Full wwPDB X-ray Structure Validation Report (i)

Oct 18, 2023 – 06:36 PM EDT

PDB ID	:	1UC5
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 (i) 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 (i)) were used in the production of this report:

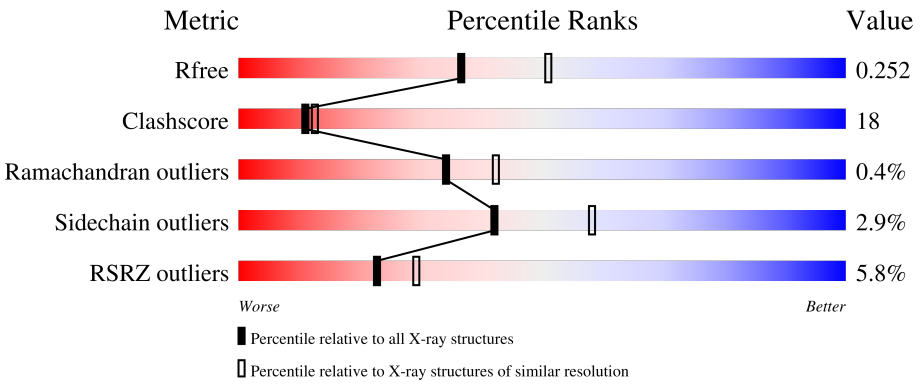
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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 <=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	5%, 70%, 29%, • •
1	L	554	4%, 67%, 31%, • •
2	B	224	53%, 25%, •, 21%
2	E	224	12%, 43%, 34%, •, 21%
3	G	173	7%, 51%, 26%, •, 21%

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Mol	Chain	Length	Quality of chain
3	M	173	5% 55% 21% • 21%

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	NH4	A	1605	-	-	-	X
5	NH4	L	2605	-	-	-	X
7	CNC	B	1601	X	-	-	-
7	CNC	E	2601	X	-	-	-

2 Entry composition (i)

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

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

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

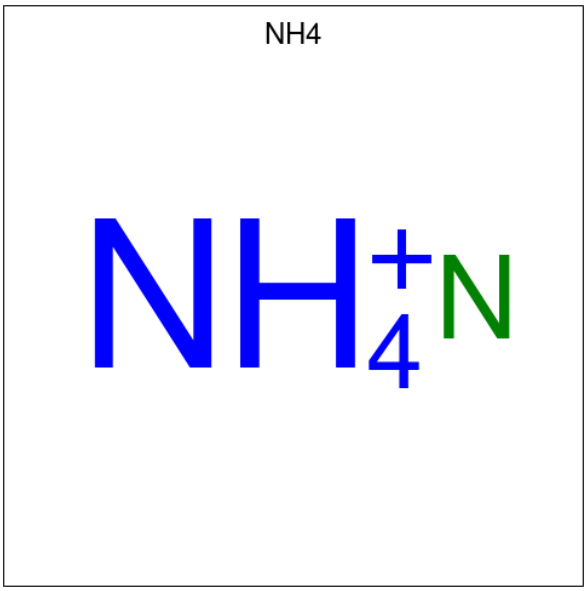
- Molecule 3 is a protein called diol dehydrase gamma subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	G	137	1093	681	195	214	3	0	0	0
3	M	137	1092	681	195	213	3	0	0	0

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

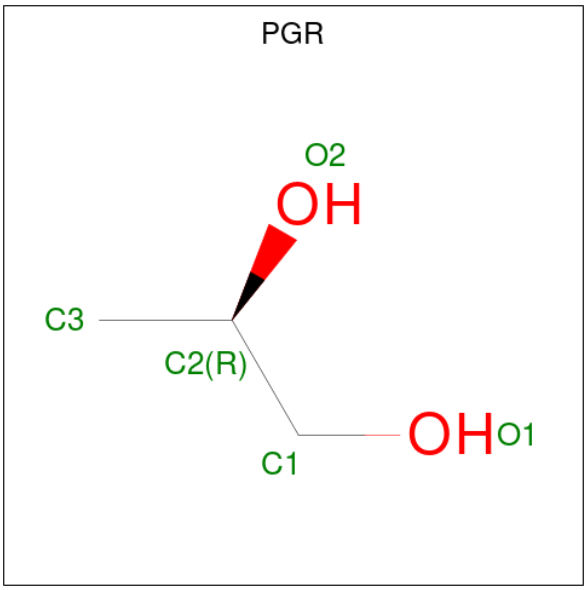
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	K		
4	A	1	1	1	0	0
4	L	1	1	1	0	0

- Molecule 5 is AMMONIUM ION (three-letter code: NH4) (formula: H_4N).



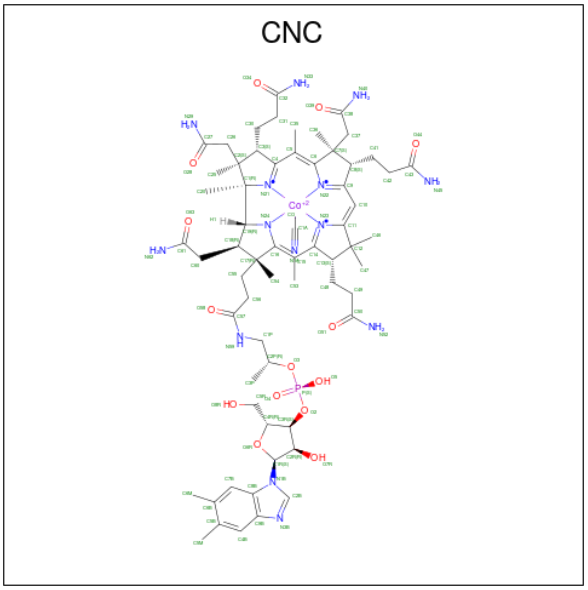
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total N 1 1	0	0
5	A	1	Total N 1 1	0	0
5	L	1	Total N 1 1	0	0
5	L	1	Total N 1 1	0	0

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



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

- Molecule 7 is CYANOCOBALAMIN (three-letter code: CNC) (formula: $C_{63}H_{89}CoN_{14}O_{14}P$).



