:HA	2:E:219:GLU:O	2.13	0.48
5:A:601:COY:H552	5:A:601:COY:H531	1.94	0.48
1:L:140:GLN:HE21	1:L:141:GLN:H	1.61	0.48
1:L:177[B]:ARG:HG2	1:L:461:GLN:CG	2.43	0.48
1:A:20:VAL:HG13	1:L:550:PRO:HG3	1.96	0.48
1:A:406:GLU:HG3	1:A:407:ASP:N	2.27	0.48
1:A:441:TYR:CG	1:L:1:MET:HG2	2.48	0.48
2:E:69:PRO:HA	2:E:106:ARG:HD3	1.94	0.48
1:A:222:THR:HB	5:A:601:COY:H721	1.95	0.48
1:L:429:PRO:HA	1:L:430:PRO:HD3	1.77	0.48
1:L:461:GLN:NE2	1:L:461:GLN:HA	2.29	0.48
1:L:186:LEU:CD2	1:L:199:THR:HB	2.44	0.48
1:A:177[B]:ARG:HG2	1:A:461:GLN:CD	2.38	0.48
1:L:69:TYR:HB2	1:L:289:ALA:HB1	1.95	0.48
2:E:109:LYS:HG2	2:E:214:GLY:N	2.29	0.48
2:E:94:GLY:O	2:E:97:GLU:OE2	2.31	0.48
2:B:50:GLU:HG2	2:B:220:LEU:CD2	2.44	0.47
7:A:1113:HOH:O	2:B:197:GLN:HG3	2.14	0.47
1:L:452:ASN:ND2	1:L:454:VAL:HG23	2.29	0.47
3:M:66:LEU:HA	3:M:66:LEU:HD23	1.71	0.47
5:L:601:COY:C6	5:L:601:COY:H4B	2.45	0.47
1:A:140:GLN:HE22	1:A:361[B]:SER:HB2	1.78	0.47
5:L:601:COY:N3B	5:L:601:COY:H202	2.29	0.47
1:A:331:ALA:HA	1:A:359:PHE:HB2	1.97	0.47
2:E:112:ASP:O	2:E:116:VAL:HG13	2.15	0.47
1:L:179:ALA:HB3	1:L:180:PRO:HD3	1.96	0.46
2:E:199:LYS:HE2	2:E:203:LEU:HD11	1.97	0.46
3:G:77:GLN:NE2	7:G:226:HOH:O	2.42	0.46
1:L:152:VAL:HG21	1:L:431:ILE:HG23	1.97	0.46
2:E:55:ARG:NH2	2:E:56:GLN:HB2	2.29	0.46
2:E:119:GLU:OE2	2:E:217:PRO:HG3	2.15	0.46
2:E:178:ARG:NH1	2:E:178:ARG:HG3	2.30	0.46
3:M:60:THR:HB	7:M:221:HOH:O	2.15	0.46
5:A:601:COY:H473	5:A:601:COY:H491	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:212:VAL:HA	7:E:245:HOH:O	2.16	0.46
1:A:82:MET:HE3	7:A:1178:HOH:O	2.16	0.46
2:E:177:LYS:HG2	2:E:179:GLU:HB2	1.98	0.46
2:E:178:ARG:HG3	2:E:178:ARG:HH11	1.80	0.46
2:E:174:ARG:HH11	2:E:179:GLU:CG	2.25	0.46
3:M:100:ARG:HD3	3:M:103:MET:HE1	1.97	0.46
1:A:306:PRO:O	1:A:312:GLY:HA3	2.16	0.46
3:G:54[B]:LYS:HD2	3:G:58:ASN:HD22	1.81	0.46
1:L:262:SER:HA	7:L:606:HOH:O	2.15	0.46
1:A:369:ASN:HD22	1:A:369:ASN:HA	1.57	0.46
1:L:331:ALA:HA	1:L:359:PHE:HB2	1.98	0.45
1:A:2:ARG:NH1	1:L:405:GLU:OE1	2.50	0.45
1:A:299:SER:OG	1:A:303:ILE:HA	2.15	0.45
1:L:429:PRO:HD3	1:L:459:PHE:CG	2.51	0.45
1:L:370:TYR:OH	1:L:444:GLY:HA3	2.17	0.45
2:E:62:GLU:OE2	2:E:125:GLY:N	2.50	0.45
1:L:430:PRO:O	1:L:451:ARG:NH2	2.50	0.45
5:L:601:COY:H301	2:E:153:LEU:CD2	2.46	0.45
3:M:55:THR:OG1	3:M:59:LYS:O	2.30	0.45
3:M:69:VAL:HG23	3:M:74:VAL:HG22	1.98	0.45
1:L:549:ASP:OD2	1:L:551:ASN:ND2	2.50	0.45
2:E:51:VAL:HG11	2:E:221:ARG:HD2	1.99	0.45
2:B:60:GLN:NE2	7:B:435:HOH:O	2.48	0.45
3:G:80:ARG:NH2	7:G:325:HOH:O	2.49	0.45
1:L:192:VAL:CG1	1:L:414:LYS:HD2	2.43	0.45
3:G:170:LYS:HE2	7:G:300:HOH:O	2.17	0.45
1:L:487:GLN:NE2	1:L:491:ASN:OD1	2.50	0.45
2:E:163:GLU:N	7:E:301:HOH:O	2.50	0.45
3:M:71:SER:O	3:M:72:ASN:HB2	2.16	0.45
3:M:80:ARG:NH1	7:M:266:HOH:O	2.50	0.45
