



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 06:31 PM UTC

PDB ID : 8U6J / pdb_00008u6j
Title : Crystal Structure of HIV-1 Reverse Transcriptase in Complex with N-(2-(5-chloro-2-((2-cyanoindolizin-8-yl)oxy)phenoxy)ethyl)-N-methylacrylamide (JLJ746), a non-nucleoside inhibitor
Authors : Prucha, G.; Henry, S.; Jorgensen, W.L.; Anderson, K.S.
Deposited on : 2023-09-13
Resolution : 2.64 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

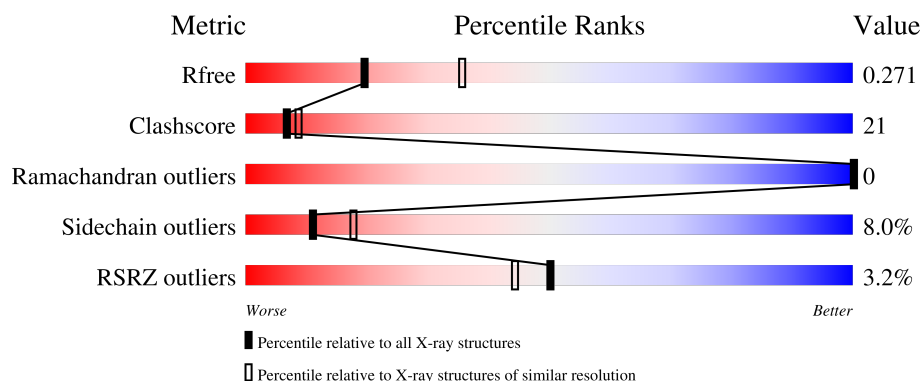
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.64 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	2053 (2.66-2.62)
Clashscore	190562	2097 (2.66-2.62)
Ramachandran outliers	187476	2066 (2.66-2.62)
Sidechain outliers	187428	2066 (2.66-2.62)
RSRZ outliers	180081	2052 (2.66-2.62)

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

Mol	Chain	Length	Quality of chain
1	A	557	4% 60% 34% • •
2	B	428	2% 59% 34% • 5%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7344 atoms, of which 18 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	543	Total	C	N	O	S	0	0	0
			4124	2670	674	774	6			

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

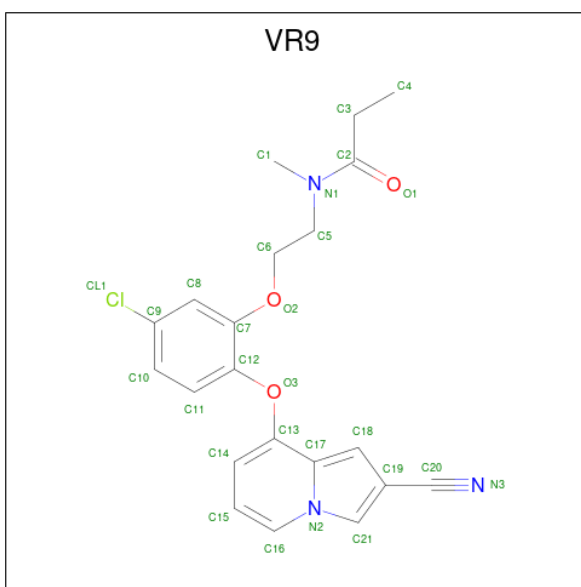
- Molecule 2 is a protein called p51 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	408	Total	C	N	O	S	0	0	0
			3162	2051	515	591	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-(5-chloro-2-{[(4R)-2-cyanoindolizin-8-yl]oxy}phenoxy)ethyl]-N-methylpropanamide (CCD ID: VR9) (formula: C₂₁H₂₀ClN₃O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Cl	H	N	O	0	0
			46	21	1	18	3	3		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

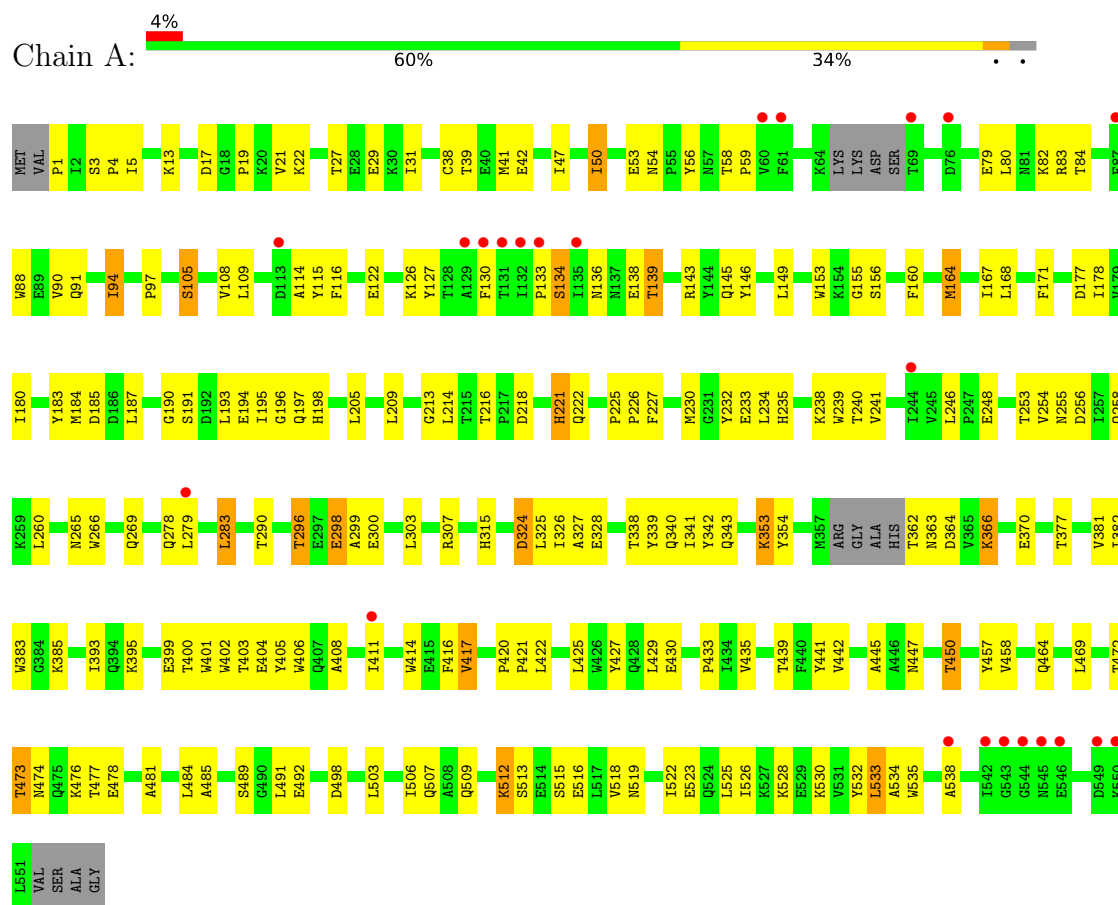
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total	O	0	0
			3	3		
5	B	8	Total	O	0	0
			8	8		

