Full wwPDB X-ray Structure Validation Report (i)

Nov 14, 2023 – 11:18 AM JST

PDB ID	:	5Z97
Title	:	Crystal structure of a lactonase double mutant in complex with ligand N
Authors	:	Zheng, Y.Y.; Liu, W.D.; Chen, C.C.; Guo, R.T.
Deposited on	:	2018-02-02
Resolution	:	2.32 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:

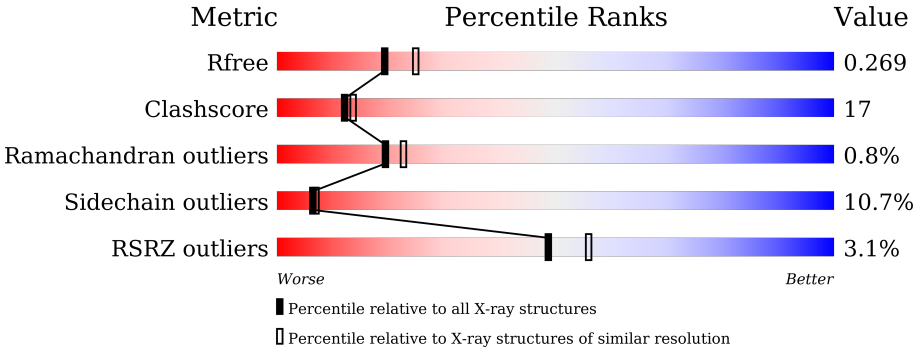
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.32 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	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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	263	79% 20% •
1	B	263	80% 19% •
1	C	263	71% 25% •
1	D	263	12% 41% 46% 12% •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8498 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.

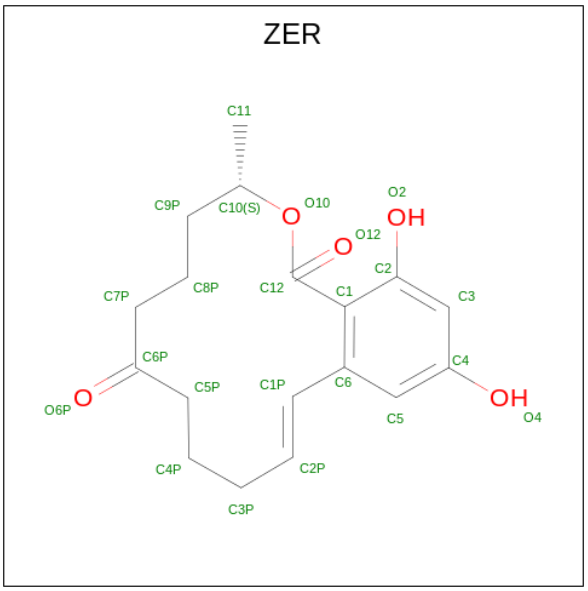
- Molecule 1 is a protein called Lactonase for protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	263	2048	1300	347	392	9	0	0	0
1	B	263	2048	1300	347	392	9	0	0	0
1	C	263	2048	1300	347	392	9	0	0	0
1	D	261	2030	1288	344	389	9	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

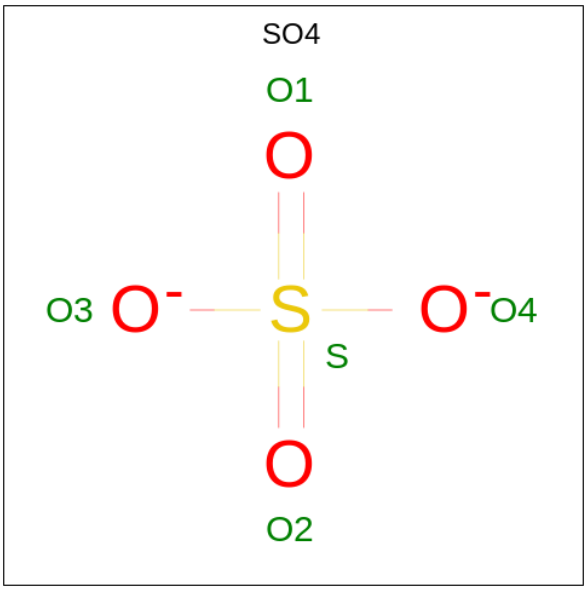
Chain	Residue	Modelled	Actual	Comment	Reference
A	105	ALA	SER	engineered mutation	UNP A0A0D2ILK1
A	160	ALA	TYR	engineered mutation	UNP A0A0D2ILK1
B	105	ALA	SER	engineered mutation	UNP A0A0D2ILK1
B	160	ALA	TYR	engineered mutation	UNP A0A0D2ILK1
C	105	ALA	SER	engineered mutation	UNP A0A0D2ILK1
C	160	ALA	TYR	engineered mutation	UNP A0A0D2ILK1
D	105	ALA	SER	engineered mutation	UNP A0A0D2ILK1
D	160	ALA	TYR	engineered mutation	UNP A0A0D2ILK1

- Molecule 2 is (3S,11E)-14,16-dihydroxy-3-methyl-3,4,5,6,9,10-hexahydro-1H-2-benzoxacyclo tetradecine-1,7(8H)-dione (three-letter code: ZER) (formula: $C_{18}H_{22}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	23	18	5	0	0
			Total	C	O		
2	B	1	23	18	5	0	0
			Total	C	O		
2	C	1	23	18	5	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
3	A	1	5	4	1	0	0

- Molecule 4 is water.

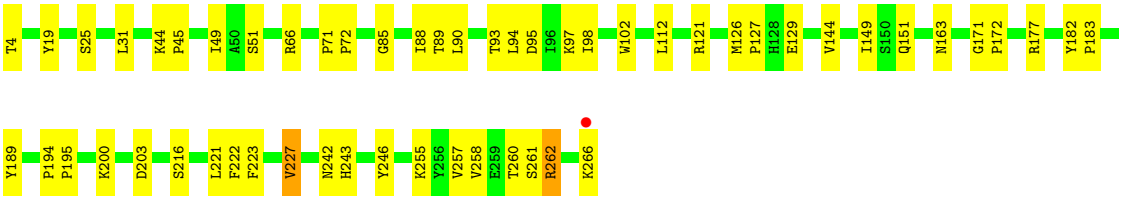
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	74	74	74	0	0
			Total	O		
4	B	97	97	97	0	0
			Total	O		
4	C	59	59	59	0	0
			Total	O		
4	D	20	20	20	0	0

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.

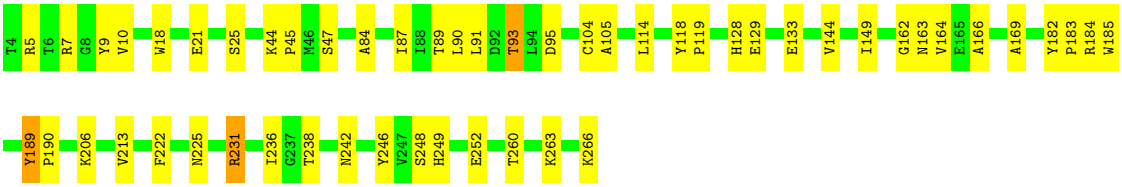
• Molecule 1: Lactonase for protein

Chain A:



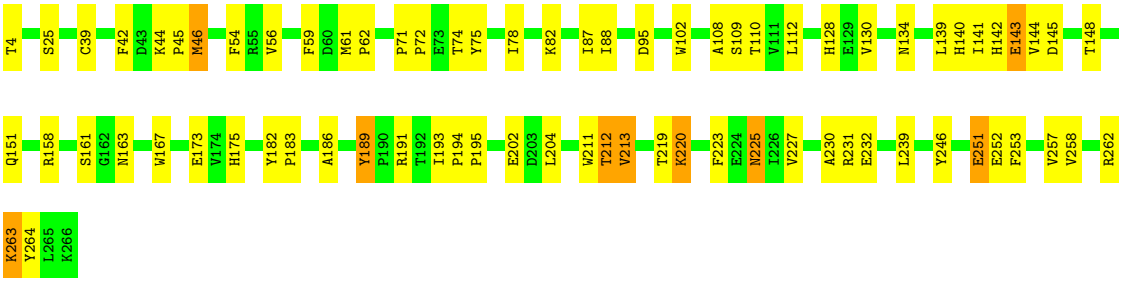
• Molecule 1: Lactonase for protein

Chain B:



