Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 02:15 pm GMT

PDB ID	:	1UON
Title	:	REOVIRUS POLYMERASE LAMBDA-3 LOCALIZED BY ELECTRON CRYOMICROSCOPY OF VIRIONS AT 7.6-A RESOLUTION
Authors	:	Zhang, X.; Walker, S.B.; Chipman, P.R.; Nibert, M.L.; Baker, T.S.
Deposited on	:	2003-09-21
Resolution	:	7.60 Å(reported)
Based on initial model	:	1UON

This is a Full wwPDB EM Validation Report for a publicly released PDB/EMDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

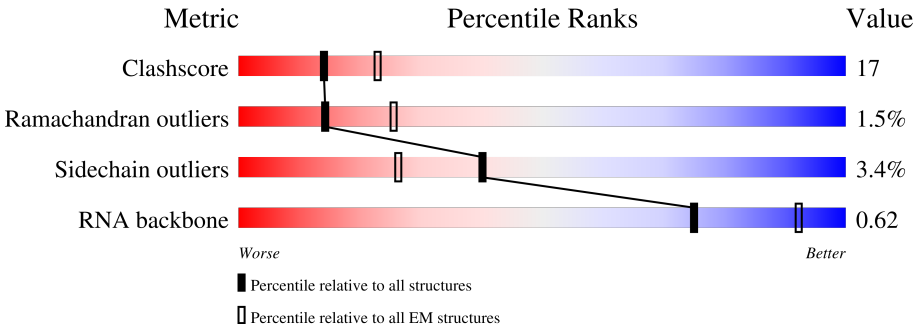
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 7.60 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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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%

Mol	Chain	Length	Quality of chain
1	A	1267	68% 30% .
2	B	5	20% 80%
3	C	8	75% 25%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10703 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 MINOR CORE PROTEIN LAMBDA 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1264	9986	6369	1712	1841	64	0	0

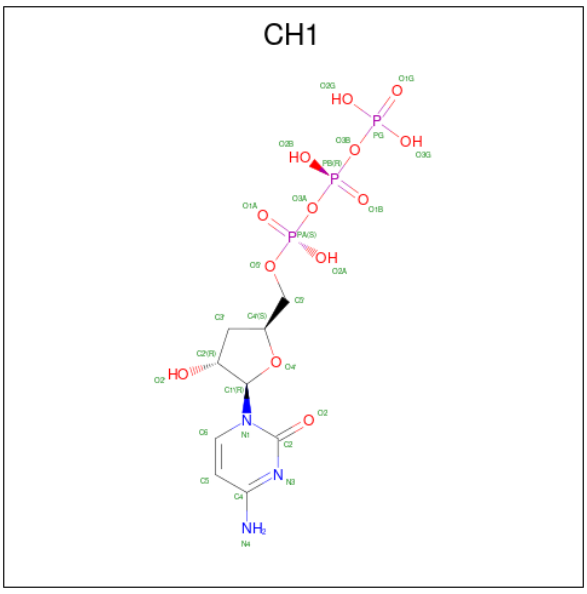
- Molecule 2 is a RNA chain called 5'-R(*GP*GP*GP*GP*GP*)-3'.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	5	116	50	25	36	5	0	0

- Molecule 3 is a RNA chain called 5'-R(*UP*AP*GP*CP*CP*CP*CP*CP*)-3'.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	C	8	165	74	27	56	8	0	0

- Molecule 4 is 3'-DEOXY-CYTIDINE-5'-TRIPHOSPHATE (three-letter code: CH1) (formula: $C_9H_{16}N_3O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			84	27	9	39	9	
4	A	1	Total	C	N	O	P	0
			84	27	9	39	9	
4	A	1	Total	C	N	O	P	0
			84	27	9	39	9	

- Molecule 5 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		AltConf
5	A	2	Total	Mn	0
			2	2	

- Molecule 6 is water.

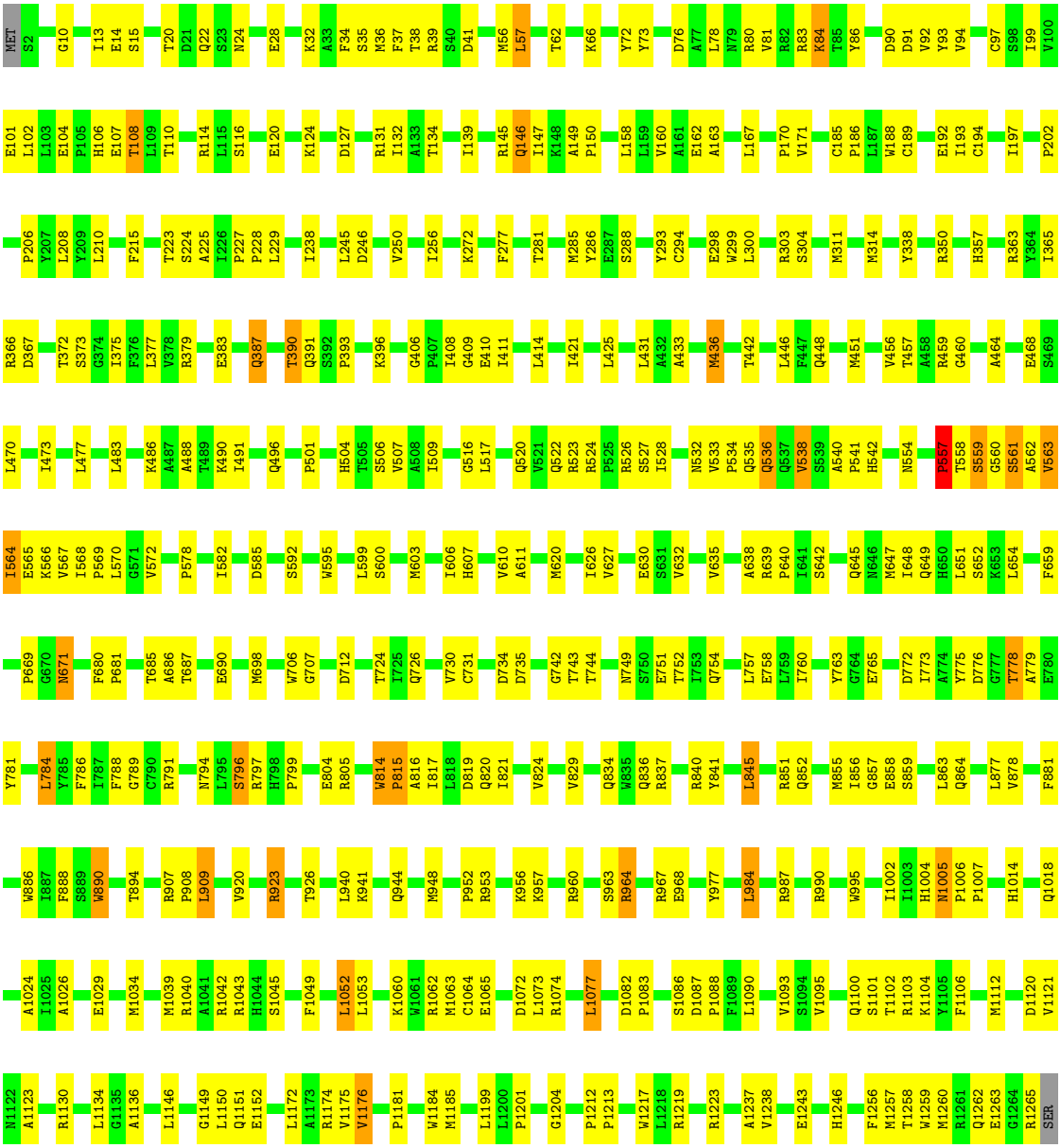
Mol	Chain	Residues	Atoms		AltConf
6	A	340	Total	O	0
			340	340	
6	B	4	Total	O	0
			4	4	
6	C	6	Total	O	0
			6	6	

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. 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. 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.

