



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 09:49 PM EDT

PDB ID : 1UC4 / pdb_00001uc4
Title : Structure of diol dehydratase complexed with (S)-1,2-propanediol
Authors : Shibata, N.; Nakanishi, Y.; Fukuoka, M.; Yamanishi, M.; Yasuoka, N.; Toraya, T.
Deposited on : 2003-04-08
Resolution : 1.80 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

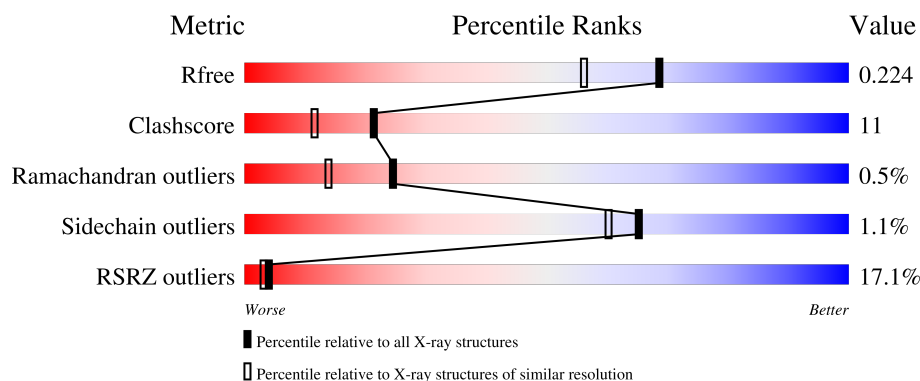
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	2% 84% 14% ..
1	L	554	21% 76% 22% ..
2	B	224	9% 62% 17% 21%
2	E	224	49% 45% 31% 21%
3	G	173	5% 71% 8% 21%

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Mol	Chain	Length	Quality of chain
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
7	CNC	B	2601	X	-	-	-
7	CNC	E	3601	X	-	-	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 14904 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	0	0
			4201	2620	727	825	29			
1	L	551	Total	C	N	O	S	0	0	0
			4201	2620	727	825	29			

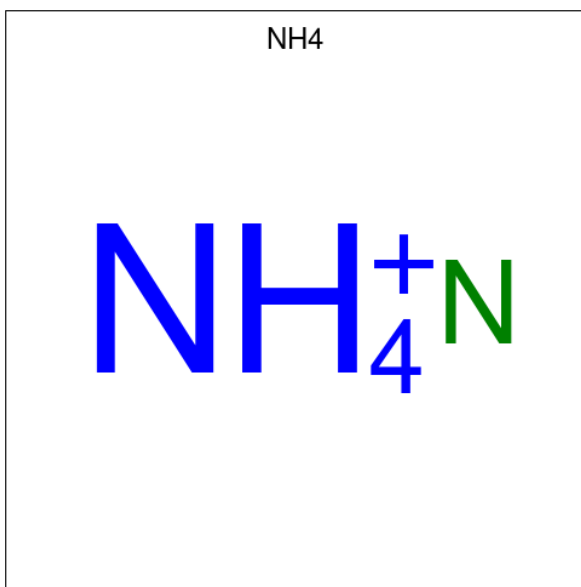
- Molecule 2 is a protein called diol dehydrase beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	178	Total	C	N	O	S	0	0	0
			1358	859	244	253	2			
2	E	176	Total	C	N	O	S	0	0	0
			1349	854	242	251	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	137	Total	C	N	O	S	0	0	0
			1093	681	195	214	3			
3	M	137	Total	C	N	O	S	0	0	0
			1093	681	195	214	3			

- Molecule 4 is AMMONIUM ION (CCD ID: NH4) (formula: H₄N).

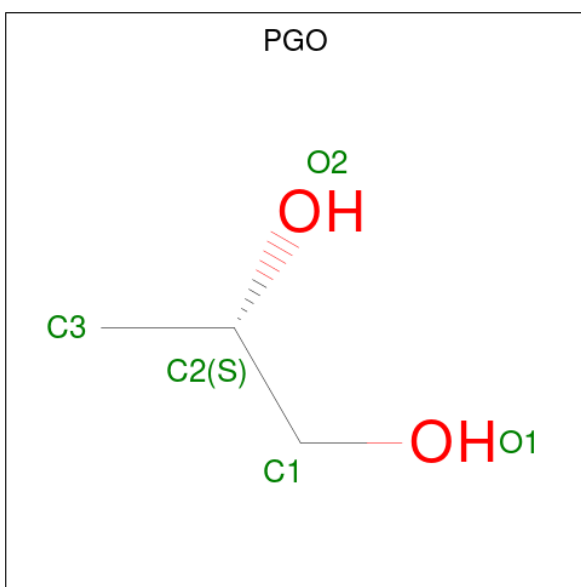


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total N 1 1	0	0
4	A	1	Total N 1 1	0	0
4	L	1	Total N 1 1	0	0
4	L	1	Total N 1 1	0	0

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

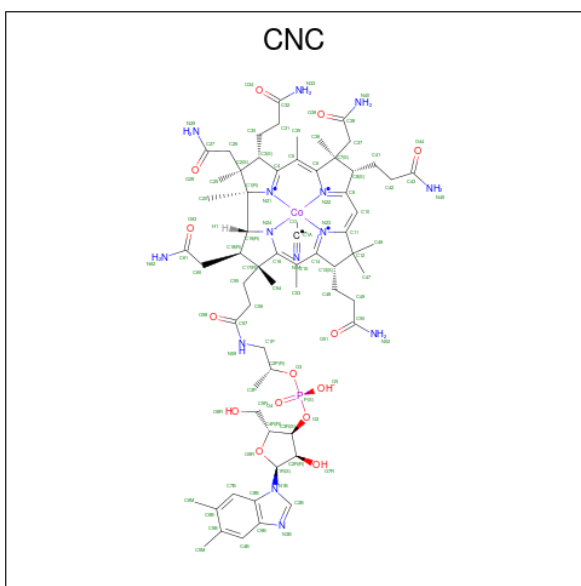
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total K 1 1	0	0
5	L	1	Total K 1 1	0	0

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



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

- Molecule 7 is CYANOCOBALAMIN (CCD ID: CNC) (formula: $\text{C}_{63}\text{H}_{89}\text{CoN}_{14}\text{O}_{14}\text{P}$).



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

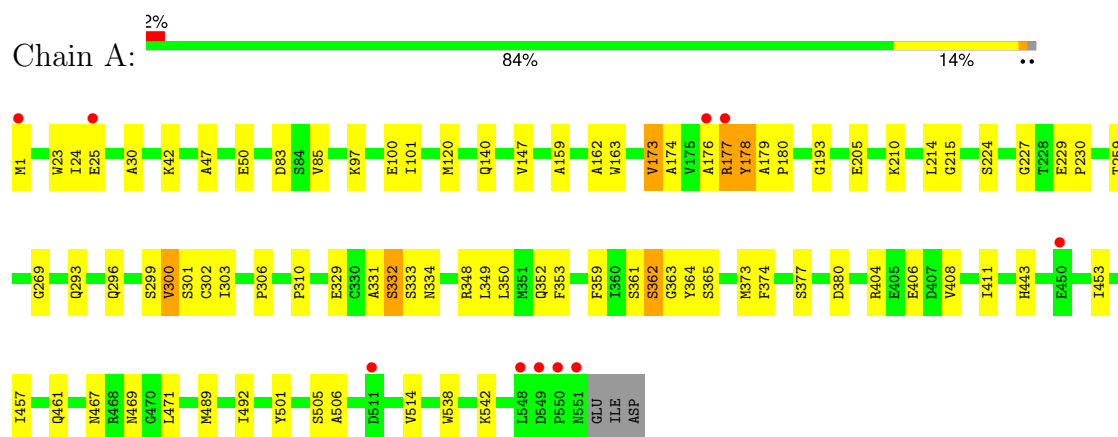
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	543	Total 543	O 543	0	0
8	B	141	Total 141	O 141	0	0
8	G	185	Total 185	O 185	0	0
8	L	360	Total 360	O 360	0	0
8	E	55	Total 55	O 55	0	0
8	M	127	Total 127	O 127	0	0

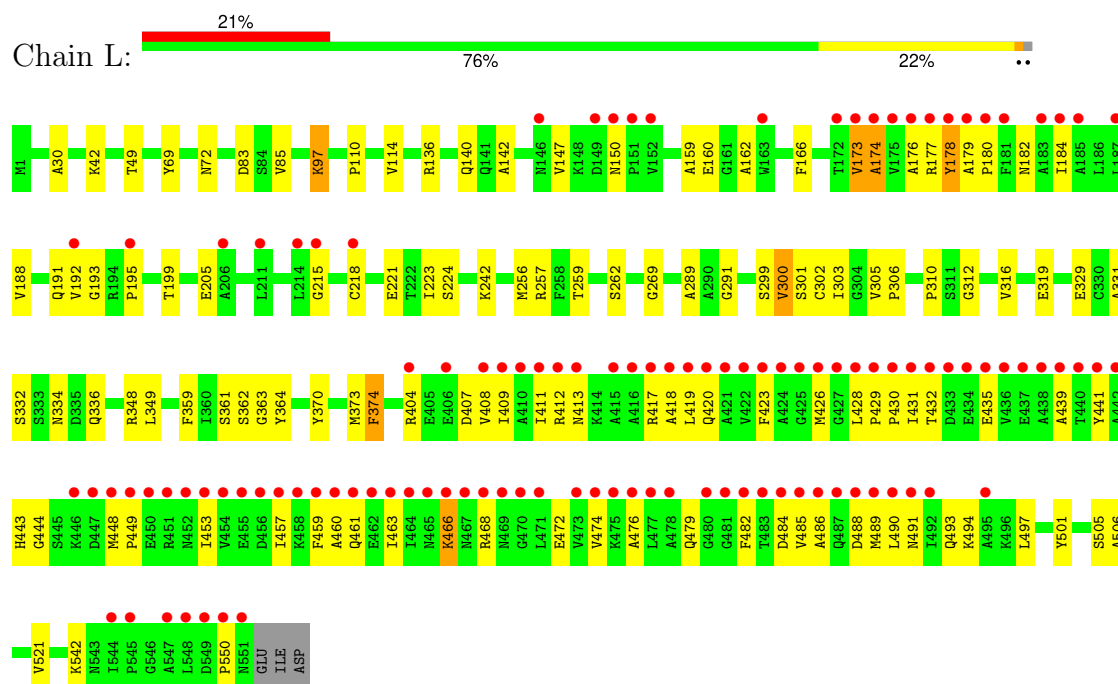
3 Residue-property plots

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.