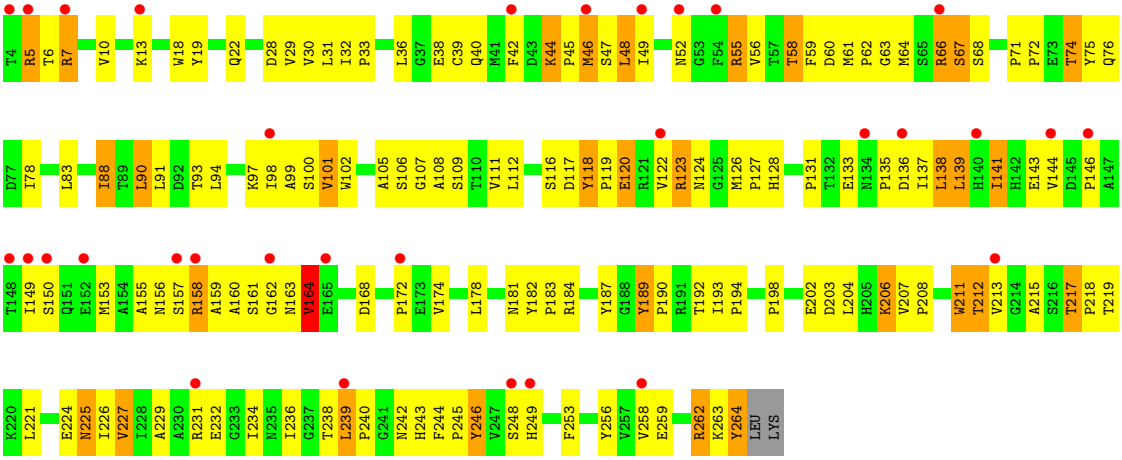
• Molecule 1: Lactonase for protein

Chain C:



• Molecule 1: Lactonase for protein

Chain D:


T4 R5 T6 R7 V10 K13 W18 Y19 Q22 D28 V29 V30 L31 I32 P33 L36 G37 E38 C39 Q40 M41 F42 D43 K44 P45 M46 S47 L48 I49 N52 G53 F54 R55 V56 T57 T58 F59 D60 M61 P62 G63 M64 S65 R66 S67 S68 P71 P72 E73 T74 Y75 Q76
D77 I78 L83 I88 T89 L90 L91 D92 T93 L94 K97 I98 A99 S100 V101 W102 A105 S106 G107 A108 S109 T110 V111 L112 S116 D117 Y118 P119 E120 R121 V122 R123 N124 G125 M126 P127 H128 P131 T132 E133 N134 P135 D136 I137 L138 L139 H140 I141 H142 E143 V144 D145 P146 A147
T148 I149 S150 Q151 E152 M153 A154 A155 N156 S157 R158 A159 A160 S161 G162 N163 V164 E165 D168 P172 E173 V174 L178 N181 Y182 P183 R184 Y187 G188 Y189 P190 R191 T192 I193 P194 P198 E202 D203 L204 H205 K206 V207 P208 W211 T212 V213 G214 A215 S216 T217 P218 T219
K220 L221 E224 N225 I226 V227 I228 A229 A230 R231 E232 G233 I234 N235 I236 G237 T238 L239 P240 G241 N242 H243 F244 P245 Y246 V247 S248 H249 F253 Y256 V257 V258 E259 R262 K263 Y264 LEU LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	44.32Å 110.52Å 127.78Å 90.00° 99.93° 90.00°	Depositor
Resolution (Å)	25.00 – 2.32 24.93 – 2.32	Depositor EDS
% Data completeness (in resolution range)	94.9 (25.00-2.32) 94.7 (24.93-2.32)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.87 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.210 , 0.266 0.217 , 0.269	Depositor DCC
R_{free} test set	2490 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	40.1	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 25.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	0.277 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	8498	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.25% 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: ZER, SO4

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	0.54	0/2106	0.60	0/2875
1	B	0.50	0/2106	0.58	0/2875
1	C	0.43	0/2106	0.58	0/2875
1	D	0.43	0/2088	0.63	0/2853
All	All	0.48	0/8406	0.60	0/11478

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	2048	0	1989	31	0
1	B	2048	0	1989	31	0
1	C	2048	0	1989	53	0
1	D	2030	0	1965	164	0
2	A	23	0	21	3	0
2	B	23	0	21	0	0
2	C	23	0	21	3	0
3	A	5	0	0	0	0
4	A	74	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	97	0	0	2	0
4	C	59	0	0	2	0
4	D	20	0	0	2	0
All	All	8498	0	7995	277	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 17.

