



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2021 – 10:34 AM EDT

PDB ID : 1EGM  
Title : CRYSTAL STRUCTURE OF DIOL DEHYDRATASE-CYANOCOBALAMIN COMPLEX AT 100K.  
Authors : Masuda, J.; Shibata, N.; Toraya, T.; Morimoto, Y.; Yasuoka, N.  
Deposited on : 2000-02-15  
Resolution : 1.85 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.1  
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) : 2.23.1

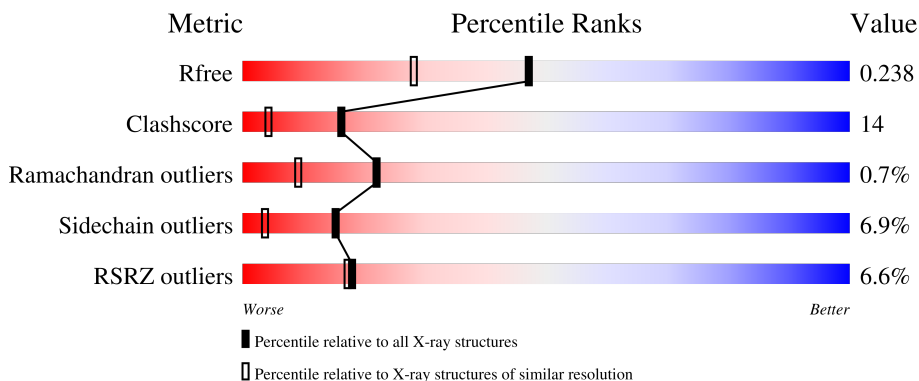
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	554	
1	L	554	
2	B	224	
2	E	224	
3	G	173	

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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
5	CNC	A	601	X	-	-	-
5	CNC	L	601	X	-	-	-

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 14737 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
			Total	C	N	O	S			
1	A	551	Total	C	N	O	S	0	2	0
			4209	2625	727	828	29			
1	L	551	Total	C	N	O	S	0	1	0
			4206	2623	727	827	29			

- Molecule 2 is a protein called PROPANEDIOL DEHYDRATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	178	Total	C	N	O	S	0	0	0
			1358	859	244	253	2			
2	E	177	Total	C	N	O	S	0	0	0
			1353	856	243	252	2			

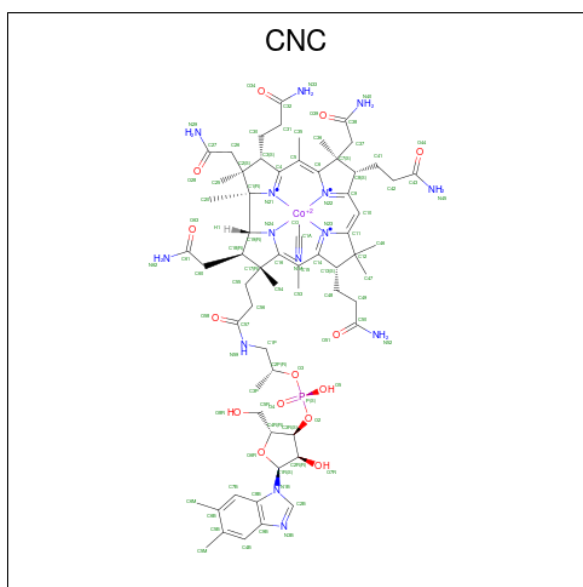
- Molecule 3 is a protein called PROPANEDIOL DEHYDRATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	G	137	Total	C	N	O	S	0	3	0
			1108	691	196	218	3			
3	M	137	Total	C	N	O	S	0	1	0
			1098	684	195	216	3			

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

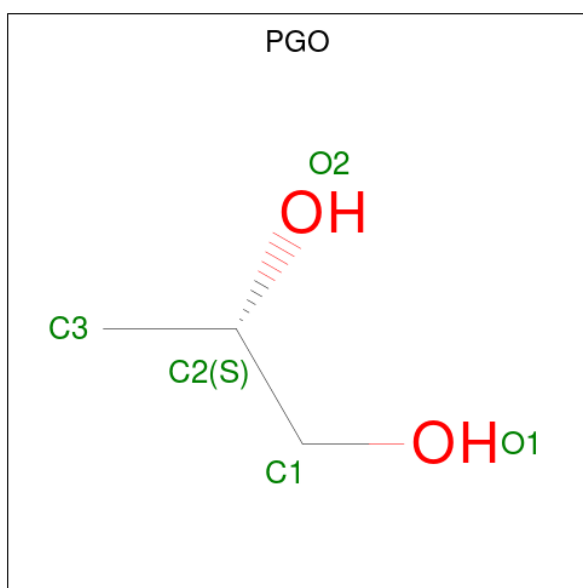
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total	K	0
			1	1	
4	L	1	Total	K	0
			1	1	

- Molecule 5 is CYANOCOBALAMIN (three-letter code: CNC) (formula: C<sub>63</sub>H<sub>89</sub>CoN<sub>14</sub>O<sub>14</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	Co	N	O			P
5	A	1	91	62	1	13	14	1	0	0
5	L	1	91	62	1	13	14	1	0	0

- Molecule 6 is S-1,2-PROPANEDIOL (three-letter code: PGO) (formula:  $C_3H_8O_2$ ).



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

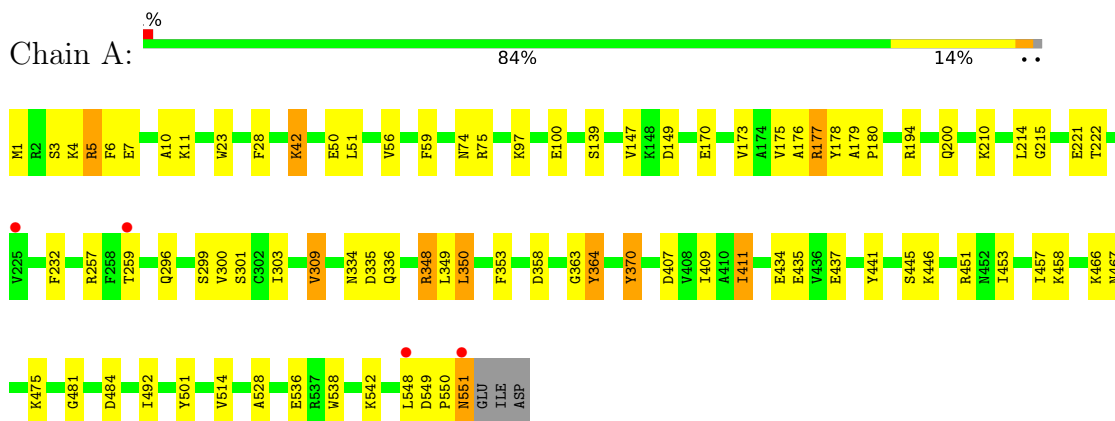
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	490	Total O 490 490	0	0
7	B	118	Total O 118 118	0	0
7	G	152	Total O 152 152	0	0
7	L	319	Total O 319 319	0	0
7	E	37	Total O 37 37	0	0
7	M	95	Total O 95 95	0	0

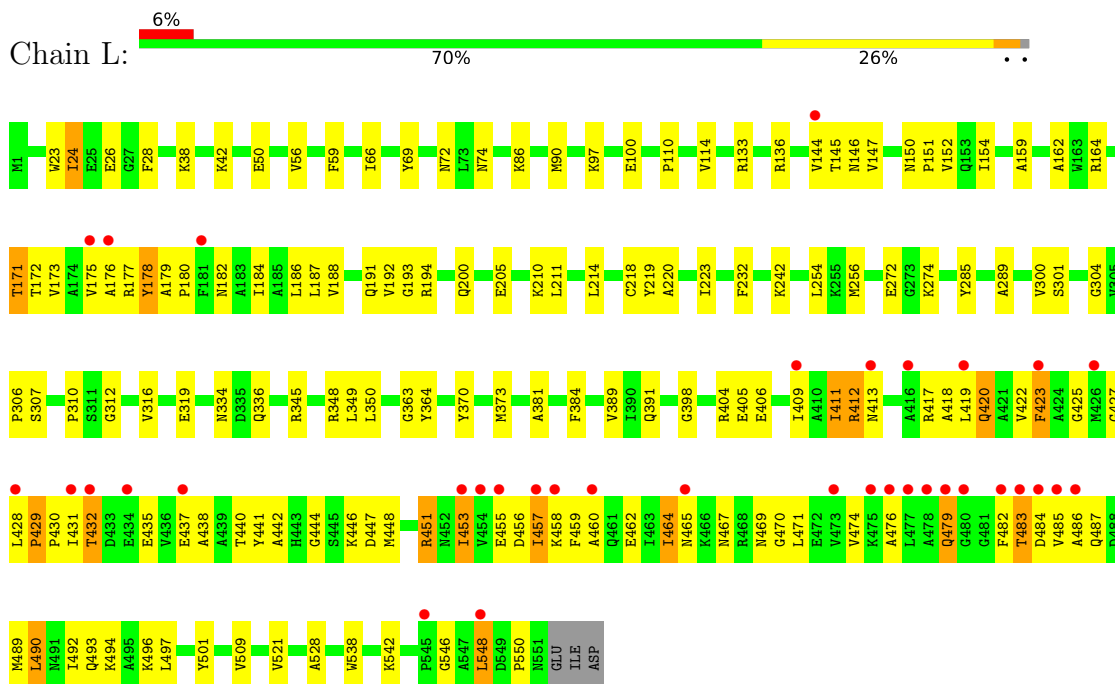
### 3 Residue-property plots [i](#)