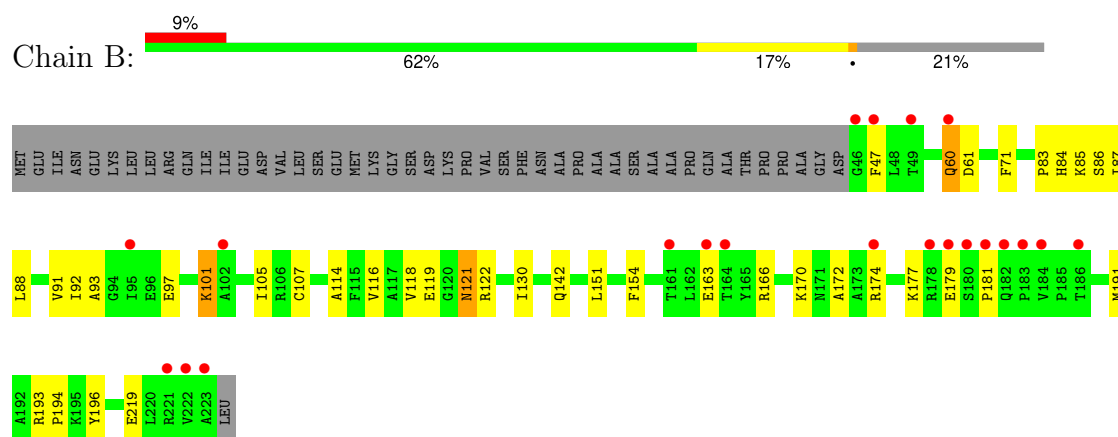
- Molecule 1: diol dehydrase alpha subunit



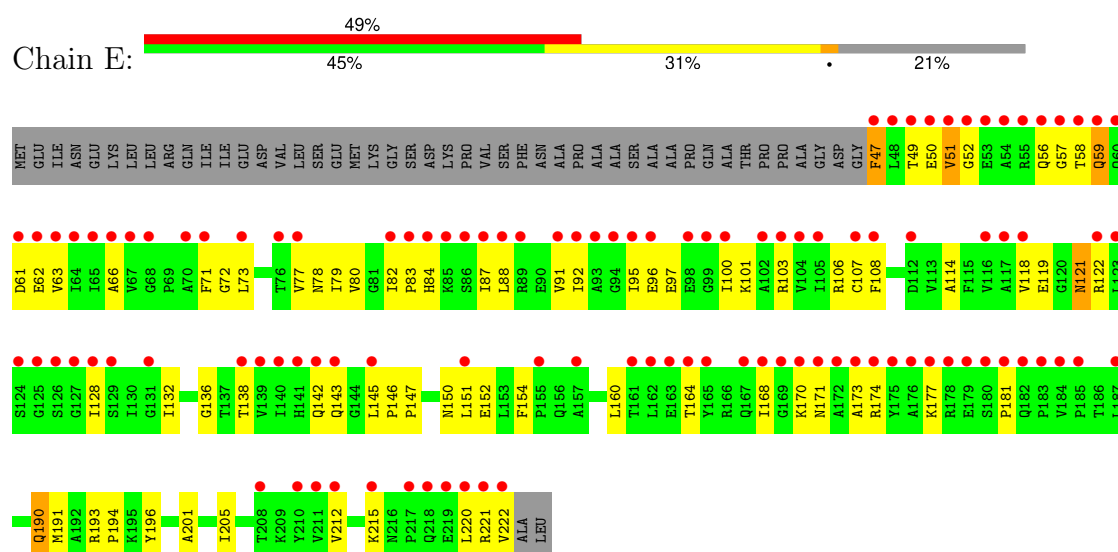
- Molecule 1: diol dehydrase alpha subunit



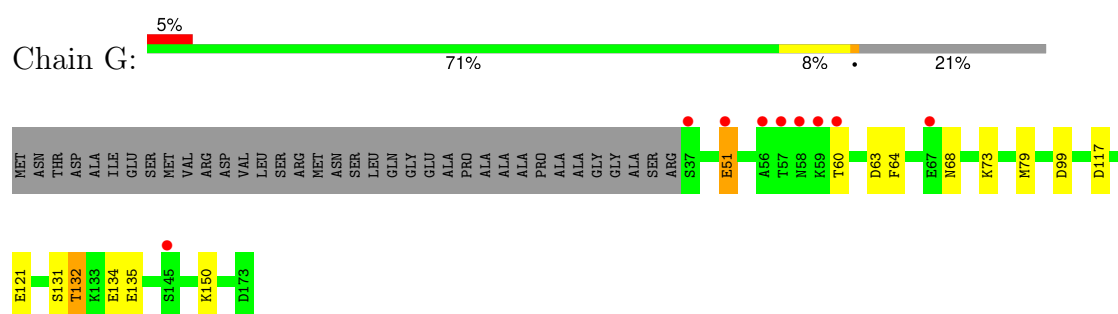
- Molecule 2: diol dehydrase beta subunit



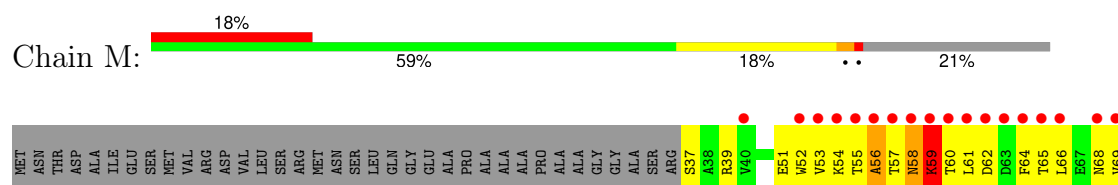
• Molecule 2: diol dehydrase beta subunit



• Molecule 3: diol dehydrase gamma subunit



• Molecule 3: diol dehydrase gamma subunit





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.83Å 121.95Å 208.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.92 – 1.80 36.92 – 1.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (36.92-1.80) 82.8 (36.92-1.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 1.81Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.195 , 0.230 0.189 , 0.224	Depositor DCC
R_{free} test set	14380 reflections (9.96%)	wwPDB-VP
Wilson B-factor (Å ²)	18.8	Xtriage
Anisotropy	0.893	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 57.1	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	0.95	EDS
Total number of atoms	14904	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% 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: PGO, NH4, K, CNC

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	0.40	0/4273	0.93	17/5787 (0.3%)
1	L	0.36	0/4273	0.92	14/5787 (0.2%)
2	B	0.35	0/1380	0.92	4/1868 (0.2%)
2	E	0.31	0/1371	0.88	4/1856 (0.2%)
3	G	0.35	0/1108	0.86	3/1497 (0.2%)
3	M	0.32	0/1108	0.83	1/1497 (0.1%)
All	All	0.36	0/13513	0.91	43/18292 (0.2%)

There are no bond length outliers.

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	332	SER	N-CA-C	9.46	125.36	110.70
1	A	269	GLY	N-CA-C	9.07	127.43	115.36
1	A	224	SER	N-CA-C	8.91	123.06	110.50
1	L	224	SER	N-CA-C	8.60	122.63	110.50
2	E	154	PHE	CA-C-N	8.27	128.47	119.87
2	E	154	PHE	C-N-CA	8.27	128.47	119.87
1	L	269	GLY	N-CA-C	8.01	125.62	115.21
1	A	443	HIS	N-CA-C	-7.50	104.10	113.55
2	B	154	PHE	CA-C-N	7.30	128.56	120.45
2	B	154	PHE	C-N-CA	7.30	128.56	120.45
1	A	173	VAL	N-CA-C	6.89	118.40	108.48
1	A	174	ALA	N-CA-C	-6.83	103.63	112.23
1	L	443	HIS	N-CA-C	-6.72	105.61	113.88
1	A	332	SER	N-CA-C	6.62	124.90	110.80
1	A	30	ALA	N-CA-C	6.59	118.12	111.07
1	A	364	TYR	N-CA-C	-6.37	100.99	110.23
1	L	506	ALA	N-CA-C	6.21	119.35	110.10
3	G	132	THR	N-CA-C	-6.15	101.42	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	374	PHE	N-CA-C	-6.05	105.20	112.59
2	E	196	TYR	N-CA-C	5.80	122.19	114.12
1	A	24	ILE	N-CA-C	5.80	117.23	110.62
1	A	101	ILE	N-CA-C	5.79	116.44	110.82
1	L	174	ALA	N-CA-C	-5.75	104.99	112.23
1	A	227	GLY	N-CA-C	5.67	122.75	115.32
1	L	364	TYR	N-CA-C	-5.54	101.64	109.96
1	L	30	ALA	N-CA-C	5.52	117.38	111.36
2	E	136	GLY	N-CA-C	5.51	120.23	113.79
1	L	97	LYS	N-CA-C	5.42	117.29	110.24
1	A	506	ALA	N-CA-C	5.41	118.17	110.10
3	M	73	LYS	N-CA-C	-5.36	106.69	113.18
1	A	293	GLN	N-CA-C	5.34	118.02	111.82
1	A	469	ASN	N-CA-C	5.32	118.61	110.36
1	A	362	SER	N-CA-C	-5.32	103.62	111.81
3	G	131	SER	N-CA-C	5.31	118.23	109.85
1	L	173	VAL	N-CA-C	5.24	116.20	108.45
1	A	374	PHE	N-CA-C	-5.22	105.36	112.26
2	B	196	TYR	N-CA-C	5.14	121.27	114.12
2	B	116	VAL	N-CA-C	-5.13	105.50	110.42
3	G	99	ASP	N-CA-C	5.10	116.84	111.28
1	L	150	ASN	CA-C-N	5.04	124.65	119.05
1	L	150	ASN	C-N-CA	5.04	124.65	119.05
1	A	120	MET	N-CA-C	5.04	118.28	110.17
1	L	362	SER	N-CA-C	-5.00	104.10	111.81

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	4201	0	4140	50	0
1	L	4201	0	4140	95	0
2	B	1358	0	1408	29	0
2	E	1349	0	1400	67	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	1093	0	1101	10	0
3	M	1093	0	1101	45	0
4	A	2	0	0	0	0
4	L	2	0	0	0	0
5	A	1	0	0	0	0
5	L	1	0	0	0	0
6	A	5	0	6	0	0
6	L	5	0	6	0	0
7	B	91	0	87	4	0
7	E	91	0	87	6	0
8	A	543	0	0	4	0
8	B	141	0	0	1	0
8	E	55	0	0	1	0
8	G	185	0	0	3	0
8	L	360	0	0	7	0
8	M	127	0	0	1	0
All	All	14904	0	13476	294	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 11.