All (277) 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:D:135:PRO:HD2	1:D:138:LEU:HD11	1.23	1.09
1:D:75:TYR:C	1:D:78:ILE:HD11	1.76	1.05
1:D:162:GLY:HA3	1:D:248:SER:HB2	1.44	0.96
1:D:49:ILE:CD1	1:D:258:VAL:HG13	1.95	0.94
1:D:160:ALA:O	1:D:242:ASN:HB2	1.66	0.94
1:A:126:MET:SD	1:A:260:THR:HG21	2.07	0.93
1:C:212:THR:HG21	1:C:239:LEU:HG	1.51	0.93
1:D:99:ALA:O	1:D:123:ARG:HB3	1.67	0.93
1:C:230:ALA:HB2	1:D:227:VAL:HG12	1.51	0.90
1:D:49:ILE:HD13	1:D:258:VAL:HG13	1.53	0.90
1:D:62:PRO:HB2	1:D:74:THR:CG2	2.04	0.88
1:D:135:PRO:HD2	1:D:138:LEU:CD1	2.02	0.88
1:D:124:ASN:ND2	1:D:264:TYR:CE1	2.42	0.88
1:D:207:VAL:HB	1:D:208:PRO:HD2	1.53	0.87
1:D:62:PRO:HB2	1:D:74:THR:HG23	1.58	0.86
1:D:62:PRO:CB	1:D:74:THR:CG2	2.53	0.85
1:C:223:PHE:O	1:C:227:VAL:HG23	1.77	0.84
1:D:66:ARG:HG2	1:D:66:ARG:HH21	1.42	0.84
1:D:135:PRO:O	1:D:139:LEU:HD12	1.77	0.84
1:D:75:TYR:CA	1:D:78:ILE:HD11	2.07	0.84
1:D:227:VAL:O	1:D:231:ARG:HG3	1.78	0.83
1:B:252:GLU:N	1:B:252:GLU:OE1	2.12	0.83
1:D:28:ASP:HA	1:D:55:ARG:O	1.80	0.82
1:D:29:VAL:HG22	1:D:100:SER:HB2	1.61	0.82
1:D:62:PRO:HB3	1:D:74:THR:HG21	1.62	0.82
1:D:29:VAL:O	1:D:56:VAL:HA	1.79	0.81
1:D:28:ASP:OD1	1:D:55:ARG:HG2	1.80	0.81
1:D:49:ILE:CD1	1:D:258:VAL:CG1	2.59	0.80
1:D:207:VAL:HB	1:D:208:PRO:CD	2.11	0.79
1:D:135:PRO:HG3	1:D:221:LEU:HD21	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:39:CYS:HB2	1:D:58:THR:HG23	1.62	0.79
1:D:72:PRO:HA	1:D:75:TYR:CZ	2.18	0.78
1:C:252:GLU:N	1:C:252:GLU:OE1	2.17	0.77
1:A:243:HIS:CD2	2:A:301:ZER:H6	2.20	0.77
1:D:137:ILE:HG13	1:D:138:LEU:HG	1.67	0.77
1:D:99:ALA:C	1:D:123:ARG:HB3	2.04	0.77
1:D:160:ALA:O	1:D:243:HIS:N	2.13	0.77
1:D:75:TYR:HA	1:D:78:ILE:HD11	1.66	0.76
1:C:223:PHE:CE1	1:C:227:VAL:HG21	2.22	0.75
1:D:29:VAL:O	1:D:56:VAL:HG23	1.86	0.75
1:C:142:HIS:CD2	1:C:191:ARG:HD3	2.23	0.74
1:D:66:ARG:HG2	1:D:66:ARG:NH2	1.98	0.74
1:D:135:PRO:HB2	1:D:137:ILE:HG12	1.70	0.74
1:D:141:ILE:HD13	1:D:149:ILE:HG12	1.68	0.74
1:B:260:THR:O	1:B:263:LYS:HG2	1.87	0.73
1:D:39:CYS:O	1:D:42:PHE:HB2	1.89	0.73
1:D:88:ILE:HG13	1:D:118:TYR:CD2	2.24	0.73
1:C:42:PHE:O	1:C:46:MET:HB2	1.90	0.72
1:D:28:ASP:OD1	1:D:55:ARG:HB3	1.90	0.72
1:D:39:CYS:HB2	1:D:58:THR:CG2	2.18	0.72
1:D:182:TYR:HB2	1:D:183:PRO:HD3	1.70	0.72
1:D:107:GLY:O	1:D:111:VAL:HG23	1.89	0.72
1:D:62:PRO:HB3	1:D:74:THR:CG2	2.20	0.71
1:D:211:TRP:HB3	1:D:236:ILE:HD12	1.72	0.71
1:D:158:ARG:HD2	1:D:158:ARG:C	2.10	0.71
1:D:112:LEU:HB2	1:D:198:PRO:HG2	1.74	0.70
1:D:135:PRO:O	1:D:139:LEU:CD1	2.38	0.70
1:D:29:VAL:N	1:D:55:ARG:O	2.24	0.70
1:D:135:PRO:CD	1:D:138:LEU:HD11	2.14	0.69
1:D:36:LEU:O	1:D:181:ASN:ND2	2.25	0.69
1:D:44:LYS:HB2	1:D:45:PRO:CD	2.23	0.69
1:D:60:ASP:OD2	1:D:66:ARG:HB2	1.93	0.69
1:D:62:PRO:CB	1:D:74:THR:HG23	2.19	0.69
1:D:100:SER:OG	1:D:123:ARG:HG2	1.93	0.69
1:D:88:ILE:HD13	1:D:91:LEU:HD12	1.74	0.68
1:D:62:PRO:CB	1:D:74:THR:HG21	2.23	0.67
1:D:75:TYR:C	1:D:78:ILE:CD1	2.61	0.67
1:D:217:THR:HG22	1:D:218:PRO:HD2	1.76	0.67
1:B:144:VAL:HG23	1:B:149:ILE:HG13	1.77	0.66
1:A:4:THR:HG22	1:C:151:GLN:OE1	1.94	0.66
1:D:10:VAL:HG21	1:D:94:LEU:HD21	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:30:VAL:C	1:D:31:LEU:HD23	2.16	0.66
1:D:52:ASN:OD1	1:D:262:ARG:NH2	2.29	0.66
1:D:7:ARG:HD2	1:D:19:TYR:OH	1.96	0.66
1:D:39:CYS:CB	1:D:58:THR:HG23	2.25	0.66
1:D:76:GLN:N	1:D:78:ILE:HD11	2.10	0.66
1:D:161:SER:O	1:D:248:SER:HB3	1.96	0.65
1:D:44:LYS:HB2	1:D:45:PRO:HD3	1.79	0.65
1:D:227:VAL:O	1:D:231:ARG:CG	2.44	0.65
1:A:126:MET:SD	1:A:260:THR:CG2	2.84	0.64
1:D:189:TYR:H	1:D:190:PRO:HD2	1.61	0.64
1:D:259:GLU:HA	1:D:262:ARG:HG3	1.79	0.64
1:D:28:ASP:OD1	1:D:55:ARG:CG	2.47	0.63
1:A:144:VAL:HG23	1:A:149:ILE:HG13	1.81	0.63
1:D:144:VAL:HG23	1:D:149:ILE:HG13	1.81	0.63
1:D:120:GLU:CD	1:D:120:GLU:H	2.02	0.62
1:C:72:PRO:HA	1:C:75:TYR:CZ	2.35	0.61
1:C:220:LYS:HG2	1:D:215:ALA:HB1	1.83	0.61
1:D:207:VAL:CB	1:D:208:PRO:CD	2.77	0.61
1:A:257:VAL:O	1:A:260:THR:HG22	2.00	0.61
1:D:160:ALA:C	1:D:242:ASN:HB2	2.21	0.61
1:D:204:LEU:CD2	1:D:234:ILE:HD11	2.31	0.61
1:D:206:LYS:HA	1:D:206:LYS:NZ	2.16	0.60
1:D:49:ILE:HD11	1:D:258:VAL:CG1	2.30	0.60
1:A:85:GLY:O	1:A:89:THR:HG23	2.01	0.60
1:D:39:CYS:HA	1:D:42:PHE:HD2	1.67	0.60
1:D:207:VAL:CB	1:D:208:PRO:HD2	2.28	0.60
2:C:301:ZER:O10	2:C:301:ZER:H11	2.01	0.59
1:D:49:ILE:HD12	1:D:49:ILE:O	2.02	0.59
1:D:155:ALA:O	1:D:158:ARG:HG3	2.03	0.59
1:A:4:THR:N	4:A:401:HOH:O	2.34	0.59
1:D:40:GLN:HG3	1:D:40:GLN:O	2.02	0.59
1:D:128:HIS:ND1	1:D:212:THR:O	2.35	0.59
1:D:66:ARG:HH21	1:D:66:ARG:CG	2.13	0.59
1:D:164:VAL:O	1:D:168:ASP:OD1	2.21	0.58
1:C:175:HIS:ND1	4:C:401:HOH:O	2.32	0.58
1:D:160:ALA:O	1:D:242:ASN:CB	2.48	0.58
1:A:243:HIS:HD2	2:A:301:ZER:H6	1.67	0.58
1:D:90:LEU:O	1:D:90:LEU:HG	1.99	0.58
1:A:260:THR:HG23	1:A:261:SER:N	2.18	0.58
1:D:204:LEU:HG	1:D:234:ILE:HD11	1.84	0.57
1:C:75:TYR:HA	1:C:78:ILE:HD11	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:38:GLU:CD	1:D:40:GLN:HB3	2.25	0.57
1:D:39:CYS:SG	1:D:58:THR:HG23	2.44	0.57
1:D:116:SER:HB2	1:D:203:ASP:HB3	1.85	0.57
1:D:99:ALA:O	1:D:123:ARG:CB	2.48	0.57
1:D:88:ILE:HG13	1:D:118:TYR:CE2	2.40	0.56
1:D:28:ASP:OD1	1:D:55:ARG:CB	2.53	0.56
1:D:64:MET:HB3	1:D:181:ASN:ND2	2.20	0.56
1:B:128:HIS:CD2	1:B:129:GLU:HG3	2.40	0.56
1:D:52:ASN:OD1	1:D:52:ASN:O	2.23	0.56
1:D:31:LEU:HD23	1:D:31:LEU:N	2.20	0.55
1:A:182:TYR:HB2	1:A:183:PRO:HD3	1.87	0.55
1:C:128:HIS:ND1	1:C:212:THR:HB	2.21	0.55
1:D:153:MET:HE3	1:D:153:MET:HA	1.88	0.55
1:C:213:VAL:HG12	1:D:219:THR:HG21	1.87	0.54
1:D:63:GLY:HA3	1:D:75:TYR:CD2	2.42	0.54
1:B:231:ARG:NE	4:B:405:HOH:O	2.39	0.54
1:B:44:LYS:N	1:B:45:PRO:CD	2.70	0.54
1:C:182:TYR:HB2	1:C:183:PRO:HD3	1.90	0.54
1:C:134:ASN:ND2	2:C:301:ZER:O4	2.39	0.53
1:D:161:SER:O	1:D:248:SER:CB	2.55	0.53
1:D:105:ALA:O	1:D:108:ALA:HB3	2.08	0.53
1:D:45:PRO:HA	1:D:48:LEU:HD22	1.91	0.53
1:D:238:THR:O	1:D:239:LEU:HD12	2.09	0.52
1:D:60:ASP:HB2	1:D:67:SER:OG	2.10	0.52
1:D:189:TYR:N	1:D:190:PRO:HD2	2.23	0.52
1:D:136:ASP:HA	1:D:139:LEU:HD13	1.91	0.52
1:C:213:VAL:CG1	1:D:219:THR:HG21	2.41	0.51
1:D:206:LYS:HA	1:D:206:LYS:CE	2.40	0.51
1:D:118:TYR:N	1:D:118:TYR:CD1	2.79	0.51
1:C:142:HIS:CE1	1:C:143:GLU:HG2	2.47	0.50