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: PROPANEDIOL DEHYDRATASE

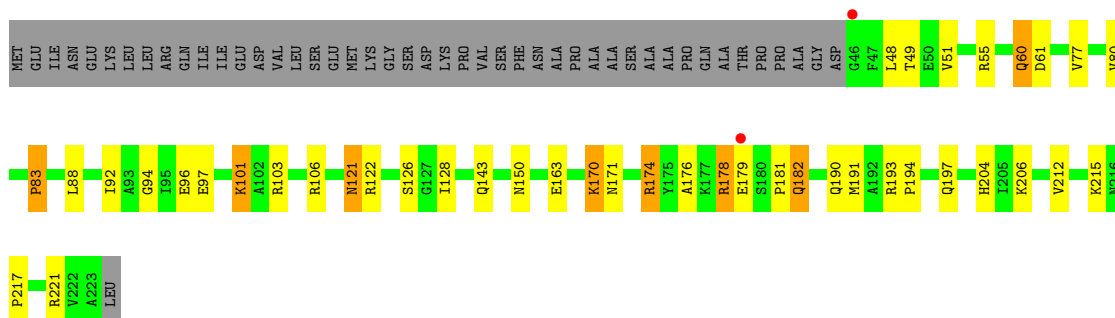


- Molecule 1: PROPANEDIOL DEHYDRATASE

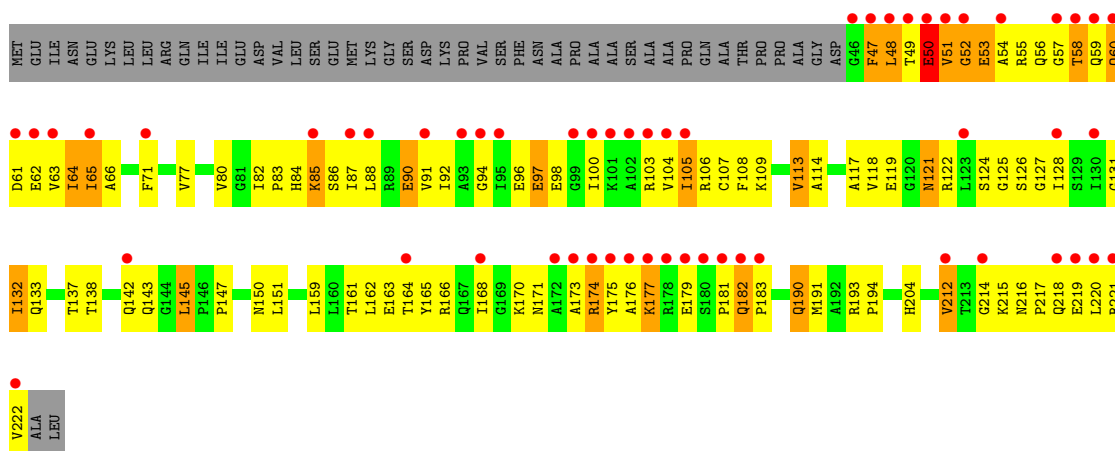


- Molecule 2: PROPANEDIOL DEHYDRATASE

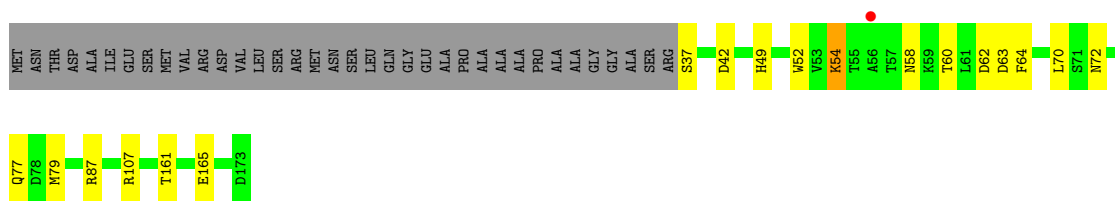




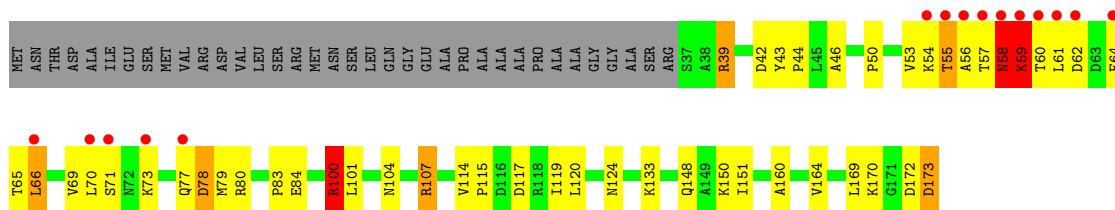
● Molecule 2: PROPANEDIOL DEHYDRATASE



● Molecule 3: PROPANEDIOL DEHYDRATASE



● Molecule 3: PROPANEDIOL DEHYDRATASE





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.00Å 121.60Å 207.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.85 36.43 – 1.85	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-1.85) 88.6 (36.43-1.85)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.91 (at 1.85Å)	Xtrriage
Refinement program	SHELXL-97, CNS	Depositor
R, $R_{free}$	0.182 , 0.249 0.176 , 0.238	Depositor DCC
$R_{free}$ test set	7100 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.3	Xtrriage
Anisotropy	0.733	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 86.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	14737	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.66% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PGO, 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	0.36	1/4289 (0.0%)	1.00	9/5809 (0.2%)
1	L	0.33	0/4282	1.00	6/5799 (0.1%)
2	B	0.32	0/1380	0.95	0/1868
2	E	0.31	0/1375	0.86	0/1861
3	G	0.33	0/1135	1.02	4/1532 (0.3%)
3	M	0.31	0/1117	1.04	3/1509 (0.2%)
All	All	0.34	1/13578 (0.0%)	0.99	22/18378 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	309	VAL	CB-CG2	-5.71	1.40	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	364	TYR	CB-CG-CD1	9.35	126.61	121.00
1	A	75	ARG	NE-CZ-NH1	-9.11	115.75	120.30
1	L	164	ARG	NE-CZ-NH1	8.20	124.40	120.30
1	A	364	TYR	CG-CD1-CE1	7.91	127.62	121.30
1	L	164	ARG	CD-NE-CZ	7.25	133.76	123.60
1	A	370	TYR	CB-CG-CD1	7.01	125.21	121.00
3	M	107	ARG	NE-CZ-NH1	-6.27	117.17	120.30
3	G	87	ARG	CD-NE-CZ	6.09	132.12	123.60
3	G	87	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	L	133	ARG	NE-CZ-NH2	-5.91	117.35	120.30
1	L	364	TYR	CB-CG-CD1	5.90	124.54	121.00
3	M	107	ARG	NE-CZ-NH2	5.88	123.24	120.30
1	A	257	ARG	NE-CZ-NH1	5.53	123.07	120.30
3	M	100	ARG	CD-NE-CZ	5.38	131.13	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	484	ASP	CB-CG-OD1	5.35	123.11	118.30
3	G	107	ARG	NE-CZ-NH1	-5.31	117.64	120.30
1	A	5	ARG	CD-NE-CZ	5.28	130.99	123.60
1	A	364	TYR	CD1-CE1-CZ	-5.19	115.13	119.80
3	G	87	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	A	194	ARG	CD-NE-CZ	5.13	130.78	123.60
1	L	345	ARG	NE-CZ-NH1	-5.03	117.78	120.30
1	L	412	ARG	NE-CZ-NH1	-5.01	117.79	120.30

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	4209	0	4145	56	0
1	L	4206	0	4142	136	0
2	B	1358	0	1408	35	0
2	E	1353	0	1403	112	0
3	G	1108	0	1114	11	0
3	M	1098	0	1103	48	0
4	A	1	0	0	0	0
4	L	1	0	0	0	0
5	A	91	0	87	6	0
5	L	91	0	87	11	0
6	A	5	0	6	0	0
6	L	5	0	6	0	0
7	A	490	0	0	10	0
7	B	118	0	0	8	0
7	E	37	0	0	3	0
7	G	152	0	0	2	0
7	L	319	0	0	13	0
7	M	95	0	0	3	0
All	All	14737	0	13501	390	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 14.

