Full wwPDB X-ray Structure Validation Report ⓘ

Oct 30, 2023 – 05:35 PM EDT

PDB ID	:	8U6E
Title	:	Crystal Structure of HIV-1 Reverse Transcriptase in Complex with N-(4-chloro-3-(3-chloro-5-cyanophenoxy)phenethyl)-N-methylacrylamide (JLJ738), a non-nucleoside inhibitor
Authors	:	Prucha, G.; Henry, S.; Jorgensen, W.L.; Anderson, K.S.
Deposited on	:	2023-09-13
Resolution	:	2.31 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 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:

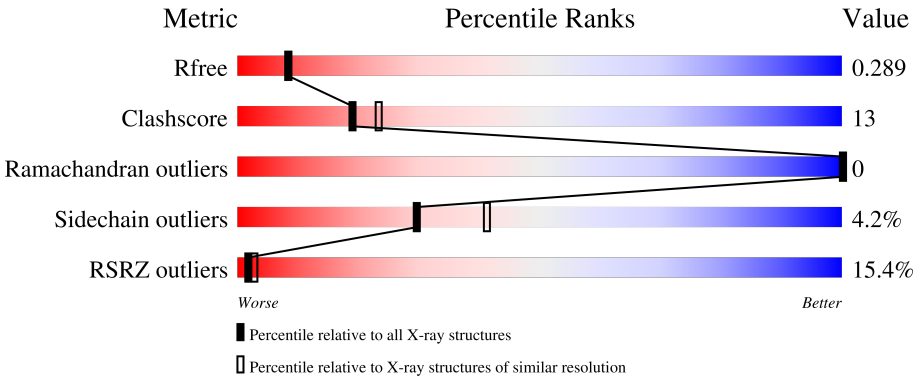
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.31 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	557	18% 70% 25%
2	B	428	11% 68% 26% 5%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7453 atoms, of which 16 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	541	Total	C	N	O	S	0	2	0
			4154	2684	691	771	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

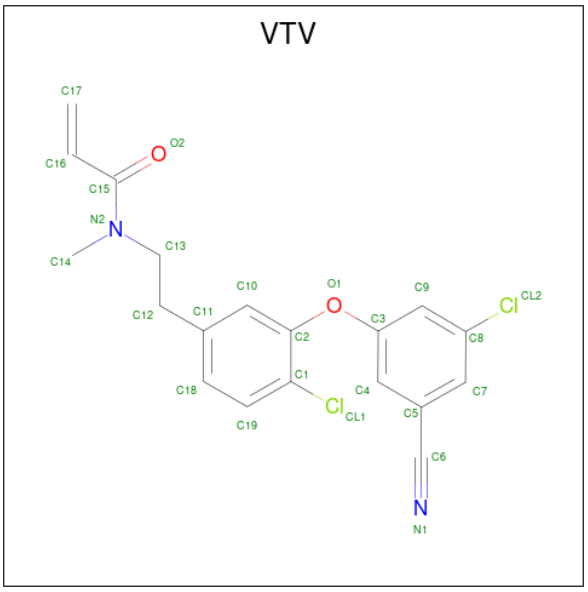
- Molecule 2 is a protein called p51 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	405	Total	C	N	O	S	0	1	0
			3229	2101	535	588	5			

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 N-{2-[4-chloro-3-(3-chloro-5-cyanophenoxy)phenyl]ethyl}-N-methylprop-2-enamide (three-letter code: VTV) (formula: $C_{19}H_{16}Cl_2N_2O_2$) (labeled as "Ligand of Interest" by depositor).

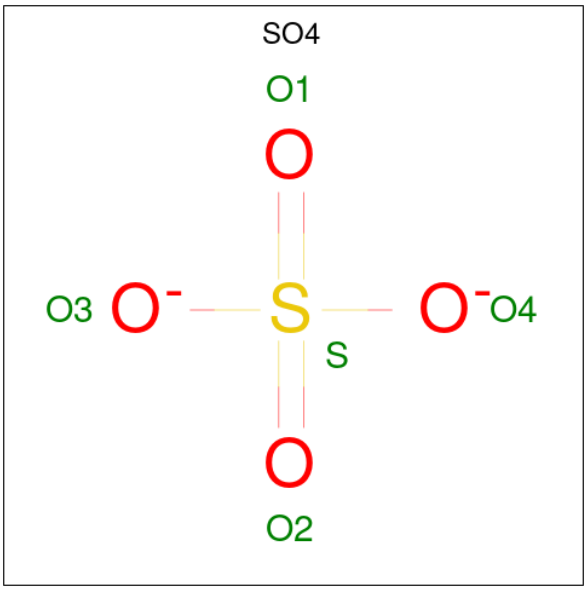


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Cl	H	N	O	0	0
			41	19	2	16	2	2		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 6 is water.

