Full wwPDB X-ray Structure Validation Report ⓘ

Dec 9, 2021 – 05:58 pm GMT

PDB ID	:	7Q1C
Title	:	Crystal structure of Trypanosoma cruzi histone deacetylase DAC2 complexed with a hydroxamate inhibitor
Authors	:	Ramos-Morales, E.; Marek, M.; Romier, C.
Deposited on	:	2021-10-18
Resolution	:	2.30 Å(reported)

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

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

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

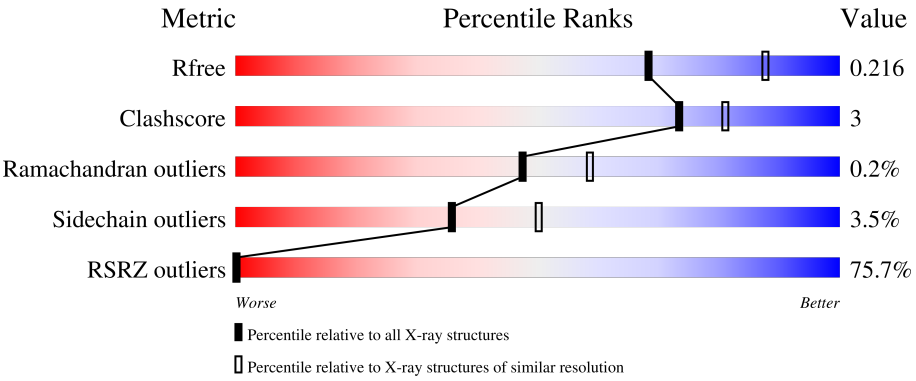
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.24
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.24

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	467	70% 81% 10% • 9%
1	B	467	69% 82% 9% • 9%

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
4	T56	A	504	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6752 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 Histone deacetylase DAC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	427	Total	C	N	O	S	0	2	0
			3251	2079	569	584	19			
1	B	426	Total	C	N	O	S	0	0	0
			3227	2065	561	582	19			

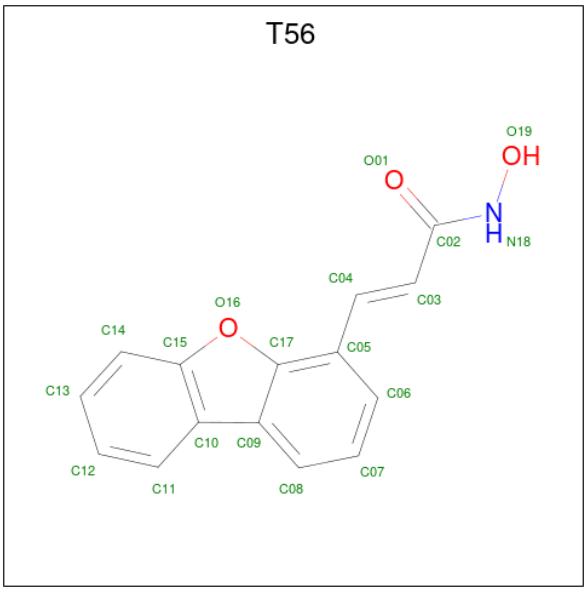
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	K	0	0
			2	2		
3	B	2	Total	K	0	0
			2	2		

- Molecule 4 is (E)-3-dibenzofuran-4-yl-N-oxidanyl-prop-2-enamide (three-letter code: T56) (formula: $C_{15}H_{11}NO_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 19 15 1 3	0	0
4	B	1	Total C N O 19 15 1 3	0	0

- Molecule 5 is water.

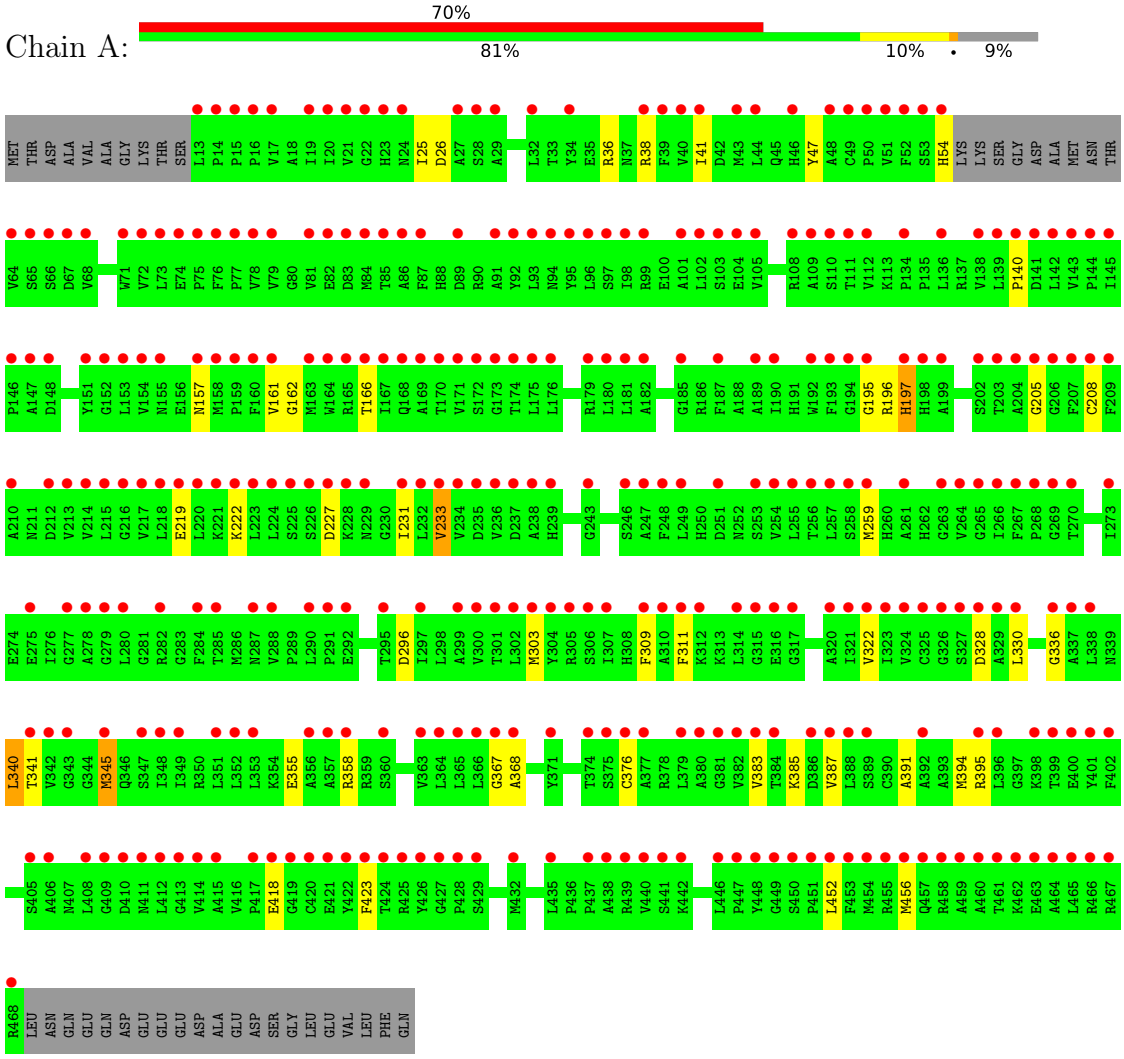
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	109	Total O 109 109	0	0
5	B	121	Total O 121 121	0	0

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.

