



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 17, 2023 – 12:17 PM EDT

PDB ID : 1UC4
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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

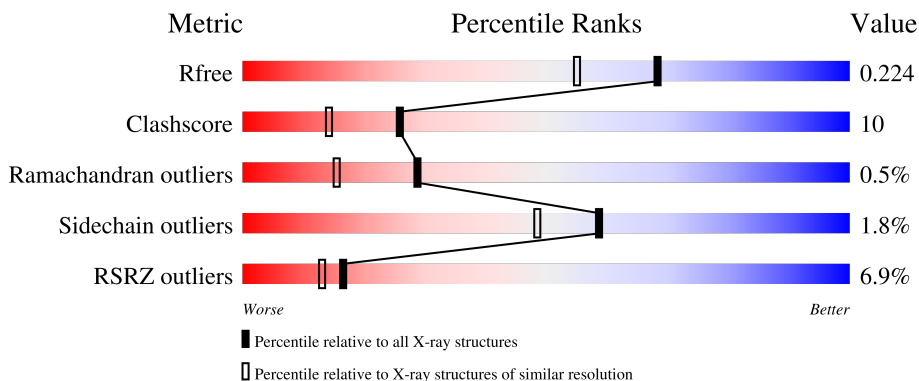
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (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	 86% 12% ..
1	L	554	 8% 79% 20% ..
2	B	224	 62% 16% • 21%
2	E	224	 25% 46% 30% • 21%
3	G	173	 72% 7% • 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 [i](#)

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
			Total	C	N	O	S			
1	A	551	4201	2620	727	825	29	0	0	0
1	L	551	4201	2620	727	825	29	0	0	0

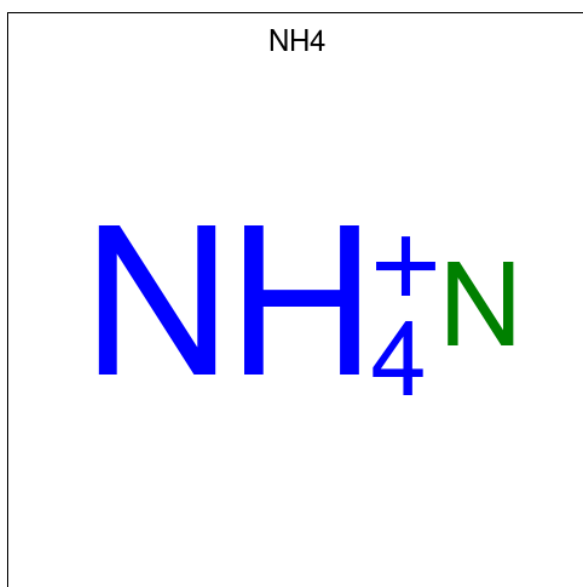
- Molecule 2 is a protein called diol dehydrase beta subunit.

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

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

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

- Molecule 4 is AMMONIUM ION (three-letter code: NH4) (formula: H₄N).

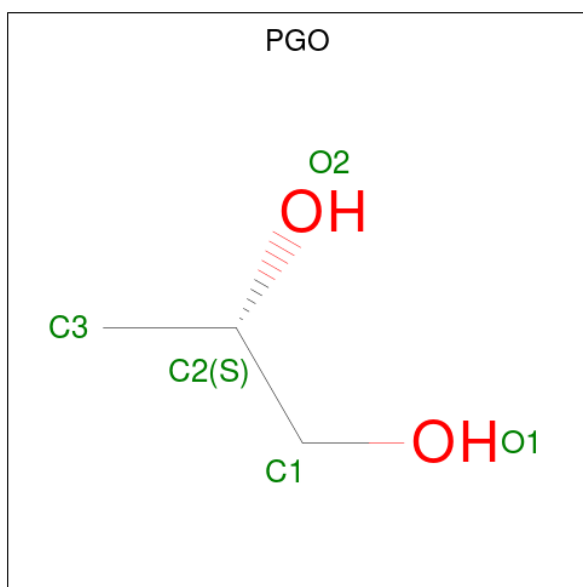


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total N 1 1	0	0
4	A	1	Total N 1 1	0	0
4	L	1	Total N 1 1	0	0
4	L	1	Total N 1 1	0	0

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

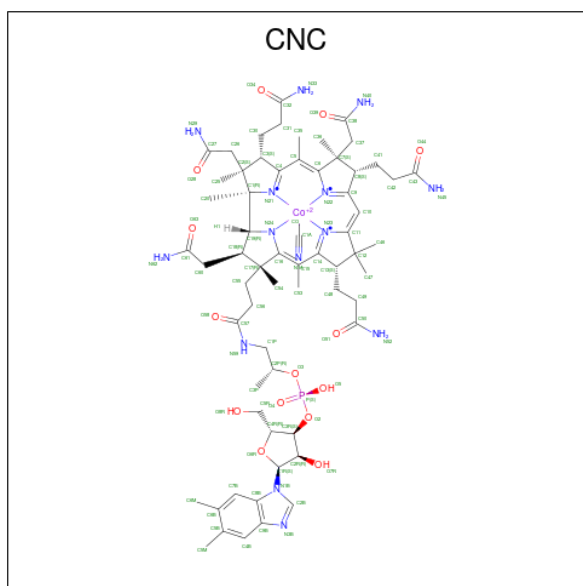
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total K 1 1	0	0
5	L	1	Total K 1 1	0	0

- Molecule 6 is S-1,2-PROPANEDIOL (three-letter code: 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 CYANOCOBALAMIN (three-letter code: CNC) (formula: $C_{63}H_{89}CoN_{14}O_{14}P$).