All (294) 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)
1:A:193:GLY:HA2	1:A:411:ILE:HD11	1.32	1.07
1:L:493:GLN:HG2	3:M:79:MET:HE2	1.39	1.03
2:E:174:ARG:HG2	2:E:181:PRO:HB3	1.50	0.91
2:B:121:ASN:C	2:B:121:ASN:HD22	1.79	0.90
2:E:190:GLN:H	2:E:190:GLN:HE21	1.21	0.88
2:E:190:GLN:H	2:E:190:GLN:NE2	1.79	0.79
3:M:60:THR:HG22	3:M:62:ASP:H	1.48	0.79
2:E:78:ASN:ND2	2:E:82:ILE:HB	1.99	0.78
3:G:60:THR:HG22	3:G:63:ASP:CG	2.11	0.75
1:L:179:ALA:HB3	1:L:180:PRO:HD3	1.71	0.71
2:E:49:THR:OG1	2:E:221:ARG:HB3	1.91	0.71
3:M:54:LYS:HG2	3:M:55:THR:H	1.55	0.70
1:L:497:LEU:HD22	3:M:55:THR:HG22	1.74	0.69
7:B:2601:CNC:H552	7:B:2601:CNC:H531	1.74	0.69
3:G:117:ASP:O	3:G:121:GLU:HG3	1.93	0.68
8:L:3854:HOH:O	2:E:190:GLN:HG3	1.92	0.68
1:L:159:ALA:HB1	1:L:411:ILE:HG22	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:106:ARG:HB2	2:E:220:LEU:HD11	1.77	0.67
7:E:3601:CNC:H552	7:E:3601:CNC:H531	1.76	0.67
2:E:121:ASN:HD22	2:E:122:ARG:N	1.93	0.67
1:A:163:TRP:HB2	1:A:411:ILE:HD13	1.77	0.66
1:L:476:ALA:HA	1:L:479:GLN:HE21	1.60	0.66
2:E:121:ASN:HD22	2:E:121:ASN:C	2.03	0.66
2:E:190:GLN:HE21	2:E:190:GLN:N	1.93	0.65
2:E:77:VAL:HG12	2:E:83:PRO:HA	1.79	0.65
2:E:78:ASN:HD21	2:E:82:ILE:HB	1.60	0.65
3:M:55:THR:HG21	3:M:64:PHE:CZ	2.33	0.64
1:A:489:MET:O	1:A:492:ILE:HG22	1.97	0.64
3:M:59:LYS:NZ	3:M:59:LYS:HB3	2.13	0.64
7:B:2601:CNC:H362	7:B:2601:CNC:H351	1.78	0.63
1:A:177:ARG:HB2	1:A:457:ILE:HG23	1.80	0.63
1:L:331:ALA:HA	1:L:359:PHE:HB2	1.80	0.63
7:E:3601:CNC:H362	7:E:3601:CNC:H351	1.81	0.63
1:L:490:LEU:O	1:L:494:LYS:HG3	1.99	0.63
1:L:140:GLN:OE1	1:L:361:SER:HB2	1.99	0.62
3:M:56:ALA:HB2	3:M:80:ARG:HB2	1.81	0.62
2:B:163:GLU:HG3	8:B:2614:HOH:O	1.99	0.62
2:B:174:ARG:HD2	2:B:181:PRO:HB3	1.83	0.61
1:L:259:THR:HG22	8:L:3888:HOH:O	2.00	0.61
2:E:108:PHE:HB3	2:E:212:VAL:HG12	1.81	0.61
2:B:121:ASN:C	2:B:121:ASN:ND2	2.52	0.60
1:L:474:VAL:HG11	1:L:490:LEU:HD21	1.84	0.60
1:A:159:ALA:HB1	1:A:411:ILE:HG12	1.82	0.60
1:L:301:SER:HB3	7:E:3601:CNC:H532	1.83	0.60
1:L:494:LYS:NZ	1:L:494:LYS:HB3	2.16	0.60
2:E:212:VAL:HG11	2:E:215:LYS:HD3	1.84	0.60
2:E:164:THR:O	2:E:168:ILE:HG13	2.02	0.60
2:E:132:ILE:HG12	2:E:138:THR:HG23	1.83	0.59
3:M:144:GLU:HG3	3:M:150:LYS:HE3	1.84	0.59
1:A:42:LYS:HD3	1:A:50:GLU:CD	2.28	0.59
3:M:54:LYS:CD	3:M:58:ASN:HA	2.32	0.59
2:B:177:LYS:HE2	2:B:179:GLU:OE2	2.03	0.58
1:L:408:VAL:O	1:L:412:ARG:HG2	2.03	0.58
1:L:420:GLN:HA	1:L:431:ILE:HD12	1.84	0.58
3:M:132:THR:OG1	3:M:135:GLU:HG3	2.02	0.58
1:L:177:ARG:HA	1:L:461:GLN:NE2	2.18	0.58
3:G:60:THR:HG22	3:G:63:ASP:OD2	2.04	0.58
2:E:63:VAL:HG23	2:E:100:ILE:HG21	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:VAL:O	1:A:411:ILE:HG22	2.04	0.58
1:A:163:TRP:HB2	1:A:411:ILE:CD1	2.33	0.58
3:M:148:GLN:HA	3:M:150:LYS:NZ	2.19	0.58
2:E:122:ARG:HA	2:E:143:GLN:NE2	2.19	0.58
2:E:59:GLN:HB2	2:E:61:ASP:OD1	2.04	0.57
3:G:134:GLU:HG2	8:G:333:HOH:O	2.03	0.57
1:A:25:GLU:CD	1:A:25:GLU:H	2.12	0.57
2:E:114:ALA:O	2:E:118:VAL:HG23	2.04	0.57
1:A:214:LEU:HD21	1:A:467:ASN:HD22	1.70	0.57
2:B:174:ARG:CD	2:B:181:PRO:HB3	2.35	0.57
1:L:69:TYR:HB2	1:L:289:ALA:HB1	1.86	0.57
2:E:87:ILE:O	2:E:91:VAL:HG23	2.05	0.57
1:A:461:GLN:NE2	8:A:3148:HOH:O	2.38	0.56
2:E:121:ASN:O	2:E:143:GLN:HB2	2.05	0.56
1:L:221:GLU:HG3	1:L:257:ARG:HD2	1.88	0.56
1:A:179:ALA:HB3	1:A:180:PRO:HD3	1.88	0.55
2:B:121:ASN:HD22	2:B:122:ARG:N	2.03	0.55
1:L:463:ILE:HG23	1:L:468:ARG:HB2	1.87	0.55
1:A:147:VAL:HG12	1:A:373:MET:HE1	1.87	0.55
3:M:54:LYS:HD2	3:M:58:ASN:HA	1.87	0.55
1:L:199:THR:H	1:L:218:CYS:HB2	1.72	0.55
1:L:173:VAL:HG12	1:L:182:ASN:ND2	2.21	0.55
1:L:466:LYS:NZ	1:L:466:LYS:HB3	2.22	0.55
2:E:88:LEU:O	2:E:92:ILE:HG13	2.06	0.54
1:A:140:GLN:OE1	1:A:361:SER:HB2	2.08	0.54
2:B:191:MET:C	2:B:194:PRO:HD2	2.32	0.54
7:B:2601:CNC:C2B	7:B:2601:CNC:H492	2.38	0.54
1:L:159:ALA:HB1	1:L:411:ILE:CG2	2.37	0.54
2:E:121:ASN:C	2:E:121:ASN:ND2	2.65	0.54
3:G:60:THR:HG23	3:G:63:ASP:H	1.72	0.54
1:L:485:VAL:O	1:L:489:MET:HG2	2.08	0.54
1:L:453:ILE:O	1:L:457:ILE:HG13	2.08	0.53
3:M:53:VAL:HG12	3:M:54:LYS:N	2.23	0.53
2:B:193:ARG:HB3	2:B:194:PRO:HD3	1.91	0.53
1:L:439:ALA:HB2	1:L:448:MET:HE1	1.91	0.53
2:E:79:ILE:HG23	2:E:80:VAL:HG13	1.90	0.53
1:L:188:VAL:O	1:L:192:VAL:HG23	2.10	0.52
1:L:334:ASN:ND2	1:L:348:ARG:HD3	2.24	0.52
2:E:193:ARG:HB3	2:E:194:PRO:HD3	1.90	0.52
1:A:1:MET:HG2	1:L:441:TYR:CE2	2.44	0.52
1:A:408:VAL:HA	1:A:411:ILE:HG22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:370:TYR:OH	1:L:444:GLY:HA3	2.09	0.52
2:E:170:LYS:O	2:E:174:ARG:HB2	2.10	0.52
3:M:100:ARG:HG3	3:M:100:ARG:HH11	1.74	0.52
1:L:205:GLU:HG2	8:E:3633:HOH:O	2.09	0.52
1:L:484:ASP:OD1	1:L:485:VAL:HG23	2.10	0.52
3:M:100:ARG:HG3	3:M:100:ARG:NH1	2.25	0.52
3:G:64:PHE:CE1	3:G:79:MET:HG2	2.44	0.51
3:G:51:GLU:CD	3:G:51:GLU:H	2.17	0.51
1:A:404:ARG:HH21	1:A:406:GLU:CD	2.19	0.51
1:L:160:GLU:HG3	1:L:408:VAL:HG13	1.93	0.51
2:E:191:MET:C	2:E:194:PRO:HD2	2.36	0.51
1:A:97:LYS:HB2	1:A:100:GLU:HG3	1.93	0.51
1:A:299:SER:OG	1:A:303:ILE:HA	2.10	0.51
1:A:329:GLU:OE2	1:A:505:SER:HA	2.11	0.51
2:B:97:GLU:OE1	2:B:170:LYS:HE2	2.11	0.51
2:B:105:ILE:HG22	2:B:219:GLU:HA	1.92	0.51
1:L:110:PRO:O	1:L:114:VAL:HG23	2.11	0.51
2:E:121:ASN:ND2	2:E:122:ARG:HG3	2.26	0.51
1:L:69:TYR:HB3	3:M:100:ARG:NH1	2.26	0.50
1:L:413:ASN:O	1:L:417:ARG:HG2	2.11	0.50
2:E:150:ASN:HD22	2:E:152:GLU:C	2.20	0.50
1:L:493:GLN:O	1:L:497:LEU:HG	2.10	0.50
2:B:107:CYS:HB3	2:B:119:GLU:OE1	2.11	0.50
1:L:180:PRO:HG2	1:L:460:ALA:O	2.12	0.50
1:L:418:ALA:HA	1:L:482:PHE:CE2	2.46	0.50
1:A:205:GLU:HG2	8:A:2621:HOH:O	2.12	0.50
2:E:114:ALA:HB2	7:E:3601:CNC:HM62	1.93	0.50
1:L:484:ASP:OD1	1:L:485:VAL:N	2.46	0.49
1:A:215:GLY:HA2	8:A:2817:HOH:O	2.12	0.49
1:L:223:ILE:HG22	1:L:242:LYS:HD2	1.94	0.49
1:L:409:ILE:HD13	1:L:441:TYR:HE1	1.78	0.49
2:E:57:GLY:O	2:E:58:THR:HB	2.12	0.49
1:A:310:PRO:HG2	1:L:542:LYS:HD2	1.94	0.49
2:B:142:GLN:NE2	2:B:151:LEU:HD21	2.28	0.49
2:E:72:GLY:C	2:E:73:LEU:HD12	2.38	0.49
1:L:428:LEU:O	1:L:429:PRO:C	2.55	0.49
2:E:128:ILE:HD12	2:E:128:ILE:N	2.28	0.48
3:M:57:THR:HG23	3:M:77:GLN:O	2.13	0.48
3:M:57:THR:HG1	3:M:59:LYS:HE2	1.78	0.48
3:M:148:GLN:HA	3:M:150:LYS:HZ3	1.77	0.48
1:L:305:VAL:HB	1:L:306:PRO:CD	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:429:PRO:HD3	1:L:459:PHE:CD2	2.47	0.48
2:B:83:PRO:HG2	2:B:86:SER:OG	2.14	0.48
3:M:144:GLU:HG3	3:M:150:LYS:CE	2.42	0.48
1:L:428:LEU:HD23	1:L:459:PHE:HD2	1.78	0.48
3:M:55:THR:HB	3:M:78:ASP:O	2.13	0.48
2:E:100:ILE:HG13	2:E:173:ALA:HB1	1.94	0.48
1:A:259:THR:CG2	1:A:296:GLN:HE21	2.26	0.48
1:A:350:LEU:HA	1:A:353:PHE:HB3	1.94	0.48
3:M:56:ALA:O	3:M:57:THR:HG23	2.13	0.48
3:M:39:ARG:HH11	3:M:39:ARG:HG2	1.78	0.48
