



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:01 AM UTC

PDB ID : 7U5Z / pdb_00007u5z
Title : Crystal Structure of HIV-1 Reverse Transcriptase in Complex with JLJ353
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Deposited on : 2022-03-03
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 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

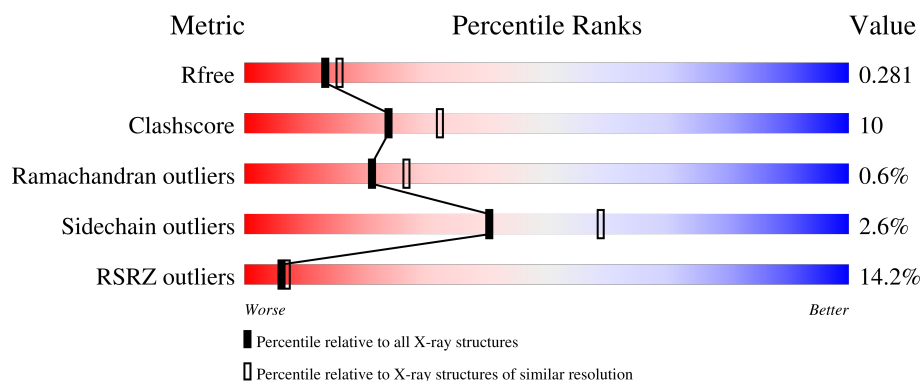
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 $\leq 5\%$. 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	15% 74% 23% ..
2	B	428	11% 72% 20% 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7758 atoms, of which 10 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	2	0
			4350	2818	719	805	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

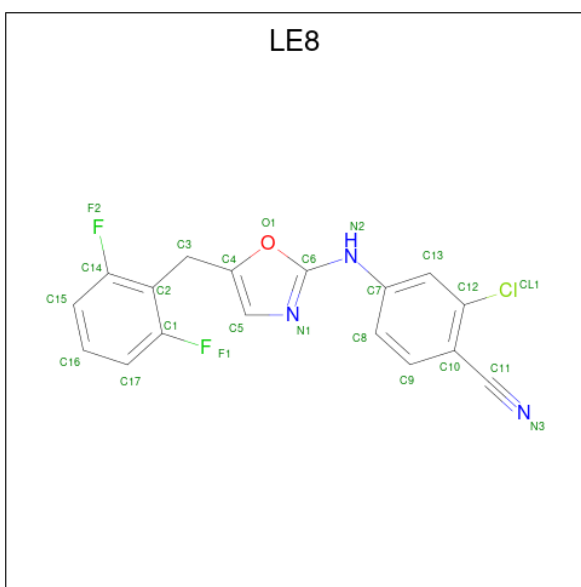
- Molecule 2 is a protein called p51 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	402	Total	C	N	O	S	0	3	0
			3294	2144	542	602	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 2-chloro-4-({5-[(2,6-difluorophenyl)methyl]-1,3-oxazol-2-yl}amino)benzonitrile (CCD ID: LE8) (formula: C₁₇H₁₀ClF₂N₃O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	A	1	Total	C	Cl	F	H	N	O	0	0
			34	17	1	2	10	3	1		

