



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:57 PM UTC

PDB ID : 8U6T / pdb_00008u6t
Title : Crystal Structure of HIV-1 Reverse Transcriptase in Complex with 5-(2-(2-(3-acryloyl-2-oxo-2,3-dihydro-1H-benzo[d]imidazol-1-yl)ethoxy)phenoxy)-2-naphthonitrile (JLJ758), a non-nucleoside inhibitor
Authors : Prucha, G.; Henry, S.; Jorgensen, W.L.; Anderson, K.S.
Deposited on : 2023-09-13
Resolution : 2.25 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

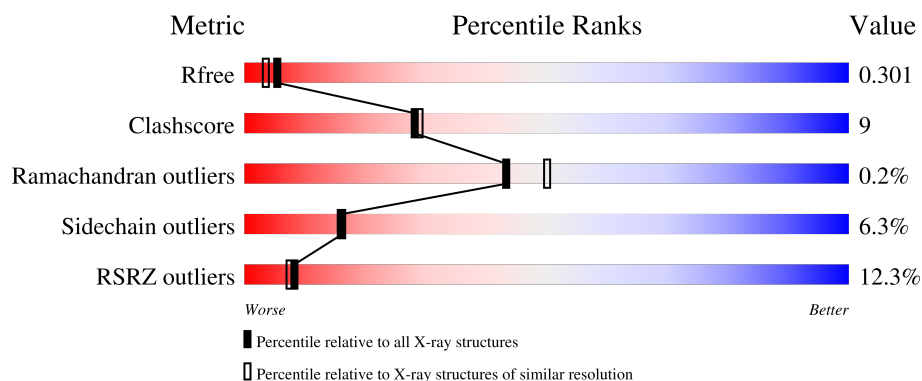
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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}	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	556	13% 78% 17% • •
2	B	428	11% 74% 17% • 6%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7735 atoms, of which 21 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	549	Total	C	N	O	S	0	0	0
			4348	2813	724	804	7			

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

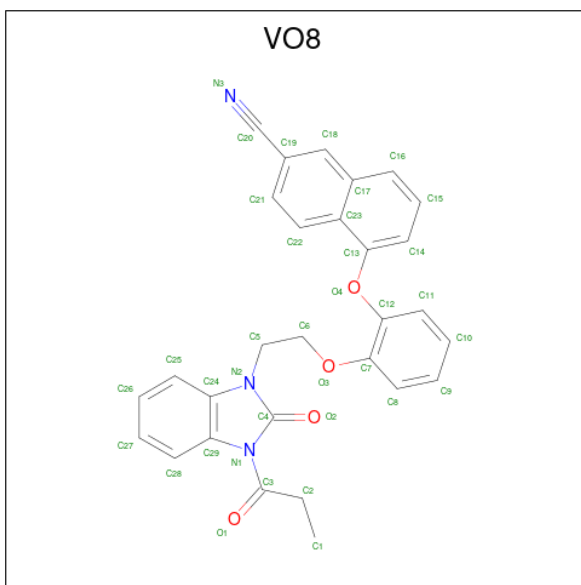
- Molecule 2 is a protein called p51 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	401	Total	C	N	O	S	0	2	0
			3278	2133	538	601	6			

There is a discrepancy between the modelled and reference sequences:

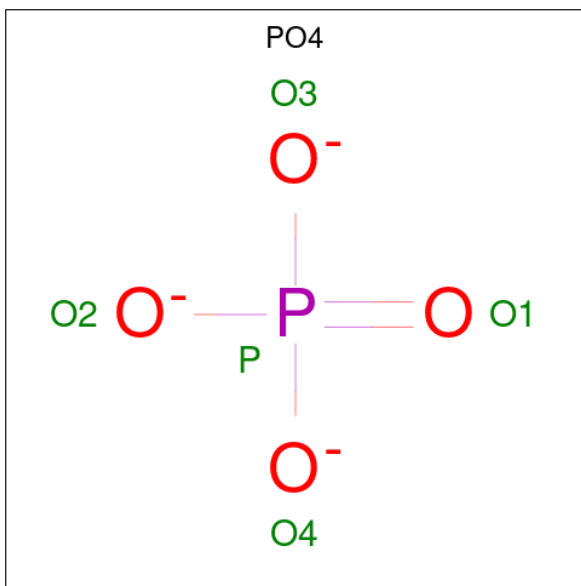
Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 3 is 5-(2-{2-[2-oxo-3-(prop-2-enoyl)-2,3-dihydro-1H-benzimidazol-1-yl]ethoxy}phenoxy)naphthalene-2-carbonitrile (CCD ID: VO8) (formula: C₂₉H₂₃N₃O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	
			57	29	21	3	4	
							0	0

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	Mg 1	0	0
5	B	1	Total 1	Mg 1	0	0