2:E:47:PHE:O	2:E:222:VAL:HA	2.14	0.47
1:L:486:ALA:O	1:L:489:MET:HB2	2.13	0.47
2:B:93:ALA:HB3	2:B:166:ARG:HH12	1.78	0.47
2:B:93:ALA:CB	2:B:166:ARG:HH12	2.27	0.47
2:E:142:GLN:NE2	2:E:151:LEU:HD21	2.28	0.47
2:E:107:CYS:HB3	2:E:119:GLU:OE1	2.14	0.47
2:E:108:PHE:HB3	2:E:212:VAL:CG1	2.44	0.47
1:A:538:TRP:O	1:A:542:LYS:HG3	2.14	0.47
1:L:453:ILE:HG22	1:L:457:ILE:CD1	2.45	0.47
3:G:132:THR:OG1	3:G:135:GLU:HG3	2.14	0.47
1:L:426:MET:HE3	1:L:472:GLU:HB2	1.96	0.47
1:L:486:ALA:HB1	3:M:66:LEU:HD21	1.97	0.47
2:E:57:GLY:O	2:E:58:THR:CB	2.62	0.47
2:E:59:GLN:NE2	2:E:59:GLN:N	2.63	0.47
3:M:55:THR:C	3:M:57:THR:H	2.23	0.47
1:A:210:LYS:O	1:A:210:LYS:HD3	2.14	0.47
1:L:419:LEU:HD11	1:L:423:PHE:HE1	1.80	0.47
1:A:300:VAL:HG12	1:A:301:SER:N	2.30	0.47
1:L:42:LYS:HG2	1:L:49:THR:OG1	2.16	0.46
3:M:59:LYS:HB3	3:M:59:LYS:HZ3	1.80	0.46
1:A:514:VAL:HG12	8:G:203:HOH:O	2.14	0.46
1:L:162:ALA:HB3	1:L:193:GLY:HA3	1.97	0.46
1:L:173:VAL:HG12	1:L:182:ASN:CG	2.40	0.46
2:B:83:PRO:HG2	2:B:86:SER:CB	2.45	0.46
3:M:60:THR:HG22	3:M:61:LEU:N	2.29	0.46
1:L:83:ASP:OD2	1:L:85:VAL:HB	2.15	0.46
2:E:92:ILE:O	2:E:96:GLU:HG3	2.16	0.46
2:B:130:ILE:HD11	2:B:172:ALA:CB	2.46	0.46
1:L:291:GLY:HA2	3:M:100:ARG:HB3	1.98	0.46
1:A:42:LYS:HB2	1:A:50:GLU:HB3	1.97	0.46
1:L:334:ASN:ND2	1:L:349:LEU:HA	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:118:VAL:O	2:E:121:ASN:ND2	2.49	0.46
2:B:88:LEU:O	2:B:92:ILE:HG13	2.15	0.46
7:B:2601:CNC:H291	7:B:2601:CNC:H251	1.81	0.45
7:E:3601:CNC:O6R	7:E:3601:CNC:H492	2.16	0.45
1:A:334:ASN:ND2	1:A:348:ARG:HD3	2.31	0.45
1:A:334:ASN:ND2	1:A:349:LEU:HA	2.31	0.45
3:M:54:LYS:HG2	3:M:55:THR:N	2.29	0.45
1:A:23:TRP:HB2	1:L:550:PRO:HG3	1.98	0.45
2:B:61:ASP:CG	2:B:101:LYS:HE2	2.42	0.45
1:L:174:ALA:HB2	1:L:373:MET:HE2	1.98	0.45
2:E:201:ALA:O	2:E:205:ILE:HG13	2.17	0.45
1:A:365:SER:HB2	1:A:377:SER:HB3	1.98	0.45
1:L:173:VAL:HG21	1:L:176:ALA:HA	1.99	0.45
1:L:184:ILE:O	1:L:188:VAL:HG23	2.17	0.45
3:M:58:ASN:C	3:M:59:LYS:HD2	2.42	0.45
2:B:60:GLN:O	2:B:60:GLN:HG2	2.17	0.45
1:L:147:VAL:O	1:L:147:VAL:HG22	2.17	0.45
3:M:56:ALA:CB	3:M:80:ARG:HB2	2.46	0.45
1:L:262:SER:HA	8:L:3677:HOH:O	2.16	0.44
1:A:331:ALA:HA	1:A:359:PHE:HB2	1.99	0.44
1:L:299:SER:OG	1:L:303:ILE:HA	2.17	0.44
2:E:100:ILE:CG1	2:E:173:ALA:HB1	2.47	0.44
3:M:68:ASN:HB3	3:M:74:VAL:HG23	1.98	0.44
2:E:97:GLU:OE1	2:E:170:LYS:HE2	2.17	0.44
3:M:57:THR:CG2	3:M:77:GLN:HG2	2.47	0.44
1:A:302:CYS:O	1:A:306:PRO:HD2	2.17	0.44
1:L:306:PRO:O	1:L:312:GLY:HA3	2.17	0.44
3:M:51:GLU:HG2	3:M:52:TRP:HD1	1.83	0.44
1:L:426:MET:HE3	1:L:472:GLU:CB	2.47	0.44
2:E:96:GLU:HA	2:E:100:ILE:O	2.17	0.44
2:B:71:PHE:CE1	2:B:84:HIS:HB3	2.53	0.44
1:L:215:GLY:HA2	8:L:3817:HOH:O	2.17	0.44
1:L:316:VAL:O	1:L:319:GLU:HG2	2.16	0.44
2:E:212:VAL:HG11	2:E:215:LYS:CD	2.48	0.44
2:B:174:ARG:HD2	2:B:181:PRO:CB	2.46	0.44
2:B:83:PRO:HG2	2:B:86:SER:HB2	1.99	0.44
1:L:336:GLN:HE22	1:L:374:PHE:HB3	1.82	0.44
2:E:49:THR:HG1	2:E:221:ARG:HB3	1.83	0.44
3:M:55:THR:OG1	3:M:59:LYS:HD3	2.18	0.44
1:A:178:TYR:CE2	1:A:453:ILE:HG23	2.53	0.43
2:E:150:ASN:ND2	2:E:152:GLU:C	2.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:150:LYS:HE2	8:G:314:HOH:O	2.17	0.43
1:L:474:VAL:CG1	1:L:490:LEU:HD21	2.47	0.43
3:M:55:THR:HG21	3:M:64:PHE:CE2	2.53	0.43
2:B:60:GLN:CD	2:B:60:GLN:H	2.26	0.43
1:L:432:THR:HG1	1:L:435:GLU:HG3	1.84	0.43
1:L:486:ALA:HB3	3:M:66:LEU:HD11	2.00	0.43
2:E:142:GLN:HG2	2:E:145:LEU:HD22	2.00	0.43
1:L:302:CYS:O	1:L:306:PRO:HD2	2.18	0.43
2:E:91:VAL:O	2:E:95:ILE:HG13	2.18	0.43
1:L:300:VAL:HG12	1:L:301:SER:N	2.34	0.43
2:E:56:GLN:HG3	2:E:57:GLY:N	2.32	0.43
2:E:160:LEU:HD22	2:E:164:THR:HG21	2.00	0.43
3:M:75:THR:HB	8:M:254:HOH:O	2.17	0.43
3:G:68:ASN:OD1	3:G:73:LYS:HD3	2.18	0.43
1:L:173:VAL:HG11	1:L:179:ALA:HA	1.99	0.43
1:L:142:ALA:HB2	1:L:166:PHE:CE1	2.54	0.42
2:E:100:ILE:HG22	2:E:101:LYS:N	2.34	0.42
2:B:122:ARG:HG2	2:B:122:ARG:HH11	1.84	0.42
2:E:71:PHE:CE1	2:E:84:HIS:HB3	2.54	0.42
2:E:106:ARG:HD2	2:E:108:PHE:CZ	2.55	0.42
1:L:72:ASN:CG	8:L:3783:HOH:O	2.63	0.42
1:L:136:ARG:HD2	1:L:521:VAL:O	2.19	0.42
1:A:178:TYR:HE2	1:A:453:ILE:HG23	1.84	0.42
1:A:83:ASP:OD2	1:A:85:VAL:HB	2.19	0.42
2:E:212:VAL:HG13	2:E:215:LYS:HB3	2.00	0.42
1:L:453:ILE:HG22	1:L:457:ILE:HD11	2.02	0.42
2:E:174:ARG:HG2	2:E:174:ARG:HH11	1.85	0.42
1:A:229:GLU:N	1:A:230:PRO:HD2	2.34	0.42
1:A:471:LEU:HD23	1:A:471:LEU:HA	1.91	0.42
1:A:47:ALA:HB3	8:A:2974:HOH:O	2.19	0.42
1:A:365:SER:HB3	1:A:380:ASP:HA	2.02	0.42
2:B:47:PHE:CE2	2:B:85:LYS:HA	2.55	0.42
1:A:162:ALA:HB3	1:A:193:GLY:HA3	2.01	0.41
1:L:404:ARG:CB	1:L:404:ARG:HH11	2.33	0.41
2:E:142:GLN:O	2:E:142:GLN:HG3	2.18	0.41
1:L:97:LYS:HG3	8:L:3886:HOH:O	2.20	0.41
2:E:77:VAL:HG12	2:E:83:PRO:CA	2.50	0.41
1:A:334:ASN:HD21	1:A:349:LEU:HA	1.85	0.41
1:L:223:ILE:HG13	1:L:256:MET:HE2	2.02	0.41
2:E:170:LYS:HG3	2:E:171:ASN:N	2.36	0.41
3:M:65:THR:O	3:M:69:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:407:ASP:O	1:L:411:ILE:HG12	2.19	0.41
3:M:39:ARG:HG2	3:M:39:ARG:NH1	2.35	0.41
1:A:173:VAL:HG21	1:A:176:ALA:HA	2.02	0.41
1:A:332:SER:HB2	1:A:352:GLN:HG2	2.02	0.41
1:L:334:ASN:HD21	1:L:349:LEU:HA	1.85	0.41
2:E:66:ALA:HB1	2:E:107:CYS:SG	2.61	0.41
3:M:37:SER:HB2	3:M:91:SER:OG	2.19	0.41
2:B:87:ILE:O	2:B:91:VAL:HG23	2.20	0.41
1:L:191:GLN:OE1	1:L:195:PRO:HA	2.20	0.41
1:L:494:LYS:HB3	1:L:494:LYS:HZ3	1.84	0.41
1:L:429:PRO:HA	1:L:430:PRO:HD2	1.86	0.41
7:E:3601:CNC:H531	7:E:3601:CNC:C55	2.48	0.41
3:M:100:ARG:HA	3:M:100:ARG:NE	2.35	0.41
1:L:488:ASP:HA	1:L:491:ASN:HD22	1.85	0.41
8:L:3782:HOH:O	3:M:100:ARG:HD3	2.20	0.41
1:A:300:VAL:HG12	1:A:301:SER:H	1.85	0.41
1:L:177:ARG:CB	1:L:457:ILE:HG23	2.50	0.41
2:E:62:GLU:OE2	2:E:103:ARG:NH2	2.54	0.41
1:A:542:LYS:HD2	1:L:310:PRO:HG2	2.03	0.41
1:L:142:ALA:HB2	1:L:166:PHE:CD1	2.56	0.41
1:L:448:MET:HA	1:L:449:PRO:HD3	1.92	0.41
2:E:146:PRO:HA	2:E:147:PRO:HD3	1.97	0.41
1:A:333:SER:HA	1:A:362:SER:OG	2.21	0.40
1:L:476:ALA:HA	1:L:479:GLN:NE2	2.32	0.40
2:B:114:ALA:O	2:B:118:VAL:HG23	2.21	0.40
1:L:329:GLU:OE2	1:L:505:SER:HA	2.22	0.40
3:M:71:SER:O	3:M:72:ASN:HB2	2.21	0.40
2:E:100:ILE:HD11	2:E:177:LYS:CG	2.51	0.40
3:M:51:GLU:H	3:M:51:GLU:CD	2.29	0.40
1:L:178:TYR:HE2	1:L:453:ILE:HG23	1.87	0.40
2:E:51:VAL:HG12	2:E:52:GLY:N	2.35	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	549/554 (99%)	523 (95%)	24 (4%)	2 (0%)	30	19
1	L	549/554 (99%)	522 (95%)	25 (5%)	2 (0%)	30	19
2	B	176/224 (79%)	171 (97%)	5 (3%)	0	100	100
2	E	174/224 (78%)	161 (92%)	11 (6%)	2 (1%)	11	3
3	G	135/173 (78%)	133 (98%)	2 (2%)	0	100	100
3	M	135/173 (78%)	125 (93%)	7 (5%)	3 (2%)	5	1
All	All	1718/1902 (90%)	1635 (95%)	74 (4%)	9 (0%)	24	14

