



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 01:43 AM UTC

PDB ID : 1UC5 / pdb_00001uc5
Title : Structure of diol dehydratase complexed with (R)-1,2-propanediol
Authors : Shibata, N.; Nakanishi, Y.; Fukuoka, M.; Yamanishi, M.; Yasuoka, N.; Toraya, T.
Deposited on : 2003-04-08
Resolution : 2.30 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	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

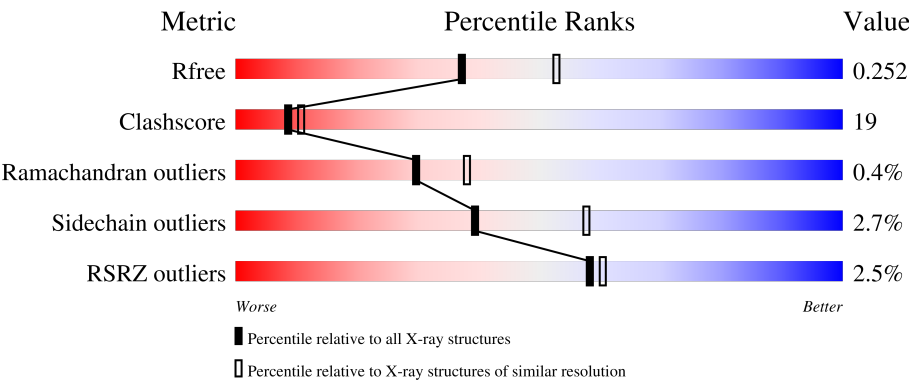
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	% 68%31%..
1	L	554	64%32%..
2	B	224	5% 51%27%.21%
2	E	224	4% 42%35%.21%
3	G	173	6% 51%25%.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	1601	X	-	-	-
7	CNC	E	2601	X	-	-	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 14220 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	177	Total	C	N	O	S	0	0	0
			1353	856	243	252	2			

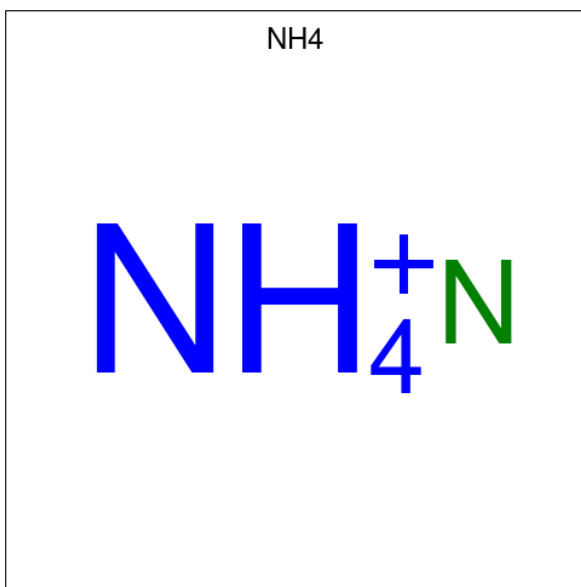
- Molecule 3 is a protein called diol dehydrase gamma subunit.

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
			1092	681	195	213	3			

- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

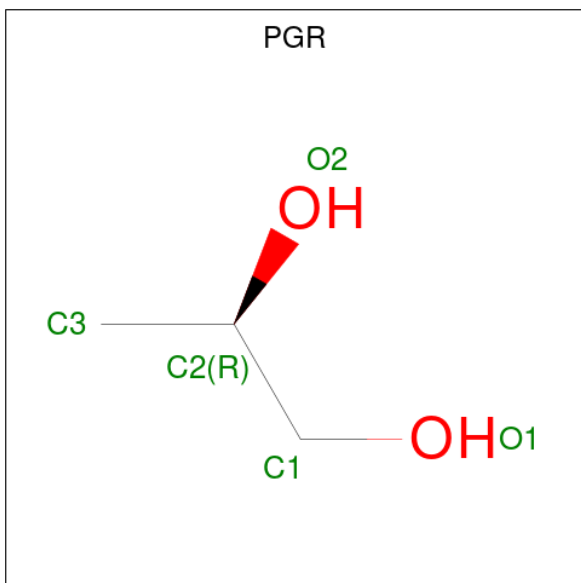
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total	0	0
			1 K		
4	L	1	Total	0	0
			1 K		

- Molecule 5 is AMMONIUM ION (CCD ID: NH4) (formula: H₄N).



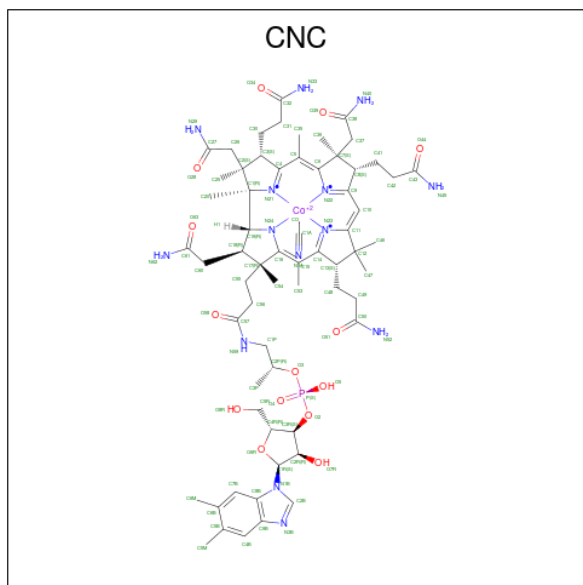
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total N 1 1	0	0
5	A	1	Total N 1 1	0	0
5	L	1	Total N 1 1	0	0
5	L	1	Total N 1 1	0	0

- Molecule 6 is R-1,2-PROPANEDIOL (CCD ID: PGR) (formula: $C_3H_8O_2$).



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: $C_{63}H_{89}CoN_{14}O_{14}P$).



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

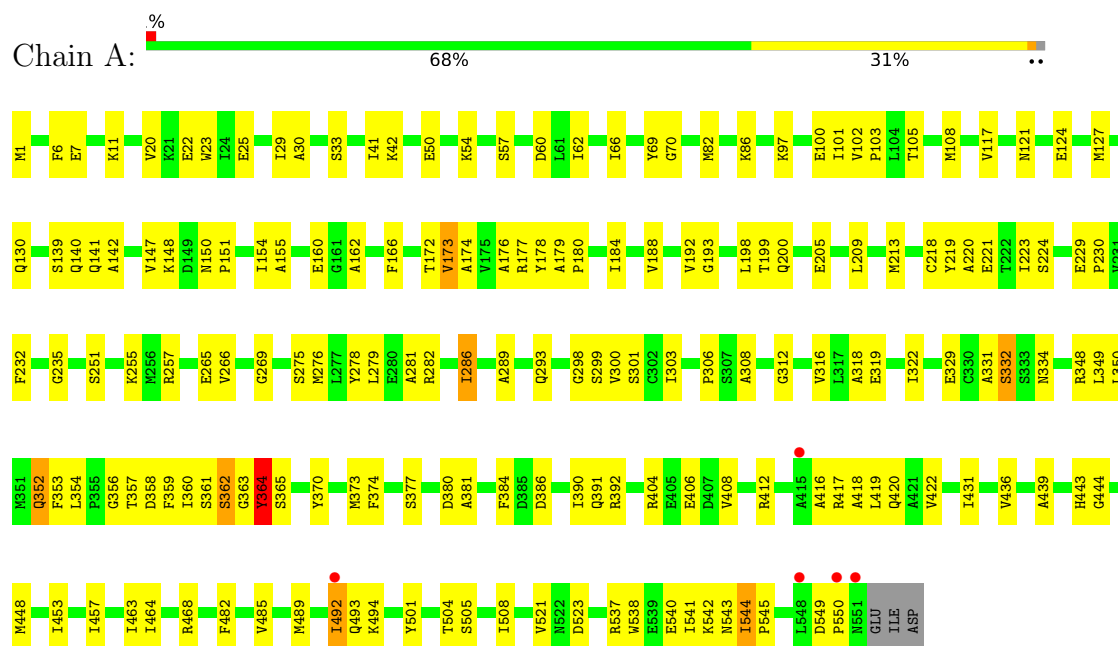
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	267	Total O 267 267	0	0
8	B	72	Total O 72 72	0	0
8	G	70	Total O 70 70	0	0
8	L	227	Total O 227 227	0	0
8	E	23	Total O 23 23	0	0
8	M	65	Total O 65 65	0	0

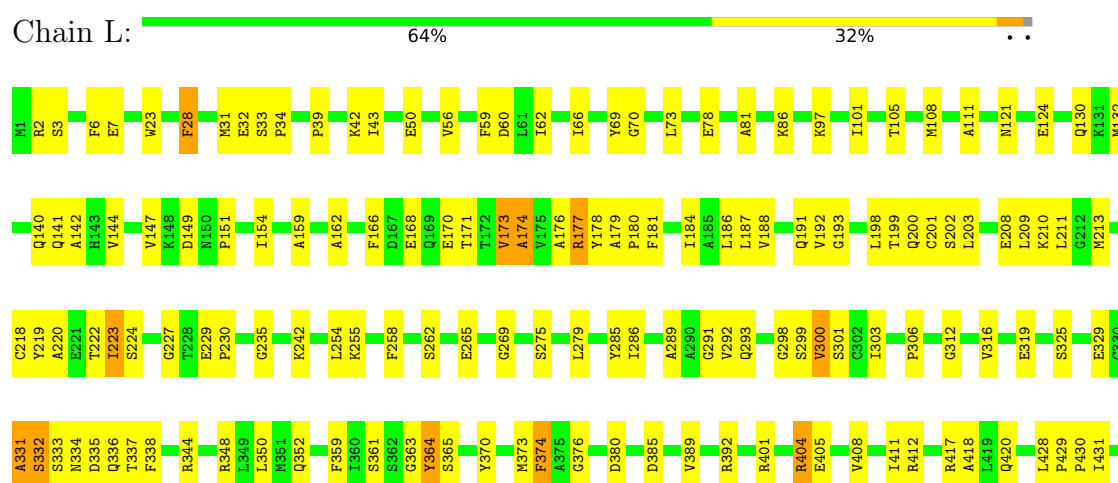
3 Residue-property plots

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

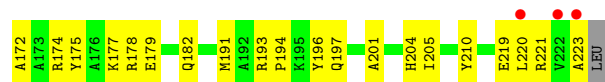
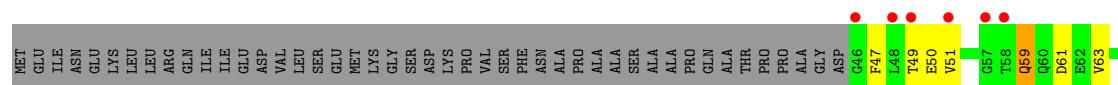