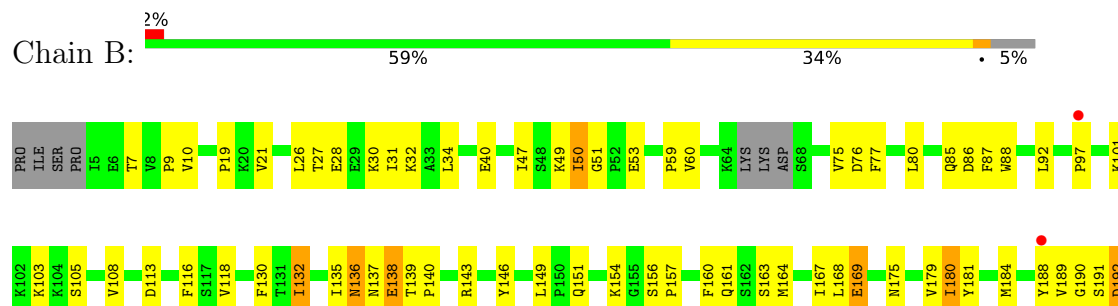
3 Residue-property plots

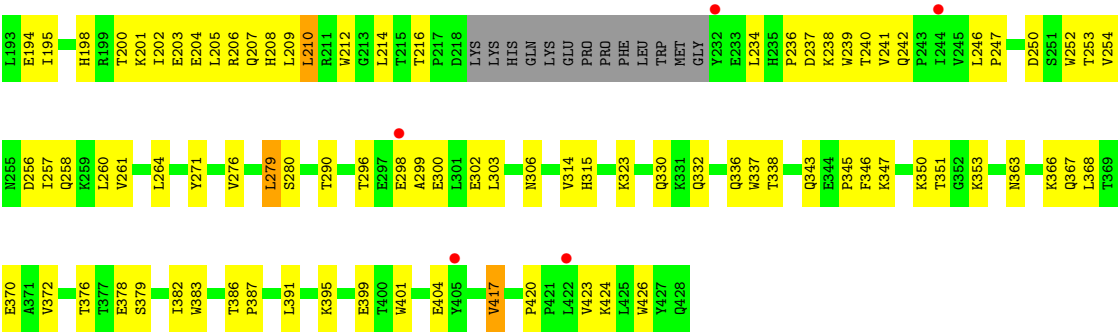
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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	224.43Å 69.63Å 105.06Å 90.00° 105.89° 90.00°	Depositor
Resolution (Å)	43.26 – 2.64 43.26 – 2.64	Depositor EDS
% Data completeness (in resolution range)	96.8 (43.26-2.64) 96.8 (43.26-2.64)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 2.65Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487)	Depositor
R, R_{free}	0.239 , 0.274 0.241 , 0.271	Depositor DCC
R_{free} test set	2000 reflections (4.33%)	wwPDB-VP
Wilson B-factor (Å ²)	82.3	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 67.1	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	0.95	EDS
Total number of atoms	7344	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: VR9, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.40	0/4236	0.54	0/5811
2	B	0.44	0/3254	0.57	0/4458
All	All	0.42	0/7490	0.55	0/10269

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	4124	0	3855	192	0
2	B	3162	0	2956	125	0
3	A	28	18	0	0	0
4	B	1	0	0	0	0
5	A	3	0	0	1	0
5	B	8	0	0	0	0
All	All	7326	18	6811	302	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 21.