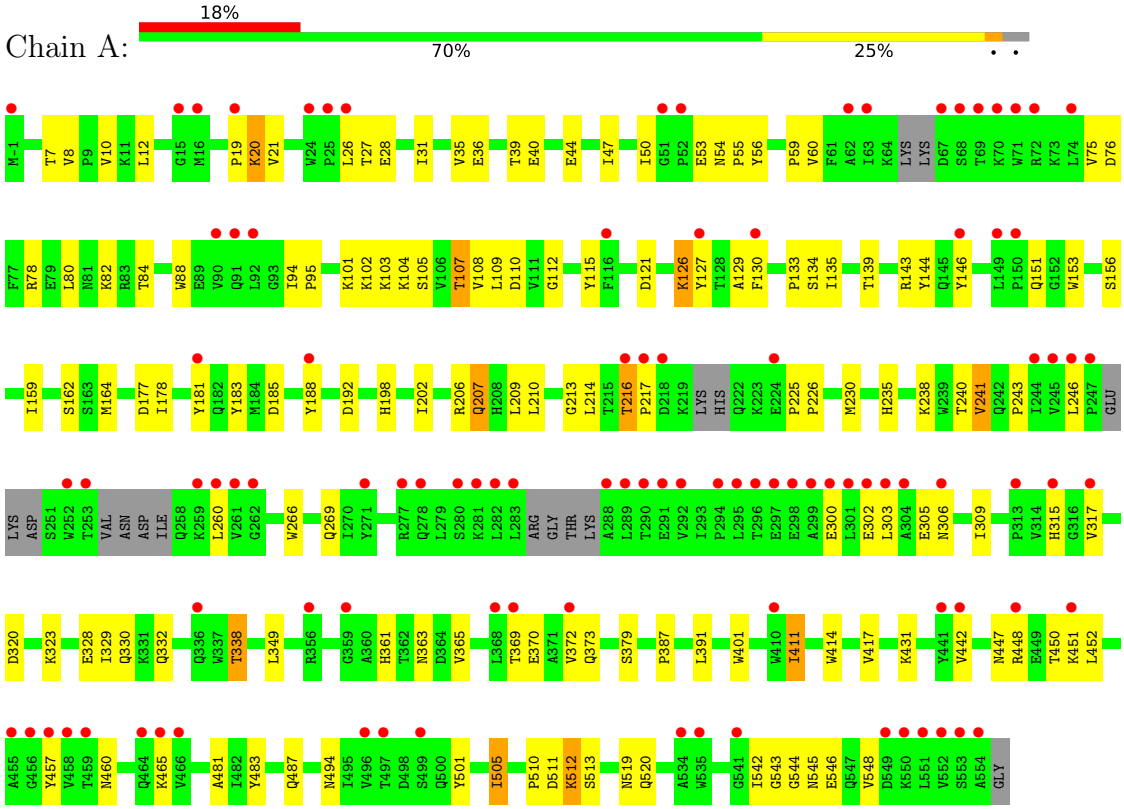
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	16	Total O 16 16	0	0
6	B	7	Total O 7 7	0	0

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.

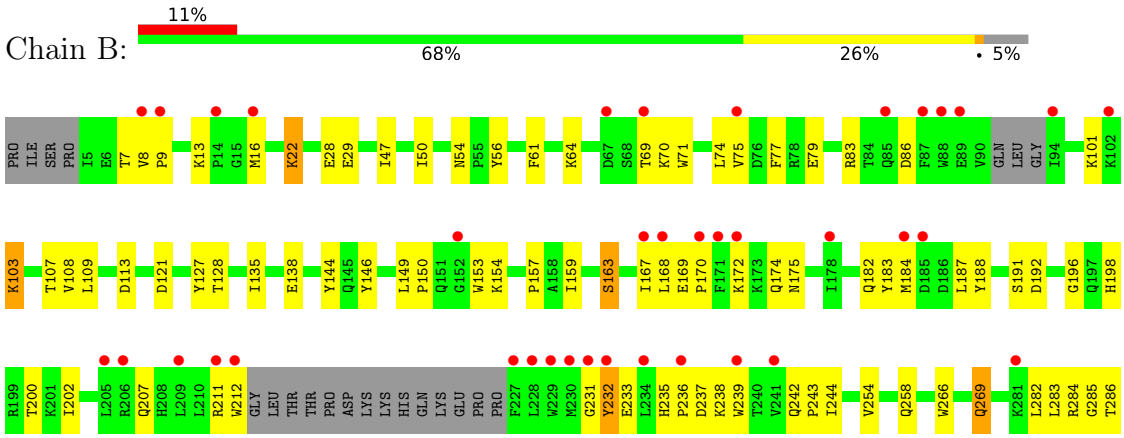
• Molecule 1: Reverse transcriptase/ribonuclease H

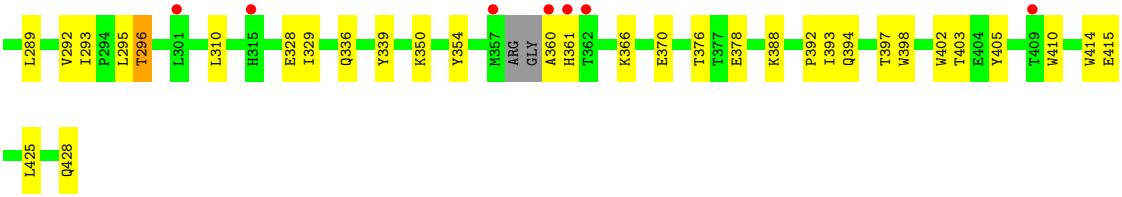
Chain A:



• Molecule 2: p51 RT

Chain B:




L289
V292
I293
P294
L295
T296
L301
L310
H315
E328
I329
Q336
Y339
K350
Y354
M357
ARG
GLY
A360
H361
T362
K366
E370
T376
T377
E378
K388
P392
I393
Q394
T397
W398
W402
T403
E404
Y405
T409
W410
W414
E415
L425
Q428