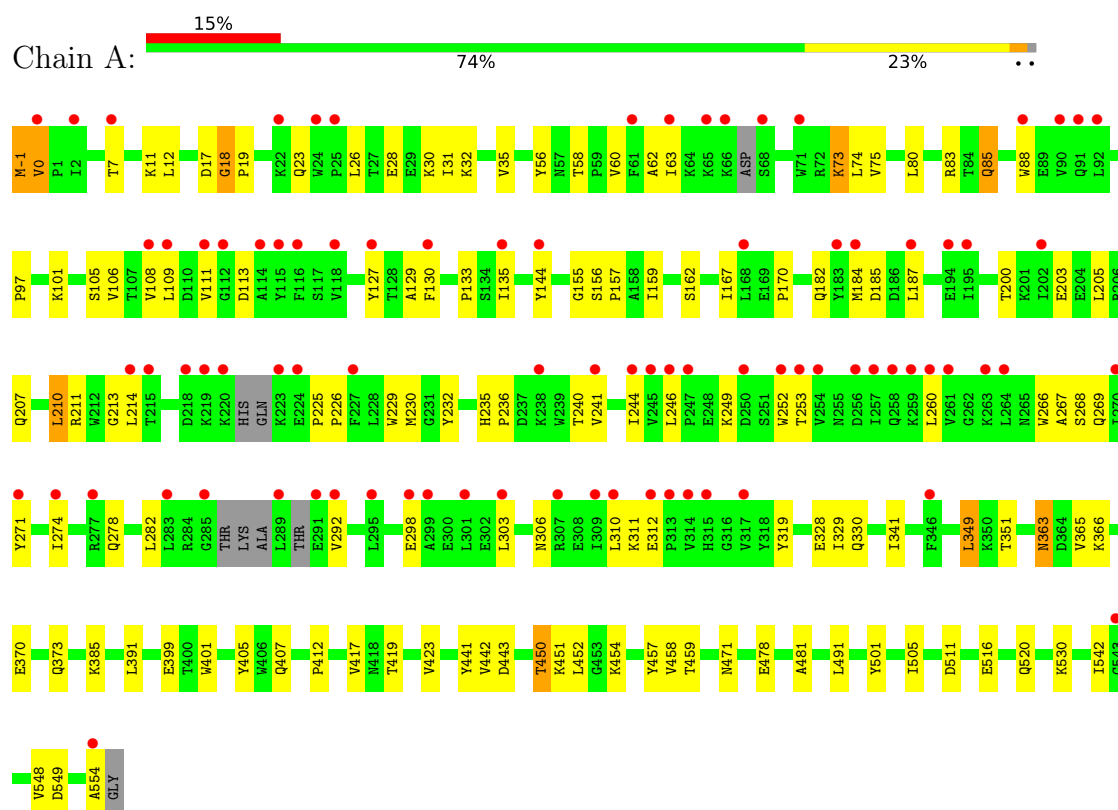
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	54	Total	O	0	0
			54	54		
4	B	26	Total	O	0	0
			26	26		

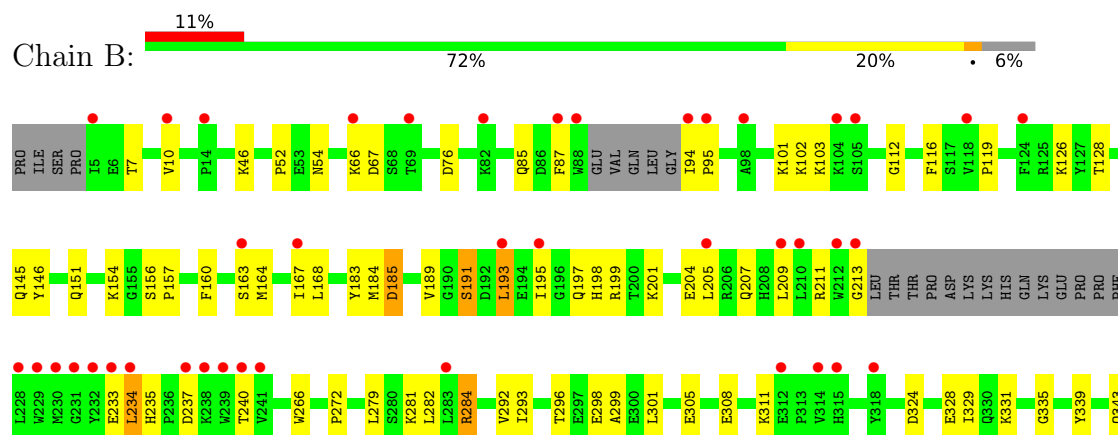
3 Residue-property plots

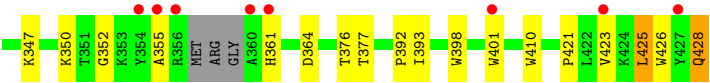
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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	162.87Å 73.54Å 109.23Å 90.00° 100.47° 90.00°	Depositor
Resolution (Å)	48.90 – 2.30 48.90 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.90-2.30) 99.3 (48.90-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.233 , 0.280 0.236 , 0.281	Depositor DCC
R_{free} test set	2749 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	61.3	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 39.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7758	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.44% 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: LE8

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	2/4468 (0.0%)	0.61	2/6087 (0.0%)
2	B	0.39	0/3392	0.58	0/4612
All	All	0.41	2/7860 (0.0%)	0.59	2/10699 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	211[A]	ARG	C-O	6.72	1.32	1.24
1	A	211[B]	ARG	C-O	6.72	1.32	1.24

