Full wwPDB X-ray Structure Validation Report (i)

Oct 23, 2023 – 02:43 PM EDT

PDB ID	:	2ZLG
Title	:	The Structual Basis for Peptidomimetic Inhibition of Eukaryotic Ribonucleotide Reductase
Authors	:	Xu, H.; Fairman, J.W.; Wijerathna, S.R.; LaMacchia, J.; Kreischer, N.R.; Helmbrecht, E.; Cooperman, B.S.; Dealwis, C.
Deposited on	:	2008-04-09
Resolution	:	2.52 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:

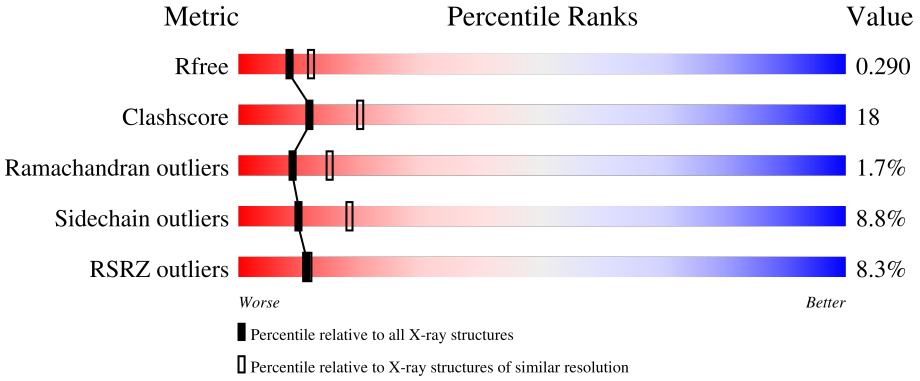
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.52 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	5743 (2.54-2.50)
Clashscore	141614	6463 (2.54-2.50)
Ramachandran outliers	138981	6335 (2.54-2.50)
Sidechain outliers	138945	6337 (2.54-2.50)
RSRZ outliers	127900	5630 (2.54-2.50)

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	888	6% 49% 20% • 26%

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
2	MRT	A	889	-	-	-	X

2 Entry composition (i)

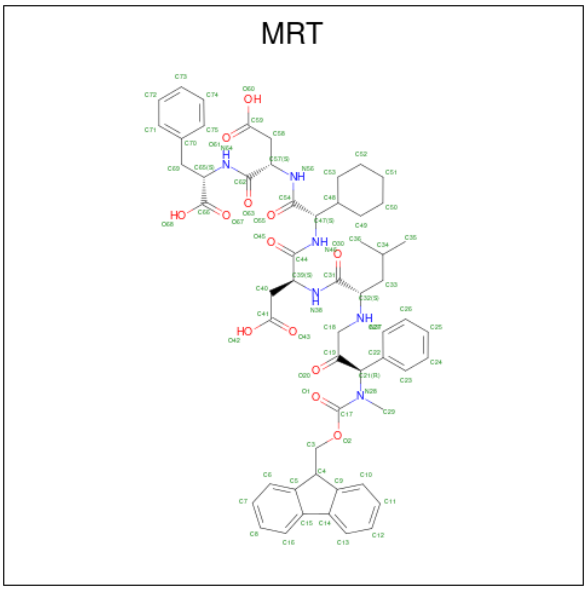
There are 4 unique types of molecules in this entry. The entry contains 5407 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Ribonucleoside-diphosphate reductase large chain 1.

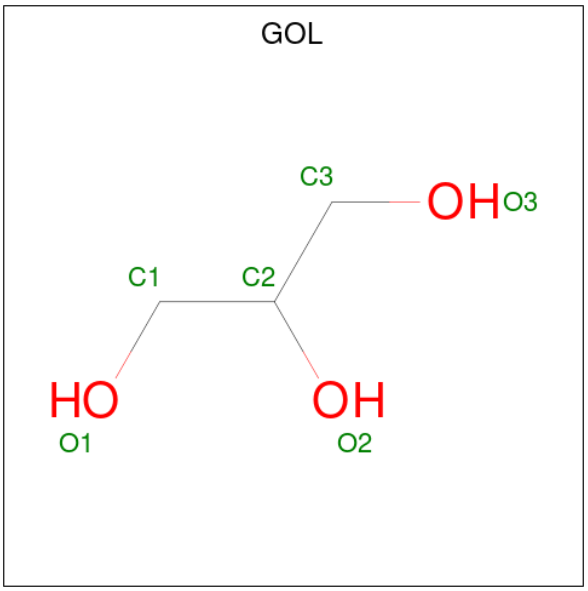
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	654	5228	3333	887	977	31	0	0	0

- Molecule 2 is (5R,9S,12S,15S,18S,21S)-21-benzyl-12,18-bis(carboxymethyl)-15-cyclohexyl-1-(9H-fluoren-9-yl)-4-methyl-9-(2-methylpropyl)-3,6,10,13,16,19-hexaoxo-5-phenyl-2-oxa-4,8,11,14,17,20-hexaazadocosan-22-oic acid (three-letter code: MRT) (formula: $C_{56}H_{66}N_6O_{13}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	75	56	6	13	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is water.