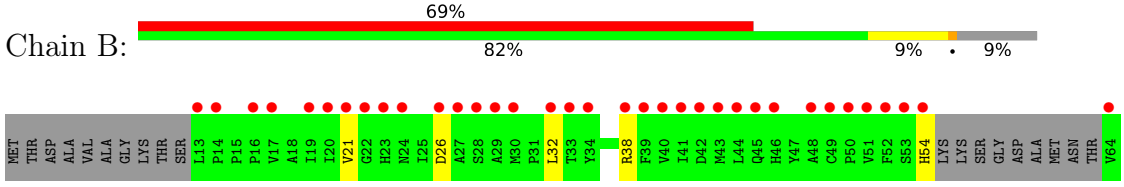
• Molecule 1: Histone deacetylase DAC2

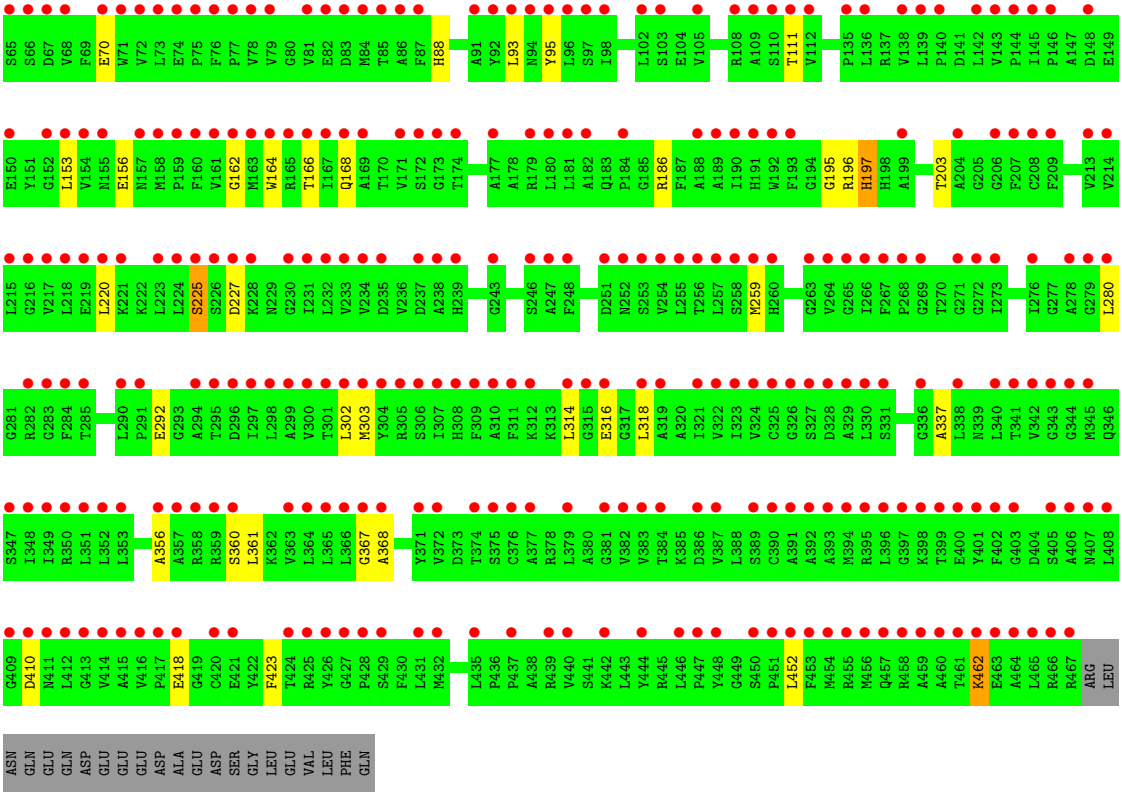
Chain A:



• Molecule 1: Histone deacetylase DAC2

Chain B:




S65 S66 D67 V68 F69 E70 W71 V72 L73 E74 P75 F76 P77 V78 V79 G80 V81 E82 D83 M84 T85 A86 F87 H88 A91 Y92 L93 N94 Y95 L96 S97 I98 L102 S103 E104 V105 R108 A109 S110 T111 V112 P135 L136 R137 V138 L139 P140 D141 L142 V143 P144 I145 P146 A147 D148 E149
E150 Y151 G152 L153 V154 N155 E156 N157 M158 P159 F160 V161 G162 M163 W164 R165 T166 I167 Q168 A169 T170 V171 S172 G173 T174 A177 A178 R179 L180 L181 A182 Q183 P184 G185 R186 F187 A188 A189 I190 H191 W192 F193 G194 G195 R196 H197 H198 A199 T203 A204 G205 G206 F207 C208 F209 V213 V214
L215 G216 V217 L218 E219 L220 K221 K222 L223 L224 S225 S226 D227 K228 N229 G230 I231 L232 V233 V234 D235 V236 D237 A238 H239 G243 S246 A247 F248 D251 N252 S253 V254 L255 T256 L257 S258 M259 H260 G263 V264 G265 I266 F267 P268 G269 T270 G271 G272 I273 I276 G277 A278 G279 L280
G281 R282 G283 F284 T285 L290 P291 E292 G293 A294 T295 D296 I297 L298 A299 V300 T301 L302 M303 Y304 R305 S306 I307 H308 F309 A310 F311 K312 K313 L314 G315 E316 G317 L318 A319 A320 I321 V322 I323 V324 C325 G326 S327 D328 A329 L330 S331 G336 A337 L338 N339 L340 T341 V342 G343 G344 M345 Q346
S347 I348 I349 R350 L351 L352 L353 A356 A357 R358 R359 S360 L361 K362 V363 L364 L365 L366 G367 A368 Y371 V372 D373 T374 S375 C376 A377 R378 L379 A380 G381 V382 V383 T384 K385 D386 V387 L388 S389 C390 A391 A392 A393 M394 R395 L396 G397 K398 T399 E400 Y401 F402 G403 D404 S405 A406 N407 L408
G409 D410 W411 L412 G413 V414 A415 V416 P417 E418 G419 C420 E421 Y422 F423 T424 R425 Y426 G427 P428 S429 F430 L431 M432 L435 P436 P437 A438 R439 V440 S441 K442 L443 Y444 R445 L446 P447 Y448 G449 S450 P451 L452 F453 M454 R455 M456 Q457 R458 A459 A460 T461 K462 E463 A464 L465 R466 R467 ARG LEU
ASN GLN GLU GLN ASP GLU GLU GLU ASP ALA GLU ASP SER GLY LEU GLU VAL LEU PHE GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	66.07Å 95.35Å 96.92Å 90.00° 103.50° 90.00°	Depositor
Resolution (Å)	48.11 – 2.30 48.11 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.11-2.30) 99.8 (48.11-2.30)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.61 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.19rc4_4035, PHENIX 1.19rc4_4035	Depositor
R, R_{free}	0.196 , 0.224 0.188 , 0.216	Depositor DCC
R_{free} test set	2623 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	36.6	Xtriage
Anisotropy	0.526	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6752	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.16% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: T56, ZN, K