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	211[A]	ARG	CA-C-O	7.67	128.79	120.20
1	A	211[B]	ARG	CA-C-O	7.67	128.79	120.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4350	0	4287	92	0
2	B	3294	0	3276	66	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	24	10	0	1	0
4	A	54	0	0	3	0
4	B	26	0	0	0	0
All	All	7748	10	7563	154	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (154) 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:11:LYS:O	1:A:85:GLN:HG2	1.83	0.78
2:B:393:ILE:HD13	2:B:398:TRP:HB2	1.66	0.76
1:A:28:GLU:HG3	1:A:135:ILE:HD12	1.67	0.75
2:B:128:THR:OG1	2:B:146:TYR:HB2	1.90	0.71
1:A:458:VAL:HG22	1:A:548:VAL:HB	1.77	0.67
2:B:425:LEU:O	2:B:428:GLN:HG3	1.96	0.65
2:B:279:LEU:HA	2:B:282:LEU:HD12	1.79	0.64
2:B:183:TYR:CE2	2:B:184:MET:HG2	2.35	0.62
1:A:405:TYR:CE2	1:A:407:GLN:HB2	2.37	0.60
2:B:10:VAL:HG13	2:B:87:PHE:HZ	1.67	0.59
1:A:23:GLN:OE1	1:A:60:VAL:HG12	2.03	0.59
1:A:278:GLN:O	1:A:282:LEU:HG	2.03	0.58
2:B:233:GLU:O	2:B:234:LEU:HB2	2.02	0.58
1:A:417:VAL:HG22	1:A:419:THR:HG23	1.87	0.57
2:B:207:GLN:O	2:B:211:ARG:HB2	2.05	0.57
1:A:17:ASP:O	1:A:83:ARG:HD3	2.04	0.57
2:B:240:THR:O	2:B:350:LYS:HG2	2.05	0.56
1:A:311:LYS:HG3	1:A:312:GLU:N	2.20	0.56
1:A:260:LEU:HD21	1:A:303:LEU:HD13	1.85	0.56
2:B:335:GLY:O	2:B:355:ALA:HA	2.06	0.56
1:A:240:THR:HG23	1:A:241:VAL:O	2.06	0.55
1:A:244:ILE:CD1	1:A:267:ALA:HB2	2.36	0.55
2:B:234:LEU:HD11	2:B:377:THR:CG2	2.36	0.55
2:B:163:SER:O	2:B:167:ILE:HG13	2.07	0.55
1:A:73:LYS:HE2	1:A:75:VAL:CG2	2.38	0.54
2:B:126:LYS:HA	2:B:145:GLN:OE1	2.06	0.54
1:A:109:LEU:HD11	1:A:205:LEU:HD23	1.89	0.54
1:A:412:PRO:HD3	2:B:401:TRP:CZ2	2.44	0.53
1:A:478:GLU:HG2	4:A:717:HOH:O	2.09	0.53
2:B:331:LYS:NZ	2:B:364:ASP:OD2	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:ILE:HD12	1:A:267:ALA:HB2	1.88	0.53
1:A:246:LEU:CD1	1:A:310:LEU:HD12	2.39	0.52
2:B:339:TYR:CZ	2:B:352:GLY:HA3	2.44	0.52
1:A:12:LEU:HD11	1:A:127:TYR:CE1	2.45	0.52
2:B:301:LEU:HG	2:B:305:GLU:OE2	2.09	0.52
2:B:195:ILE:HD11	2:B:199:ARG:NH2	2.24	0.52
1:A:31:ILE:O	1:A:35:VAL:HG23	2.09	0.52
1:A:111:VAL:HG22	1:A:185:ASP:O	2.10	0.52
1:A:225:PRO:HG2	1:A:236:PRO:HG3	1.92	0.52
2:B:164:MET:O	2:B:168:LEU:HG	2.09	0.51
1:A:443:ASP:HB2	1:A:548:VAL:HG13	1.92	0.51
2:B:209:LEU:O	2:B:213:GLY:N	2.44	0.51
1:A:97:PRO:HG2	1:A:232:TYR:CD1	2.46	0.51
1:A:30:LYS:HE3	1:A:62:ALA:HB3	1.91	0.51
1:A:207:GLN:O	1:A:210:LEU:HB2	2.11	0.51