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

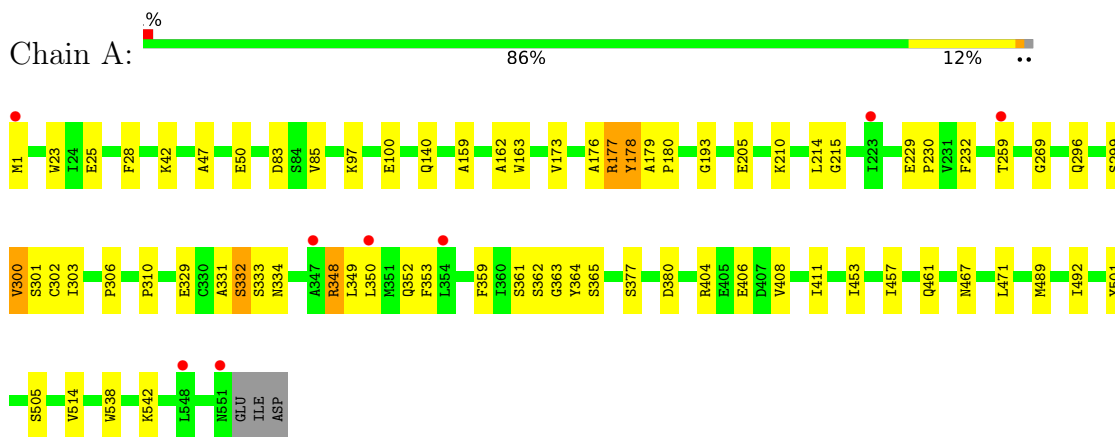
- Molecule 8 is water.

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

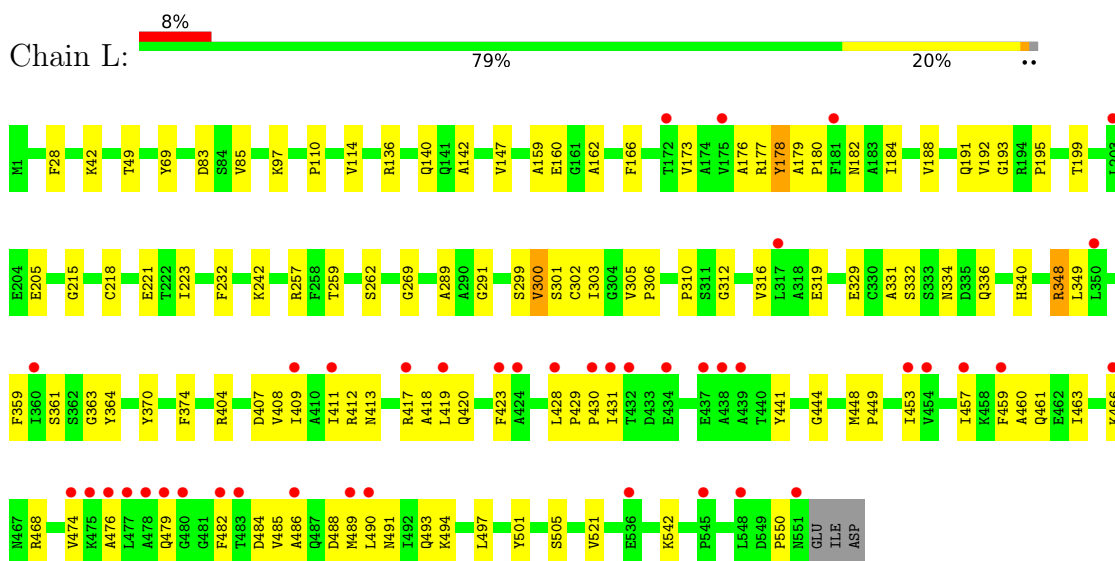
3 Residue-property plots [i](#)

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.

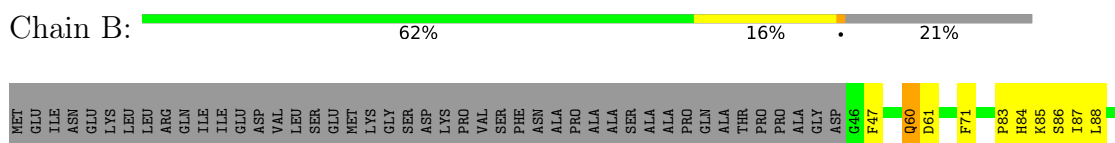
- Molecule 1: diol dehydrase alpha subunit