All (302) 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:458:VAL:HG22	1:A:464:GLN:HG2	1.36	1.05
2:B:50:ILE:HD12	2:B:51:GLY:H	1.24	0.96
1:A:278:GLN:HG2	1:A:298:GLU:HB2	1.48	0.96
1:A:253:THR:HG23	1:A:256:ASP:H	1.39	0.87
2:B:180:ILE:HG12	2:B:189:VAL:HG12	1.57	0.86
1:A:91:GLN:HE21	2:B:137:ASN:HB3	1.42	0.83
1:A:411:ILE:O	1:A:411:ILE:HG23	1.80	0.81
1:A:532:TYR:CE2	1:A:534:ALA:HB2	2.16	0.80
1:A:240:THR:HG1	1:A:315:HIS:HD1	1.21	0.79
2:B:50:ILE:HD12	2:B:51:GLY:N	1.96	0.79
1:A:324:ASP:O	1:A:343:GLN:HG2	1.84	0.78
1:A:91:GLN:NE2	2:B:137:ASN:HB3	2.00	0.76
2:B:50:ILE:CD1	2:B:51:GLY:H	1.99	0.74
1:A:253:THR:HG22	1:A:256:ASP:CG	2.14	0.73
2:B:132:ILE:HD12	2:B:132:ILE:N	2.05	0.72
1:A:134:SER:HB3	1:A:139:THR:OG1	1.89	0.72
2:B:253:THR:O	2:B:257:ILE:HG12	1.88	0.72
1:A:473:THR:HG23	1:A:476:LYS:CB	2.20	0.71
1:A:516:GLU:HA	1:A:519:ASN:HD22	1.55	0.71
1:A:88:TRP:CZ2	2:B:143:ARG:HD3	2.26	0.71
2:B:101:LYS:O	2:B:236:PRO:HB2	1.90	0.71
2:B:368:LEU:O	2:B:372:VAL:HG23	1.91	0.71
2:B:108:VAL:HG22	2:B:188:TYR:CD2	2.27	0.70
1:A:366:LYS:HE2	1:A:405:TYR:OH	1.91	0.70
1:A:246:LEU:HD22	1:A:260:LEU:CD1	2.22	0.69
1:A:105:SER:HB2	1:A:198:HIS:CE1	2.27	0.69
1:A:3:SER:HB3	1:A:5:ILE:HD12	1.74	0.69
2:B:350:LYS:HE3	2:B:378:GLU:OE1	1.93	0.69
1:A:164:MET:HE2	1:A:164:MET:HA	1.77	0.67
2:B:85:GLN:HA	2:B:88:TRP:NE1	2.09	0.67
2:B:296:THR:HG22	2:B:298:GLU:N	2.10	0.67
1:A:503:LEU:HD22	1:A:535:TRP:HB2	1.76	0.66
1:A:164:MET:HE1	1:A:214:LEU:HD13	1.78	0.66
2:B:10:VAL:HG22	2:B:87:PHE:CZ	2.30	0.65
1:A:58:THR:HG23	1:A:59:PRO:HD2	1.78	0.65
2:B:189:VAL:HG21	2:B:202:ILE:HD12	1.78	0.65
2:B:10:VAL:HG22	2:B:87:PHE:CE2	2.32	0.64
2:B:189:VAL:HG21	2:B:202:ILE:CD1	2.27	0.64
2:B:401:TRP:HE3	2:B:404:GLU:HG3	1.63	0.64
1:A:489:SER:OG	1:A:528:LYS:HE3	1.98	0.64
1:A:39:THR:HG23	1:A:42:GLU:OE1	1.97	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:ILE:HD11	1:A:183:TYR:CE1	2.33	0.63
1:A:241:VAL:HG13	1:A:266:TRP:HE1	1.63	0.63
1:A:130:PHE:O	1:A:143:ARG:HD2	1.99	0.63
1:A:79:GLU:HG3	1:A:83:ARG:NH1	2.14	0.63
2:B:27:THR:OG1	2:B:30:LYS:HG3	1.99	0.63
2:B:103:LYS:HE2	2:B:179:VAL:HG23	1.81	0.62
2:B:246:LEU:HD11	2:B:264:LEU:HD21	1.81	0.62
2:B:332:GLN:HB2	2:B:336:GLN:O	1.99	0.62
2:B:302:GLU:O	2:B:306:ASN:ND2	2.33	0.61
1:A:439:THR:HG22	1:A:441:TYR:CE1	2.35	0.61
2:B:296:THR:HG22	2:B:299:ALA:H	1.65	0.61
1:A:254:VAL:HG13	1:A:283:LEU:HD21	1.83	0.60
1:A:3:SER:HB3	1:A:5:ILE:CD1	2.31	0.60
2:B:366:LYS:O	2:B:370:GLU:HG3	2.02	0.60
2:B:118:VAL:HG11	2:B:149:LEU:HD11	1.83	0.60
2:B:210:LEU:HD22	2:B:214:LEU:O	2.00	0.60
1:A:134:SER:O	1:A:136:ASN:N	2.34	0.60
1:A:324:ASP:N	1:A:324:ASP:OD1	2.33	0.60
1:A:115:TYR:CD2	1:A:156:SER:HB3	2.35	0.60
1:A:3:SER:OG	1:A:5:ILE:HG13	2.01	0.60
1:A:411:ILE:O	1:A:411:ILE:CG2	2.49	0.60
1:A:518:VAL:O	1:A:522:ILE:HG13	2.01	0.60
2:B:175:ASN:OD1	2:B:201:LYS:HE3	2.02	0.60
1:A:194:GLU:CD	1:A:196:GLY:H	2.10	0.60
1:A:533:LEU:HD12	1:A:534:ALA:H	1.67	0.59
1:A:469:LEU:HB3	1:A:472:THR:HG21	1.84	0.59
1:A:84:THR:HG21	1:A:153:TRP:HE1	1.66	0.59
1:A:290:THR:O	1:A:290:THR:HG22	2.02	0.59
1:A:382:ILE:HG23	2:B:136:ASN:HD21	1.67	0.59
1:A:382:ILE:HG23	2:B:136:ASN:ND2	2.17	0.59
1:A:114:ALA:HB1	1:A:160:PHE:CE1	2.38	0.59
1:A:533:LEU:HD12	1:A:534:ALA:N	2.18	0.59
1:A:3:SER:OG	1:A:4:PRO:HD2	2.02	0.58
2:B:237:ASP:OD1	2:B:238:LYS:N	2.36	0.58
1:A:27:THR:HG22	1:A:29:GLU:N	2.18	0.58
1:A:447:ASN:CG	1:A:450:THR:HG23	2.28	0.58
2:B:27:THR:O	2:B:31:ILE:HD12	2.04	0.58
2:B:138:GLU:HG3	2:B:139:THR:HG23	1.85	0.58
1:A:105:SER:HB2	1:A:198:HIS:ND1	2.19	0.57
1:A:21:VAL:CG1	1:A:59:PRO:HD3	2.34	0.57
1:A:164:MET:HE1	1:A:214:LEU:CD1	2.34	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:SER:OG	1:A:198:HIS:ND1	2.27	0.57
1:A:41:MET:HG3	1:A:47:ILE:HD11	1.85	0.57
1:A:38:CYS:O	1:A:47:ILE:HD11	2.05	0.56
1:A:205:LEU:CD2	1:A:209:LEU:HD11	2.35	0.56
1:A:435:VAL:CG1	2:B:290:THR:HG21	2.35	0.56
1:A:13:LYS:HE3	1:A:82:LYS:O	2.06	0.56
1:A:341:ILE:HG21	1:A:383:TRP:CH2	2.41	0.56
1:A:180:ILE:CG2	1:A:187:LEU:HD22	2.36	0.56
1:A:88:TRP:CE2	2:B:143:ARG:HD3	2.41	0.56
1:A:233:GLU:N	1:A:240:THR:O	2.25	0.56
1:A:420:PRO:HA	1:A:422:LEU:N	2.21	0.56
1:A:492:GLU:HG2	1:A:530:LYS:HB2	1.87	0.56
1:A:27:THR:O	1:A:31:ILE:HG13	2.06	0.55
1:A:406:TRP:CD1	2:B:420:PRO:HB3	2.42	0.55
2:B:236:PRO:HA	2:B:239:TRP:CD2	2.42	0.55
1:A:241:VAL:HG13	1:A:266:TRP:NE1	2.22	0.55
1:A:246:LEU:HD22	1:A:260:LEU:HD12	1.88	0.55
2:B:253:THR:H	2:B:256:ASP:HB2	1.72	0.55
1:A:408:ALA:HB2	2:B:337:TRP:HH2	1.72	0.54
2:B:105:SER:O	2:B:190:GLY:HA2	2.07	0.54
2:B:169:GLU:HA	2:B:169:GLU:OE1	2.08	0.54