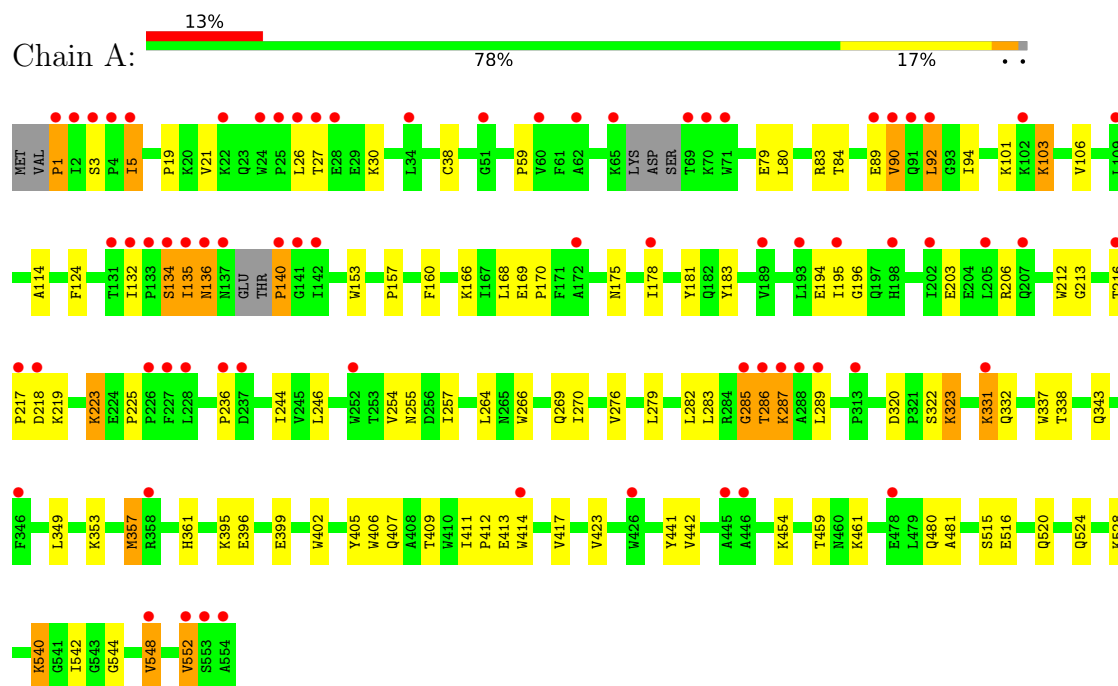
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	20	Total 20	O 20	0	0
6	B	15	Total 15	O 15	0	0

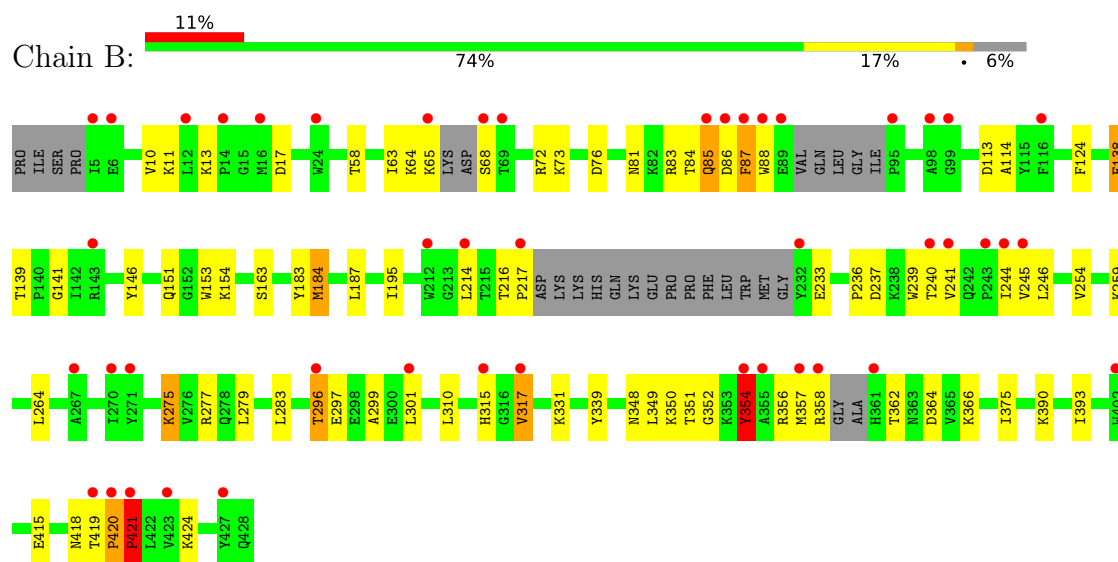
3 Residue-property plots [i](#)