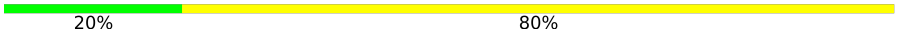
- Molecule 1: MINOR CORE PROTEIN LAMBDA 3

Chain A: 



• Molecule 2: 5'-R(*GP*GP*GP*GP*GP*)-3'

Chain B:



• Molecule 3: 5'-R(*UP*AP*GP*CP*CP*CP*CP*CP*)-3'

Chain C:

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	1.00Å 1.00Å 1.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 7.60	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-7.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10703	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CH1, MN

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	0.38	0/10239	0.61	1/13905 (0.0%)
2	B	0.81	1/130 (0.8%)	0.68	0/201
3	C	0.52	0/182	0.71	0/280
All	All	0.39	1/10551 (0.0%)	0.61	1/14386 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1272	G	OP3-P	-7.08	1.52	1.61

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	408	ILE	N-CA-C	-5.48	96.20	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9986	0	9903	356	0
2	B	116	0	56	7	0
3	C	165	0	88	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	84	0	36	3	0
5	A	2	0	0	0	0
6	A	340	0	0	8	0
6	B	4	0	0	0	0
6	C	6	0	0	0	0
All	All	10703	0	10083	357	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 (357) 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:223:THR:HG22	1:A:225:ALA:H	1.14	1.12
1:A:1112:MET:HE1	1:A:1150:LEU:HD11	1.31	1.08
1:A:562:ALA:HB2	2:B:1274:G:H21	1.22	1.04
1:A:410:GLU:H	1:A:649:GLN:NE2	1.58	1.01
1:A:724:THR:HG22	1:A:726:GLN:H	1.31	0.96
1:A:749:ASN:HD21	1:A:751:GLU:HB3	1.31	0.96
1:A:81:VAL:H	1:A:671:ASN:HD21	1.09	0.95
1:A:22:GLN:NE2	1:A:878:VAL:H	1.66	0.94
1:A:146:GLN:HE22	1:A:805:ARG:H	1.08	0.94
1:A:561:SER:HB3	1:A:566:LYS:HE2	1.54	0.89
1:A:410:GLU:H	1:A:649:GLN:HE22	1.12	0.89
1:A:743:THR:HG22	1:A:744:THR:H	1.37	0.86
1:A:562:ALA:HB2	2:B:1274:G:N2	1.91	0.86
1:A:1005:ASN:HB2	1:A:1130:ARG:HH22	1.41	0.84
1:A:856:ILE:HB	1:A:859:SER:HB2	1.61	0.83
1:A:563:VAL:O	1:A:564:ILE:HG22	1.80	0.82
1:A:78:LEU:HD12	1:A:80:ARG:NH2	1.96	0.80
1:A:851:ARG:HH11	1:A:864:GLN:HE21	1.29	0.80
1:A:907:ARG:HB3	1:A:908:PRO:HD3	1.64	0.79
1:A:536:GLN:HE22	1:A:685:THR:H	1.30	0.78
1:A:1004:HIS:C	1:A:1006:PRO:HD3	2.05	0.77
1:A:1201:PRO:HB2	1:A:1204:GLY:O	1.84	0.77
1:A:522:GLN:HE22	1:A:796:SER:HB3	1.47	0.76
1:A:1005:ASN:HD21	1:A:1263:GLU:HB3	1.49	0.75
1:A:167:LEU:HD23	1:A:837:ARG:HD2	1.68	0.75
1:A:425:LEU:HD13	1:A:698:MET:HE3	1.67	0.74
1:A:379:ARG:HH12	1:A:387:GLN:NE2	1.84	0.74
1:A:814:TRP:HB3	1:A:815:PRO:HD3	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:821:ILE:HG23	1:A:845:LEU:HD13	1.70	0.74
1:A:39:ARG:HH11	1:A:39:ARG:HG2	1.53	0.74
1:A:81:VAL:H	1:A:671:ASN:ND2	1.85	0.74
1:A:749:ASN:HD22	1:A:752:THR:H	1.33	0.73
1:A:114:ARG:HB2	1:A:215:PHE:CE1	2.24	0.73
1:A:603:MET:HE3	1:A:648:ILE:HG23	1.71	0.72
1:A:1072:ASP:OD1	1:A:1074:ARG:HD3	1.89	0.72
1:A:1087:ASP:HB3	1:A:1088:PRO:HD3	1.72	0.72
1:A:104:GLU:HG3	1:A:116:SER:HA	1.71	0.72
1:A:410:GLU:N	1:A:649:GLN:NE2	2.37	0.72
1:A:285:MET:HG3	1:A:365:ILE:HD11	1.70	0.72
1:A:363:ARG:HH22	1:A:834:GLN:HE22	1.38	0.72
1:A:167:LEU:HD21	1:A:840:ARG:CZ	2.20	0.72
1:A:22:GLN:HE21	1:A:878:VAL:H	1.38	0.71
1:A:749:ASN:ND2	1:A:752:THR:H	1.89	0.71
1:A:957:LYS:HE3	1:A:1026:ALA:HB2	1.73	0.70
1:A:561:SER:HB3	1:A:566:LYS:CE	2.21	0.70
1:A:743:THR:HG22	1:A:744:THR:N	2.07	0.70
1:A:223:THR:HG22	1:A:225:ALA:N	1.99	0.69
1:A:114:ARG:HB2	1:A:215:PHE:HE1	1.56	0.69
1:A:557:PRO:HD2	1:A:731:CYS:O	1.93	0.69
1:A:536:GLN:HA	1:A:536:GLN:HE21	1.58	0.69
1:A:227:PRO:HB2	1:A:228:PRO:HD3	1.75	0.68
1:A:1005:ASN:ND2	1:A:1263:GLU:HB3	2.09	0.68
1:A:171:VAL:HG11	1:A:1090:LEU:HD11	1.77	0.67
1:A:66:LYS:HB3	1:A:97:CYS:HA	1.77	0.67
1:A:410:GLU:N	1:A:649:GLN:HE22	1.90	0.67
1:A:776:ASP:OD1	1:A:778:THR:HB	1.93	0.67
1:A:92:VAL:HG11	1:A:383:GLU:HB3	1.77	0.66
1:A:281:THR:O	1:A:285:MET:HG2	1.96	0.65
1:A:73:TYR:HB3	1:A:132:ILE:HD12	1.78	0.65
1:A:926:THR:HG21	1:A:1246:HIS:CG	2.32	0.65
1:A:92:VAL:CG1	1:A:383:GLU:HB3	2.27	0.65
1:A:94:VAL:HG22	1:A:139:ILE:HG23	1.78	0.65
1:A:532:ASN:OD1	1:A:535:GLN:HG3	1.97	0.65
1:A:754:GLN:HE21	1:A:775:TYR:HD2	1.41	0.65
1:A:779:ALA:HB3	1:A:786:PHE:HB2	1.79	0.64
1:A:815:PRO:HG2	1:A:1034:MET:CE	2.27	0.64
1:A:81:VAL:N	1:A:671:ASN:HD21	1.89	0.63
1:A:724:THR:HG22	1:A:726:GLN:N	2.09	0.63