- Molecule 1: diol dehydrase alpha subunit



- Molecule 2: diol dehydrase beta subunit



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 36.91 – 1.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (36.92-1.80) 82.8 (36.91-1.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 1.81Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.195 , 0.230 0.188 , 0.224	Depositor DCC
R_{free} test set	14380 reflections (9.96%)	wwPDB-VP
Wilson B-factor (Å ²)	18.8	Xtrriage
Anisotropy	0.893	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 63.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: K, CNC, NH4, 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	0.33	0/4273	0.61	2/5787 (0.0%)
1	L	0.30	0/4273	0.58	2/5787 (0.0%)
2	B	0.28	0/1380	0.58	0/1868
2	E	0.26	0/1371	0.52	0/1856
3	G	0.29	0/1108	0.53	0/1497
3	M	0.28	0/1108	0.50	0/1497
All	All	0.30	0/13513	0.58	4/18292 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	269	GLY	N-CA-C	5.73	127.43	113.10
1	L	332	SER	N-CA-C	5.32	125.36	111.00
1	A	332	SER	N-CA-C	5.15	124.90	111.00
1	L	269	GLY	N-CA-C	5.01	125.62	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4201	0	4140	49	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	4201	0	4140	90	0
2	B	1358	0	1408	28	0
2	E	1349	0	1400	66	0
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	6	0
8	M	127	0	0	1	0
All	All	14904	0	13476	283	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 10.

All (283) 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
2:E:174:ARG:HG2	2:E:181:PRO:HB3	1.50	0.91
2:E:190:GLN:H	2:E:190:GLN:HE21	1.21	0.88
2:B:121:ASN:C	2:B:121:ASN:HD22	1.79	0.85
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
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:G:60:THR:HG22	3:G:63:ASP:CG	2.11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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	0.61
2:E:121:ASN:HD22	2:E:121:ASN:C	2.03	0.61
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:63:VAL:HG23	2:E:100:ILE:HG21	1.85	0.58
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
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:L:493:GLN:HG2	3:M:79:MET:CE	2.36	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
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:42:LYS:HD3	1:A:50:GLU:CD	2.28	0.54
1:A:140:GLN:OE1	1:A:361:SER:HB2	2.08	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
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
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:A:25:GLU:CD	1:A:25:GLU:H	2.12	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
1:L:370:TYR:OH	1:L:444:GLY:HA3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:E:114:ALA:HB2	7:E:3601:CNC:HM62	1.91	0.51
1:L:160:GLU:HG3	1:L:408:VAL:HG13	1.93	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:121:ASN:C	2:E:121:ASN:ND2	2.65	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
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
2:B:191:MET:C	2:B:194:PRO:HD2	2.32	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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:51:GLU:CD	3:G:51:GLU:H	2.17	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
3:M:57:THR:HG1	3:M:59:LYS:HE2	1.80	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: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
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
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
2:E:191:MET:C	2:E:194:PRO:HD2	2.36	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
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
1:A:404:ARG:HH21	1:A:406:GLU:CD	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:L:493:GLN:HG2	3:M:79:MET:HE1	1.99	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
2:E:150:ASN:HD22	2:E:152:GLU:C	2.20	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
2:E:72:GLY:C	2:E:73:LEU:HD12	2.38	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:428:LEU:O	1:L:429:PRO:C	2.55	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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:136:ARG:HD2	1:L:521:VAL:O	2.19	0.42
3:M:55:THR:C	3:M:57:THR:H	2.23	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:173:VAL:HG12	1:L:182:ASN:CG	2.40	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
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
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
1:L:493:GLN:HG2	3:M:79:MET:HE2	2.03	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:191:GLN:OE1	1:L:195:PRO:HA	2.20	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:B:61:ASP:CG	2:B:101:LYS:HE2	2.42	0.40
2:E:100:ILE:HD11	2:E:177:LYS:CG	2.51	0.40
1:L:178:TYR:HE2	1:L:453:ILE:HG23	1.87	0.40
1:L:340:HIS:CD2	2:E:195:LYS:HZ2	2.38	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 [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	549/554 (99%)	523 (95%)	24 (4%)	2 (0%)	34 21
1	L	549/554 (99%)	522 (95%)	25 (5%)	2 (0%)	34 21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	176/224 (79%)	171 (97%)	5 (3%)	0	100	100
2	E	174/224 (78%)	161 (92%)	11 (6%)	2 (1%)	14	4
3	G	135/173 (78%)	133 (98%)	2 (2%)	0	100	100
3	M	135/173 (78%)	125 (93%)	7 (5%)	3 (2%)	6	1
All	All	1718/1902 (90%)	1635 (95%)	74 (4%)	9 (0%)	29	15

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 [i](#)

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%)	443 (98%)	7 (2%)	62	54
1	L	450/453 (99%)	444 (99%)	6 (1%)	69	62
2	B	146/183 (80%)	142 (97%)	4 (3%)	44	31
2	E	146/183 (80%)	142 (97%)	4 (3%)	44	31
3	G	116/141 (82%)	115 (99%)	1 (1%)	78	75
3	M	116/141 (82%)	113 (97%)	3 (3%)	46	32
All	All	1424/1554 (92%)	1399 (98%)	25 (2%)	59	48

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	PHE
1	A	177	ARG
1	A	178	TYR
1	A	232	PHE
1	A	348	ARG
1	A	364	TYR
1	A	501	TYR
2	B	60	GLN
2	B	101	LYS
2	B	121	ASN
2	B	150	ASN
3	G	51	GLU
1	L	28	PHE
1	L	178	TYR
1	L	232	PHE
1	L	348	ARG
1	L	364	TYR
1	L	501	TYR
2	E	47	PHE
2	E	59	GLN
2	E	121	ASN
2	E	190	GLN
3	M	39	ARG
3	M	59	LYS
3	M	100	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) 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	543	ASN
2	B	75	GLN
2	B	121	ASN
2	B	142	GLN
2	B	204	HIS
3	G	58	ASN
1	L	45	ASN
1	L	74	ASN
1	L	334	ASN