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



• 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	222.15Å 67.27Å 103.26Å 90.00° 108.10° 90.00°	Depositor
Resolution (Å)	36.98 – 2.25 36.98 – 2.25	Depositor EDS
% Data completeness (in resolution range)	98.8 (36.98-2.25) 98.8 (36.98-2.25)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 2.24Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.247 , 0.287 0.278 , 0.301	Depositor DCC
R_{free} test set	2000 reflections (2.89%)	wwPDB-VP
Wilson B-factor (Å ²)	58.5	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 53.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7735	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% 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: MG, PO4, VO8

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	0.53	0/4461	0.76	4/6078 (0.1%)
2	B	0.53	2/3376 (0.1%)	0.73	7/4595 (0.2%)
All	All	0.53	2/7837 (0.0%)	0.75	11/10673 (0.1%)

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

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	138[A]	GLU	C-O	7.06	1.32	1.24
2	B	138[B]	GLU	C-O	7.06	1.32	1.24

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	285	GLY	N-CA-C	-9.20	103.25	114.66
2	B	138[A]	GLU	CA-C-O	8.00	129.03	120.55
2	B	138[B]	GLU	CA-C-O	8.00	129.03	120.55
2	B	141	GLY	CA-C-O	-5.91	118.38	122.22
2	B	420	PRO	N-CA-C	5.69	117.64	110.70
2	B	421	PRO	CA-N-CD	-5.24	104.67	112.00
1	A	287	LYS	N-CA-C	5.22	116.89	108.08
2	B	354[A]	TYR	CA-C-O	5.21	126.58	120.80
2	B	354[B]	TYR	CA-C-O	5.21	126.58	120.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	286	THR	N-CA-C	5.11	121.67	110.80
1	A	287	LYS	CB-CA-C	-5.11	110.71	116.63

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	225	PRO	Peptide

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	4348	0	4293	71	0
2	B	3278	0	3235	67	0
3	A	36	21	0	4	0
4	A	15	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	20	0	0	1	0
6	B	15	0	0	2	0
All	All	7714	21	7528	136	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 9.