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	163.37Å 74.02Å 109.14Å 90.00° 100.32° 90.00°	Depositor
Resolution (Å)	30.71 – 2.31 30.71 – 2.31	Depositor EDS
% Data completeness (in resolution range)	99.8 (30.71-2.31) 99.8 (30.71-2.31)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.24 (at 2.31Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487)	Depositor
R, R_{free}	0.236 , 0.293 0.235 , 0.289	Depositor DCC
R_{free} test set	1999 reflections (3.54%)	wwPDB-VP
Wilson B-factor (Å^2)	65.2	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 55.0	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	0.94	EDS
Total number of atoms	7453	wwPDB-VP
Average B, all atoms (Å^2)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.26% 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: VTV, MG, 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	0.43	0/4264	0.58	0/5829
2	B	0.48	0/3321	0.61	0/4528
All	All	0.45	0/7585	0.59	0/10357

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	4154	0	3915	114	0
2	B	3229	0	3125	87	0
3	A	25	16	0	1	0
4	A	1	0	0	0	0
5	A	5	0	0	0	0
6	A	16	0	0	2	0
6	B	7	0	0	0	0
All	All	7437	16	7040	188	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 13.

All (188) 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:28:GLU:HG3	1:A:135:ILE:HD12	1.35	1.04
2:B:360:ALA:HB2	2:B:366:LYS:HD2	1.48	0.94
1:A:542:ILE:HG13	2:B:283:LEU:HD12	1.50	0.91
2:B:282:LEU:HD11	2:B:296:THR:CG2	2.03	0.87
1:A:372:VAL:HG11	1:A:411:ILE:HD12	1.59	0.83
1:A:36:GLU:O	1:A:39:THR:HG22	1.82	0.78
1:A:300:GLU:HA	1:A:303:LEU:HB3	1.66	0.78
1:A:260:LEU:HD23	1:A:260:LEU:O	1.85	0.76
2:B:282:LEU:HD21	2:B:295:LEU:HD23	1.65	0.76
2:B:360:ALA:CB	2:B:366:LYS:HD2	2.17	0.75
2:B:282:LEU:CD2	2:B:295:LEU:HD23	2.19	0.73
1:A:542:ILE:HG13	2:B:283:LEU:CD1	2.19	0.73
1:A:107:THR:HG1	1:A:198:HIS:HE2	1.35	0.72
1:A:328:GLU:HG2	1:A:330:GLN:NE2	2.04	0.72
1:A:26:LEU:HB2	1:A:31:ILE:HD11	1.70	0.72
1:A:447:ASN:OD1	1:A:450:THR:HG23	1.90	0.72
2:B:282:LEU:HD11	2:B:296:THR:HG23	1.72	0.70
1:A:104:LYS:HG3	1:A:192:ASP:HA	1.73	0.68
2:B:244:ILE:HB	2:B:310:LEU:HD22	1.76	0.68
1:A:302:GLU:O	1:A:306:ASN:N	2.25	0.68
1:A:12:LEU:HD11	1:A:127:TYR:CE1	2.29	0.67
1:A:238:LYS:HD2	1:A:315[A]:HIS:ND1	2.09	0.66
1:A:27:THR:O	1:A:31:ILE:HD12	1.95	0.66
1:A:330:GLN:HB2	1:A:338:THR:HG22	1.79	0.65
2:B:107:THR:HA	2:B:232:TYR:O	1.97	0.65
2:B:233:GLU:O	2:B:233:GLU:HG2	1.98	0.64
2:B:167:ILE:HD12	2:B:212:TRP:HB3	1.80	0.63
1:A:206:ARG:HB3	1:A:216:THR:HG21	1.82	0.61
2:B:329:ILE:O	2:B:392:PRO:HG3	2.00	0.61
1:A:94:ILE:HG21	1:A:230:MET:CE	2.31	0.61
2:B:198:HIS:O	2:B:202:ILE:HG12	2.01	0.61
1:A:329:ILE:HD12	1:A:391:LEU:HD22	1.83	0.60
2:B:238:LYS:HD2	2:B:350:LYS:NZ	2.16	0.60
2:B:163:SER:O	2:B:167:ILE:HG12	2.02	0.59
1:A:21:VAL:HB	1:A:59:PRO:HD3	1.83	0.59
2:B:196:GLY:O	2:B:200:THR:HG23	2.02	0.59
1:A:94:ILE:HD12	1:A:95:PRO:O	2.02	0.59
1:A:266:TRP:O	1:A:269:GLN:HG2	2.02	0.59
2:B:16:MET:HE1	2:B:83:ARG:HA	1.85	0.59
1:A:328:GLU:HG2	1:A:330:GLN:HE22	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:ILE:O	1:A:546:GLU:N	2.35	0.58
2:B:360:ALA:HB2	2:B:366:LYS:CD	2.28	0.58
1:A:373:GLN:NE2	2:B:397:THR:HG23	2.19	0.58
1:A:543:GLY:HA3	2:B:283:LEU:O	2.03	0.58