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	0.42	0/3330	0.62	0/4519
1	B	0.40	0/3300	0.60	0/4480
All	All	0.41	0/6630	0.61	0/8999

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

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	3251	0	3283	24	0
1	B	3227	0	3251	19	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	19	0	0	0	0
4	B	19	0	0	0	0
5	A	109	0	0	1	0
5	B	121	0	0	3	0
All	All	6752	0	6534	43	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 3.

All (43) 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:355:GLU:OE1	1:A:358:ARG:NH1	2.22	0.73
1:B:70:GLU:OE1	1:B:186:ARG:NH2	2.23	0.72
1:A:26:ASP:OD2	1:A:38:ARG:NH2	2.27	0.67
1:B:156:GLU:OE2	5:B:602:HOH:O	2.14	0.65
1:A:233:VAL:HB	1:A:322:VAL:HG22	1.84	0.58
1:A:196:ARG:NH2	5:A:602:HOH:O	2.25	0.57
1:B:162:GLY:O	1:B:166:THR:HG23	2.04	0.57
1:B:292:GLU:HG3	1:B:337:ALA:HB1	1.87	0.56
1:A:196:ARG:HB3	1:A:208:CYS:HB3	1.88	0.54
1:B:356:ALA:HA	1:B:361:LEU:HD12	1.90	0.54
1:A:162:GLY:O	1:A:166:THR:HG23	2.09	0.53
1:A:47:TYR:CE2	1:A:385:LYS:HD2	2.45	0.52
1:B:225:SER:OG	1:B:227:ASP:OD1	2.28	0.51
1:B:196:ARG:NH1	5:B:607:HOH:O	2.38	0.51
1:B:418:GLU:HA	1:B:423:PHE:CD2	2.46	0.50
1:A:25:ILE:HD11	1:A:38:ARG:HG2	1.97	0.47
1:B:259:MET:HB2	1:B:303:MET:SD	2.54	0.47
1:B:88:HIS:HB2	1:B:93:LEU:HD11	1.97	0.47
1:B:95:TYR:HE2	1:B:153:LEU:HD12	1.79	0.46
1:A:296:ASP:OD2	1:A:341:THR:OG1	2.23	0.46
1:A:140:PRO:HD2	1:A:161:VAL:HB	1.98	0.46
1:B:314:LEU:HD13	1:B:318:LEU:HD12	1.99	0.45
1:A:157:ASN:HD21	1:A:205:GLY:HA2	1.82	0.45
1:A:311:PHE:CZ	1:A:355:GLU:HG2	2.52	0.45
1:B:302:LEU:HD13	1:B:452:LEU:HD21	1.99	0.44
1:B:164:TRP:O	1:B:168:GLN:HG3	2.17	0.44
1:A:197:HIS:H	1:A:197:HIS:CD2	2.35	0.44
1:B:26:ASP:OD2	1:B:38:ARG:NH2	2.25	0.44
1:A:418:GLU:HA	1:A:423:PHE:CD1	2.53	0.43
1:B:337:ALA:N	5:B:601:HOH:O	2.05	0.43
1:A:195:GLY:HA3	1:A:367:GLY:O	2.20	0.42
1:A:259:MET:HB2	1:A:303:MET:SD	2.59	0.42
1:B:195:GLY:HA3	1:B:367:GLY:O	2.20	0.42
1:B:462:LYS:HB3	1:B:462:LYS:HZ2	1.84	0.42
1:A:328:ASP:O	1:A:336:GLY:HA3	2.20	0.41
1:A:383:VAL:O	1:A:387:VAL:HG23	2.21	0.41
1:A:330:LEU:HD21	1:A:345:MET:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:MET:HE2	1:A:394:MET:HB2	1.49	0.41
1:A:340:LEU:N	1:A:340:LEU:HD23	2.36	0.41
1:B:197:HIS:CD2	1:B:197:HIS:H	2.37	0.41
1:A:36:ARG:HD2	1:A:376:CYS:SG	2.61	0.41
1:A:219:GLU:OE1	1:A:222:LYS:HD3	2.21	0.40
1:A:391:ALA:O	1:A:395:ARG:HG2	2.21	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	425/467 (91%)	415 (98%)	9 (2%)	1 (0%)	47	58
1	B	422/467 (90%)	410 (97%)	11 (3%)	1 (0%)	47	58
All	All	847/934 (91%)	825 (97%)	20 (2%)	2 (0%)	47	58

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	368	ALA
1	B	368	ALA

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	343/374 (92%)	332 (97%)	11 (3%)	39	54
1	B	340/374 (91%)	327 (96%)	13 (4%)	33	47
All	All	683/748 (91%)	659 (96%)	24 (4%)	36	50

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	ILE
1	A	54	HIS
1	A	197	HIS
1	A	227	ASP
1	A	231	ILE
1	A	233	VAL
1	A	309	PHE
1	A	340	LEU
1	A	345	MET
1	A	452	LEU
1	A	456	MET
1	B	21	VAL
1	B	32	LEU
1	B	54	HIS
1	B	111	THR
1	B	197	HIS
1	B	203	THR
1	B	220	LEU
1	B	225	SER
1	B	280	LEU
1	B	316	GLU
1	B	360	SER
1	B	410	ASP
1	B	462	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 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	T56	B	504	2	17,21,21	2.60	6 (35%)	20,29,29	1.46	4 (20%)
4	T56	A	504	2	17,21,21	2.45	6 (35%)	20,29,29	1.29	3 (15%)