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Mol	Chain	Res	Type
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	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

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 monosaccharides 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
6	PGO	L	3602	5	3,4,4	0.16	0	1,4,4	0.13	0
6	PGO	A	2602	5	3,4,4	0.22	0	1,4,4	0.06	0
7	CNC	B	2601	-	89,101,103	1.33	10 (11%)	139,166,171	1.08	10 (7%)
7	CNC	E	3601	-	89,101,103	1.34	8 (8%)	139,166,171	1.16	12 (8%)

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	B	2601	-	1/1/36/38	7/52/223/235	0/3/11/11
6	PGO	A	2602	5	-	0/2/2/2	-
7	CNC	E	3601	-	1/1/36/38	10/52/223/235	0/3/11/11
6	PGO	L	3602	5	-	0/2/2/2	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	E	3601	CNC	C5M-C5B	-5.52	1.40	1.51
7	B	2601	CNC	C5M-C5B	-5.36	1.40	1.51
7	E	3601	CNC	C14-N23	4.15	1.41	1.30
7	B	2601	CNC	C14-N23	3.83	1.40	1.30
7	B	2601	CNC	O58-C57	3.04	1.29	1.23
7	E	3601	CNC	O58-C57	2.90	1.29	1.23
7	E	3601	CNC	C13-C14	2.86	1.59	1.51
7	B	2601	CNC	C48-C49	2.72	1.61	1.52
7	B	2601	CNC	C9-N22	2.46	1.36	1.30
7	B	2601	CNC	C13-C14	2.41	1.58	1.51
7	E	3601	CNC	C48-C49	2.41	1.60	1.52
7	B	2601	CNC	C30-C3	2.36	1.60	1.54
7	E	3601	CNC	C9-N22	2.35	1.36	1.30
7	B	2601	CNC	C48-C13	2.32	1.59	1.54
7	E	3601	CNC	C30-C3	2.21	1.59	1.54
7	E	3601	CNC	C7-C6	2.21	1.59	1.54
7	B	2601	CNC	C7-C6	2.04	1.59	1.54
7	B	2601	CNC	C41-C8	2.01	1.59	1.54

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	2601	CNC	C41-C8-C9	-3.53	104.98	111.19
7	E	3601	CNC	C26-C2-C1	3.41	115.31	110.01
7	E	3601	CNC	C41-C8-C9	-3.30	105.38	111.19
7	E	3601	CNC	C56-C55-C17	3.15	121.59	115.52
7	B	2601	CNC	C18-C19-N24	3.04	106.71	101.88
7	B	2601	CNC	C56-C55-C17	2.93	121.16	115.52
7	E	3601	CNC	C11-N23-C14	2.85	107.39	106.31
7	E	3601	CNC	C7-C37-C38	2.81	122.72	114.25
7	E	3601	CNC	C18-C19-N24	2.79	106.31	101.88
7	B	2601	CNC	C55-C17-C16	2.71	122.06	116.24
7	B	2601	CNC	C11-N23-C14	2.70	107.33	106.31
7	B	2601	CNC	C7-C37-C38	2.66	122.26	114.25
7	E	3601	CNC	C47-C12-C46	-2.52	105.09	109.35
7	E	3601	CNC	C19-N24-C16	-2.51	107.91	111.96
7	B	2601	CNC	C4B-C9B-C8B	-2.42	118.63	121.10
7	E	3601	CNC	C55-C17-C16	2.40	121.41	116.24
7	E	3601	CNC	C4B-C9B-C8B	-2.38	118.66	121.10
7	B	2601	CNC	C47-C12-C46	-2.37	105.35	109.35
7	E	3601	CNC	O58-C57-C56	-2.35	117.72	122.02
7	B	2601	CNC	O58-C57-C56	-2.33	117.75	122.02
7	B	2601	CNC	C19-N24-C16	-2.23	108.35	111.96
7	E	3601	CNC	C12-C11-N23	2.03	113.68	111.48

All (2) chirality outliers are listed below:

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

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	2601	CNC	C12-C13-C48-C49
7	E	3601	CNC	C4-C3-C30-C31
7	E	3601	CNC	C2-C3-C30-C31
7	B	2601	CNC	C2-C26-C27-N29
7	B	2601	CNC	C2-C26-C27-O28
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