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	51	VAL
3	M	58	ASN
3	M	59	LYS
1	A	363	GLY
1	L	363	GLY
2	E	50	GLU
3	M	56	ALA
1	A	300	VAL
1	L	300	VAL

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	450/453 (99%)	447 (99%)	3 (1%)	76	73
1	L	450/453 (99%)	447 (99%)	3 (1%)	76	73
2	B	146/183 (80%)	143 (98%)	3 (2%)	47	36
2	E	146/183 (80%)	142 (97%)	4 (3%)	39	27
3	G	116/141 (82%)	115 (99%)	1 (1%)	70	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	M	116/141 (82%)	114 (98%)	2 (2%)	53 45
All	All	1424/1554 (92%)	1408 (99%)	16 (1%)	65 60

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	177	ARG
1	A	178	TYR
1	A	501	TYR
2	B	60	GLN
2	B	101	LYS
2	B	121	ASN
3	G	51	GLU
1	L	178	TYR
1	L	466	LYS
1	L	501	TYR
2	E	47	PHE
2	E	59	GLN
2	E	121	ASN
2	E	190	GLN
3	M	59	LYS
3	M	100	ARG

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	74	ASN
1	A	334	ASN
1	A	352	GLN
1	A	465	ASN
1	A	467	ASN
1	A	487	GLN
1	A	534	GLN
1	A	543	ASN
2	B	59	GLN
2	B	75	GLN
2	B	121	ASN
2	B	142	GLN
2	B	171	ASN
2	B	204	HIS
3	G	47	ASN

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Mol	Chain	Res	Type
1	L	45	ASN
1	L	74	ASN
1	L	334	ASN
1	L	352	GLN
1	L	461	GLN
1	L	465	ASN
1	L	467	ASN
1	L	479	GLN
1	L	543	ASN
2	E	56	GLN
2	E	59	GLN
2	E	60	GLN
2	E	75	GLN
2	E	121	ASN
2	E	142	GLN
2	E	143	GLN
2	E	150	ASN
2	E	182	GLN
2	E	190	GLN
3	M	77	GLN
3	M	124	ASN
3	M	148	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 4 are modelled with single atom and 2 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$
7	CNC	B	2601	-	94,101,103	1.36	11 (11%)	150,166,171	1.07	9 (6%)
7	CNC	E	3601	-	94,101,103	1.37	11 (11%)	150,166,171	1.15	11 (7%)
6	PGO	L	3602	5	4,4,4	0.67	0	4,4,4	0.68	0
6	PGO	A	2602	5	4,4,4	0.65	0	4,4,4	0.66	0