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	T56	B	504	2	-	2/7/7/7	0/3/3/3
4	T56	A	504	2	-	2/7/7/7	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	504	T56	C02-N18	8.56	1.47	1.33
4	A	504	T56	C02-N18	7.53	1.46	1.33
4	A	504	T56	O01-C02	-3.17	1.18	1.24
4	B	504	T56	O01-C02	-2.98	1.18	1.24
4	A	504	T56	C05-C04	2.78	1.53	1.47
4	A	504	T56	C10-C15	-2.71	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	504	T56	C05-C04	2.64	1.53	1.47
4	A	504	T56	C03-C02	2.64	1.53	1.48
4	A	504	T56	C09-C17	-2.62	1.37	1.43
4	B	504	T56	C03-C02	2.41	1.53	1.48
4	B	504	T56	C10-C15	-2.39	1.38	1.43
4	B	504	T56	C09-C17	-2.07	1.39	1.43

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	504	T56	O19-N18-C02	3.73	128.63	119.62
4	A	504	T56	C05-C04-C03	-3.36	121.68	126.93
4	B	504	T56	C04-C03-C02	-2.90	115.90	121.56
4	B	504	T56	C05-C04-C03	-2.69	122.72	126.93
4	A	504	T56	O19-N18-C02	2.44	125.50	119.62
4	A	504	T56	C03-C02-N18	2.30	118.96	114.38
4	B	504	T56	C06-C05-C04	-2.24	117.22	120.64

There are no chirality outliers.

All (4) torsion outliers are listed below:

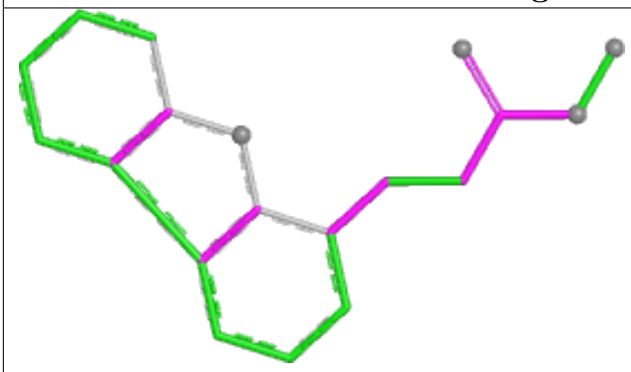
Mol	Chain	Res	Type	Atoms
4	A	504	T56	N18-C02-C03-C04
4	B	504	T56	N18-C02-C03-C04
4	A	504	T56	O01-C02-C03-C04
4	B	504	T56	O01-C02-C03-C04

There are no ring outliers.

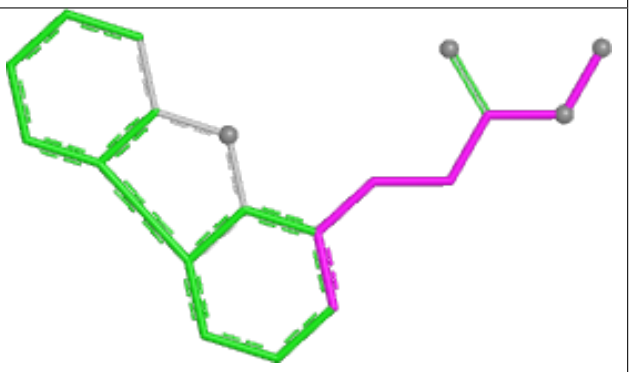
No monomer is involved in short contacts.

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.