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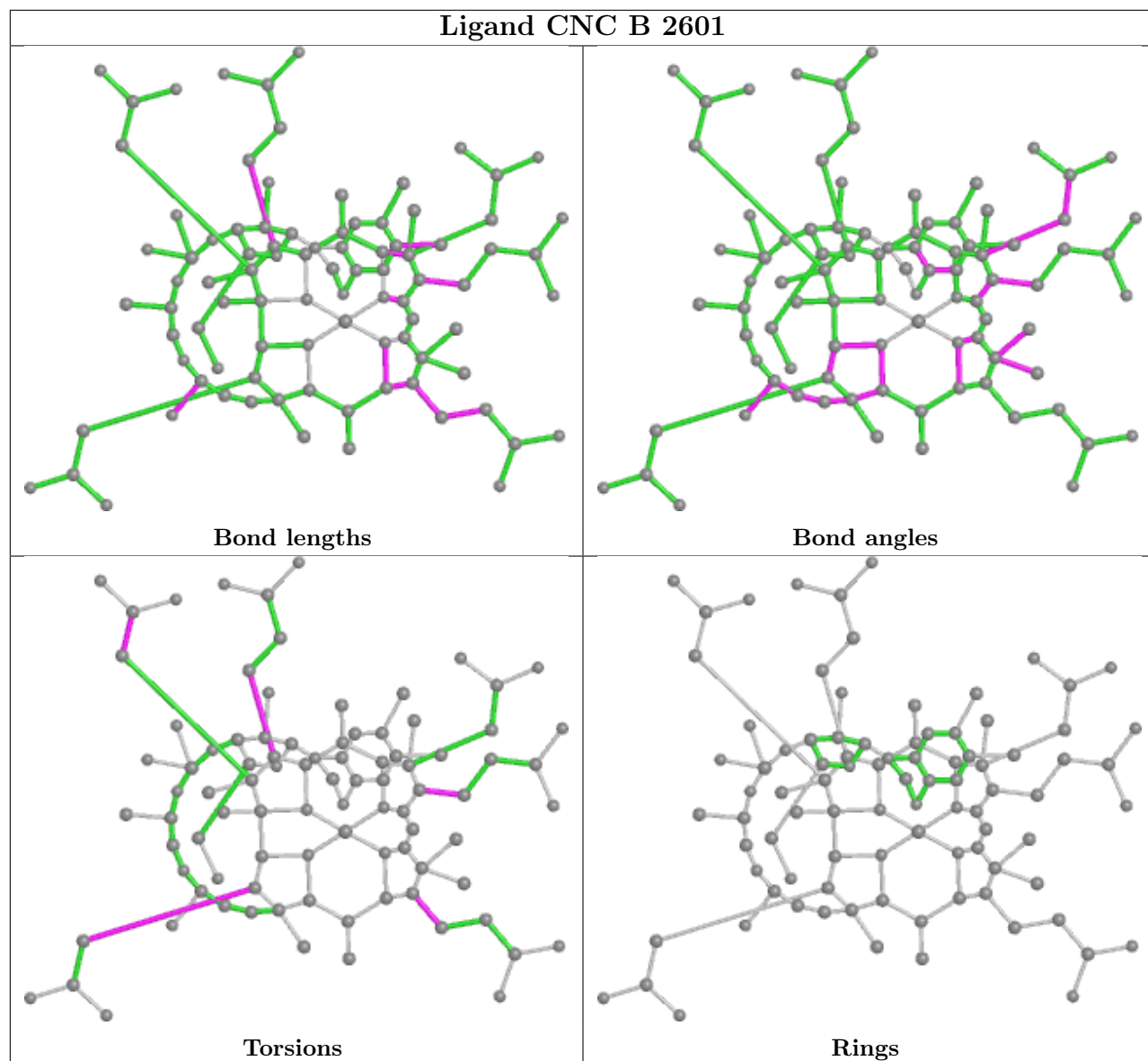
Mol	Chain	Res	Type	Atoms
7	E	3601	CNC	C19-C18-C60-C61
7	B	2601	CNC	C42-C41-C8-C9
7	E	3601	CNC	C12-C13-C48-C49
7	B	2601	CNC	C2-C3-C30-C31
7	E	3601	CNC	C3-C2-C26-C27
7	B	2601	CNC	C17-C18-C60-C61