All (136) 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)
2:B:13:LYS:HZ1	2:B:85:GLN:HB3	1.14	1.08
3:A:601:VO8:O2	3:A:601:VO8:C1	2.10	0.99
1:A:175:ASN:HB3	1:A:178:ILE:HD13	1.48	0.96
2:B:13:LYS:HE2	2:B:86:ASP:H	1.31	0.94
2:B:13:LYS:NZ	2:B:85:GLN:HB3	1.91	0.83
1:A:406:TRP:CH2	2:B:418:ASN:HA	2.16	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:114:ALA:HB2	2:B:214:LEU:HG	1.61	0.81
1:A:454:LYS:HG3	1:A:552:VAL:HG22	1.62	0.79
2:B:85:GLN:HA	2:B:88:TRP:CE2	2.19	0.78
2:B:85:GLN:HA	2:B:88:TRP:NE1	2.04	0.72
1:A:90:VAL:HG21	1:A:157:PRO:HB2	1.72	0.71
1:A:203:GLU:OE2	1:A:206:ARG:NH1	2.22	0.71
2:B:241:VAL:HG22	2:B:350:LYS:HA	1.71	0.71
2:B:420:PRO:HD2	2:B:421:PRO:HD2	1.73	0.70
1:A:343:GLN:HG3	1:A:349:LEU:HD21	1.75	0.69
2:B:13:LYS:HE2	2:B:86:ASP:N	2.06	0.68
3:A:601:VO8:C1	3:A:601:VO8:C4	2.72	0.68
2:B:65:LYS:C	2:B:68:SER:HB3	2.20	0.67
1:A:254:VAL:HB	1:A:289:LEU:HA	1.77	0.66
2:B:354[B]:TYR:HE2	2:B:375:ILE:HG13	1.61	0.66
1:A:3:SER:CB	1:A:5:ILE:HG13	2.27	0.65
1:A:80:LEU:O	1:A:84:THR:HG23	1.98	0.64
2:B:85:GLN:HB2	2:B:88:TRP:CZ2	2.33	0.63
1:A:194:GLU:O	1:A:195:ILE:C	2.41	0.63
1:A:136:ASN:HD22	1:A:140:PRO:HG3	1.65	0.61
2:B:354[B]:TYR:CE2	2:B:375:ILE:HG13	2.36	0.61
1:A:175:ASN:HB3	1:A:178:ILE:CD1	2.27	0.61
1:A:79:GLU:OE2	1:A:83:ARG:NH1	2.32	0.61
2:B:73:LYS:NZ	2:B:146:TYR:OH	2.36	0.59
1:A:38:CYS:SG	1:A:132:ILE:HD11	2.43	0.58
1:A:255:ASN:HB2	1:A:289:LEU:HB3	1.86	0.58
2:B:275:LYS:HD3	2:B:277:ARG:H	1.67	0.58
2:B:357:MET:O	2:B:358:ARG:C	2.46	0.58
2:B:10:VAL:HA	2:B:87:PHE:CE2	2.39	0.57
1:A:1:PRO:O	1:A:213:GLY:HA3	2.04	0.57
1:A:331:LYS:HG2	1:A:337:TRP:CZ3	2.39	0.57
1:A:331:LYS:HD2	1:A:423:VAL:HG22	1.85	0.57
2:B:424:LYS:NZ	6:B:602:HOH:O	2.32	0.57
1:A:84:THR:HG21	1:A:153:TRP:HE1	1.69	0.57
1:A:402:TRP:HB2	1:A:409:THR:HG21	1.86	0.56
2:B:11:LYS:HB2	2:B:87:PHE:CE1	2.39	0.56
1:A:285:GLY:O	1:A:287:LYS:N	2.39	0.56
2:B:88:TRP:CG	2:B:154:LYS:HB3	2.40	0.56
2:B:317:VAL:HG21	2:B:348:ASN:O	2.05	0.55
2:B:420:PRO:CD	2:B:421:PRO:HD2	2.35	0.55
1:A:169:GLU:N	1:A:170:PRO:HD2	2.23	0.54
2:B:88:TRP:CZ2	2:B:154:LYS:HD2	2.44	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:254:VAL:HG13	2:B:283:LEU:HD22	1.91	0.53
1:A:194:GLU:O	1:A:196:GLY:N	2.42	0.52
2:B:244:ILE:HB	2:B:310:LEU:HD22	1.91	0.52
1:A:405:TYR:CE2	1:A:407:GLN:HB3	2.44	0.51
2:B:17:ASP:O	2:B:83:ARG:NE	2.38	0.51
2:B:390:LYS:NZ	2:B:415:GLU:OE2	2.41	0.51
2:B:317:VAL:HG22	2:B:349:LEU:HD23	1.93	0.51
1:A:254:VAL:HG13	1:A:283:LEU:HD22	1.93	0.51
1:A:540:LYS:HB2	1:A:542:ILE:CD1	2.42	0.50
1:A:84:THR:CG2	1:A:124:PHE:HZ	2.24	0.50
1:A:134:SER:O	1:A:135:ILE:C	2.54	0.50
2:B:10:VAL:HG11	2:B:153:TRP:CH2	2.47	0.50
2:B:317:VAL:CG2	2:B:349:LEU:HD23	2.42	0.49
2:B:88:TRP:CZ2	2:B:154:LYS:CD	2.95	0.49
2:B:88:TRP:CD1	2:B:154:LYS:HB2	2.48	0.48
1:A:412:PRO:O	1:A:414:TRP:HD1	1.96	0.48
2:B:64:LYS:HB3	2:B:68:SER:HB2	1.94	0.48
1:A:257:ILE:HB	1:A:283:LEU:HD21	1.96	0.48
2:B:85:GLN:O	2:B:86:ASP:C	2.55	0.48
2:B:420:PRO:O	2:B:421:PRO:C	2.55	0.48
1:A:3:SER:CB	1:A:212:TRP:O	2.62	0.48
1:A:21:VAL:HB	1:A:59:PRO:HD3	1.95	0.48
1:A:540:LYS:HB2	1:A:542:ILE:HD12	1.95	0.48