• Molecule 1: diol dehydrase alpha subunit

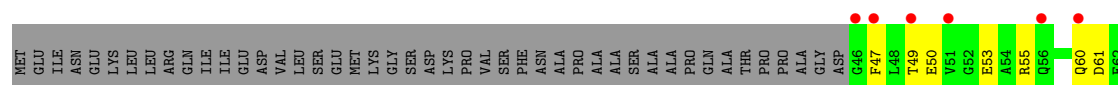




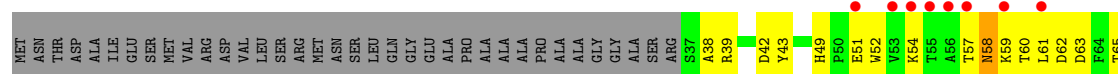
• Molecule 2: diol dehydrase beta subunit



• Molecule 2: diol dehydrase beta subunit

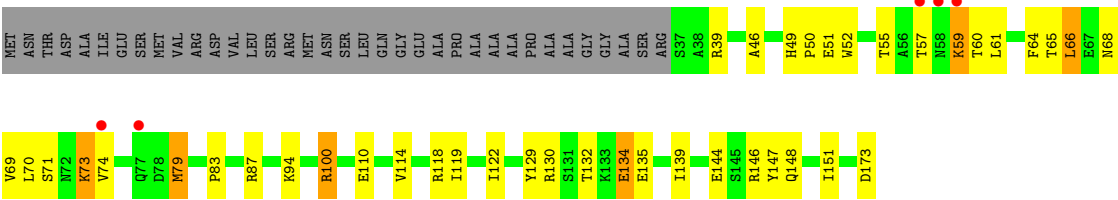


• Molecule 3: diol dehydrase gamma subunit



• 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	74.64Å 122.27Å 207.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.85 – 2.30 46.85 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (46.85-2.30) 83.1 (46.85-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.29Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.208 , 0.255 0.204 , 0.252	Depositor DCC
R_{free} test set	8020 reflections (10.11%)	wwPDB-VP
Wilson B-factor (Å ²)	25.1	Xtriage
Anisotropy	1.325	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 46.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14220	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% 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: CNC, K, PGR, NH4

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	0.43	0/4273	0.98	17/5787 (0.3%)
1	L	0.42	0/4273	0.98	14/5787 (0.2%)
2	B	0.41	0/1380	1.02	4/1868 (0.2%)
2	E	0.39	0/1375	0.99	5/1861 (0.3%)
3	G	0.41	0/1108	0.89	1/1497 (0.1%)
3	M	0.39	0/1107	0.93	2/1495 (0.1%)
All	All	0.41	0/13516	0.97	43/18295 (0.2%)

There are no bond length outliers.

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	154	PHE	CA-C-N	11.42	131.74	119.87
2	B	154	PHE	C-N-CA	11.42	131.74	119.87
1	A	224	SER	N-CA-C	9.10	122.73	110.35
1	L	224	SER	N-CA-C	8.84	122.37	110.35
2	E	154	PHE	CA-C-N	8.50	129.56	120.12
2	E	154	PHE	C-N-CA	8.50	129.56	120.12
1	L	269	GLY	N-CA-C	8.37	125.05	115.08
1	A	269	GLY	N-CA-C	8.05	124.66	115.08
1	A	443	HIS	N-CA-C	-8.01	103.98	114.31
1	L	443	HIS	N-CA-C	-7.41	104.75	114.31
1	L	332	SER	N-CA-C	7.34	122.07	110.70
1	L	174	ALA	N-CA-C	-7.15	102.89	111.69
1	A	173	VAL	N-CA-C	6.78	119.29	108.85
1	L	374	PHE	N-CA-C	-6.58	104.57	112.59
1	A	174	ALA	N-CA-C	-6.50	103.70	111.69
1	A	374	PHE	N-CA-C	-6.40	104.78	112.59
1	A	332	SER	N-CA-C	6.07	123.73	110.80
1	L	173	VAL	N-CA-C	5.99	118.08	108.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	364	TYR	N-CA-C	-5.95	101.04	109.96
1	L	364	TYR	N-CA-C	-5.90	101.11	109.96
1	A	235	GLY	N-CA-C	-5.84	107.67	115.32
3	M	73	LYS	N-CA-C	-5.78	105.48	112.54
1	L	235	GLY	N-CA-C	-5.76	107.78	115.32
2	B	136	GLY	N-CA-C	5.72	120.48	113.79
3	M	79	MET	N-CA-C	5.68	118.99	112.57
2	E	196	TYR	N-CA-C	5.58	121.88	114.12
2	E	136	GLY	N-CA-C	5.54	120.28	113.79
1	A	362	SER	N-CA-C	-5.51	103.32	111.81
1	A	549	ASP	CA-C-N	5.51	125.86	119.47
1	A	549	ASP	C-N-CA	5.51	125.86	119.47
1	A	60	ASP	N-CA-C	-5.48	101.89	110.17
3	G	73	LYS	N-CA-C	-5.45	105.89	112.54
1	A	70	GLY	N-CA-C	5.44	121.40	114.66
1	L	331	ALA	N-CA-C	-5.38	97.74	107.75
1	A	232	PHE	N-CA-C	-5.38	105.50	111.36
1	L	227	GLY	N-CA-C	5.28	120.55	114.16
1	L	60	ASP	N-CA-C	-5.14	102.42	110.17
2	B	81	GLY	N-CA-C	5.09	121.82	115.21
1	A	286	ILE	N-CA-C	-5.06	105.45	110.62
1	A	30	ALA	N-CA-C	5.06	116.48	111.07
1	L	202	SER	N-CA-C	5.04	116.48	108.67
2	E	151	LEU	N-CA-C	-5.04	106.82	113.12
1	L	70	GLY	N-CA-C	5.01	121.89	115.32

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	130	0
1	L	4201	0	4140	160	0
2	B	1358	0	1408	51	0
2	E	1353	0	1403	79	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	1093	0	1101	44	0
3	M	1092	0	1101	49	0
4	A	1	0	0	0	0
4	L	1	0	0	0	0
5	A	2	0	0	0	0
5	L	2	0	0	1	0
6	A	5	0	6	0	0
6	L	5	0	6	0	0
7	B	91	0	87	6	0
7	E	91	0	87	8	0
8	A	267	0	0	14	0
8	B	72	0	0	4	0
8	E	23	0	0	2	0
8	G	70	0	0	1	0
8	L	227	0	0	11	0
8	M	65	0	0	3	0
All	All	14220	0	13479	506	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 19.

