



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 31, 2021 – 02:56 PM EDT

PDB ID : 2ZD1
Title : Crystal Structure of HIV-1 Reverse Transcriptase (RT) in Complex with
TMC278 (Rilpivirine), A Non-nucleoside RT Inhibitor
Authors : Das, K.; Bauman, J.D.; Clark Jr., A.D.; Shatkin, A.J.; Arnold, E.
Deposited on : 2007-11-16
Resolution : 1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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 : 2.23.2
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) : 2.23.2

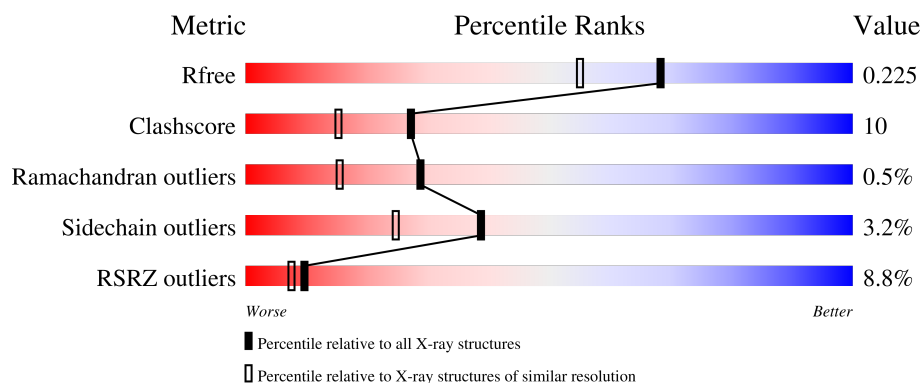
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	557	<div> <div>6%</div> <div>80%</div> <div>18%</div> <div>..</div> </div>
2	B	428	<div> <div>11%</div> <div>73%</div> <div>21%</div> <div>..</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8581 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 Reverse transcriptase/ribonuclease H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	554	Total	C	N	O	S	0	0	0
			4505	2917	748	832	8			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP P03366
A	0	VAL	-	expression tag	UNP P03366
A	172	ALA	LYS	engineered mutation	UNP P03366
A	173	ALA	LYS	engineered mutation	UNP P03366
A	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 2 is a protein called p51 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	412	Total	C	N	O	S	0	0	0
			3413	2225	564	617	7			

There is a discrepancy between the modelled and reference sequences:

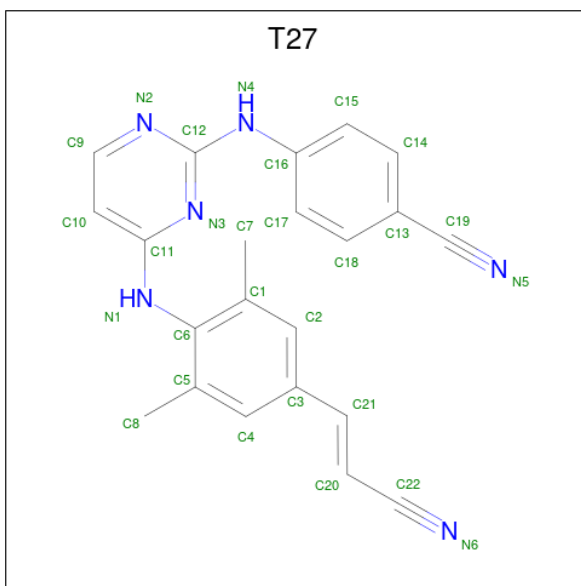
Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 4 is 4-{[4-({4-[(E)-2-cyanoethenyl]-2,6-dimethylphenyl}amino)pyrimidin-2-yl]amino}benzonitrile (three-letter code: T27) (formula: $C_{22}H_{18}N_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			28	22	6		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			4	2	2		