2:B:132:ILE:N	2:B:132:ILE:CD1	2.71	0.54
1:A:427:TYR:CE2	1:A:525:LEU:HD13	2.43	0.54
2:B:118:VAL:HB	2:B:149:LEU:HD12	1.89	0.54
1:A:325:LEU:HD21	1:A:383:TRP:CE3	2.43	0.53
2:B:189:VAL:HG23	2:B:189:VAL:O	2.08	0.53
2:B:160:PHE:HE2	2:B:164:MET:HE2	1.73	0.53
1:A:53:GLU:H	1:A:53:GLU:CD	2.17	0.53
2:B:323:LYS:HB2	2:B:343:GLN:NE2	2.24	0.53
1:A:240:THR:OG1	1:A:315:HIS:ND1	2.27	0.53
1:A:474:ASN:O	1:A:478:GLU:HG3	2.09	0.53
2:B:60:VAL:HG11	2:B:130:PHE:CD2	2.44	0.53
1:A:27:THR:HG22	1:A:29:GLU:H	1.74	0.53
1:A:298:GLU:H	1:A:298:GLU:CD	2.12	0.52
2:B:205:LEU:O	2:B:209:LEU:HG	2.09	0.52
2:B:376:THR:HG23	2:B:386:THR:HG22	1.90	0.52
1:A:532:TYR:HE2	1:A:534:ALA:HB2	1.70	0.52
2:B:203:GLU:O	2:B:207:GLN:HG2	2.09	0.52
1:A:21:VAL:HG11	1:A:59:PRO:HD3	1.92	0.52
1:A:353:LYS:NZ	5:A:701:HOH:O	2.31	0.52
1:A:512:LYS:HG2	1:A:513:SER:H	1.75	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:279:LEU:N	2:B:279:LEU:HD23	2.25	0.52
2:B:296:THR:HB	2:B:299:ALA:HB3	1.92	0.51
1:A:439:THR:HG22	1:A:441:TYR:HE1	1.75	0.51
2:B:254:VAL:O	2:B:258:GLN:HG3	2.10	0.51
1:A:253:THR:CG2	1:A:256:ASP:H	2.18	0.51
1:A:326:ILE:HD12	1:A:342:TYR:O	2.11	0.51
2:B:279:LEU:HD22	2:B:299:ALA:HB1	1.92	0.51
2:B:332:GLN:HG3	2:B:338:THR:HG23	1.93	0.51
1:A:91:GLN:NE2	2:B:137:ASN:O	2.44	0.51
1:A:296:THR:HG22	1:A:299:ALA:CB	2.41	0.51
1:A:265:ASN:OD1	1:A:353:LYS:HE3	2.11	0.50
1:A:354:TYR:OH	1:A:370:GLU:OE1	2.28	0.50
1:A:240:THR:HG22	1:A:241:VAL:N	2.27	0.50
2:B:88:TRP:CH2	2:B:154:LYS:HD3	2.46	0.50
1:A:50:ILE:HD12	1:A:143:ARG:HB3	1.93	0.50
1:A:522:ILE:O	1:A:526:ILE:HG23	2.12	0.50
2:B:279:LEU:CD2	2:B:299:ALA:HB1	2.42	0.50
2:B:350:LYS:CE	2:B:378:GLU:OE1	2.59	0.50
1:A:458:VAL:HG22	1:A:464:GLN:CG	2.25	0.50
2:B:160:PHE:CE2	2:B:164:MET:HE2	2.47	0.50
1:A:246:LEU:O	1:A:307:ARG:NH2	2.45	0.50
1:A:382:ILE:HA	2:B:136:ASN:HD22	1.77	0.50
1:A:429:LEU:HD21	1:A:506:ILE:HG22	1.94	0.50
2:B:208:HIS:O	2:B:212:TRP:HD1	1.95	0.49
2:B:191:SER:OG	2:B:198:HIS:ND1	2.26	0.49
2:B:138:GLU:CG	2:B:139:THR:HG23	2.42	0.49
1:A:47:ILE:HG22	1:A:145:GLN:O	2.12	0.49
1:A:400:THR:O	1:A:403:THR:HG22	2.12	0.49
1:A:515:SER:O	1:A:519:ASN:ND2	2.45	0.49
1:A:180:ILE:HG21	1:A:187:LEU:HD22	1.94	0.49
1:A:512:LYS:HD3	1:A:513:SER:N	2.28	0.49
1:A:97:PRO:HG2	1:A:232:TYR:CD1	2.48	0.48
1:A:233:GLU:O	1:A:239:TRP:HA	2.13	0.48
1:A:235:HIS:HB2	1:A:238:LYS:HG2	1.94	0.48
2:B:423:VAL:O	2:B:426:TRP:HB2	2.13	0.48
1:A:3:SER:CB	1:A:5:ILE:CD1	2.92	0.48
2:B:194:GLU:O	2:B:195:ILE:C	2.56	0.48
2:B:296:THR:CG2	2:B:299:ALA:H	2.26	0.48
2:B:257:ILE:O	2:B:261:VAL:HG22	2.13	0.48
2:B:118:VAL:CG1	2:B:149:LEU:HD11	2.44	0.47
1:A:445:ALA:O	1:A:477:THR:HG21	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:TRP:CZ3	1:A:155:GLY:HA3	2.48	0.47
2:B:314:VAL:HG12	2:B:315:HIS:N	2.29	0.47
1:A:94:ILE:HD11	1:A:183:TYR:CZ	2.50	0.47
1:A:326:ILE:CD1	1:A:343:GLN:HA	2.44	0.47
1:A:406:TRP:CE2	2:B:420:PRO:HB3	2.49	0.47
2:B:85:GLN:HG3	2:B:88:TRP:CZ2	2.50	0.47
1:A:17:ASP:OD1	1:A:56:TYR:HE1	1.96	0.47
1:A:205:LEU:HD23	1:A:209:LEU:CD1	2.45	0.47
2:B:156:SER:N	2:B:157:PRO:HD2	2.29	0.47
1:A:91:GLN:OE1	2:B:140:PRO:HA	2.15	0.47
2:B:189:VAL:CG2	2:B:202:ILE:CD1	2.91	0.47
1:A:116:PHE:CE1	1:A:146:TYR:HE2	2.32	0.47
1:A:492:GLU:HA	1:A:530:LYS:O	2.15	0.47
2:B:247:PRO:O	2:B:252:TRP:HH2	1.98	0.47
1:A:136:ASN:C	1:A:138:GLU:H	2.23	0.46
1:A:126:LYS:HE3	1:A:127:TYR:CZ	2.50	0.46
1:A:523:GLU:O	1:A:526:ILE:HG13	2.15	0.46
1:A:5:ILE:CD1	1:A:167:ILE:HD11	2.46	0.46
1:A:303:LEU:O	1:A:307:ARG:HG3	2.15	0.46
1:A:420:PRO:HA	1:A:421:PRO:C	2.41	0.46
1:A:296:THR:HG22	1:A:299:ALA:HB3	1.98	0.46
1:A:439:THR:CG2	1:A:441:TYR:HE1	2.28	0.46
1:A:485:ALA:O	1:A:489:SER:HB3	2.16	0.46
1:A:512:LYS:HG2	1:A:519:ASN:OD1	2.16	0.46
2:B:26:LEU:O	2:B:31:ILE:HD11	2.16	0.46
1:A:439:THR:CG2	1:A:441:TYR:CE1	2.98	0.46
1:A:377:THR:O	1:A:381:VAL:HG23	2.15	0.46
2:B:363:ASN:O	2:B:367:GLN:HG3	2.16	0.46
2:B:296:THR:HB	2:B:299:ALA:CB	2.46	0.46
1:A:80:LEU:O	1:A:84:THR:HG23	2.15	0.45
1:A:183:TYR:OH	1:A:230:MET:HE2	2.16	0.45
1:A:515:SER:OG	1:A:518:VAL:HG23	2.16	0.45
2:B:168:LEU:HD13	2:B:180:ILE:HG21	1.98	0.45
2:B:395:LYS:HE3	2:B:399:GLU:OE2	2.16	0.45
1:A:180:ILE:N	1:A:180:ILE:HD12	2.31	0.45
2:B:132:ILE:HD12	2:B:132:ILE:H	1.80	0.45
2:B:198:HIS:O	2:B:202:ILE:HG12	2.16	0.45
1:A:164:MET:SD	1:A:168:LEU:CD1	3.04	0.45
2:B:303:LEU:HD12	2:B:303:LEU:O	2.15	0.45
1:A:58:THR:CG2	1:A:59:PRO:HD2	2.45	0.45
1:A:225:PRO:HA	1:A:226:PRO:C	2.42	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:88:TRP:CZ2	2:B:154:LYS:HD3	2.52	0.45
2:B:296:THR:O	2:B:300:GLU:HB2	2.17	0.45