1:A:754:GLN:O	1:A:758:GLU:HG3	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:851:ARG:HH11	1:A:864:GLN:NE2	1.96	0.63
1:A:24:ASN:O	1:A:28:GLU:HG3	1.98	0.63
1:A:995:TRP:CZ2	1:A:1006:PRO:HG3	2.33	0.63
1:A:1064:CYS:HB3	1:A:1065:GLU:OE2	1.98	0.63
1:A:433:ALA:HB1	1:A:610:VAL:HG23	1.81	0.63
1:A:146:GLN:HE22	1:A:805:ARG:N	1.90	0.63
1:A:1062:ARG:HG3	1:A:1243:GLU:HB2	1.81	0.63
1:A:76:ASP:OD2	1:A:80:ARG:NH1	2.32	0.63
1:A:393:PRO:HG3	1:A:592:SER:HA	1.80	0.63
1:A:146:GLN:NE2	1:A:805:ARG:H	1.88	0.62
1:A:558:THR:O	1:A:559:SER:HB3	2.00	0.62
1:A:570:LEU:HD21	1:A:730:VAL:HG21	1.82	0.62
1:A:83:ARG:HG2	1:A:92:VAL:HA	1.82	0.61
1:A:393:PRO:CG	1:A:592:SER:HA	2.29	0.61
1:A:372:THR:HB	1:A:796:SER:OG	2.00	0.61
1:A:542:HIS:NE2	1:A:690:GLU:CG	2.63	0.61
1:A:120:GLU:O	1:A:124:LYS:HG3	1.99	0.61
1:A:167:LEU:HD21	1:A:840:ARG:NH2	2.16	0.60
1:A:952:PRO:HG2	1:A:956:LYS:HE3	1.83	0.60
1:A:562:ALA:CB	2:B:1274:G:H21	2.07	0.59
1:A:1029:GLU:N	1:A:1029:GLU:OE1	2.36	0.59
1:A:542:HIS:NE2	1:A:690:GLU:HG3	2.17	0.58
1:A:293:TYR:CZ	1:A:1074:ARG:NH2	2.71	0.58
1:A:451:MET:HA	1:A:451:MET:CE	2.34	0.58
1:A:409:GLY:HA3	1:A:649:GLN:NE2	2.19	0.58
1:A:377:LEU:HD12	1:A:377:LEU:H	1.68	0.58
1:A:501:PRO:HD2	1:A:504:HIS:HD2	1.67	0.58
1:A:829:VAL:HG13	1:A:890:TRP:CE2	2.39	0.57
1:A:797:ARG:C	1:A:799:PRO:HD3	2.24	0.57
1:A:194:CYS:SG	1:A:206:PRO:HG2	2.45	0.57
1:A:560:GLY:O	2:B:1276:G:H1'	2.04	0.57
1:A:566:LYS:HD2	1:A:784:LEU:HD23	1.86	0.57
1:A:851:ARG:NH1	1:A:864:GLN:HE21	2.01	0.57
1:A:794:ASN:OD1	1:A:796:SER:HB2	2.04	0.57
1:A:522:GLN:NE2	1:A:796:SER:HB3	2.18	0.57
1:A:815:PRO:HG2	1:A:1034:MET:HE3	1.87	0.57
1:A:724:THR:HG23	1:A:726:GLN:OE1	2.04	0.56
1:A:202:PRO:HD2	6:A:1412:HOH:O	2.05	0.56
1:A:501:PRO:HD2	1:A:504:HIS:CD2	2.40	0.56
1:A:193:ILE:HD13	1:A:229:LEU:HD21	1.88	0.56
1:A:836:GLN:HG2	1:A:886:TRP:CE3	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:855:MET:CE	1:A:858:GLU:H	2.19	0.56
1:A:1176:VAL:O	1:A:1176:VAL:HG13	2.06	0.56
1:A:1040:ARG:HG3	1:A:1043:ARG:NH2	2.21	0.56
1:A:856:ILE:HB	1:A:859:SER:CB	2.35	0.56
1:A:13:ILE:HD13	1:A:163:ALA:HB3	1.88	0.55
1:A:562:ALA:O	1:A:565:GLU:HB3	2.06	0.55
1:A:20:THR:HG21	6:A:1543:HOH:O	2.06	0.55
1:A:926:THR:CG2	1:A:1246:HIS:CG	2.90	0.55
1:A:944:GLN:HB3	1:A:948:MET:CE	2.37	0.55
1:A:957:LYS:O	1:A:960:ARG:HG3	2.06	0.55
1:A:1082:ASP:HB2	1:A:1083:PRO:CD	2.37	0.55
4:A:1301:CH1:HN41	3:C:1285:G:H1	1.55	0.55
1:A:659:PHE:CZ	1:A:681:PRO:HG2	2.41	0.55
1:A:724:THR:CG2	1:A:726:GLN:H	2.13	0.55
1:A:814:TRP:O	1:A:815:PRO:C	2.45	0.55
1:A:595:TRP:CE2	1:A:600:SER:HB3	2.42	0.54
1:A:1065:GLU:H	1:A:1065:GLU:CD	2.09	0.54
1:A:188:TRP:CZ2	1:A:192:GLU:HG3	2.43	0.54
1:A:926:THR:HG21	1:A:1246:HIS:ND1	2.22	0.54
1:A:957:LYS:HE2	1:A:1024:ALA:O	2.06	0.54
1:A:193:ILE:O	1:A:197:ILE:HG13	2.08	0.54
1:A:22:GLN:HE22	1:A:878:VAL:H	1.52	0.54
1:A:566:LYS:CD	1:A:784:LEU:HD23	2.37	0.54
1:A:516:GLY:HA3	1:A:528:ILE:HG22	1.89	0.54
1:A:561:SER:O	1:A:565:GLU:HB3	2.08	0.54
1:A:92:VAL:HG13	1:A:383:GLU:CG	2.38	0.54
1:A:606:ILE:O	1:A:610:VAL:HB	2.08	0.54
1:A:607:HIS:HB2	1:A:648:ILE:HG21	1.89	0.54
1:A:603:MET:CE	1:A:648:ILE:HG23	2.38	0.54
1:A:819:ASP:OD1	1:A:953:ARG:NH1	2.40	0.54
1:A:532:ASN:OD1	1:A:534:PRO:HD2	2.08	0.53
1:A:107:GLU:O	1:A:108:THR:CB	2.55	0.53
1:A:564:ILE:HG21	1:A:1185:MET:HB3	1.89	0.53
1:A:167:LEU:HD23	1:A:837:ARG:CD	2.37	0.53
1:A:1073:LEU:HG	1:A:1093:VAL:HG11	1.90	0.53
1:A:944:GLN:HB3	1:A:948:MET:HE2	1.91	0.52
1:A:62:THR:O	1:A:66:LYS:HE2	2.09	0.52
1:A:81:VAL:HG13	1:A:132:ILE:HD13	1.91	0.52
1:A:1005:ASN:N	1:A:1006:PRO:HD3	2.24	0.52
1:A:436:MET:O	1:A:436:MET:HE2	2.09	0.52
1:A:1052:LEU:HD21	1:A:1176:VAL:HG22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:LEU:HD12	1:A:377:LEU:N	2.25	0.52
1:A:446:LEU:HD13	1:A:1149:GLY:HA3	1.92	0.52
1:A:743:THR:CG2	1:A:744:THR:H	2.16	0.52
1:A:406:GLY:HA3	1:A:630:GLU:O	2.10	0.52
1:A:170:PRO:HG3	1:A:886:TRP:HB2	1.91	0.52
1:A:540:ALA:HB3	1:A:541:PRO:HD3	1.91	0.51
1:A:566:LYS:HD2	1:A:784:LEU:CD2	2.40	0.51
1:A:784:LEU:HD12	1:A:786:PHE:CZ	2.46	0.51
1:A:814:TRP:O	1:A:817:ILE:HG22	2.10	0.51
1:A:1219:ARG:O	1:A:1223:ARG:HG3	2.10	0.51
1:A:14:GLU:C	1:A:20:THR:HG22	2.31	0.51
1:A:32:LYS:O	1:A:36:MET:HG3	2.11	0.51
1:A:470:LEU:HD23	1:A:477:LEU:HD21	1.92	0.51
1:A:984:LEU:O	1:A:987:ARG:HB2	2.11	0.51