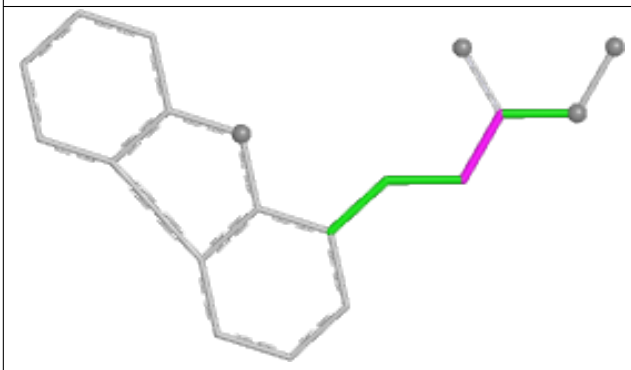
Ligand T56 B 504



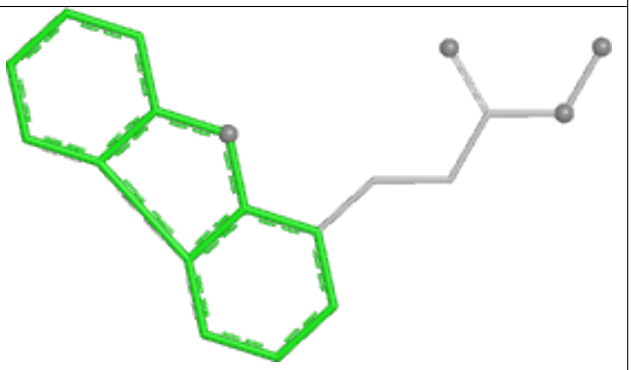
Bond lengths



Bond angles

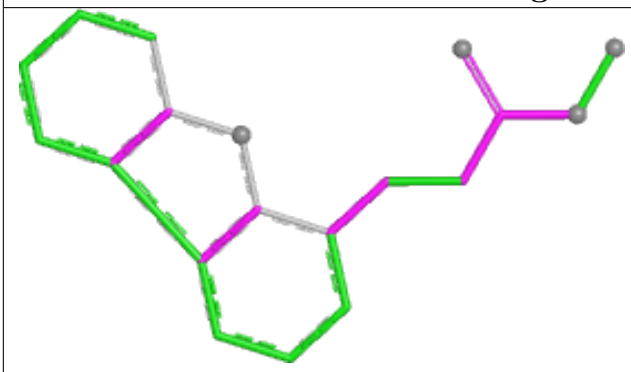


Torsions

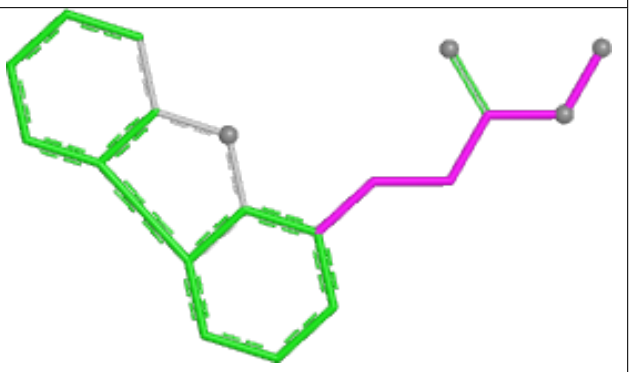


Rings

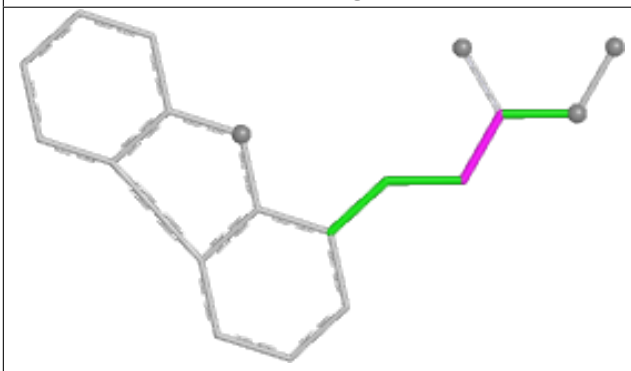
Ligand T56 A 504



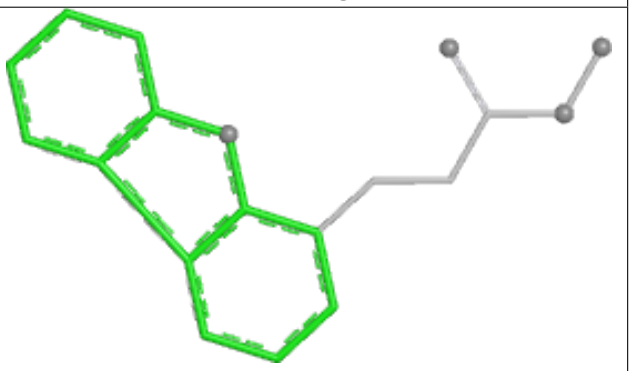
Bond lengths



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.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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, 95^{th} 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	427/467 (91%)	2.92	325 (76%)	0	0	28, 39, 72, 127	0
1	B	426/467 (91%)	3.03	321 (75%)	0	0	29, 41, 77, 118	0
All	All	853/934 (91%)	2.98	646 (75%)	0	0	28, 40, 75, 127	0

All (646) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	460	ALA	12.3
1	A	465	LEU	11.9
1	B	465	LEU	11.7
1	A	464	ALA	10.7
1	B	64	VAL	10.0
1	B	463	GLU	9.9
1	A	459	ALA	9.8
1	B	461	THR	9.4
1	A	467	ARG	9.4
1	A	461	THR	9.2
1	B	460	ALA	8.4
1	B	226	SER	7.8
1	B	466	ARG	7.8
1	A	264	VAL	7.7
1	B	280	LEU	7.2
1	B	396	LEU	7.1
1	A	226	SER	7.0
1	B	399	THR	7.0
1	B	110	SER	6.8
1	A	64	VAL	6.7
1	B	464	ALA	6.7
1	B	279	GLY	6.7
1	B	54	HIS	6.6
1	B	410	ASP	6.6