1:D:117:ASP:C	1:D:119:PRO:HD3	2.32	0.50
1:D:215:ALA:N	1:D:239:LEU:O	2.45	0.50
1:C:158:ARG:HG3	1:C:167:TRP:CD1	2.46	0.50
1:D:71:PRO:O	1:D:74:THR:HB	2.12	0.50
1:C:72:PRO:HA	1:C:75:TYR:CE1	2.47	0.50
1:D:76:GLN:N	1:D:78:ILE:CD1	2.75	0.49
1:D:217:THR:CG2	1:D:218:PRO:HD2	2.41	0.49
1:C:102:TRP:CD1	1:C:102:TRP:C	2.85	0.49
1:D:120:GLU:OE2	1:D:120:GLU:N	2.42	0.49
1:D:141:ILE:O	1:D:141:ILE:HG23	2.12	0.49
1:B:9:TYR:HA	1:B:18:TRP:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:204:LEU:CG	1:D:234:ILE:HD11	2.42	0.49
1:D:40:GLN:HG2	1:D:174:VAL:HG21	1.93	0.49
1:A:260:THR:CG2	1:A:261:SER:N	2.75	0.49
1:D:28:ASP:CA	1:D:55:ARG:O	2.55	0.49
1:B:95:ASP:CG	1:B:95:ASP:O	2.51	0.49
1:C:108:ALA:HB1	1:C:130:VAL:HG22	1.95	0.49
1:D:31:LEU:HB3	1:D:42:PHE:CE1	2.47	0.48
1:A:258:VAL:O	1:A:262:ARG:HB2	2.13	0.48
1:D:172:PRO:HD3	4:D:312:HOH:O	2.12	0.48
1:D:153:MET:HA	1:D:156:ASN:HB2	1.95	0.48
1:C:194:PRO:HB2	1:C:195:PRO:HD3	1.94	0.48
1:D:78:ILE:HG23	1:D:83:LEU:HG	1.94	0.48
1:B:44:LYS:HB2	1:B:45:PRO:HD3	1.95	0.47
1:D:124:ASN:ND2	1:D:264:TYR:CD1	2.82	0.47
1:B:5:ARG:NH1	1:B:21:GLU:OE1	2.47	0.47
1:C:263:LYS:HE3	1:C:264:TYR:CZ	2.50	0.47
1:D:248:SER:OG	1:D:249:HIS:N	2.47	0.47
1:C:87:ILE:HD12	1:C:110:THR:HG21	1.96	0.47
1:C:145:ASP:OD1	1:C:148:THR:CB	2.62	0.47
1:D:112:LEU:HD21	1:D:127:PRO:HG3	1.95	0.47
1:C:193:ILE:N	1:C:194:PRO:CD	2.78	0.47
1:B:189:TYR:HB2	1:B:190:PRO:HD3	1.97	0.47
1:D:19:TYR:CD1	1:D:19:TYR:C	2.88	0.47
1:D:193:ILE:HB	1:D:194:PRO:HD3	1.97	0.47
1:C:142:HIS:NE2	1:C:191:ARG:HD3	2.29	0.47
1:A:44:LYS:N	1:A:45:PRO:HD2	2.30	0.47
1:B:18:TRP:CD2	1:B:90:LEU:HD22	2.50	0.47
1:C:194:PRO:HB2	1:C:195:PRO:CD	2.44	0.46
1:C:232:GLU:OE1	1:C:232:GLU:HA	2.15	0.46
1:D:99:ALA:O	1:D:123:ARG:N	2.39	0.46
1:A:31:LEU:HD23	1:A:102:TRP:HB3	1.96	0.46
1:B:185:TRP:CH2	1:B:190:PRO:HG3	2.51	0.46
1:D:18:TRP:HA	1:D:67:SER:HB3	1.97	0.46
1:D:32:ILE:HD12	1:D:101:VAL:HG12	1.97	0.46
1:D:66:ARG:HD3	4:D:302:HOH:O	2.16	0.46
1:D:211:TRP:CE3	1:D:229:ALA:HB2	2.51	0.46
1:A:112:LEU:HD21	1:A:127:PRO:HG3	1.97	0.46
1:C:211:TRP:NE1	1:C:225:ASN:OD1	2.39	0.46
1:D:88:ILE:CD1	1:D:91:LEU:HD12	2.44	0.46
1:C:61:MET:HB3	1:C:62:PRO:CD	2.45	0.46
1:C:108:ALA:CB	1:C:130:VAL:HG22	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:153:MET:HE3	1:D:153:MET:CA	2.45	0.46
1:C:54:PHE:CD1	1:C:54:PHE:N	2.84	0.45
1:B:213:VAL:O	1:B:238:THR:HA	2.15	0.45
1:D:33:PRO:HA	1:D:42:PHE:HE2	1.81	0.45
1:C:193:ILE:HB	1:C:194:PRO:HD3	1.97	0.45
1:D:221:LEU:HA	1:D:221:LEU:HD23	1.67	0.45
1:B:162:GLY:HA2	1:B:242:ASN:OD1	2.17	0.45
1:D:124:ASN:ND2	1:D:264:TYR:HE1	2.07	0.45
1:A:262:ARG:HD3	1:A:262:ARG:HA	1.76	0.45
1:C:44:LYS:N	1:C:45:PRO:CD	2.79	0.45
1:C:251:GLU:H	1:C:251:GLU:HG2	1.45	0.45
1:B:118:TYR:N	1:B:119:PRO:CD	2.79	0.45
1:B:129:GLU:HB3	1:B:222:PHE:CE2	2.51	0.45
1:D:29:VAL:O	1:D:56:VAL:CG2	2.63	0.45
1:D:239:LEU:HG	1:D:240:PRO:HD2	1.99	0.45
1:C:158:ARG:O	1:C:161:SER:OG	2.32	0.45
1:A:177:ARG:HD3	4:A:453:HOH:O	2.17	0.45
1:D:213:VAL:O	1:D:238:THR:HA	2.17	0.45
1:B:248:SER:HG	1:B:249:HIS:CE1	2.27	0.44
1:C:112:LEU:HA	1:C:112:LEU:HD23	1.75	0.44
1:A:200:LYS:HB2	1:A:203:ASP:OD2	2.17	0.44
1:D:29:VAL:O	1:D:56:VAL:CA	2.60	0.44
1:B:7:ARG:NH2	4:B:408:HOH:O	2.49	0.44
1:B:105:ALA:HA	1:B:129:GLU:O	2.18	0.44
1:D:158:ARG:HD2	1:D:159:ALA:N	2.33	0.44
1:C:141:ILE:HG23	1:C:186:ALA:HB1	1.99	0.44
1:B:89:THR:O	1:B:93:THR:HG23	2.18	0.44
1:B:222:PHE:O	1:B:225:ASN:HB2	2.18	0.43
1:D:204:LEU:CD2	1:D:232:GLU:HG3	2.48	0.43
1:A:45:PRO:O	1:A:49:ILE:HD12	2.18	0.43
1:D:178:LEU:HD23	1:D:178:LEU:HA	1.80	0.43
1:D:225:ASN:N	1:D:225:ASN:HD22	2.16	0.43
1:C:253:PHE:O	1:C:257:VAL:HG23	2.18	0.43
1:A:98:ILE:HD12	1:A:121:ARG:C	2.39	0.43
1:C:145:ASP:OD1	1:C:148:THR:OG1	2.23	0.43
1:A:223:PHE:CE1	1:A:227:VAL:HG11	2.53	0.43
1:D:32:ILE:HG23	1:D:61:MET:CE	2.49	0.43
1:D:131:PRO:O	1:D:194:PRO:HA	2.19	0.43
1:B:104:CYS:HA	1:B:128:HIS:O	2.19	0.43
1:C:46:MET:HG2	1:C:56:VAL:HG11	1.99	0.43
2:C:301:ZER:O10	2:C:301:ZER:C1P	2.64	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:TYR:CE2	1:A:66:ARG:CZ	3.01	0.42
1:D:5:ARG:HA	1:D:22:GLN:O	2.19	0.42
1:D:160:ALA:HB1	1:D:243:HIS:HB2	2.00	0.42
1:C:78:ILE:HG13	1:C:189:TYR:CE1	2.54	0.42
1:D:42:PHE:O	1:D:46:MET:N	2.52	0.42
1:D:243:HIS:C	1:D:245:PRO:HD3	2.39	0.42
1:C:139:LEU:HD22	1:C:140:HIS:CE1	2.53	0.42
1:A:88:ILE:HD13	1:A:88:ILE:HA	1.85	0.42
1:B:166:ALA:HA	1:B:169:ALA:HB3	2.02	0.42
2:A:301:ZER:O10	2:A:301:ZER:H11	2.19	0.42
1:C:4:THR:N	4:C:408:HOH:O	2.51	0.42
1:A:194:PRO:N	1:A:195:PRO:CD	2.82	0.42
1:C:145:ASP:OD1	1:C:148:THR:HB	2.19	0.42
1:A:216:SER:HB2	1:A:242:ASN:OD1	2.20	0.42
1:D:33:PRO:HA	1:D:42:PHE:CE2	2.54	0.42
1:D:246:TYR:HB3	1:D:253:PHE:CE2	2.54	0.42
1:C:39:CYS:HB3	1:C:59:PHE:O	2.20	0.42
1:C:258:VAL:O	1:C:262:ARG:HB3	2.20	0.41
1:D:102:TRP:HE3	1:D:126:MET:HG3	1.84	0.41
1:A:71:PRO:HA	1:A:72:PRO:HD3	1.84	0.41
1:A:171:GLY:HA2	1:A:172:PRO:HD3	1.84	0.41
1:D:118:TYR:N	1:D:119:PRO:HD3	2.35	0.41
1:D:49:ILE:HD11	1:D:258:VAL:HG12	2.02	0.41
1:B:84:ALA:HB1	1:B:114:LEU:HD23	2.03	0.41
1:B:119:PRO:HG3	1:B:206:LYS:HD3	2.02	0.41
1:B:149:ILE:HG21	1:B:183:PRO:HA	2.02	0.41
1:A:221:LEU:HD23	1:A:221:LEU:HA	1.92	0.41
1:B:87:ILE:O	1:B:91:LEU:HG	2.21	0.41
1:D:10:VAL:CG1	1:D:93:THR:HG21	2.50	0.41
1:D:72:PRO:HA	1:D:75:TYR:CE1	2.55	0.41
1:C:42:PHE:C	1:C:45:PRO:HD2	2.40	0.41
1:C:134:ASN:HD21	1:C:194:PRO:HG3	1.85	0.41
1:B:44:LYS:N	1:B:45:PRO:HD2	2.35	0.41
1:C:71:PRO:HD2	1:C:74:THR:HG21	2.03	0.41
1:B:182:TYR:HB2	1:B:183:PRO:HD3	2.02	0.41
1:D:244:PHE:O	1:D:248:SER:N	2.46	0.41
1:A:129:GLU:HB3	1:A:222:PHE:CZ	2.56	0.40
1:D:49:ILE:HD11	1:D:258:VAL:HG13	1.86	0.40
1:C:142:HIS:ND1	1:C:143:GLU:HG2	2.37	0.40
1:B:144:VAL:CG2	1:B:149:ILE:HG13	2.48	0.40
1:D:146:PRO:HG3	1:D:187:TYR:OH	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:LEU:HD11	1:A:94:LEU:HD11	2.03	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	261/263 (99%)	253 (97%)	6 (2%)	2 (1%)	19	23
1	B	261/263 (99%)	251 (96%)	8 (3%)	2 (1%)	19	23
1	C	261/263 (99%)	251 (96%)	8 (3%)	2 (1%)	19	23
1	D	259/263 (98%)	232 (90%)	25 (10%)	2 (1%)	19	23
All	All	1042/1052 (99%)	987 (95%)	47 (4%)	8 (1%)	19	23