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
7	CNC	E	3601	-	1/1/36/38	11/56/223/235	0/3/11/11
6	PGO	L	3602	5	-	0/2/2/2	-
6	PGO	A	2602	5	-	0/2/2/2	-
7	CNC	B	2601	-	1/1/36/38	8/56/223/235	0/3/11/11

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	E	3601	CNC	C5M-C5B	-5.90	1.40	1.51
7	B	2601	CNC	C5M-C5B	-5.72	1.40	1.51
7	E	3601	CNC	C14-N23	4.44	1.41	1.30
7	B	2601	CNC	C14-N23	4.09	1.40	1.30
7	B	2601	CNC	O58-C57	3.12	1.29	1.23
7	E	3601	CNC	O58-C57	2.98	1.29	1.23
7	E	3601	CNC	C13-C14	2.97	1.59	1.51
7	B	2601	CNC	C48-C49	2.82	1.61	1.52
7	E	3601	CNC	C2B-N3B	2.63	1.36	1.31
7	B	2601	CNC	C9-N22	2.62	1.36	1.30
7	B	2601	CNC	C2B-N3B	2.56	1.36	1.31
7	B	2601	CNC	C13-C14	2.51	1.58	1.51
7	E	3601	CNC	C9-N22	2.50	1.36	1.30
7	E	3601	CNC	C48-C49	2.49	1.60	1.52
7	B	2601	CNC	C30-C3	2.42	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	2601	CNC	C48-C13	2.38	1.59	1.54
7	E	3601	CNC	C30-C3	2.27	1.59	1.54
7	E	3601	CNC	C7-C6	2.22	1.59	1.54
7	B	2601	CNC	C41-C8	2.07	1.59	1.54
7	E	3601	CNC	C17-C18	2.07	1.58	1.54
7	B	2601	CNC	C7-C6	2.05	1.59	1.54
7	E	3601	CNC	C48-C13	2.03	1.59	1.54

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	2601	CNC	C41-C8-C9	-3.56	104.98	111.19
7	E	3601	CNC	C26-C2-C1	3.44	115.31	110.00
7	E	3601	CNC	C41-C8-C9	-3.33	105.38	111.19
7	E	3601	CNC	C56-C55-C17	3.12	121.59	115.58
7	B	2601	CNC	C18-C19-N24	3.01	106.71	101.92
7	B	2601	CNC	C56-C55-C17	2.89	121.16	115.58
7	E	3601	CNC	C11-N23-C14	2.85	107.39	106.31
7	E	3601	CNC	C7-C37-C38	2.85	122.72	114.28
7	E	3601	CNC	C18-C19-N24	2.76	106.31	101.92
7	B	2601	CNC	C55-C17-C16	2.71	122.06	116.17
7	B	2601	CNC	C11-N23-C14	2.70	107.33	106.31
7	B	2601	CNC	C7-C37-C38	2.70	122.26	114.28
7	E	3601	CNC	C47-C12-C46	-2.60	105.09	109.41
7	E	3601	CNC	C19-N24-C16	-2.54	107.91	111.96
7	B	2601	CNC	C47-C12-C46	-2.45	105.35	109.41
7	E	3601	CNC	C55-C17-C16	2.41	121.41	116.17
7	E	3601	CNC	O58-C57-C56	-2.37	117.72	122.02
7	B	2601	CNC	O58-C57-C56	-2.36	117.75	122.02
7	B	2601	CNC	C19-N24-C16	-2.26	108.35	111.96
7	E	3601	CNC	C12-C11-N23	2.05	113.68	111.49

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	B	2601	CNC	N24
7	E	3601	CNC	N24

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	2601	CNC	C12-C13-C48-C49

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Mol	Chain	Res	Type	Atoms
7	E	3601	CNC	C4-C3-C30-C31
7	B	2601	CNC	C2-C26-C27-N29
7	B	2601	CNC	C2-C26-C27-O28
7	E	3601	CNC	C2-C3-C30-C31
7	E	3601	CNC	C13-C48-C49-C50
7	E	3601	CNC	C1-C2-C26-C27
7	E	3601	CNC	C25-C2-C26-C27
7	E	3601	CNC	C17-C18-C60-C61
7	E	3601	CNC	C42-C41-C8-C9
7	B	2601	CNC	C19-C18-C60-C61
7	E	3601	CNC	C19-C18-C60-C61
7	B	2601	CNC	C42-C41-C8-C9
7	B	2601	CNC	C2-C3-C30-C31
7	E	3601	CNC	C3R-O2-P-O4
7	E	3601	CNC	C3-C2-C26-C27
7	B	2601	CNC	C17-C18-C60-C61
7	B	2601	CNC	C4-C3-C30-C31
7	E	3601	CNC	C12-C13-C48-C49

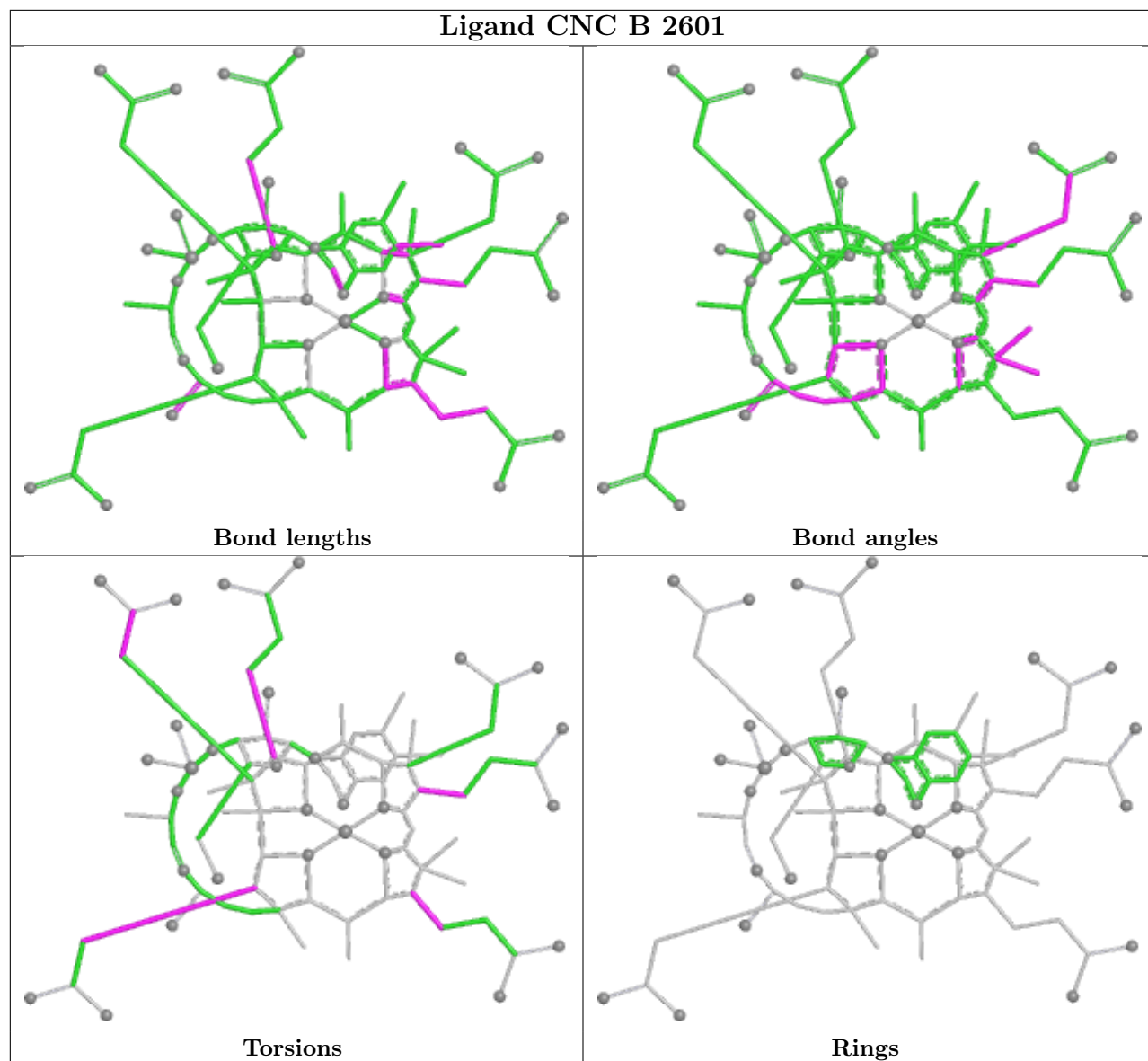
There are no ring outliers.