1:A:31:ILE:CD1	1:A:133:PRO:HG2	2.46	0.45
2:B:154:LYS:HE3	2:B:184:MET:HE2	1.98	0.45
2:B:206:ARG:NH1	2:B:216:THR:HG22	2.32	0.45
1:A:21:VAL:CG1	1:A:22:LYS:N	2.80	0.45
1:A:108:VAL:O	1:A:109:LEU:HD23	2.17	0.45
1:A:399:GLU:HA	1:A:402:TRP:CD1	2.52	0.45
1:A:442:VAL:HB	1:A:481:ALA:HB1	1.99	0.45
1:A:94:ILE:HD11	1:A:183:TYR:OH	2.17	0.45
1:A:341:ILE:HD12	1:A:341:ILE:HG23	1.79	0.45
2:B:201:LYS:NZ	2:B:204:GLU:OE1	2.46	0.45
1:A:235:HIS:HB2	1:A:238:LYS:CG	2.45	0.44
1:A:447:ASN:HB3	1:A:450:THR:OG1	2.17	0.44
1:A:183:TYR:CE2	1:A:184:MET:HG3	2.53	0.44
1:A:328:GLU:O	1:A:339:TYR:HA	2.16	0.44
2:B:7:THR:O	2:B:9:PRO:HD3	2.17	0.44
1:A:395:LYS:HA	1:A:414:TRP:HH2	1.83	0.44
2:B:53:GLU:OE1	2:B:53:GLU:N	2.49	0.44
2:B:76:ASP:OD1	2:B:76:ASP:C	2.61	0.44
1:A:362:THR:HG22	1:A:363:ASN:N	2.33	0.44
1:A:205:LEU:HD23	1:A:209:LEU:HG	2.00	0.44
1:A:404:GLU:HA	1:A:404:GLU:OE1	2.18	0.44
2:B:49:LYS:HA	2:B:143:ARG:O	2.18	0.44
2:B:60:VAL:HG13	2:B:130:PHE:HB2	1.99	0.44
1:A:164:MET:HE3	1:A:164:MET:HB2	1.84	0.44
2:B:116:PHE:CZ	2:B:151:GLN:HG3	2.53	0.44
1:A:90:VAL:O	1:A:91:GLN:C	2.61	0.44
2:B:391:LEU:O	2:B:417:VAL:HG12	2.17	0.44
2:B:206:ARG:HH12	2:B:216:THR:C	2.25	0.44
2:B:345:PRO:HB2	2:B:346:PHE:CD2	2.53	0.44
2:B:28:GLU:HB2	2:B:135:ILE:HD11	2.00	0.43
1:A:395:LYS:HA	1:A:414:TRP:CH2	2.53	0.43
1:A:1:PRO:HD2	1:A:213:GLY:HA2	1.99	0.43
2:B:47:ILE:HG22	2:B:146:TYR:HA	2.00	0.43
2:B:75:VAL:HG11	2:B:77:PHE:CZ	2.54	0.43
1:A:442:VAL:HG12	1:A:457:TYR:HB3	2.01	0.43
2:B:163:SER:O	2:B:167:ILE:HG13	2.19	0.43
1:A:227:PHE:HB2	1:A:234:LEU:HB2	1.99	0.43
2:B:179:VAL:O	2:B:189:VAL:HA	2.17	0.43
1:A:484:LEU:HA	1:A:484:LEU:HD23	1.71	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:246:LEU:HD23	2:B:246:LEU:HA	1.68	0.43
1:A:115:TYR:O	1:A:149:LEU:HB2	2.19	0.43
1:A:171:PHE:CD1	1:A:171:PHE:C	2.97	0.43
1:A:184:MET:HB2	1:A:185:ASP:H	1.63	0.43
1:A:266:TRP:O	1:A:269:GLN:HG2	2.18	0.43
1:A:435:VAL:HG12	2:B:290:THR:HG21	2.00	0.43
2:B:92:LEU:O	2:B:161:GLN:NE2	2.52	0.43
2:B:379:SER:OG	2:B:387:PRO:HD3	2.19	0.43
1:A:338:THR:HG22	1:A:340:GLN:NE2	2.34	0.42
2:B:21:VAL:HB	2:B:59:PRO:HD3	2.01	0.42
1:A:134:SER:HB3	1:A:139:THR:CB	2.48	0.42
1:A:425:LEU:HD23	1:A:425:LEU:HA	1.88	0.42
1:A:498:ASP:HB2	1:A:538:ALA:HB2	2.01	0.42
2:B:296:THR:HG22	2:B:298:GLU:H	1.84	0.42
1:A:258:GLN:CG	1:A:283:LEU:HD11	2.49	0.42
2:B:19:PRO:HG3	2:B:80:LEU:HB2	2.00	0.42
1:A:183:TYR:CD2	1:A:184:MET:HG3	2.55	0.42
1:A:512:LYS:CG	1:A:513:SER:H	2.31	0.42
1:A:53:GLU:OE1	1:A:53:GLU:N	2.38	0.42
1:A:116:PHE:HE1	1:A:146:TYR:HE2	1.66	0.42
1:A:235:HIS:HB2	1:A:238:LYS:O	2.20	0.42
1:A:79:GLU:OE2	1:A:83:ARG:NH1	2.52	0.42
1:A:327:ALA:HB2	1:A:341:ILE:CD1	2.50	0.42
2:B:382:ILE:HG22	2:B:383:TRP:CD2	2.55	0.42
2:B:154:LYS:CE	2:B:184:MET:HE2	2.50	0.41
1:A:416:PHE:CD1	1:A:417:VAL:N	2.88	0.41
2:B:315:HIS:O	2:B:347:LYS:NZ	2.52	0.41
2:B:242:GLN:HG2	2:B:351:THR:O	2.20	0.41
2:B:97:PRO:HG3	2:B:181:TYR:HB2	2.02	0.41
1:A:303:LEU:HD12	1:A:303:LEU:HA	1.93	0.41
1:A:3:SER:C	1:A:5:ILE:H	2.29	0.41
1:A:433:PRO:HD3	1:A:532:TYR:CZ	2.56	0.41
2:B:241:VAL:HG22	2:B:350:LYS:HA	2.03	0.41
1:A:164:MET:CE	1:A:214:LEU:HD13	2.49	0.41
1:A:235:HIS:N	1:A:238:LYS:O	2.53	0.41
2:B:34:LEU:HD23	2:B:34:LEU:HA	1.75	0.41
2:B:157:PRO:HG3	2:B:184:MET:HA	2.03	0.41
2:B:258:GLN:HA	2:B:261:VAL:HG22	2.02	0.41
2:B:330:GLN:OE1	2:B:338:THR:OG1	2.29	0.41
1:A:19:PRO:O	1:A:56:TYR:HB3	2.21	0.41
1:A:105:SER:O	1:A:190:GLY:HA2	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:TYR:N	1:A:115:TYR:CD1	2.89	0.41
1:A:164:MET:SD	1:A:187:LEU:HD11	2.61	0.41
1:A:491:LEU:H	1:A:491:LEU:HD22	1.86	0.41
2:B:132:ILE:CD1	2:B:132:ILE:H	2.33	0.41
1:A:50:ILE:CD1	1:A:143:ARG:HB3	2.50	0.40
1:A:171:PHE:HD1	1:A:171:PHE:O	2.03	0.40
1:A:246:LEU:HD22	1:A:260:LEU:HD13	2.02	0.40
1:A:457:TYR:O	1:A:458:VAL:HG23	2.21	0.40
1:A:193:LEU:HB3	1:A:197:GLN:HB2	2.03	0.40
1:A:205:LEU:HD23	1:A:209:LEU:HD11	2.03	0.40
1:A:526:ILE:HD12	1:A:526:ILE:C	2.47	0.40
2:B:192:ASP:OD1	2:B:192:ASP:N	2.54	0.40
1:A:218:ASP:CB	1:A:221:HIS:CE1	3.04	0.40
1:A:435:VAL:HG13	2:B:290:THR:HG21	2.03	0.40
1:A:507:GLN:C	1:A:509:GLN:H	2.30	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	537/557 (96%)	504 (94%)	33 (6%)	0	100	100
2	B	402/428 (94%)	382 (95%)	20 (5%)	0	100	100
All	All	939/985 (95%)	886 (94%)	53 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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	408/495 (82%)	374 (92%)	34 (8%)	10	16
2	B	318/390 (82%)	294 (92%)	24 (8%)	12	20
All	All	726/885 (82%)	668 (92%)	58 (8%)	11	18