All (506) 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:L:453:ILE:HD13	1:L:453:ILE:H	1.14	1.08
1:A:62:ILE:HG23	1:A:286:ILE:HD11	1.41	0.99
2:E:122:ARG:HA	2:E:143:GLN:HE21	1.27	0.97
2:B:121:ASN:C	2:B:121:ASN:HD22	1.74	0.94
2:E:174:ARG:HG2	2:E:181:PRO:HB3	1.49	0.94
1:L:438:ALA:C	1:L:448:MET:HE1	1.95	0.91
2:E:190:GLN:H	2:E:190:GLN:HE21	1.11	0.91
1:L:31:MET:HG3	1:L:32:GLU:HG3	1.52	0.91
2:E:121:ASN:HD22	2:E:122:ARG:N	1.69	0.90
2:E:121:ASN:HD22	2:E:121:ASN:C	1.81	0.88
1:A:489:MET:O	1:A:493:GLN:HG2	1.75	0.86
1:L:477:LEU:HD12	1:L:489:MET:HE2	1.59	0.84
2:E:47:PHE:CD2	2:E:85:LYS:HD3	2.14	0.83
1:L:442:ALA:HB2	1:L:448:MET:HE3	1.60	0.82
3:G:81:ILE:HD12	3:G:86:LEU:HG	1.61	0.81
1:L:173:VAL:HG21	1:L:176:ALA:HA	1.63	0.81
3:G:60:THR:HG22	3:G:63:ASP:CG	2.06	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:489:MET:O	1:A:492:ILE:HG22	1.83	0.79
2:B:140:ILE:HD11	2:B:168:ILE:HG23	1.65	0.79
1:L:453:ILE:H	1:L:453:ILE:CD1	1.90	0.78
1:L:171:THR:HG22	1:L:186:LEU:HD22	1.64	0.78
1:L:493:GLN:OE1	1:L:496:LYS:HD3	1.85	0.75
1:A:220:ALA:HB1	1:A:223:ILE:HD11	1.68	0.75
1:L:499:GLY:HA2	8:L:2729:HOH:O	1.87	0.74
3:G:118:ARG:O	3:G:122:ILE:HG12	1.87	0.74
1:A:23:TRP:HB2	1:L:550:PRO:HG3	1.68	0.74
1:A:282:ARG:O	1:A:286:ILE:HG12	1.88	0.74
2:B:103:ARG:HD2	2:B:219:GLU:OE1	1.88	0.74
2:E:164:THR:O	2:E:168:ILE:HG12	1.88	0.73
1:L:198:LEU:HD21	1:L:508:ILE:HD13	1.69	0.73
3:M:100:ARG:HG3	3:M:100:ARG:HH11	1.53	0.72
2:B:121:ASN:HD22	2:B:122:ARG:N	1.87	0.72
1:A:172:THR:OG1	7:B:1601:CNC:N29	2.21	0.71
1:L:199:THR:H	1:L:218:CYS:HB2	1.55	0.71
3:M:57:THR:HG22	3:M:57:THR:O	1.89	0.71
2:B:121:ASN:C	2:B:121:ASN:ND2	2.49	0.70
1:A:42:LYS:HB2	1:A:50:GLU:HB3	1.72	0.70
1:A:121:ASN:OD1	1:A:124:GLU:HG3	1.91	0.69
2:B:51:VAL:HG23	2:B:51:VAL:O	1.92	0.69
2:E:190:GLN:H	2:E:190:GLN:NE2	1.87	0.69
7:E:2601:CNC:H552	7:E:2601:CNC:H531	1.74	0.69
3:G:134:GLU:CD	3:G:134:GLU:H	2.01	0.69
3:M:122:ILE:HD12	3:M:139:ILE:HG23	1.74	0.68
2:B:61:ASP:OD2	2:B:101:LYS:HE3	1.93	0.68
1:L:66:ILE:HD12	1:L:285:TYR:HB3	1.76	0.68
7:B:1601:CNC:H531	7:B:1601:CNC:H552	1.76	0.68
1:A:420:GLN:HA	1:A:431:ILE:HD12	1.76	0.68
2:E:53:GLU:HB3	2:E:55:ARG:HH12	1.58	0.67
2:E:122:ARG:HA	2:E:143:GLN:NE2	2.05	0.67
1:L:223:ILE:N	1:L:223:ILE:HD12	2.10	0.67
3:M:100:ARG:HG3	3:M:100:ARG:NH1	2.10	0.67
1:L:42:LYS:HB3	1:L:50:GLU:HB3	1.76	0.67
2:B:177:LYS:HE2	2:B:179:GLU:OE2	1.96	0.66
3:G:157:ARG:HD2	8:G:203:HOH:O	1.95	0.66
1:A:86:LYS:HB2	8:A:1854:HOH:O	1.95	0.66
1:L:140:GLN:OE1	1:L:361:SER:HB2	1.95	0.66
3:G:60:THR:HG23	3:G:63:ASP:H	1.61	0.66
3:M:68:ASN:HB3	3:M:74:VAL:HG23	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:88:LEU:O	2:B:92:ILE:HG12	1.96	0.66
2:E:154:PHE:CE2	2:E:168:ILE:HD12	2.31	0.66
2:E:150:ASN:HD22	2:E:152:GLU:N	1.94	0.66
1:L:477:LEU:CD1	1:L:489:MET:HE2	2.26	0.65
3:M:64:PHE:HE1	3:M:79:MET:HG2	1.60	0.65
2:E:95:ILE:HD13	2:E:169:GLY:O	1.97	0.65
1:L:453:ILE:HD13	1:L:453:ILE:N	2.00	0.65
3:M:49:HIS:HB3	3:M:52:TRP:CD1	2.32	0.65
3:M:59:LYS:HB3	3:M:59:LYS:HZ3	1.62	0.65
2:E:121:ASN:C	2:E:121:ASN:ND2	2.49	0.64
1:L:42:LYS:CB	1:L:50:GLU:HB3	2.28	0.64
1:A:392:ARG:CD	1:A:544:ILE:HD12	2.28	0.64
1:L:121:ASN:OD1	1:L:124:GLU:HG3	1.99	0.63
3:M:39:ARG:HH11	3:M:39:ARG:HG2	1.63	0.63
7:B:1601:CNC:H362	7:B:1601:CNC:H351	1.80	0.63
2:E:142:GLN:HB3	2:E:145:LEU:HD22	1.79	0.63
1:L:105:THR:HA	1:L:108:MET:HE3	1.79	0.63
1:L:220:ALA:HB1	1:L:223:ILE:HD11	1.80	0.62
1:A:179:ALA:HB3	1:A:180:PRO:HD3	1.80	0.62
1:A:493:GLN:HB3	8:A:1737:HOH:O	1.99	0.62
1:L:484:ASP:OD1	1:L:485:VAL:HG23	1.98	0.62
2:E:63:VAL:HG23	2:E:100:ILE:HG21	1.80	0.62
2:B:119:GLU:HG2	8:B:1651:HOH:O	2.00	0.62
2:B:201:ALA:O	2:B:205:ILE:HG12	1.99	0.62
2:E:89:ARG:HH21	2:E:90:GLU:HG2	1.64	0.62
7:E:2601:CNC:H362	7:E:2601:CNC:H351	1.82	0.62
1:A:209:LEU:O	1:A:213:MET:HG3	1.99	0.62
1:L:331:ALA:HA	1:L:359:PHE:HB2	1.81	0.62
3:M:147:TYR:C	3:M:148:GLN:HG2	2.24	0.62
1:A:147:VAL:HG12	1:A:373:MET:HE1	1.82	0.62
2:B:63:VAL:HG23	2:B:100:ILE:HG21	1.80	0.62
1:L:329:GLU:OE2	1:L:505:SER:HA	1.99	0.62
3:M:59:LYS:HB3	3:M:59:LYS:NZ	2.15	0.62
1:A:184:ILE:O	1:A:188:VAL:HG23	2.00	0.62
1:A:331:ALA:HA	1:A:359:PHE:HB2	1.82	0.62
2:E:88:LEU:O	2:E:92:ILE:HG12	1.99	0.62
8:L:2759:HOH:O	3:M:100:ARG:HD3	2.00	0.62
3:M:132:THR:OG1	3:M:134:GLU:HG3	1.99	0.62
1:L:210:LYS:NZ	1:L:467:ASN:HD21	1.98	0.61
1:L:473:VAL:HG12	1:L:489:MET:HE1	1.82	0.61
2:E:191:MET:C	2:E:194:PRO:HD2	2.25	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:GLU:HG3	8:A:1645:HOH:O	1.99	0.61
1:L:66:ILE:HD12	1:L:285:TYR:CB	2.30	0.61
3:G:51:GLU:CD	3:G:51:GLU:H	2.09	0.61
1:L:493:GLN:HE21	3:M:79:MET:HB3	1.65	0.61
3:M:65:THR:O	3:M:69:VAL:HG23	2.00	0.60
1:A:223:ILE:HD12	1:A:223:ILE:N	2.17	0.60
1:L:392:ARG:CD	1:L:544:ILE:HD12	2.31	0.60
3:G:57:THR:HG21	3:G:78:ASP:OD1	2.00	0.60
1:A:162:ALA:HB3	1:A:193:GLY:HA3	1.84	0.60
3:M:118:ARG:O	3:M:122:ILE:HG12	2.01	0.60
1:A:494:LYS:HE3	3:G:61:LEU:O	2.01	0.60
1:L:69:TYR:HB2	1:L:289:ALA:HB1	1.82	0.60
1:A:97:LYS:O	1:A:101:ILE:HG12	2.02	0.60
1:L:418:ALA:HA	1:L:482:PHE:CE2	2.37	0.60
1:A:148:LYS:HE3	8:A:1821:HOH:O	2.02	0.59
1:L:265:GLU:HG2	1:L:279:LEU:HD13	1.84	0.59
2:E:190:GLN:HE21	2:E:190:GLN:N	1.92	0.59
2:B:193:ARG:HG3	2:B:197:GLN:HB2	1.84	0.59
1:L:442:ALA:CB	1:L:448:MET:HE3	2.30	0.59
1:L:177:ARG:HB3	1:L:457:ILE:HG23	1.83	0.59
1:A:105:THR:HA	1:A:108:MET:HE3	1.85	0.59
1:L:507:ILE:C	1:L:508:ILE:HD12	2.28	0.59
1:A:140:GLN:OE1	1:A:361:SER:HB2	2.03	0.59
2:B:118:VAL:O	2:B:122:ARG:HG3	2.03	0.59
3:G:122:ILE:HD12	3:G:139:ILE:HG23	1.85	0.59
1:L:448:MET:HE2	1:L:448:MET:HA	1.85	0.59
1:A:180:PRO:HG3	1:A:464:ILE:HD11	1.84	0.59
3:M:66:LEU:HD22	3:M:70:LEU:HG	1.84	0.59
1:A:86:LYS:HG3	8:A:1827:HOH:O	2.03	0.59
1:L:392:ARG:HD3	1:L:544:ILE:HD12	1.85	0.59
1:L:439:ALA:N	1:L:448:MET:HE1	2.18	0.58
1:L:474:VAL:HG22	1:L:489:MET:HE3	1.84	0.58
1:A:418:ALA:O	1:A:422:VAL:HG23	2.04	0.58
2:B:59:GLN:NE2	2:B:101:LYS:NZ	2.52	0.58
3:G:43:TYR:HB2	3:G:92:ILE:HD13	1.86	0.58
1:A:418:ALA:HA	1:A:482:PHE:CE2	2.39	0.58
3:G:133:LYS:HD2	3:G:164:VAL:HG21	1.84	0.58
1:A:439:ALA:HB2	1:A:448:MET:HE1	1.86	0.58
2:E:49:THR:OG1	2:E:221:ARG:HB3	2.04	0.57
3:M:114:VAL:HB	3:M:119:ILE:HD11	1.86	0.57
2:E:71:PHE:CE1	2:E:84:HIS:HB3	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:104:VAL:HG12	2:E:220:LEU:HD12	1.85	0.57
1:L:179:ALA:HB3	1:L:180:PRO:HD3	1.85	0.57
3:M:64:PHE:CE1	3:M:79:MET:HG2	2.39	0.57
1:A:97:LYS:HB2	1:A:100:GLU:HG3	1.86	0.57
1:A:392:ARG:HD3	1:A:544:ILE:HD12	1.86	0.57
2:B:59:GLN:NE2	2:B:101:LYS:HZ1	2.03	0.56
2:B:130:ILE:HD11	2:B:172:ALA:HB2	1.87	0.56
1:L:62:ILE:O	1:L:66:ILE:HG12	2.05	0.56
1:A:199:THR:H	1:A:218:CYS:HB2	1.69	0.56
3:G:146:ARG:HG2	3:G:147:TYR:CE2	2.40	0.56
3:M:144:GLU:O	3:M:148:GLN:HA	2.04	0.56
2:B:87:ILE:O	2:B:91:VAL:HG23	2.05	0.56
1:L:336:GLN:HE22	1:L:374:PHE:HB3	1.68	0.56
3:M:60:THR:HG22	3:M:61:LEU:N	2.19	0.56
1:L:159:ALA:HB1	1:L:411:ILE:HG22	1.87	0.56
2:E:83:PRO:HG2	2:E:86:SER:OG	2.05	0.56
1:L:408:VAL:O	1:L:412:ARG:HG2	2.05	0.56
1:A:266:VAL:HG23	8:A:1707:HOH:O	2.06	0.56
1:A:316:VAL:O	1:A:319:GLU:HG2	2.06	0.56
1:L:219:TYR:HB2	1:L:255:LYS:O	2.06	0.56
1:L:392:ARG:HD2	1:L:544:ILE:HG23	1.88	0.56
1:L:533:LEU:HD11	1:L:541:ILE:HD12	1.87	0.56
1:L:62:ILE:HG23	1:L:286:ILE:HD11	1.88	0.56
1:L:147:VAL:HG22	2:E:186:THR:HB	1.88	0.56
1:L:209:LEU:O	1:L:213:MET:HG3	2.06	0.56
1:L:493:GLN:HG2	8:L:2831:HOH:O	2.05	0.56
1:A:33:SER:HB3	1:A:275:SER:HB3	1.87	0.55
1:A:220:ALA:CB	1:A:223:ILE:HD11	2.35	0.55
1:A:139:SER:HA	8:A:1729:HOH:O	2.07	0.55