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

- Molecule 8 is water.

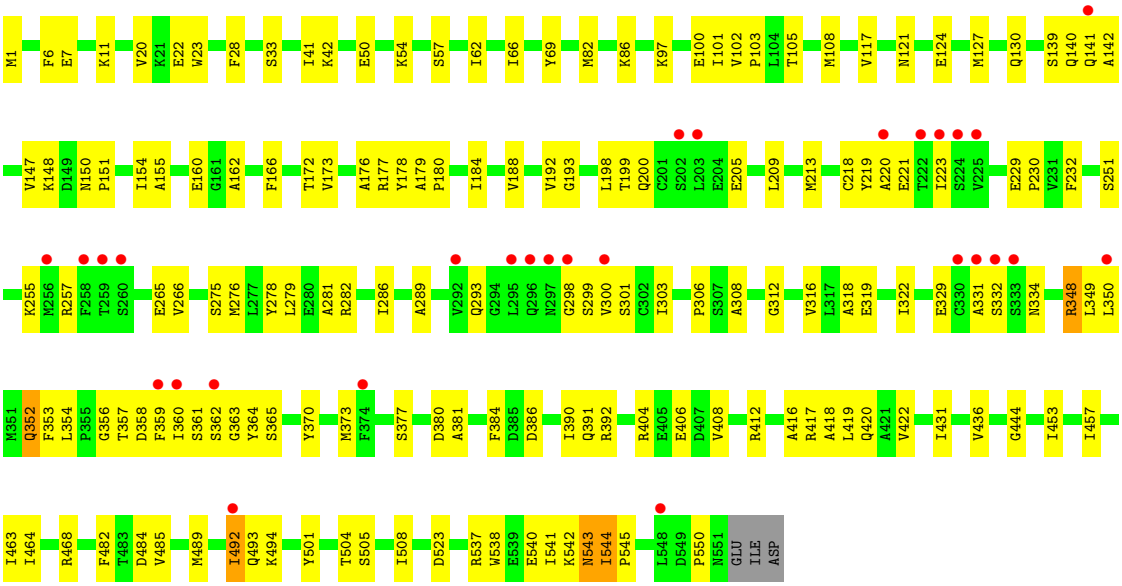
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	267	267	267	0	0
			Total	O		
8	B	72	72	72	0	0
			Total	O		
8	G	70	70	70	0	0
			Total	O		
8	L	227	227	227	0	0
			Total	O		
8	E	23	23	23	0	0
			Total	O		
8	M	65	65	65	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

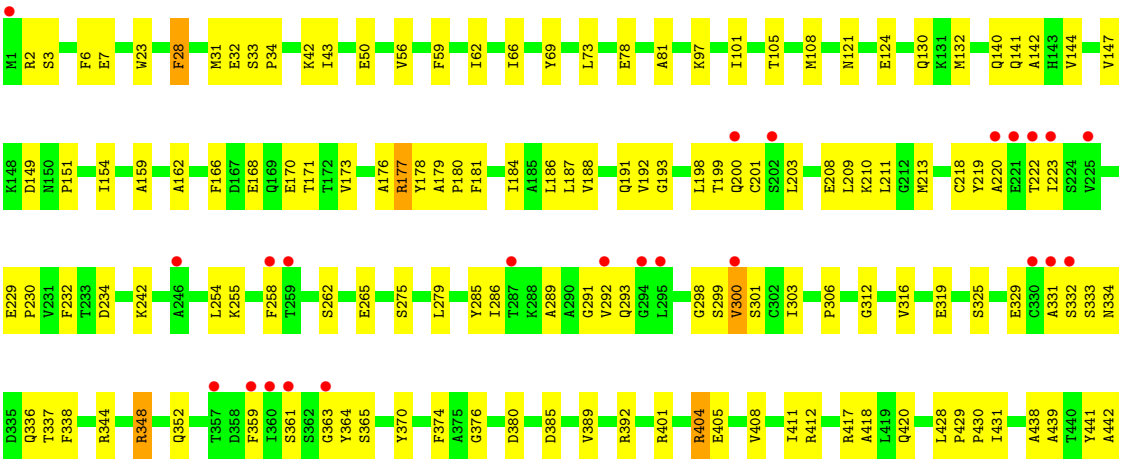
- Molecule 1: diol dehydrase alpha subunit

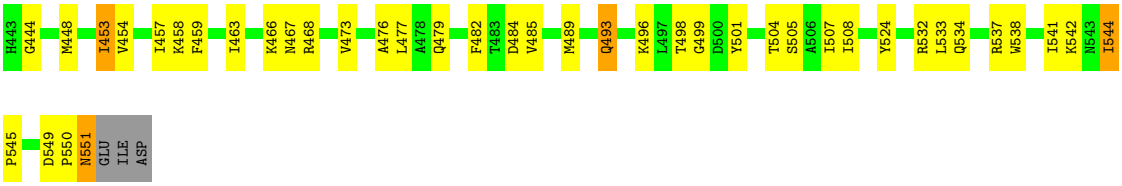
Chain A:



- Molecule 1: diol dehydrase alpha subunit

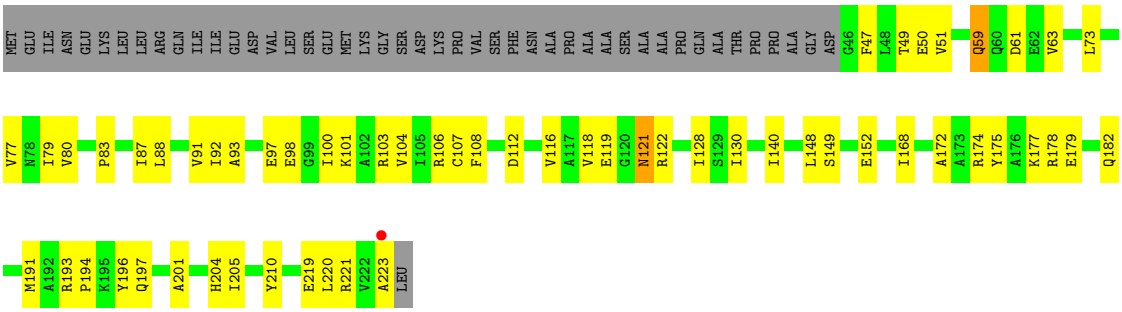
Chain L:





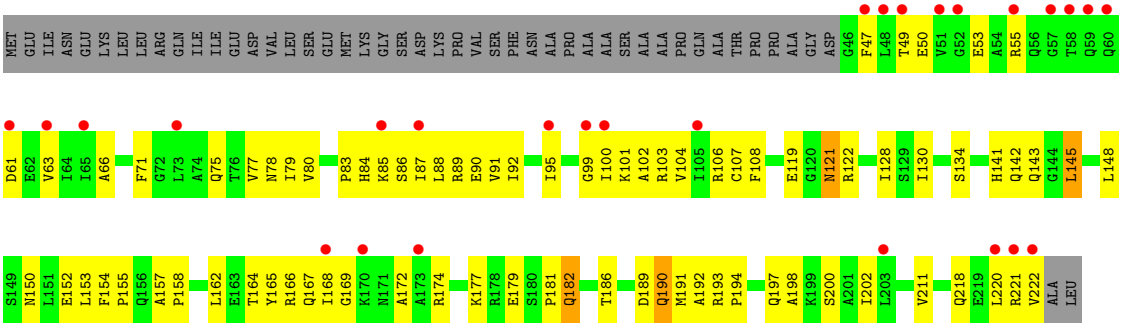
• Molecule 2: diol dehydrase beta subunit

Chain B:



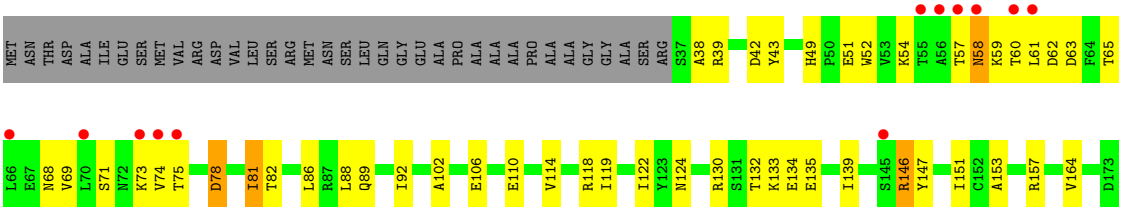
• Molecule 2: diol dehydrase beta subunit

Chain E:



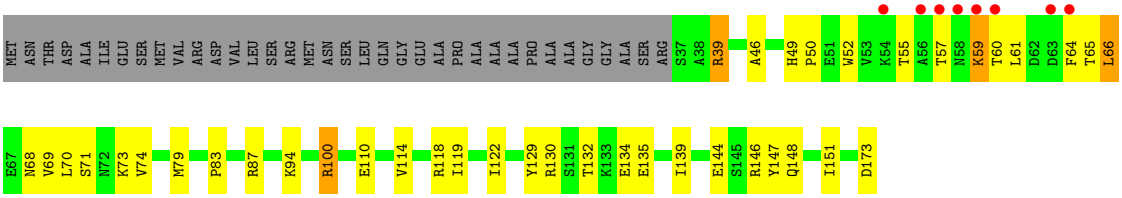
• Molecule 3: diol dehydrase gamma subunit

Chain G:



• Molecule 3: diol dehydrase gamma subunit

Chain M:


MET
ASN
THR
ASP
ALA
ILE
GLU
SER
MET
VAL
ARG
ASP
VAL
LEU
SER
ARG
MET
ASN
SER
LEU
GLN
GLY
GLU
ALA
PRO
ALA
ALA
ALA
PRO
ALA
ALA
GLY
GLY
ALA
SER
ARG
S37
A38
R39
A46
H49
P50
E51
W52
V53
K54
T55
A56
T57
N58
K59
T60
L61
D62
D63
F64
T65
L66
E67
N68
V69
L70
S71
N72
K73
V74
M79
P83
R87
K94
R100
E110
V114
R118
I119
I122
Y129
R130
S131
T132
K133
E134
E135
I139
E144
S145
R146
Y147
Q148
I151
D173

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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)	0.31 , 45.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: CNC, PGR, K, 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	0.35	0/4273	0.63	0/5787
1	L	0.34	0/4273	0.62	0/5787
2	B	0.33	0/1380	0.61	0/1868
2	E	0.31	0/1375	0.60	0/1861
3	G	0.33	0/1108	0.57	0/1497
3	M	0.33	0/1107	0.57	0/1495
All	All	0.34	0/13516	0.61	0/18295

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4201	0	4140	124	0
1	L	4201	0	4140	154	0
2	B	1358	0	1408	51	0
2	E	1353	0	1403	76	0
3	G	1093	0	1101	44	0
3	M	1092	0	1101	47	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	489	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 18.