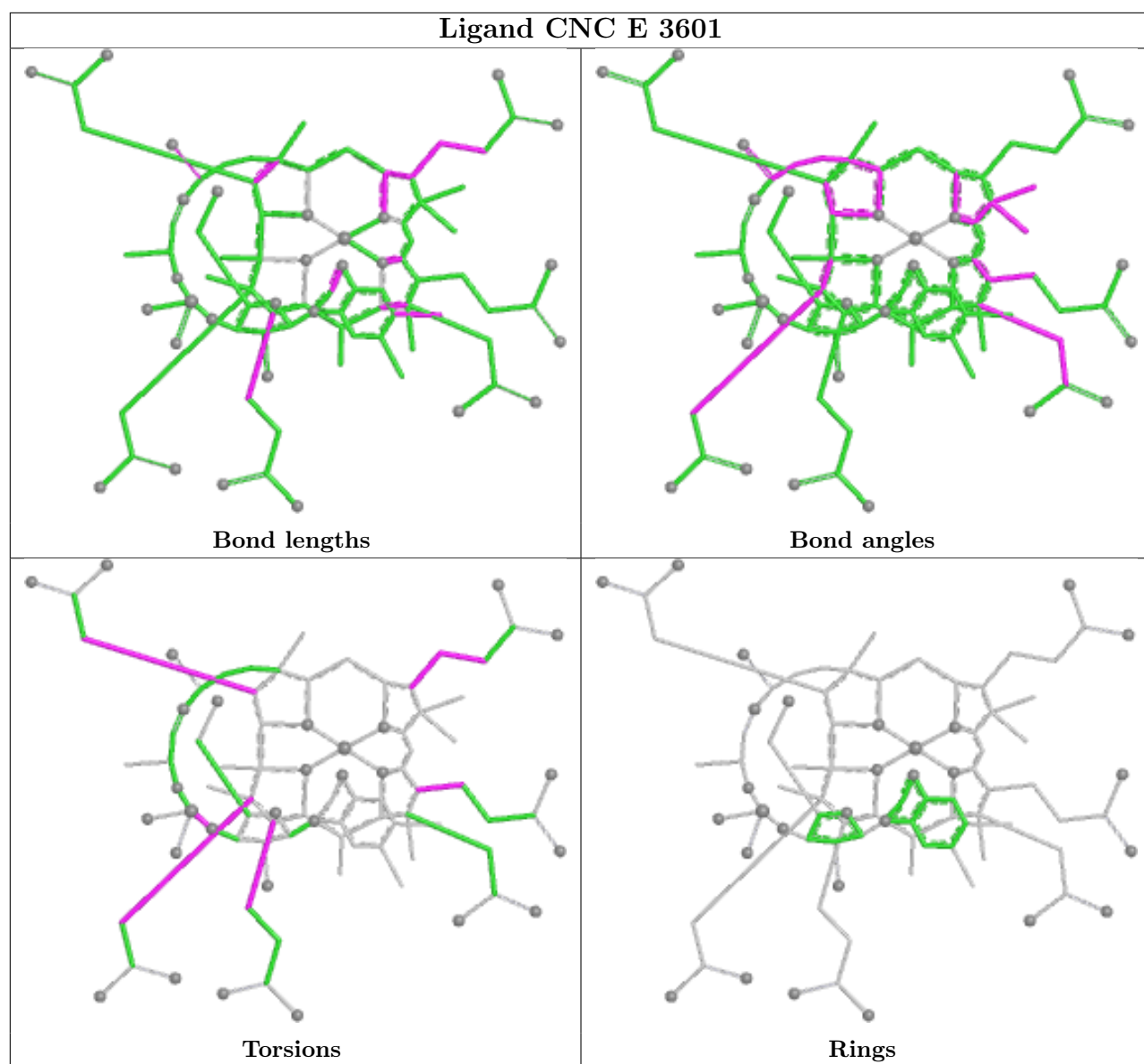
2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	2601	CNC	4	0
7	E	3601	CNC	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 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 CNC B 2601





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	551/554 (99%)	-0.06	10 (1%) 67 68	11, 18, 30, 66	2 (0%)
1	L	551/554 (99%)	0.88	116 (21%) 2 2	14, 23, 65, 80	1 (0%)
2	B	178/224 (79%)	0.81	21 (11%) 9 7	17, 29, 48, 54	0
2	E	176/224 (78%)	2.30	109 (61%) 0 0	22, 50, 98, 111	0
3	G	137/173 (79%)	0.37	9 (6%) 24 23	15, 23, 38, 47	3 (2%)
3	M	137/173 (79%)	1.40	31 (22%) 2 1	17, 29, 69, 82	1 (0%)
All	All	1730/1902 (90%)	0.72	296 (17%) 4 3	11, 23, 65, 111	7 (0%)

All (296) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	M	56	ALA	8.6
1	L	478	ALA	7.5
2	E	51	VAL	7.2
3	M	57	THR	6.4
1	L	482	PHE	6.0
3	M	55	THR	5.8
3	M	60	THR	5.8
1	L	436	VAL	5.8
2	E	127	GLY	5.5
1	L	429	PRO	5.4
1	L	459	PHE	5.4
1	L	481	GLY	5.3
1	L	476	ALA	5.3
1	L	454	VAL	5.3
1	L	431	ILE	5.3
1	L	410	ALA	5.3
1	L	438	ALA	5.2
1	L	175	VAL	5.1
2	E	49	THR	5.0

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Mol	Chain	Res	Type	RSRZ
2	E	128	ILE	5.0
1	L	423	PHE	5.0
1	L	550	PRO	5.0
2	E	220	LEU	4.9
3	M	66	LEU	4.9
1	L	457	ILE	4.8
1	L	480	GLY	4.8
3	M	58	ASN	4.7
1	L	421	ALA	4.6
1	L	422	VAL	4.6
1	L	477	LEU	4.6
1	L	489	MET	4.6
1	L	483	THR	4.6
2	E	92	ILE	4.5
2	E	47	PHE	4.5
2	E	212	VAL	4.5
1	L	176	ALA	4.5
1	L	181	PHE	4.4
1	L	149	ASP	4.4
1	L	439	ALA	4.4
1	L	442	ALA	4.4
3	M	62	ASP	4.4
1	L	428	LEU	4.4
3	M	65	THR	4.4
1	L	424	ALA	4.4
2	E	54	ALA	4.4
1	L	430	PRO	4.3
1	L	473	VAL	4.3
1	L	449	PRO	4.3
1	L	490	LEU	4.3
2	E	95	ILE	4.3
1	L	464	ILE	4.3
3	M	73	LYS	4.2
2	E	48	LEU	4.2
3	M	61	LEU	4.2
2	E	63	VAL	4.2
1	L	453	ILE	4.2
3	M	76	ALA	4.1
3	M	59	LYS	4.0
2	E	65	ILE	4.0
1	L	474	VAL	4.0
1	L	425	GLY	4.0

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Mol	Chain	Res	Type	RSRZ
2	E	176	ALA	4.0
2	E	184	VAL	4.0
3	M	70	LEU	3.9
2	B	223	ALA	3.9
1	L	427	GLY	3.9
1	L	487	GLN	3.9
1	L	174	ALA	3.8
3	M	68	ASN	3.8
2	E	131	GLY	3.8
1	L	415	ALA	3.8
1	L	460	ALA	3.8
1	L	433	ASP	3.8
1	L	183	ALA	3.7
2	E	172	ALA	3.7
3	M	72	ASN	3.7
1	A	548	LEU	3.7
1	L	548	LEU	3.7
1	L	441	TYR	3.7
1	L	434	GLU	3.7
3	M	74	VAL	3.7
3	G	58	ASN	3.6
2	E	217	PRO	3.6
2	E	105	ILE	3.6
2	E	64	ILE	3.5
2	E	164	THR	3.5
3	M	75	THR	3.5
2	E	52	GLY	3.5
1	L	417	ARG	3.5
1	L	451	ARG	3.5
1	L	485	VAL	3.5
2	E	91	VAL	3.5
2	E	138	THR	3.4
2	E	183	PRO	3.4
1	L	551	ASN	3.4
2	B	222	VAL	3.4
2	E	222	VAL	3.4
2	E	58	THR	3.4
3	M	69	VAL	3.4
3	M	78	ASP	3.4
1	L	419	LEU	3.4
2	B	46	GLY	3.4
2	E	173	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
2	E	50	GLU	3.3
1	L	488	ASP	3.3
2	E	208	THR	3.3
3	M	54	LYS	3.3
2	E	66	ALA	3.3
1	L	455	GLU	3.3
2	E	107	CYS	3.3
2	E	88	LEU	3.3
2	E	140	ILE	3.2
2	E	151	LEU	3.2
1	L	432	THR	3.2
1	L	450	GLU	3.2
2	E	57	GLY	3.2
2	E	169	GLY	3.2
1	L	465	ASN	3.2
1	L	409	ILE	3.1
2	E	171	ASN	3.1
2	E	67	VAL	3.1
2	E	68	GLY	3.1
3	M	63	ASP	3.1
1	L	491	ASN	3.1
2	E	125	GLY	3.1
2	E	182	GLN	3.1
1	L	547	ALA	3.1
2	E	181	PRO	3.1
2	E	175	TYR	3.1
1	L	152	VAL	3.1
1	L	173	VAL	3.1
2	E	170	LYS	3.1
2	E	99	GLY	3.1
1	L	178	TYR	3.0
1	L	192	VAL	3.0
1	L	452	ASN	3.0
1	L	172	THR	3.0
2	E	185	PRO	3.0
1	L	195	PRO	3.0
2	E	83	PRO	2.9
1	L	435	GLU	2.9
2	E	124	SER	2.9
2	E	118	VAL	2.9
2	E	165	TYR	2.9
2	E	102	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
2	E	87	ILE	2.9
1	L	471	LEU	2.9
1	L	150	ASN	2.9
2	E	141	HIS	2.9
1	L	461	GLN	2.9
2	E	221	ARG	2.8
1	A	551	ASN	2.8
2	B	164	THR	2.8
2	E	60	GLN	2.8
2	B	183	PRO	2.8
2	E	215	LYS	2.8
1	L	484	ASP	2.8
1	L	549	ASP	2.8
1	L	486	ALA	2.8
3	G	56	ALA	2.8
3	M	64	PHE	2.8
1	A	177	ARG	2.8
2	B	60	GLN	2.8
2	E	89	ARG	2.8
2	E	73	LEU	2.8
2	E	163	GLU	2.8
1	L	411	ILE	2.8
2	E	100	ILE	2.8
1	A	550	PRO	2.8
2	B	184	VAL	2.8
2	E	70	ALA	2.7
2	E	96	GLU	2.7
2	E	76	THR	2.7
1	L	456	ASP	2.7
1	L	151	PRO	2.7
2	B	186	THR	2.7
2	E	180	SER	2.7
1	L	413	ASN	2.7
1	L	206	ALA	2.7
2	E	61	ASP	2.7
2	E	218	GLN	2.7
2	E	145	LEU	2.7
1	L	470	GLY	2.6
2	E	77	VAL	2.6
1	L	447	ASP	2.6
1	L	462	GLU	2.6
2	B	163	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	L	463	ILE	2.6
2	B	221	ARG	2.6
2	E	56	GLN	2.6
2	E	59	GLN	2.6
2	B	179	GLU	2.6
2	B	102	ALA	2.6
3	G	57	THR	2.6
2	E	108	PHE	2.6
1	A	176	ALA	2.6
2	E	104	VAL	2.6
2	E	86	SER	2.6
3	G	37	SER	2.6
2	E	98	GLU	2.5
2	E	168	ILE	2.5
1	L	408	VAL	2.5
3	M	117	ASP	2.5
1	L	475	LYS	2.5
1	L	187	LEU	2.5
3	M	77	GLN	2.5
2	E	210	TYR	2.5
1	L	440	THR	2.5
2	E	161	THR	2.5
2	E	162	LEU	2.4
1	A	450	GLU	2.4
2	E	179	GLU	2.4
3	G	51	GLU	2.4
1	L	492	ILE	2.4
1	L	179	ALA	2.4
3	M	40	VAL	2.4
2	E	55	ARG	2.4
3	M	124	ASN	2.4
1	L	416	ALA	2.4
2	B	178	ARG	2.4
1	L	215	GLY	2.4
1	L	426	MET	2.4
3	M	79	MET	2.4
1	L	184	ILE	2.4
1	L	468	ARG	2.4
2	E	82	ILE	2.4
2	B	95	ILE	2.3
2	E	93	ALA	2.3
1	L	146	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	L	180	PRO	2.3
2	E	84	HIS	2.3
2	E	211	VAL	2.3
3	G	145	SER	2.3
3	M	71	SER	2.3
1	A	549	ASP	2.3
2	E	103	ARG	2.3
2	E	62	GLU	2.3
2	E	123	LEU	2.3
1	L	418	ALA	2.3
1	A	1	MET	2.3
2	E	116	VAL	2.3
2	B	49	THR	2.3
1	L	466	LYS	2.3
1	L	545	PRO	2.3
2	E	178	ARG	2.3
3	G	67	GLU	2.3
1	L	211	LEU	2.3
1	L	214	LEU	2.3
2	B	180	SER	2.2
2	E	142	GLN	2.2
2	E	139	VAL	2.2
2	E	177	LYS	2.2
3	G	59	LYS	2.2
1	L	177	ARG	2.2
2	E	122	ARG	2.2
3	G	60	THR	2.2
1	A	511	ASP	2.2
1	L	163	TRP	2.2
2	E	71	PHE	2.2
1	L	544	ILE	2.2
1	L	446	LYS	2.2
2	E	85	LYS	2.2
1	A	25	GLU	2.2
2	E	117	ALA	2.2
2	E	157	ALA	2.2
3	M	52	TRP	2.2
1	L	412	ARG	2.2
1	L	448	MET	2.2
2	E	143	GLN	2.2
2	E	167	GLN	2.2
2	B	161	THR	2.2