1:A:299:SER:OG	1:A:303:ILE:HA	2.06	0.55
1:A:334:ASN:ND2	1:A:349:LEU:HA	2.21	0.55
2:E:148:LEU:HD13	7:E:2601:CNC:H411	1.88	0.55
3:M:151:ILE:N	3:M:151:ILE:HD12	2.22	0.55
2:B:59:GLN:HE21	2:B:101:LYS:NZ	2.05	0.55
3:G:132:THR:OG1	3:G:135:GLU:HG3	2.07	0.55
3:G:68:ASN:C	3:G:74:VAL:HG22	2.32	0.55
1:A:485:VAL:O	1:A:489:MET:HG2	2.07	0.55
1:A:82:MET:HE3	1:A:86:LYS:NZ	2.22	0.55
1:A:173:VAL:HG21	1:A:176:ALA:HA	1.88	0.55
1:L:56:VAL:HA	1:L:59:PHE:CD1	2.42	0.55
3:M:122:ILE:HD12	3:M:139:ILE:CG2	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:141:GLN:HG3	1:L:168:GLU:HB3	1.87	0.54
2:E:61:ASP:O	2:E:100:ILE:HG23	2.07	0.54
1:A:356:GLY:HA2	1:A:360:ILE:HD11	1.89	0.54
1:L:428:LEU:HD22	1:L:459:PHE:HB3	1.90	0.54
2:E:79:ILE:HG23	2:E:80:VAL:HG13	1.89	0.54
1:L:162:ALA:HB3	1:L:193:GLY:HA3	1.89	0.54
2:B:50:GLU:HG2	2:B:220:LEU:CD2	2.37	0.54
2:E:86:SER:HB3	2:E:162:LEU:HD11	1.88	0.54
1:A:7:GLU:O	1:A:11:LYS:HG3	2.08	0.54
1:A:329:GLU:OE2	1:A:505:SER:HA	2.08	0.54
1:L:332:SER:HB2	1:L:352:GLN:HG2	1.89	0.54
1:L:545:PRO:HG2	8:L:2664:HOH:O	2.08	0.54
1:A:69:TYR:HB2	1:A:289:ALA:HB1	1.90	0.53
1:A:188:VAL:O	1:A:192:VAL:HG23	2.07	0.53
1:L:484:ASP:OD1	1:L:485:VAL:N	2.38	0.53
1:A:180:PRO:O	1:A:184:ILE:HG13	2.08	0.53
3:G:74:VAL:HA	3:G:78:ASP:OD2	2.08	0.53
1:L:184:ILE:O	1:L:188:VAL:HG23	2.09	0.53
1:A:453:ILE:O	1:A:457:ILE:HG12	2.08	0.53
1:L:208:GLU:OE1	5:L:2605:NH4:N	2.42	0.53
3:M:39:ARG:HG2	3:M:39:ARG:NH1	2.24	0.53
1:L:453:ILE:HD11	2:E:182:GLN:OE1	2.09	0.53
3:M:46:ALA:O	3:M:50:PRO:HG3	2.09	0.53
3:M:129:TYR:CD2	3:M:173:ASP:HB3	2.43	0.53
1:L:33:SER:CB	1:L:275:SER:HB3	2.39	0.53
2:E:174:ARG:HG2	2:E:181:PRO:CB	2.31	0.53
1:A:334:ASN:ND2	1:A:348:ARG:HD3	2.24	0.52
3:G:134:GLU:CD	3:G:134:GLU:N	2.67	0.52
2:B:130:ILE:HD11	2:B:172:ALA:CB	2.39	0.52
1:L:466:LYS:HB2	1:L:466:LYS:NZ	2.24	0.52
1:A:334:ASN:HD21	1:A:349:LEU:HA	1.75	0.52
1:A:357:THR:H	1:A:360:ILE:HD13	1.75	0.52
3:M:132:THR:OG1	3:M:135:GLU:HG3	2.09	0.52
1:A:386:ASP:O	1:A:390:ILE:HG12	2.10	0.52
1:A:390:ILE:HD11	1:L:344:ARG:HA	1.91	0.52
1:L:299:SER:OG	1:L:303:ILE:HA	2.10	0.52
1:A:198:LEU:HD21	1:A:508:ILE:HD13	1.92	0.52
2:B:210:TYR:HA	8:B:1639:HOH:O	2.10	0.52
1:L:370:TYR:OH	1:L:444:GLY:HA3	2.09	0.52
1:A:54:LYS:HG3	8:A:1804:HOH:O	2.09	0.52
2:B:77:VAL:HG12	2:B:83:PRO:HA	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:57:THR:O	3:M:57:THR:CG2	2.57	0.51
2:B:191:MET:C	2:B:194:PRO:HD2	2.34	0.51
2:E:100:ILE:HD11	2:E:177:LYS:HD2	1.91	0.51
2:E:193:ARG:HB3	2:E:194:PRO:HD3	1.92	0.51
1:L:210:LYS:HZ1	1:L:467:ASN:HD21	1.58	0.51
1:A:538:TRP:CE2	1:A:542:LYS:HD3	2.45	0.51
1:L:508:ILE:HD12	1:L:508:ILE:N	2.26	0.51
2:E:99:GLY:C	2:E:100:ILE:HD12	2.34	0.51
1:A:1:MET:HB3	8:A:1831:HOH:O	2.10	0.51
1:A:318:ALA:O	1:A:322:ILE:HG12	2.10	0.51
1:A:356:GLY:HA2	1:A:360:ILE:CD1	2.40	0.51
3:G:49:HIS:HB3	3:G:52:TRP:CD1	2.45	0.51
3:G:54:LYS:HD3	3:G:59:LYS:O	2.11	0.51
1:L:463:ILE:HG23	1:L:468:ARG:HB2	1.91	0.51
2:E:100:ILE:CD1	2:E:177:LYS:HD2	2.41	0.50
1:L:538:TRP:O	1:L:542:LYS:HG3	2.12	0.50
3:G:60:THR:HG22	3:G:63:ASP:OD2	2.12	0.50
2:B:107:CYS:HB3	2:B:119:GLU:OE1	2.12	0.50
2:E:193:ARG:HG3	2:E:197:GLN:HB2	1.92	0.50
2:B:193:ARG:HB3	2:B:194:PRO:HD3	1.94	0.50
1:L:291:GLY:HA2	3:M:100:ARG:HB3	1.92	0.50
1:L:300:VAL:HG12	1:L:301:SER:N	2.26	0.50
1:A:20:VAL:HG22	1:A:308:ALA:HB1	1.93	0.50
1:A:545:PRO:HG2	8:A:1728:HOH:O	2.11	0.50
7:E:2601:CNC:H492	7:E:2601:CNC:O6R	2.11	0.50
1:A:82:MET:HE3	1:A:86:LYS:HZ1	1.77	0.50
1:A:417:ARG:NH1	1:A:417:ARG:HB2	2.27	0.50
1:L:473:VAL:CG1	1:L:489:MET:HE1	2.40	0.50
1:L:132:MET:HE3	1:L:325:SER:HA	1.94	0.49
1:A:42:LYS:HD3	1:A:50:GLU:CD	2.38	0.49
2:B:112:ASP:O	2:B:116:VAL:HG23	2.13	0.49
1:L:187:LEU:O	1:L:191:GLN:HG2	2.11	0.49
1:A:370:TYR:OH	1:A:444:GLY:HA3	2.12	0.49
1:L:149:ASP:O	1:L:151:PRO:HD3	2.11	0.49
1:L:493:GLN:OE1	1:L:493:GLN:HA	2.12	0.49
2:B:47:PHE:O	2:B:223:ALA:N	2.43	0.49
1:A:298:GLY:N	1:A:319:GLU:OE2	2.40	0.49
3:M:147:TYR:O	3:M:148:GLN:HG2	2.11	0.49
1:A:391:GLN:NE2	1:A:541:ILE:HD12	2.28	0.49
1:A:102:VAL:HB	1:A:103:PRO:HD3	1.93	0.49
1:L:142:ALA:HB2	1:L:166:PHE:CD1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:108:PHE:O	2:E:211:VAL:HG13	2.13	0.49
2:E:179:GLU:HB3	8:E:2623:HOH:O	2.12	0.49
2:B:100:ILE:HD13	2:B:177:LYS:HD2	1.95	0.48
3:G:146:ARG:O	3:G:146:ARG:HG3	2.11	0.48
1:L:223:ILE:N	1:L:223:ILE:CD1	2.76	0.48
2:E:153:LEU:HG	2:E:155:PRO:HD3	1.95	0.48
2:B:100:ILE:CD1	2:B:177:LYS:HD2	2.44	0.48
3:G:75:THR:N	3:G:78:ASP:OD2	2.39	0.48
2:E:47:PHE:O	2:E:222:VAL:HA	2.13	0.48
1:L:177:ARG:HD2	1:L:457:ILE:CG2	2.43	0.48
1:L:223:ILE:HG22	1:L:242:LYS:HD2	1.94	0.48
2:B:93:ALA:O	2:B:97:GLU:HB2	2.13	0.48
1:L:130:GLN:NE2	1:L:524:TYR:CZ	2.81	0.48
1:L:334:ASN:ND2	1:L:348:ARG:HD3	2.28	0.48
2:E:87:ILE:HG23	2:E:165:TYR:CG	2.48	0.48
2:E:198:ALA:O	2:E:202:ILE:HG12	2.13	0.48
2:E:47:PHE:HE2	2:E:88:LEU:HD23	1.79	0.48
2:B:100:ILE:HD11	2:B:177:LYS:HG3	1.96	0.48
1:L:429:PRO:HD3	1:L:459:PHE:CG	2.49	0.48
1:A:417:ARG:CB	1:A:417:ARG:HH11	2.27	0.48
1:L:549:ASP:C	1:L:551:ASN:H	2.21	0.48
2:E:95:ILE:HG21	2:E:102:ALA:HB2	1.96	0.48
1:A:150:ASN:O	1:A:154:ILE:HG12	2.14	0.47
2:B:122:ARG:HG2	2:B:122:ARG:HH11	1.79	0.47
3:G:38:ALA:HB2	3:G:52:TRP:HZ3	1.79	0.47
1:L:142:ALA:HB2	1:L:166:PHE:CE1	2.49	0.47
1:L:337:THR:HG23	1:L:376:GLY:C	2.39	0.47
1:L:420:GLN:HA	1:L:431:ILE:HD12	1.96	0.47
3:M:110:GLU:OE2	3:M:151:ILE:HD13	2.14	0.47
1:L:453:ILE:O	1:L:457:ILE:HG12	2.14	0.47
3:M:83:PRO:O	3:M:87:ARG:HG3	2.14	0.47
2:B:104:VAL:HG12	2:B:220:LEU:HD12	1.97	0.47
1:L:81:ALA:HB3	8:L:2725:HOH:O	2.14	0.47
1:A:142:ALA:HB2	1:A:166:PHE:CD1	2.49	0.47
1:A:373:MET:HA	1:A:373:MET:HE2	1.97	0.47
3:G:68:ASN:O	3:G:74:VAL:HG22	2.15	0.47
1:L:33:SER:HB3	1:L:275:SER:HB3	1.96	0.47
1:L:97:LYS:O	1:L:101:ILE:HG12	2.14	0.47
1:L:300:VAL:HG12	1:L:301:SER:H	1.79	0.47
1:L:420:GLN:HB3	8:L:2817:HOH:O	2.13	0.47
3:M:60:THR:CG2	3:M:61:LEU:N	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:98:GLU:OE1	2:B:174:ARG:HD3	2.15	0.47
3:G:71:SER:OG	3:G:73:LYS:HG3	2.14	0.47
2:E:174:ARG:NH1	2:E:181:PRO:HB3	2.30	0.47
2:E:189:ASP:HB3	2:E:192:ALA:HB2	1.97	0.47
2:B:140:ILE:HG13	2:B:152:GLU:HB2	1.96	0.47
1:A:257:ARG:HH21	1:A:329:GLU:CD	2.23	0.46
2:E:107:CYS:HB3	2:E:119:GLU:OE1	2.15	0.46
3:M:151:ILE:CD1	3:M:151:ILE:H	2.28	0.46
2:E:87:ILE:HG23	2:E:165:TYR:CD2	2.50	0.46
2:E:100:ILE:HD11	2:E:177:LYS:CG	2.45	0.46
1:A:332:SER:HB2	1:A:352:GLN:HG2	1.96	0.46
1:A:147:VAL:HG12	1:A:373:MET:CE	2.45	0.46
2:E:91:VAL:O	2:E:95:ILE:HG12	2.15	0.46
1:A:251:SER:HA	3:G:86:LEU:HD11	1.96	0.46
1:A:550:PRO:HB3	2:E:202:ILE:HD12	1.97	0.46
1:A:350:LEU:HA	1:A:353:PHE:HB3	1.97	0.46
1:L:220:ALA:CB	1:L:223:ILE:HD11	2.45	0.46
2:E:174:ARG:HD2	2:E:179:GLU:OE1	2.15	0.46
1:A:1:MET:HG2	1:L:441:TYR:CZ	2.51	0.46
3:G:153:ALA:O	3:G:157:ARG:HG3	2.16	0.46
1:L:370:TYR:CD1	1:L:370:TYR:C	2.93	0.46
1:A:489:MET:HE3	1:A:489:MET:HB3	1.90	0.46
1:L:23:TRP:HB3	1:L:28:PHE:HB2	1.98	0.46
1:A:29:ILE:C	1:A:276:MET:HE3	2.41	0.46
3:G:122:ILE:HD12	3:G:139:ILE:CG2	2.46	0.46
1:L:262:SER:HA	8:L:2672:HOH:O	2.14	0.46
1:A:141:GLN:HB3	1:A:362:SER:HA	1.98	0.45
1:L:2:ARG:HD2	8:L:2741:HOH:O	2.15	0.45
2:E:47:PHE:HD2	2:E:222:VAL:HG13	1.81	0.45
1:A:293:GLN:OE1	1:A:504:THR:HA	2.16	0.45
1:A:365:SER:HB2	1:A:377:SER:HB3	1.98	0.45
1:A:543:ASN:C	1:A:543:ASN:ND2	2.72	0.45
1:L:177:ARG:CB	1:L:457:ILE:HG23	2.46	0.45
3:G:39:ARG:O	3:G:42:ASP:N	2.48	0.45
1:L:334:ASN:ND2	1:L:348:ARG:CZ	2.79	0.45
1:L:550:PRO:O	1:L:551:ASN:HB2	2.16	0.45
3:M:71:SER:OG	3:M:73:LYS:HG3	2.17	0.45
1:L:33:SER:OG	1:L:34:PRO:HD2	2.17	0.45