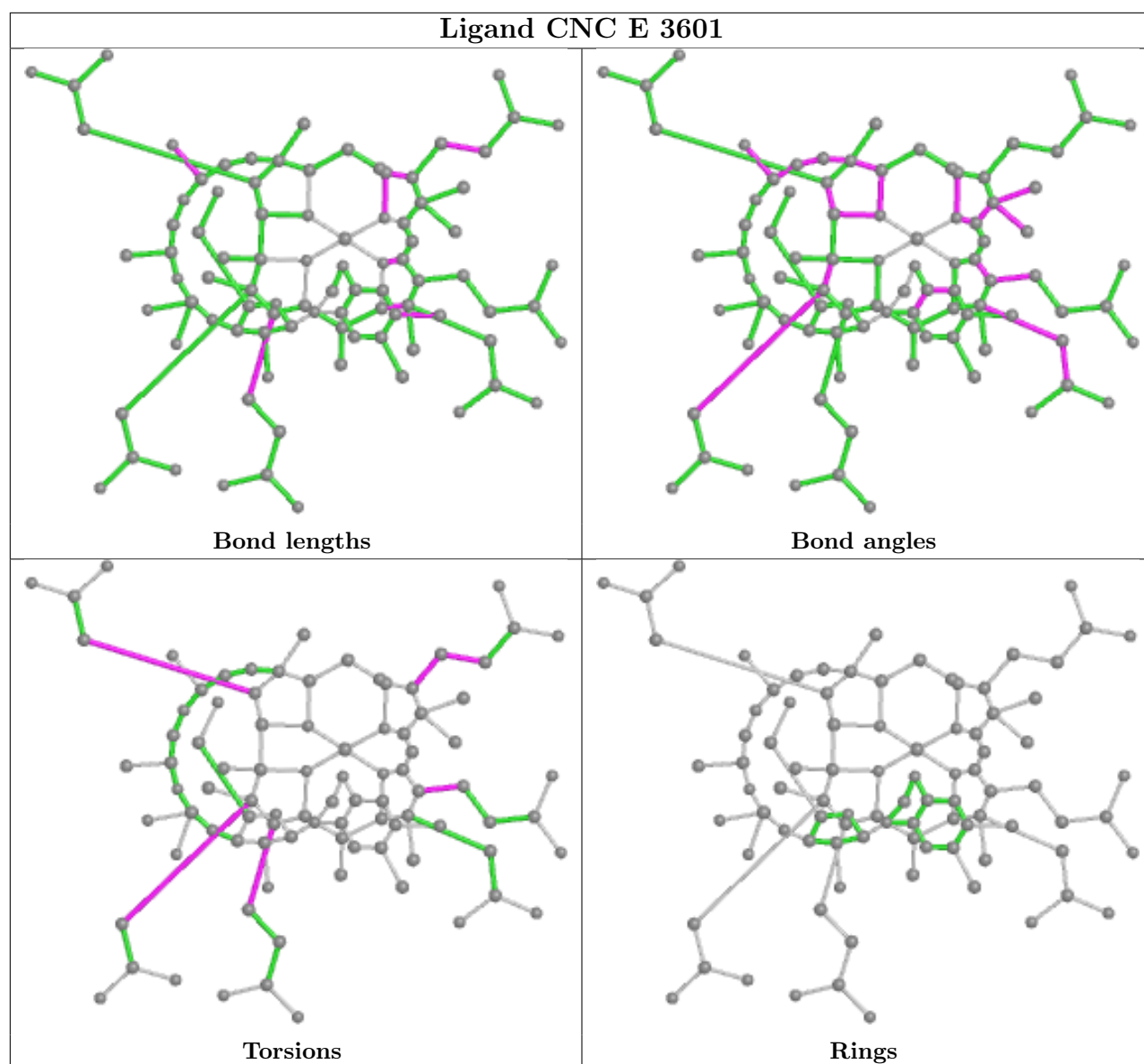
There are no ring outliers.

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.





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%)	-0.12	8 (1%) 73 70	13, 18, 30, 66	2 (0%)
1	L	551/554 (99%)	0.37	42 (7%) 13 10	14, 23, 65, 80	1 (0%)
2	B	178/224 (79%)	-0.07	0 100 100	17, 29, 48, 54	0
2	E	176/224 (78%)	1.57	56 (31%) 0 0	22, 50, 98, 111	0
3	G	137/173 (79%)	-0.17	0 100 100	15, 23, 38, 47	3 (2%)
3	M	137/173 (79%)	0.50	14 (10%) 6 5	22, 29, 69, 82	1 (0%)
All	All	1730/1902 (90%)	0.26	120 (6%) 16 13	13, 24, 65, 111	7 (0%)

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	51	VAL	8.3
2	E	47	PHE	7.9
3	M	57	THR	6.7
2	E	54	ALA	6.7
2	E	99	GLY	6.5
3	M	66	LEU	5.9
1	L	482	PHE	5.7
3	M	55	THR	5.6
2	E	60	GLN	5.5
1	L	454	VAL	5.5
2	E	95	ILE	5.3
3	M	56	ALA	5.2
2	E	100	ILE	5.1
2	E	63	VAL	4.9
2	E	93	ALA	4.7
2	E	61	ASP	4.5
1	L	439	ALA	4.4
2	E	58	THR	4.3
2	E	102	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
3	M	58	ASN	4.3
2	E	222	VAL	4.3
2	E	173	ALA	4.3
1	A	259	THR	4.2
1	L	428	LEU	4.1
2	E	59	GLN	4.0
1	L	459	PHE	4.0
2	E	50	GLU	4.0
2	E	48	LEU	4.0
1	L	483	THR	3.9
2	E	97	GLU	3.9
1	L	453	ILE	3.7
1	L	431	ILE	3.7
2	E	178	ARG	3.7
2	E	170	LYS	3.7
2	E	128	ILE	3.6
3	M	59	LYS	3.6
2	E	179	GLU	3.5
1	L	551	ASN	3.4
2	E	174	ARG	3.4
1	L	434	GLU	3.4
3	M	62	ASP	3.4
2	E	220	LEU	3.4
2	E	98	GLU	3.3
2	E	218	GLN	3.3
1	A	350	LEU	3.3
1	L	490	LEU	3.3
2	E	172	ALA	3.3
1	L	181	PHE	3.2
2	E	105	ILE	3.2
2	E	177	LYS	3.2
1	L	175	VAL	3.2
2	E	101	LYS	3.1
2	E	91	VAL	3.1
2	E	49	THR	3.0
1	A	551	ASN	3.0
2	E	62	GLU	3.0
3	M	70	LEU	3.0
1	L	479	GLN	2.9
2	E	221	ARG	2.8
2	E	53	GLU	2.8
1	L	424	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
2	E	89	ARG	2.8
2	E	127	GLY	2.7
1	A	548	LEU	2.7
2	E	87	ILE	2.7
2	E	175	TYR	2.6
1	A	347	ALA	2.6
1	L	411	ILE	2.6
2	E	56	GLN	2.6
1	L	480	GLY	2.6
1	L	486	ALA	2.6
1	L	409	ILE	2.6
2	E	55	ARG	2.5
1	L	419	LEU	2.5
1	L	545	PRO	2.5
2	E	181	PRO	2.5
1	L	457	ILE	2.5
1	L	417	ARG	2.5
1	L	317	LEU	2.5
1	L	350	LEU	2.5
1	L	548	LEU	2.5
2	E	125	GLY	2.5
2	E	94	GLY	2.4
1	L	423	PHE	2.4
3	M	61	LEU	2.4
1	L	430	PRO	2.4
2	E	83	PRO	2.4
1	L	438	ALA	2.3
1	L	437	GLU	2.3
2	E	57	GLY	2.3
2	E	85	LYS	2.3
3	M	54	LYS	2.3
2	E	64	ILE	2.3
1	L	489	MET	2.3
1	A	223	ILE	2.3
2	E	176	ALA	2.3
1	L	466	LYS	2.2
1	L	474	VAL	2.2
1	L	172	THR	2.2
1	L	476	ALA	2.2
1	L	360	ILE	2.2
3	M	37	SER	2.2
1	L	478	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	1	MET	2.1
1	A	354	LEU	2.1
1	L	432	THR	2.1
2	E	86	SER	2.1
2	E	84	HIS	2.1
2	E	126	SER	2.1
2	E	163	GLU	2.1
2	E	92	ILE	2.1
2	E	166	ARG	2.1
1	L	203	LEU	2.1
1	L	477	LEU	2.1
1	L	536	GLU	2.0
3	M	60	THR	2.0
2	E	212	VAL	2.0
1	L	475	LYS	2.0
3	M	73	LYS	2.0
3	M	71	SER	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 monosaccharides 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.