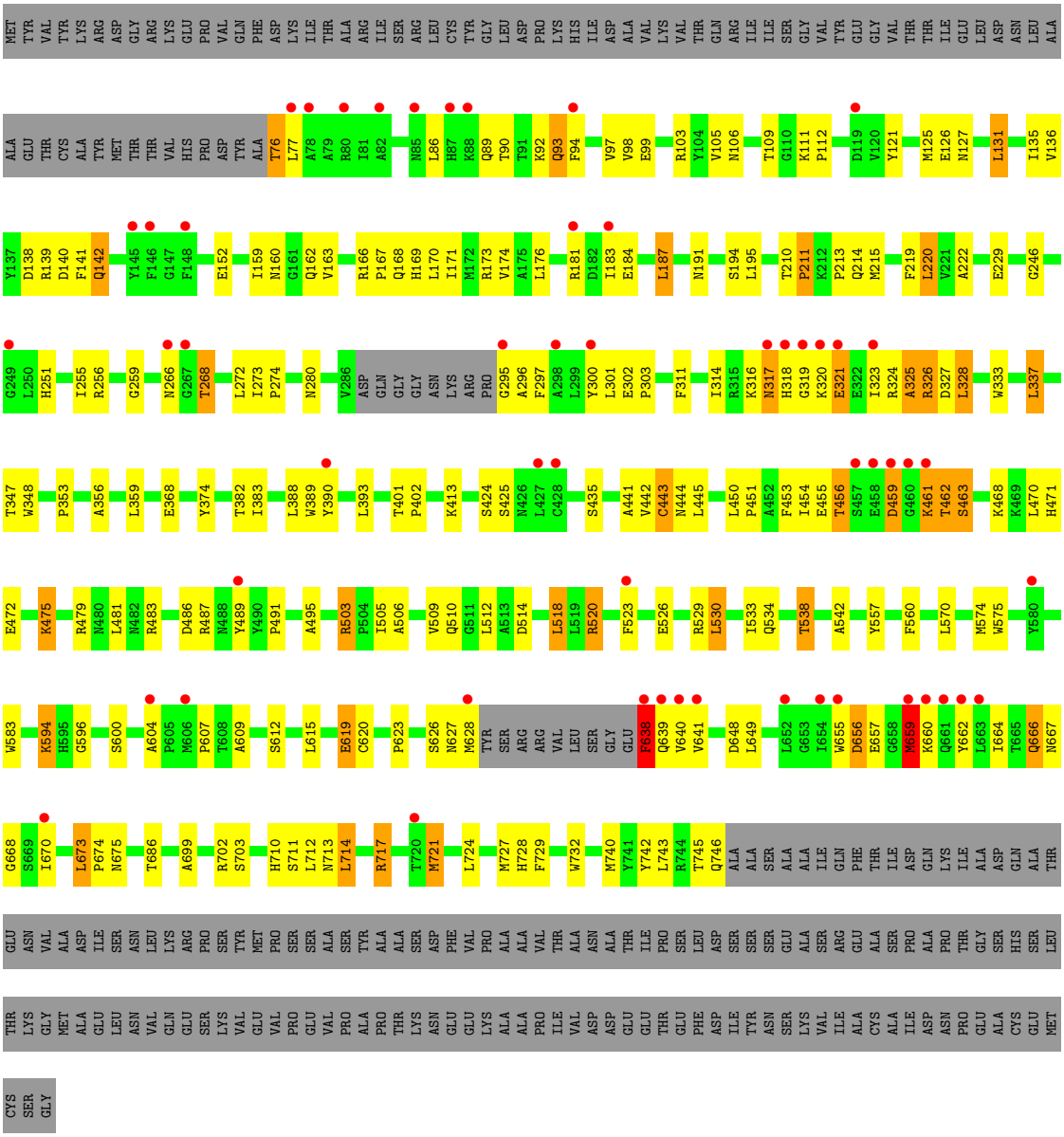
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	92	92	92	0	0

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: Ribonucleoside-diphosphate reductase large chain 1

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	107.79Å 116.56Å 63.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.60 – 2.52 49.59 – 2.52	Depositor EDS
% Data completeness (in resolution range)	97.0 (49.60-2.52) 97.0 (49.59-2.52)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.11 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0007	Depositor
R, R_{free}	0.216 , 0.292 0.214 , 0.290	Depositor DCC
R_{free} test set	1359 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	52.6	Xtriage
Anisotropy	0.742	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 50.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5407	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% 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: MRT, GOL

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	0/5347	0.56	1/7238 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	638	PHE	N-CA-C	-6.95	92.25	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	462	THR	Peptide
1	A	638	PHE	Peptide