1:A:40:GLU:O	1:A:44:GLU:HG3	2.04	0.57
2:B:108:VAL:O	2:B:231:GLY:HA2	2.04	0.57
2:B:393:ILE:HD13	2:B:398:TRP:HB2	1.86	0.56
1:A:329:ILE:HD12	1:A:391:LEU:CD2	2.35	0.56
2:B:75:VAL:HG11	2:B:77:PHE:CZ	2.41	0.56
1:A:370:GLU:OE2	2:B:394[A]:GLN:NE2	2.31	0.56
1:A:20:LYS:NZ	1:A:55:PRO:HB2	2.21	0.55
1:A:320:ASP:OD2	1:A:323:LYS:NZ	2.36	0.55
1:A:181[B]:TYR:CE2	1:A:183:TYR:HB2	2.42	0.55
2:B:242:GLN:HA	2:B:242:GLN:OE1	2.06	0.55
1:A:543:GLY:CA	2:B:283:LEU:O	2.55	0.55
1:A:54:ASN:OD1	1:A:56:TYR:N	2.33	0.55
2:B:154:LYS:O	2:B:157:PRO:HD2	2.06	0.55
1:A:494:ASN:HB3	2:B:289:LEU:HD12	1.89	0.55
2:B:292:VAL:O	2:B:293:ILE:HD13	2.07	0.55
1:A:26:LEU:HB2	1:A:31:ILE:CD1	2.37	0.55
2:B:266:TRP:O	2:B:269:GLN:HG3	2.07	0.55
2:B:235:HIS:O	2:B:237:ASP:N	2.40	0.54
2:B:79:GLU:OE2	2:B:83:ARG:NH1	2.39	0.54
1:A:60:VAL:HG23	1:A:75:VAL:HG22	1.90	0.54
2:B:28:GLU:HB2	2:B:135:ILE:HD11	1.90	0.54
2:B:366:LYS:O	2:B:370:GLU:HG3	2.07	0.54
2:B:402:TRP:CZ3	2:B:403:THR:HG22	2.43	0.54
1:A:7:THR:HG21	1:A:121:ASP:HA	1.88	0.53
1:A:305:GLU:O	1:A:309:ILE:N	2.38	0.53
1:A:543:GLY:N	2:B:283:LEU:O	2.41	0.53
2:B:47:ILE:HD12	2:B:144:TYR:CD1	2.42	0.53
1:A:28:GLU:HG3	1:A:135:ILE:CD1	2.24	0.53
2:B:388:LYS:HE2	2:B:415:GLU:OE2	2.08	0.53
2:B:425:LEU:O	2:B:428:GLN:HG2	2.07	0.53
1:A:130:PHE:CZ	1:A:144:TYR:HB2	2.43	0.53
1:A:460:ASN:HA	2:B:286:THR:O	2.08	0.53
1:A:10:VAL:HG21	1:A:153:TRP:HH2	1.73	0.53
1:A:94:ILE:HG21	1:A:230:MET:HE3	1.90	0.53
1:A:451:LYS:N	1:A:451:LYS:HD3	2.22	0.53
1:A:361:HIS:ND1	1:A:513:SER:OG	2.37	0.53
1:A:181[A]:TYR:HE1	2:B:138:GLU:HG2	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:TYR:OH	1:A:156:SER:HB3	2.10	0.52
2:B:101:LYS:O	2:B:236:PRO:HB2	2.09	0.52
2:B:402:TRP:CH2	2:B:403:THR:HG22	2.44	0.52
1:A:164:MET:HA	1:A:164:MET:HE2	1.92	0.52
2:B:61:PHE:CZ	2:B:74:LEU:HD23	2.44	0.52
2:B:354:TYR:OH	2:B:378:GLU:OE2	2.22	0.52
1:A:465:LYS:NZ	6:A:702:HOH:O	2.42	0.52
1:A:31:ILE:O	1:A:35:VAL:HG23	2.09	0.52
1:A:332:GLN:HG3	1:A:338:THR:HB	1.93	0.51
2:B:169:GLU:N	2:B:170:PRO:HD2	2.25	0.51
1:A:54:ASN:ND2	1:A:126:LYS:O	2.42	0.51
1:A:501:TYR:CE1	1:A:505:ILE:HD11	2.47	0.50
1:A:511:ASP:O	1:A:512:LYS:HD3	2.11	0.50
1:A:542:ILE:O	1:A:542:ILE:HG22	2.11	0.50
1:A:110:ASP:O	1:A:217:PRO:HD2	2.12	0.50
1:A:94:ILE:HG21	1:A:230:MET:HE2	1.93	0.50
1:A:108:VAL:HG22	1:A:188:TYR:CD2	2.48	0.49
1:A:109:LEU:HD12	1:A:109:LEU:N	2.27	0.49
1:A:202:ILE:O	1:A:206:ARG:HG3	2.13	0.49
1:A:213:GLY:C	1:A:214:LEU:HD23	2.33	0.49
1:A:103:LYS:H	3:A:601:VTV:C14	2.25	0.49
1:A:544:GLY:N	2:B:285:GLY:O	2.45	0.48
1:A:84:THR:HG21	1:A:153:TRP:CZ2	2.48	0.48
1:A:513:SER:N	1:A:519:ASN:OD1	2.44	0.48
1:A:207:GLN:O	1:A:210:LEU:HB2	2.14	0.48
1:A:411:ILE:HG22	1:A:414:TRP:CD1	2.49	0.48
2:B:103:LYS:O	2:B:236:PRO:HG2	2.12	0.48
2:B:376:THR:HG21	2:B:410:TRP:CZ3	2.49	0.48
2:B:239:TRP:HD1	2:B:242:GLN:OE1	1.97	0.48
1:A:543:GLY:HA3	2:B:284:ARG:HA	1.95	0.48
2:B:8:VAL:HG13	2:B:9:PRO:HD2	1.95	0.48
2:B:187:LEU:HD12	2:B:187:LEU:HA	1.65	0.48
1:A:450:THR:OG1	1:A:452:LEU:HB2	2.14	0.48
1:A:363:ASN:HA	1:A:511:ASP:OD1	2.14	0.47
2:B:366:LYS:HD3	2:B:370:GLU:OE2	2.14	0.47
1:A:47:ILE:HG22	1:A:146:TYR:HA	1.96	0.47
1:A:50:ILE:HG12	1:A:143:ARG:HB3	1.96	0.47
2:B:56:TYR:CZ	2:B:127:TYR:HE1	2.33	0.47