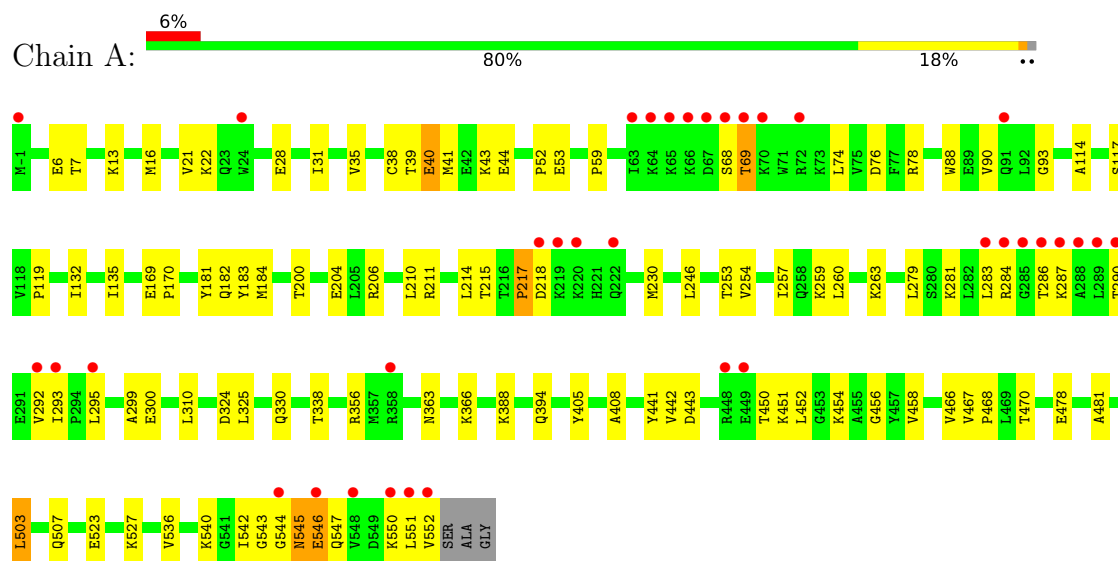
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	375	Total	O	0	0
			375	375		
6	B	251	Total	O	0	0
			251	251		

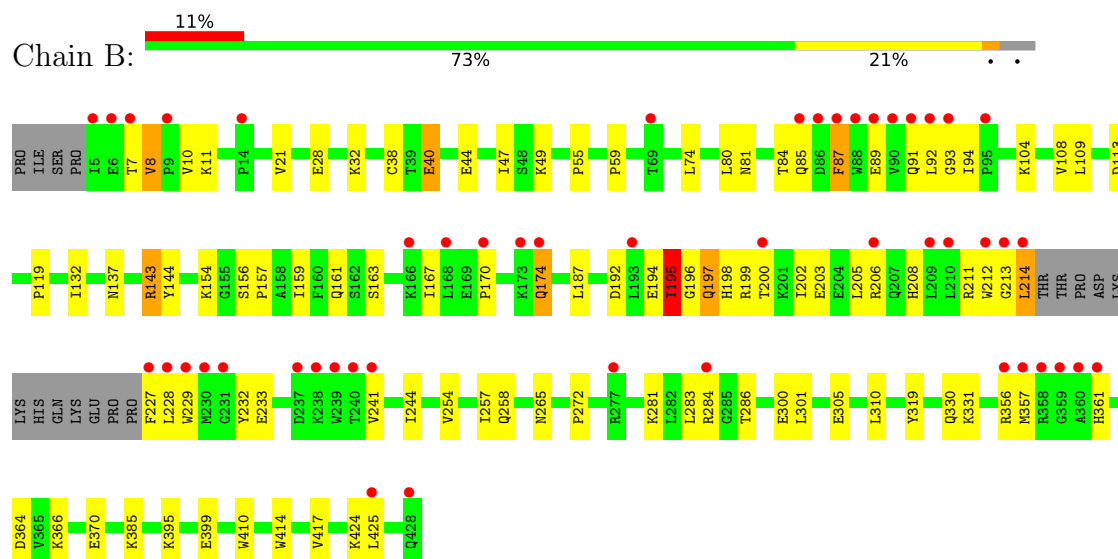
3 Residue-property plots [i](#)

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: Reverse transcriptase/ribonuclease H



• Molecule 2: p51 RT



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	163.37Å 73.26Å 110.07Å 90.00° 100.07° 90.00°	Depositor
Resolution (Å)	40.00 – 1.80 38.36 – 1.79	Depositor EDS
% Data completeness (in resolution range)	95.2 (40.00-1.80) 94.1 (38.36-1.79)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 1.79Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.220 , 0.248 0.216 , 0.225	Depositor DCC
R_{free} test set	2283 reflections (2.02%)	wwPDB-VP
Wilson B-factor (Å ²)	25.6	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 48.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8581	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, T27, 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	0.40	0/4623	0.63	1/6284 (0.0%)
2	B	0.38	0/3511	0.61	2/4768 (0.0%)
All	All	0.39	0/8134	0.62	3/11052 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	325	LEU	CA-CB-CG	7.37	132.25	115.30
2	B	143	ARG	NE-CZ-NH2	-6.06	117.27	120.30
2	B	143	ARG	NE-CZ-NH1	5.24	122.92	120.30

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	4505	0	4562	92	0
2	B	3413	0	3443	75	0
3	A	5	0	0	0	0
4	A	28	0	18	1	0
5	B	4	0	6	0	0
6	A	375	0	0	9	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	251	0	0	8	0
All	All	8581	0	8029	162	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 10.