1:L:380:ASP:OD1	1:L:380:ASP:C	2.58	0.45
1:A:117:VAL:HG21	1:A:322:ILE:HD11	1.98	0.45
3:G:57:THR:O	3:G:58:ASN:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:68:ASN:HB3	3:G:74:VAL:HG22	1.98	0.45
2:B:106:ARG:HD2	2:B:108:PHE:CZ	2.51	0.45
2:B:204:HIS:HD2	8:B:1630:HOH:O	1.98	0.45
1:L:42:LYS:HB2	1:L:50:GLU:HB3	1.99	0.45
3:M:55:THR:HG22	8:M:235:HOH:O	2.16	0.45
3:G:110:GLU:OE2	3:G:151:ILE:HG12	2.17	0.45
1:L:188:VAL:O	1:L:192:VAL:HG23	2.17	0.45
1:L:447:ASP:O	1:L:448:MET:HE2	2.17	0.45
1:A:219:TYR:HB2	1:A:255:LYS:O	2.17	0.45
2:B:50:GLU:HG2	2:B:220:LEU:HD21	1.99	0.45
2:E:50:GLU:HG3	2:E:218:GLN:HB3	1.99	0.45
2:E:71:PHE:CD1	2:E:71:PHE:C	2.94	0.45
1:A:23:TRP:HB2	1:L:550:PRO:CG	2.43	0.44
1:A:543:ASN:C	1:A:543:ASN:HD22	2.23	0.44
2:E:77:VAL:HG12	2:E:83:PRO:HA	1.98	0.44
2:E:100:ILE:HD12	2:E:100:ILE:N	2.33	0.44
2:E:130:ILE:HD11	2:E:172:ALA:CB	2.47	0.44
1:A:160:GLU:OE1	1:A:412:ARG:HD2	2.18	0.44
3:M:55:THR:C	3:M:57:THR:H	2.24	0.44
1:L:210:LYS:NZ	1:L:467:ASN:ND2	2.64	0.44
3:G:124:ASN:O	3:G:130:ARG:HG3	2.17	0.44
1:L:222:THR:O	7:E:2601:CNC:N40	2.51	0.44
1:L:404:ARG:CB	1:L:404:ARG:HH11	2.31	0.44
2:E:60:GLN:C	2:E:60:GLN:CD	2.86	0.44
1:A:142:ALA:HB2	1:A:166:PHE:CE1	2.53	0.44
1:A:265:GLU:HG2	1:A:279:LEU:HD13	2.00	0.44
3:G:54:LYS:O	3:G:82:THR:HG21	2.17	0.44
1:L:33:SER:HB2	1:L:275:SER:HB3	2.00	0.44
1:L:170:GLU:HB2	1:L:200:GLN:CG	2.47	0.44
3:M:146:ARG:HD2	3:M:147:TYR:CE2	2.52	0.44
1:A:538:TRP:O	1:A:542:LYS:HG3	2.18	0.44
1:A:6:PHE:CZ	1:L:405:GLU:HA	2.53	0.44
1:A:205:GLU:OE1	1:A:205:GLU:HA	2.18	0.44
1:A:365:SER:HB3	1:A:380:ASP:HA	2.00	0.44
1:L:454:VAL:HG23	2:E:182:GLN:NE2	2.33	0.44
2:E:66:ALA:HB1	2:E:107:CYS:SG	2.58	0.44
2:E:157:ALA:N	2:E:158:PRO:CD	2.81	0.44
1:A:278:TYR:O	1:A:281:ALA:HB3	2.17	0.44
2:B:106:ARG:HD2	2:B:108:PHE:CE2	2.53	0.44
2:B:128:ILE:HD12	2:B:128:ILE:N	2.32	0.44
7:B:1601:CNC:H531	7:B:1601:CNC:C55	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:65:THR:OG1	3:G:68:ASN:ND2	2.51	0.44
1:L:39:PRO:HG3	1:L:111:ALA:C	2.43	0.44
2:E:83:PRO:HG2	2:E:86:SER:CB	2.48	0.44
2:E:63:VAL:HG13	2:E:128:ILE:HG22	2.00	0.43
1:A:540:GLU:HG3	8:A:1866:HOH:O	2.19	0.43
2:B:73:LEU:HD13	8:B:1655:HOH:O	2.16	0.43
1:L:144:VAL:HG12	1:L:154:ILE:HG23	1.98	0.43
1:L:429:PRO:HA	1:L:430:PRO:HD2	1.74	0.43
3:M:57:THR:HB	3:M:59:LYS:HG2	1.98	0.43
1:A:127:MET:O	1:A:130:GLN:HG2	2.19	0.43
2:B:175:TYR:O	2:B:178:ARG:HD3	2.18	0.43
1:L:151:PRO:HG2	1:L:181:PHE:HD2	1.82	0.43
2:E:75:GLN:NE2	2:E:134:SER:HB3	2.34	0.43
3:M:100:ARG:HD2	8:M:182:HOH:O	2.16	0.43
1:A:1:MET:HG2	1:L:441:TYR:CE2	2.54	0.43
2:E:191:MET:HA	2:E:191:MET:HE2	2.00	0.43
3:G:52:TRP:HE3	3:G:88:LEU:HD13	1.84	0.43
3:M:151:ILE:HD12	3:M:151:ILE:H	1.83	0.43
1:L:408:VAL:O	1:L:412:ARG:CG	2.65	0.43
2:E:47:PHE:HD1	2:E:47:PHE:H	1.67	0.43
1:L:56:VAL:HA	1:L:59:PHE:CE1	2.54	0.43
3:M:49:HIS:HB3	3:M:52:TRP:CG	2.54	0.43
1:L:174:ALA:HA	1:L:373:MET:HE2	1.99	0.43
3:M:151:ILE:N	3:M:151:ILE:CD1	2.81	0.43
1:A:229:GLU:N	1:A:230:PRO:HD2	2.33	0.43
1:A:489:MET:O	1:A:492:ILE:CG2	2.61	0.43
1:A:523:ASP:OD1	1:A:523:ASP:N	2.51	0.43
1:L:78:GLU:HB2	8:L:2696:HOH:O	2.18	0.43
3:G:49:HIS:HB3	3:G:52:TRP:CG	2.54	0.43
1:L:385:ASP:HB2	8:L:2608:HOH:O	2.19	0.43
1:L:417:ARG:HE	1:L:417:ARG:HB2	1.60	0.43
2:E:142:GLN:O	2:E:145:LEU:HB2	2.18	0.43
1:L:303:ILE:HG23	1:L:338:PHE:HB3	2.00	0.42
1:L:333:SER:O	1:L:361:SER:HA	2.19	0.42
3:M:57:THR:HG22	3:M:59:LYS:HD3	2.01	0.42
1:A:62:ILE:O	1:A:66:ILE:HG13	2.19	0.42
3:G:89:GLN:OE1	3:G:89:GLN:HA	2.18	0.42
1:L:242:LYS:HD3	1:L:242:LYS:HA	1.77	0.42
1:L:463:ILE:HA	1:L:468:ARG:HD3	2.00	0.42
7:E:2601:CNC:H531	7:E:2601:CNC:C55	2.45	0.42
1:A:306:PRO:O	1:A:312:GLY:HA3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:537:ARG:CZ	1:A:541:ILE:HD11	2.49	0.42
1:A:544:ILE:HB	1:A:545:PRO:HD2	2.01	0.42
1:L:258:PHE:CZ	1:L:292:VAL:HG21	2.54	0.42
1:L:549:ASP:C	1:L:551:ASN:N	2.78	0.42
1:A:200:GLN:HE22	1:A:221:GLU:HB3	1.85	0.42
2:B:79:ILE:HG23	2:B:80:VAL:HG13	2.01	0.42
2:B:127:GLY:C	2:B:128:ILE:HD12	2.45	0.42
2:B:148:LEU:HD13	7:B:1601:CNC:H411	1.99	0.42
1:L:254:LEU:HD21	8:L:2778:HOH:O	2.19	0.42
1:L:316:VAL:O	1:L:319:GLU:HG2	2.19	0.42
1:L:335:ASP:C	1:L:336:GLN:HG2	2.44	0.42
7:E:2601:CNC:H421	7:E:2601:CNC:C10	2.49	0.42
1:A:25:GLU:N	1:A:25:GLU:CD	2.78	0.42
1:L:223:ILE:CG2	1:L:242:LYS:HD2	2.49	0.42
1:L:229:GLU:HB3	1:L:230:PRO:HD3	2.01	0.42
1:A:381:ALA:HA	1:A:384:PHE:CE2	2.54	0.42
1:L:298:GLY:N	1:L:319:GLU:OE2	2.48	0.42
1:L:476:ALA:HA	1:L:479:GLN:HG2	2.02	0.42
2:E:100:ILE:HG22	2:E:101:LYS:O	2.20	0.42
2:E:200:SER:HB2	7:E:2601:CNC:H3P1	2.01	0.42
1:A:350:LEU:O	1:A:354:LEU:HG	2.20	0.42
1:L:159:ALA:HB1	1:L:411:ILE:CG2	2.50	0.42
1:L:293:GLN:OE1	1:L:504:THR:HA	2.19	0.42
1:L:306:PRO:O	1:L:312:GLY:HA3	2.20	0.42
2:B:106:ARG:HB2	2:B:220:LEU:HD11	2.01	0.42
1:L:43:ILE:HD13	1:L:73:LEU:HB3	2.01	0.42
1:L:258:PHE:CE2	1:L:292:VAL:HG21	2.55	0.42
1:L:365:SER:O	1:L:380:ASP:HA	2.20	0.42
2:E:106:ARG:HB2	2:E:220:LEU:HD11	2.02	0.42
2:E:174:ARG:HG3	2:E:179:GLU:HB2	2.01	0.42
2:E:162:LEU:HD23	2:E:162:LEU:HA	1.85	0.42
1:A:364:TYR:CD1	1:A:364:TYR:C	2.97	0.42
1:L:334:ASN:ND2	1:L:348:ARG:NH1	2.68	0.42
1:L:550:PRO:O	1:L:551:ASN:CB	2.68	0.42
2:E:90:GLU:OE1	2:E:166:ARG:HD2	2.20	0.42
1:A:301:SER:HB3	7:B:1601:CNC:H532	2.02	0.41
1:L:201:CYS:SG	1:L:203:LEU:HD21	2.60	0.41
1:A:155:ALA:HB2	1:A:419:LEU:HD22	2.02	0.41
1:A:408:VAL:HG21	1:L:6:PHE:CZ	2.55	0.41
3:G:135:GLU:O	3:G:139:ILE:HG13	2.19	0.41
1:A:489:MET:C	1:A:492:ILE:HG22	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:49:THR:HG21	2:B:221:ARG:HH12	1.85	0.41
1:L:3:SER:O	1:L:7:GLU:HG3	2.20	0.41
2:E:78:ASN:HD21	2:E:80:VAL:HG22	1.85	0.41
3:M:57:THR:CG2	3:M:59:LYS:HD3	2.50	0.41
1:A:151:PRO:HB3	8:A:1636:HOH:O	2.19	0.41
2:E:121:ASN:OD1	2:E:143:GLN:HA	2.20	0.41
3:G:102:ALA:O	3:G:106:GLU:HG2	2.21	0.41
1:L:229:GLU:N	1:L:230:PRO:CD	2.83	0.41
1:L:473:VAL:HG12	1:L:489:MET:CE	2.49	0.41
1:A:416:ALA:HB3	1:A:436:VAL:HG13	2.01	0.41
1:A:463:ILE:HG23	1:A:468:ARG:HB2	2.03	0.41
3:G:57:THR:O	3:G:58:ASN:CB	2.69	0.41
2:B:130:ILE:HD13	2:B:168:ILE:HG22	2.01	0.41
1:L:385:ASP:O	1:L:389:VAL:HG23	2.20	0.41
2:E:77:VAL:HG22	8:E:2620:HOH:O	2.20	0.41
3:M:94:LYS:HB3	8:M:215:HOH:O	2.20	0.41
1:A:404:ARG:HB3	1:A:406:GLU:HG2	2.03	0.41
3:G:62:ASP:O	3:G:65:THR:HG23	2.21	0.41
3:G:114:VAL:HB	3:G:119:ILE:HD11	2.03	0.41
1:L:532:ARG:O	1:L:534:GLN:HG2	2.21	0.41
2:E:167:GLN:OE1	2:E:167:GLN:HA	2.20	0.41
3:M:147:TYR:O	3:M:148:GLN:CG	2.69	0.41
1:A:57:SER:HB3	8:A:1749:HOH:O	2.19	0.41
2:B:79:ILE:HD11	2:B:196:TYR:HB3	2.02	0.41
2:B:100:ILE:HD11	2:B:177:LYS:CG	2.51	0.41
3:G:65:THR:O	3:G:69:VAL:HG23	2.20	0.41
1:L:211:LEU:HD23	1:L:211:LEU:HA	1.88	0.41
1:A:276:MET:SD	1:A:306:PRO:HB3	2.61	0.41
1:L:401:ARG:HB3	1:L:537:ARG:HH12	1.86	0.41
1:A:139:SER:HB3	1:A:358:ASP:O	2.21	0.40
3:M:130:ARG:HH11	3:M:130:ARG:HG2	1.86	0.40
1:A:42:LYS:HD3	1:A:50:GLU:OE2	2.21	0.40
2:E:47:PHE:CG	2:E:85:LYS:HD3	2.55	0.40
1:A:173:VAL:CG2	1:A:176:ALA:HA	2.51	0.40
3:M:51:GLU:CD	3:M:51:GLU:H	2.29	0.40
1:A:176:ALA:HB3	8:A:1672:HOH:O	2.21	0.40
1:A:221:GLU:HG3	1:A:257:ARG:HD2	2.03	0.40
1:L:173:VAL:CG2	1:L:176:ALA:HA	2.41	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%)	518 (94%)	28 (5%)	3 (0%)	24	31
1	L	549/554 (99%)	517 (94%)	29 (5%)	3 (0%)	24	31
2	B	176/224 (79%)	167 (95%)	9 (5%)	0	100	100
2	E	175/224 (78%)	168 (96%)	7 (4%)	0	100	100
3	G	135/173 (78%)	131 (97%)	3 (2%)	1 (1%)	18	23
3	M	135/173 (78%)	130 (96%)	5 (4%)	0	100	100
All	All	1719/1902 (90%)	1631 (95%)	81 (5%)	7 (0%)	30	38