2:B:13:LYS:CE	2:B:86:ASP:H	2.17	0.48
1:A:19:PRO:HG3	1:A:80:LEU:HB2	1.95	0.47
2:B:81:ASN:HB3	2:B:154:LYS:HD2	1.95	0.47
1:A:266:TRP:O	1:A:269:GLN:HG2	2.14	0.47
1:A:279:LEU:O	1:A:282:LEU:HB2	2.15	0.47
1:A:320:ASP:C	1:A:322:SER:H	2.23	0.47
1:A:402:TRP:HB2	1:A:409:THR:CG2	2.44	0.47
1:A:544:GLY:O	1:A:548:VAL:HG23	2.15	0.47
1:A:246:LEU:HD11	1:A:264:LEU:HD21	1.97	0.47
1:A:357:MET:HB3	1:A:357:MET:HE3	1.62	0.47
1:A:407:GLN:HG2	2:B:393:ILE:HA	1.95	0.47
2:B:85:GLN:HA	2:B:88:TRP:CD1	2.49	0.47
1:A:103:LYS:O	3:A:601:VO8:C1	2.63	0.46
1:A:166:LYS:HA	1:A:169:GLU:HG3	1.97	0.46
2:B:10:VAL:HG11	2:B:153:TRP:HH2	1.80	0.46
2:B:216:THR:O	2:B:217:PRO:C	2.58	0.46
2:B:418:ASN:C	2:B:420:PRO:HD3	2.40	0.46
2:B:195:ILE:HD11	2:B:233:GLU:OE1	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:LEU:O	1:A:169:GLU:C	2.58	0.45
1:A:402:TRP:CE3	1:A:411:ILE:HG21	2.50	0.45
1:A:194:GLU:C	1:A:196:GLY:N	2.70	0.45
1:A:395:LYS:HE2	1:A:399:GLU:OE1	2.16	0.45
2:B:236:PRO:HA	2:B:239:TRP:CD2	2.52	0.45
1:A:94:ILE:HG22	1:A:183:TYR:CE1	2.52	0.45
2:B:183:TYR:CE2	2:B:184:MET:HG3	2.51	0.45
1:A:441:TYR:O	1:A:548:VAL:HG21	2.16	0.44
1:A:442:VAL:HB	1:A:481:ALA:HB1	1.99	0.44
1:A:461:LYS:HE2	6:A:707:HOH:O	2.17	0.44
1:A:181:TYR:CE2	2:B:138[A]:GLU:HG2	2.52	0.44
1:A:216:THR:HB	1:A:217:PRO:HD2	1.99	0.44
2:B:13:LYS:HE3	2:B:85:GLN:N	2.33	0.44
2:B:356:ARG:NH1	2:B:362:THR:HB	2.33	0.44
1:A:136:ASN:HB2	1:A:140:PRO:HG3	2.00	0.44
2:B:356:ARG:HH12	2:B:366:LYS:HZ3	1.65	0.44
1:A:94:ILE:HG22	1:A:183:TYR:HE1	1.83	0.43
2:B:419:THR:N	2:B:420:PRO:HD3	2.32	0.43
1:A:323:LYS:O	1:A:343:GLN:NE2	2.52	0.43
1:A:524:GLN:O	1:A:528:LYS:HG2	2.18	0.43
1:A:454:LYS:HD2	1:A:552:VAL:O	2.19	0.43
1:A:135:ILE:H	1:A:135:ILE:HD13	1.83	0.42
1:A:218:ASP:O	1:A:219:LYS:C	2.62	0.42
2:B:58:THR:HG23	2:B:76:ASP:O	2.19	0.42
2:B:85:GLN:CB	2:B:88:TRP:CZ2	3.02	0.42
1:A:135:ILE:HG12	1:A:136:ASN:H	1.84	0.42
1:A:516:GLU:O	1:A:520:GLN:HG3	2.20	0.42
2:B:241:VAL:HG13	2:B:351:THR:HG23	2.02	0.42
2:B:84:THR:HG21	2:B:124:PHE:HZ	1.85	0.42
1:A:84:THR:HG21	1:A:124:PHE:HZ	1.84	0.41
2:B:259:LYS:NZ	6:B:601:HOH:O	2.31	0.41
1:A:114:ALA:HB1	1:A:160:PHE:CE1	2.55	0.41
1:A:134:SER:CB	1:A:140:PRO:HA	2.51	0.41
2:B:72:ARG:NH2	2:B:151:GLN:OE1	2.53	0.41
1:A:27:THR:OG1	1:A:30:LYS:HG3	2.21	0.41
1:A:223:LYS:H	1:A:223:LYS:HG2	1.65	0.41
2:B:296:THR:HG22	2:B:297:GLU:H	1.86	0.41
1:A:236:PRO:HA	3:A:601:VO8:C3	2.51	0.41
2:B:88:TRP:CE2	2:B:154:LYS:CD	3.04	0.41
2:B:88:TRP:CE2	2:B:154:LYS:HD2	2.56	0.41
2:B:246:LEU:HD11	2:B:264:LEU:HD21	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:279:LEU:HD23	2:B:299:ALA:HB1	2.03	0.41
2:B:331:LYS:NZ	2:B:364:ASP:OD2	2.44	0.41
2:B:420:PRO:N	2:B:421:PRO:HD2	2.36	0.41
1:A:92:LEU:H	1:A:92:LEU:HG	1.30	0.41
1:A:406:TRP:CZ3	2:B:418:ASN:HA	2.56	0.41
2:B:339:TYR:CZ	2:B:352:GLY:HA3	2.55	0.41
2:B:88:TRP:CH2	2:B:154:LYS:HD3	2.57	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	543/556 (98%)	513 (94%)	29 (5%)	1 (0%)	43	50
2	B	393/428 (92%)	378 (96%)	14 (4%)	1 (0%)	36	40
All	All	936/984 (95%)	891 (95%)	43 (5%)	2 (0%)	43	50