2:B:254:VAL:O	2:B:258:GLN:HG3	2.14	0.47
2:B:366:LYS:HG3	2:B:405:TYR:CD1	2.50	0.47
2:B:16:MET:HE3	2:B:83:ARG:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:HIS:HB2	1:A:238:LYS:O	2.15	0.47
2:B:108:VAL:HG22	2:B:188:TYR:CD2	2.50	0.47
1:A:31:ILE:HG12	1:A:133:PRO:O	2.15	0.46
1:A:129:ALA:HA	1:A:144:TYR:O	2.15	0.46
1:A:501:TYR:O	1:A:505:ILE:HD12	2.15	0.46
2:B:13:LYS:CB	2:B:16:MET:HE2	2.45	0.46
2:B:182:GLN:HG3	2:B:187:LEU:HD13	1.96	0.46
2:B:64:LYS:HE3	2:B:71:TRP:CE2	2.50	0.46
1:A:365:VAL:HG11	1:A:401:TRP:CG	2.51	0.46
1:A:442:VAL:HB	1:A:481:ALA:HB1	1.98	0.46
1:A:447:ASN:OD1	1:A:450:THR:N	2.30	0.46
2:B:7:THR:HB	2:B:121:ASP:HA	1.96	0.46
1:A:465:LYS:NZ	6:A:701:HOH:O	2.29	0.46
1:A:483:TYR:CE1	1:A:520:GLN:HB3	2.51	0.46
1:A:240:THR:HG23	1:A:241:VAL:O	2.15	0.46
2:B:150:PRO:HG2	2:B:153:TRP:HB2	1.98	0.46
2:B:286:THR:O	2:B:286:THR:HG22	2.16	0.46
2:B:167:ILE:HG23	2:B:212:TRP:HB2	1.99	0.45
1:A:7:THR:CG2	1:A:121:ASP:HA	2.46	0.45
1:A:241:VAL:O	1:A:243:PRO:HD3	2.16	0.45
2:B:74:LEU:HD12	2:B:75:VAL:N	2.32	0.45
1:A:19:PRO:O	1:A:56:TYR:HA	2.17	0.45
2:B:74:LEU:HD12	2:B:75:VAL:H	1.81	0.45
2:B:22:LYS:HD3	2:B:22:LYS:HA	1.65	0.45
1:A:379:SER:CB	1:A:387:PRO:HD3	2.47	0.45
2:B:336:GLN:HA	2:B:354:TYR:O	2.17	0.45
1:A:134:SER:CB	1:A:139:THR:HG22	2.47	0.44
1:A:483:TYR:CE2	1:A:487:GLN:OE1	2.70	0.44
2:B:168:LEU:O	2:B:172:LYS:HD3	2.17	0.44
2:B:207:GLN:O	2:B:211:ARG:HG3	2.16	0.44
2:B:328:GLU:O	2:B:339:TYR:HA	2.17	0.44
1:A:238:LYS:HE3	1:A:315[A]:HIS:CE1	2.53	0.43
2:B:128:THR:OG1	2:B:146:TYR:HB2	2.18	0.43
1:A:545:ASN:HA	1:A:548:VAL:HG12	2.00	0.43
1:A:88:TRP:HB2	2:B:54:ASN:O	2.19	0.43
1:A:177:ASP:OD1	1:A:177:ASP:N	2.49	0.43
1:A:417:VAL:O	1:A:417:VAL:HG13	2.19	0.43
1:A:457:TYR:C	1:A:457:TYR:CD1	2.92	0.43
1:A:78:ARG:O	1:A:82:LYS:HG3	2.19	0.43
1:A:317:VAL:HG23	1:A:349:LEU:HD23	2.00	0.43
1:A:80:LEU:HD12	1:A:80:LEU:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:239:TRP:HE1	2:B:243:PRO:HD3	1.83	0.42
1:A:369:THR:O	1:A:373:GLN:HG2	2.19	0.42
1:A:8:VAL:HG21	1:A:159:ILE:HG23	2.01	0.42
1:A:130:PHE:CE1	1:A:144:TYR:HB2	2.55	0.42
2:B:149:LEU:HD21	2:B:159:ILE:HG21	2.01	0.42
2:B:174:GLN:HG2	2:B:175:ASN:OD1	2.19	0.42
1:A:112:GLY:HA2	1:A:185:ASP:CG	2.39	0.42
1:A:361:HIS:HB3	1:A:510:PRO:HB3	2.02	0.42
2:B:183:TYR:CE2	2:B:184:MET:HG2	2.55	0.42
2:B:238:LYS:HD2	2:B:350:LYS:HZ1	1.85	0.42
2:B:191:SER:HG	2:B:198:HIS:CE1	2.36	0.41
1:A:76:ASP:OD1	1:A:78:ARG:HB2	2.20	0.41
2:B:50:ILE:HD12	2:B:54:ASN:HB3	2.01	0.41
1:A:102:LYS:HB2	1:A:102:LYS:HE3	1.93	0.41
2:B:70:LYS:HD2	2:B:70:LYS:HA	1.68	0.41
2:B:167:ILE:O	2:B:167:ILE:HG22	2.21	0.41
1:A:181[B]:TYR:HE2	1:A:183:TYR:HB2	1.85	0.41
1:A:209:LEU:HB3	1:A:214:LEU:HB2	2.03	0.41
1:A:225:PRO:HD2	1:A:226:PRO:HD2	2.03	0.41
1:A:225:PRO:N	1:A:226:PRO:HD2	2.35	0.41
1:A:246:LEU:CB	1:A:260:LEU:HD12	2.50	0.41
2:B:292:VAL:C	2:B:293:ILE:HD13	2.41	0.41
1:A:108:VAL:C	1:A:109:LEU:HD12	2.42	0.40
1:A:50:ILE:CG1	1:A:143:ARG:HB3	2.52	0.40
2:B:109:LEU:HA	2:B:109:LEU:HD13	1.77	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	531/557 (95%)	509 (96%)	22 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	398/428 (93%)	371 (93%)	27 (7%)	0	100 100
All	All	929/985 (94%)	880 (95%)	49 (5%)	0	100 100