All (390) 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:60:GLN:HG2	2:B:126:SER:HA	1.44	0.99
2:E:190:GLN:H	2:E:190:GLN:HE21	1.10	0.92
2:E:77:VAL:HG12	2:E:83:PRO:HA	1.58	0.84
3:M:56:ALA:HB2	3:M:80:ARG:HB2	1.59	0.82
2:B:174:ARG:HB2	2:B:181:PRO:HG3	1.62	0.81
1:L:146:ASN:HD21	1:L:150:ASN:HB3	1.44	0.81
1:L:175:VAL:HG11	1:L:457:ILE:HD11	1.64	0.79
1:L:470:GLY:O	1:L:474:VAL:HG23	1.83	0.79
1:L:428:LEU:HD23	1:L:459:PHE:HD2	1.45	0.79
2:E:128:ILE:HD13	2:E:176:ALA:HA	1.62	0.79
1:L:432:THR:HG23	1:L:435:GLU:OE1	1.84	0.79
1:A:23:TRP:HB2	1:L:550:PRO:HG3	1.66	0.78
1:A:259[A]:THR:HG22	1:A:296:GLN:HB3	1.65	0.78
3:M:66:LEU:O	3:M:70:LEU:HG	1.84	0.78
2:B:171:ASN:HA	2:B:174:ARG:HG3	1.64	0.78
3:M:57:THR:HG23	3:M:77:GLN:O	1.84	0.77
1:A:221:GLU:O	1:A:259[A]:THR:HG23	1.85	0.77
2:B:61:ASP:O	2:B:101:LYS:HD2	1.85	0.76
2:E:108:PHE:HB3	2:E:212:VAL:HG13	1.66	0.76
3:M:54:LYS:HZ1	3:M:58:ASN:HB2	1.52	0.75
1:L:205:GLU:HG2	7:L:908:HOH:O	1.85	0.74
7:L:792:HOH:O	3:M:100:ARG:HD3	1.88	0.73
1:L:180:PRO:HG2	1:L:460:ALA:O	1.89	0.73
2:E:64:ILE:HG13	2:E:124:SER:HB2	1.71	0.73
1:L:97:LYS:HB2	1:L:100[B]:GLU:HG3	1.71	0.72
1:L:171:THR:HB	1:L:186:LEU:HD22	1.70	0.72
2:E:190:GLN:H	2:E:190:GLN:NE2	1.87	0.71
3:M:59:LYS:NZ	3:M:59:LYS:HB3	2.06	0.71
2:E:71:PHE:HE1	2:E:88:LEU:HD22	1.55	0.71
2:E:104:VAL:O	2:E:220:LEU:HB2	1.91	0.71
1:L:423:PHE:HB2	1:L:431:ILE:HD12	1.73	0.70
3:M:65:THR:O	3:M:69:VAL:HG23	1.91	0.70
1:L:484:ASP:OD1	1:L:485:VAL:HG23	1.91	0.70
1:L:413:ASN:O	1:L:417:ARG:HG3	1.92	0.69
2:E:174:ARG:HG3	2:E:179:GLU:HB2	1.75	0.69
2:E:49:THR:OG1	2:E:221:ARG:HB3	1.93	0.68
2:E:66:ALA:HA	2:E:105:ILE:O	1.92	0.68
2:E:62:GLU:OE2	2:E:124:SER:HA	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:184:ILE:O	1:L:188:VAL:HG23	1.92	0.68
2:E:53:GLU:HA	2:E:218:GLN:HA	1.77	0.67
2:B:190:GLN:HG2	7:B:308:HOH:O	1.94	0.67
2:E:122:ARG:HA	2:E:143:GLN:NE2	2.10	0.67
7:L:876:HOH:O	2:E:190:GLN:HG3	1.94	0.66
1:L:486:ALA:HB1	3:M:66:LEU:HD21	1.77	0.66
2:E:51:VAL:O	2:E:219:GLU:HB3	1.95	0.66
2:E:132:ILE:HG23	2:E:138:THR:OG1	1.95	0.66
1:A:407:ASP:O	1:A:411:ILE:HD12	1.96	0.66
1:L:187:LEU:O	1:L:191:GLN:HG2	1.96	0.65
2:E:87:ILE:O	2:E:91:VAL:HG23	1.97	0.65
3:M:100:ARG:HG3	3:M:100:ARG:HH11	1.62	0.65
1:L:453:ILE:HD11	2:E:183:PRO:HD2	1.78	0.65
2:B:55:ARG:HG3	7:B:250:HOH:O	1.97	0.65
1:A:97:LYS:HB2	1:A:100[B]:GLU:HG3	1.79	0.64
1:L:173:VAL:HG12	1:L:182:ASN:ND2	2.11	0.64
3:M:71:SER:OG	3:M:73:LYS:HG3	1.98	0.64
2:E:142:GLN:NE2	2:E:151:LEU:HD21	2.13	0.64
1:L:152:VAL:HG22	1:L:431:ILE:HG12	1.80	0.64
1:L:146:ASN:ND2	1:L:150:ASN:HB3	2.13	0.64
2:E:177:LYS:HB2	2:E:179:GLU:OE1	1.97	0.63
1:L:72:ASN:OD1	1:L:74:ASN:HB2	1.99	0.63
2:E:161:THR:OG1	2:E:163:GLU:HB2	1.98	0.63
5:L:601:CNC:HM62	2:E:114:ALA:HB2	1.80	0.63
2:E:215:LYS:HZ1	2:E:218:GLN:HG2	1.64	0.63
2:E:113:VAL:HG23	2:E:133:GLN:HG3	1.80	0.63
3:M:84[A]:GLU:HG2	7:M:186:HOH:O	1.98	0.63
1:A:551:ASN:H	1:A:551:ASN:ND2	1.96	0.63
1:A:214:LEU:HD21	1:A:467:ASN:HA	1.81	0.62
1:L:147:VAL:HA	1:L:373:MET:SD	2.40	0.62
1:A:1:MET:HG2	1:L:441:TYR:CE2	2.34	0.62
1:L:175:VAL:O	1:L:178:TYR:HB2	2.00	0.62
1:L:538:TRP:O	1:L:542:LYS:HG3	1.99	0.62
3:M:39:ARG:O	3:M:42:ASP:HB2	1.99	0.62
1:L:159:ALA:HB1	1:L:411:ILE:HG22	1.81	0.62
1:L:334:ASN:HD21	1:L:349:LEU:HA	1.64	0.62
1:L:497:LEU:HD22	3:M:55:THR:HG22	1.81	0.61
3:M:54:LYS:NZ	3:M:58:ASN:HB2	2.13	0.61
2:E:127:GLY:O	2:E:142:GLN:HA	2.01	0.61
1:L:453:ILE:O	1:L:457:ILE:HB	1.99	0.61
1:A:6:PHE:CG	1:L:405:GLU:HG3	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:180:PRO:O	1:L:184:ILE:HD12	2.01	0.61
2:E:47:PHE:HB3	2:E:85:LYS:HE3	1.81	0.61
1:L:459:PHE:O	1:L:462:GLU:HB3	2.01	0.61
2:E:90:GLU:O	2:E:166:ARG:HA	2.01	0.61
1:L:370:TYR:OH	1:L:444:GLY:HA3	2.01	0.61
3:G:64:PHE:CE1	3:G:79:MET:HG2	2.36	0.60
2:B:49:THR:HB	2:B:221:ARG:HB3	1.83	0.60
1:L:453:ILE:O	1:L:453:ILE:HG12	2.02	0.60
2:B:51:VAL:HG11	2:B:221:ARG:HB2	1.84	0.60
2:E:174:ARG:O	2:E:179:GLU:HB2	2.02	0.60
1:L:188:VAL:O	1:L:192:VAL:HG23	2.02	0.59
2:B:97:GLU:OE1	2:B:170:LYS:HE2	2.02	0.59
2:E:212:VAL:HG22	2:E:215:LYS:HB2	1.83	0.59
1:L:432:THR:O	1:L:435:GLU:HB2	2.03	0.59
1:L:469:ASN:OD1	1:L:471:LEU:HB2	2.02	0.59
1:L:493:GLN:HB3	7:L:824:HOH:O	2.02	0.59
2:E:190:GLN:HE21	2:E:190:GLN:N	1.90	0.59
1:A:334:ASN:HD21	1:A:349:LEU:HA	1.67	0.59
2:E:90:GLU:HA	2:E:90:GLU:OE2	2.03	0.59
2:B:92:ILE:O	2:B:96:GLU:HG3	2.03	0.58
1:L:419:LEU:O	1:L:423:PHE:HB2	2.02	0.58
2:E:108:PHE:HB3	2:E:212:VAL:CG1	2.34	0.58
5:L:601:CNC:N29	5:L:601:CNC:H3	2.18	0.58
2:E:174:ARG:HB3	2:E:181:PRO:HG3	1.85	0.58
1:L:484:ASP:O	1:L:487:GLN:HB3	2.04	0.57
2:E:60:GLN:HA	2:E:126:SER:HA	1.86	0.57
3:M:107:ARG:HG2	3:M:151:ILE:HG22	1.85	0.57
5:A:601:CNC:H362	5:A:601:CNC:H351	1.85	0.57
5:A:601:CNC:C2B	5:A:601:CNC:H492	2.35	0.57
1:L:223:ILE:HG22	1:L:242:LYS:HD2	1.87	0.57
1:L:485:VAL:O	1:L:489:MET:HG3	2.04	0.57
1:A:528:ALA:HA	7:L:849:HOH:O	2.05	0.56
3:G:77:GLN:HG2	7:G:299:HOH:O	2.05	0.56
2:E:51:VAL:HG12	2:E:219:GLU:HB3	1.87	0.56
1:A:334:ASN:ND2	1:A:349:LEU:HA	2.21	0.56
1:A:7:GLU:O	1:A:11:LYS:HG3	2.05	0.56
2:B:121:ASN:ND2	2:B:143:GLN:HA	2.21	0.56
2:E:94:GLY:HA2	2:E:97:GLU:OE1	2.05	0.56
2:E:47:PHE:O	2:E:222:VAL:HA	2.05	0.56
1:L:427:GLY:O	1:L:459:PHE:HE2	1.89	0.56
5:L:601:CNC:H362	5:L:601:CNC:H351	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:334:ASN:ND2	1:L:349:LEU:HA	2.21	0.56
1:L:173:VAL:HG21	1:L:176:ALA:HA	1.87	0.56
5:L:601:CNC:O39	5:L:601:CNC:H361	2.04	0.56
3:M:59:LYS:HD3	3:M:78:ASP:HB3	1.88	0.56
1:A:10:ALA:HB3	7:A:1076:HOH:O	2.06	0.55
1:L:420:GLN:HA	1:L:431:ILE:HB	1.88	0.55
1:A:475:LYS:HG2	3:G:70:LEU:HD23	1.88	0.55
3:M:53:VAL:O	3:M:54:LYS:HG3	2.05	0.55
2:B:170:LYS:O	2:B:174:ARG:HG2	2.06	0.55
2:E:191:MET:HE1	2:E:194:PRO:HG2	1.88	0.55
1:L:546:GLY:O	1:L:548:LEU:HD23	2.06	0.55
1:L:420:GLN:HB2	1:L:431:ILE:CG2	2.37	0.55