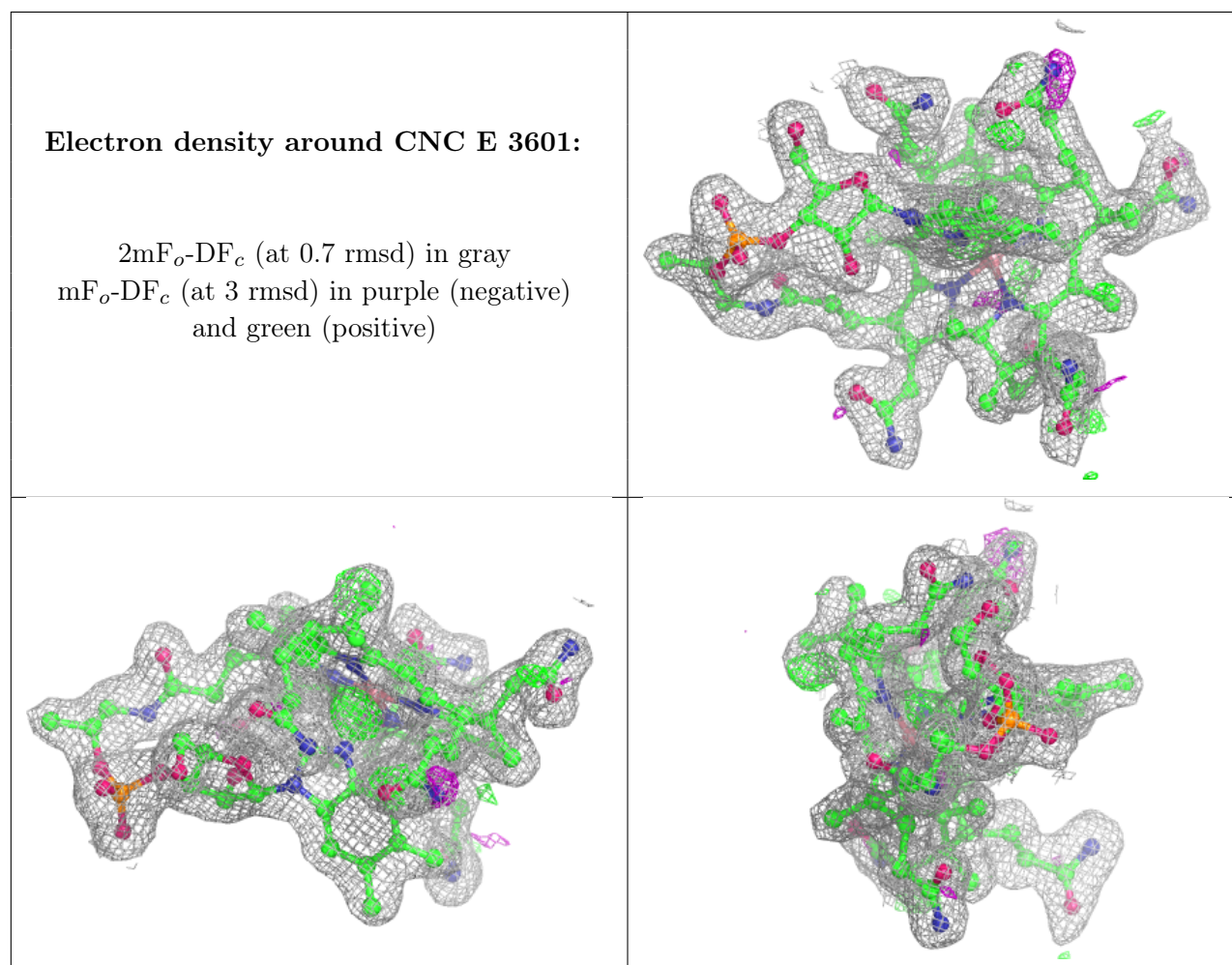
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	CNC	E	3601	91/93	0.94	0.15	22,27,35,40	0
6	PGO	L	3602	5/5	0.95	0.19	22,23,24,24	0
7	CNC	B	2601	91/93	0.96	0.13	14,17,26,32	0
4	NH4	L	3605	1/1	0.96	0.26	30,30,30,30	0
6	PGO	A	2602	5/5	0.97	0.24	14,15,16,16	0
4	NH4	L	3604	1/1	0.97	0.24	16,16,16,16	0