2:B:157:ALA:HA	2:B:160:LEU:HD22	1.98	0.45
3:M:74:VAL:HA	3:M:78:ASP:OD1	2.16	0.45
3:M:94:LYS:NZ	7:M:286:HOH:O	2.50	0.45
3:M:117:ASP:N	3:M:117:ASP:OD1	2.50	0.45
1:A:461:GLN:NE2	7:A:1134:HOH:O	2.49	0.45
2:B:88:LEU:HD12	2:B:88:LEU:HA	1.89	0.45
1:A:38:LYS:HE2	7:A:942:HOH:O	2.17	0.44
1:A:177[A]:ARG:NH2	7:A:1181:HOH:O	2.50	0.44
1:L:274:LYS:NZ	7:L:936:HOH:O	2.50	0.44
1:L:549:ASP:HA	1:L:550:PRO:HD3	1.70	0.44
2:E:47:PHE:CE1	2:E:85:LYS:HA	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:174:ARG:HB2	2:E:181:PRO:HG3	1.99	0.44
3:M:54:LYS:HG2	3:M:55:THR:O	2.16	0.44
2:E:72:GLY:N	2:E:84:HIS:HD2	2.15	0.44
1:A:550:PRO:CG	1:L:23:TRP:HB2	2.45	0.44
3:G:64:PHE:CE2	3:G:79:MET:HG2	2.52	0.44
3:G:142:ASP:OD1	3:G:146[A]:ARG:NH1	2.50	0.44
1:L:175:VAL:O	1:L:175:VAL:HG13	2.17	0.44
1:L:493:GLN:H	1:L:493:GLN:HG2	1.51	0.44
2:E:127:GLY:O	2:E:142:GLN:HA	2.17	0.44
1:A:302:CYS:O	1:A:306:PRO:HD2	2.17	0.44
1:A:329:GLU:OE2	1:A:505:SER:HA	2.17	0.44
3:G:39:ARG:NH1	7:G:309:HOH:O	2.50	0.44
3:G:157:ARG:NH2	7:G:290:HOH:O	2.50	0.44
2:E:141:HIS:NE2	2:E:149:SER:O	2.50	0.44
3:G:42:ASP:C	3:G:48:LYS:HG3	2.43	0.44
3:G:168:LYS:NZ	7:G:274:HOH:O	2.50	0.44
1:L:432:THR:OG1	1:L:434:GLU:HG3	2.18	0.44
3:M:51:GLU:H	3:M:51:GLU:CD	2.26	0.44
1:A:538:TRP:CE2	1:A:542:LYS:HD2	2.52	0.44
2:E:90:GLU:O	2:E:166:ARG:HD2	2.18	0.44
1:L:16:GLN:NE2	7:L:1093:HOH:O	2.50	0.44
1:L:468:ARG:HD2	1:L:472:GLU:OE1	2.18	0.44
2:E:122:ARG:HD2	2:E:122:ARG:HA	1.66	0.44
3:M:107:ARG:HH11	3:M:107:ARG:HD3	1.61	0.44
1:L:177[B]:ARG:HG2	1:L:461:GLN:CD	2.43	0.43
1:L:429:PRO:HD3	1:L:459:PHE:CD2	2.53	0.43
1:A:177[A]:ARG:NH1	7:A:1265:HOH:O	2.50	0.43
1:L:177[A]:ARG:HG2	1:L:461:GLN:CG	2.48	0.43
1:A:97:LYS:HB2	1:A:100[A]:GLU:CG	2.36	0.43
3:M:57:THR:HG21	3:M:59:LYS:HD2	2.00	0.43
2:E:195[A]:LYS:HE3	2:E:196:TYR:OH	2.18	0.43
1:L:435:GLU:OE2	1:L:451:ARG:NE	2.50	0.43
1:L:432:THR:OG1	1:L:435:GLU:HG3	2.18	0.43
2:E:90:GLU:O	2:E:166:ARG:HA	2.19	0.43
5:A:601:COY:H601	5:A:601:COY:H262	2.01	0.43
5:A:601:COY:C6	5:A:601:COY:H4B	2.49	0.43
3:G:75:THR:OG1	3:G:77:GLN:HG2	2.18	0.43
1:L:24:ILE:N	1:L:24:ILE:HD13	2.34	0.43
1:L:435:GLU:HG2	1:L:449:PRO:HG2	2.00	0.43
1:A:441:TYR:CE2	1:L:1:MET:HG2	2.54	0.43
2:B:77:VAL:HG12	2:B:83:PRO:HA	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:62:GLU:HA	2:E:100:ILE:HG23	1.99	0.43
3:M:66:LEU:HD22	3:M:70:LEU:HD13	2.00	0.43
1:A:174:ALA:HA	1:A:373:MET:HE2	1.99	0.42
1:A:215:GLY:HA2	7:A:791:HOH:O	2.19	0.42
1:L:174:ALA:HA	1:L:373:MET:HE2	2.01	0.42
2:E:49:THR:HG22	2:E:51:VAL:CG1	2.48	0.42
2:E:114:ALA:O	2:E:118:VAL:HG23	2.19	0.42
1:A:140:GLN:HE21	1:A:140:GLN:CA	2.32	0.42
5:A:601:COY:H202	5:A:601:COY:N3B	2.34	0.42
1:L:173:VAL:CG2	1:L:176:ALA:HA	2.37	0.42
2:E:53:GLU:HG3	2:E:218:GLN:NE2	2.35	0.42