1:A:1112:MET:HE1	1:A:1150:LEU:CD1	2.22	0.51
1:A:1002:ILE:HD13	1:A:1136:ALA:HB2	1.94	0.50
1:A:34:PHE:CZ	1:A:160:VAL:HG21	2.46	0.50
1:A:561:SER:HB2	2:B:1275:G:H2'	1.93	0.50
1:A:940:LEU:O	1:A:941:LYS:HB2	2.11	0.50
1:A:39:ARG:HH11	1:A:39:ARG:CG	2.22	0.50
1:A:857:GLY:C	1:A:859:SER:H	2.15	0.50
1:A:1258:THR:HG23	1:A:1262:GLN:NE2	2.27	0.50
1:A:303:ARG:HG3	1:A:303:ARG:HH11	1.77	0.50
1:A:411:ILE:C	1:A:411:ILE:HD12	2.32	0.50
1:A:1174:ARG:HB2	6:A:1401:HOH:O	2.10	0.50
1:A:436:MET:HE2	1:A:436:MET:C	2.32	0.50
1:A:298:GLU:HB2	1:A:311:MET:CE	2.42	0.49
1:A:523:ARG:HG2	1:A:524:ARG:N	2.28	0.49
1:A:778:THR:CG2	1:A:779:ALA:N	2.75	0.49
1:A:425:LEU:HB2	1:A:698:MET:HE3	1.94	0.49
1:A:578:PRO:HB2	1:A:742:GLY:HA3	1.93	0.49
1:A:245:LEU:HD22	1:A:367:ASP:HA	1.93	0.49
1:A:464:ALA:O	1:A:468:GLU:HG2	2.12	0.49
1:A:509:ILE:HD13	1:A:538:VAL:HG21	1.94	0.49
1:A:572:VAL:HG13	1:A:789:GLY:O	2.12	0.49
1:A:582:ILE:HG21	1:A:757:LEU:CD2	2.42	0.49
1:A:686:ALA:O	1:A:690:GLU:HB2	2.12	0.49
1:A:557:PRO:HG3	1:A:781:TYR:OH	2.13	0.49
1:A:881:PHE:O	1:A:909:LEU:HD12	2.12	0.49
1:A:436:MET:HE1	1:A:442:THR:HG21	1.94	0.48
1:A:409:GLY:HA3	1:A:627:VAL:HG21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:749:ASN:ND2	1:A:751:GLU:HB3	2.14	0.48
1:A:1199:LEU:HD12	1:A:1219:ARG:HD3	1.94	0.48
1:A:523:ARG:HG2	1:A:524:ARG:H	1.77	0.48
1:A:1120:ASP:HB3	1:A:1123:ALA:CB	2.43	0.48
1:A:568:ILE:N	1:A:569:PRO:CD	2.76	0.48
1:A:92:VAL:HG13	1:A:383:GLU:HG3	1.94	0.48
1:A:272:LYS:HD3	1:A:338:TYR:OH	2.14	0.48
1:A:470:LEU:CD2	1:A:477:LEU:HD21	2.44	0.48
1:A:299:TRP:CD2	1:A:303:ARG:HG2	2.49	0.48
1:A:446:LEU:HD22	1:A:1149:GLY:C	2.34	0.48
1:A:815:PRO:HB2	1:A:953:ARG:O	2.14	0.48
1:A:1082:ASP:HB2	1:A:1083:PRO:HD2	1.95	0.48
1:A:35:SER:HB3	4:A:1302:CH1:H1'	1.96	0.48
1:A:599:LEU:O	1:A:603:MET:HG2	2.14	0.48
1:A:582:ILE:HG21	1:A:757:LEU:HD21	1.96	0.47
1:A:104:GLU:CG	1:A:116:SER:HA	2.43	0.47
1:A:396:LYS:HD2	1:A:765:GLU:HB3	1.96	0.47
1:A:542:HIS:NE2	1:A:690:GLU:HG2	2.28	0.47
1:A:223:THR:HG21	6:A:1452:HOH:O	2.14	0.47
1:A:13:ILE:HD13	1:A:163:ALA:CB	2.45	0.47
1:A:83:ARG:NH1	1:A:84:LYS:O	2.48	0.47
1:A:760:ILE:O	1:A:763:TYR:HB3	2.14	0.47
1:A:957:LYS:HD2	1:A:957:LYS:N	2.30	0.47
1:A:528:ILE:HG12	3:C:1285:G:C5	2.50	0.47
1:A:632:VAL:HB	1:A:635:VAL:HB	1.96	0.47
1:A:1134:LEU:HA	1:A:1257:MET:HE3	1.97	0.46
1:A:149:ALA:HB1	1:A:150:PRO:CD	2.45	0.46
1:A:1172:LEU:O	1:A:1175:VAL:HG13	2.14	0.46
1:A:565:GLU:OE1	1:A:1103:ARG:HB2	2.16	0.46
1:A:595:TRP:HA	1:A:599:LEU:HB2	1.97	0.46
1:A:964:ARG:O	1:A:968:GLU:HG3	2.16	0.46
1:A:15:SER:N	1:A:20:THR:HG22	2.31	0.46
1:A:238:ILE:HD12	1:A:841:TYR:CZ	2.51	0.46
1:A:538:VAL:HG13	1:A:651:LEU:HB2	1.96	0.46
1:A:743:THR:CG2	1:A:744:THR:N	2.78	0.46
1:A:784:LEU:HD22	1:A:784:LEU:HA	1.79	0.46
1:A:1146:LEU:HD21	1:A:1152:GLU:HG2	1.98	0.46
1:A:92:VAL:CG1	1:A:92:VAL:O	2.64	0.46
1:A:101:GLU:HG2	1:A:102:LEU:HG	1.97	0.46
1:A:477:LEU:HB3	1:A:496:GLN:HB3	1.97	0.46
1:A:1005:ASN:O	1:A:1007:PRO:HD3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:GLU:O	1:A:108:THR:HB	2.16	0.45
1:A:246:ASP:O	1:A:250:VAL:HG23	2.16	0.45
1:A:561:SER:HB3	2:B:1275:G:O2'	2.16	0.45
1:A:734:ASP:OD1	4:A:1301:CH1:H5'2	2.16	0.45
1:A:459:ARG:HG3	3:C:1286:C:OP2	2.16	0.45
1:A:706:TRP:O	1:A:707:GLY:C	2.55	0.45
1:A:149:ALA:HB1	1:A:150:PRO:HD2	1.98	0.45
1:A:486:LYS:HE2	1:A:488:ALA:HB3	1.98	0.45
1:A:561:SER:O	1:A:562:ALA:HB3	2.16	0.45
1:A:1102:THR:O	1:A:1106:PHE:HD2	2.00	0.45
1:A:106:HIS:CE1	1:A:108:THR:HB	2.51	0.45
1:A:72:TYR:O	1:A:83:ARG:HD2	2.16	0.45
1:A:784:LEU:CD1	1:A:791:ARG:HD2	2.46	0.45
1:A:457:THR:O	1:A:491:ILE:HG13	2.16	0.45
1:A:856:ILE:O	1:A:856:ILE:HG22	2.16	0.45
1:A:1077:LEU:HD13	1:A:1077:LEU:HA	1.79	0.45
1:A:907:ARG:HH12	1:A:1060:LYS:HE3	1.82	0.45
1:A:457:THR:C	1:A:491:ILE:HG13	2.38	0.45
1:A:563:VAL:O	1:A:564:ILE:CG2	2.60	0.45
1:A:886:TRP:HA	6:A:1527:HOH:O	2.15	0.44
1:A:1095:VAL:HG23	1:A:1237:ALA:HB2	1.99	0.44
1:A:208:LEU:HB2	1:A:210:LEU:HD21	1.99	0.44
1:A:995:TRP:HZ2	1:A:1006:PRO:HG3	1.79	0.44
1:A:127:ASP:O	1:A:131:ARG:HG3	2.17	0.44
1:A:303:ARG:HH11	1:A:303:ARG:CG	2.30	0.44
1:A:517:LEU:HD23	1:A:527:SER:HA	2.00	0.44
1:A:38:THR:O	1:A:41:ASP:HB2	2.18	0.44
1:A:162:GLU:OE1	1:A:837:ARG:NH2	2.50	0.44
1:A:223:THR:CG2	1:A:224:SER:N	2.81	0.44
1:A:373:SER:OG	1:A:375:ILE:HG12	2.18	0.44