1:A:111:VAL:O	1:A:111:VAL:HG23	2.11	0.51
1:A:266:TRP:O	1:A:269:GLN:HG2	2.11	0.51
1:A:451:LYS:HB3	1:A:471:ASN:HA	1.93	0.50
1:A:454:LYS:NZ	1:A:554:ALA:HB3	2.27	0.50
2:B:112:GLY:HA3	2:B:185:ASP:HB3	1.93	0.50
2:B:112:GLY:CA	2:B:185:ASP:HB3	2.41	0.50
1:A:246:LEU:HD11	1:A:310:LEU:HD12	1.94	0.50
1:A:155:GLY:O	1:A:159:ILE:HG13	2.12	0.50
2:B:201:LYS:O	2:B:204:GLU:HB2	2.12	0.49
2:B:292:VAL:C	2:B:293:ILE:HD13	2.37	0.49
2:B:195:ILE:O	2:B:198:HIS:HB3	2.13	0.49
1:A:19:PRO:HG3	1:A:80:LEU:HB2	1.95	0.49
1:A:74:LEU:C	1:A:74:LEU:HD23	2.37	0.49
2:B:329:ILE:O	2:B:392:PRO:HG3	2.12	0.49
1:A:246:LEU:HG	1:A:310:LEU:HD12	1.93	0.49
1:A:253:THR:HA	1:A:292:VAL:HA	1.93	0.49
1:A:167:ILE:O	1:A:170:PRO:HD2	2.13	0.48
2:B:189:VAL:HG21	2:B:205:LEU:HD23	1.94	0.48
2:B:282:LEU:HD11	2:B:299:ALA:HB1	1.95	0.48
1:A:184:MET:H	1:A:184:MET:HE2	1.79	0.48
1:A:423:VAL:O	4:A:701:HOH:O	2.20	0.48
2:B:103:LYS:HB3	2:B:191:SER:O	2.14	0.48
1:A:226:PRO:HB3	1:A:235:HIS:CD2	2.49	0.48
1:A:73:LYS:HE2	1:A:75:VAL:HG23	1.96	0.48
2:B:46:LYS:HE2	2:B:116:PHE:HB3	1.96	0.47
1:A:58:THR:N	1:A:129:ALA:O	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:THR:O	1:A:203:GLU:HB2	2.14	0.47
1:A:109:LEU:CD1	1:A:205:LEU:HD23	2.45	0.47
1:A:319:TYR:OH	1:A:385:LYS:HE2	2.15	0.47
2:B:421:PRO:HB3	2:B:423:VAL:HG12	1.96	0.47
1:A:130:PHE:CZ	1:A:144:TYR:HB2	2.50	0.47
2:B:7:THR:HG22	2:B:119:PRO:HG2	1.97	0.47
1:A:267:ALA:HB1	1:A:271:TYR:HD2	1.79	0.47
1:A:329:ILE:HD12	1:A:391:LEU:HD22	1.96	0.47
2:B:195:ILE:HD11	2:B:199:ARG:HH21	1.81	0.46
1:A:450:THR:OG1	1:A:452:LEU:HB2	2.15	0.46
2:B:428:GLN:HE21	2:B:428:GLN:HB2	1.52	0.46
1:A:252:TRP:CZ3	1:A:260:LEU:HD22	2.50	0.46
1:A:311:LYS:CG	1:A:312:GLU:N	2.78	0.46
1:A:373:GLN:OE1	2:B:401:TRP:NE1	2.36	0.46
1:A:182:GLN:HB2	1:A:187:LEU:CD2	2.46	0.46
1:A:329:ILE:HD12	1:A:391:LEU:CD2	2.45	0.46
2:B:282:LEU:HD21	2:B:296:THR:HG23	1.98	0.46
2:B:281:LYS:O	2:B:284:ARG:HB2	2.16	0.45
1:A:229:TRP:CD2	1:A:230:MET:HG2	2.51	0.45
1:A:306:ASN:O	1:A:310:LEU:HG	2.17	0.45
2:B:101:LYS:HE2	2:B:102:LYS:HE3	1.98	0.45
1:A:23:GLN:HG3	1:A:133:PRO:HG3	1.99	0.45
2:B:308:GLU:HA	2:B:311:LYS:HD3	1.99	0.45
2:B:151:GLN:HB3	2:B:185:ASP:OD2	2.17	0.45
1:A:63:ILE:HG13	1:A:63:ILE:O	2.17	0.45
1:A:328:GLU:HG2	1:A:330:GLN:NE2	2.32	0.45
1:A:246:LEU:CG	1:A:310:LEU:HD12	2.48	0.44
2:B:156:SER:N	2:B:157:PRO:HD2	2.33	0.44
2:B:191:SER:OG	2:B:193:LEU:HG	2.18	0.44
1:A:111:VAL:HG22	1:A:185:ASP:C	2.43	0.44