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	ILE
1	A	54	ASN
1	A	94	ILE
1	A	105	SER
1	A	122	GLU
1	A	134	SER
1	A	139	THR
1	A	164	MET
1	A	177	ASP
1	A	178	ILE
1	A	195	ILE
1	A	216	THR
1	A	221	HIS
1	A	222	GLN
1	A	248	GLU
1	A	255	ASN
1	A	279	LEU
1	A	283	LEU
1	A	296	THR
1	A	298	GLU
1	A	300	GLU
1	A	324	ASP
1	A	353	LYS
1	A	364	ASP
1	A	366	LYS
1	A	385	LYS
1	A	393	ILE
1	A	401	TRP
1	A	417	VAL
1	A	430	GLU
1	A	450	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	473	THR
1	A	512	LYS
1	A	533	LEU
2	B	32	LYS
2	B	40	GLU
2	B	50	ILE
2	B	86	ASP
2	B	113	ASP
2	B	132	ILE
2	B	136	ASN
2	B	138	GLU
2	B	169	GLU
2	B	180	ILE
2	B	192	ASP
2	B	200	THR
2	B	210	LEU
2	B	234	LEU
2	B	240	THR
2	B	250	ASP
2	B	260	LEU
2	B	271	TYR
2	B	276	VAL
2	B	279	LEU
2	B	280	SER
2	B	353	LYS
2	B	417	VAL
2	B	424	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	147	ASN
1	A	242	GLN
1	A	340	GLN
1	A	343	GLN
1	A	487	GLN
1	A	519	ASN
2	B	136	ASN
2	B	147	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	VR9	A	601	-	30,30,30	4.01	11 (36%)	35,41,41	2.96	9 (25%)