All (489) 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:E:174:ARG:HG2	2:E:181:PRO:HB3	1.49	0.94
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:B:121:ASN:C	2:B:121:ASN:HD22	1.74	0.90
1:A:489:MET:O	1:A:493:GLN:HG2	1.75	0.86
2:E:47:PHE:CD2	2:E:85:LYS:HD3	2.14	0.83
2:E:121:ASN:HD22	2:E:121:ASN:C	1.81	0.83
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
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
3:G:60:THR:HG22	3:G:63:ASP:CG	2.06	0.75
1:A:220:ALA:HB1	1:A:223:ILE:HD11	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:L:438:ALA:HB1	1:L:448:MET:HE1	1.73	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
1:L:473:VAL:HG12	1:L:489:MET:HE1	1.75	0.68
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
1:A:147:VAL:HG12	1:A:373:MET:HE1	1.78	0.66
2:E:121:ASN:C	2:E:121:ASN:ND2	2.49	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
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
3:M:64:PHE:HE1	3:M:79:MET:HG2	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:134:GLU:CD	3:G:134:GLU:H	2.01	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: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
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:NZ	3:M:59:LYS:HB3	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:177:ARG:HB3	1:L:457:ILE:HG23	1.83	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: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: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
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
3:M:147:TYR:C	3:M:148:GLN:HG2	2.24	0.57
2:E:71:PHE:CE1	2:E:84:HIS:HB3	2.39	0.57
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: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
3:G:51:GLU:CD	3:G:51:GLU:H	2.09	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:E:191:MET:C	2:E:194:PRO:HD2	2.25	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
1:A:485:VAL:O	1:A:489:MET:HG2	2.07	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
2:B:121:ASN:C	2:B:121:ASN:ND2	2.49	0.54
3:M:122:ILE:HD12	3:M:139:ILE:CG2	2.36	0.54
1:L:141:GLN:HG3	1:L:168:GLU:HB3	1.87	0.54
1:L:507:ILE:C	1:L:508:ILE:HD12	2.28	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
3:M:59:LYS:HB3	3:M:59:LYS:HZ3	1.73	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:L:438:ALA:CB	1:L:448:MET:HE1	2.39	0.53
3:M:39:ARG:HG2	3:M:39:ARG:NH1	2.24	0.53
1:L:439:ALA:HA	1:L:448:MET:HE3	1.91	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
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:105:THR:HA	1:A:108:MET:HE3	1.92	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
3:M:57:THR:O	3:M:57:THR:CG2	2.57	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
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
3:M:147:TYR:O	3:M:148:GLN:HG2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:G:68:ASN:C	3:G:74:VAL:HG22	2.32	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:417:ARG:NH1	1:A:417:ARG:HB2	2.27	0.50
1:L:442:ALA:HB2	1:L:448:MET:CE	2.42	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
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
2:B:59:GLN:NE2	2:B:101:LYS:HZ1	2.11	0.49
1:L:142:ALA:HB2	1:L:166:PHE:CD1	2.47	0.49
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
1:L:442:ALA:HB2	1:L:448:MET:HE3	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:191:MET:C	2:B:194:PRO:HD2	2.34	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
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
1:A:373:MET:HA	1:A:373:MET:HE2	1.96	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
3:G:134:GLU:CD	3:G:134:GLU:N	2.67	0.47
1:L:142:ALA:HB2	1:L:166:PHE:CE1	2.49	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
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
2:E:99:GLY:C	2:E:100:ILE:HD12	2.34	0.47
3:M:60:THR:CG2	3:M:61:LEU:N	2.77	0.47
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:132:MET:HE3	1:L:325:SER:HA	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:23:TRP:HB3	1:L:28:PHE:HB2	1.98	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: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: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
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
1:L:438:ALA:C	1:L:448:MET:HE3	2.36	0.45
3:M:55:THR:HG22	8:M:235:HOH:O	2.16	0.45
1:A:42:LYS:HD3	1:A:50:GLU:CD	2.38	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: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
1:A:23:TRP:HB2	1:L:550:PRO:CG	2.43	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:404:ARG:CB	1:L:404:ARG:HH11	2.31	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
3:G:65:THR:OG1	3:G:68:ASN:ND2	2.51	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
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
1:L:549:ASP:C	1:L:551:ASN:H	2.21	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:L:337:THR:HG23	1:L:376:GLY:C	2.39	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:A:543:ASN:C	1:A:543:ASN:ND2	2.72	0.42
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
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: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: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
7:E:2601:CNC:H421	7:E:2601:CNC:C10	2.49	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
2:B:59:GLN:NE2	2:B:101:LYS:HZ2	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:257:ARG:HH21	1:A:329:GLU:CD	2.23	0.42
2:E:162:LEU:HD23	2:E:162:LEU:HA	1.85	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
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
1:A:543:ASN:C	1:A:543:ASN:HD22	2.23	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:105:THR:HA	1:L:108:MET:HE3	2.01	0.41
1:L:229:GLU:N	1:L:230:PRO:CD	2.83	0.41
1:L:370:TYR:CD1	1:L:370:TYR:C	2.93	0.41
1:A:82:MET:HE2	1:A:86:LYS:HE2	2.02	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
1:L:477:LEU:HD12	1:L:489:MET:HE1	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:484:ASP:N	1:A:484:ASP:OD1	2.54	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
1:L:380:ASP:OD1	1:L:380:ASP:C	2.58	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
1:L:438:ALA:O	1:L:448:MET:HE3	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
1:L:438:ALA:C	1:L:448:MET:CE	2.90	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 (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	549/554 (99%)	518 (94%)	28 (5%)	3 (0%)	29	35
1	L	549/554 (99%)	517 (94%)	29 (5%)	3 (0%)	29	35
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%)	22	26
3	M	135/173 (78%)	130 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1719/1902 (90%)	1631 (95%)	81 (5%)	7 (0%)	34 42

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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	450/453 (99%)	439 (98%)	11 (2%)	49 66
1	L	450/453 (99%)	436 (97%)	14 (3%)	40 55
2	B	146/183 (80%)	142 (97%)	4 (3%)	44 61
2	E	146/183 (80%)	140 (96%)	6 (4%)	30 43
3	G	116/141 (82%)	113 (97%)	3 (3%)	46 63
3	M	116/141 (82%)	112 (97%)	4 (3%)	37 51
All	All	1424/1554 (92%)	1382 (97%)	42 (3%)	42 58

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	PHE
1	A	41	ILE
1	A	178	TYR
1	A	232	PHE
1	A	348	ARG

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Mol	Chain	Res	Type
1	A	352	GLN
1	A	364	TYR
1	A	492	ILE
1	A	501	TYR
1	A	543	ASN
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	178	TYR
1	L	232	PHE
1	L	234	ASP
1	L	348	ARG
1	L	364	TYR
1	L	404	ARG
1	L	453	ILE
1	L	458	LYS
1	L	493	GLN
1	L	498	THR
1	L	501	TYR
1	L	544	ILE
1	L	551	ASN
2	E	103	ARG
2	E	121	ASN
2	E	141	HIS
2	E	145	LEU
2	E	182	GLN
2	E	190	GLN
3	M	39	ARG
3	M	59	LYS
3	M	66	LEU
3	M	100	ARG