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	58	ASN
1	A	363	GLY
1	L	177	ARG
1	L	363	GLY
1	A	177	ARG
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%)	442 (98%)	8 (2%)	51	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	450/453 (99%)	435 (97%)	15 (3%)	33	50
2	B	146/183 (80%)	142 (97%)	4 (3%)	39	58
2	E	146/183 (80%)	141 (97%)	5 (3%)	32	49
3	G	116/141 (82%)	113 (97%)	3 (3%)	40	59
3	M	116/141 (82%)	112 (97%)	4 (3%)	32	49
All	All	1424/1554 (92%)	1385 (97%)	39 (3%)	39	58

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	ILE
1	A	178	TYR
1	A	352	GLN
1	A	364	TYR
1	A	492	ILE
1	A	501	TYR
1	A	521	VAL
1	A	544	ILE
2	B	59	GLN
2	B	121	ASN
2	B	149	SER
2	B	182	GLN
3	G	78	ASP
3	G	81	ILE
3	G	146	ARG
1	L	28	PHE
1	L	86	LYS
1	L	178	TYR
1	L	223	ILE
1	L	350	LEU
1	L	364	TYR
1	L	404	ARG
1	L	453	ILE
1	L	458	LYS
1	L	466	LYS
1	L	493	GLN
1	L	498	THR
1	L	501	TYR
1	L	544	ILE
1	L	551	ASN