3:M:82:THR:HB	3:M:83:PRO:HD2	2.01	0.42
1:L:489:MET:O	1:L:493:GLN:HG2	2.19	0.42
2:E:60:GLN:HA	2:E:125:GLY:O	2.19	0.42
2:E:95:ILE:CG2	2:E:100:ILE:HG22	2.50	0.42
1:A:408:VAL:HA	1:A:411:ILE:HG22	2.01	0.42
5:A:601:COY:H531	5:A:601:COY:C55	2.49	0.42
5:L:601:COY:H3P1	2:E:200:SER:HB2	2.01	0.42
2:E:117:ALA:HB1	2:E:141:HIS:HB2	2.02	0.42
3:M:134:GLU:CD	3:M:134:GLU:H	2.27	0.42
3:M:157:ARG:HD2	7:M:224:HOH:O	2.19	0.42
1:A:414:LYS:NZ	7:A:1240:HOH:O	2.49	0.42
1:L:97:LYS:HB2	1:L:97:LYS:HE3	1.80	0.42
5:L:601:COY:C2B	5:L:601:COY:H202	2.50	0.42
2:E:177:LYS:HG3	2:E:179:GLU:HB2	2.01	0.42
2:E:191:MET:C	2:E:194:PRO:HD2	2.45	0.42
3:G:41:SER:O	3:G:48:LYS:HE2	2.20	0.41
2:E:59:GLN:HG2	2:E:61:ASP:H	1.85	0.41
2:E:130:ILE:HD11	2:E:172:ALA:CB	2.50	0.41
1:L:72:ASN:HB3	1:L:107:ALA:HA	2.03	0.41
1:L:280:GLU:O	1:L:283:CYS:HB2	2.20	0.41
1:L:432:THR:OG1	1:L:434:GLU:OE2	2.30	0.41
1:L:1:MET:HE3	1:L:1:MET:HB2	1.61	0.41
7:A:1142:HOH:O	2:B:204:HIS:HE1	2.04	0.41
1:A:86:LYS:HA	1:A:86:LYS:HD3	1.59	0.41
1:A:334:ASN:OD1	1:A:349:LEU:HA	2.20	0.41
2:B:64:ILE:HD13	2:B:103:ARG:HB3	2.03	0.41
3:G:54[B]:LYS:HE3	3:G:54[B]:LYS:HB3	1.76	0.41
1:L:162:ALA:HB3	1:L:193:GLY:HA3	2.02	0.41
3:M:144:GLU:O	3:M:148:GLN:HA	2.21	0.41
1:L:175:VAL:HG11	1:L:457:ILE:HD11	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:497:LEU:HD21	3:M:79:MET:CA	2.37	0.41
2:E:82:ILE:HA	2:E:83:PRO:HD3	1.95	0.41
2:E:139:VAL:O	2:E:139:VAL:HG13	2.20	0.41
2:E:90:GLU:HB3	2:E:166:ARG:HB2	2.02	0.41
1:L:114:VAL:HG13	1:L:277:LEU:HD13	2.03	0.41
1:L:470:GLY:O	1:L:474:VAL:HG23	2.20	0.41
2:E:221:ARG:O	2:E:222:VAL:O	2.39	0.41
1:L:434:GLU:HG3	1:L:434:GLU:H	1.64	0.41
1:L:496:LYS:HB3	1:L:496:LYS:HE2	1.80	0.41
3:M:100:ARG:NE	3:M:100:ARG:HA	2.36	0.41
1:A:38:LYS:HG3	1:A:39:PRO:HD2	2.03	0.40
5:A:601:COY:O28	5:A:601:COY:H3	2.20	0.40
1:L:140:GLN:HE21	1:L:141:GLN:N	2.19	0.40
1:A:3:SER:O	1:A:7:GLU:HG3	2.21	0.40
3:G:52:TRP:O	3:G:54[A]:LYS:HE3	2.21	0.40
1:L:184:ILE:O	1:L:188:VAL:HG23	2.21	0.40
1:L:300:VAL:HG12	1:L:301:SER:N	2.36	0.40
3:G:44:PRO:O	3:G:48:LYS:HG2	2.21	0.40
1:L:180:PRO:HG3	1:L:464:ILE:HD11	2.03	0.40
1:L:202:SER:O	1:L:203:LEU:HD23	2.22	0.40
1:L:302:CYS:O	1:L:306:PRO:HD2	2.21	0.40
2:E:174:ARG:CD	2:E:179:GLU:HG2	2.48	0.40
2:E:175:TYR:CE1	2:E:181:PRO:HD2	2.56	0.40
2:E:222:VAL:HG13	2:E:223:ALA:N	2.36	0.40
3:G:118:ARG:NH2	7:G:262:HOH:O	2.50	0.40
1:L:420:GLN:HA	1:L:431:ILE:HD12	2.03	0.40
1:L:536:GLU:HG2	7:L:1059:HOH:O	2.21	0.40
2:E:128:ILE:CD1	2:E:175:TYR:HB3	2.52	0.40
1:L:140:GLN:HE21	1:L:140:GLN:CA	2.34	0.40
1:L:152:VAL:HG22	1:L:431:ILE:CD1	2.52	0.40
2:E:122:ARG:NH1	2:E:122:ARG:HG3	2.37	0.40
3:M:146:ARG:HH11	3:M:146:ARG:HD3	1.75	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries

of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	553/554 (100%)	533 (96%)	18 (3%)	2 (0%)	30	15
1	L	555/554 (100%)	536 (97%)	17 (3%)	2 (0%)	30	15
2	B	180/224 (80%)	176 (98%)	4 (2%)	0	100	100
2	E	177/224 (79%)	163 (92%)	12 (7%)	2 (1%)	11	2
3	G	139/173 (80%)	136 (98%)	2 (1%)	1 (1%)	18	7
3	M	137/173 (79%)	134 (98%)	2 (2%)	1 (1%)	18	7
All	All	1741/1902 (92%)	1678 (96%)	55 (3%)	8 (0%)	24	11

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	222	VAL
3	G	56	ALA
3	M	55	THR
1	A	300	VAL
1	L	300	VAL
1	A	363	GLY
1	L	363	GLY
2	E	47	PHE

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%)	433 (95%)	21 (5%)	24	6
1	L	456/453 (101%)	412 (90%)	44 (10%)	8	1
2	B	150/183 (82%)	132 (88%)	18 (12%)	5	0
2	E	147/183 (80%)	112 (76%)	35 (24%)	1	0
3	G	120/141 (85%)	105 (88%)	15 (12%)	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	M	118/141 (84%)	102 (86%)	16 (14%)	3	0
All	All	1445/1554 (93%)	1296 (90%)	149 (10%)	7	0

All (149) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	VAL
1	A	38	LYS
1	A	42	LYS
1	A	73	LEU
1	A	86	LYS
1	A	140	GLN
1	A	173	VAL
1	A	178	TYR
1	A	198	LEU
1	A	210[A]	LYS
1	A	210[B]	LYS
1	A	211	LEU
1	A	245	LEU
1	A	326	LEU
1	A	350	LEU
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	97	GLU
2	B	121	ASN
2	B	122	ARG
2	B	150	ASN
2	B	160	LEU
2	B	167	GLN
2	B	178	ARG
2	B	180	SER
2	B	182	GLN
2	B	190[A]	GLN
2	B	190[B]	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
3	G	74	VAL
3	G	94	LYS
3	G	124[A]	ASN
3	G	124[B]	ASN
3	G	126	LEU
3	G	134	GLU
3	G	146[A]	ARG
3	G	146[B]	ARG
3	G	150	LYS
1	L	1	MET
1	L	9	LEU
1	L	13	PRO
1	L	20	VAL
1	L	24	ILE
1	L	25	GLU
1	L	42	LYS
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	218	CYS
1	L	277	LEU
1	L	326	LEU
1	L	411	ILE
1	L	414	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	434	GLU
1	L	450	GLU
1	L	452	ASN
1	L	453	ILE
1	L	454	VAL
1	L	455	GLU
1	L	457	ILE
1	L	466	LYS
1	L	468	ARG
1	L	471	LEU
1	L	487	GLN
1	L	489	MET
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	49	THR
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	67	VAL
2	E	80	VAL
2	E	85	LYS
2	E	88	LEU
2	E	89	ARG
2	E	97	GLU
2	E	98	GLU
2	E	100	ILE
2	E	106	ARG
2	E	113	VAL
2	E	116	VAL
2	E	121	ASN
2	E	122	ARG
2	E	129	SER
2	E	132	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	141	HIS
2	E	143	GLN
2	E	145	LEU
2	E	150	ASN
2	E	167	GLN
2	E	170	LYS
2	E	174	ARG
2	E	177	LYS
2	E	179	GLU
2	E	180	SER
2	E	182	GLN
2	E	219	GLU
2	E	222	VAL
3	M	45	LEU
3	M	57	THR
3	M	59	LYS
3	M	66	LEU
3	M	67	GLU
3	M	69	VAL
3	M	70	LEU
3	M	74	VAL
3	M	77	GLN
3	M	88	LEU
3	M	127	ARG
3	M	134	GLU
3	M	146	ARG
3	M	148	GLN
3	M	150	LYS
3	M	161	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	479	GLN
1	A	493	GLN
1	A	534	GLN
2	B	59	GLN
2	B	121	ASN
2	B	167	GLN
2	B	204	HIS
3	G	58	ASN
3	G	77	GLN
1	L	35	ASN
1	L	45	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	479	GLN
1	L	487	GLN
1	L	534	GLN
1	L	551	ASN
2	E	59	GLN
2	E	60	GLN
2	E	84	HIS
2	E	121	ASN
2	E	143	GLN
2	E	150	ASN
2	E	171	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 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	$\# Z > 2$
6	PGO	A	602	4	4,4,4	0.88	0	4,4,4	0.61	0
5	COY	L	601	-	108,118,118	0.88	2 (1%)	160,192,192	1.20	13 (8%)
6	PGO	L	602	4	4,4,4	0.93	0	4,4,4	0.56	0
5	COY	A	601	-	108,118,118	0.85	2 (1%)	160,192,192	1.12	16 (10%)

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	A	602	4	-	0/2/2/2	-
5	COY	L	601	-	2/2/36/38	8/61/241/241	0/5/13/13
6	PGO	L	602	4	-	0/2/2/2	-
5	COY	A	601	-	2/2/36/38	9/61/241/241	0/5/13/13

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	601	COY	O58-C57	2.68	1.28	1.23
5	A	601	COY	O58-C57	2.43	1.28	1.23
5	L	601	COY	C6-C5	-2.27	1.38	1.44
5	A	601	COY	C6-C5	-2.18	1.38	1.44