All (162) 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:7:THR:HG22	1:A:119:PRO:HG2	1.48	0.95
2:B:89:GLU:HB2	2:B:91:GLN:HG2	1.49	0.94
2:B:84:THR:HG23	2:B:154:LYS:HE2	1.50	0.93
1:A:6:GLU:H	1:A:6:GLU:CD	1.75	0.89
2:B:143:ARG:HD3	6:B:436:HOH:O	1.74	0.87
1:A:454:LYS:NZ	1:A:552:VAL:HB	1.88	0.87
1:A:466:VAL:HG22	1:A:550:LYS:NZ	1.95	0.81
1:A:542:ILE:O	1:A:545:ASN:HB2	1.83	0.79
1:A:544:GLY:HA2	2:B:286:THR:HG22	1.64	0.78
1:A:466:VAL:HG22	1:A:550:LYS:HZ3	1.51	0.74
2:B:163:SER:O	2:B:167:ILE:HG13	1.87	0.74
1:A:543:GLY:N	2:B:283:LEU:O	2.21	0.74
2:B:109:LEU:HD21	2:B:206:ARG:HH21	1.53	0.73
1:A:454:LYS:HZ1	1:A:552:VAL:HB	1.52	0.72
2:B:11:LYS:O	2:B:85:GLN:HG2	1.89	0.72
1:A:456:GLY:HA3	1:A:550:LYS:NZ	2.08	0.69
1:A:38:CYS:SG	1:A:132:ILE:HD11	2.34	0.68
2:B:357:MET:HG3	2:B:357:MET:O	1.93	0.67
2:B:195:ILE:HD11	2:B:199:ARG:CZ	2.26	0.66
2:B:10:VAL:HG22	2:B:87:PHE:CZ	2.32	0.65
2:B:174:GLN:O	2:B:174:GLN:HG3	1.97	0.64
2:B:241:VAL:HG22	6:B:644:HOH:O	1.97	0.64
2:B:7:THR:HG22	2:B:119:PRO:HG2	1.80	0.64
6:A:842:HOH:O	2:B:49:LYS:HE3	1.98	0.64
1:A:253:THR:HG22	1:A:292:VAL:HG22	1.80	0.63
2:B:10:VAL:HG13	2:B:87:PHE:CE1	2.33	0.63
1:A:478:GLU:HG2	6:A:800:HOH:O	1.97	0.62
1:A:88:TRP:CD1	2:B:143:ARG:HD2	2.34	0.62
2:B:10:VAL:HG22	2:B:87:PHE:HZ	1.63	0.62
2:B:84:THR:CG2	2:B:154:LYS:HE2	2.28	0.62
2:B:203:GLU:OE1	2:B:206:ARG:HD2	2.00	0.62
1:A:454:LYS:HZ2	1:A:552:VAL:HB	1.63	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:GLY:HA3	1:A:550:LYS:HZ2	1.63	0.61
2:B:424:LYS:HD2	6:B:508:HOH:O	2.00	0.61
1:A:547:GLN:HG2	1:A:551:LEU:HD21	1.83	0.60
1:A:254:VAL:HG22	1:A:293:ILE:HD11	1.84	0.60
1:A:441:TYR:CG	1:A:544:GLY:HA3	2.38	0.59
2:B:104:LYS:HG2	2:B:192:ASP:OD1	2.02	0.59
1:A:28:GLU:HG3	1:A:135:ILE:HD12	1.85	0.59
2:B:213:GLY:O	2:B:214:LEU:HB3	2.02	0.57
2:B:319:TYR:OH	2:B:385:LYS:HE2	2.04	0.57
1:A:552:VAL:HG11	6:A:740:HOH:O	2.05	0.57
2:B:194:GLU:O	2:B:196:GLY:N	2.38	0.56
6:A:877:HOH:O	2:B:137:ASN:HB3	2.05	0.56
2:B:89:GLU:N	2:B:89:GLU:OE1	2.38	0.56
2:B:425:LEU:HD23	2:B:425:LEU:O	2.06	0.56
1:A:544:GLY:O	1:A:546:GLU:N	2.37	0.55
1:A:295:LEU:HB3	1:A:300:GLU:OE1	2.06	0.55
1:A:452:LEU:CD2	1:A:470:THR:HG22	2.36	0.55
1:A:542:ILE:O	1:A:545:ASN:CB	2.52	0.55
1:A:90:VAL:HG23	6:B:467:HOH:O	2.07	0.55
1:A:546:GLU:O	1:A:546:GLU:HG2	2.07	0.55
1:A:546:GLU:O	1:A:546:GLU:CG	2.55	0.54
1:A:286:THR:OG1	1:A:287:LYS:N	2.41	0.54
1:A:536:VAL:HB	1:A:542:ILE:HD12	1.90	0.54