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Mol	Chain	Res	Type
2	E	121	ASN
2	E	141	HIS
2	E	145	LEU
2	E	182	GLN
2	E	190	GLN
3	M	59	LYS
3	M	66	LEU
3	M	100	ARG
3	M	134	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
1	A	320	ASN
1	A	334	ASN
1	A	352	GLN
1	A	465	ASN
1	A	467	ASN
1	A	543	ASN
2	B	59	GLN
2	B	75	GLN
2	B	121	ASN
2	B	142	GLN
2	B	167	GLN
2	B	204	HIS
2	B	216	ASN
3	G	47	ASN
3	G	68	ASN
3	G	72	ASN
3	G	124	ASN
1	L	16	GLN
1	L	45	ASN
1	L	74	ASN
1	L	130	GLN
1	L	320	ASN
1	L	334	ASN
1	L	352	GLN
1	L	465	ASN
1	L	467	ASN
1	L	513	GLN
1	L	543	ASN

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Mol	Chain	Res	Type
2	E	59	GLN
2	E	75	GLN
2	E	121	ASN
2	E	143	GLN
2	E	150	ASN
2	E	190	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 2 are monoatomic and 4 are modelled with single atom - 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	1601	-	94,101,103	1.34	11 (11%)	150,166,171	1.08	10 (6%)
7	CNC	E	2601	-	94,101,103	1.37	9 (9%)	150,166,171	1.16	13 (8%)
6	PGR	L	2602	4	4,4,4	0.57	0	4,4,4	0.78	0
6	PGR	A	1602	4	4,4,4	0.66	0	4,4,4	0.64	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	B	1601	-	1/1/36/38	10/56/223/235	0/3/11/11
6	PGR	L	2602	4	-	0/2/2/2	-
6	PGR	A	1602	4	-	0/2/2/2	-
7	CNC	E	2601	-	1/1/36/38	11/56/223/235	0/3/11/11

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	E	2601	CNC	C5M-C5B	-6.07	1.39	1.51
7	B	1601	CNC	C5M-C5B	-5.85	1.40	1.51
7	E	2601	CNC	C14-N23	4.43	1.41	1.30
7	B	1601	CNC	C14-N23	4.11	1.40	1.30
7	E	2601	CNC	C13-C14	3.22	1.59	1.51
7	E	2601	CNC	C2B-N3B	2.83	1.37	1.31
7	B	1601	CNC	O58-C57	2.81	1.28	1.23
7	B	1601	CNC	C48-C49	2.81	1.61	1.52
7	E	2601	CNC	O58-C57	2.68	1.28	1.23
7	B	1601	CNC	C2B-N3B	2.66	1.36	1.31
7	B	1601	CNC	C13-C14	2.52	1.58	1.51
7	B	1601	CNC	C9-N22	2.39	1.36	1.30
7	E	2601	CNC	C9-N22	2.34	1.36	1.30
7	E	2601	CNC	C48-C49	2.31	1.59	1.52
7	B	1601	CNC	C41-C8	2.28	1.59	1.54
7	B	1601	CNC	C30-C3	2.15	1.59	1.54
7	E	2601	CNC	C48-C13	2.15	1.59	1.54
7	B	1601	CNC	C7B-C6B	2.13	1.42	1.39
7	E	2601	CNC	C41-C8	2.07	1.59	1.54
7	B	1601	CNC	C48-C13	2.06	1.59	1.54

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	E	2601	CNC	C41-C8-C9	-3.46	105.16	111.19
7	E	2601	CNC	C56-C55-C17	3.09	121.55	115.58
7	B	1601	CNC	C56-C55-C17	3.07	121.51	115.58
7	B	1601	CNC	C18-C19-N24	2.98	106.67	101.92
7	E	2601	CNC	C26-C2-C1	2.95	114.56	110.00
7	B	1601	CNC	C11-N23-C14	2.91	107.41	106.31
7	B	1601	CNC	C41-C8-C9	-2.90	106.13	111.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	E	2601	CNC	C18-C19-N24	2.79	106.36	101.92
7	E	2601	CNC	C55-C17-C16	2.76	122.18	116.17
7	B	1601	CNC	C7-C37-C38	2.74	122.38	114.28
7	E	2601	CNC	C47-C12-C46	-2.69	104.94	109.41
7	E	2601	CNC	C11-N23-C14	2.67	107.32	106.31
7	B	1601	CNC	C19-N24-C16	-2.61	107.78	111.96
7	E	2601	CNC	C7-C37-C38	2.60	121.97	114.28
7	E	2601	CNC	C19-N24-C16	-2.60	107.81	111.96
7	E	2601	CNC	C12-C11-N23	2.57	114.24	111.49
7	B	1601	CNC	O58-C57-C56	-2.47	117.54	122.02
7	B	1601	CNC	C47-C12-C46	-2.44	105.36	109.41
7	B	1601	CNC	C55-C17-C16	2.28	121.13	116.17
7	E	2601	CNC	O58-C57-C56	-2.10	118.21	122.02
7	E	2601	CNC	C9-N22-C6	2.09	107.79	105.28
7	E	2601	CNC	C36-C7-C8	-2.06	108.25	112.05
7	B	1601	CNC	C9-N22-C6	2.03	107.72	105.28

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	B	1601	CNC	N24
7	E	2601	CNC	N24

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	1601	CNC	C1-C2-C26-C27
7	B	1601	CNC	C25-C2-C26-C27
7	B	1601	CNC	C3-C2-C26-C27
7	E	2601	CNC	O6R-C4R-C5R-O8R
7	B	1601	CNC	C4-C3-C30-C31
7	B	1601	CNC	C2-C26-C27-N29
7	E	2601	CNC	C13-C48-C49-C50
7	B	1601	CNC	C2-C26-C27-O28
7	B	1601	CNC	C2-C3-C30-C31
7	E	2601	CNC	C4-C3-C30-C31
7	E	2601	CNC	C1-C2-C26-C27
7	E	2601	CNC	C25-C2-C26-C27
7	E	2601	CNC	C2-C3-C30-C31
7	E	2601	CNC	C17-C18-C60-C61
7	E	2601	CNC	C3R-C4R-C5R-O8R
7	B	1601	CNC	C13-C48-C49-C50

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Mol	Chain	Res	Type	Atoms
7	B	1601	CNC	C12-C13-C48-C49
7	B	1601	CNC	C19-C18-C60-C61
7	E	2601	CNC	C19-C18-C60-C61
7	E	2601	CNC	C3-C2-C26-C27
7	E	2601	CNC	C12-C13-C48-C49

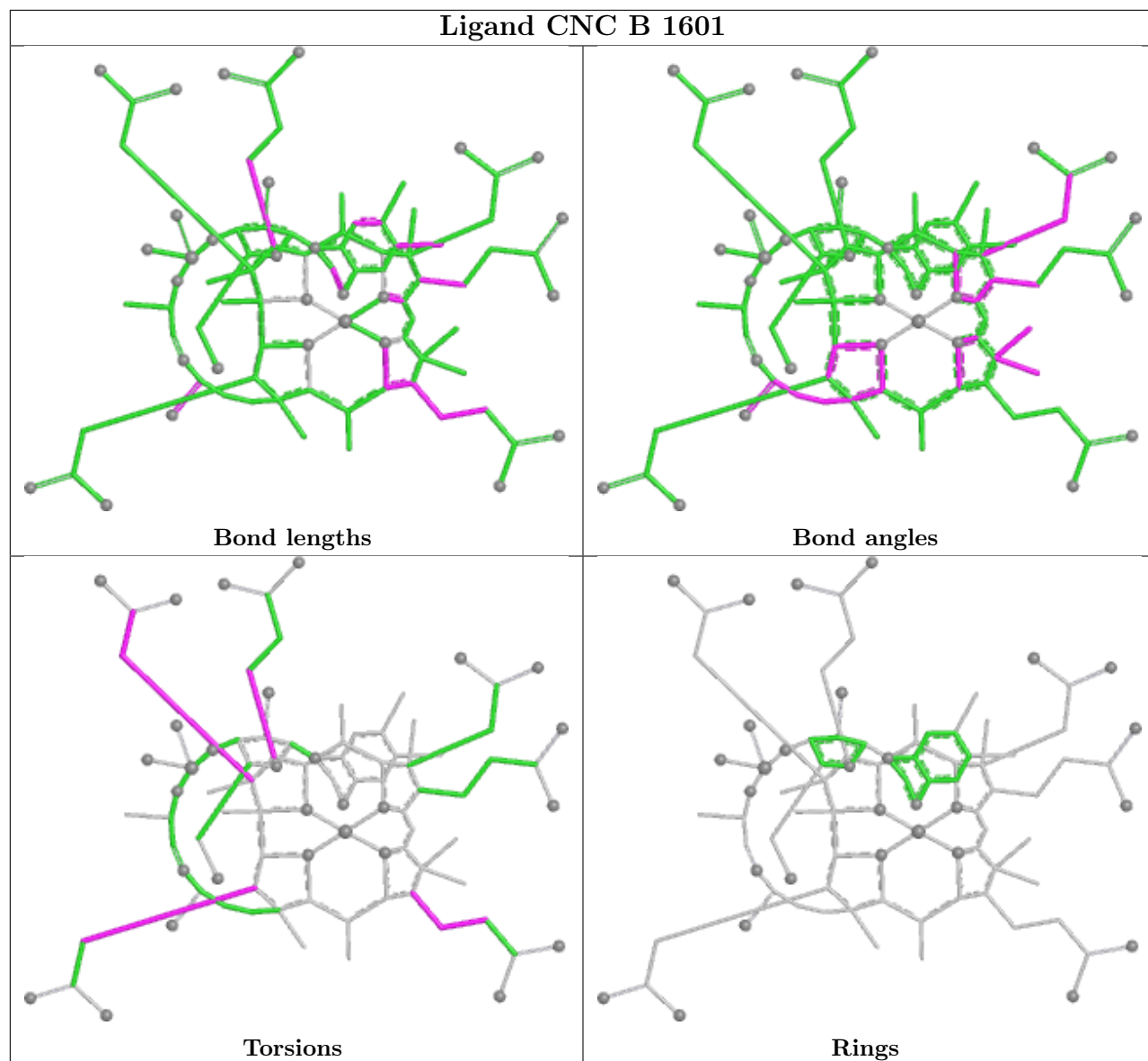
There are no ring outliers.