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	5228	0	5173	173	0
2	A	75	0	63	15	0
3	A	12	0	16	0	0
4	A	92	0	0	5	0
All	All	5407	0	5252	185	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 (185) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:729:PHE:HA	4:A:919:HOH:O	1.57	1.05
1:A:337:LEU:HG	1:A:368:GLU:HG2	1.44	0.96
1:A:297:PHE:HB2	1:A:328:LEU:HD12	1.46	0.93
1:A:319:GLY:HA2	1:A:324:ARG:HH11	1.32	0.93
1:A:538:THR:HG22	1:A:583:TRP:HE1	1.36	0.89
1:A:316:LYS:HG2	1:A:318:HIS:CE1	2.08	0.88
1:A:717:ARG:O	1:A:746:GLN:HA	1.76	0.84
1:A:673:LEU:HD23	1:A:674:PRO:HD2	1.58	0.83
1:A:86:LEU:HD11	1:A:163:VAL:HG11	1.60	0.82
1:A:732:TRP:HB3	4:A:919:HOH:O	1.78	0.82
1:A:106:ASN:HB3	1:A:109:THR:HG22	1.60	0.81
2:A:889:MRT:H29	2:A:889:MRT:C18	2.11	0.80
1:A:319:GLY:HA2	1:A:324:ARG:NH1	1.95	0.80
2:A:889:MRT:H4	2:A:889:MRT:C29	2.11	0.80
1:A:538:THR:CG2	1:A:583:TRP:HE1	1.95	0.80
1:A:159:ILE:HG23	1:A:160:ASN:H	1.48	0.78
2:A:889:MRT:H29	2:A:889:MRT:H18	1.65	0.78
2:A:889:MRT:H4	2:A:889:MRT:N28	1.98	0.77
1:A:461:LYS:HG2	1:A:461:LYS:O	1.84	0.76
2:A:889:MRT:C54	2:A:889:MRT:HN64	1.96	0.76
2:A:889:MRT:H4	2:A:889:MRT:H29B	1.66	0.76
1:A:220:LEU:HB2	1:A:441:ALA:HB3	1.68	0.75
1:A:326:ARG:HB3	1:A:326:ARG:NH1	2.03	0.74
1:A:159:ILE:CG2	1:A:160:ASN:H	2.02	0.73
1:A:280:ASN:HA	1:A:328:LEU:HD21	1.70	0.73
1:A:109:THR:HG23	1:A:111:LYS:H	1.54	0.72
1:A:183:ILE:O	1:A:187:LEU:HD22	1.89	0.71
1:A:170:LEU:HD22	1:A:173:ARG:NH2	2.04	0.71
1:A:699:ALA:HA	1:A:702:ARG:NH1	2.06	0.71
1:A:159:ILE:HG23	1:A:160:ASN:N	2.07	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:745:THR:O	1:A:746:GLN:HG2	1.94	0.67
2:A:889:MRT:O1	2:A:889:MRT:H27	1.93	0.67
1:A:560:PHE:CZ	1:A:596:GLY:HA2	2.30	0.66
1:A:721:MET:HB3	2:A:889:MRT:C8	2.26	0.66
1:A:462:THR:O	1:A:463:SER:HB2	1.95	0.66
1:A:393:LEU:HD13	1:A:721:MET:HG3	1.78	0.65
1:A:509:VAL:O	1:A:620:CYS:HA	1.97	0.64
1:A:401:THR:HB	1:A:402:PRO:HA	1.80	0.64
1:A:106:ASN:HB3	1:A:109:THR:CG2	2.28	0.63
1:A:90:THR:HG21	1:A:166:ARG:HG3	1.80	0.63
1:A:141:PHE:O	1:A:142:GLN:HG3	1.97	0.63
1:A:538:THR:HG22	1:A:583:TRP:NE1	2.11	0.63
1:A:534:GLN:O	1:A:538:THR:HG23	1.99	0.61
1:A:170:LEU:O	1:A:174:VAL:HG23	2.01	0.61
1:A:721:MET:HB3	2:A:889:MRT:H8	1.81	0.61
1:A:702:ARG:HH11	1:A:710:HIS:HE1	1.50	0.60
1:A:210:THR:HB	1:A:211:PRO:HD2	1.84	0.60
1:A:280:ASN:CA	1:A:328:LEU:HD21	2.31	0.60
1:A:140:ASP:OD2	1:A:168:GLN:HG2	2.03	0.59
1:A:136:VAL:HG12	1:A:138:ASP:HB2	1.85	0.59
1:A:481:LEU:HB3	1:A:505:ILE:HD12	1.84	0.59
1:A:468:LYS:O	1:A:472:GLU:HG3	2.03	0.59
1:A:483:ARG:NH2	1:A:487:ARG:HD2	2.17	0.59
1:A:159:ILE:CG2	1:A:160:ASN:N	2.64	0.58
1:A:444:ASN:C	1:A:445:LEU:HD23	2.24	0.58
1:A:475:LYS:O	1:A:479:ARG:HG3	2.04	0.57
1:A:662:TYR:O	1:A:666:GLN:HB2	2.03	0.57
1:A:670:ILE:HA	1:A:673:LEU:HD12	1.87	0.57