There are no Ramachandran outliers to report.

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	413/495 (83%)	395 (96%)	18 (4%)	28 39
2	B	335/390 (86%)	322 (96%)	13 (4%)	32 45
All	All	748/885 (84%)	717 (96%)	31 (4%)	30 43

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LYS
1	A	53	GLU
1	A	101	LYS
1	A	105	SER
1	A	107	THR
1	A	126	LYS
1	A	151	GLN
1	A	162	SER
1	A	178	ILE
1	A	207	GLN
1	A	216	THR
1	A	241	VAL
1	A	338	THR
1	A	411	ILE
1	A	431	LYS
1	A	448	ARG
1	A	505	ILE
1	A	512	LYS

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Mol	Chain	Res	Type
2	B	22	LYS
2	B	29	GLU
2	B	69	THR
2	B	86	ASP
2	B	103	LYS
2	B	113	ASP
2	B	163	SER
2	B	192	ASP
2	B	232	TYR
2	B	269	GLN
2	B	296	THR
2	B	361	HIS
2	B	414	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	182	GLN
1	A	474	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 1 is 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	$\#\|Z\| > 2$
3	VTV	A	601	-	26,26,26	1.82	5 (19%)	35,35,35	1.15	2 (5%)
5	SO4	A	603	-	4,4,4	0.20	0	6,6,6	0.39	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
3	VTV	A	601	-	-	5/17/17/17	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	VTV	C15-N2	7.25	1.45	1.35
3	A	601	VTV	C5-C6	3.58	1.52	1.44
3	A	601	VTV	C1-CL1	2.30	1.79	1.73
3	A	601	VTV	O2-C15	-2.17	1.18	1.23
3	A	601	VTV	C8-CL2	2.15	1.79	1.74

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	601	VTV	C16-C15-N2	2.86	124.04	118.00
3	A	601	VTV	C18-C11-C10	2.31	121.77	118.54

There are no chirality outliers.

All (5) torsion outliers are listed below:

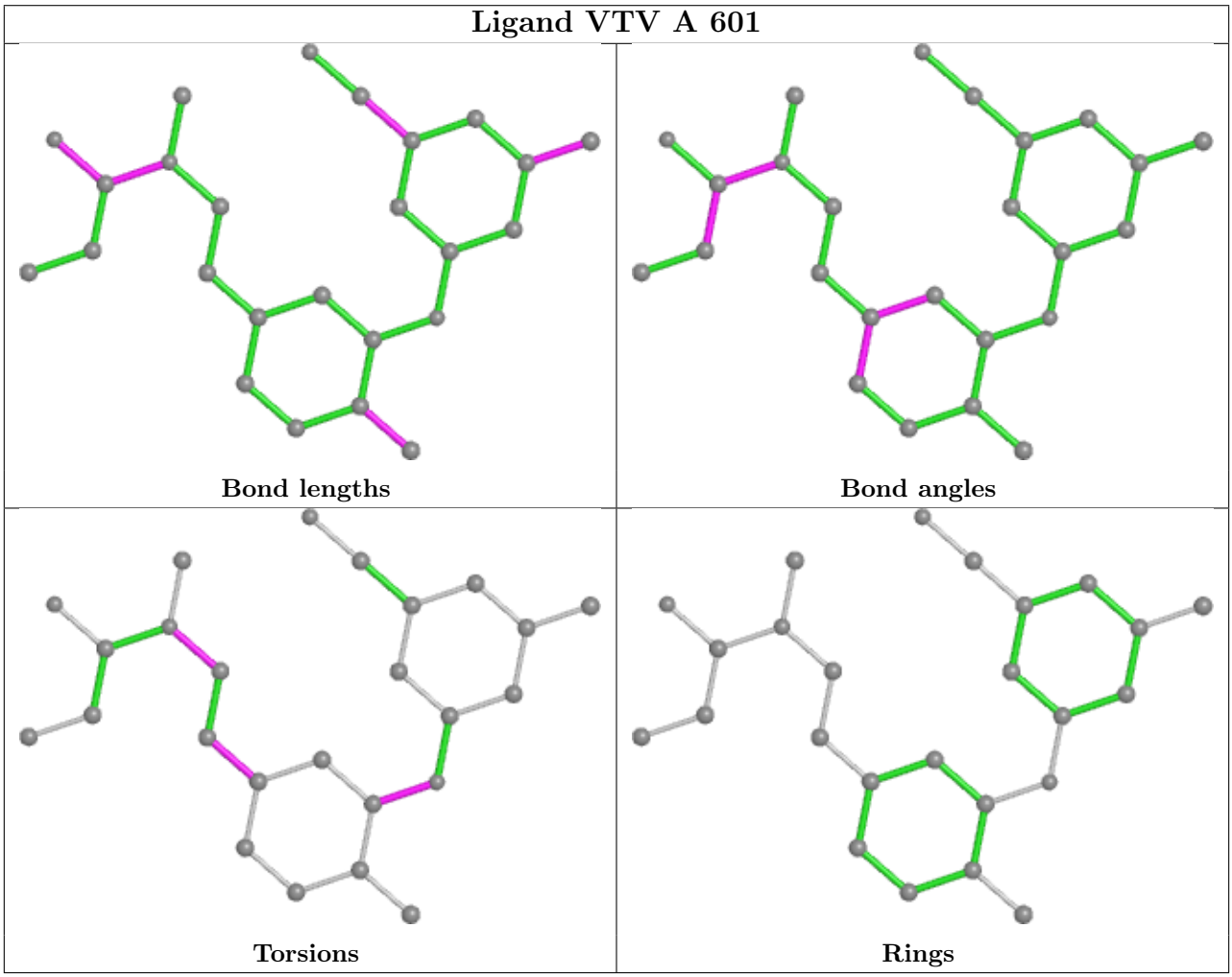
Mol	Chain	Res	Type	Atoms
3	A	601	VTV	C12-C13-N2-C15
3	A	601	VTV	C12-C13-N2-C14
3	A	601	VTV	C18-C11-C12-C13
3	A	601	VTV	C10-C11-C12-C13
3	A	601	VTV	C1-C2-O1-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	VTV	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 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.