1:A:585:ASP:HB3	1:A:772:ASP:HB3	1.98	0.44
1:A:855:MET:HE3	1:A:858:GLU:H	1.81	0.44
1:A:863:LEU:CD2	1:A:1039:MET:HE2	2.48	0.44
1:A:1172:LEU:HD21	1:A:1217:TRP:HA	1.98	0.44
1:A:106:HIS:HE1	1:A:108:THR:HB	1.83	0.44
1:A:749:ASN:HD22	1:A:752:THR:N	2.07	0.44
1:A:1150:LEU:HD12	1:A:1150:LEU:N	2.32	0.44
1:A:39:ARG:HG2	1:A:39:ARG:NH1	2.28	0.44
1:A:561:SER:CB	1:A:566:LYS:HE2	2.35	0.44
1:A:814:TRP:O	1:A:816:ALA:N	2.51	0.44
1:A:855:MET:O	1:A:856:ILE:HD13	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:TYR:CB	1:A:132:ILE:HD12	2.47	0.43
1:A:84:LYS:HD2	1:A:86:TYR:CZ	2.53	0.43
1:A:425:LEU:HB2	1:A:698:MET:CE	2.48	0.43
1:A:820:GLN:O	1:A:824:VAL:HG23	2.18	0.43
1:A:256:ILE:HD12	1:A:277:PHE:CE2	2.52	0.43
1:A:554:ASN:HB2	6:A:1551:HOH:O	2.17	0.43
1:A:557:PRO:O	1:A:557:PRO:HG2	2.18	0.43
1:A:421:ILE:HD12	1:A:421:ILE:HA	1.88	0.43
1:A:533:VAL:HB	1:A:534:PRO:HD3	1.99	0.43
1:A:757:LEU:HD22	1:A:773:ILE:HG21	2.00	0.43
1:A:294:CYS:SG	1:A:314:MET:HB3	2.59	0.43
1:A:659:PHE:CZ	1:A:681:PRO:CG	3.02	0.43
1:A:1086:SER:O	1:A:1090:LEU:HG	2.19	0.43
1:A:642:SER:OG	1:A:645:GLN:HG3	2.18	0.43
1:A:15:SER:HA	1:A:20:THR:HG22	1.99	0.43
1:A:814:TRP:CB	1:A:815:PRO:HD3	2.45	0.43
1:A:460:GLY:N	3:C:1285:G:H5"	2.34	0.43
1:A:814:TRP:CD2	1:A:852:GLN:HB2	2.53	0.43
1:A:73:TYR:HB2	1:A:132:ILE:HG23	1.99	0.43
1:A:456:VAL:HG21	1:A:977:TYR:CE2	2.54	0.43
1:A:542:HIS:CE1	1:A:690:GLU:HG3	2.54	0.42
1:A:1014:HIS:O	1:A:1018:GLN:HG3	2.19	0.42
1:A:1120:ASP:HB3	1:A:1123:ALA:HB2	2.00	0.42
1:A:286:TYR:C	1:A:288:SER:N	2.71	0.42
1:A:749:ASN:ND2	1:A:752:THR:N	2.63	0.42
1:A:1052:LEU:HD13	1:A:1259:TRP:CG	2.53	0.42
1:A:448:GLN:NE2	1:A:620:MET:H	2.16	0.42
1:A:814:TRP:CG	1:A:815:PRO:N	2.82	0.42
1:A:83:ARG:HG3	1:A:83:ARG:HH11	1.85	0.42
1:A:357:HIS:CE1	1:A:788:PHE:HB2	2.54	0.42
1:A:520:GLN:NE2	1:A:523:ARG:HD3	2.35	0.42
1:A:390:THR:HG22	1:A:391:GLN:N	2.34	0.42
1:A:473:ILE:HG21	1:A:507:VAL:HG11	2.01	0.42
1:A:654:LEU:HD21	1:A:659:PHE:CE1	2.55	0.42
1:A:560:GLY:HA3	2:B:1275:G:N2	2.34	0.42
1:A:877:LEU:HB2	1:A:888:PHE:CD2	2.54	0.42
1:A:78:LEU:HD12	1:A:80:ARG:CZ	2.50	0.42
1:A:170:PRO:CG	1:A:886:TRP:HB2	2.49	0.42
1:A:350:ARG:HD2	6:A:1524:HOH:O	2.19	0.42
1:A:528:ILE:HD12	1:A:528:ILE:HA	1.88	0.42
1:A:603:MET:HE3	1:A:652:SER:OG	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:855:MET:HE1	1:A:858:GLU:H	1.83	0.42
1:A:90:ASP:O	1:A:92:VAL:N	2.50	0.42
1:A:158:LEU:HD22	1:A:238:ILE:HD13	2.02	0.42
1:A:245:LEU:CD2	1:A:367:ASP:HA	2.50	0.42
1:A:829:VAL:HG13	1:A:890:TRP:NE1	2.34	0.42
1:A:147:ILE:HD12	1:A:149:ALA:O	2.21	0.41
1:A:114:ARG:HG3	1:A:114:ARG:HH11	1.85	0.41
1:A:923:ARG:CB	1:A:923:ARG:HH11	2.33	0.41
1:A:1256:PHE:O	1:A:1260:MET:HG3	2.21	0.41
1:A:56:MET:HG2	1:A:188:TRP:CE2	2.55	0.41
1:A:538:VAL:HG22	1:A:647:MET:HA	2.02	0.41
1:A:541:PRO:HB2	1:A:648:ILE:HD11	2.01	0.41
1:A:680:PHE:HA	1:A:681:PRO:HD3	1.85	0.41
1:A:814:TRP:HB3	1:A:815:PRO:CD	2.45	0.41
1:A:1262:GLN:HG2	1:A:1265:ARG:NH1	2.36	0.41
1:A:145:ARG:O	1:A:805:ARG:HD2	2.20	0.41
1:A:626:ILE:CG2	1:A:638:ALA:HB1	2.50	0.41
1:A:1043:ARG:HD3	6:A:1659:HOH:O	2.20	0.41
1:A:1049:PHE:CG	1:A:1053:LEU:HD23	2.55	0.41
1:A:167:LEU:N	1:A:167:LEU:HD22	2.36	0.41
1:A:93:TYR:CD1	1:A:379:ARG:HB3	2.55	0.41
1:A:524:ARG:HG2	1:A:524:ARG:HH11	1.85	0.41
1:A:639:ARG:HA	1:A:640:PRO:HD3	1.93	0.41
1:A:1052:LEU:HD12	1:A:1052:LEU:HA	1.87	0.41
1:A:814:TRP:CB	1:A:815:PRO:CD	2.98	0.41
1:A:817:ILE:O	1:A:821:ILE:HG12	2.21	0.41
1:A:460:GLY:O	1:A:490:LYS:NZ	2.53	0.40
1:A:564:ILE:HD12	1:A:564:ILE:HA	1.97	0.40
1:A:948:MET:HE1	1:A:1042:ARG:HG3	2.03	0.40
1:A:57:LEU:HD21	1:A:189:CYS:SG	2.62	0.40
1:A:304:SER:O	1:A:1104:LYS:HE3	2.22	0.40
1:A:1212:PRO:HA	1:A:1213:PRO:HD3	1.92	0.40
1:A:134:THR:CG2	1:A:669:PRO:HG2	2.51	0.40
1:A:451:MET:HA	1:A:451:MET:HE3	2.03	0.40
1:A:523:ARG:HG2	1:A:523:ARG:HH11	1.85	0.40
1:A:1181:PRO:HD2	1:A:1184:TRP:CE3	2.57	0.40
1:A:393:PRO:HG2	1:A:592:SER:HA	2.03	0.40
1:A:483:LEU:HD21	1:A:967:ARG:HA	2.04	0.40
1:A:66:LYS:HA	1:A:66:LYS:HD3	1.84	0.40
1:A:185:CYS:HB3	1:A:186:PRO:HD3	2.03	0.40
1:A:520:GLN:NE2	1:A:526:ARG:NH1	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1100:GLN:CG	1:A:1101:SER:N	2.84	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 PDB entries followed by that with respect to all EM entries.