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	601	COY	C54-C17-C18	-3.41	108.10	112.99
5	A	601	COY	C8B-N1B-C1R	3.37	131.11	125.41
5	A	601	COY	C55-C17-C16	3.35	123.15	116.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	601	COY	C12-C11-C10	3.33	128.51	123.35
5	A	601	COY	C41-C8-C9	-3.24	105.53	111.19
5	L	601	COY	C53-C15-C14	-3.11	113.50	118.59
5	L	601	COY	C56-C57-N59	3.10	122.00	116.34
5	A	601	COY	O58-C57-C56	-3.01	116.57	122.02
5	L	601	COY	C53-C15-C16	2.99	125.43	120.36
5	L	601	COY	C5-C6-N22	-2.90	120.46	126.52
5	A	601	COY	C35-C5-C6	2.81	125.14	120.36
5	A	601	COY	C14-N23-C11	2.79	109.25	105.44
5	L	601	COY	O58-C57-C56	-2.79	116.96	122.02
5	L	601	COY	C41-C8-C9	-2.71	106.46	111.19
5	L	601	COY	C60-C61-N62	2.48	122.13	116.19
5	L	601	COY	C8B-N1B-C1R	2.41	129.49	125.41
5	A	601	COY	C35-C5-C4	-2.34	113.78	118.42
5	L	601	COY	C55-C17-C16	2.31	121.11	116.59
5	A	601	COY	C47-C12-C13	2.23	121.78	112.74
5	A	601	COY	C1R-N1B-C2B	-2.22	122.16	127.09
5	A	601	COY	C5-C6-N22	-2.21	121.90	126.52
5	A	601	COY	C71-N9A-C4A	-2.18	123.07	126.63
5	A	601	COY	C30-C3-C4	2.13	113.80	108.51
5	A	601	COY	C9B-C8B-N1B	2.12	106.24	105.30
5	L	601	COY	C71-N9A-C4A	-2.08	123.23	126.63
5	A	601	COY	C15-C16-N24	-2.08	119.47	122.42
5	A	601	COY	C12-C11-C10	2.05	126.54	123.35
5	L	601	COY	C10-C11-N23	-2.05	120.99	124.27
5	A	601	COY	C54-C17-C18	-2.02	110.08	112.99

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	601	COY	N24
5	A	601	COY	N21
5	L	601	COY	N24
5	L	601	COY	N21

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	601	COY	C12-C13-C48-C49
5	A	601	COY	C71-C72-C73-C74
5	L	601	COY	C71-C72-C73-C74
5	L	601	COY	C30-C31-C32-O34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	L	601	COY	C30-C31-C32-N33
5	A	601	COY	C30-C31-C32-O34
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	C12-C13-C48-C49
5	L	601	COY	C8-C41-C42-C43
5	A	601	COY	C72-C71-N9A-C4A
5	L	601	COY	C72-C71-N9A-C4A
5	L	601	COY	C3R-O2-P-O4
5	A	601	COY	C17-C18-C60-C61
5	L	601	COY	C19-C18-C60-C61
5	A	601	COY	C72-C71-N9A-C8A

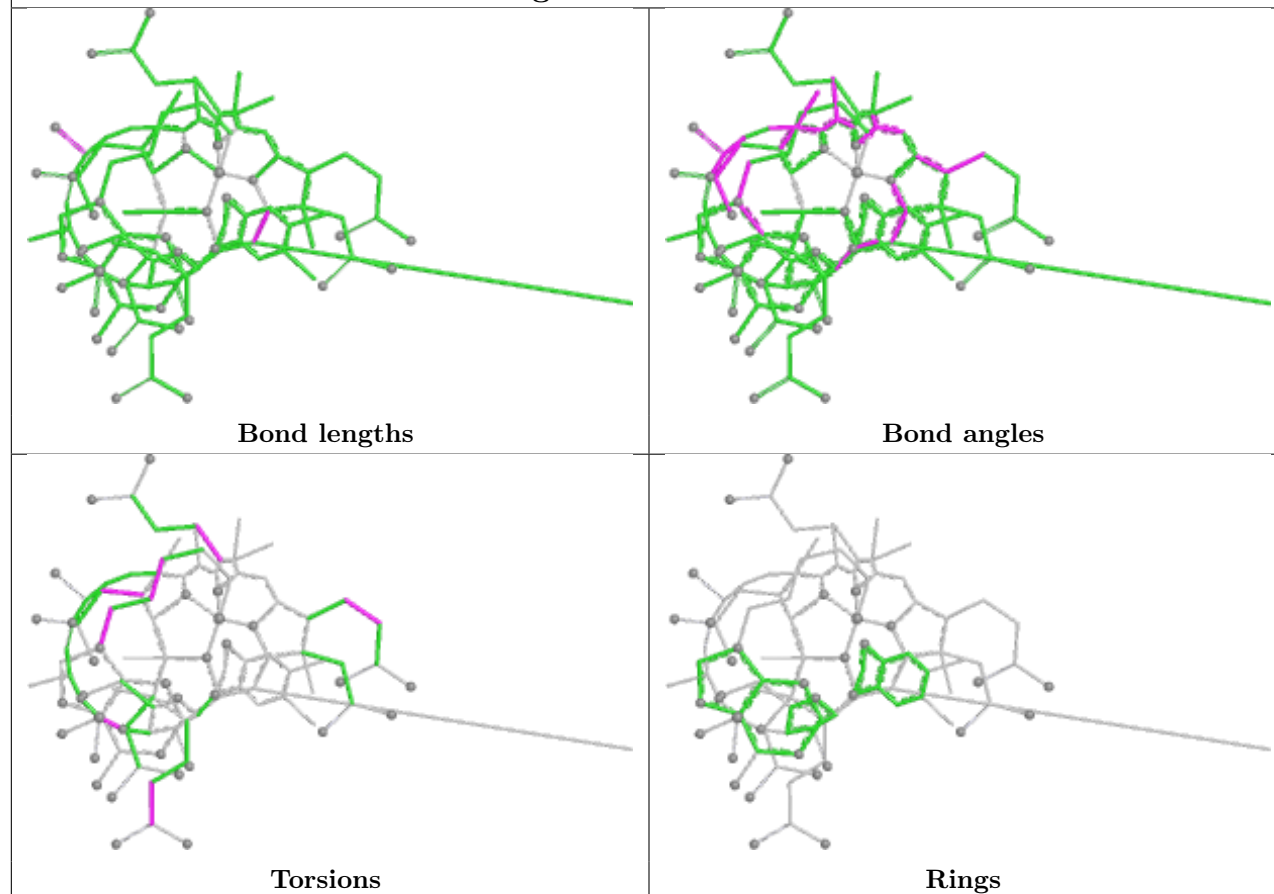
There are no ring outliers.