2:B:91:GLN:O	2:B:92:LEU:HB2	2.08	0.54
1:A:230:MET:HA	1:A:230:MET:HE2	1.90	0.54
1:A:200:THR:O	1:A:204:GLU:HG3	2.08	0.53
2:B:361:HIS:O	2:B:361:HIS:CD2	2.61	0.53
1:A:114:ALA:HA	1:A:214:LEU:HD22	1.89	0.53
1:A:466:VAL:HG22	1:A:550:LYS:HZ2	1.72	0.52
1:A:536:VAL:HB	1:A:542:ILE:CD1	2.39	0.52
2:B:254:VAL:O	2:B:258:GLN:HG3	2.08	0.52
2:B:108:VAL:HB	2:B:232:TYR:HB3	1.91	0.52
1:A:503:LEU:O	1:A:507:GLN:HG3	2.09	0.52
2:B:301:LEU:O	2:B:305:GLU:HG3	2.09	0.52
2:B:366:LYS:O	2:B:370:GLU:HG3	2.09	0.51
1:A:169:GLU:HB3	1:A:170:PRO:CD	2.40	0.51
2:B:197:GLN:HA	2:B:200:THR:HG23	1.91	0.51
1:A:546:GLU:N	1:A:546:GLU:OE1	2.42	0.51
1:A:52:PRO:HD2	1:A:53:GLU:OE2	2.11	0.51
1:A:40:GLU:HG3	1:A:41:MET:N	2.25	0.51
2:B:91:GLN:NE2	2:B:93:GLY:HA2	2.25	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:GLU:CD	1:A:6:GLU:N	2.56	0.51
1:A:210:LEU:HD21	1:A:215:THR:HG22	1.93	0.50
2:B:195:ILE:HD11	2:B:199:ARG:NE	2.26	0.50
2:B:81:ASN:HA	2:B:84:THR:HG22	1.92	0.50
1:A:458:VAL:HG13	1:A:546:GLU:HG3	1.94	0.50
2:B:91:GLN:C	2:B:93:GLY:H	2.14	0.50
1:A:90:VAL:O	1:A:90:VAL:HG22	2.12	0.50
1:A:181:TYR:CE2	1:A:183:TYR:HB2	2.47	0.50
1:A:547:GLN:O	1:A:551:LEU:HG	2.12	0.50
2:B:196:GLY:O	2:B:200:THR:HG23	2.12	0.50
1:A:31:ILE:O	1:A:35:VAL:HG23	2.13	0.49
1:A:441:TYR:HB3	1:A:544:GLY:O	2.12	0.49
1:A:74:LEU:O	1:A:74:LEU:HD23	2.13	0.49
1:A:253:THR:HA	1:A:292:VAL:HA	1.95	0.49
2:B:89:GLU:HB2	2:B:91:GLN:CG	2.34	0.48
1:A:76:ASP:OD1	1:A:78:ARG:HG3	2.12	0.48
1:A:230:MET:HE3	6:A:671:HOH:O	2.14	0.48
1:A:246:LEU:HD11	1:A:310:LEU:HD12	1.95	0.48
1:A:443:ASP:HB3	1:A:546:GLU:OE2	2.14	0.48
2:B:395:LYS:HE3	2:B:399:GLU:OE2	2.13	0.48
1:A:450:THR:O	1:A:451:LYS:HB2	2.14	0.48
2:B:10:VAL:HG13	2:B:87:PHE:CZ	2.48	0.47
1:A:263:LYS:HE3	6:A:806:HOH:O	2.14	0.47
1:A:246:LEU:HD22	1:A:260:LEU:CD1	2.44	0.47
1:A:324:ASP:OD2	1:A:388:LYS:HD2	2.14	0.47
1:A:117:SER:O	1:A:119:PRO:HD3	2.15	0.47
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.97	0.47
1:A:454:LYS:HB2	1:A:550:LYS:HB3	1.96	0.47
1:A:330:GLN:OE1	1:A:338:THR:HG23	2.15	0.46
2:B:195:ILE:O	2:B:195:ILE:HG13	2.15	0.46
1:A:39:THR:O	1:A:43:LYS:HG3	2.16	0.46
1:A:13:LYS:HD2	1:A:16:MET:HE1	1.97	0.46
1:A:53:GLU:H	1:A:53:GLU:CD	2.18	0.46
1:A:408:ALA:HB1	2:B:364:ASP:HB3	1.98	0.46
1:A:523:GLU:HG2	1:A:527:LYS:HE3	1.98	0.45
2:B:197:GLN:H	2:B:197:GLN:HG2	1.52	0.45
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.97	0.45
1:A:544:GLY:CA	2:B:286:THR:HG22	2.41	0.45