2:A:889:MRT:H71	2:A:889:MRT:C66	2.35	0.57
1:A:99:GLU:O	1:A:103:ARG:HG2	2.04	0.57
1:A:183:ILE:HG22	1:A:187:LEU:CD2	2.35	0.56
1:A:326:ARG:HB3	1:A:326:ARG:HH11	1.68	0.56
1:A:456:THR:HA	1:A:463:SER:HA	1.87	0.56
1:A:297:PHE:HB2	1:A:328:LEU:CD1	2.28	0.56
1:A:714:LEU:HB3	1:A:727:MET:HE3	1.87	0.56
1:A:702:ARG:HH11	1:A:710:HIS:CE1	2.24	0.56
1:A:251:HIS:HB3	1:A:424:SER:HB3	1.86	0.55
1:A:259:GLY:HA2	1:A:268:THR:HB	1.88	0.55
1:A:557:TYR:CE1	1:A:600:SER:HB3	2.42	0.55
1:A:76:THR:HG23	1:A:77:LEU:H	1.72	0.54
1:A:140:ASP:OD2	1:A:167:PRO:HB2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:724:LEU:HD22	1:A:728:HIS:NE2	2.22	0.54
1:A:105:VAL:HG22	1:A:112:PRO:HA	1.89	0.54
1:A:628:MET:HE1	1:A:664:ILE:HA	1.90	0.54
1:A:628:MET:CE	1:A:664:ILE:HA	2.37	0.54
1:A:211:PRO:O	1:A:213:PRO:HD3	2.09	0.53
1:A:510:GLN:HE22	1:A:615:LEU:HB2	1.74	0.52
1:A:639:GLN:HG3	1:A:640:VAL:H	1.74	0.52
1:A:523:PHE:CE1	1:A:623:PRO:HG3	2.45	0.52
1:A:246:GLY:O	1:A:295:GLY:HA3	2.10	0.52
1:A:94:PHE:O	1:A:97:VAL:HG22	2.10	0.52
1:A:656:ASP:H	1:A:659:MET:HG3	1.75	0.52
1:A:314:ILE:HG23	1:A:325:ALA:HB3	1.91	0.52
1:A:316:LYS:HG2	1:A:318:HIS:NE2	2.24	0.51
1:A:699:ALA:HA	1:A:702:ARG:HH11	1.76	0.51
2:A:889:MRT:H29	2:A:889:MRT:N37	2.25	0.51
1:A:389:TRP:NE1	1:A:393:LEU:HD11	2.26	0.51
1:A:255:ILE:HG21	1:A:272:LEU:HD23	1.92	0.50
1:A:721:MET:CB	2:A:889:MRT:H8	2.40	0.50
1:A:639:GLN:CG	1:A:640:VAL:H	2.24	0.50
1:A:732:TRP:HE3	4:A:919:HOH:O	1.92	0.50
2:A:889:MRT:O1	2:A:889:MRT:C27	2.59	0.50
1:A:166:ARG:HB2	1:A:169:HIS:ND1	2.27	0.50
1:A:296:ALA:C	1:A:297:PHE:HD2	2.15	0.50
1:A:109:THR:HG23	1:A:111:LYS:N	2.22	0.50
1:A:530:LEU:O	1:A:534:GLN:HG3	2.11	0.50
1:A:255:ILE:HB	1:A:272:LEU:HD21	1.94	0.50
1:A:510:GLN:HE22	1:A:612:SER:HA	1.77	0.50
1:A:348:TRP:O	1:A:383:ILE:HG12	2.12	0.49
1:A:520:ARG:NH2	1:A:648:ASP:OD2	2.45	0.49
1:A:170:LEU:HD22	1:A:173:ARG:HH21	1.74	0.49
1:A:300:TYR:OH	1:A:425:SER:HB3	2.13	0.49
1:A:443:CYS:HA	4:A:922:HOH:O	2.12	0.49
1:A:607:PRO:HD3	1:A:711:SER:OG	2.13	0.49
1:A:713:ASN:ND2	1:A:742:TYR:HB2	2.28	0.48
1:A:106:ASN:CB	1:A:109:THR:HG22	2.36	0.48
1:A:318:HIS:O	1:A:318:HIS:ND1	2.44	0.48
1:A:529:ARG:O	1:A:533:ILE:HG13	2.14	0.48
1:A:575:TRP:CZ2	1:A:703:SER:HB3	2.48	0.48
1:A:660:LYS:O	1:A:664:ILE:HG13	2.14	0.48
1:A:510:GLN:HA	1:A:620:CYS:HA	1.96	0.48
1:A:594:LYS:HE3	1:A:594:LYS:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:TYR:CE1	1:A:125:MET:HE2	2.49	0.48
1:A:167:PRO:O	1:A:171:ILE:HG13	2.14	0.48
1:A:127:ASN:HB2	1:A:131:LEU:CD2	2.43	0.47
1:A:506:ALA:HB1	1:A:604:ALA:HB3	1.95	0.47
1:A:471:HIS:CD2	1:A:542:ALA:HB2	2.49	0.47
1:A:453:PHE:CE2	1:A:470:LEU:HA	2.50	0.47
1:A:609:ALA:H	1:A:619:GLU:CD	2.18	0.47
1:A:220:LEU:HD13	1:A:425:SER:O	2.15	0.47
1:A:656:ASP:OD2	1:A:656:ASP:N	2.47	0.46
1:A:523:PHE:CZ	1:A:623:PRO:HG3	2.50	0.46