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	1262/1267 (100%)	1169 (93%)	74 (6%)	19 (2%)	10 46

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	108	THR
1	A	559	SER
1	A	561	SER
1	A	814	TRP
1	A	564	ILE
1	A	963	SER
1	A	91	ASP
1	A	557	PRO
1	A	567	VAL
1	A	687	THR
1	A	964	ARG
1	A	110	THR
1	A	99	ILE
1	A	146	GLN
1	A	611	ALA
1	A	815	PRO
1	A	10	GLY
1	A	1005	ASN
1	A	563	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 PDB entries followed by that with respect to all EM entries.

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	1081/1083 (100%)	1044 (97%)	37 (3%)	37 60

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	PHE
1	A	57	LEU
1	A	84	LYS
1	A	300	LEU
1	A	366	ARG
1	A	387	GLN
1	A	390	THR
1	A	414	LEU
1	A	431	LEU
1	A	436	MET
1	A	506	SER
1	A	536	GLN
1	A	538	VAL
1	A	557	PRO
1	A	671	ASN
1	A	712	ASP
1	A	735	ASP
1	A	778	THR
1	A	784	LEU
1	A	796	SER
1	A	804	GLU
1	A	845	LEU
1	A	890	TRP
1	A	894	THR
1	A	909	LEU
1	A	920	VAL
1	A	923	ARG
1	A	984	LEU
1	A	990	ARG
1	A	1045	SER

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Mol	Chain	Res	Type
1	A	1052	LEU
1	A	1063	MET
1	A	1077	LEU
1	A	1121	VAL
1	A	1151	GLN
1	A	1176	VAL
1	A	1238	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	121	ASN
1	A	146	GLN
1	A	283	HIS
1	A	296	ASN
1	A	387	GLN
1	A	448	GLN
1	A	504	HIS
1	A	520	GLN
1	A	522	GLN
1	A	536	GLN
1	A	649	GLN
1	A	664	ASN
1	A	671	ASN
1	A	675	HIS
1	A	710	HIS
1	A	728	ASN
1	A	749	ASN
1	A	754	GLN
1	A	834	GLN
1	A	864	GLN
1	A	969	GLN
1	A	980	GLN
1	A	1004	HIS
1	A	1005	ASN
1	A	1165	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	4/5 (80%)	0	0
3	C	7/8 (87%)	0	0
All	All	11/13 (84%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
4	CH1	A	1302	-	24,29,29	1.16	3 (12%)	33,45,45	2.79	15 (45%)
4	CH1	A	1303	-	24,29,29	1.13	2 (8%)	33,45,45	2.72	15 (45%)
4	CH1	A	1301	5	24,29,29	1.15	1 (4%)	33,45,45	2.84	15 (45%)