2:B:88:LEU:O	2:B:92:ILE:HG13	2.07	0.55
2:E:182:GLN:HG3	2:E:183:PRO:HD2	1.89	0.55
1:L:428:LEU:HD23	1:L:459:PHE:CD2	2.35	0.55
1:L:487:GLN:N	3:M:66:LEU:HD11	2.22	0.55
3:M:56:ALA:HB3	3:M:77:GLN:O	2.07	0.55
2:B:51:VAL:CG1	2:B:221:ARG:HB2	2.37	0.54
2:E:219:GLU:HG3	2:E:220:LEU:H	1.72	0.54
1:L:136:ARG:HD2	1:L:521:VAL:O	2.06	0.54
1:L:86:LYS:HE3	1:L:90:MET:SD	2.47	0.54
2:E:47:PHE:O	2:E:222:VAL:O	2.25	0.54
1:L:489:MET:O	1:L:493:GLN:HG2	2.08	0.54
2:E:48:LEU:HD21	2:E:88:LEU:HD23	1.89	0.54
7:A:867:HOH:O	2:B:204:HIS:HE1	1.89	0.54
2:E:109:LYS:HG3	2:E:215:LYS:O	2.08	0.53
2:E:65:ILE:CG2	2:E:104:VAL:HG22	2.38	0.53
3:G:60:THR:HG23	3:G:63:ASP:H	1.74	0.53
1:L:24:ILE:HG13	7:L:844:HOH:O	2.09	0.53
2:E:66:ALA:HB1	2:E:107:CYS:SG	2.48	0.53
2:E:174:ARG:HG2	2:E:181:PRO:HB3	1.91	0.53
5:A:601:CNC:H251	5:A:601:CNC:H291	1.72	0.53
1:L:66:ILE:HG12	1:L:285:TYR:HB3	1.90	0.53
2:E:77:VAL:HG12	2:E:83:PRO:CA	2.36	0.53
1:A:23:TRP:CE3	1:L:550:PRO:HB2	2.44	0.53
1:A:259[A]:THR:CG2	1:A:296:GLN:HE21	2.22	0.52
1:A:1:MET:HG2	1:L:441:TYR:CD2	2.44	0.52
1:L:423:PHE:CB	1:L:431:ILE:HD12	2.40	0.52
1:L:476:ALA:HA	1:L:479:GLN:HG2	1.91	0.52
1:L:162:ALA:HB3	1:L:193:GLY:HA3	1.92	0.52
1:L:487:GLN:O	1:L:490:LEU:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:57:THR:OG1	3:M:78:ASP:HA	2.10	0.52
3:M:54:LYS:CE	3:M:58:ASN:HB2	2.39	0.52
1:A:453:ILE:HG23	1:A:457:ILE:HD12	1.91	0.52
2:B:48:LEU:HB2	7:B:335:HOH:O	2.10	0.52
5:L:601:CNC:C2B	5:L:601:CNC:H492	2.40	0.52
2:E:64:ILE:HG13	2:E:124:SER:CB	2.38	0.52
2:E:106:ARG:HD2	2:E:108:PHE:CE2	2.45	0.52
1:A:4:LYS:HD2	1:L:447:ASP:OD2	2.09	0.52
1:L:438:ALA:HB1	1:L:448:MET:HE2	1.92	0.52
2:E:58:THR:HG22	2:E:58:THR:O	2.10	0.52
1:A:175:VAL:CG1	1:A:177:ARG:HH11	2.23	0.51
1:A:514:VAL:HG12	7:A:774:HOH:O	2.09	0.51
1:A:538:TRP:O	1:A:542:LYS:HG3	2.10	0.51
3:G:161:THR:O	3:G:165[A]:GLU:HG3	2.10	0.51
2:E:142:GLN:CG	2:E:145:LEU:HD22	2.40	0.51
1:A:179:ALA:HB3	1:A:180:PRO:HD3	1.93	0.51
1:A:551:ASN:H	1:A:551:ASN:HD22	1.57	0.51
1:L:42:LYS:HB3	1:L:50:GLU:HB3	1.91	0.51
1:L:179:ALA:HB3	1:L:180:PRO:HD3	1.92	0.51
1:L:429:PRO:HD3	1:L:459:PHE:CD2	2.46	0.51
1:L:429:PRO:HG2	1:L:456:ASP:OD1	2.10	0.51
2:E:50:GLU:O	2:E:219:GLU:O	2.29	0.51
2:B:163:GLU:HG3	7:B:236:HOH:O	2.11	0.51
2:B:94:GLY:O	2:B:97:GLU:HB3	2.11	0.51
2:E:71:PHE:CE1	2:E:88:LEU:HD22	2.40	0.51
2:E:219:GLU:HG3	2:E:220:LEU:N	2.26	0.51
5:L:601:CNC:H2R	2:E:137:THR:HG21	1.93	0.50
3:M:100:ARG:HG3	3:M:100:ARG:NH1	2.25	0.50
3:M:115:PRO:HB3	7:M:213:HOH:O	2.10	0.50
1:A:458:LYS:HB2	7:A:1083:HOH:O	2.12	0.50
1:A:550:PRO:HG2	1:L:23:TRP:HB2	1.94	0.50
1:A:542:LYS:HD2	1:L:310:PRO:HG2	1.93	0.50
2:E:51:VAL:O	2:E:51:VAL:HG12	2.11	0.50
2:E:47:PHE:HZ	2:E:84:HIS:HB3	1.77	0.50
1:A:1:MET:HG2	1:L:441:TYR:CZ	2.47	0.49
1:L:435:GLU:OE2	1:L:451:ARG:HD2	2.12	0.49
1:L:194:ARG:HH12	1:L:509:VAL:HA	1.77	0.49
2:E:51:VAL:O	2:E:52:GLY:O	2.30	0.49
2:E:56:GLN:HG3	2:E:57:GLY:N	2.25	0.49
2:E:86:SER:HB3	2:E:162:LEU:HD11	1.93	0.49
2:E:48:LEU:HD21	2:E:88:LEU:CD2	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:142:GLN:HG3	2:E:142:GLN:O	2.11	0.49
3:M:57:THR:O	3:M:58:ASN:O	2.30	0.49
7:A:789:HOH:O	1:L:528:ALA:HA	2.11	0.49
2:E:164:THR:O	2:E:168:ILE:HD12	2.13	0.49
3:M:55:THR:HG21	3:M:64:PHE:CZ	2.48	0.49
2:E:109:LYS:HE2	2:E:214:GLY:C	2.33	0.49
5:A:601:CNC:H552	5:A:601:CNC:H531	1.94	0.49
2:E:175:TYR:CZ	2:E:181:PRO:HG2	2.48	0.49
1:A:149:ASP:HB2	7:A:859:HOH:O	2.13	0.48
1:L:489:MET:HE3	7:L:764:HOH:O	2.14	0.48
2:E:173:ALA:O	2:E:176:ALA:HB3	2.13	0.48
3:M:160:ALA:O	3:M:164:VAL:HG23	2.14	0.48
1:L:23:TRP:CZ2	1:L:26:GLU:HG3	2.48	0.48
3:M:54:LYS:HE3	3:M:58:ASN:HB2	1.94	0.48
2:E:113:VAL:CG2	2:E:133:GLN:HG3	2.44	0.48
2:E:117:ALA:HB2	2:E:131:GLY:HA3	1.95	0.48
1:L:97:LYS:HB2	1:L:100[B]:GLU:CG	2.39	0.48
1:L:404:ARG:HD2	1:L:406:GLU:OE2	2.14	0.48
2:E:114:ALA:O	2:E:118:VAL:HG23	2.14	0.48
2:E:132:ILE:HG12	2:E:138:THR:HG23	1.94	0.48
3:G:42:ASP:HB3	3:G:49:HIS:CD2	2.49	0.48
1:L:389:VAL:HG23	7:L:776:HOH:O	2.14	0.48
3:M:59:LYS:O	3:M:60:THR:OG1	2.29	0.48
1:L:306:PRO:O	1:L:312:GLY:HA3	2.14	0.48
2:E:92:ILE:O	2:E:96:GLU:HG3	2.13	0.48
1:A:42:LYS:HD3	1:A:50:GLU:HB3	1.96	0.47
1:L:431:ILE:HG22	1:L:431:ILE:O	2.13	0.47
2:E:50:GLU:O	2:E:51:VAL:HB	2.13	0.47
3:M:100:ARG:HD2	3:M:100:ARG:N	2.29	0.47
1:L:177:ARG:NH2	2:E:151:LEU:HB3	2.30	0.47
2:E:83:PRO:HG2	2:E:86:SER:OG	2.15	0.47
1:L:145:THR:HG21	1:L:172:THR:HG22	1.96	0.47
1:A:299:SER:OG	1:A:303:ILE:HA	2.14	0.47
2:E:48:LEU:HD23	2:E:222:VAL:HG22	1.97	0.47
3:M:83:PRO:HG2	3:M:84[B]:GLU:OE1	2.15	0.46
1:L:56:VAL:HA	1:L:59:PHE:CD1	2.50	0.46
1:L:69:TYR:HB2	1:L:289:ALA:HB1	1.95	0.46
5:A:601:CNC:N3B	5:A:601:CNC:H202	2.30	0.46
3:G:60:THR:HG23	3:G:62:ASP:N	2.31	0.46
1:L:42:LYS:CB	1:L:50:GLU:HB3	2.45	0.46
1:L:86:LYS:O	1:L:86:LYS:HG2	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:159:ALA:HB1	1:L:411:ILE:CG2	2.45	0.46
2:E:121:ASN:HD22	2:E:122:ARG:N	2.14	0.46
2:B:77:VAL:HG12	2:B:83:PRO:HA	1.96	0.46
3:G:72:ASN:HB3	7:G:314:HOH:O	2.15	0.46
1:A:177:ARG:CD	1:A:177:ARG:H	2.29	0.46
1:L:146:ASN:HD21	1:L:150:ASN:CB	2.21	0.46
5:A:601:CNC:H251	5:A:601:CNC:N29	2.31	0.46
1:L:316:VAL:O	1:L:319:GLU:HG2	2.16	0.46
1:L:409:ILE:HG23	1:L:440:THR:HG22	1.96	0.45
1:L:442:ALA:HB2	1:L:448:MET:HE1	1.98	0.45
2:E:63:VAL:HG23	2:E:100:ILE:HG21	1.98	0.45
1:A:147:VAL:HG22	1:A:445:SER:OG	2.16	0.45
1:A:334:ASN:ND2	1:A:348:ARG:HD3	2.30	0.45
2:E:82:ILE:HG21	2:E:162:LEU:HD21	1.97	0.45
2:E:105:ILE:HG13	2:E:217:PRO:HB3	1.99	0.45
2:E:174:ARG:HA	2:E:179:GLU:OE1	2.17	0.45
2:B:60:GLN:OE1	2:B:178:ARG:NH2	2.50	0.45
2:B:122:ARG:NH2	7:B:287:HOH:O	2.50	0.45
2:E:171:ASN:OD1	2:E:181:PRO:HB2	2.17	0.45
1:A:74:ASN:ND2	7:A:877:HOH:O	2.50	0.45
2:B:182:GLN:NE2	7:B:300:HOH:O	2.50	0.45
3:G:60:THR:HG22	3:G:63:ASP:CG	2.37	0.45
1:L:336:GLN:OE1	2:E:193:ARG:NH1	2.50	0.45
1:L:486:ALA:C	3:M:66:LEU:HD11	2.37	0.45