1:A:18:GLY:HA3	1:A:56:TYR:CE1	2.53	0.44
2:B:191:SER:HB3	2:B:198:HIS:CE1	2.52	0.44
1:A:26:LEU:HD22	1:A:30:LYS:HE2	2.00	0.44
1:A:491:LEU:HD23	1:A:491:LEU:HA	1.78	0.44
1:A:268:SER:HA	1:A:274:ILE:HD12	2.00	0.44
2:B:94:ILE:HG13	2:B:95:PRO:HD2	1.99	0.44
2:B:425:LEU:H	2:B:425:LEU:HG	1.58	0.44
1:A:106:VAL:HG11	3:A:601:LE8:CL1	2.55	0.43
2:B:101:LYS:HG3	2:B:102:LYS:HG3	1.99	0.43
2:B:197:GLN:O	2:B:201:LYS:HG2	2.18	0.43
1:A:213:GLY:C	1:A:214:LEU:HD23	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:ASP:OD2	1:A:549:ASP:HA	2.18	0.43
2:B:292:VAL:O	2:B:293:ILE:HD13	2.18	0.43
1:A:501:TYR:CZ	1:A:505:ILE:HD11	2.54	0.43
2:B:282:LEU:HD11	2:B:299:ALA:CB	2.48	0.43
2:B:339:TYR:CE1	2:B:352:GLY:HA3	2.53	0.43
1:A:101:LYS:N	1:A:101:LYS:HD3	2.34	0.43
1:A:162:SER:OG	2:B:52:PRO:HG3	2.18	0.43
1:A:246:LEU:HG	1:A:310:LEU:CD1	2.49	0.42
2:B:324:ASP:O	2:B:343:GLN:HG2	2.19	0.42
2:B:66:LYS:O	2:B:67:ASP:HB2	2.19	0.42
2:B:193:LEU:HG	2:B:193:LEU:H	1.67	0.42
1:A:88:TRP:HB2	2:B:54:ASN:O	2.20	0.42
1:A:108:VAL:HA	1:A:187:LEU:O	2.19	0.42
1:A:441:TYR:O	1:A:457:TYR:HA	2.18	0.42
1:A:244:ILE:HG22	1:A:310:LEU:HD13	2.01	0.42
1:A:298:GLU:N	1:A:298:GLU:OE1	2.52	0.42
1:A:341:ILE:O	1:A:349:LEU:HD12	2.19	0.42
2:B:266:TRP:CE3	2:B:426:TRP:HB3	2.55	0.42
1:A:365:VAL:HG11	1:A:401:TRP:CG	2.54	0.42
2:B:298:GLU:O	2:B:299:ALA:C	2.62	0.42
2:B:94:ILE:HG12	2:B:95:PRO:O	2.19	0.42
2:B:234:LEU:HD11	2:B:377:THR:HG21	2.02	0.42
1:A:28:GLU:O	1:A:32:LYS:HG3	2.20	0.41
1:A:156:SER:HB2	1:A:157:PRO:HD3	2.01	0.41
1:A:363:ASN:HA	1:A:511:ASP:OD1	2.19	0.41
1:A:363:ASN:OD1	1:A:363:ASN:C	2.62	0.41
1:A:366:LYS:O	1:A:370:GLU:HG3	2.20	0.41
1:A:516:GLU:O	1:A:520:GLN:HG3	2.20	0.41
2:B:154:LYS:HA	2:B:184:MET:HE1	2.02	0.41
2:B:328:GLU:O	2:B:339:TYR:HA	2.21	0.41
1:A:442:VAL:HB	1:A:481:ALA:HB1	2.02	0.41
1:A:530:LYS:HA	4:A:710:HOH:O	2.20	0.41
2:B:76:ASP:OD1	2:B:76:ASP:C	2.60	0.41
2:B:282:LEU:CD2	2:B:296:THR:HG23	2.51	0.41
1:A:-1:MET:HE3	1:A:0:VAL:O	2.21	0.41
1:A:249:LYS:O	1:A:252:TRP:NE1	2.53	0.41
1:A:269:GLN:HA	1:A:351:THR:O	2.21	0.41
1:A:454:LYS:HZ2	1:A:554:ALA:HB3	1.85	0.41
2:B:376:THR:HG21	2:B:410:TRP:CZ3	2.56	0.41
2:B:160:PHE:O	2:B:160:PHE:CD1	2.74	0.40
1:A:442:VAL:HG12	1:A:457:TYR:HB3	2.03	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	542/557 (97%)	522 (96%)	19 (4%)	1 (0%)	43	55
2	B	397/428 (93%)	364 (92%)	28 (7%)	5 (1%)	9	10
All	All	939/985 (95%)	886 (94%)	47 (5%)	6 (1%)	21	27