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	541/557 (97%)	1.02	101 (18%) 1 1	44, 83, 134, 161	0
2	B	405/428 (94%)	0.80	45 (11%) 5 8	46, 73, 119, 158	0
All	All	946/985 (96%)	0.93	146 (15%) 2 3	44, 78, 126, 161	0

All (146) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	296	THR	12.5
1	A	301	LEU	7.8
1	A	292	VAL	7.7
1	A	294	PRO	7.7
2	B	239	TRP	6.9
2	B	87	PHE	6.8
1	A	295	LEU	6.7
1	A	297	GLU	6.4
1	A	288	ALA	6.4
1	A	289	LEU	6.2
2	B	229	TRP	6.0
1	A	298	GLU	5.8
1	A	69	THR	5.8
2	B	88	TRP	5.4
1	A	68	SER	5.3
2	B	232	TYR	5.3
1	A	262	GLY	5.2
2	B	209	LEU	5.1
2	B	85	GLN	5.0
1	A	554	ALA	4.7
1	A	290	THR	4.7
2	B	171	PHE	4.6
1	A	90	VAL	4.6
1	A	261	VAL	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	116	PHE	4.5
1	A	181[A]	TYR	4.5
1	A	299	ALA	4.4
1	A	24	TRP	4.4
1	A	282	LEU	4.4
2	B	227	PHE	4.2
1	A	217	PRO	4.1
1	A	553	SER	4.1
1	A	246	LEU	4.1
1	A	313	PRO	4.1
2	B	14	PRO	4.0
1	A	315[A]	HIS	4.0
1	A	458	VAL	3.9
1	A	252	TRP	3.9
2	B	212	TRP	3.8
1	A	549	ASP	3.8
1	A	304	ALA	3.8
1	A	280	SER	3.7
2	B	357	MET	3.7
2	B	360	ALA	3.6
2	B	231	GLY	3.6
1	A	127	TYR	3.6
1	A	52	PRO	3.5
2	B	168	LEU	3.5
1	A	260	LEU	3.4
1	A	63	ILE	3.3
1	A	67	ASP	3.3
1	A	457	TYR	3.3
1	A	71	TRP	3.3
2	B	236	PRO	3.3
2	B	409	THR	3.3
1	A	291	GLU	3.2
2	B	241	VAL	3.2
2	B	178	ILE	3.2
1	A	72	ARG	3.2
1	A	218	ASP	3.1
1	A	551	LEU	3.1
1	A	19	PRO	3.1
1	A	271	TYR	3.0
1	A	442	VAL	3.0
1	A	466	VAL	3.0
2	B	89	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	91	GLN	2.9
1	A	306	ASN	2.9
1	A	534	ALA	2.9
2	B	230	MET	2.9
2	B	9	PRO	2.8
1	A	216	THR	2.8
1	A	62	ALA	2.8
1	A	-1	MET	2.8
1	A	281	LYS	2.8
2	B	75	VAL	2.8
1	A	441	TYR	2.7
1	A	550	LYS	2.7
2	B	301	LEU	2.7
1	A	92	LEU	2.6
1	A	303	LEU	2.6
2	B	94	ILE	2.6
1	A	149	LEU	2.6
1	A	283	LEU	2.6
1	A	278	GLN	2.5
1	A	26	LEU	2.5
1	A	277	ARG	2.5
1	A	259	LYS	2.4
1	A	300	GLU	2.4
1	A	245	VAL	2.4
1	A	535	TRP	2.4
2	B	170	PRO	2.4
1	A	464	GLN	2.4
2	B	16	MET	2.4
1	A	302	GLU	2.4
1	A	16	MET	2.4
1	A	74	LEU	2.3
1	A	70	LYS	2.3
2	B	152	GLY	2.3
2	B	205	LEU	2.3
2	B	69	THR	2.3
1	A	15	GLY	2.3
2	B	185	ASP	2.3
1	A	130	PHE	2.3
1	A	451	LYS	2.3
1	A	336	GLN	2.3
1	A	359	GLY	2.3
1	A	496	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	361	HIS	2.2
1	A	247	PRO	2.2
1	A	51	GLY	2.2
1	A	455	ALA	2.2
1	A	552	VAL	2.2
1	A	497	THR	2.2
2	B	102	LYS	2.2
2	B	234	LEU	2.2
1	A	465	LYS	2.2
2	B	206	ARG	2.2
1	A	188	TYR	2.1
2	B	362	THR	2.1
1	A	224	GLU	2.1
2	B	228	LEU	2.1
2	B	281	LYS	2.1
2	B	167	ILE	2.1
1	A	150	PRO	2.1
1	A	368	LEU	2.1
2	B	184	MET	2.1
1	A	410	TRP	2.1
2	B	211	ARG	2.1
1	A	456	GLY	2.1
1	A	253	THR	2.1
2	B	8	VAL	2.1
1	A	25	PRO	2.1
1	A	499	SER	2.1
1	A	541	GLY	2.1
2	B	172	LYS	2.1
2	B	67	ASP	2.1
1	A	459	THR	2.1
1	A	372	VAL	2.1
1	A	146	TYR	2.1
2	B	315	HIS	2.1
1	A	448	ARG	2.1
1	A	244	ILE	2.0
1	A	317	VAL	2.0
1	A	356	ARG	2.0
1	A	369	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)