2:B:60:GLN:NE2	2:B:176:ALA:O	2.50	0.45
1:L:391:GLN:OE1	1:L:398:GLY:N	2.50	0.45
1:L:254:LEU:HD21	7:L:835:HOH:O	2.16	0.45
2:E:100:ILE:HD11	2:E:177:LYS:HD2	1.98	0.45
3:G:54:LYS:NZ	3:G:58:ASN:O	2.50	0.45
2:E:85:LYS:HE2	2:E:85:LYS:HB3	1.28	0.45
3:M:170:LYS:HB2	3:M:170:LYS:HE3	1.48	0.45
2:E:47:PHE:CZ	2:E:84:HIS:HB3	2.53	0.44
1:L:172:THR:OG1	5:L:601:CNC:N29	2.50	0.44
1:L:272:GLU:O	1:L:274:LYS:HG2	2.17	0.44
2:E:220:LEU:HD23	2:E:220:LEU:HA	1.79	0.44
3:M:107:ARG:HG2	3:M:151:ILE:CG2	2.46	0.44
2:E:87:ILE:HA	2:E:162:LEU:HD22	1.98	0.44
1:A:370:TYR:CZ	1:A:446:LYS:HG3	2.53	0.44
2:B:191:MET:C	2:B:194:PRO:HD2	2.38	0.44
2:B:217:PRO:HD2	7:B:302:HOH:O	2.18	0.44
2:B:174:ARG:HE	2:B:174:ARG:HB3	1.62	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:72:ASN:ND2	7:L:794:HOH:O	2.50	0.44
1:L:422:VAL:HG12	1:L:423:PHE:N	2.33	0.44
1:L:435:GLU:OE2	1:L:451:ARG:HG3	2.18	0.44
5:L:601:CNC:H552	5:L:601:CNC:H531	1.98	0.44
2:E:47:PHE:CG	2:E:85:LYS:HE3	2.53	0.44
2:E:65:ILE:HG22	2:E:104:VAL:HG13	2.00	0.44
2:E:128:ILE:HD13	2:E:176:ALA:CA	2.41	0.44
1:L:110:PRO:O	1:L:114:VAL:HG23	2.18	0.44
1:L:301:SER:HB3	5:L:601:CNC:H532	2.00	0.44
1:L:429:PRO:HA	1:L:430:PRO:HD2	1.72	0.44
1:L:493:GLN:HG2	1:L:493:GLN:H	1.57	0.44
2:E:62:GLU:CD	2:E:125:GLY:H	2.19	0.44
1:A:434:GLU:HB2	7:A:1070:HOH:O	2.17	0.44
2:B:212:VAL:HG12	2:B:215:LYS:HB2	2.00	0.44
2:E:159:LEU:N	2:E:159:LEU:HD23	2.33	0.44
3:M:120:LEU:O	3:M:124:ASN:ND2	2.50	0.44
3:M:169:LEU:O	3:M:172:ASP:HB2	2.17	0.44
1:A:173:VAL:HG21	1:A:176:ALA:HA	1.99	0.43
1:A:222:THR:HA	1:A:259[A]:THR:CG2	2.48	0.43
1:L:151:PRO:HA	1:L:154:ILE:HD12	1.99	0.43
2:E:54:ALA:O	2:E:55:ARG:HG2	2.17	0.43
2:E:204:HIS:HD2	7:E:231:HOH:O	2.01	0.43
2:B:106:ARG:HG3	2:B:106:ARG:HH11	1.83	0.43
1:L:272:GLU:HG2	7:L:821:HOH:O	2.16	0.43
1:L:370:TYR:CZ	1:L:446:LYS:HD2	2.53	0.43
1:L:404:ARG:HD2	1:L:406:GLU:CD	2.38	0.43
1:L:442:ALA:HB2	1:L:448:MET:CE	2.48	0.43
1:A:56:VAL:HA	1:A:59:PHE:CD1	2.52	0.43
2:B:193:ARG:HG3	2:B:197:GLN:HB2	1.99	0.43
2:B:193:ARG:HB3	2:B:194:PRO:HD3	2.01	0.43
3:M:173:ASP:OD1	3:M:173:ASP:N	2.50	0.43
1:A:177:ARG:H	1:A:177:ARG:HD2	1.84	0.43
1:L:425:GLY:HA3	7:L:870:HOH:O	2.19	0.43
1:L:432:THR:O	1:L:435:GLU:N	2.51	0.43
1:L:447:ASP:N	1:L:447:ASP:OD1	2.50	0.43
2:E:145:LEU:HD12	2:E:145:LEU:HA	1.79	0.43
2:E:119:GLU:OE2	2:E:217:PRO:HG3	2.19	0.43
1:L:173:VAL:HG23	1:L:173:VAL:O	2.17	0.43
3:M:101:LEU:O	3:M:104:ASN:HB3	2.18	0.43
1:A:215:GLY:HA2	7:A:827:HOH:O	2.19	0.43
1:L:492:ILE:O	1:L:496:LYS:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:601:CNC:H1R	7:E:248:HOH:O	2.18	0.43
2:E:106:ARG:HD2	2:E:108:PHE:CZ	2.54	0.43
2:E:119:GLU:HA	2:E:122:ARG:HH21	1.83	0.42
1:L:220:ALA:O	1:L:256:MET:HA	2.19	0.42
2:E:87:ILE:HG23	2:E:165:TYR:CD1	2.55	0.42
2:E:142:GLN:HE21	2:E:145:LEU:HD22	1.84	0.42
2:E:212:VAL:HG11	2:E:215:LYS:HD3	2.02	0.42
1:A:409:ILE:HD13	1:A:441:TYR:HE1	1.83	0.42
1:L:489:MET:HE3	1:L:489:MET:HB3	1.96	0.42
1:A:23:TRP:HB2	1:L:550:PRO:CG	2.43	0.42
1:A:335:ASP:OD1	1:A:335:ASP:N	2.49	0.42
2:E:85:LYS:H	2:E:85:LYS:HG2	1.19	0.42
3:M:114:VAL:HB	3:M:119:ILE:HD11	2.01	0.42
1:L:404:ARG:HH11	1:L:406:GLU:CD	2.23	0.42
3:M:46:ALA:O	3:M:50:PRO:HG3	2.20	0.42
1:L:406:GLU:H	1:L:406:GLU:HG2	1.66	0.42
1:L:200:GLN:HG2	1:L:219:TYR:CZ	2.55	0.42
1:L:418:ALA:HA	1:L:482:PHE:CE2	2.55	0.42
1:L:490:LEU:HD13	1:L:490:LEU:HA	1.72	0.42
3:M:60:THR:HG22	3:M:61:LEU:N	2.34	0.42
1:A:301:SER:HA	1:A:336:GLN:HG3	2.02	0.42
3:M:39:ARG:NH1	3:M:39:ARG:HG2	2.35	0.41
1:A:549:ASP:OD1	1:A:551:ASN:ND2	2.50	0.41
1:L:304:GLY:HA2	1:L:307:SER:HG	1.85	0.41
1:A:50:GLU:HG2	1:A:51:LEU:N	2.35	0.41
1:L:411:ILE:N	1:L:411:ILE:HD13	2.35	0.41
2:E:65:ILE:HG22	2:E:65:ILE:O	2.20	0.41
2:E:147:PRO:HD2	7:E:229:HOH:O	2.20	0.41
1:L:171:THR:HG23	1:L:172:THR:N	2.34	0.41
1:L:211:LEU:HD23	1:L:464:ILE:HD11	2.00	0.41
3:M:133:LYS:HD2	3:M:164:VAL:HG21	2.03	0.41
1:A:170:GLU:HB2	1:A:200:GLN:NE2	2.36	0.41
2:E:94:GLY:O	2:E:97:GLU:OE1	2.38	0.41
3:M:107:ARG:HH11	3:M:107:ARG:HD3	1.55	0.41
1:L:144:VAL:HB	1:L:186:LEU:HD13	2.02	0.41
2:E:174:ARG:HG2	2:E:181:PRO:CB	2.49	0.41
1:A:481:GLY:HA2	7:A:1002:HOH:O	2.21	0.41
1:L:205:GLU:HA	1:L:205:GLU:OE1	2.21	0.41
1:L:429:PRO:HG3	1:L:455:GLU:HG3	2.03	0.41
1:A:259[A]:THR:HG21	1:A:296:GLN:HE21	1.85	0.41
2:B:103:ARG:HH11	2:B:103:ARG:HD2	1.72	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:122:ARG:HG2	2:B:122:ARG:HH11	1.86	0.41
3:G:49:HIS:HB3	3:G:52:TRP:CG	2.56	0.41
1:L:72:ASN:HB2	7:L:793:HOH:O	2.20	0.41
1:L:210:LYS:NZ	1:L:467:ASN:HD21	2.18	0.41
1:L:497:LEU:HD21	3:M:79:MET:C	2.41	0.41
5:L:601:CNC:H531	5:L:601:CNC:C55	2.51	0.41
2:E:165:TYR:HA	2:E:168:ILE:HD12	2.02	0.41
2:E:215:LYS:NZ	2:E:216:ASN:O	2.54	0.41
1:A:3:SER:OG	1:A:5:ARG:HB3	2.21	0.41
1:L:420:GLN:NE2	1:L:431:ILE:O	2.49	0.41
2:E:87:ILE:HG12	2:E:165:TYR:CE2	2.55	0.41
1:A:139:SER:HB3	1:A:358:ASP:O	2.21	0.40
1:A:350:LEU:HA	1:A:353:PHE:HB3	2.02	0.40
2:B:206:LYS:HG2	7:B:328:HOH:O	2.21	0.40
2:E:108:PHE:HE1	2:E:218:GLN:H	1.67	0.40
1:A:435:GLU:OE2	1:A:451:ARG:NH1	2.50	0.40
2:B:60:GLN:HE21	2:B:60:GLN:HB3	1.68	0.40
2:B:179:GLU:O	2:B:181:PRO:HD3	2.22	0.40
1:L:497:LEU:HD13	3:M:55:THR:CG2	2.51	0.40
2:E:215:LYS:HZ2	2:E:215:LYS:HG2	1.75	0.40
1:L:381:ALA:HA	1:L:384:PHE:CE2	2.56	0.40
3:M:151:ILE:HD12	7:M:192:HOH:O	2.21	0.40
1:L:486:ALA:HB3	3:M:66:LEU:HD11	2.03	0.40
3:M:43:TYR:CG	3:M:44:PRO:HA	2.56	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	551/554 (100%)	531 (96%)	18 (3%)	2 (0%)	34 19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	550/554 (99%)	516 (94%)	30 (6%)	4 (1%)	22	9
2	B	176/224 (79%)	169 (96%)	7 (4%)	0	100	100
2	E	175/224 (78%)	158 (90%)	13 (7%)	4 (2%)	6	1
3	G	138/173 (80%)	135 (98%)	3 (2%)	0	100	100
3	M	136/173 (79%)	131 (96%)	3 (2%)	2 (2%)	10	2
All	All	1726/1902 (91%)	1640 (95%)	74 (4%)	12 (1%)	22	9