2 monomers are involved in 22 short contacts:

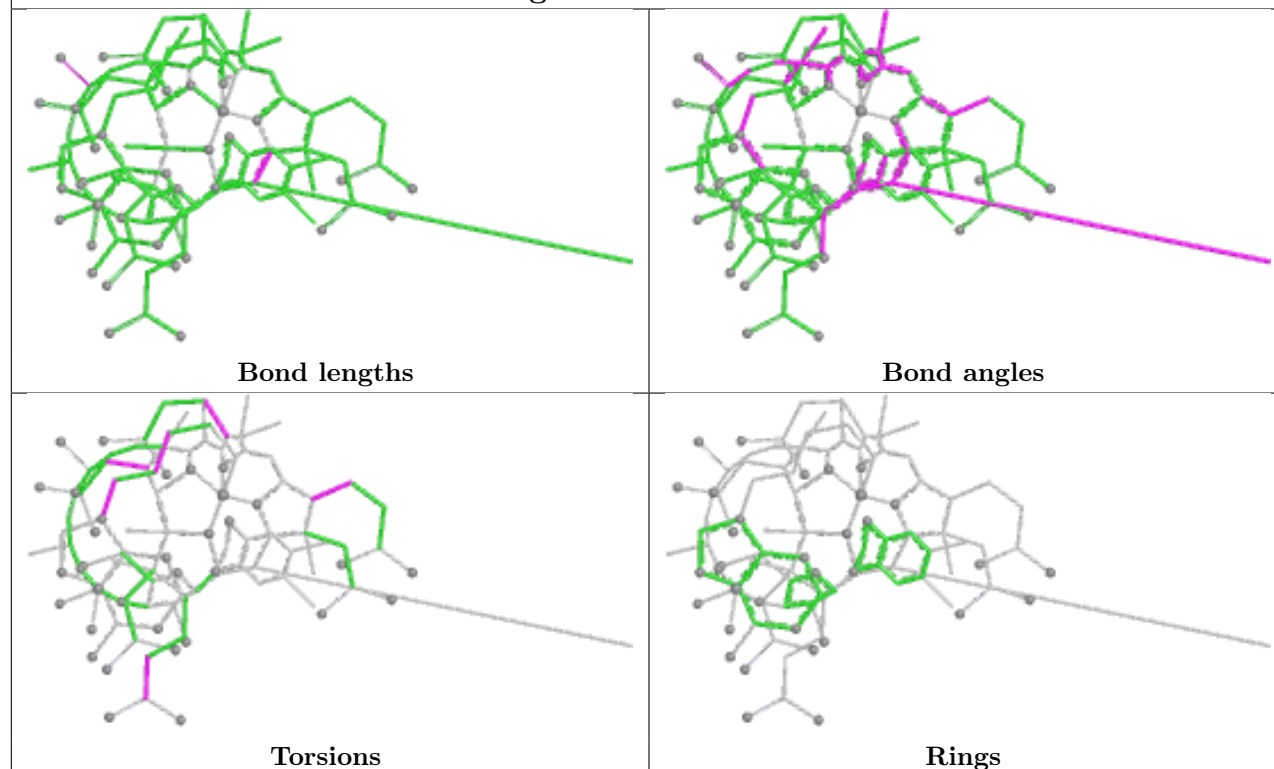
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	601	COY	11	0
5	A	601	COY	11	0

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

Ligand COY L 601



Ligand COY A 601



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(Å ²)	Q<0.9
1	A	551/554 (99%)	-0.70	2 (0%) 88 91	8, 12, 26, 74	4 (0%)
1	L	551/554 (99%)	-0.23	17 (3%) 51 58	8, 16, 45, 74	7 (1%)
2	B	178/224 (79%)	-0.22	2 (1%) 78 83	10, 19, 36, 56	4 (2%)
2	E	178/224 (79%)	1.20	37 (20%) 2 3	12, 37, 80, 104	1 (0%)
3	G	137/173 (79%)	-0.22	4 (2%) 53 60	11, 17, 38, 58	4 (2%)
3	M	137/173 (79%)	0.29	15 (10%) 10 12	12, 21, 63, 108	2 (1%)
All	All	1732/1902 (91%)	-0.19	77 (4%) 39 45	8, 17, 48, 108	22 (1%)