1:A:302:GLU:HG2	1:A:333:TRP:HB3	1.97	0.46
1:A:450:LEU:HB2	1:A:451:PRO:HD3	1.98	0.46
1:A:483:ARG:NH2	1:A:487:ARG:CD	2.77	0.46
1:A:337:LEU:HG	1:A:368:GLU:CG	2.31	0.46
1:A:317:ASN:ND2	1:A:317:ASN:C	2.69	0.46
1:A:538:THR:HB	1:A:583:TRP:NE1	2.31	0.46
1:A:445:LEU:HD22	1:A:506:ALA:HB3	1.98	0.46
1:A:655:TRP:HA	1:A:659:MET:HG3	1.98	0.46
1:A:273:ILE:HG21	1:A:323:ILE:HD12	1.97	0.46
1:A:627:ASN:HB2	1:A:668:GLY:O	2.16	0.46
1:A:454:ILE:HD13	1:A:518:LEU:HB3	1.97	0.45
1:A:570:LEU:O	1:A:574:MET:HG3	2.16	0.45
1:A:413:LYS:HE3	1:A:575:TRP:CE2	2.51	0.45
1:A:92:LYS:O	1:A:93:GLN:CB	2.64	0.45
1:A:740:MET:SD	1:A:743:LEU:HD23	2.57	0.45
1:A:109:THR:HG23	1:A:111:LYS:HG3	1.99	0.45
1:A:166:ARG:HG3	1:A:169:HIS:CE1	2.52	0.45
1:A:510:GLN:NE2	1:A:612:SER:HA	2.32	0.45
1:A:510:GLN:NE2	1:A:615:LEU:HB2	2.32	0.45
1:A:273:ILE:HB	1:A:274:PRO:HD3	1.98	0.45
1:A:326:ARG:HB3	1:A:326:ARG:CZ	2.47	0.45
1:A:673:LEU:HD23	1:A:674:PRO:CD	2.37	0.44
1:A:126:GLU:OE1	1:A:181:ARG:NH1	2.50	0.44
1:A:251:HIS:HE1	1:A:435:SER:OG	2.00	0.44
1:A:557:TYR:CZ	1:A:600:SER:HB3	2.52	0.44
1:A:222:ALA:HA	1:A:251:HIS:CE1	2.53	0.44
1:A:486:ASP:CG	1:A:503:ARG:HH22	2.21	0.44
1:A:518:LEU:HD12	1:A:518:LEU:HA	1.65	0.44
1:A:649:LEU:HD13	1:A:655:TRP:CE3	2.52	0.44
2:A:889:MRT:C54	2:A:889:MRT:N64	2.67	0.44
1:A:139:ARG:HD3	1:A:194:SER:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:HIS:HD2	4:A:909:HOH:O	2.00	0.43
1:A:538:THR:HB	1:A:583:TRP:CE2	2.53	0.43
1:A:670:ILE:O	1:A:673:LEU:HB2	2.18	0.43
1:A:311:PHE:O	1:A:314:ILE:HG12	2.17	0.43
1:A:489:TYR:O	1:A:489:TYR:CD2	2.72	0.43
1:A:213:PRO:HB2	1:A:215:MET:CE	2.49	0.43
1:A:256:ARG:HA	1:A:353:PRO:HD2	2.01	0.43
1:A:314:ILE:HD13	1:A:314:ILE:HA	1.83	0.43
1:A:302:GLU:HA	1:A:303:PRO:HD3	1.87	0.42
1:A:347:THR:HB	1:A:382:THR:CG2	2.49	0.42
1:A:713:ASN:HD22	1:A:713:ASN:HA	1.67	0.42
1:A:526:GLU:OE1	1:A:529:ARG:HD3	2.19	0.42
1:A:714:LEU:HD12	1:A:714:LEU:HA	1.80	0.42
1:A:94:PHE:O	1:A:98:VAL:HG23	2.19	0.42
1:A:356:ALA:HB1	1:A:374:TYR:CD1	2.55	0.42
1:A:106:ASN:OD1	1:A:109:THR:HG22	2.20	0.41
2:A:889:MRT:H27	2:A:889:MRT:H29A	2.02	0.41
1:A:317:ASN:C	1:A:317:ASN:HD22	2.24	0.41
1:A:455:GLU:O	1:A:463:SER:HA	2.19	0.41
1:A:135:ILE:HG23	1:A:168:GLN:HB3	2.02	0.41
1:A:111:LYS:HA	1:A:112:PRO:HD2	1.85	0.41
1:A:280:ASN:HA	1:A:328:LEU:CD2	2.45	0.41
1:A:319:GLY:HA2	1:A:324:ARG:HD2	2.02	0.41
1:A:393:LEU:HD22	1:A:724:LEU:HB3	2.03	0.41
1:A:486:ASP:OD2	1:A:503:ARG:NH2	2.54	0.41
1:A:219:PHE:HA	1:A:441:ALA:O	2.21	0.41
1:A:390:TYR:CD1	1:A:390:TYR:C	2.94	0.41
1:A:714:LEU:HD23	1:A:727:MET:HE2	2.03	0.41
1:A:191:ASN:O	1:A:195:LEU:HG	2.22	0.40
1:A:538:THR:CG2	1:A:583:TRP:NE1	2.72	0.40
1:A:442:VAL:HG21	1:A:495:ALA:HB1	2.03	0.40
1:A:489:TYR:CD2	1:A:489:TYR:C	2.95	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	648/888 (73%)	595 (92%)	42 (6%)	11 (2%)	9 15