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	50	GLU
2	E	52	GLY
2	E	58	THR
3	M	58	ASN
1	L	483	THR
1	A	300	VAL
1	L	300	VAL
1	L	363	GLY
1	L	429	PRO
2	E	51	VAL
1	A	363	GLY
3	M	59	LYS

### 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	452/453 (100%)	434 (96%)	18 (4%)	31	14
1	L	451/453 (100%)	423 (94%)	28 (6%)	18	5
2	B	146/183 (80%)	135 (92%)	11 (8%)	13	3
2	E	146/183 (80%)	119 (82%)	27 (18%)	1	0
3	G	119/141 (84%)	117 (98%)	2 (2%)	60	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	M	117/141 (83%)	105 (90%)	12 (10%)	7 1
All	All	1431/1554 (92%)	1333 (93%)	98 (7%)	15 4

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	PHE
1	A	42	LYS
1	A	177	ARG
1	A	178	TYR
1	A	210	LYS
1	A	232	PHE
1	A	309	VAL
1	A	348	ARG
1	A	350	LEU
1	A	364	TYR
1	A	411	ILE
1	A	437	GLU
1	A	466	LYS
1	A	492	ILE
1	A	501	TYR
1	A	536	GLU
1	A	548	LEU
1	A	551	ASN
2	B	60	GLN
2	B	80	VAL
2	B	83	PRO
2	B	101	LYS
2	B	121	ASN
2	B	128	ILE
2	B	150	ASN
2	B	170	LYS
2	B	174	ARG
2	B	178	ARG
2	B	182	GLN
3	G	37	SER
3	G	54	LYS
1	L	24	ILE
1	L	28	PHE
1	L	38	LYS
1	L	171	THR
1	L	178	TYR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	L	214	LEU
1	L	218	CYS
1	L	232	PHE
1	L	348	ARG
1	L	350	LEU
1	L	411	ILE
1	L	412	ARG
1	L	420	GLN
1	L	423	PHE
1	L	432	THR
1	L	437	GLU
1	L	451	ARG
1	L	453	ILE
1	L	457	ILE
1	L	458	LYS
1	L	464	ILE
1	L	465	ASN
1	L	479	GLN
1	L	483	THR
1	L	490	LEU
1	L	494	LYS
1	L	501	TYR
1	L	548	LEU
2	E	47	PHE
2	E	48	LEU
2	E	50	GLU
2	E	53	GLU
2	E	59	GLN
2	E	60	GLN
2	E	61	ASP
2	E	64	ILE
2	E	65	ILE
2	E	80	VAL
2	E	85	LYS
2	E	90	GLU
2	E	97	GLU
2	E	98	GLU
2	E	103	ARG
2	E	105	ILE
2	E	113	VAL
2	E	121	ASN
2	E	132	ILE

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Mol	Chain	Res	Type
2	E	145	LEU
2	E	150	ASN
2	E	170	LYS
2	E	174	ARG
2	E	177	LYS
2	E	182	GLN
2	E	190	GLN
2	E	212	VAL
3	M	39	ARG
3	M	55	THR
3	M	58	ASN
3	M	59	LYS
3	M	62	ASP
3	M	66	LEU
3	M	78	ASP
3	M	100	ARG
3	M	117	ASP
3	M	148	GLN
3	M	150	LYS
3	M	173	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) 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	543	ASN
1	A	551	ASN
2	B	59	GLN
2	B	75	GLN
2	B	121	ASN
2	B	142	GLN
2	B	182	GLN
2	B	204	HIS
1	L	74	ASN
1	L	334	ASN
1	L	352	GLN
1	L	461	GLN
1	L	465	ASN
1	L	467	ASN

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Mol	Chain	Res	Type
1	L	513	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
2	E	218	GLN
3	M	58	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 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	$\# Z  > 2$
5	CNC	A	601	-	80,101,103	0.99	4 (5%)	101,166,171	1.17	10 (9%)
6	PGO	L	602	4	3,4,4	0.49	0	1,4,4	0.08	0
6	PGO	A	602	4	3,4,4	0.60	0	1,4,4	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	CNC	L	601	-	80,101,103	0.91	4 (5%)	101,166,171	1.29	14 (13%)

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
5	CNC	A	601	-	1/1/36/38	6/51/223/235	0/3/11/11
6	PGO	L	602	4	-	2/2/2/2	-
6	PGO	A	602	4	-	0/2/2/2	-
5	CNC	L	601	-	1/1/36/38	10/51/223/235	0/3/11/11

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	601	CNC	C17-C18	2.78	1.58	1.54
5	A	601	CNC	C17-C18	2.60	1.57	1.54
5	A	601	CNC	C20-C1	-2.47	1.48	1.53
5	A	601	CNC	O58-C57	2.40	1.28	1.23
5	L	601	CNC	O58-C57	2.31	1.28	1.23
5	L	601	CNC	C11-C10	-2.14	1.37	1.40
5	A	601	CNC	C11-C10	-2.08	1.37	1.40
5	L	601	CNC	C20-C1	-2.06	1.49	1.53

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	601	CNC	C55-C17-C16	4.14	123.70	109.92
5	L	601	CNC	C54-C17-C18	-3.73	107.47	112.98
5	A	601	CNC	C55-C17-C16	3.66	122.11	109.92
5	A	601	CNC	C16-C15-C14	-2.88	119.78	124.27
5	A	601	CNC	C2P-C1P-N59	2.79	117.05	112.93
5	A	601	CNC	C6-C5-C4	-2.74	119.99	124.27
5	A	601	CNC	C13-C14-C15	-2.74	121.74	131.68
5	L	601	CNC	C16-C15-C14	-2.68	120.08	124.27
5	A	601	CNC	C3-C4-C5	-2.59	122.28	131.68
5	L	601	CNC	C1-C19-C18	-2.55	117.72	121.93
5	L	601	CNC	C13-C14-C15	-2.51	122.58	131.68
5	L	601	CNC	C56-C55-C17	2.41	120.16	115.50
5	L	601	CNC	C4B-C9B-C8B	-2.39	118.66	121.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	601	CNC	C20-C1-C19	2.37	111.64	109.36
5	L	601	CNC	O58-C57-C56	-2.35	117.72	122.02
5	L	601	CNC	C5-C6-N22	-2.33	120.56	124.81
5	L	601	CNC	C56-C57-N59	2.32	120.33	116.42
5	L	601	CNC	C6-C5-C4	-2.28	120.71	124.27
5	A	601	CNC	C4B-C9B-C8B	-2.23	118.82	121.10
5	A	601	CNC	C25-C2-C3	-2.18	112.26	115.58
5	A	601	CNC	O5-P-O3	2.18	115.37	106.78
5	L	601	CNC	C3-C4-C5	-2.09	124.09	131.68
5	L	601	CNC	C36-C7-C8	-2.09	108.34	112.11
5	A	601	CNC	C12-C11-C10	2.08	128.17	124.64

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	601	CNC	N24
5	L	601	CNC	N24

All (18) torsion outliers are listed below:

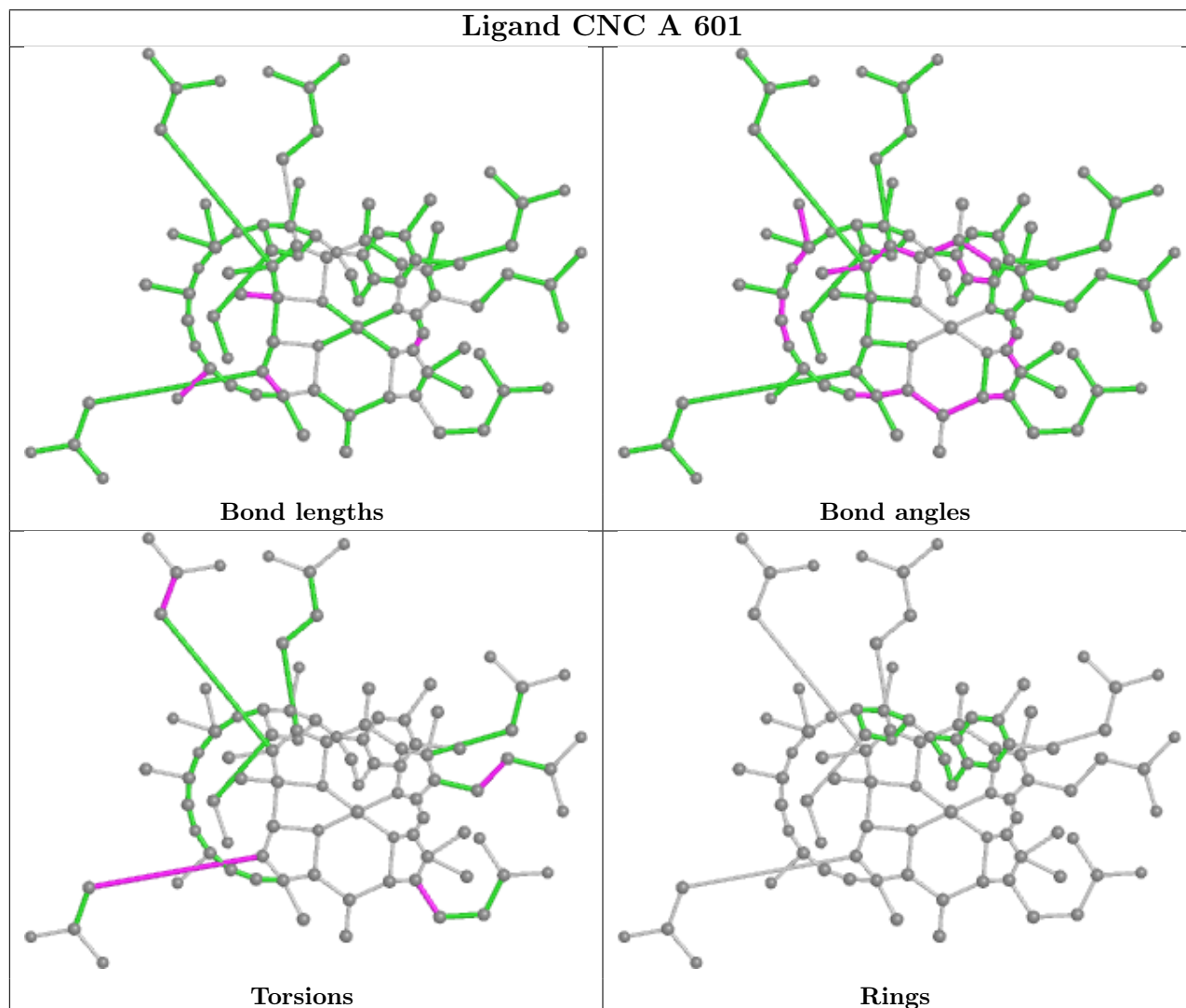
Mol	Chain	Res	Type	Atoms
5	A	601	CNC	C2-C26-C27-O28
5	L	601	CNC	C1-C2-C26-C27
5	L	601	CNC	C25-C2-C26-C27
5	L	601	CNC	C3-C2-C26-C27
6	L	602	PGO	O1-C1-C2-C3
6	L	602	PGO	O1-C1-C2-O2
5	A	601	CNC	C2-C26-C27-N29
5	A	601	CNC	C12-C13-C48-C49
5	L	601	CNC	C2-C26-C27-N29
5	L	601	CNC	C2-C26-C27-O28
5	L	601	CNC	C30-C31-C32-O34
5	L	601	CNC	C30-C31-C32-N33
5	L	601	CNC	C4-C3-C30-C31
5	A	601	CNC	C19-C18-C60-C61
5	L	601	CNC	C17-C18-C60-C61
5	L	601	CNC	C19-C18-C60-C61
5	A	601	CNC	C8-C41-C42-C43
5	A	601	CNC	C17-C18-C60-C61

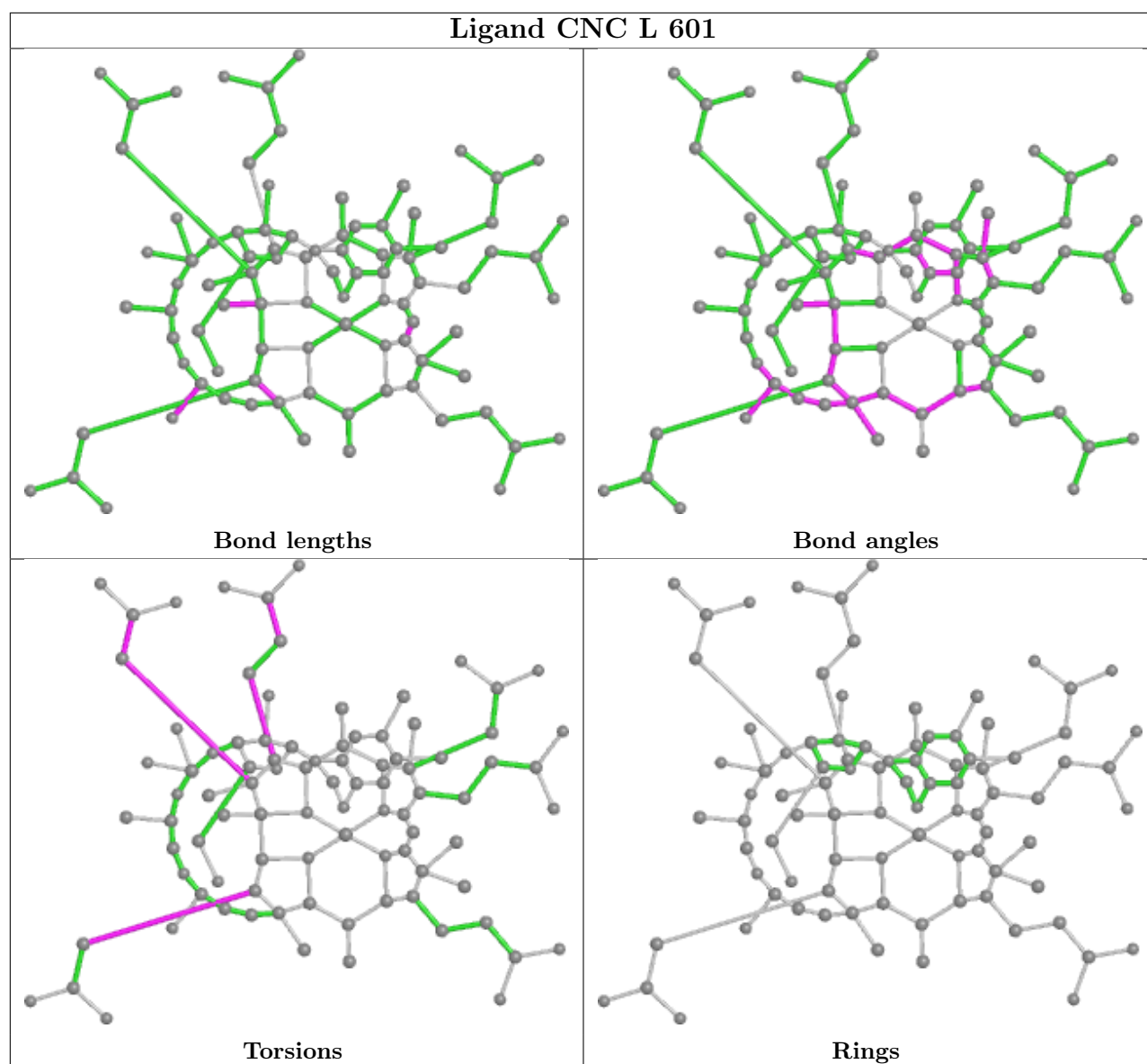
There are no ring outliers.

2 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	601	CNC	6	0
5	L	601	CNC	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.





## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	551/554 (99%)	-0.29	4 (0%) 87 88	10, 17, 34, 86	0
1	L	551/554 (99%)	0.20	36 (6%) 18 18	10, 24, 68, 100	0
2	B	178/224 (79%)	-0.14	2 (1%) 80 81	15, 28, 51, 78	0
2	E	177/224 (79%)	1.57	56 (31%) 0 0	21, 49, 100, 112	0
3	G	137/173 (79%)	-0.39	1 (0%) 87 88	14, 22, 44, 70	0
3	M	137/173 (79%)	0.33	15 (10%) 5 5	19, 30, 70, 95	0
All	All	1731/1902 (91%)	0.11	114 (6%) 18 17	10, 23, 65, 112	0

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	51	VAL	7.9
3	M	66	LEU	7.6
1	L	454	VAL	7.1
2	E	100	ILE	6.6
2	E	47	PHE	6.4
1	L	477	LEU	5.9
3	M	55	THR	5.9
1	L	486	ALA	5.2
2	E	58	THR	5.1
1	L	453	ILE	5.1
1	L	482	PHE	4.6
3	M	57	THR	4.6
2	E	48	LEU	4.5
2	E	221	ARG	4.5
2	E	104	VAL	4.5
3	M	56	ALA	4.4
2	E	54	ALA	4.4
2	E	93	ALA	4.4
2	E	91	VAL	4.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	E	179	GLU	4.3
2	E	52	GLY	4.2
2	E	57	GLY	4.2
1	L	428	LEU	4.1
2	E	65	ILE	4.1
2	E	168	ILE	4.1
2	E	49	THR	4.1
1	L	426	MET	4.1
3	M	58	ASN	3.9
2	E	180	SER	3.8
1	L	458	LYS	3.8
1	L	457	ILE	3.7
2	E	222	VAL	3.7
2	E	128	ILE	3.7
2	E	61	ASP	3.7
2	E	181	PRO	3.7
2	E	59	GLN	3.6
2	E	60	GLN	3.6
1	L	423	PHE	3.5
2	E	87	ILE	3.5
2	E	62	GLU	3.5
3	M	64	PHE	3.5
2	E	95	ILE	3.4
2	E	220	LEU	3.4
2	E	99	GLY	3.3
1	L	483	THR	3.3
2	E	175	TYR	3.2
2	E	214	GLY	3.2
1	L	485	VAL	3.2
1	L	409	ILE	3.2
3	G	56	ALA	3.1
3	M	59	LYS	3.1
2	E	105	ILE	3.0
2	E	173	ALA	3.0
3	M	70	LEU	3.0
2	E	177	LYS	2.9
1	L	431	ILE	2.9
2	E	50	GLU	2.9
1	A	548	LEU	2.9
2	E	46	GLY	2.9
1	L	419	LEU	2.9
2	E	85	LYS	2.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	551	ASN	2.8
2	E	71	PHE	2.8
2	E	219	GLU	2.8
1	L	434	GLU	2.8
1	L	437	GLU	2.8
2	E	101	LYS	2.7
2	E	178	ARG	2.7
1	L	432	THR	2.7
1	L	548	LEU	2.7
2	E	123	LEU	2.7
3	M	60	THR	2.7
2	E	172	ALA	2.6
1	A	259[A]	THR	2.6
3	M	54	LYS	2.6
3	M	73	LYS	2.6
2	E	182	GLN	2.6
1	L	416	ALA	2.6
3	M	77	GLN	2.6
2	E	174	ARG	2.5
1	L	479	GLN	2.5
1	L	176	ALA	2.5
1	L	478	ALA	2.5
2	E	63	VAL	2.5
1	L	455	GLU	2.5
1	L	476	ALA	2.4
2	E	88	LEU	2.4
1	L	484	ASP	2.4
3	M	61	LEU	2.4
1	L	473	VAL	2.4
2	B	46	GLY	2.4
2	E	103	ARG	2.4
1	L	465	ASN	2.4
1	L	460	ALA	2.4
2	E	183	PRO	2.4
1	L	181	PHE	2.3
3	M	71	SER	2.3
2	E	164	THR	2.3
2	E	130	ILE	2.3
1	L	144	VAL	2.3
1	L	175	VAL	2.3
2	E	142	GLN	2.2
1	L	413	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	L	545	PRO	2.2
2	E	102	ALA	2.2
2	E	176	ALA	2.1
2	E	218	GLN	2.1
3	M	62	ASP	2.1
1	A	225	VAL	2.1
1	L	475	LYS	2.1
2	E	94	GLY	2.1
2	B	179	GLU	2.0
2	E	212	VAL	2.0
1	L	480	GLY	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](#)

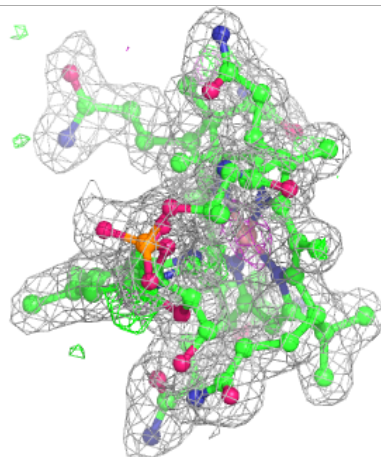
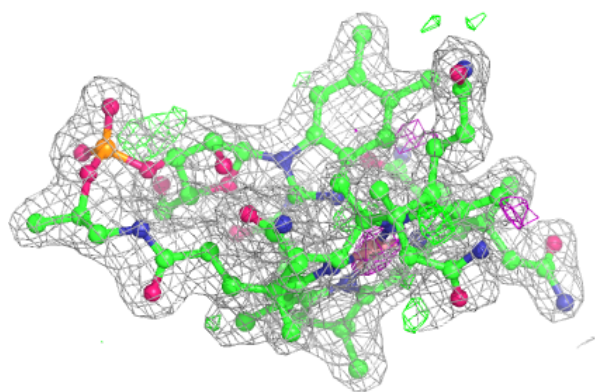
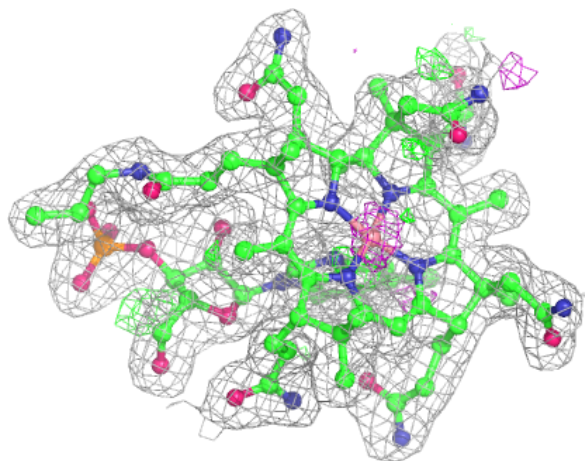
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

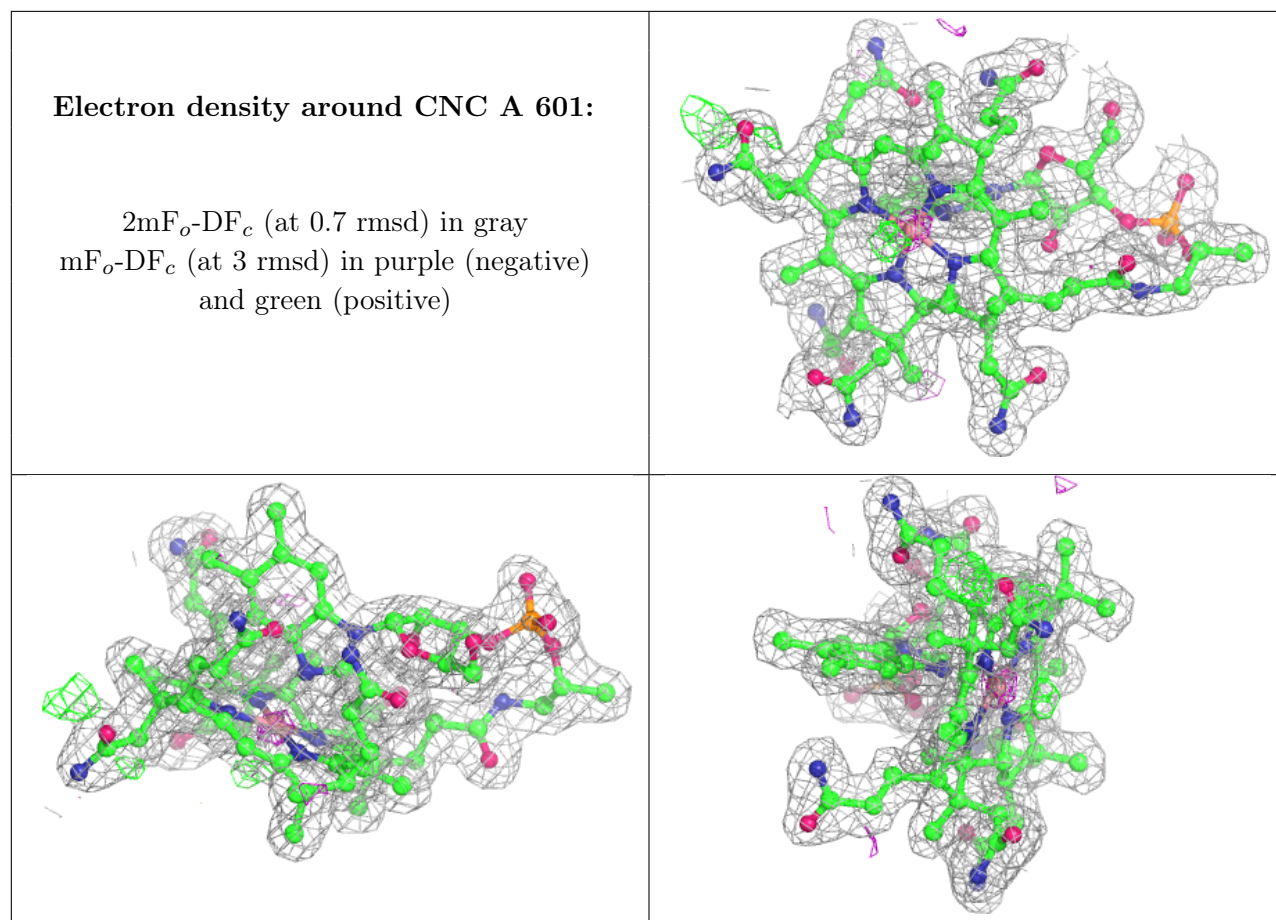
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	PGO	L	602	5/5	0.94	0.17	24,24,26,29	0
5	CNC	L	601	91/93	0.95	0.13	16,28,44,67	0
6	PGO	A	602	5/5	0.97	0.17	11,11,14,17	0
5	CNC	A	601	91/93	0.98	0.12	9,17,25,51	0
4	K	A	603	1/1	0.99	0.09	13,13,13,13	0
4	K	L	603	1/1	0.99	0.08	20,20,20,20	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 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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.