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
4	CH1	A	1302	-	-	6/22/34/34	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CH1	A	1303	-	-	8/22/34/34	0/2/2/2
4	CH1	A	1301	5	-	5/22/34/34	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1302	CH1	C6-C5	2.64	1.41	1.35
4	A	1301	CH1	C6-C5	2.62	1.41	1.35
4	A	1303	CH1	C6-C5	2.46	1.40	1.35
4	A	1302	CH1	PG-O1G	2.14	1.57	1.50
4	A	1303	CH1	PB-O1B	2.03	1.58	1.50
4	A	1302	CH1	PB-O1B	2.01	1.58	1.50

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1303	CH1	O3G-PG-O1G	-7.66	80.70	110.68
4	A	1302	CH1	O3G-PG-O1G	-7.37	81.81	110.68
4	A	1301	CH1	O3G-PG-O1G	-7.33	81.97	110.68
4	A	1301	CH1	O3G-PG-O3B	-6.68	82.22	104.64
4	A	1302	CH1	O3G-PG-O3B	-6.61	82.48	104.64
4	A	1303	CH1	O3G-PG-O3B	-6.32	83.45	104.64
4	A	1301	CH1	O3G-PG-O2G	-5.16	87.91	107.64
4	A	1303	CH1	O3G-PG-O2G	-5.13	88.04	107.64
4	A	1302	CH1	O3G-PG-O2G	-5.11	88.09	107.64
4	A	1302	CH1	O2-C2-N3	-4.97	114.25	122.33
4	A	1301	CH1	O2-C2-N3	-4.95	114.27	122.33
4	A	1303	CH1	O2-C2-N3	-4.81	114.50	122.33
4	A	1302	CH1	C3'-C4'-C5'	-4.23	104.77	113.11
4	A	1301	CH1	C3'-C4'-C5'	-4.10	105.01	113.11
4	A	1301	CH1	O4'-C1'-C2'	-3.98	102.77	106.51
4	A	1303	CH1	C3'-C4'-C5'	-3.84	105.53	113.11
4	A	1302	CH1	O4'-C1'-C2'	-3.76	102.97	106.51
4	A	1301	CH1	PB-O3A-PA	-3.51	120.77	132.83
4	A	1301	CH1	O4'-C4'-C5'	3.35	115.02	109.52
4	A	1302	CH1	PB-O3B-PG	-3.15	122.03	132.83
4	A	1303	CH1	PB-O3A-PA	-3.11	122.15	132.83
4	A	1303	CH1	O4'-C4'-C5'	3.03	114.50	109.52
4	A	1302	CH1	PB-O3A-PA	-3.02	122.46	132.83
4	A	1301	CH1	PB-O3B-PG	-3.00	122.54	132.83
4	A	1303	CH1	O4'-C1'-C2'	-2.91	103.77	106.51
4	A	1302	CH1	C6-N1-C2	-2.82	115.61	120.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1301	CH1	C6-N1-C2	-2.79	115.66	120.49
4	A	1303	CH1	C6-N1-C2	-2.77	115.68	120.49
4	A	1302	CH1	O4'-C4'-C5'	2.75	114.04	109.52
4	A	1302	CH1	O2G-PG-O3B	2.71	113.71	104.64
4	A	1301	CH1	O2G-PG-O3B	2.70	113.69	104.64
4	A	1303	CH1	O3B-PG-O1G	2.53	125.24	111.19
4	A	1303	CH1	O2G-PG-O3B	2.43	112.78	104.64
4	A	1303	CH1	PB-O3B-PG	-2.40	124.60	132.83
4	A	1302	CH1	O3B-PG-O1G	2.35	124.24	111.19
4	A	1301	CH1	O3B-PG-O1G	2.32	124.05	111.19
4	A	1301	CH1	O4'-C1'-N1	2.28	113.56	108.36
4	A	1302	CH1	N1-C2-N3	2.26	122.92	118.81
4	A	1303	CH1	N1-C2-N3	2.24	122.89	118.81
4	A	1302	CH1	O4'-C1'-N1	2.22	113.44	108.36
4	A	1301	CH1	N1-C2-N3	2.20	122.81	118.81
4	A	1301	CH1	O2G-PG-O1G	2.10	118.92	110.68
4	A	1302	CH1	O2G-PG-O1G	2.07	118.80	110.68
4	A	1303	CH1	O4'-C1'-N1	2.03	112.99	108.36
4	A	1303	CH1	O2G-PG-O1G	2.02	118.61	110.68

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1301	CH1	C3'-C4'-C5'-O5'
4	A	1301	CH1	O4'-C4'-C5'-O5'
4	A	1301	CH1	C5'-O5'-PA-O1A
4	A	1302	CH1	C3'-C4'-C5'-O5'
4	A	1302	CH1	O4'-C4'-C5'-O5'
4	A	1302	CH1	C5'-O5'-PA-O2A
4	A	1302	CH1	C5'-O5'-PA-O3A
4	A	1303	CH1	C3'-C4'-C5'-O5'
4	A	1303	CH1	O4'-C4'-C5'-O5'
4	A	1303	CH1	C5'-O5'-PA-O1A
4	A	1303	CH1	C5'-O5'-PA-O3A
4	A	1302	CH1	C4'-C5'-O5'-PA
4	A	1303	CH1	PG-O3B-PB-O3A
4	A	1301	CH1	C5'-O5'-PA-O3A
4	A	1302	CH1	C5'-O5'-PA-O1A
4	A	1301	CH1	PB-O3A-PA-O2A
4	A	1303	CH1	PB-O3A-PA-O1A
4	A	1303	CH1	PG-O3B-PB-O1B

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Mol	Chain	Res	Type	Atoms
4	A	1303	CH1	PG-O3B-PB-O2B