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	93	GLN
1	A	142	GLN
1	A	325	ALA
1	A	459	ASP
1	A	717	ARG
1	A	321	GLU
1	A	659	MET
1	A	656	ASP
1	A	268	THR
1	A	461	LYS
1	A	211	PRO

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	567/761 (74%)	517 (91%)	50 (9%)	10 18

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	THR
1	A	89	GLN
1	A	131	LEU
1	A	152	GLU
1	A	162	GLN
1	A	176	LEU

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Mol	Chain	Res	Type
1	A	184	GLU
1	A	187	LEU
1	A	214	GLN
1	A	220	LEU
1	A	229	GLU
1	A	266	ASN
1	A	301	LEU
1	A	317	ASN
1	A	320	LYS
1	A	321	GLU
1	A	326	ARG
1	A	327	ASP
1	A	328	LEU
1	A	337	LEU
1	A	359	LEU
1	A	388	LEU
1	A	443	CYS
1	A	456	THR
1	A	459	ASP
1	A	463	SER
1	A	475	LYS
1	A	491	PRO
1	A	503	ARG
1	A	512	LEU
1	A	514	ASP
1	A	518	LEU
1	A	520	ARG
1	A	530	LEU
1	A	538	THR
1	A	594	LYS
1	A	619	GLU
1	A	626	SER
1	A	638	PHE
1	A	641	VAL
1	A	657	GLU
1	A	659	MET
1	A	666	GLN
1	A	667	ASN
1	A	673	LEU
1	A	675	ASN
1	A	686	THR
1	A	712	LEU

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Mol	Chain	Res	Type
1	A	714	LEU
1	A	721	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	HIS
1	A	127	ASN
1	A	168	GLN
1	A	251	HIS
1	A	317	ASN
1	A	386	GLN
1	A	444	ASN
1	A	482	ASN
1	A	510	GLN
1	A	595	HIS
1	A	613	GLN
1	A	692	GLN
1	A	710	HIS
1	A	713	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)

3 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	$\#\|Z\| > 2$
3	GOL	A	891	-	5,5,5	0.34	0	5,5,5	0.24	0
3	GOL	A	890	-	5,5,5	0.35	0	5,5,5	0.50	0
2	MRT	A	889	-	78,80,80	1.47	6 (7%)	97,110,110	1.91	14 (14%)

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
3	GOL	A	891	-	-	2/4/4/4	-
3	GOL	A	890	-	-	2/4/4/4	-
2	MRT	A	889	-	-	30/79/102/102	0/6/6/6

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	889	MRT	C17-N28	6.44	1.45	1.35
2	A	889	MRT	O2-C17	6.17	1.46	1.34
2	A	889	MRT	C5-C4	-4.29	1.46	1.51
2	A	889	MRT	C9-C4	-4.16	1.46	1.51
2	A	889	MRT	C9-C14	-2.56	1.37	1.40
2	A	889	MRT	C5-C15	-2.25	1.38	1.40

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	889	MRT	O2-C17-N28	7.39	120.11	111.11
2	A	889	MRT	C70-C69-C65	6.42	131.11	113.39
2	A	889	MRT	C69-C65-N64	-6.19	97.75	110.79
2	A	889	MRT	C18-N37-C32	5.96	126.51	114.01
2	A	889	MRT	C65-N64-C62	4.94	132.27	121.67
2	A	889	MRT	O2-C17-O1	-4.48	117.14	124.78
2	A	889	MRT	C22-C21-N28	3.22	117.43	111.84
2	A	889	MRT	C8-C16-C15	-3.10	116.60	120.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	889	MRT	C29-N28-C17	-3.00	111.96	120.76
2	A	889	MRT	C12-C13-C14	-2.92	116.85	120.89
2	A	889	MRT	C57-C62-N64	-2.78	110.61	116.70
2	A	889	MRT	C3-O2-C17	2.26	119.90	115.72
2	A	889	MRT	C69-C70-C75	-2.10	116.74	120.91
2	A	889	MRT	C27-C22-C21	2.04	123.74	120.71