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

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Mol	Chain	Res	Type
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	204	HIS
3	G	47	ASN
3	G	68	ASN
1	L	45	ASN
1	L	74	ASN
1	L	130	GLN
1	L	334	ASN
1	L	352	GLN
1	L	465	ASN
1	L	467	ASN
1	L	513	GLN
1	L	543	ASN
2	E	59	GLN
2	E	75	GLN
2	E	121	ASN
2	E	143	GLN
2	E	150	ASN
2	E	190	GLN
3	M	68	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 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	E	2601	-	89,101,103	1.32	8 (8%)	139,166,171	1.16	13 (9%)
6	PGR	A	1602	4	3,4,4	0.20	0	1,4,4	0.11	0
6	PGR	L	2602	4	3,4,4	0.21	0	1,4,4	0.04	0
7	CNC	B	1601	-	89,101,103	1.30	9 (10%)	139,166,171	1.09	10 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	CNC	E	2601	-	1/1/36/38	11/52/223/235	0/3/11/11
6	PGR	A	1602	4	-	0/2/2/2	-
6	PGR	L	2602	4	-	0/2/2/2	-
7	CNC	B	1601	-	1/1/36/38	10/52/223/235	0/3/11/11

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	E	2601	CNC	C5M-C5B	-5.69	1.39	1.51
7	B	1601	CNC	C5M-C5B	-5.48	1.40	1.51
7	E	2601	CNC	C14-N23	4.14	1.41	1.30
7	B	1601	CNC	C14-N23	3.84	1.40	1.30
7	E	2601	CNC	C13-C14	3.10	1.59	1.51
7	B	1601	CNC	O58-C57	2.74	1.28	1.23
7	B	1601	CNC	C48-C49	2.71	1.61	1.52
7	E	2601	CNC	O58-C57	2.61	1.28	1.23
7	B	1601	CNC	C13-C14	2.42	1.58	1.51
7	B	1601	CNC	C9-N22	2.24	1.36	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	E	2601	CNC	C48-C49	2.23	1.59	1.52
7	B	1601	CNC	C41-C8	2.22	1.59	1.54
7	E	2601	CNC	C9-N22	2.20	1.36	1.30
7	B	1601	CNC	C30-C3	2.09	1.59	1.54
7	E	2601	CNC	C48-C13	2.09	1.59	1.54
7	E	2601	CNC	C41-C8	2.02	1.59	1.54
7	B	1601	CNC	C48-C13	2.01	1.59	1.54

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	E	2601	CNC	C41-C8-C9	-3.42	105.16	111.19
7	E	2601	CNC	C56-C55-C17	3.13	121.55	115.52
7	B	1601	CNC	C56-C55-C17	3.11	121.51	115.52
7	B	1601	CNC	C18-C19-N24	3.01	106.67	101.88
7	E	2601	CNC	C26-C2-C1	2.92	114.56	110.01
7	B	1601	CNC	C11-N23-C14	2.91	107.41	106.31
7	B	1601	CNC	C41-C8-C9	-2.87	106.13	111.19
7	E	2601	CNC	C18-C19-N24	2.82	106.36	101.88
7	E	2601	CNC	C55-C17-C16	2.76	122.18	116.24
7	B	1601	CNC	C7-C37-C38	2.70	122.38	114.25
7	E	2601	CNC	C11-N23-C14	2.67	107.32	106.31
7	E	2601	CNC	C47-C12-C46	-2.61	104.94	109.35
7	B	1601	CNC	C19-N24-C16	-2.58	107.78	111.96
7	E	2601	CNC	C19-N24-C16	-2.57	107.81	111.96
7	E	2601	CNC	C7-C37-C38	2.57	121.97	114.25
7	E	2601	CNC	C12-C11-N23	2.55	114.24	111.48
7	B	1601	CNC	O58-C57-C56	-2.45	117.54	122.02
7	E	2601	CNC	C4B-C9B-C8B	-2.43	118.62	121.10
7	B	1601	CNC	C47-C12-C46	-2.36	105.36	109.35
7	B	1601	CNC	C4B-C9B-C8B	-2.34	118.70	121.10
7	B	1601	CNC	C55-C17-C16	2.27	121.13	116.24
7	E	2601	CNC	O58-C57-C56	-2.08	118.21	122.02
7	E	2601	CNC	C36-C7-C8	-2.07	108.25	112.08

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-C3-C30-C31
7	B	1601	CNC	C2-C26-C27-O28
7	E	2601	CNC	C4-C3-C30-C31
7	B	1601	CNC	C12-C13-C48-C49
7	E	2601	CNC	C1-C2-C26-C27
7	E	2601	CNC	C25-C2-C26-C27
7	E	2601	CNC	C17-C18-C60-C61
7	E	2601	CNC	C2-C3-C30-C31
7	E	2601	CNC	C3R-C4R-C5R-O8R
7	B	1601	CNC	C13-C48-C49-C50
7	B	1601	CNC	C19-C18-C60-C61
7	E	2601	CNC	C19-C18-C60-C61
7	E	2601	CNC	C12-C13-C48-C49
7	E	2601	CNC	C3-C2-C26-C27

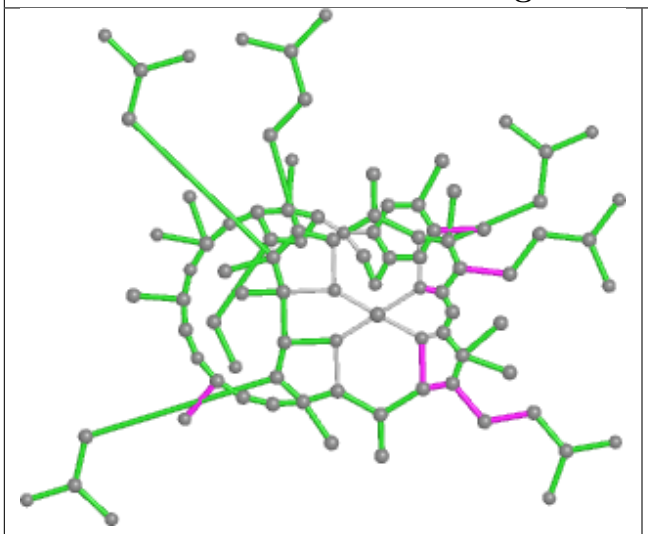
There are no ring outliers.