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Mol	Chain	Res	Type	RSRZ
1	A	463	GLU	6.4
1	B	459	ALA	6.4
1	A	74	GLU	6.3
1	B	412	LEU	6.3
1	B	227	ASP	6.2
1	B	108	ARG	6.2
1	B	213	VAL	6.1
1	B	217	VAL	6.0
1	A	466	ARG	6.0
1	A	217	VAL	5.9
1	A	110	SER	5.9
1	A	227	ASP	5.8
1	A	82	GLU	5.7
1	B	75	PRO	5.6
1	A	468	ARG	5.6
1	A	280	LEU	5.6
1	B	264	VAL	5.5
1	B	418	GLU	5.5
1	A	214	VAL	5.5
1	B	352	LEU	5.5
1	A	412	LEU	5.5
1	B	76	PHE	5.4
1	B	383	VAL	5.4
1	A	456	MET	5.4
1	B	462	LYS	5.4
1	B	299	ALA	5.4
1	A	410	ASP	5.3
1	B	414	VAL	5.3
1	B	83	ASP	5.3
1	A	83	ASP	5.3
1	A	167	ILE	5.2
1	B	223	LEU	5.2
1	B	448	TYR	5.1
1	A	76	PHE	5.1
1	B	172	SER	5.1
1	A	349	ILE	5.0
1	A	309	PHE	5.0
1	B	218	LEU	5.0
1	B	348	ILE	5.0
1	B	14	PRO	4.9
1	A	413	GLY	4.9
1	A	49	CYS	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	108	ARG	4.9
1	B	351	LEU	4.9
1	B	112	VAL	4.9
1	B	312	LYS	4.8
1	A	462	LYS	4.8
1	A	225	SER	4.8
1	B	413	GLY	4.8
1	B	214	VAL	4.8
1	A	219	GLU	4.8
1	B	136	LEU	4.8
1	A	78	VAL	4.8
1	A	54	HIS	4.8
1	B	398	LYS	4.8
1	A	326	GLY	4.8
1	B	67	ASP	4.7
1	B	216	GLY	4.7
1	A	48	ALA	4.7
1	A	112	VAL	4.7
1	B	189	ALA	4.7
1	B	53	SER	4.6
1	B	391	ALA	4.6
1	A	458	ARG	4.6
1	B	458	ARG	4.6
1	B	400	GLU	4.6
1	A	160	PHE	4.6
1	B	376	CYS	4.5
1	B	467	ARG	4.5
1	B	22	GLY	4.5
1	A	387	VAL	4.5
1	B	51	VAL	4.5
1	B	23	HIS	4.5
1	A	414	VAL	4.5
1	B	323	ILE	4.5
1	B	457	GLN	4.5
1	B	298	LEU	4.5
1	B	440	VAL	4.5
1	B	322	VAL	4.4
1	B	363	VAL	4.4
1	B	420	CYS	4.4
1	A	32	LEU	4.4
1	A	452	LEU	4.4
1	B	161	VAL	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	448	TYR	4.4
1	A	324	VAL	4.3
1	A	457	GLN	4.3
1	B	41	ILE	4.3
1	A	317	GLY	4.3
1	A	383	VAL	4.3
1	B	94	ASN	4.3
1	A	303	MET	4.3
1	B	43	MET	4.3
1	B	65	SER	4.3
1	B	360	SER	4.2
1	A	22	GLY	4.2
1	A	353	LEU	4.2
1	A	265	GLY	4.2
1	B	304	TYR	4.2
1	A	382	VAL	4.2
1	B	349	ILE	4.2
1	A	75	PRO	4.1
1	A	73	LEU	4.1
1	B	446	LEU	4.1
1	A	420	CYS	4.1
1	B	316	GLU	4.1
1	B	265	GLY	4.1
1	A	282	ARG	4.1
1	B	77	PRO	4.1
1	A	193	PHE	4.1
1	B	257	LEU	4.1
1	A	91	ALA	4.1
1	A	299	ALA	4.1
1	A	352	LEU	4.1
1	A	41	ILE	4.1
1	B	342	VAL	4.1
1	B	24	ASN	4.1
1	A	102	LEU	4.1
1	B	44	LEU	4.1
1	B	366	LEU	4.0
1	A	207	PHE	4.0
1	B	48	ALA	4.0
1	B	146	PRO	4.0
1	B	309	PHE	4.0
1	B	193	PHE	4.0
1	A	254	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	234	VAL	4.0
1	B	232	LEU	4.0
1	A	154	VAL	4.0
1	A	213	VAL	4.0
1	A	323	ILE	3.9
1	B	263	GLY	3.9
1	A	185	GLY	3.9
1	B	381	GLY	3.9
1	A	13	LEU	3.9
1	B	91	ALA	3.9
1	B	415	ALA	3.9
1	B	13	LEU	3.9
1	A	23	HIS	3.9
1	A	171	VAL	3.9
1	B	382	VAL	3.9
1	B	303	MET	3.9
1	A	95	TYR	3.9
1	B	255	LEU	3.9
1	A	161	VAL	3.9
1	A	96	LEU	3.9
1	A	221	LYS	3.8
1	B	315	GLY	3.8
1	B	411	ASN	3.8
1	B	73	LEU	3.8
1	B	207	PHE	3.8
1	B	387	VAL	3.8
1	B	180	LEU	3.8
1	B	220	LEU	3.8
1	A	77	PRO	3.8
1	B	184	PRO	3.8
1	A	395	ARG	3.8
1	B	379	LEU	3.8
1	A	375	SER	3.8
1	B	456	MET	3.8
1	A	139	LEU	3.8
1	B	307	ILE	3.7
1	A	142	LEU	3.7
1	A	304	TYR	3.7
1	A	311	PHE	3.7
1	B	74	GLU	3.7
1	A	229	ASN	3.7
1	A	450	SER	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	146	PRO	3.7
1	A	357	ALA	3.7
1	A	233	VAL	3.7
1	B	408	LEU	3.7
1	A	68	VAL	3.7
1	B	302	LEU	3.7
1	A	310	ALA	3.7
1	B	426	TYR	3.7
1	A	454	MET	3.7
1	B	215	LEU	3.7
1	B	49	CYS	3.6
1	B	96	LEU	3.6
1	B	390	CYS	3.6
1	A	222	LYS	3.6
1	B	384	THR	3.6
1	A	453	PHE	3.6
1	A	17	VAL	3.6
1	A	145	ILE	3.6
1	B	66	SER	3.6
1	B	50	PRO	3.6
1	B	225	SER	3.6
1	B	377	ALA	3.6
1	B	425	ARG	3.6
1	B	290	LEU	3.6
1	A	153	LEU	3.6
1	A	175	LEU	3.6
1	B	405	SER	3.6
1	A	379	LEU	3.6
1	A	87	PHE	3.5
1	B	453	PHE	3.5
1	B	450	SER	3.5
1	B	297	ILE	3.5
1	B	353	LEU	3.5
1	B	428	PRO	3.5
1	B	395	ARG	3.5
1	A	279	GLY	3.5
1	B	17	VAL	3.5
1	A	418	GLU	3.5
1	B	177	ALA	3.5
1	A	44	LEU	3.5
1	B	79	VAL	3.5
1	B	282	ARG	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	342	VAL	3.5
1	B	81	VAL	3.5
1	A	111	THR	3.5
1	A	182	ALA	3.5
1	A	237	ASP	3.5
1	A	440	VAL	3.5
1	B	154	VAL	3.5
1	A	220	LEU	3.4
1	A	348	ILE	3.4
1	A	21	VAL	3.4
1	A	164	TRP	3.4
1	A	266	ILE	3.4
1	B	32	LEU	3.4
1	B	364	LEU	3.4
1	A	65	SER	3.4
1	A	247	ALA	3.4
1	B	109	ALA	3.4
1	A	43	MET	3.4
1	A	302	LEU	3.4
1	A	398	LYS	3.4
1	B	326	GLY	3.4
1	B	454	MET	3.4
1	B	27	ALA	3.4
1	B	394	MET	3.4
1	B	340	LEU	3.4
1	B	324	VAL	3.3
1	A	97	SER	3.3
1	A	384	THR	3.3
1	A	81	VAL	3.3
1	A	389	SER	3.3
1	B	392	ALA	3.3
1	B	356	ALA	3.3
1	B	393	ALA	3.3
1	B	19	ILE	3.3
1	A	246	SER	3.3
1	A	316	GLU	3.3
1	B	330	LEU	3.3
1	B	402	PHE	3.3
1	B	300	VAL	3.3
1	B	386	ASP	3.3
1	A	268	PRO	3.3
1	B	233	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	278	ALA	3.2
1	A	411	ASN	3.2
1	A	159	PRO	3.2
1	A	447	PRO	3.2
1	B	417	PRO	3.2
1	B	311	PHE	3.2
1	A	109	ALA	3.2
1	B	406	ALA	3.2
1	A	338	LEU	3.2
1	A	151	TYR	3.2
1	B	143	VAL	3.2
1	A	399	THR	3.2
1	A	140	PRO	3.2
1	A	136	LEU	3.2
1	A	366	LEU	3.2
1	A	380	ALA	3.2
1	A	92	TYR	3.2
1	B	138	VAL	3.2
1	B	314	LEU	3.2
1	A	216	GLY	3.2
1	B	92	TYR	3.2
1	B	424	THR	3.2
1	A	51	VAL	3.2
1	A	405	SER	3.2
1	B	98	ILE	3.1
1	B	301	THR	3.1
1	B	437	PRO	3.1
1	A	158	MET	3.1
1	B	139	LEU	3.1
1	A	341	THR	3.1
1	A	358	ARG	3.1
1	B	190	ILE	3.1
1	B	321	ILE	3.1
1	A	322	VAL	3.1
1	B	171	VAL	3.1
1	A	218	LEU	3.1
1	B	325	CYS	3.1
1	B	82	GLU	3.1
1	A	190	ILE	3.1
1	B	173	GLY	3.1
1	B	204	ALA	3.1
1	B	256	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	407	ASN	3.1
1	B	160	PHE	3.1
1	A	439[A]	ARG	3.1
1	A	103	SER	3.1
1	B	285	THR	3.1
1	B	338	LEU	3.1
1	A	231	ILE	3.1
1	A	427	GLY	3.1
1	A	376	CYS	3.1
1	B	231	ILE	3.1
1	A	386	ASP	3.0
1	A	66	SER	3.0
1	B	221	LYS	3.0
1	A	257	LEU	3.0
1	B	158	MET	3.0
1	A	38	ARG	3.0