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	889	MRT	O1-C17-O2-C3
2	A	889	MRT	N28-C17-O2-C3
2	A	889	MRT	O1-C17-N28-C21
2	A	889	MRT	O1-C17-N28-C29
2	A	889	MRT	O2-C17-N28-C21
2	A	889	MRT	O2-C17-N28-C29
2	A	889	MRT	C62-C57-C58-C59
2	A	889	MRT	N64-C65-C69-C70
3	A	891	GOL	O1-C1-C2-C3
2	A	889	MRT	C66-C65-C69-C70
2	A	889	MRT	C4-C3-O2-C17
2	A	889	MRT	C65-C69-C70-C71
2	A	889	MRT	C65-C69-C70-C75
3	A	890	GOL	C1-C2-C3-O3
2	A	889	MRT	C57-C58-C59-O61
3	A	890	GOL	O2-C2-C3-O3
3	A	891	GOL	O1-C1-C2-O2
2	A	889	MRT	C32-C33-C34-C36
2	A	889	MRT	C32-C33-C34-C35
2	A	889	MRT	C57-C58-C59-O60
2	A	889	MRT	O30-C31-C32-N37
2	A	889	MRT	N38-C31-C32-N37
2	A	889	MRT	N38-C39-C44-O45
2	A	889	MRT	N38-C39-C44-N46
2	A	889	MRT	N37-C18-C19-O20
2	A	889	MRT	C19-C18-N37-C32
2	A	889	MRT	C44-C39-N38-C31
2	A	889	MRT	O30-C31-C32-C33
2	A	889	MRT	N28-C21-C22-C23
2	A	889	MRT	N38-C31-C32-C33
2	A	889	MRT	C39-C40-C41-O43

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Mol	Chain	Res	Type	Atoms
2	A	889	MRT	N28-C21-C22-C27
2	A	889	MRT	C40-C39-C44-O45
2	A	889	MRT	C39-C40-C41-O42

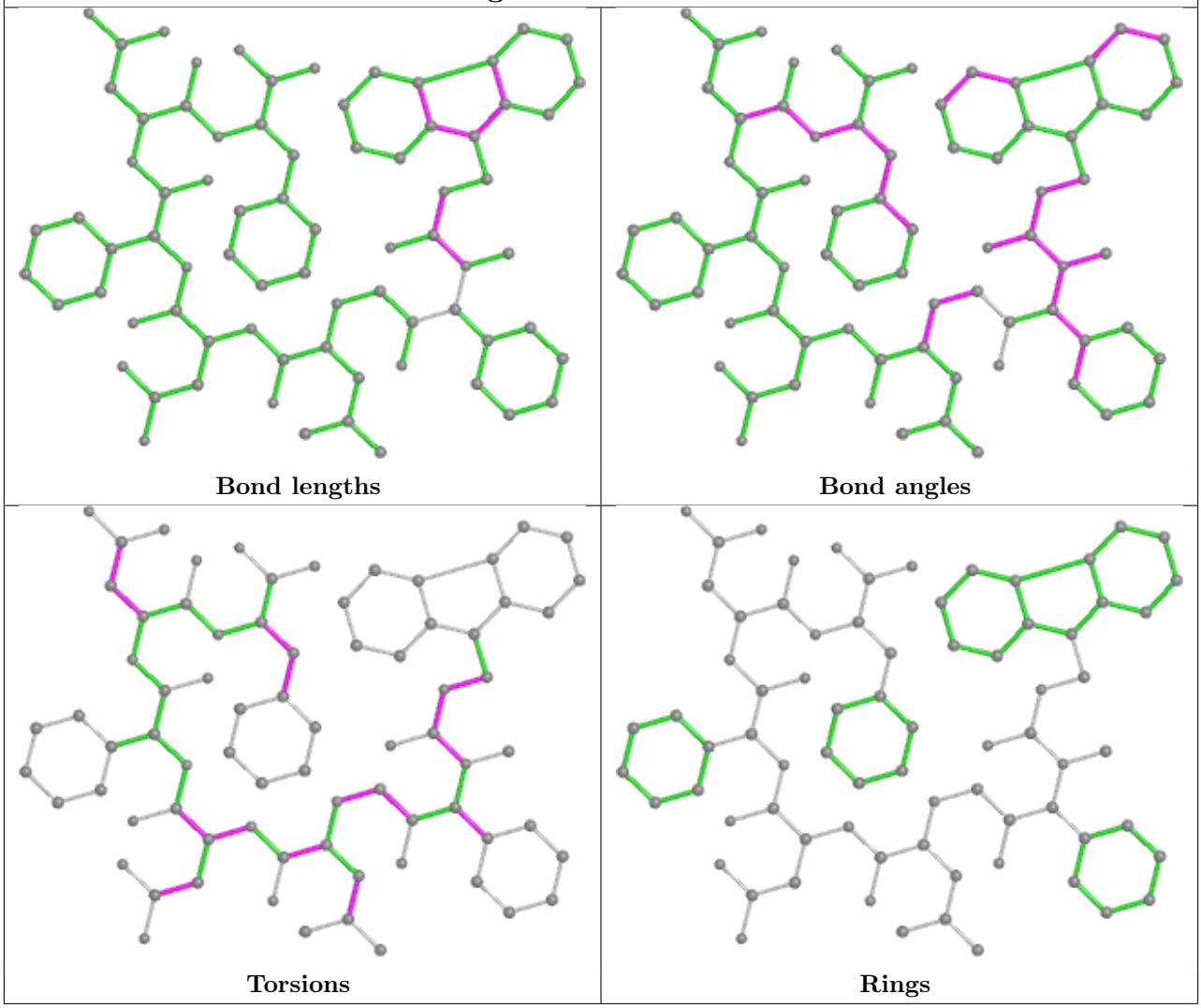
There are no ring outliers.