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	286	THR
2	B	421	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	459/495 (93%)	426 (93%)	33 (7%)	13	12
2	B	353/390 (90%)	334 (95%)	19 (5%)	20	21
All	All	812/885 (92%)	760 (94%)	52 (6%)	16	15

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	PRO
1	A	5	ILE
1	A	26	LEU
1	A	89	GLU
1	A	90	VAL
1	A	92	LEU
1	A	101	LYS
1	A	103	LYS
1	A	106	VAL
1	A	134	SER
1	A	135	ILE
1	A	136	ASN
1	A	140	PRO
1	A	223	LYS
1	A	244	ILE
1	A	270	ILE
1	A	276	VAL
1	A	323	LYS
1	A	331	LYS
1	A	332	GLN
1	A	338	THR
1	A	353	LYS
1	A	357	MET
1	A	361	HIS
1	A	396	GLU
1	A	413	GLU
1	A	417	VAL
1	A	459	THR
1	A	480	GLN
1	A	515	SER
1	A	540	LYS
1	A	548	VAL
1	A	552	VAL
2	B	63	ILE
2	B	85	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	87	PHE
2	B	113	ASP
2	B	139	THR
2	B	163	SER
2	B	184	MET
2	B	187	LEU
2	B	237	ASP
2	B	240	THR
2	B	245	VAL
2	B	275	LYS
2	B	296	THR
2	B	301	LEU
2	B	315	HIS
2	B	317	VAL
2	B	354[A]	TYR
2	B	354[B]	TYR
2	B	421	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	136	ASN
1	A	161	GLN
1	A	182	GLN
1	A	222	GLN
1	A	336	GLN
1	A	480	GLN
2	B	96	HIS
2	B	147	ASN
2	B	197	GLN
2	B	235	HIS
2	B	255	ASN
2	B	394	GLN
2	B	418	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	PO4	A	603	-	4,4,4	0.79	0	6,6,6	0.45	0
4	PO4	A	604	-	4,4,4	0.84	0	6,6,6	0.46	0
4	PO4	A	602	-	4,4,4	0.94	0	6,6,6	0.44	0
3	VO8	A	601	-	40,40,40	1.87	2 (5%)	53,56,56	1.08	1 (1%)

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	VO8	A	601	-	-	2/18/18/18	0/5/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	VO8	C2-C3	-10.42	1.34	1.51
3	A	601	VO8	C1-C2	-4.81	1.31	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	VO8	C1-C2-C3	6.44	123.98	112.69

There are no chirality outliers.

All (2) torsion outliers are listed below:

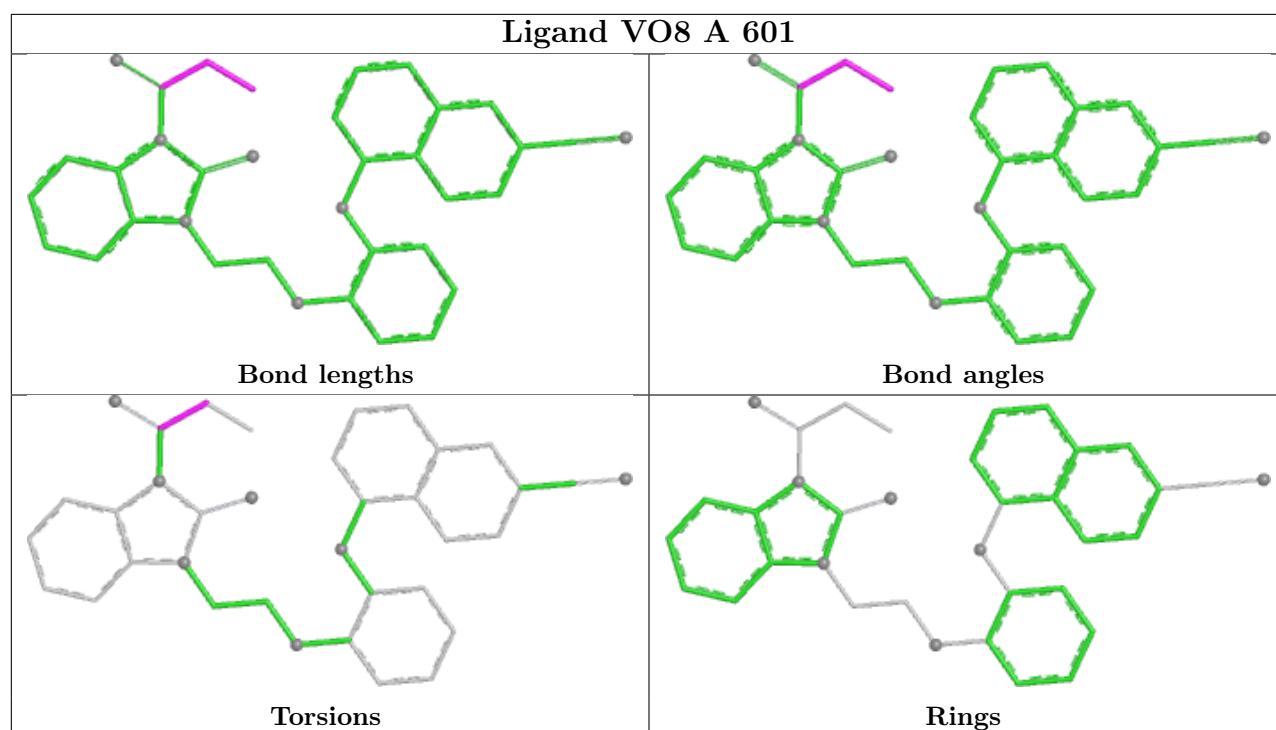
Mol	Chain	Res	Type	Atoms
3	A	601	VO8	C1-C2-C3-O1
3	A	601	VO8	C1-C2-C3-N1