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	M	57	THR	6.6
3	G	56	ALA	5.7
3	M	58	ASN	5.3
3	M	56	ALA	5.0
2	E	46	GLY	4.4
1	L	454	VAL	4.1
2	E	59	GLN	3.9
2	E	222	VAL	3.9
3	M	55	THR	3.8
1	L	548	LEU	3.8
1	L	453	ILE	3.7
2	E	95	ILE	3.6
2	E	58	THR	3.4
2	E	62	GLU	3.4
2	E	51	VAL	3.4
2	E	220	LEU	3.3
1	L	464	ILE	3.3
3	M	77	GLN	3.2
3	M	74	VAL	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	L	434	GLU	3.2
2	E	48	LEU	3.1
3	M	79	MET	3.1
2	E	221	ARG	3.1
2	E	169	GLY	3.0
2	E	179	GLU	2.9
1	A	548	LEU	2.9
2	E	60	GLN	2.9
1	L	551	ASN	2.8
1	L	465	ASN	2.8
1	L	479	GLN	2.8
2	E	47	PHE	2.7
1	L	482	PHE	2.7
3	M	64	PHE	2.7
2	E	100	ILE	2.7
2	E	177	LYS	2.7
1	L	423	PHE	2.7
2	E	57	GLY	2.7
1	L	459	PHE	2.6
3	G	53	VAL	2.6
3	M	59	LYS	2.6
2	E	117	ALA	2.5
2	E	181	PRO	2.5
2	E	94	GLY	2.5
2	E	166	ARG	2.5
3	G	57	THR	2.5
2	E	180	SER	2.5
2	E	104	VAL	2.5
3	M	62	ASP	2.4
1	A	550	PRO	2.4
3	M	60	THR	2.4
2	E	61	ASP	2.4
2	E	50	GLU	2.4
2	E	97	GLU	2.4
2	E	170	LYS	2.4
2	E	123	LEU	2.3
1	L	487	GLN	2.3
2	E	67	VAL	2.3
2	E	108	PHE	2.3
1	L	493	GLN	2.3
1	L	455	GLU	2.3
2	B	223	ALA	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	E	109	LYS	2.2
3	M	80	ARG	2.2
2	E	178	ARG	2.2
3	G	80	ARG	2.2
2	E	49	THR	2.2
3	M	54	LYS	2.2
3	M	78	ASP	2.2
2	E	212	VAL	2.1
1	L	424	ALA	2.1
2	E	122	ARG	2.1
2	E	174	ARG	2.1
2	B	60	GLN	2.1
1	L	486	ALA	2.1
1	L	483	THR	2.1
3	M	66	LEU	2.0
2	E	130	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	COY	L	601	106/106	0.97	0.07	10,20,33,53	0
6	PGO	L	602	5/5	0.97	0.06	10,11,17,21	0
6	PGO	A	602	5/5	0.98	0.06	10,10,12,19	0
5	COY	A	601	106/106	0.98	0.05	5,13,19,29	0
4	K	A	603	1/1	1.00	0.01	9,9,9,9	0
4	K	A	604	1/1	1.00	0.01	12,12,12,12	0
4	K	L	603	1/1	1.00	0.02	12,12,12,12	0

Continued on next page...

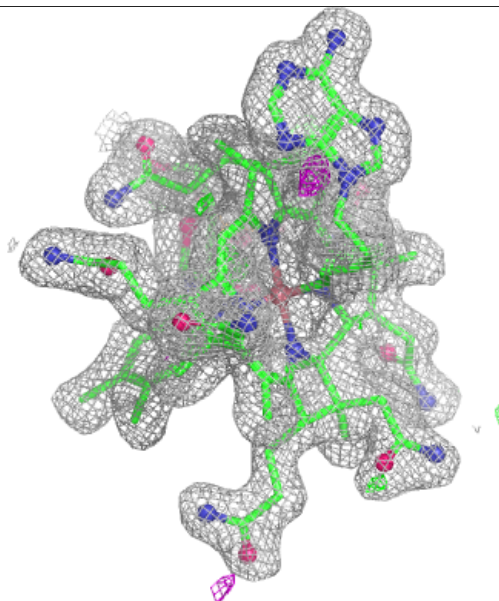
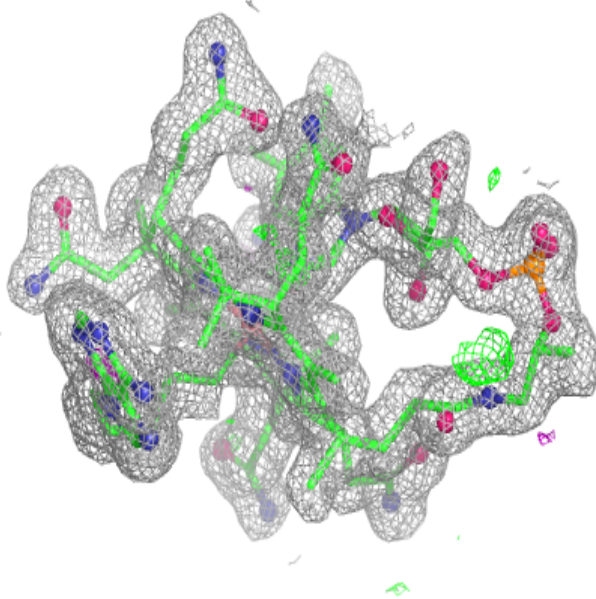
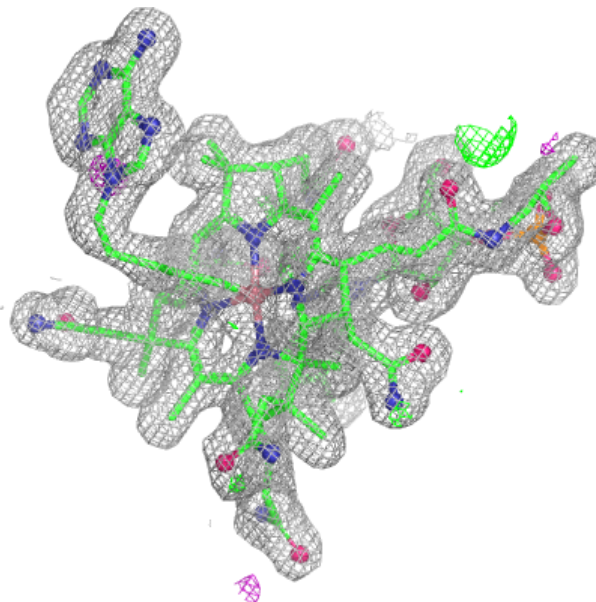
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	K	L	604	1/1	1.00	0.01	16,16,16,16	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.