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	237	ASP
2	B	85	GLN
2	B	234	LEU
2	B	272	PRO
2	B	361	HIS
1	A	18	GLY

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	460/495 (93%)	446 (97%)	14 (3%)	36	53
2	B	357/390 (92%)	350 (98%)	7 (2%)	48	67
All	All	817/885 (92%)	796 (97%)	21 (3%)	40	59

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-1	MET
1	A	0	VAL
1	A	7	THR
1	A	73	LYS
1	A	85	GLN
1	A	105	SER
1	A	113	ASP
1	A	210	LEU
1	A	349	LEU
1	A	363	ASN
1	A	399	GLU
1	A	450	THR
1	A	459	THR
1	A	542	ILE
2	B	185	ASP
2	B	191	SER
2	B	193	LEU
2	B	235	HIS
2	B	284	ARG
2	B	425	LEU
2	B	428	GLN

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 ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	LE8	A	601	-	26,26,26	1.85	1 (3%)	30,36,36	1.92	7 (23%)

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	LE8	A	601	-	-	0/10/10/10	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	LE8	C5-C4	8.72	1.39	1.34

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	LE8	O1-C4-C5	5.09	109.06	107.02
3	A	601	LE8	C4-C5-N1	-4.16	108.29	110.23
3	A	601	LE8	C10-C12-CL1	3.98	122.83	119.45
3	A	601	LE8	C14-C2-C1	3.74	119.59	114.54
3	A	601	LE8	C12-C10-C11	2.53	123.81	121.18
3	A	601	LE8	F2-C14-C2	2.52	120.78	117.64
3	A	601	LE8	C15-C14-C2	-2.19	120.01	123.99

There are no chirality outliers.

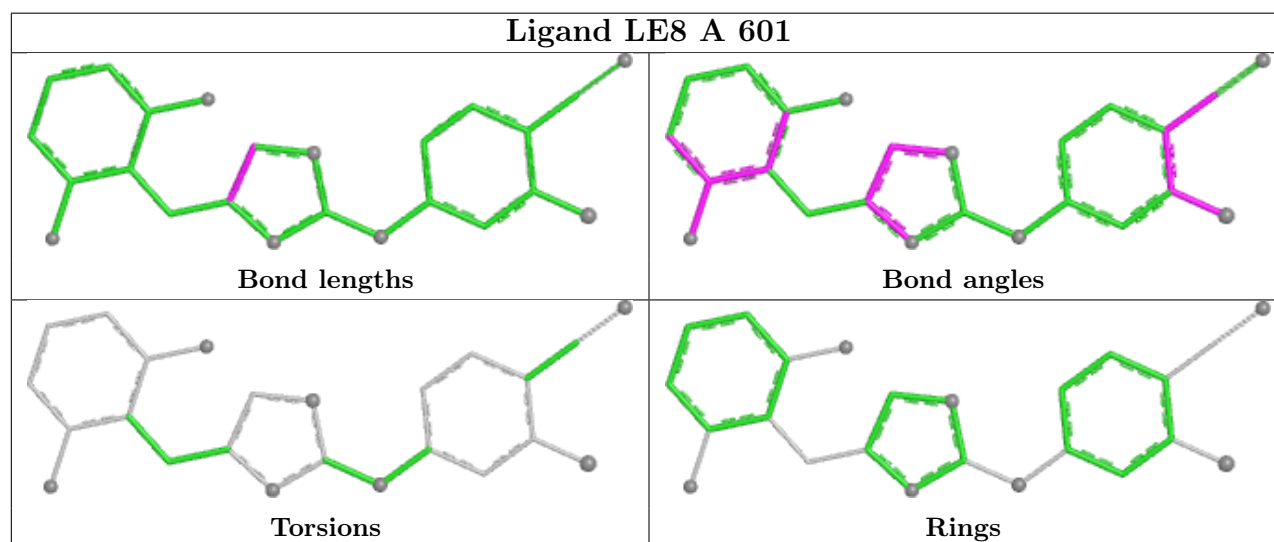
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	LE8	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [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	549/557 (98%)	0.84	86 (15%) 5 6	35, 72, 129, 162	2 (0%)
2	B	402/428 (93%)	0.83	49 (12%) 8 9	28, 67, 136, 168	3 (0%)
All	All	951/985 (96%)	0.84	135 (14%) 6 7	28, 71, 133, 168	5 (0%)