2 monomers are involved in 14 short contacts:

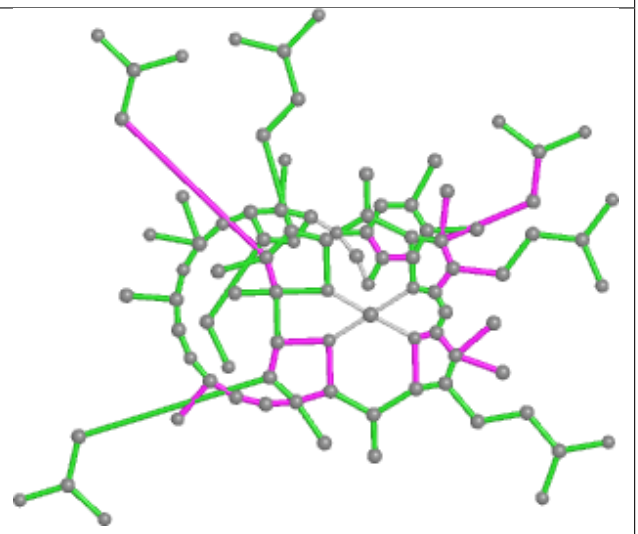
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	E	2601	CNC	8	0
7	B	1601	CNC	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

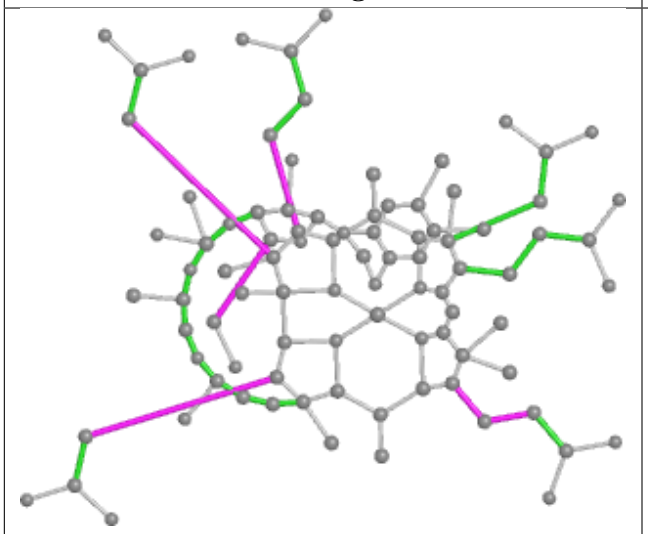
Ligand CNC E 2601



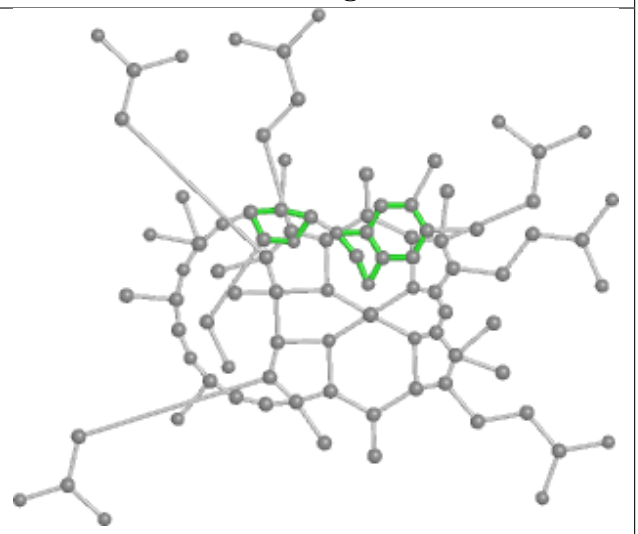
Bond lengths



Bond angles

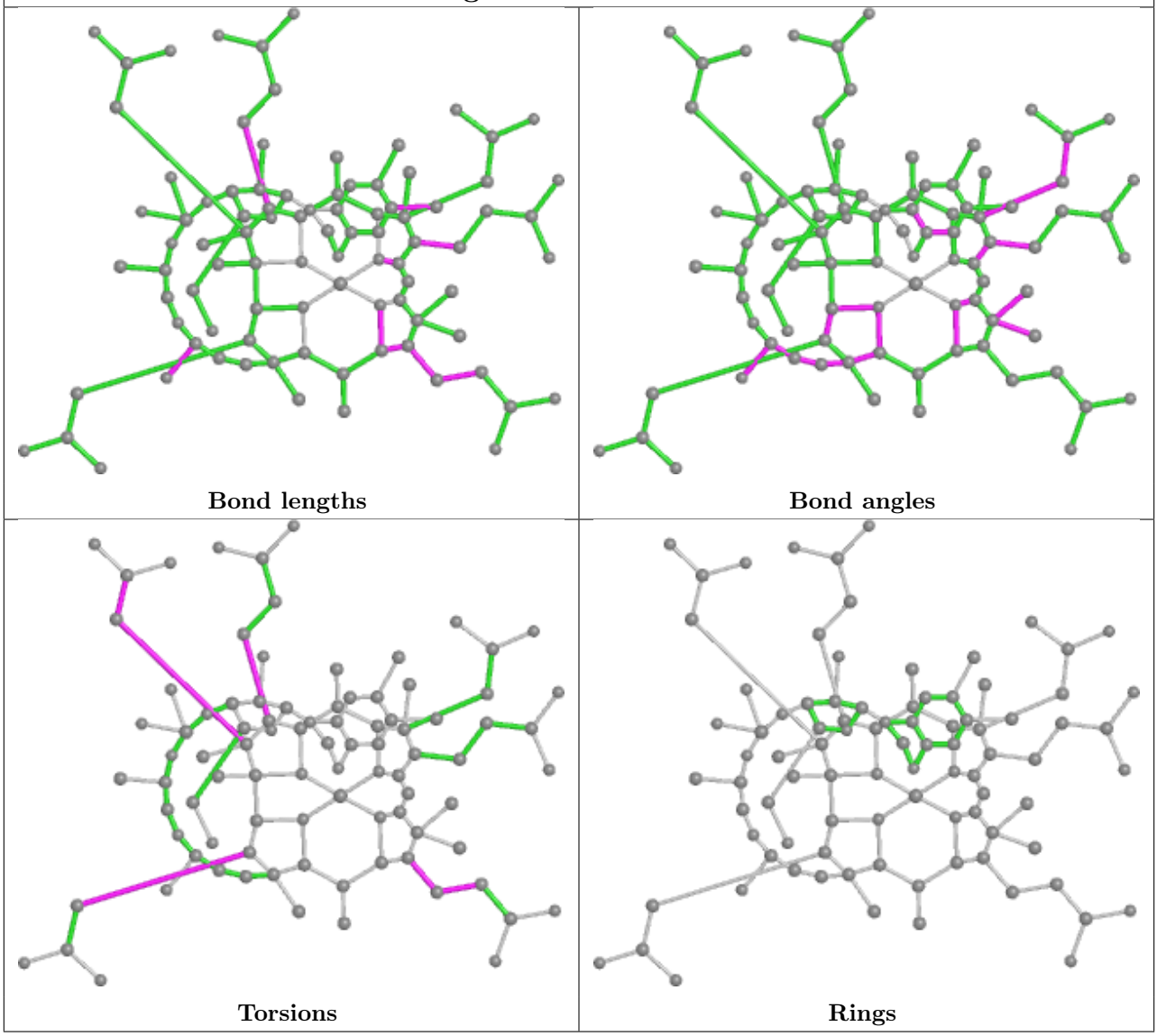


Torsions



Rings

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 (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, 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%)	0.22	29 (5%) 26 33	22, 33, 52, 84	2 (0%)
1	L	551/554 (99%)	0.23	24 (4%) 34 41	21, 34, 52, 76	1 (0%)
2	B	178/224 (79%)	0.02	1 (0%) 89 92	29, 46, 68, 76	0
2	E	177/224 (79%)	0.93	27 (15%) 2 3	34, 52, 76, 84	0
3	G	137/173 (79%)	0.41	12 (8%) 10 13	31, 42, 72, 83	3 (2%)
3	M	137/173 (79%)	0.10	8 (5%) 23 29	30, 42, 70, 79	1 (0%)
All	All	1731/1902 (91%)	0.28	101 (5%) 23 29	21, 38, 64, 84	7 (0%)

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	259	THR	6.3
3	G	56	ALA	4.8
3	G	55	THR	4.6
2	E	47	PHE	4.1
2	E	220	LEU	4.0
3	G	57	THR	3.8
1	A	223	ILE	3.8
2	E	60	GLN	3.7
2	E	48	LEU	3.6
1	A	222	THR	3.6
1	A	333	SER	3.5
1	L	295	LEU	3.4
1	L	223	ILE	3.3
2	E	55	ARG	3.3
3	M	59	LYS	3.3
3	M	58	ASN	3.3
1	L	259	THR	3.2
2	E	221	ARG	3.2
2	E	58	THR	3.2

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Mol	Chain	Res	Type	RSRZ