2:B:8:VAL:HG11	2:B:159:ILE:HG23	1.98	0.45
1:A:442:VAL:HB	1:A:481:ALA:HB1	1.99	0.45
2:B:272:PRO:HD2	6:B:589:HOH:O	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:LYS:O	1:A:284:ARG:HG3	2.17	0.44
2:B:208:HIS:HA	2:B:211:ARG:HH21	1.83	0.44
1:A:257:ILE:HB	1:A:283:LEU:HD21	2.00	0.44
4:A:557:T27:N3	4:A:557:T27:H17	2.33	0.44
1:A:21:VAL:HB	1:A:59:PRO:HD3	2.00	0.44
1:A:40:GLU:O	1:A:44:GLU:HG3	2.18	0.44
1:A:356:ARG:NH1	6:A:594:HOH:O	2.50	0.44
2:B:281:LYS:O	2:B:284:ARG:HG2	2.17	0.44
2:B:74:LEU:HD11	6:B:667:HOH:O	2.17	0.43
2:B:40:GLU:O	2:B:44:GLU:HG3	2.17	0.43
1:A:246:LEU:HD22	1:A:260:LEU:HD12	1.99	0.43
2:B:156:SER:N	2:B:157:PRO:HD2	2.34	0.43
1:A:279:LEU:HD23	1:A:299:ALA:HB1	2.00	0.43
1:A:441:TYR:CD2	1:A:544:GLY:HA3	2.53	0.43
2:B:206:ARG:NH1	2:B:229:TRP:O	2.52	0.42
2:B:202:ILE:O	2:B:205:LEU:HB3	2.20	0.42
2:B:257:ILE:HG22	2:B:283:LEU:HD11	2.00	0.42
2:B:91:GLN:OE1	2:B:161:GLN:NE2	2.42	0.42
1:A:366:LYS:HE2	1:A:405:TYR:OH	2.20	0.42
2:B:28:GLU:CG	2:B:32:LYS:HE2	2.50	0.42
2:B:187:LEU:HD12	2:B:187:LEU:HA	1.86	0.42
2:B:241:VAL:HG12	6:B:478:HOH:O	2.19	0.42
2:B:47:ILE:HD12	2:B:144:TYR:CD2	2.55	0.42
2:B:94:ILE:O	2:B:94:ILE:HG22	2.18	0.42
2:B:198:HIS:O	2:B:202:ILE:HG12	2.20	0.42
1:A:542:ILE:HG23	2:B:283:LEU:HB3	2.02	0.41
1:A:22:LYS:HG2	6:A:803:HOH:O	2.19	0.41
1:A:467:VAL:HA	1:A:468:PRO:HD3	1.90	0.41
2:B:244:ILE:HB	2:B:310:LEU:HD22	2.03	0.41
1:A:13:LYS:HB2	1:A:16:MET:HE3	2.03	0.41
1:A:206:ARG:HH22	1:A:218:ASP:HB2	1.85	0.41
1:A:74:LEU:HD23	1:A:74:LEU:C	2.41	0.41
1:A:287:LYS:O	1:A:287:LYS:HG2	2.20	0.41
1:A:363:ASN:OD1	1:A:363:ASN:C	2.59	0.41
1:A:22:LYS:O	1:A:22:LYS:HG3	2.20	0.41
1:A:182:GLN:NE2	6:A:874:HOH:O	2.54	0.41
1:A:218:ASP:OD1	1:A:218:ASP:O	2.37	0.41
1:A:547:GLN:CG	1:A:551:LEU:HD21	2.49	0.41
2:B:91:GLN:C	2:B:93:GLY:N	2.71	0.41
2:B:80:LEU:O	2:B:84:THR:HG22	2.21	0.40
2:B:109:LEU:CD2	2:B:206:ARG:HH21	2.29	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:331:LYS:NZ	2:B:364:ASP:OD2	2.46	0.40
1:A:540:LYS:HD3	1:A:540:LYS:HA	1.75	0.40
2:B:197:GLN:HA	2:B:200:THR:CG2	2.51	0.40
2:B:38:CYS:SG	2:B:132:ILE:HD11	2.62	0.40
1:A:68:SER:OG	1:A:69:THR:N	2.54	0.40
2:B:265:ASN:HB3	6:B:473:HOH:O	2.21	0.40
2:B:356:ARG:HA	2:B:356:ARG:HD3	1.83	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	552/557 (99%)	528 (96%)	21 (4%)	3 (0%)	29	15
2	B	408/428 (95%)	391 (96%)	15 (4%)	2 (0%)	29	15
All	All	960/985 (98%)	919 (96%)	36 (4%)	5 (0%)	29	15