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Mol	Chain	Res	Type	RSRZ
3	M	82	THR	2.2
2	E	126	SER	2.2
1	L	495	ALA	2.2
1	L	404	ARG	2.2
1	L	458	LYS	2.1
2	B	181	PRO	2.1
2	E	174	ARG	2.1
2	E	187	LEU	2.1
2	E	53	GLU	2.1
2	E	112	ASP	2.1
2	E	94	GLY	2.1
1	L	406	GLU	2.1
1	L	437	GLU	2.1
1	L	467	ASN	2.1
1	L	420	GLN	2.1
2	B	47	PHE	2.1
2	E	129	SER	2.1
3	M	53	VAL	2.1
1	L	185	ALA	2.1
2	E	219	GLU	2.0
1	L	469	ASN	2.0
2	B	182	GLN	2.0
1	L	218	CYS	2.0
2	E	155	PRO	2.0
2	B	174	ARG	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 oligosaccharides in this entry.

6.4 Ligands ⓘ

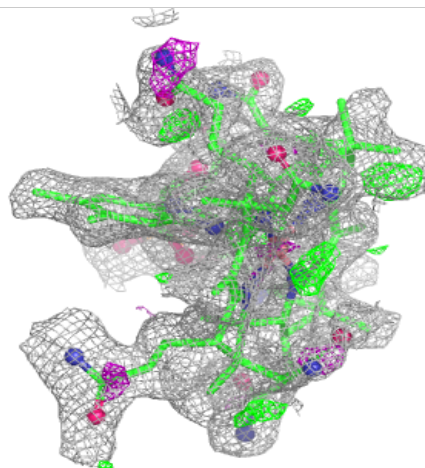
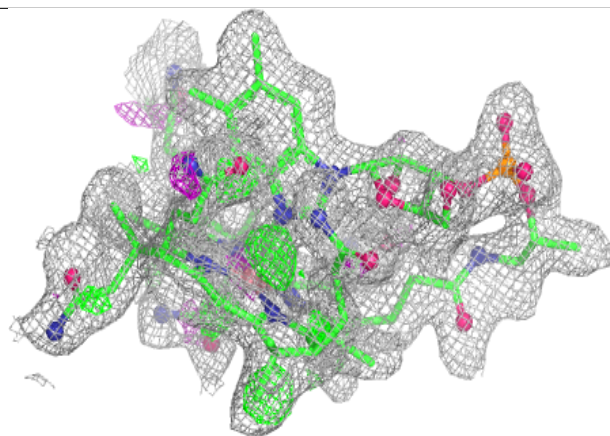
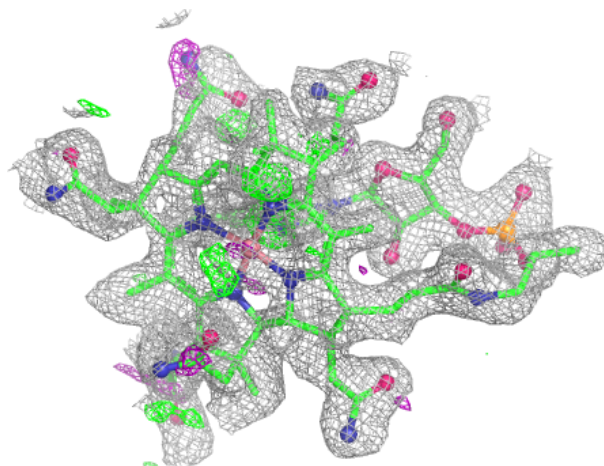
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NH4	L	3605	1/1	0.88	0.14	30,30,30,30	0
7	CNC	E	3601	91/93	0.93	0.10	22,27,35,40	0
7	CNC	B	2601	91/93	0.96	0.08	14,17,26,32	0
6	PGO	L	3602	5/5	0.96	0.08	22,23,24,24	0
6	PGO	A	2602	5/5	0.97	0.07	14,15,16,16	0
4	NH4	L	3604	1/1	0.97	0.06	16,16,16,16	0
4	NH4	A	2605	1/1	0.98	0.04	19,19,19,19	0
5	K	L	3603	1/1	0.98	0.03	20,20,20,20	0
5	K	A	2603	1/1	1.00	0.03	15,15,15,15	0
4	NH4	A	2604	1/1	1.00	0.05	14,14,14,14	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.

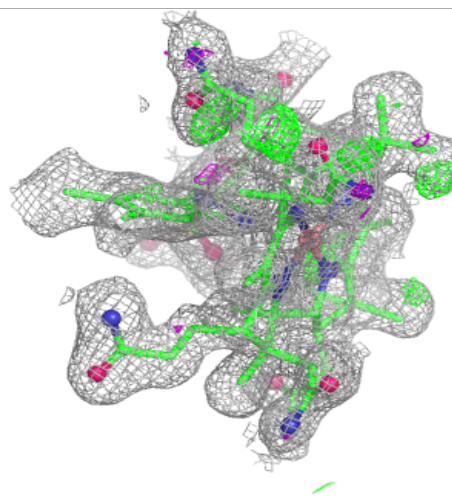
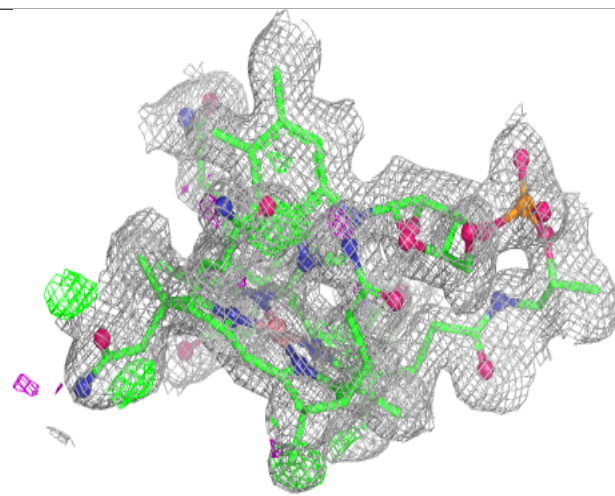
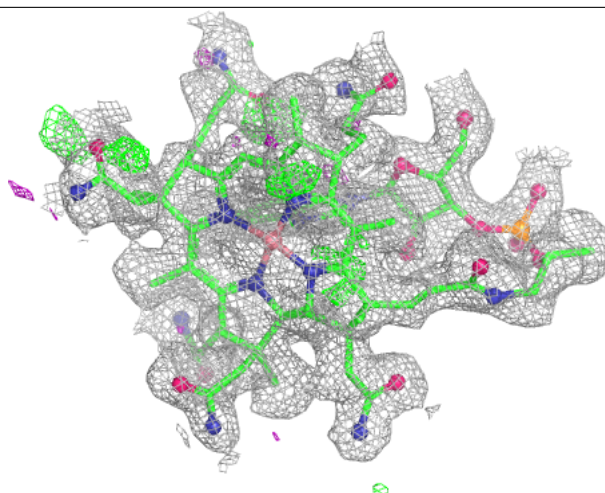
Electron density around CNC E 3601:

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 CNC B 2601:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.