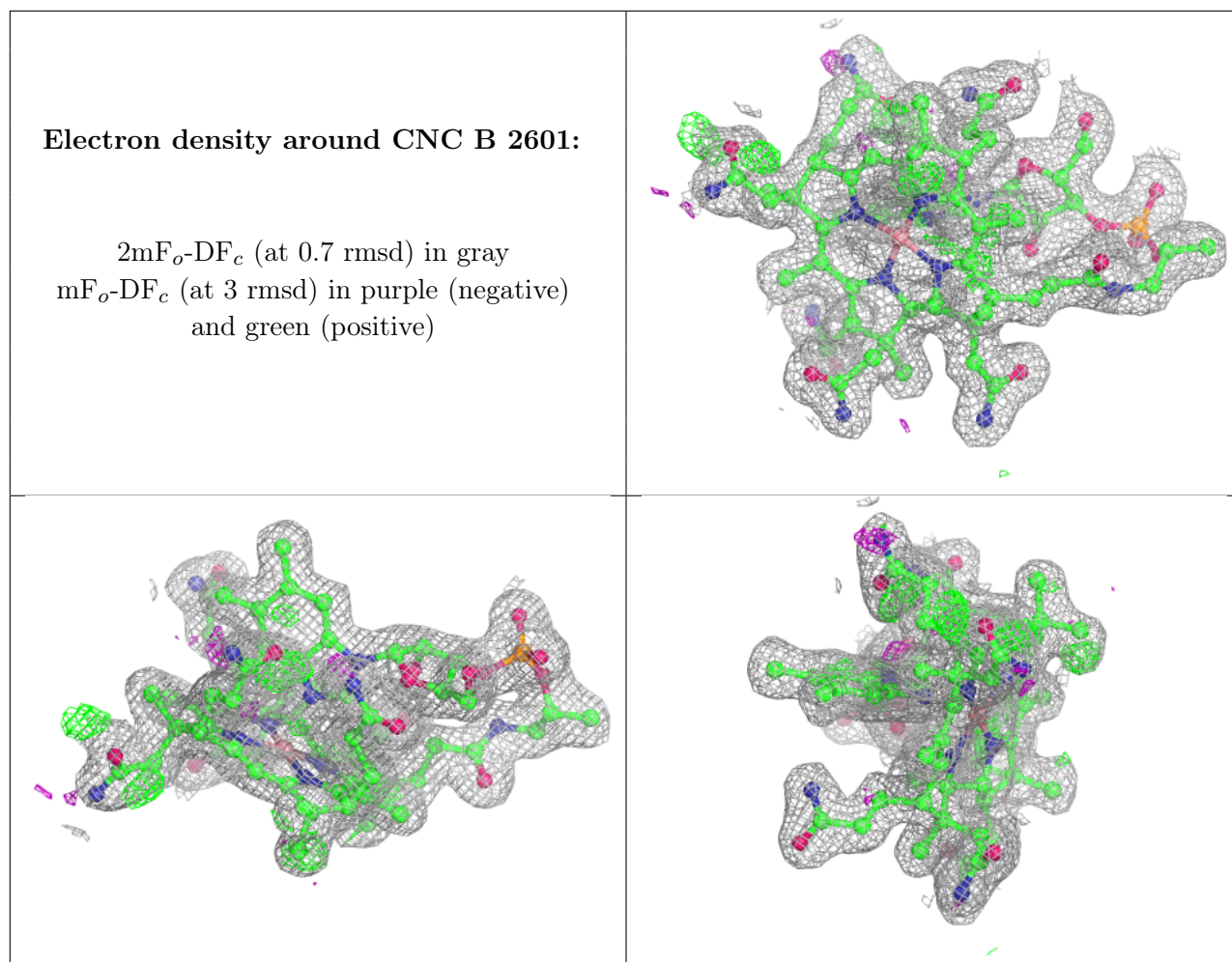
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NH4	A	2605	1/1	0.99	0.27	19,19,19,19	0
5	K	L	3603	1/1	0.99	0.10	20,20,20,20	0
4	NH4	A	2604	1/1	0.99	0.27	14,14,14,14	0
5	K	A	2603	1/1	1.00	0.14	15,15,15,15	0

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.





6.5 Other polymers [i](#)

There are no such residues in this entry.