2	E	49	THR	3.1
2	E	99	GLY	3.1
2	E	52	GLY	3.0
2	E	59	GLN	3.0
2	E	51	VAL	2.9
3	G	75	THR	2.9
1	L	222	THR	2.9
1	L	258	PHE	2.9
1	A	332	SER	2.9
2	E	57	GLY	2.9
1	L	294	GLY	2.8
2	E	63	VAL	2.8
2	E	100	ILE	2.8
2	E	168	ILE	2.8
2	E	73	LEU	2.8
1	A	548	LEU	2.7
1	A	260	SER	2.7
1	L	220	ALA	2.7
2	E	85	LYS	2.7
3	G	66	LEU	2.7
2	E	105	ILE	2.6
1	A	300	VAL	2.6
1	A	295	LEU	2.6
1	A	331	ALA	2.6
3	G	61	LEU	2.6
1	L	360	ILE	2.6
3	G	60	THR	2.5
3	G	58	ASN	2.5
1	A	224	SER	2.5
1	A	297	ASN	2.5
1	L	331	ALA	2.5
2	E	87	ILE	2.5
1	L	292	VAL	2.5
2	E	222	VAL	2.5
1	A	360	ILE	2.4
3	M	60	THR	2.4
2	E	95	ILE	2.4
1	L	246	ALA	2.4
1	L	330	CYS	2.4
2	E	61	ASP	2.4
3	G	73	LYS	2.4
3	M	54	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
3	G	70	LEU	2.4
1	A	330	CYS	2.3
1	L	357	THR	2.3
2	E	173	ALA	2.3
1	A	258	PHE	2.3
1	A	225	VAL	2.3
1	A	220	ALA	2.3
2	E	170	LYS	2.2
1	L	1	MET	2.2
2	E	203	LEU	2.2
1	A	350	LEU	2.2
1	A	202	SER	2.2
1	A	292	VAL	2.2
1	L	332	SER	2.2
2	B	223	ALA	2.2
1	A	492	ILE	2.2
1	A	256	MET	2.2
1	L	202	SER	2.2
1	A	296	GLN	2.2
1	L	225	VAL	2.2
3	G	74	VAL	2.2
1	L	359	PHE	2.2
1	A	203	LEU	2.2
1	L	300	VAL	2.1
3	M	64	PHE	2.1
1	L	361	SER	2.1
1	L	363	GLY	2.1
1	A	374	PHE	2.1
3	M	56	ALA	2.1
2	E	65	ILE	2.1
1	A	362	SER	2.1
1	L	287	THR	2.1
1	A	298	GLY	2.1
3	M	57	THR	2.1
1	A	359	PHE	2.1
1	A	141	GLN	2.0
1	L	200	GLN	2.0
1	L	221	GLU	2.0
3	G	145	SER	2.0
3	M	63	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