1	A	147	ALA	3.0
1	B	157	ASN	3.0
1	A	180	LEU	3.0
1	A	455	ARG	3.0
1	A	192	TRP	3.0
1	A	173	GLY	3.0
1	A	98	ILE	3.0
1	B	20	ILE	3.0
1	B	167	ILE	3.0
1	A	209	PHE	3.0
1	B	254	VAL	3.0
1	B	230	GLY	3.0
1	A	437	PRO	3.0
1	B	159	PRO	3.0
1	A	163	MET	3.0
1	A	351	LEU	3.0
1	A	429	SER	3.0
1	A	206	GLY	3.0
1	A	39	PHE	3.0
1	B	291	PRO	3.0
1	A	157	ASN	3.0
1	A	312	LYS	3.0
1	A	401	TYR	2.9
1	A	202	SER	2.9
1	A	166	THR	2.9
1	B	341	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	422	TYR	2.9
1	A	446	LEU	2.9
1	B	30	MET	2.9
1	B	371	TYR	2.9
1	B	435	LEU	2.9
1	B	247	ALA	2.9
1	A	263	GLY	2.9
1	B	447	PRO	2.9
1	A	138	VAL	2.9
1	B	145	ILE	2.9
1	A	402	PHE	2.9
1	B	284	PHE	2.9
1	A	347	SER	2.9
1	B	253	SER	2.9
1	B	375	SER	2.9
1	B	206	GLY	2.9
1	A	34	TYR	2.9
1	A	320	ALA	2.9
1	B	308	HIS	2.9
1	A	424	THR	2.9
1	A	234	VAL	2.9
1	A	300	VAL	2.9
1	B	452	LEU	2.9
1	A	14	PRO	2.9
1	B	421	GLU	2.9
1	A	270	THR	2.9
1	B	39	PHE	2.9
1	A	94[A]	ASN	2.9
1	A	400	GLU	2.9
1	B	163	MET	2.9
1	A	89	ASP	2.9
1	A	212	ASP	2.9
1	B	237	ASP	2.9
1	B	328	ASP	2.9
1	A	253	SER	2.8
1	B	272	GLY	2.8
1	B	228	LYS	2.8
1	A	325	CYS	2.8
1	A	273	ILE	2.8
1	A	441	SER	2.8
1	B	105	VAL	2.8
1	A	101	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	203	THR	2.8
1	A	243	GLY	2.8
1	A	381	GLY	2.8
1	B	427	GLY	2.8
1	A	321	ILE	2.8
1	A	278	ALA	2.8
1	A	438	ALA	2.8
1	A	315	GLY	2.8
1	B	327	SER	2.8
1	B	169	ALA	2.8
1	B	357	ALA	2.8
1	A	215	LEU	2.8
1	B	258	SER	2.8
1	A	417	PRO	2.8
1	B	224	LEU	2.8
1	A	371	TYR	2.8
1	A	71	TRP	2.8
1	A	189	ALA	2.7
1	A	261	ALA	2.7
1	A	29	ALA	2.7
1	B	78	VAL	2.7
1	A	84	MET	2.7
1	A	327	SER	2.7
1	B	192	TRP	2.7
1	B	142	LEU	2.7
1	A	19	ILE	2.7
1	B	152	GLY	2.7
1	B	68	VAL	2.7
1	B	102	LEU	2.7
1	A	205	GLY	2.7
1	B	336	GLY	2.7
1	A	15	PRO	2.7
1	B	153	LEU	2.7
1	A	345	MET	2.7
1	B	259	MET	2.7
1	A	144	PRO	2.7
1	B	103	SER	2.7
1	B	358	ARG	2.7
1	A	79	VAL	2.7
1	A	224	LEU	2.7
1	A	255	LEU	2.7
1	A	290	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	181	LEU	2.7
1	A	449	GLY	2.7
1	B	164	TRP	2.6
1	A	168	GLN	2.6
1	B	111	THR	2.6
1	B	439	ARG	2.6
1	A	134	PRO	2.6
1	A	20	ILE	2.6
1	A	284	PHE	2.6
1	B	219	GLU	2.6
1	B	416	VAL	2.6
1	A	53	SER	2.6
1	B	28	SER	2.6
1	A	155	ASN	2.6
1	B	29	ALA	2.6
1	B	182	ALA	2.6
1	A	28	SER	2.6
1	A	93	LEU	2.6
1	A	181	LEU	2.6
1	B	95	TYR	2.6
1	B	268	PRO	2.6
1	A	425	ARG	2.6
1	A	210	ALA	2.6
1	B	294	ALA	2.6
1	B	71	TRP	2.6
1	B	306	SER	2.6
1	A	232	LEU	2.6
1	A	169	ALA	2.6
1	B	329	ALA	2.6
1	B	276	ILE	2.6
1	A	360	SER	2.6
1	A	236	VAL	2.6
1	A	343	GLY	2.6
1	A	406	ALA	2.6
1	A	170	THR	2.5
1	A	179	ARG	2.5
1	A	328	ASP	2.5
1	B	34	TYR	2.5
1	A	24	ASN	2.5
1	A	377	ALA	2.5
1	A	195	GLY	2.5
1	B	21	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	246	SER	2.5
1	B	347	SER	2.5
1	A	85	THR	2.5
1	B	85	THR	2.5
1	A	421	GLU	2.5
1	B	296	ASP	2.5
1	A	367	GLY	2.5
1	B	93	LEU	2.5
1	B	165	ARG	2.5
1	A	40	VAL	2.5
1	A	172	SER	2.5
1	B	401	TYR	2.5
1	B	168	GLN	2.5
1	A	306	SER	2.5
1	A	415	ALA	2.5
1	A	208	CYS	2.5
1	B	252	ASN	2.5
1	B	248	PHE	2.5
1	A	256	THR	2.5
1	A	148	ASP	2.5
1	B	368	ALA	2.4
1	A	50	PRO	2.4
1	B	135	PRO	2.4
1	B	374	THR	2.4
1	B	451	PRO	2.4
1	A	228	LYS	2.4
1	A	285	THR	2.4
1	B	191	HIS	2.4
1	B	235	ASP	2.4
1	A	165	ARG	2.4
1	A	388	LEU	2.4
1	A	27	ALA	2.4
1	A	197	HIS	2.4
1	A	288	VAL	2.4
1	B	72	VAL	2.4
1	A	104	GLU	2.4
1	A	297	ILE	2.4
1	A	307	ILE	2.4
1	A	259	MET	2.4
1	A	392	ALA	2.4
1	B	199	ALA	2.4
1	B	283	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	72	VAL	2.4
1	B	179	ARG	2.4
1	B	155	ASN	2.4
1	A	86	ALA	2.4
1	B	269	GLY	2.4
1	B	455	ARG	2.4
1	B	16	PRO	2.4
1	A	374	THR	2.4
1	A	269	GLY	2.4
1	A	238	ALA	2.4
1	A	368	ALA	2.4
1	A	105	VAL	2.4
1	B	87	PHE	2.4
1	B	140	PRO	2.3
1	B	166	THR	2.3
1	B	174	THR	2.3
1	B	40	VAL	2.3
1	B	150	GLU	2.3
1	B	444	TYR	2.3
1	A	396	LEU	2.3
1	B	359	ARG	2.3
1	A	409	GLY	2.3
1	A	291	PRO	2.3
1	A	314	LEU	2.3
1	A	258	SER	2.3
1	A	330	LEU	2.3
1	A	46	HIS	2.3
1	A	248	PHE	2.3
1	B	260	HIS	2.3
1	B	305	ARG	2.3
1	B	26	ASP	2.3
1	B	148	ASP	2.3
1	A	364	LEU	2.3
1	B	295	THR	2.3
1	A	194	GLY	2.3
1	A	99	ARG	2.3
1	A	363	VAL	2.3
1	B	251	ASP	2.3
1	A	365	LEU	2.2
1	B	431	LEU	2.2
1	B	38	ARG	2.2
1	B	350	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	208	CYS	2.2
1	A	287	ASN	2.2
1	B	442	LYS	2.2
1	B	52	PHE	2.2
1	B	429	SER	2.2
1	A	204	ALA	2.2
1	B	343	GLY	2.2
1	A	198	HIS	2.2
1	B	70	GLU	2.2
1	A	329	ALA	2.2
1	B	273	ILE	2.2
1	B	318	LEU	2.2
1	A	143	VAL	2.2
1	A	423	PHE	2.2
1	A	235	ASP	2.2
1	A	295	THR	2.2
1	B	42	ASP	2.2
1	B	86	ALA	2.2
1	B	238	ALA	2.2
1	B	319	ALA	2.2
1	A	239	HIS	2.2
1	A	223	LEU	2.2
1	A	249	LEU	2.2
1	A	408	LEU	2.2
1	B	84	MET	2.2
1	A	336	GLY	2.2
1	B	162	GLY	2.2
1	B	271	GLY	2.2
1	B	344	GLY	2.2
1	A	337	ALA	2.2
1	B	45	GLN	2.2
1	B	239	HIS	2.2
1	A	435	LEU	2.2
1	A	426	TYR	2.2
1	B	389	SER	2.2
1	B	267	PHE	2.2
1	B	46	HIS	2.2
1	A	16	PRO	2.2
1	B	331	SER	2.2
1	A	277	GLY	2.2
1	B	367	GLY	2.2
1	B	397	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	187	PHE	2.1
1	A	267	PHE	2.1
1	A	199	ALA	2.1
1	B	33	THR	2.1
1	A	428	PRO	2.1
1	B	144	PRO	2.1
1	A	432	MET	2.1
1	B	243	GLY	2.1
1	A	301	THR	2.1
1	A	251	ASP	2.1
1	B	97	SER	2.1
1	A	442	LYS	2.1
1	A	141	ASP	2.1
1	A	275	GLU	2.1
1	A	451	PRO	2.1
1	B	266	ILE	2.1
1	B	365	LEU	2.1
1	A	356	ALA	2.1
1	A	419	GLY	2.1
1	A	67	ASP	2.1
1	B	372	VAL	2.1
1	A	52	PHE	2.1
1	B	345	MET	2.0
1	B	432	MET	2.0
1	A	174	THR	2.0
1	A	152	GLY	2.0
1	B	403	GLY	2.0
1	A	305	ARG	2.0
1	B	209	PHE	2.0
1	B	310	ALA	2.0
1	A	176	LEU	2.0
1	A	292	GLU	2.0
1	B	409	GLY	2.0
1	B	188	ALA	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)