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	VR9	A	601	-	-	3/16/18/18	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	VR9	C2-N1	15.36	1.53	1.34
3	A	601	VR9	C17-N2	-8.67	1.31	1.40
3	A	601	VR9	C20-C19	7.41	1.54	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	VR9	C21-N2	-5.29	1.29	1.37
3	A	601	VR9	O1-C2	-4.96	1.12	1.23
3	A	601	VR9	C4-C3	-4.63	1.31	1.51
3	A	601	VR9	C18-C19	2.56	1.44	1.40
3	A	601	VR9	C5-C6	2.13	1.57	1.50
3	A	601	VR9	C9-CL1	2.05	1.79	1.74
3	A	601	VR9	C16-C15	2.02	1.39	1.35
3	A	601	VR9	O2-C7	2.01	1.41	1.37

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	VR9	C4-C3-C2	12.00	133.71	112.69
3	A	601	VR9	C3-C2-N1	7.82	129.78	117.88
3	A	601	VR9	C16-N2-C21	-4.74	121.86	130.31
3	A	601	VR9	O1-C2-C3	-4.53	112.30	121.48
3	A	601	VR9	O1-C2-N1	-3.28	117.43	122.19
3	A	601	VR9	C1-N1-C5	3.00	121.88	115.90
3	A	601	VR9	O3-C12-C11	2.51	124.93	118.89
3	A	601	VR9	C1-N1-C2	-2.31	115.59	121.82
3	A	601	VR9	C10-C9-C8	-2.06	118.84	121.53