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	VO8	4	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 [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, 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	549/556 (98%)	0.97	71 (12%) 7 7	30, 66, 96, 117	0
2	B	401/428 (93%)	0.88	46 (11%) 9 9	30, 64, 88, 124	2 (0%)
All	All	950/984 (96%)	0.93	117 (12%) 8 7	30, 65, 94, 124	2 (0%)

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	88	TRP	7.6
2	B	354[A]	TYR	5.7
2	B	87	PHE	5.4
2	B	419	THR	5.2
2	B	241	VAL	5.2
1	A	2	ILE	5.1
2	B	95	PRO	5.0
1	A	554	ALA	4.9
1	A	140	PRO	4.8
2	B	86	ASP	4.5
1	A	1	PRO	4.5
2	B	240	THR	4.3
1	A	137	ASN	4.2
1	A	92	LEU	4.2
1	A	135	ILE	4.1
2	B	65	LYS	4.0
1	A	446	ALA	3.9
2	B	232	TYR	3.8
2	B	24	TRP	3.7
1	A	289	LEU	3.6
2	B	267	ALA	3.6
1	A	285	GLY	3.4
1	A	218	ASP	3.4
1	A	133	PRO	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	193	LEU	3.3
1	A	69	THR	3.2
2	B	116	PHE	3.2
2	B	361	HIS	3.2
1	A	70	LYS	3.1
1	A	217	PRO	3.1
2	B	420	PRO	3.1
1	A	252	TRP	3.0
2	B	317	VAL	3.0
2	B	244	ILE	3.0
2	B	270	ILE	2.9
1	A	414	TRP	2.9
1	A	60	VAL	2.9
1	A	102	LYS	2.9
1	A	34	LEU	2.9
1	A	5	ILE	2.9
2	B	214	LEU	2.9
2	B	301	LEU	2.9
2	B	315	HIS	2.8
2	B	355	ALA	2.8
2	B	89	GLU	2.8
1	A	178	ILE	2.8
1	A	195	ILE	2.8
1	A	131	THR	2.7
1	A	51	GLY	2.7
2	B	402	TRP	2.7
1	A	26	LEU	2.7
1	A	132	ILE	2.7
2	B	217	PRO	2.7
2	B	423	VAL	2.7
2	B	421	PRO	2.7
2	B	245	VAL	2.7
1	A	553	SER	2.7
2	B	271	TYR	2.6
1	A	62	ALA	2.6
1	A	227	PHE	2.6
1	A	65	LYS	2.6
1	A	141	GLY	2.6
1	A	552	VAL	2.6
1	A	202	ILE	2.6
1	A	28	GLU	2.5
1	A	236	PRO	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	357	MET	2.5
1	A	237	ASP	2.5
1	A	109	LEU	2.5
1	A	91	GLN	2.5
2	B	143	ARG	2.4
2	B	358	ARG	2.4
2	B	5	ILE	2.4
1	A	358	ARG	2.4
1	A	134	SER	2.4
1	A	346	PHE	2.4
1	A	3	SER	2.4
1	A	22	LYS	2.4
1	A	90	VAL	2.4
1	A	136	ASN	2.4
1	A	478	GLU	2.4
1	A	172	ALA	2.4
1	A	313	PRO	2.3
1	A	27	THR	2.3
1	A	426	TRP	2.3
1	A	4	PRO	2.3
2	B	69	THR	2.3
1	A	189	VAL	2.3
1	A	331	LYS	2.3
2	B	12	LEU	2.3
1	A	25	PRO	2.3
2	B	14	PRO	2.3
1	A	286	THR	2.3
2	B	6	GLU	2.3
1	A	142	ILE	2.3
1	A	287	LYS	2.2
1	A	71	TRP	2.2
2	B	296	THR	2.2
1	A	226	PRO	2.2
2	B	243	PRO	2.2
1	A	89	GLU	2.2
1	A	198	HIS	2.2
1	A	216	THR	2.2
1	A	205	LEU	2.1
2	B	98	ALA	2.1
1	A	207	GLN	2.1
2	B	99	GLY	2.1
2	B	68	SER	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	16	MET	2.1
1	A	288	ALA	2.1
1	A	445	ALA	2.1
2	B	85	GLN	2.0
1	A	228	LEU	2.0
2	B	427	TYR	2.0
1	A	548	VAL	2.0
1	A	24	TRP	2.0
2	B	212	TRP	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](#)