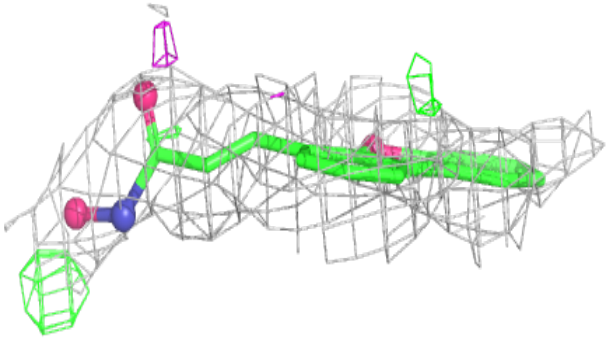
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

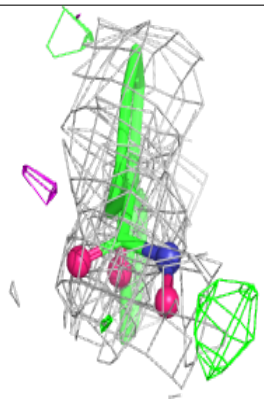
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	T56	A	504	19/19	0.56	0.42	46,87,110,111	0
4	T56	B	504	19/19	0.66	0.31	44,51,72,72	0
2	ZN	A	501	1/1	0.94	0.17	50,50,50,50	0
2	ZN	B	501	1/1	0.96	0.08	54,54,54,54	0
3	K	B	503	1/1	0.96	0.12	37,37,37,37	0
3	K	B	502	1/1	0.97	0.16	32,32,32,32	0
3	K	A	503	1/1	0.98	0.13	38,38,38,38	0
3	K	A	502	1/1	0.99	0.17	28,28,28,28	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 T56 A 504:

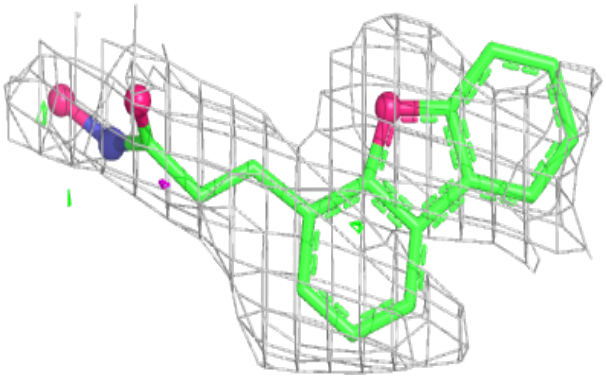
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

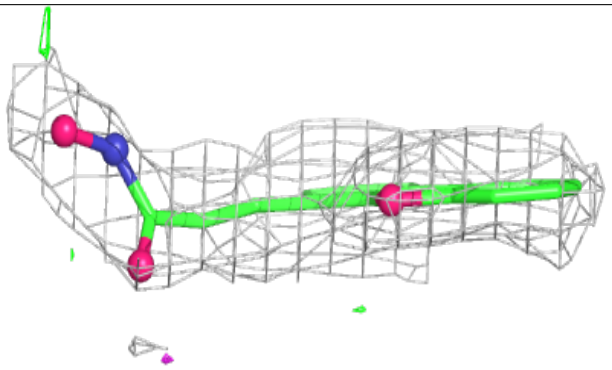


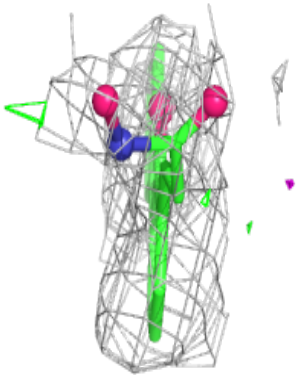


Electron density around T56 B 504:

$2mF_o$-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.