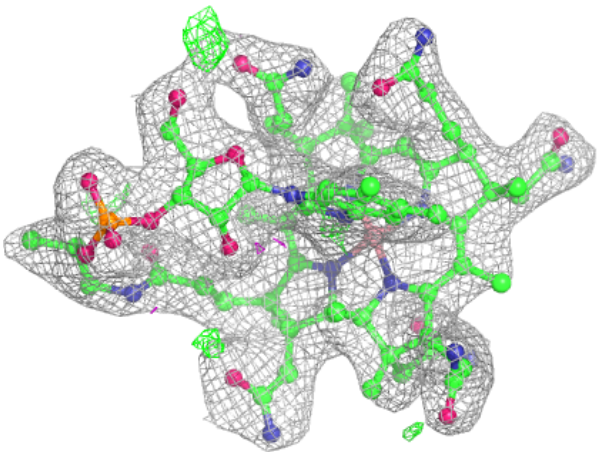
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

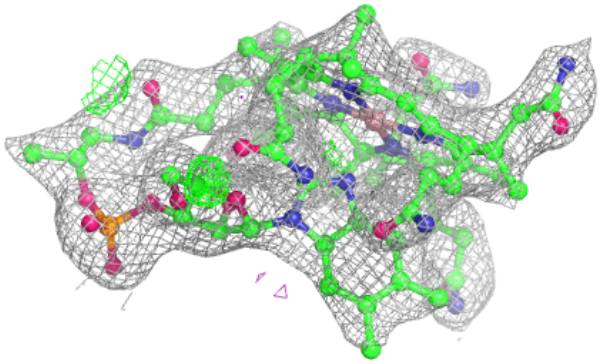
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NH4	A	1605	1/1	0.78	0.56	28,28,28,28	0
5	NH4	L	2605	1/1	0.78	0.92	38,38,38,38	0
5	NH4	A	1604	1/1	0.86	0.52	31,31,31,31	0
5	NH4	L	2604	1/1	0.93	0.14	13,13,13,13	0
7	CNC	E	2601	91/93	0.94	0.20	34,39,42,43	0
7	CNC	B	1601	91/93	0.95	0.19	23,30,36,40	0
6	PGR	A	1602	5/5	0.96	0.29	25,26,27,29	0
6	PGR	L	2602	5/5	0.96	0.30	19,20,24,27	0
4	K	A	1603	1/1	0.97	0.15	26,26,26,26	0
4	K	L	2603	1/1	0.98	0.17	27,27,27,27	0

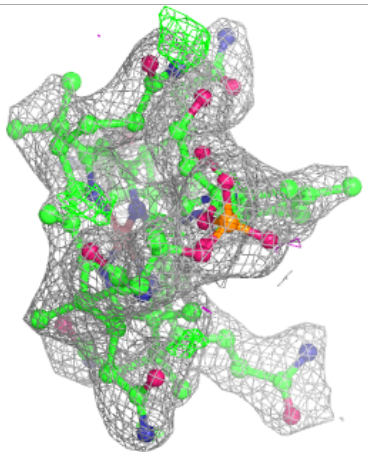
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation 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)

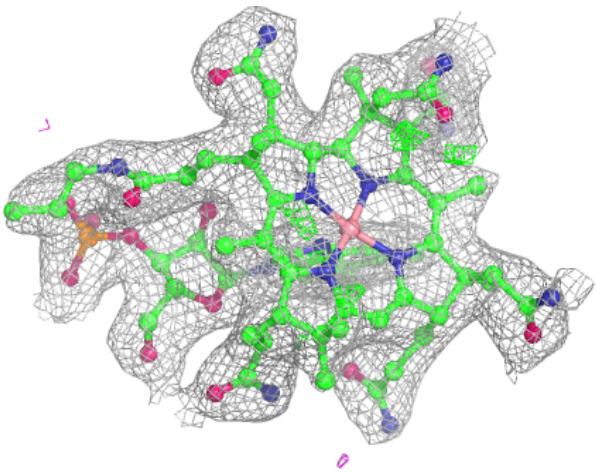


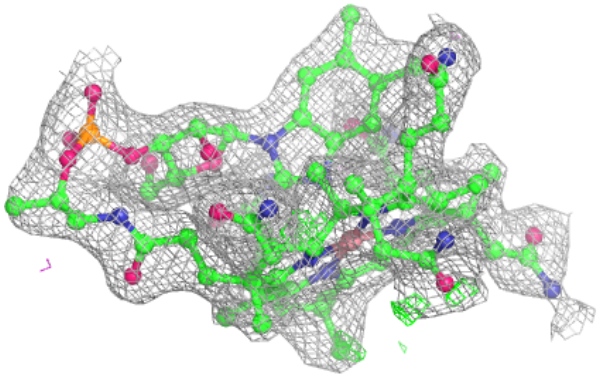


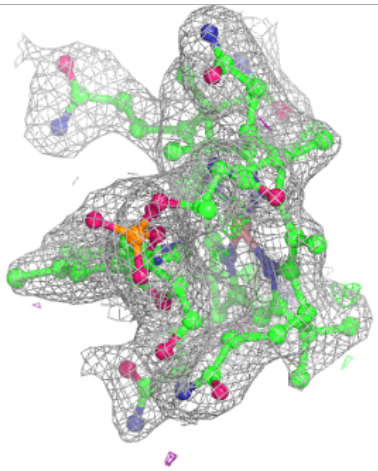


Electron density around CNC B 1601:

$2mF_o$-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.