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	163	ASN
1	D	189	TYR
1	A	189	TYR
1	C	163	ASN
1	C	189	TYR
1	D	164	VAL
1	B	163	ASN
1	B	189	TYR

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	222/222 (100%)	211 (95%)	11 (5%)	24 34
1	B	222/222 (100%)	211 (95%)	11 (5%)	24 34
1	C	222/222 (100%)	202 (91%)	20 (9%)	9 11
1	D	220/222 (99%)	167 (76%)	53 (24%)	0 0
All	All	886/888 (100%)	791 (89%)	95 (11%)	6 7

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	SER
1	A	51	SER
1	A	93	THR
1	A	95	ASP
1	A	97	LYS
1	A	151	GLN
1	A	227	VAL
1	A	246	TYR
1	A	255	LYS
1	A	262	ARG
1	A	266	LYS
1	B	10	VAL
1	B	25	SER
1	B	47	SER
1	B	93	THR
1	B	133	GLU
1	B	164	VAL
1	B	184	ARG
1	B	231	ARG
1	B	236	ILE
1	B	246	TYR
1	B	266	LYS
1	C	25	SER
1	C	46	MET
1	C	82	LYS
1	C	88	ILE
1	C	95	ASP
1	C	109	SER
1	C	143	GLU
1	C	144	VAL

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Mol	Chain	Res	Type
1	C	173	GLU
1	C	202	GLU
1	C	204	LEU
1	C	212	THR
1	C	213	VAL
1	C	219	THR
1	C	220	LYS
1	C	225	ASN
1	C	231	ARG
1	C	246	TYR
1	C	251	GLU
1	C	263	LYS
1	D	5	ARG
1	D	6	THR
1	D	7	ARG
1	D	13	LYS
1	D	44	LYS
1	D	46	MET
1	D	47	SER
1	D	48	LEU
1	D	55	ARG
1	D	58	THR
1	D	59	PHE
1	D	66	ARG
1	D	67	SER
1	D	68	SER
1	D	74	THR
1	D	88	ILE
1	D	90	LEU
1	D	97	LYS
1	D	98	ILE
1	D	101	VAL
1	D	106	SER
1	D	109	SER
1	D	118	TYR
1	D	120	GLU
1	D	122	VAL
1	D	123	ARG
1	D	133	GLU
1	D	138	LEU
1	D	139	LEU
1	D	141	ILE

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Mol	Chain	Res	Type
1	D	143	GLU
1	D	150	SER
1	D	157	SER
1	D	158	ARG
1	D	163	ASN
1	D	164	VAL
1	D	184	ARG
1	D	192	THR
1	D	202	GLU
1	D	206	LYS
1	D	211	TRP
1	D	212	THR
1	D	217	THR
1	D	224	GLU
1	D	225	ASN
1	D	226	ILE
1	D	227	VAL
1	D	239	LEU
1	D	246	TYR
1	D	256	TYR
1	D	262	ARG
1	D	263	LYS
1	D	264	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	134	ASN
1	C	205	HIS
1	D	156	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)

4 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
2	ZER	B	301	-	24,24,24	1.71	5 (20%)	32,32,32	1.14	3 (9%)
2	ZER	A	301	-	24,24,24	1.68	5 (20%)	32,32,32	1.15	3 (9%)
2	ZER	C	301	-	24,24,24	1.68	5 (20%)	32,32,32	0.94	1 (3%)
3	SO4	A	302	-	4,4,4	0.40	0	6,6,6	0.24	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
2	ZER	B	301	-	-	8/22/22/22	0/1/2/2
2	ZER	A	301	-	-	8/22/22/22	0/1/2/2
2	ZER	C	301	-	-	8/22/22/22	0/1/2/2