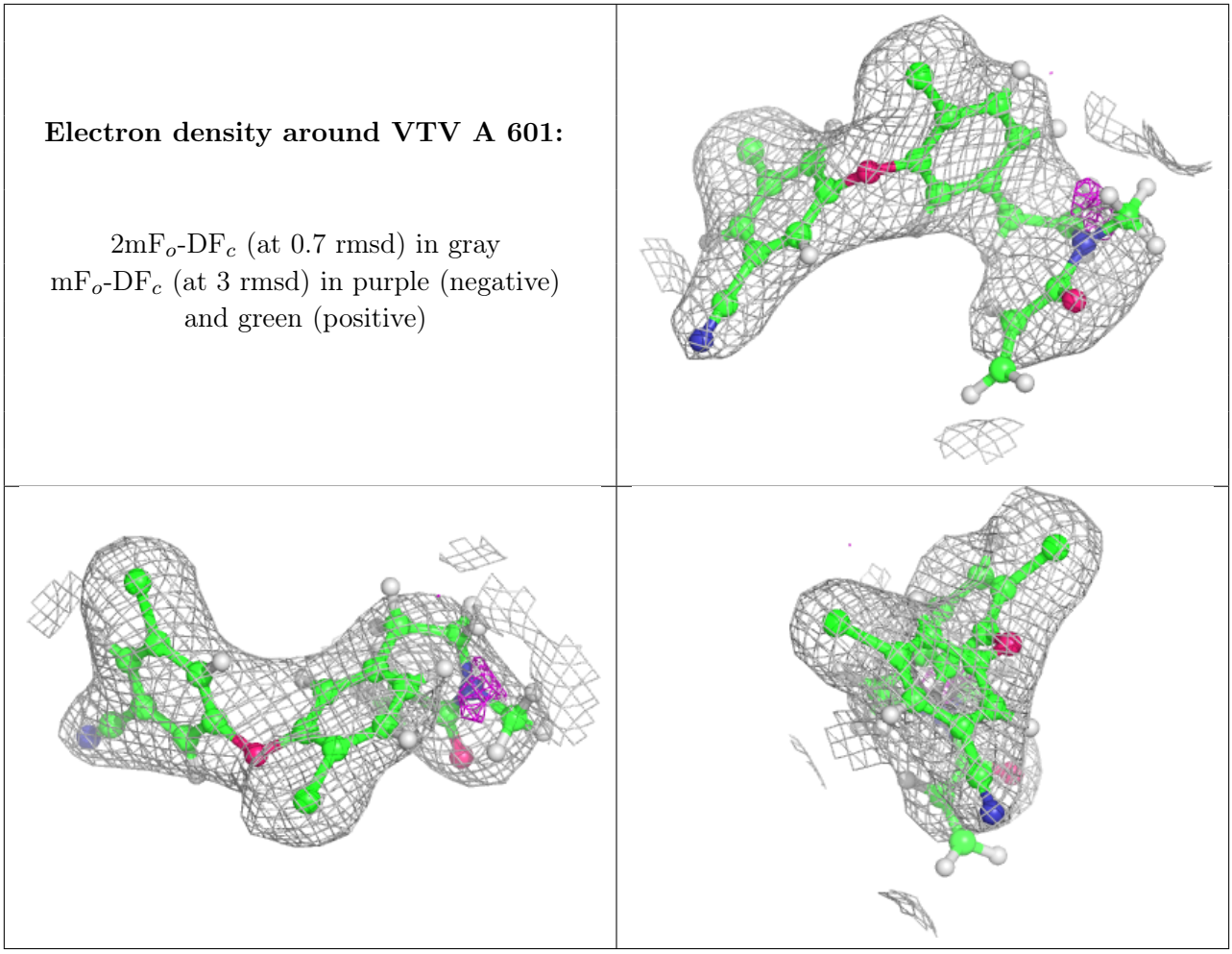
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	MG	A	602	1/1	0.81	0.34	73,73,73,73	0
5	SO4	A	603	5/5	0.88	0.23	99,101,109,128	0
3	VTV	A	601	25/25	0.94	0.17	68,81,90,104	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 VTV A 601:

$2mF_o$-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

There are no such residues in this entry.