1 monomer is involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	889	MRT	15	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 MRT A 889



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	654/888 (73%)	0.47	54 (8%) 11 11	20, 36, 73, 105	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	638	PHE	7.4
1	A	77	LEU	6.6
1	A	461	LYS	6.6
1	A	319	GLY	4.8
1	A	323	ILE	4.7
1	A	320	LYS	4.6
1	A	663	LEU	4.5
1	A	318	HIS	4.4
1	A	80	ARG	4.3
1	A	661	GLN	4.2
1	A	460	GLY	4.2
1	A	457	SER	4.2
1	A	146	PHE	3.8
1	A	88	LYS	3.6
1	A	654	ILE	3.6
1	A	655	TRP	3.5
1	A	295	GLY	3.3
1	A	78	ALA	3.3
1	A	639	GLN	3.3
1	A	459	ASP	3.3
1	A	652	LEU	3.2
1	A	489	TYR	3.2
1	A	145	TYR	3.2
1	A	428	CYS	3.2
1	A	321	GLU	3.0
1	A	662	TYR	3.0
1	A	94	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	183	ILE	2.9
1	A	181	ARG	2.9
1	A	82	ALA	2.8
1	A	660	LYS	2.8
1	A	148	PHE	2.7
1	A	85	ASN	2.6
1	A	267	GLY	2.5
1	A	266	ASN	2.5
1	A	640	VAL	2.5
1	A	670	ILE	2.4
1	A	119	ASP	2.4
1	A	87	HIS	2.4
1	A	628	MET	2.4
1	A	298	ALA	2.3
1	A	427	LEU	2.3
1	A	606	MET	2.3
1	A	317	ASN	2.3
1	A	659	MET	2.3
1	A	523	PHE	2.3
1	A	458	GLU	2.3
1	A	580	TYR	2.3
1	A	604	ALA	2.2
1	A	390	TYR	2.1
1	A	641	VAL	2.1
1	A	300	TYR	2.1
1	A	720	THR	2.0
1	A	249	GLY	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

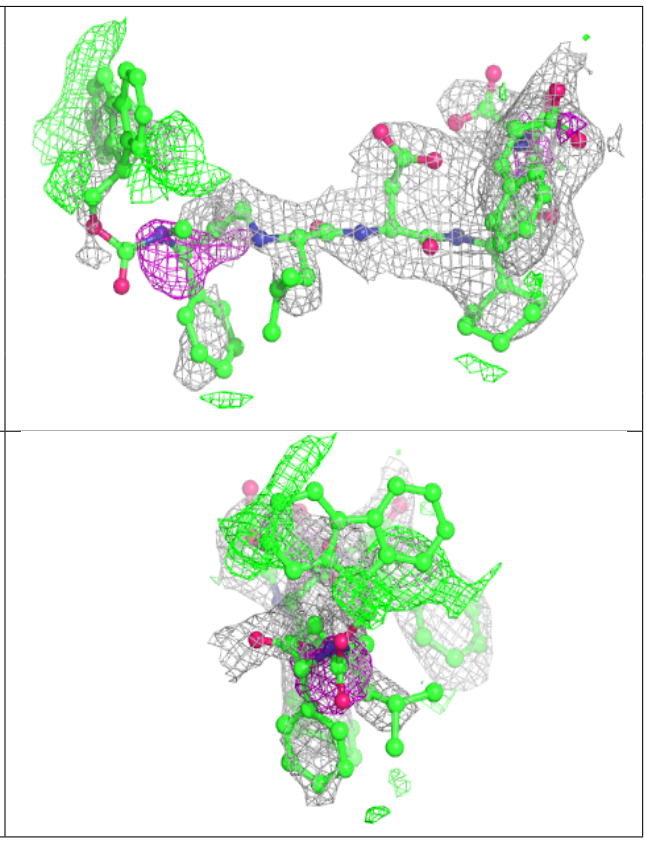
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MRT	A	889	75/75	0.65	0.45	39,75,85,89	16
3	GOL	A	891	6/6	0.81	0.19	45,47,51,61	0
3	GOL	A	890	6/6	0.86	0.22	30,44,47,47	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 MRT A 889:

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.