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	ZER	C5P-C6P	-3.95	1.41	1.50
2	C	301	ZER	C5P-C6P	-3.95	1.41	1.50
2	A	301	ZER	C6-C1P	-3.79	1.41	1.47
2	A	301	ZER	C5P-C6P	-3.77	1.41	1.50
2	C	301	ZER	C1-C12	-3.62	1.42	1.50
2	B	301	ZER	C7P-C6P	-3.53	1.42	1.50
2	A	301	ZER	C1-C12	-3.41	1.42	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	ZER	C1-C12	-3.34	1.42	1.50
2	C	301	ZER	C7P-C6P	-3.27	1.42	1.50
2	B	301	ZER	C1P-C2P	3.24	1.41	1.31
2	B	301	ZER	C6-C1P	-3.19	1.42	1.47
2	C	301	ZER	C6-C1P	-3.14	1.42	1.47
2	A	301	ZER	C1P-C2P	3.07	1.41	1.31
2	A	301	ZER	C7P-C6P	-2.95	1.43	1.50
2	C	301	ZER	C1P-C2P	2.64	1.40	1.31

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	301	ZER	C3P-C2P-C1P	-3.09	119.63	125.45
2	B	301	ZER	C7P-C6P-C5P	2.58	121.89	116.98
2	A	301	ZER	C11-C10-C9P	-2.48	107.28	113.97
2	B	301	ZER	C8P-C7P-C6P	-2.26	108.78	114.60
2	A	301	ZER	C6-C1-C2	-2.20	116.78	118.91
2	C	301	ZER	C3P-C2P-C1P	-2.07	121.55	125.45
2	A	301	ZER	O2-C2-C1	-2.01	117.38	121.14

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	ZER	C1-C12-O10-C10
2	C	301	ZER	C3P-C4P-C5P-C6P
2	B	301	ZER	C2P-C3P-C4P-C5P
2	C	301	ZER	C2P-C3P-C4P-C5P
2	A	301	ZER	C3P-C4P-C5P-C6P
2	B	301	ZER	C3P-C4P-C5P-C6P
2	B	301	ZER	C6P-C7P-C8P-C9P
2	C	301	ZER	C6P-C7P-C8P-C9P
2	A	301	ZER	C2P-C3P-C4P-C5P
2	A	301	ZER	O12-C12-O10-C10
2	A	301	ZER	C6P-C7P-C8P-C9P
2	C	301	ZER	C5P-C6P-C7P-C8P
2	C	301	ZER	C11-C10-O10-C12
2	C	301	ZER	C9P-C10-O10-C12
2	C	301	ZER	C1P-C2P-C3P-C4P
2	C	301	ZER	O6P-C6P-C7P-C8P
2	B	301	ZER	C2-C1-C12-O10
2	A	301	ZER	O6P-C6P-C7P-C8P

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Mol	Chain	Res	Type	Atoms
2	B	301	ZER	C1-C12-O10-C10
2	B	301	ZER	O6P-C6P-C7P-C8P
2	B	301	ZER	C6-C1-C12-O10
2	A	301	ZER	C7P-C8P-C9P-C10
2	B	301	ZER	C5P-C6P-C7P-C8P
2	A	301	ZER	C6-C1-C12-O10

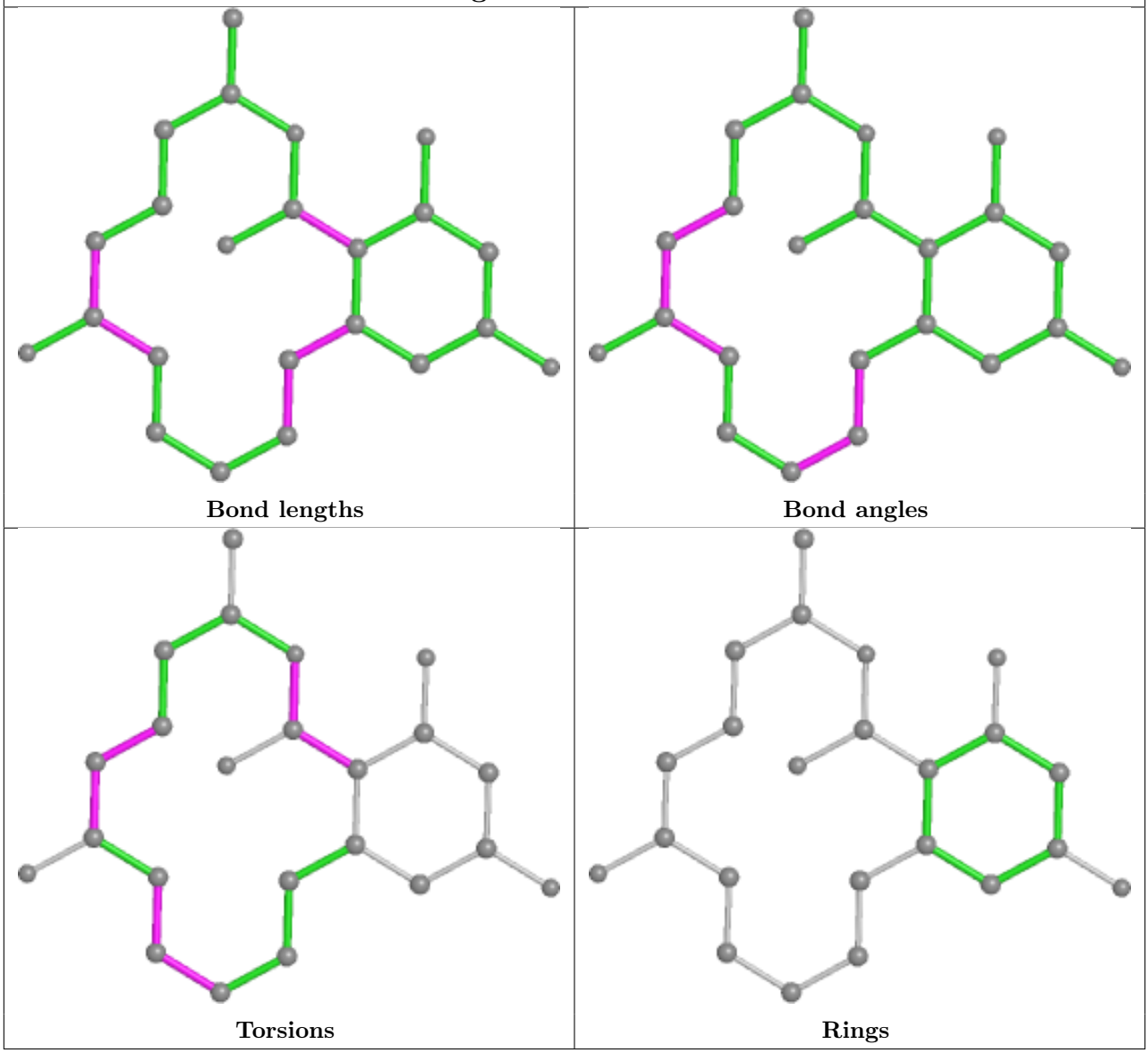
There are no ring outliers.

2 monomers are involved in 6 short contacts:

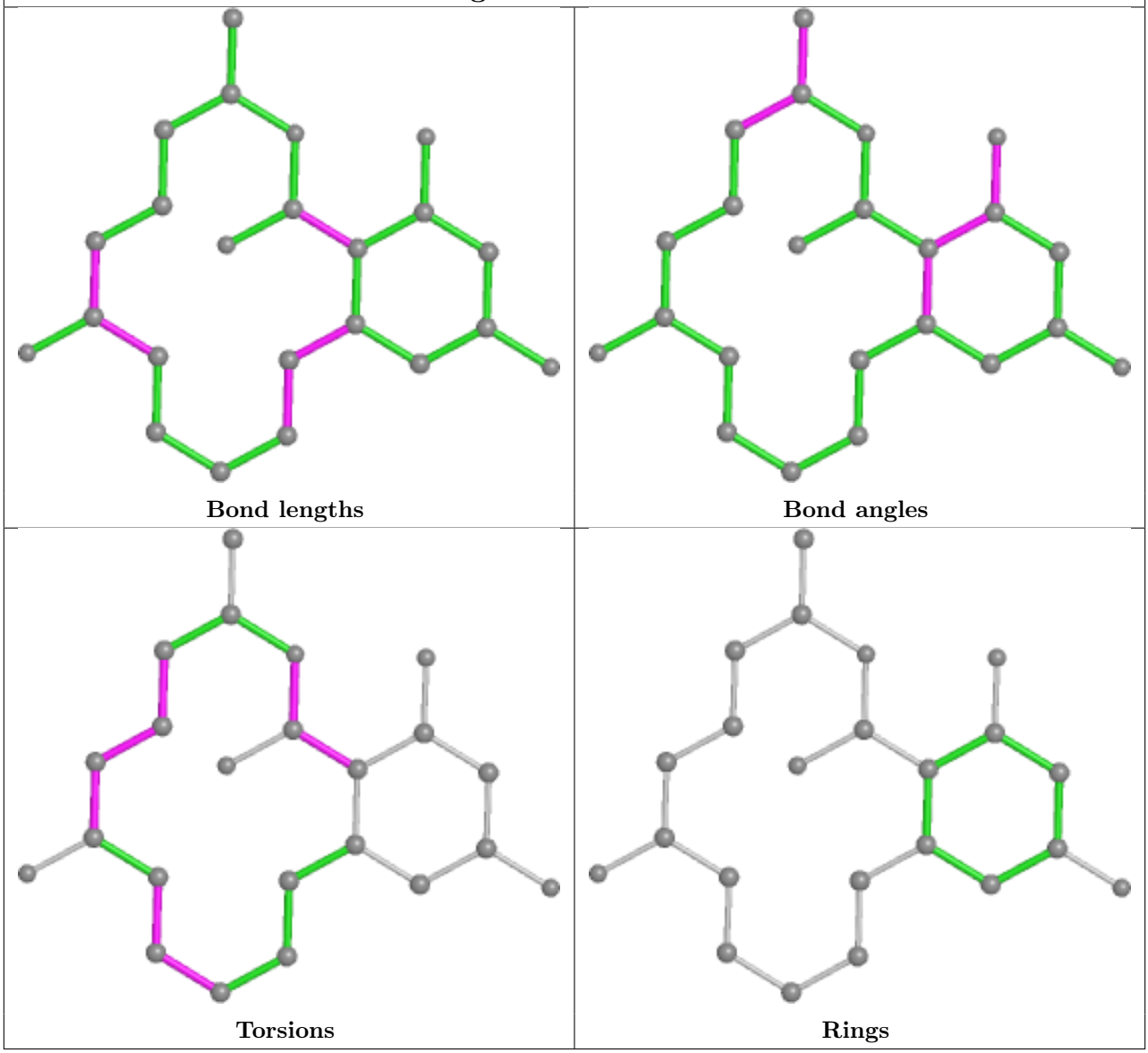
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	ZER	3	0
2	C	301	ZER	3	0

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.

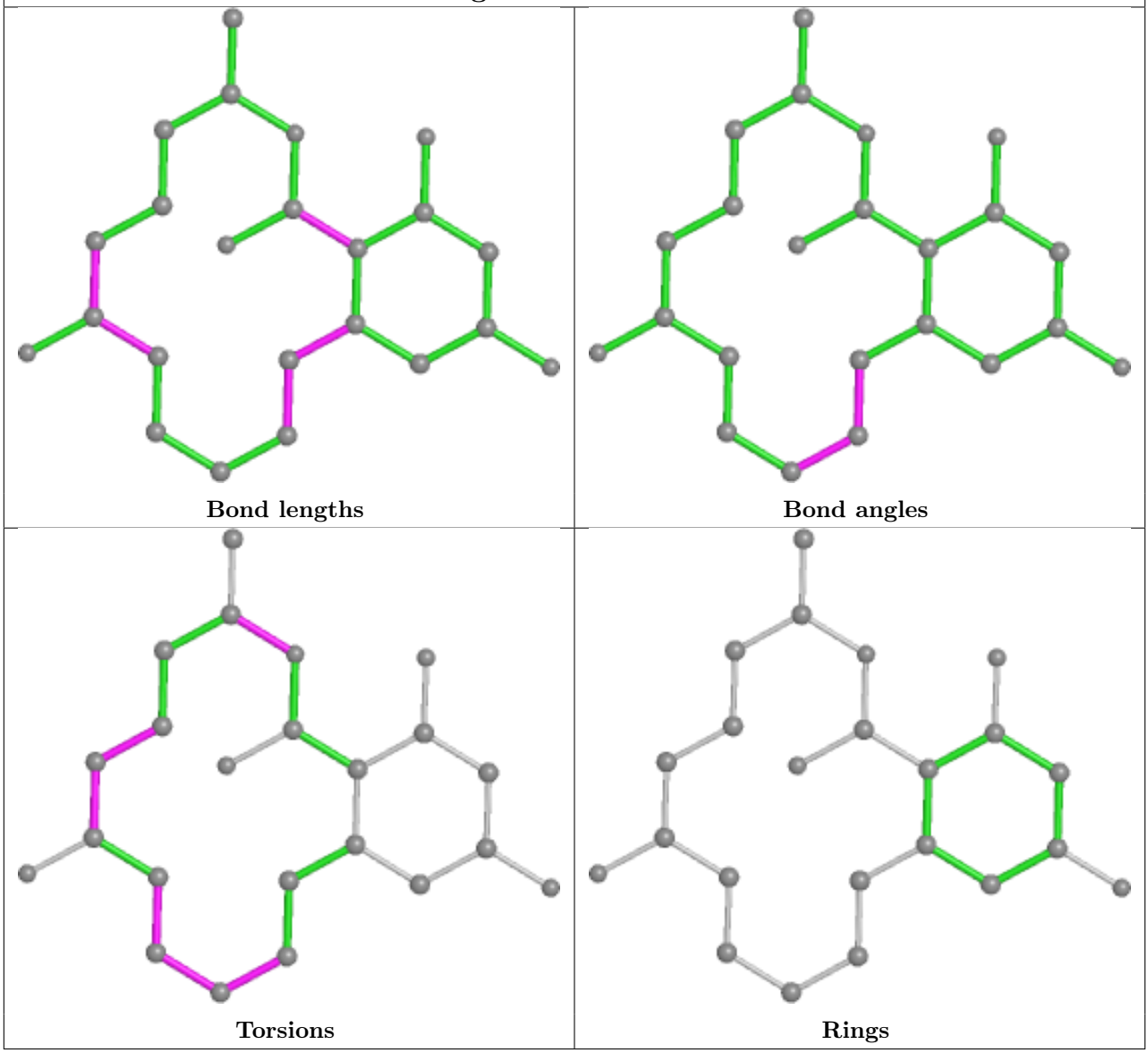
Ligand ZER B 301



Ligand ZER A 301



Ligand ZER C 301



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	263/263 (100%)	-0.36	1 (0%) 92 95	23, 36, 50, 88	0
1	B	263/263 (100%)	-0.35	0 100 100	22, 35, 49, 76	0
1	C	263/263 (100%)	-0.21	0 100 100	31, 48, 65, 81	0
1	D	261/263 (99%)	0.71	32 (12%) 4 6	34, 70, 100, 113	0
All	All	1050/1052 (99%)	-0.06	33 (3%) 49 56	22, 44, 85, 113	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	7	ARG	6.2
1	D	148	THR	4.8
1	D	144	VAL	4.7
1	D	146	PRO	4.0
1	A	266	LYS	4.0
1	D	172	PRO	3.6
1	D	98	ILE	3.4
1	D	152	GLU	3.3
1	D	162	GLY	3.1
1	D	149	ILE	3.0
1	D	249	HIS	2.9
1	D	42	PHE	2.9
1	D	140	HIS	2.9
1	D	54	PHE	2.9
1	D	150	SER	2.8
1	D	46	MET	2.8
1	D	213	VAL	2.7
1	D	231	ARG	2.7
1	D	134	ASN	2.6
1	D	4	THR	2.6
1	D	66	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	165	GLU	2.6
1	D	49	ILE	2.5
1	D	239	LEU	2.3
1	D	136	ASP	2.3
1	D	158	ARG	2.2
1	D	248	SER	2.2
1	D	5	ARG	2.1
1	D	157	SER	2.1
1	D	13	LYS	2.1
1	D	122	VAL	2.1
1	D	258	VAL	2.0
1	D	52	ASN	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)