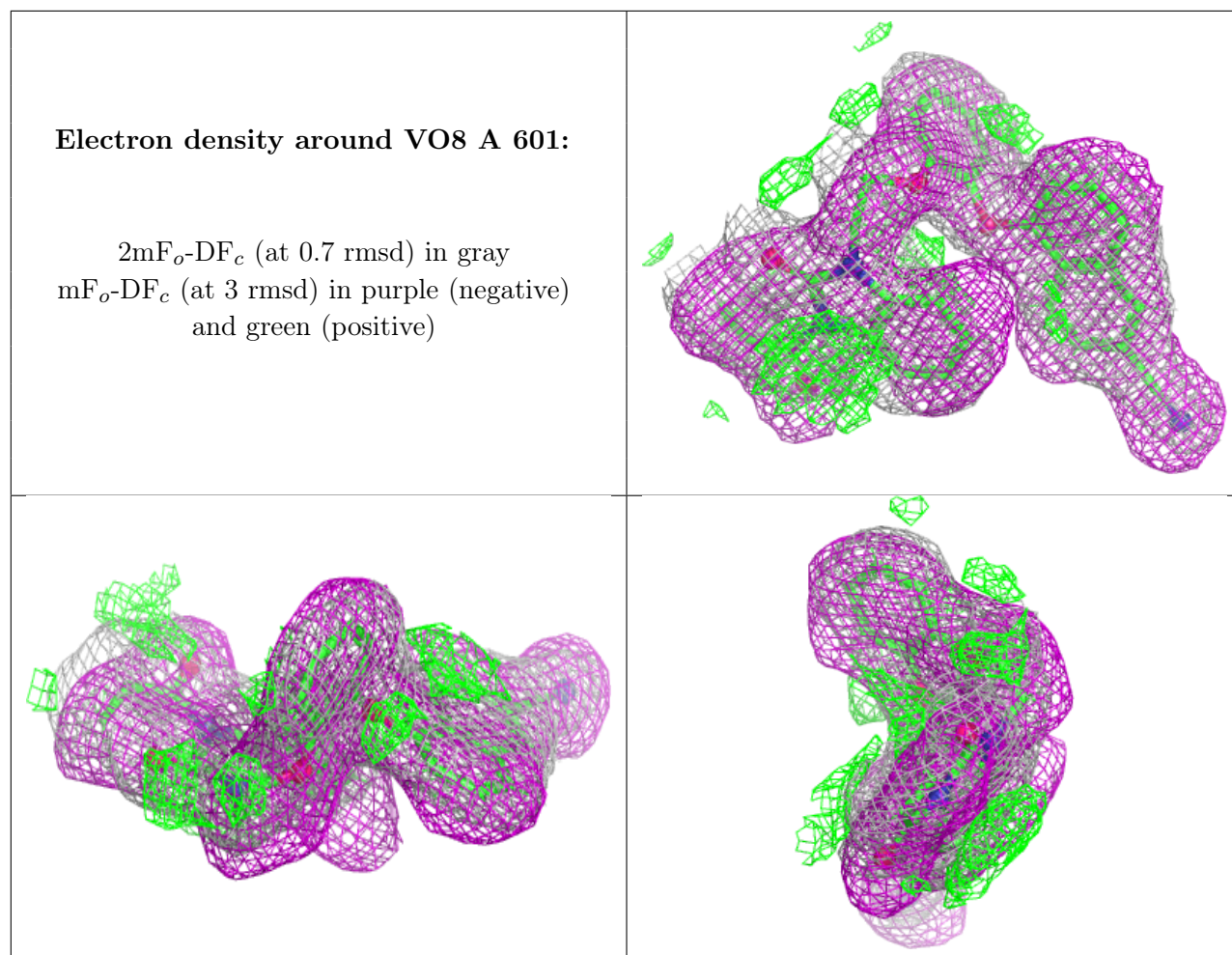
There are no oligosaccharides in this entry.

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($\text{\AA}^2$)	Q<0.9
3	VO8	A	601	36/36	0.85	0.09	0,0,0,0	0
5	MG	A	605	1/1	0.87	0.18	30,30,30,30	0
4	PO4	A	603	5/5	0.89	0.29	30,30,30,30	0
5	MG	B	501	1/1	0.93	0.22	30,30,30,30	0
4	PO4	A	602	5/5	0.96	0.22	30,30,30,30	0
4	PO4	A	604	5/5	0.97	0.13	30,30,30,30	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.