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	545	ASN
2	B	195	ILE
1	A	217	PRO
1	A	93	GLY
2	B	170	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	494/495 (100%)	484 (98%)	10 (2%)	55	44
2	B	374/390 (96%)	356 (95%)	18 (5%)	25	11
All	All	868/885 (98%)	840 (97%)	28 (3%)	39	25

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	GLU
1	A	69	THR
1	A	184	MET
1	A	211	ARG
1	A	217	PRO
1	A	259	LYS
1	A	290	THR
1	A	394	GLN
1	A	503	LEU
1	A	546	GLU
2	B	8	VAL
2	B	40	GLU
2	B	55	PRO
2	B	87	PHE
2	B	113	ASP
2	B	174	GLN
2	B	195	ILE
2	B	197	GLN
2	B	212	TRP
2	B	214	LEU
2	B	227	PHE
2	B	228	LEU
2	B	233	GLU
2	B	300	GLU
2	B	330	GLN
2	B	410	TRP
2	B	414	TRP
2	B	417	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	197	GLN
1	A	255	ASN
1	A	394	GLN
1	A	475	GLN
1	A	487	GLN
2	B	182	GLN
2	B	242	GLN
2	B	278	GLN
2	B	330	GLN
2	B	334	GLN
2	B	340	GLN
2	B	361	HIS