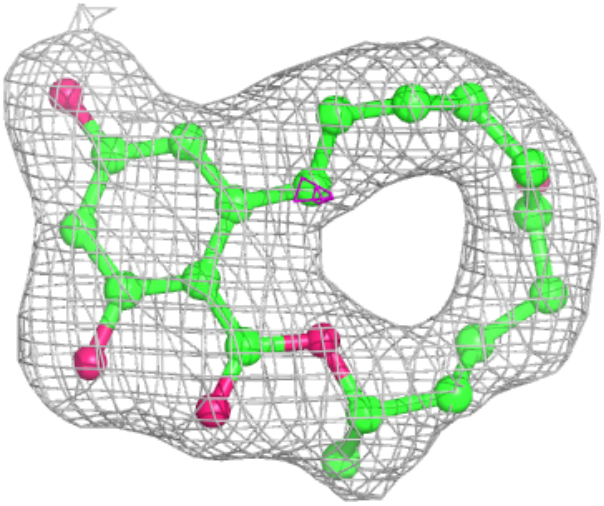
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

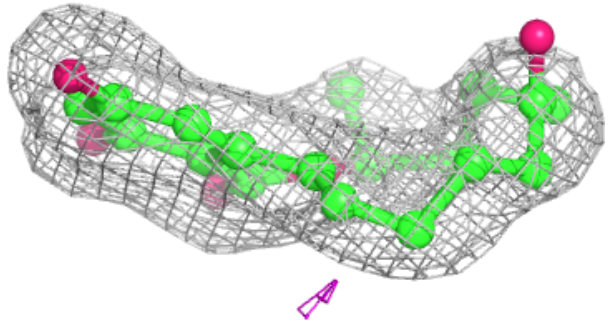
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	A	302	5/5	0.90	0.21	48,55,75,76	0
2	ZER	C	301	23/23	0.95	0.14	33,45,72,86	0
2	ZER	A	301	23/23	0.95	0.16	22,33,58,62	0
2	ZER	B	301	23/23	0.96	0.12	20,32,45,60	0

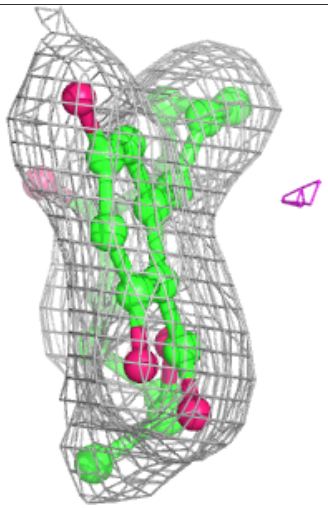
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ZER C 301:

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

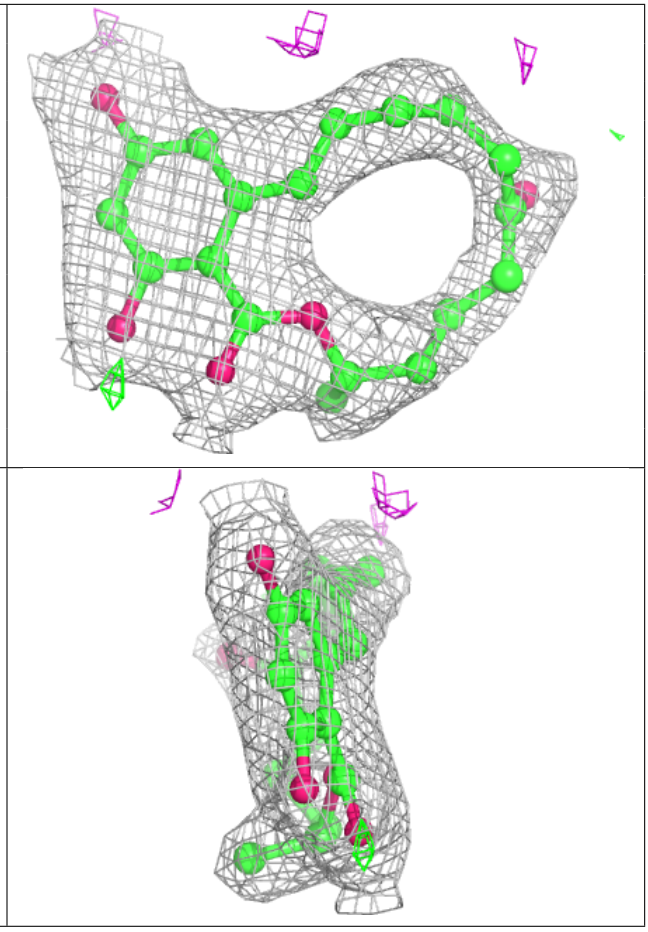


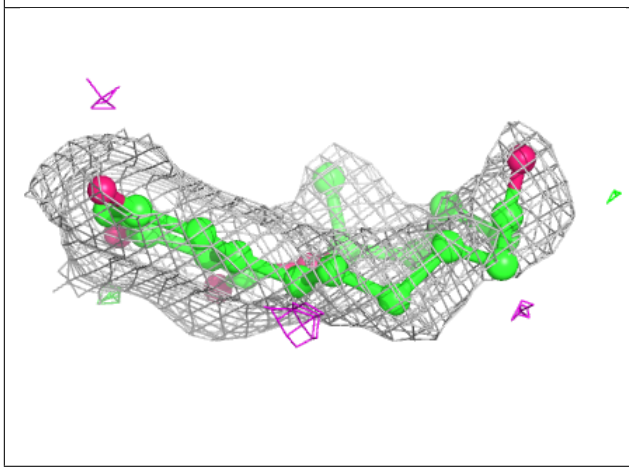




Electron density around ZER A 301:

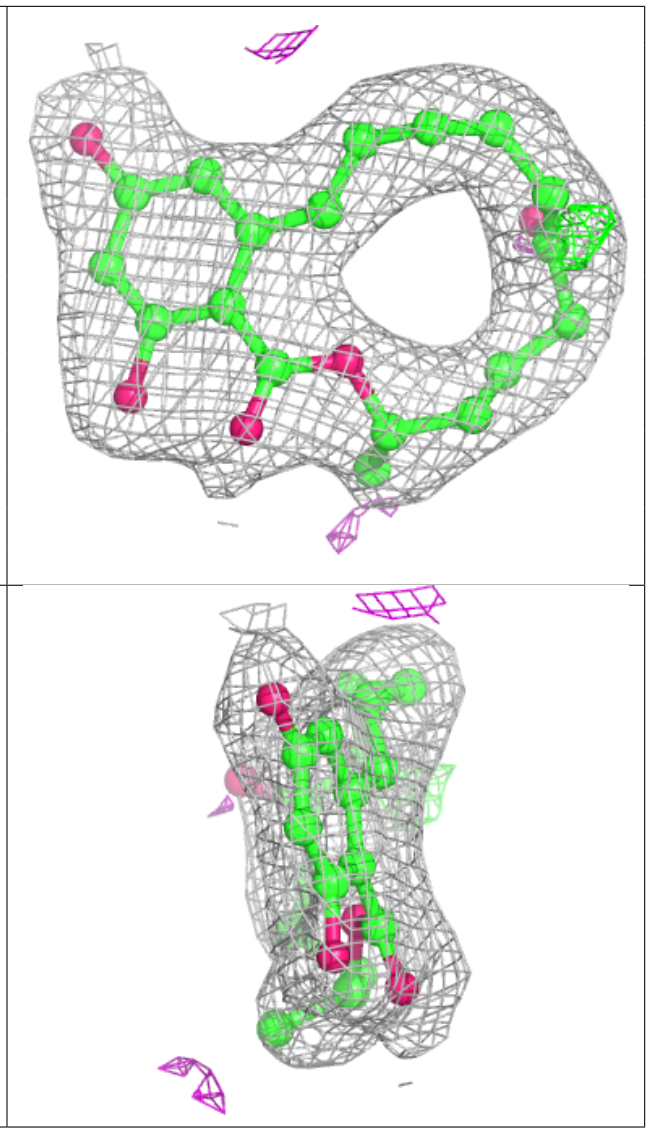
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





Electron density around ZER B 301:

$2mF_o$-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.