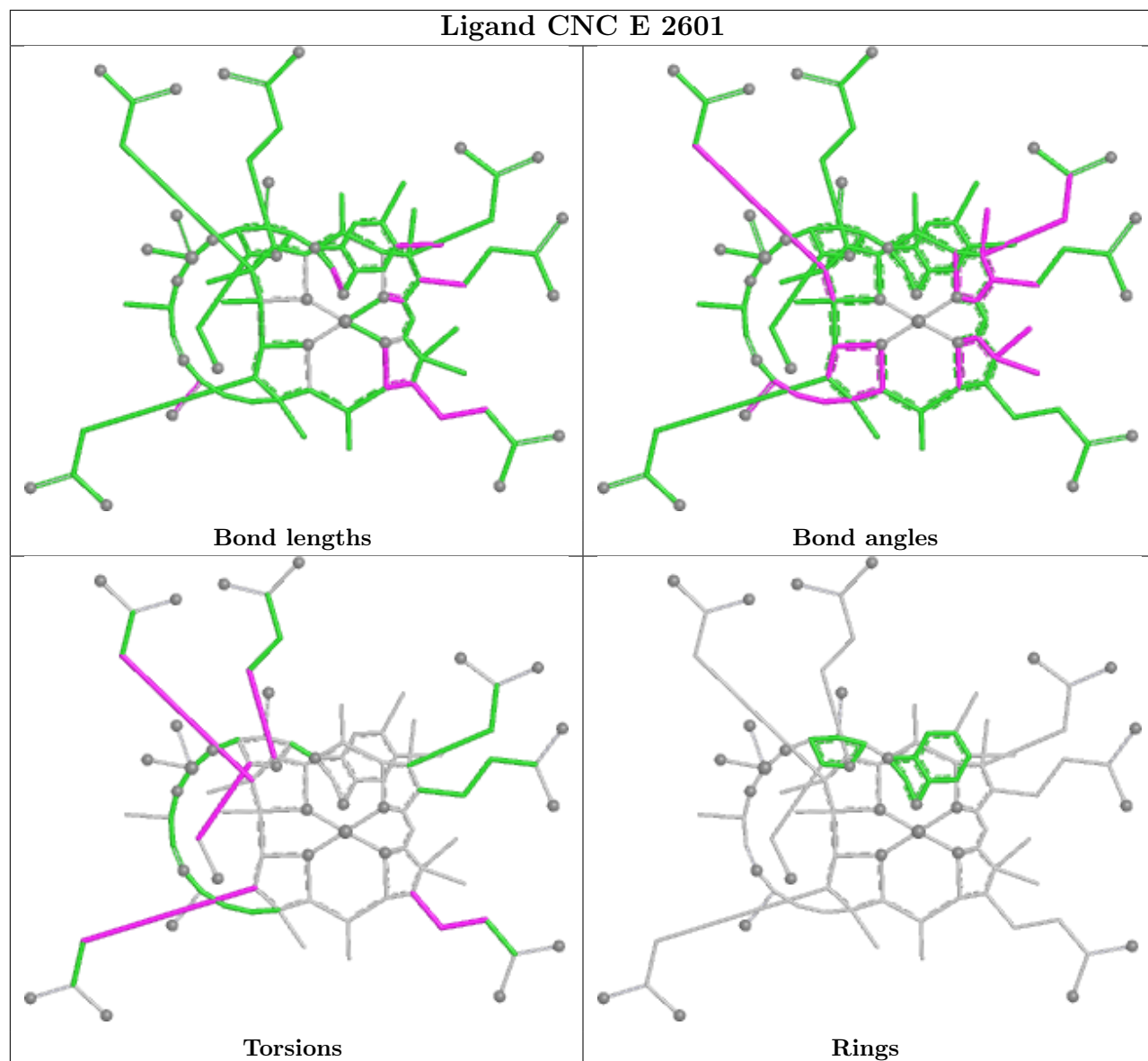
2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	1601	CNC	6	0
7	E	2601	CNC	8	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 1601





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%)	0.15	5 (0%)	81 82	19, 33, 52, 84	2 (0%)
1	L	551/554 (99%)	0.20	2 (0%)	88 89	21, 34, 52, 76	1 (0%)
2	B	178/224 (79%)	0.65	11 (6%)	26 28	29, 46, 68, 76	0
2	E	177/224 (79%)	0.89	9 (5%)	33 35	34, 52, 76, 84	0
3	G	137/173 (79%)	0.69	11 (8%)	18 20	30, 42, 72, 83	3 (2%)
3	M	137/173 (79%)	0.55	5 (3%)	46 48	24, 42, 70, 79	1 (0%)
All	All	1731/1902 (91%)	0.37	43 (2%)	58 60	19, 38, 63, 84	7 (0%)

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	222	VAL	3.4
3	G	55	THR	3.4
3	G	59	LYS	3.2
2	E	46	GLY	3.1
3	G	61	LEU	3.0
1	A	492	ILE	3.0
2	B	46	GLY	2.9
2	B	51	VAL	2.8
2	E	47	PHE	2.7
3	M	77	GLN	2.7
2	B	58	THR	2.7
3	G	51	GLU	2.7
3	G	56	ALA	2.6
3	M	57	THR	2.6
3	G	70	LEU	2.6
2	E	220	LEU	2.5
1	A	551	ASN	2.5
2	E	51	VAL	2.5
3	G	66	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	L	551	ASN	2.5
3	G	103	MET	2.5
2	E	60	GLN	2.4
1	A	548	LEU	2.4
2	B	220	LEU	2.4
3	M	59	LYS	2.3
3	G	53	VAL	2.3
2	B	48	LEU	2.3
2	B	49	THR	2.3
3	M	74	VAL	2.3
1	A	550	PRO	2.2
2	B	99	GLY	2.2
2	B	143	GLN	2.2
2	B	223	ALA	2.2
2	B	222	VAL	2.1
3	M	58	ASN	2.1
2	E	56	GLN	2.1
2	E	49	THR	2.1
3	G	57	THR	2.1
2	E	168	ILE	2.1
1	L	454	VAL	2.1
2	B	57	GLY	2.1
1	A	415	ALA	2.0
3	G	54	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

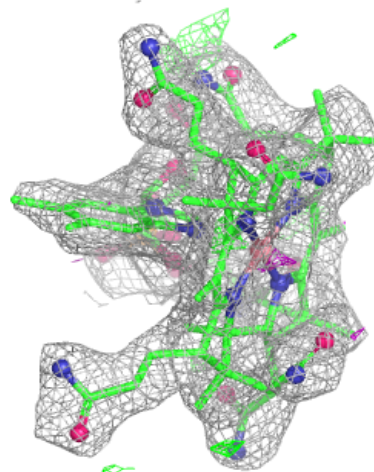
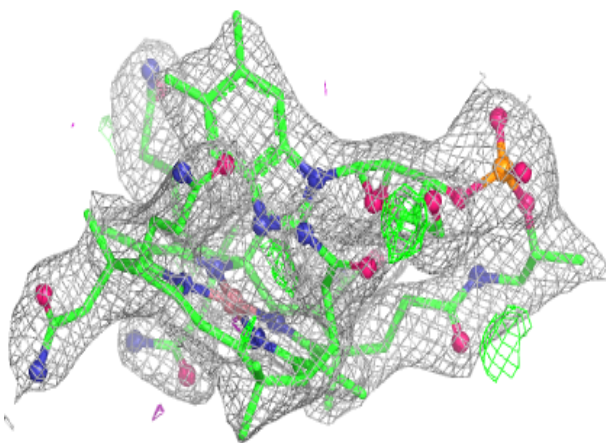
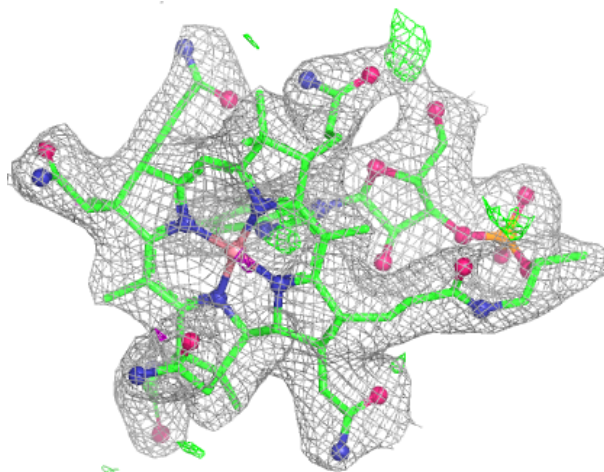
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NH4	A	1604	1/1	0.84	0.20	31,31,31,31	0
5	NH4	A	1605	1/1	0.84	0.12	28,28,28,28	0
5	NH4	L	2605	1/1	0.89	0.15	38,38,38,38	0
5	NH4	L	2604	1/1	0.93	0.13	13,13,13,13	0
6	PGR	L	2602	5/5	0.93	0.07	19,20,24,27	0
7	CNC	E	2601	91/93	0.93	0.10	34,39,42,43	0
7	CNC	B	1601	91/93	0.95	0.09	23,30,36,40	0
6	PGR	A	1602	5/5	0.96	0.07	25,26,27,29	0
4	K	A	1603	1/1	0.98	0.03	26,26,26,26	0
4	K	L	2603	1/1	0.98	0.03	27,27,27,27	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.

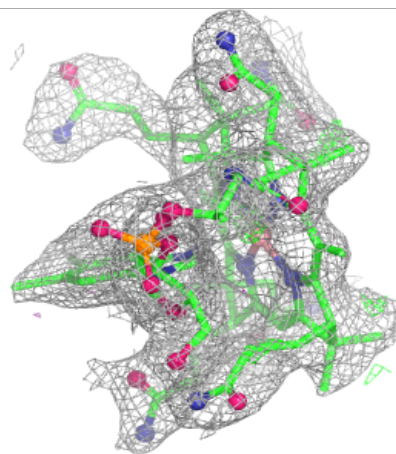
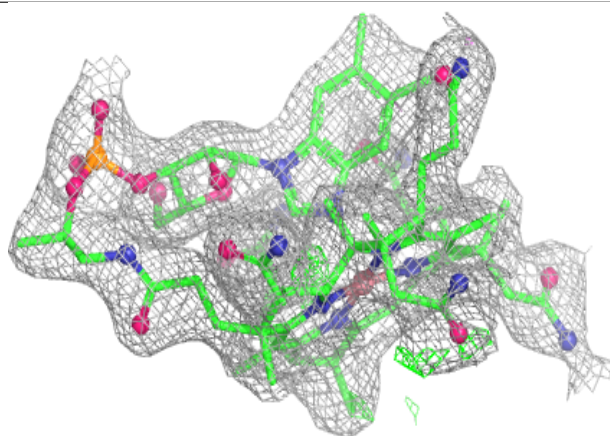
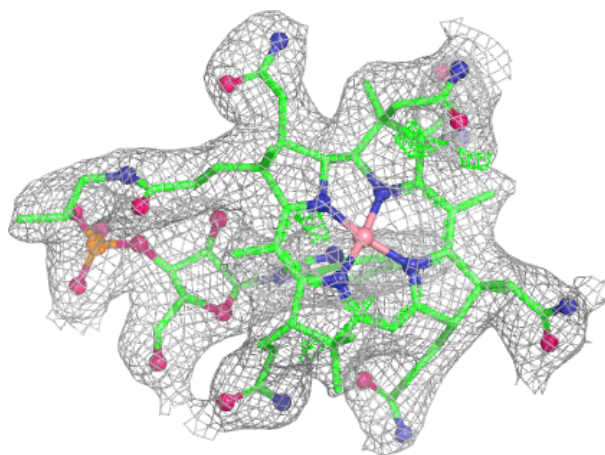
Electron density around CNC E 2601:

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 1601:

$2mF_o-DF_c$ (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.