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	$\# Z > 2$
4	T27	A	557	-	30,30,30	1.63	7 (23%)	39,40,40	1.27	3 (7%)
3	SO4	A	556	-	4,4,4	0.29	0	6,6,6	0.16	0
5	EDO	B	429	-	3,3,3	0.34	0	2,2,2	0.38	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
4	T27	A	557	-	-	2/13/14/14	0/3/3/3
5	EDO	B	429	-	-	0/1/1/1	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	557	T27	C6-C5	3.95	1.46	1.40
4	A	557	T27	C2-C1	3.24	1.44	1.39
4	A	557	T27	C17-C16	2.76	1.43	1.39
4	A	557	T27	C15-C16	2.54	1.43	1.39
4	A	557	T27	C6-C1	2.25	1.43	1.40
4	A	557	T27	C18-C17	2.17	1.42	1.38
4	A	557	T27	C2-C3	2.06	1.43	1.39

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	557	T27	N2-C12-N3	-4.50	122.29	126.55
4	A	557	T27	C9-C10-C11	-3.16	114.69	116.76
4	A	557	T27	C12-N3-C11	2.11	120.48	116.28

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	557	T27	C20-C21-C3-C4
4	A	557	T27	C20-C21-C3-C2

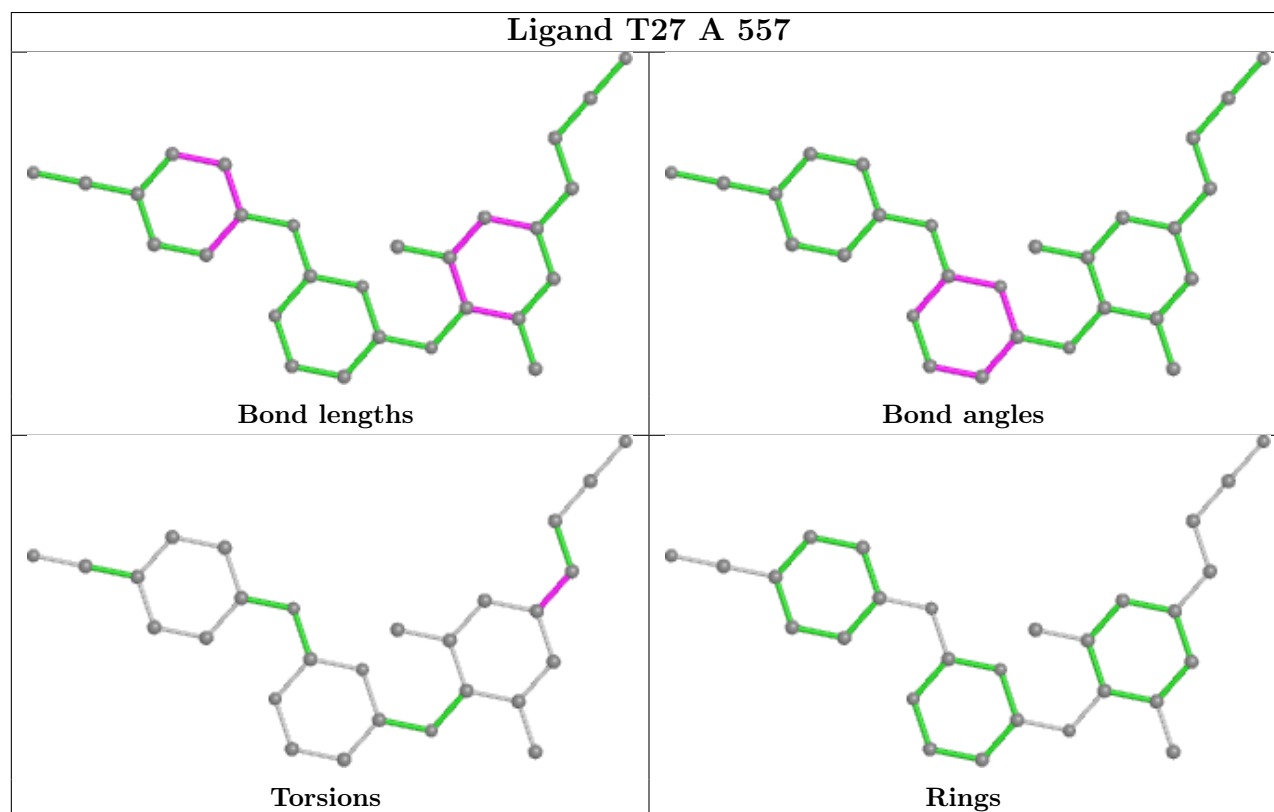
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	557	T27	1	0

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

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	554/557 (99%)	0.03	36 (6%) 18 15	16, 35, 75, 110	0
2	B	412/428 (96%)	0.44	49 (11%) 4 3	18, 37, 88, 106	0
All	All	966/985 (98%)	0.20	85 (8%) 10 7	16, 36, 84, 110	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	92	LEU	10.8
2	B	214	LEU	10.5
2	B	90	VAL	9.2
1	A	67	ASP	8.7
1	A	286	THR	8.3
2	B	93	GLY	8.1
1	A	69	THR	8.1
1	A	551	LEU	7.8
2	B	357	MET	7.4
2	B	240	THR	7.3
1	A	68	SER	6.6
2	B	91	GLN	6.5
1	A	552	VAL	6.2
2	B	358	ARG	5.6
1	A	287	LYS	5.4
1	A	285	GLY	5.4
1	A	544	GLY	5.3
2	B	5	ILE	5.2
2	B	356	ARG	4.9
2	B	88	TRP	4.7
2	B	229	TRP	4.6
1	A	70	LYS	4.4
1	A	24	TRP	4.4
2	B	238	LYS	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	227	PHE	4.4
1	A	284	ARG	4.4
2	B	173	LYS	4.3
1	A	91	GLN	4.0
2	B	212	TRP	3.9
2	B	6	GLU	3.9
2	B	241	VAL	3.8
2	B	87	PHE	3.7
2	B	359	GLY	3.7
1	A	65	LYS	3.7
1	A	222	GLN	3.6
2	B	9	PRO	3.5
1	A	550	LYS	3.5
2	B	95	PRO	3.4
1	A	290	THR	3.4
1	A	64	LYS	3.4
1	A	289	LEU	3.3
1	A	358	ARG	3.2
2	B	237	ASP	3.2
1	A	66	LYS	3.2
2	B	428	GLN	3.2
1	A	220	LYS	3.1
1	A	219	LYS	3.1
2	B	14	PRO	3.1
2	B	361	HIS	3.0
2	B	210	LEU	3.0
2	B	277	ARG	2.9
2	B	170	PRO	2.9
2	B	200	THR	2.9
2	B	69	THR	2.8
2	B	166	LYS	2.8
1	A	292	VAL	2.8
2	B	168	LEU	2.7
1	A	218	ASP	2.7
1	A	72	ARG	2.7
2	B	230	MET	2.7
2	B	206	ARG	2.7
2	B	360	ALA	2.6
1	A	548	VAL	2.6
2	B	209	LEU	2.6
2	B	425	LEU	2.6
2	B	231	GLY	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	193	LEU	2.5
1	A	-1	MET	2.5
2	B	213	GLY	2.5
2	B	85	GLN	2.5
2	B	284	ARG	2.4
1	A	283	LEU	2.4
1	A	295	LEU	2.3
1	A	546	GLU	2.3
2	B	89	GLU	2.3
2	B	174	GLN	2.2
1	A	288	ALA	2.2
2	B	86	ASP	2.2
2	B	228	LEU	2.1
2	B	239	TRP	2.1
1	A	293	ILE	2.1
1	A	449	GLU	2.1
1	A	448	ARG	2.1
1	A	63	ILE	2.0
2	B	7	THR	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](#)