There are no chirality outliers.

All (3) torsion outliers are listed below:

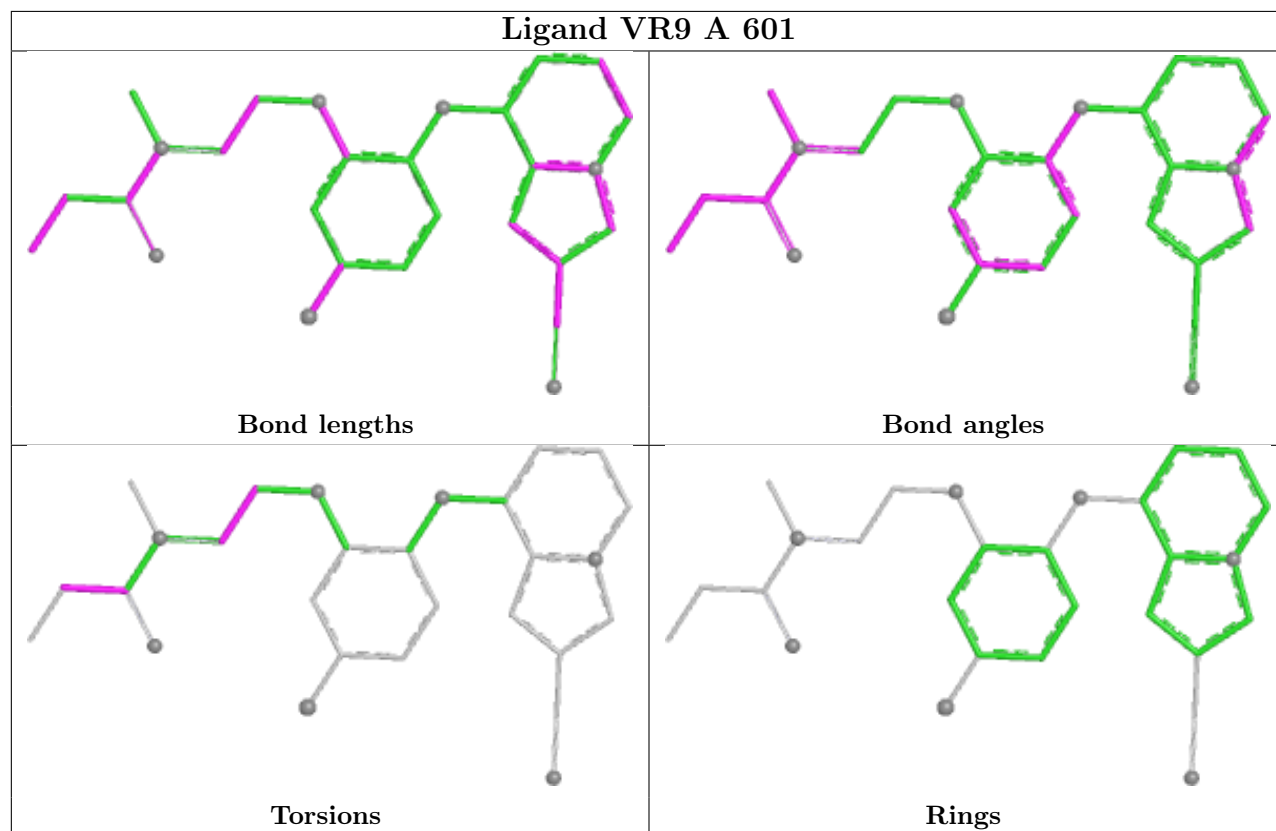
Mol	Chain	Res	Type	Atoms
3	A	601	VR9	N1-C2-C3-C4
3	A	601	VR9	N1-C5-C6-O2
3	A	601	VR9	O1-C2-C3-C4

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 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	543/557 (97%)	0.27	23 (4%) 40 34	66, 97, 143, 194	0
2	B	408/428 (95%)	0.14	7 (1%) 69 65	65, 89, 153, 174	0
All	All	951/985 (96%)	0.21	30 (3%) 50 44	65, 95, 150, 194	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	60	VAL	6.2
1	A	132	ILE	4.5
1	A	549	ASP	3.9
1	A	542	ILE	3.6
1	A	545	ASN	2.8
1	A	544	GLY	2.8
1	A	130	PHE	2.8
1	A	543	GLY	2.7
2	B	188	TYR	2.6
1	A	69	THR	2.6
1	A	61	PHE	2.6
2	B	244	ILE	2.5
1	A	244	ILE	2.5
1	A	131	THR	2.4
2	B	298	GLU	2.4
1	A	546	GLU	2.4
2	B	232	TYR	2.4
2	B	422	LEU	2.4
1	A	87	PHE	2.4
2	B	405	TYR	2.3
1	A	129	ALA	2.2
1	A	550	LYS	2.2
2	B	97	PRO	2.2
1	A	113	ASP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	538	ALA	2.1
1	A	76	ASP	2.1
1	A	135	ILE	2.1
1	A	133	PRO	2.1
1	A	279	LEU	2.1
1	A	411	ILE	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](#)

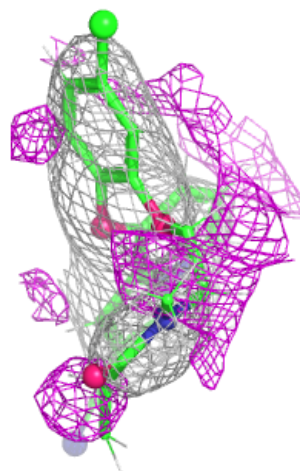
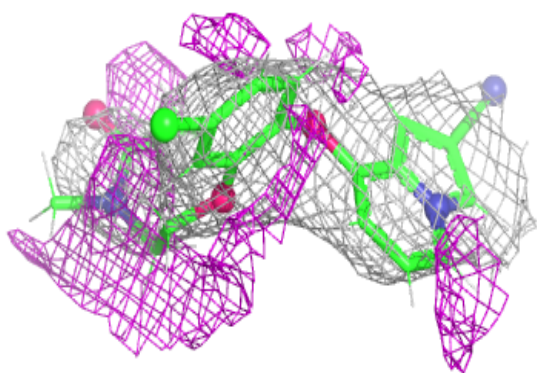
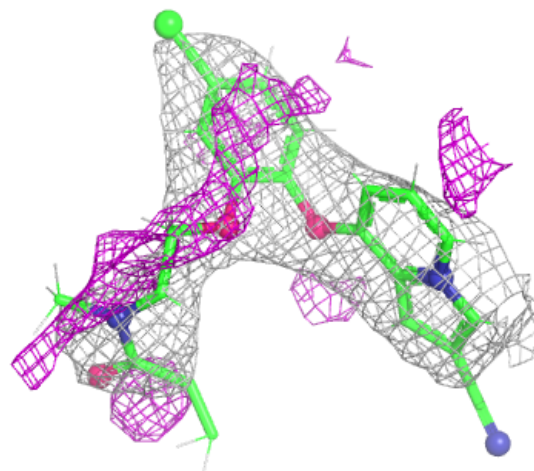
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
4	MG	B	501	1/1	0.88	0.17	84,84,84,84	0
3	VR9	A	601	28/28	0.90	0.13	80,93,110,183	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 VR9 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 [i](#)

There are no such residues in this entry.