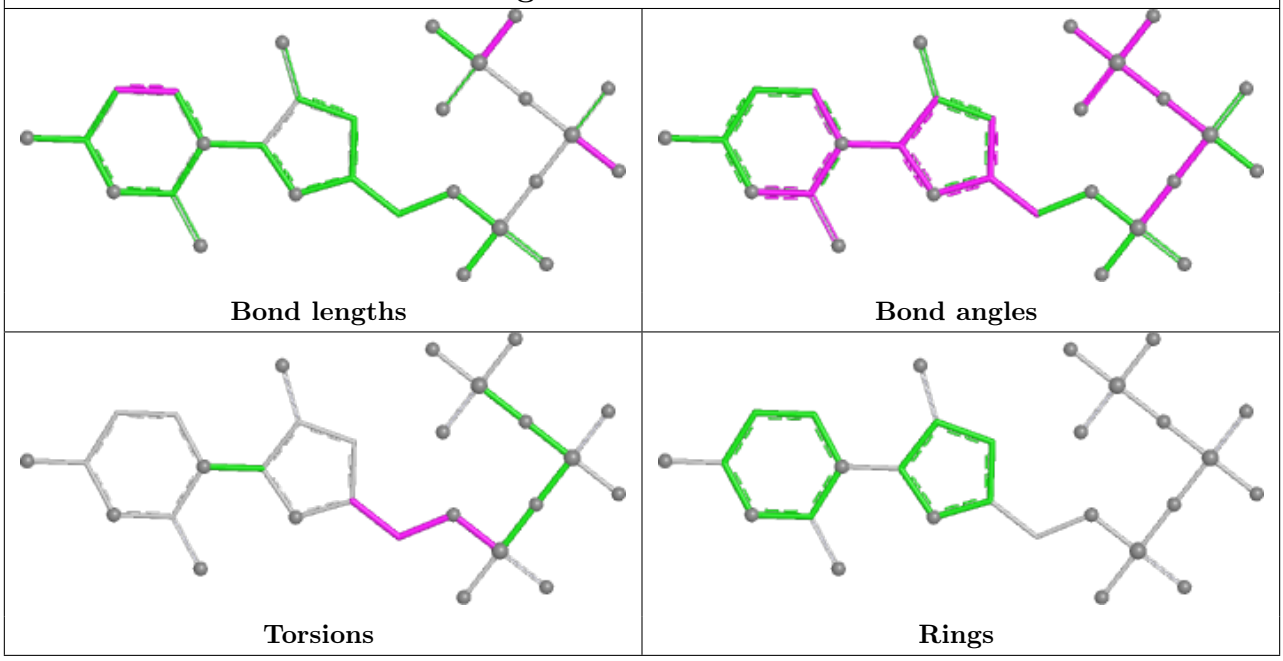
There are no ring outliers.

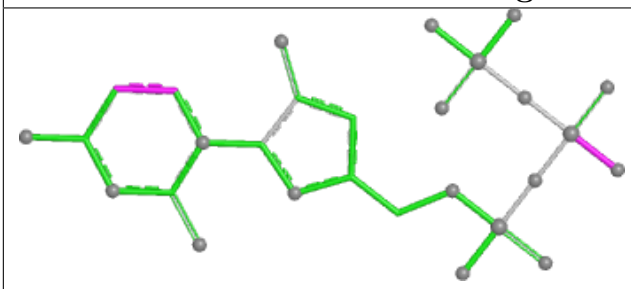
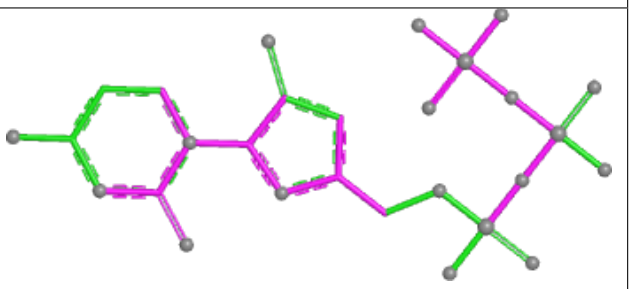
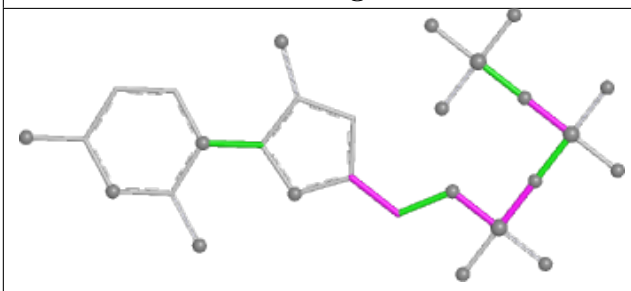
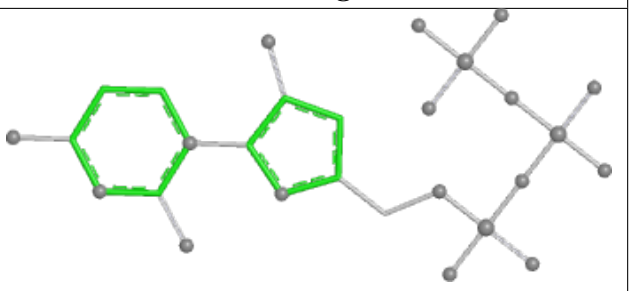
2 monomers are involved in 3 short contacts:

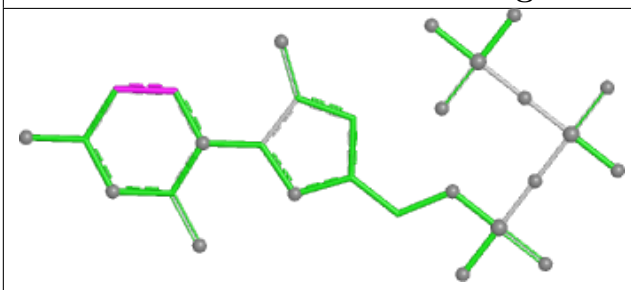
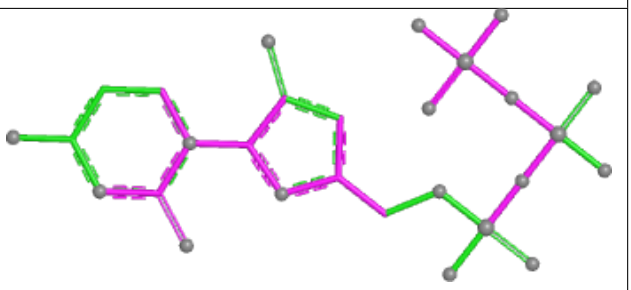
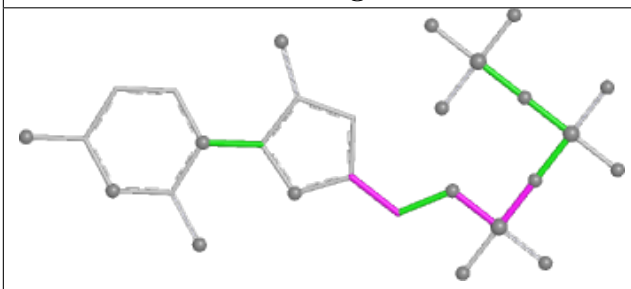
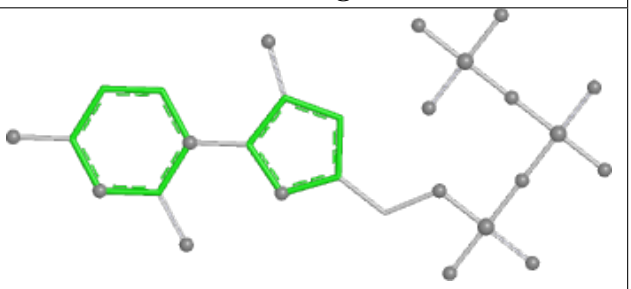
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1302	CH1	1	0
4	A	1301	CH1	2	0

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 CH1 A 1302



Ligand CH1 A 1303	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CH1 A 1301	
 Bond lengths	 Bond angles
 Torsions	 Rings

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.