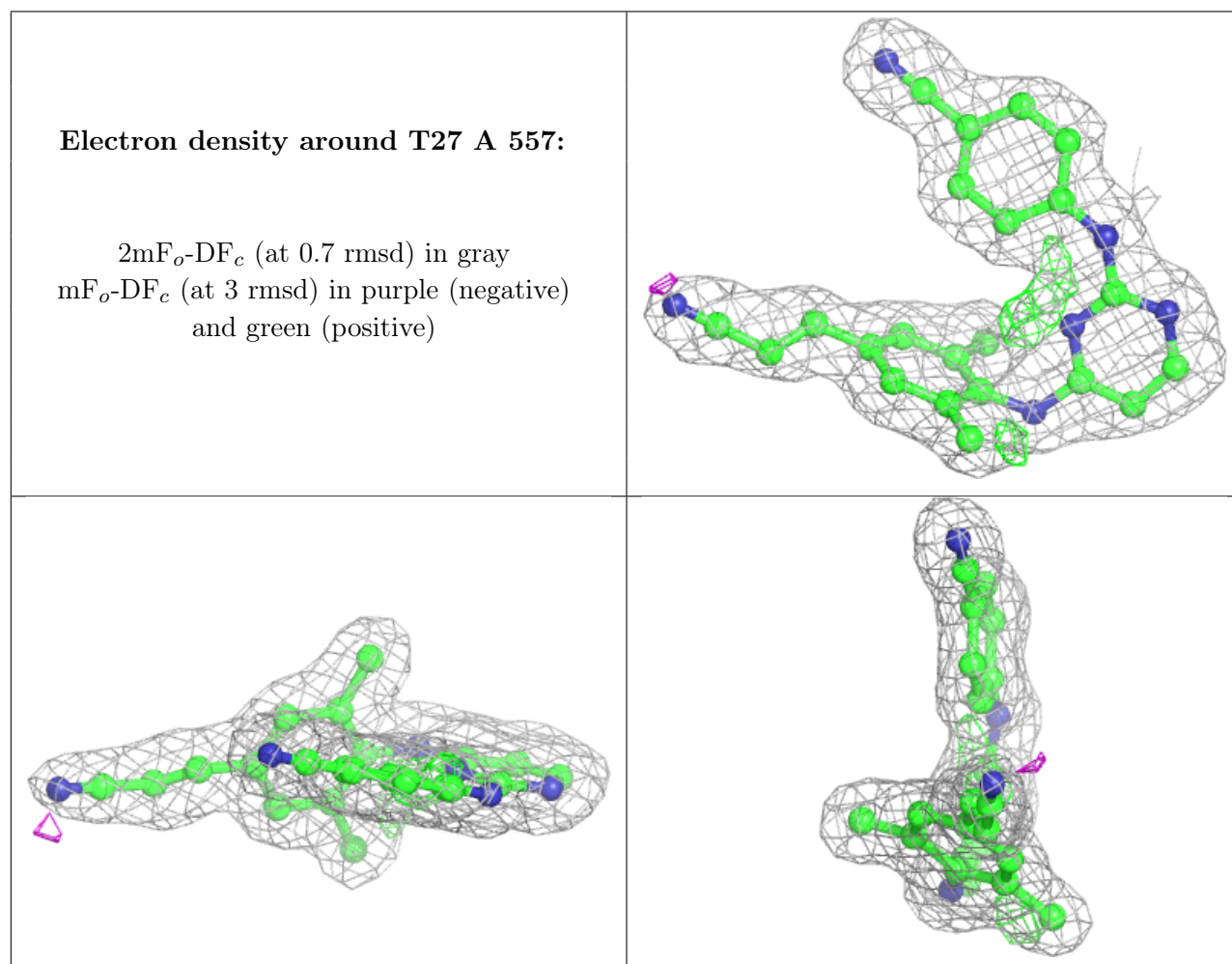
There are no monosaccharides in this entry.

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(\AA^2)	Q<0.9
5	EDO	B	429	4/4	0.85	0.26	46,51,56,59	0
3	SO4	A	556	5/5	0.87	0.15	84,86,88,89	0
4	T27	A	557	28/28	0.95	0.11	19,25,35,44	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.