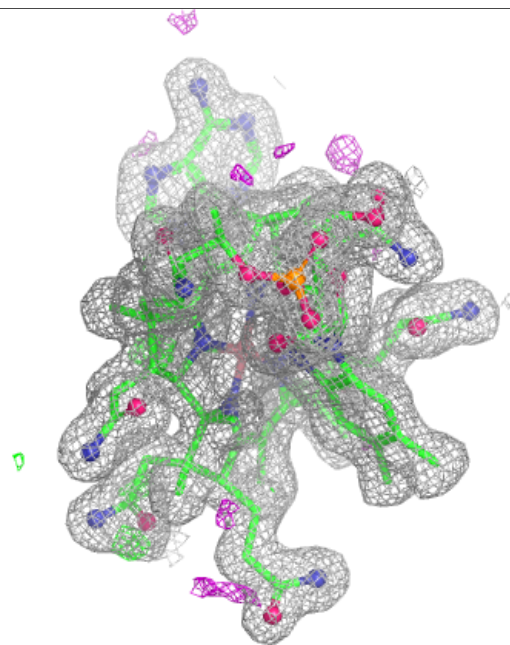
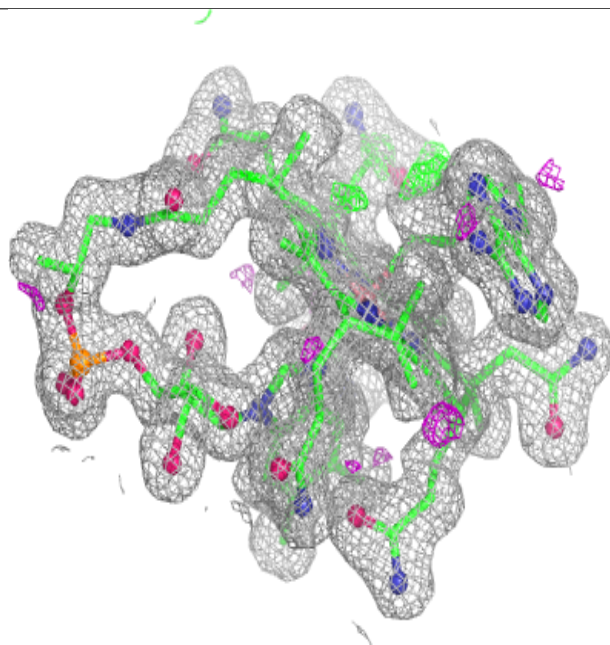
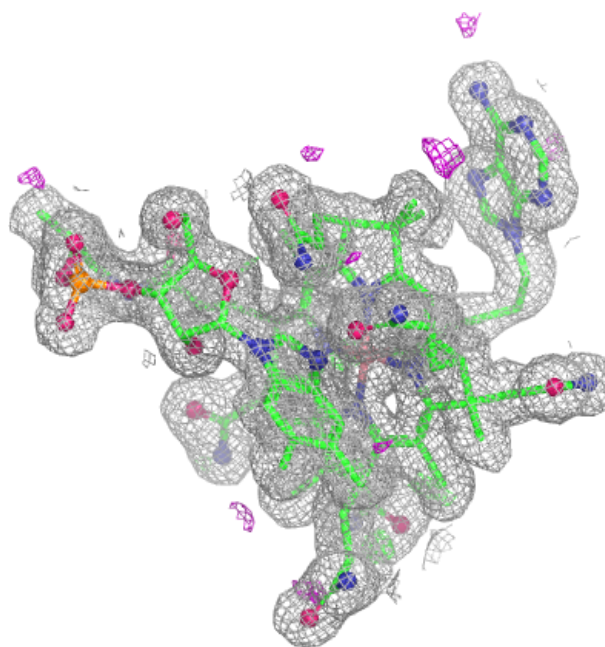
Electron density around COY L 601:

2mF_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 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.