All (135) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	228	LEU	6.0
2	B	356	ARG	5.8
2	B	233	GLU	5.6
1	A	289	LEU	5.3
2	B	87	PHE	4.9
1	A	257	ILE	4.6
1	A	223	LYS	4.6
1	A	256	ASP	4.4
1	A	285	GLY	4.3
1	A	90	VAL	4.2
1	A	315[A]	HIS	4.0
2	B	94	ILE	4.0
1	A	220	LYS	4.0
1	A	258	GLN	4.0
2	B	232	TYR	4.0
2	B	315[A]	HIS	3.9
2	B	355	ALA	3.9
2	B	241	VAL	3.9
1	A	554	ALA	3.9
1	A	543	GLY	3.9
2	B	360	ALA	3.9
1	A	115	TYR	3.8
1	A	292	VAL	3.8
1	A	24	TRP	3.8

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Mol	Chain	Res	Type	RSRZ
2	B	5	ILE	3.8
1	A	246	LEU	3.7
2	B	82	LYS	3.7
2	B	195	ILE	3.7
2	B	193	LEU	3.7
2	B	88	TRP	3.6
1	A	114	ALA	3.6
2	B	124	PHE	3.6
2	B	98	ALA	3.6
2	B	354	TYR	3.5
2	B	240	THR	3.4
1	A	260	LEU	3.3
1	A	116	PHE	3.3
1	A	291	GLU	3.3
2	B	10	VAL	3.3
1	A	244	ILE	3.3
1	A	247	PRO	3.2
2	B	229	TRP	3.2
1	A	307	ARG	3.2
1	A	314	VAL	3.2
2	B	361	HIS	3.1
1	A	214	LEU	3.1
2	B	95	PRO	3.1
1	A	245	VAL	3.1
2	B	210	LEU	3.1
2	B	238	LYS	3.1
1	A	219	LYS	3.1
1	A	254	VAL	3.0
1	A	310	LEU	3.0
1	A	317	VAL	3.0
1	A	250	ASP	3.0
1	A	183	TYR	2.9
2	B	212	TRP	2.9
1	A	63	ILE	2.9
2	B	234	LEU	2.9
2	B	237	ASP	2.9
1	A	71	TRP	2.8
1	A	309	ILE	2.8
1	A	283	LEU	2.8
2	B	230	MET	2.8
1	A	252	TRP	2.8
1	A	241	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	2	ILE	2.8
1	A	91	GLN	2.8
2	B	312	GLU	2.8
2	B	318	TYR	2.8
1	A	263	LYS	2.8
1	A	135	ILE	2.7
2	B	69	THR	2.7
2	B	66	LYS	2.7
1	A	195	ILE	2.7
2	B	427	TYR	2.7
1	A	313	PRO	2.7
1	A	295	LEU	2.7
1	A	227	PHE	2.6
1	A	109	LEU	2.6
2	B	239	TRP	2.6
2	B	401	TRP	2.6
1	A	346	PHE	2.6
1	A	215	THR	2.5
1	A	271	TYR	2.5
1	A	68	SER	2.5
1	A	92	LEU	2.5
1	A	61	PHE	2.4
1	A	261	VAL	2.4
1	A	238	LYS	2.4
2	B	118	VAL	2.4
1	A	303	LEU	2.4
1	A	264	LEU	2.4
1	A	312	GLU	2.4
2	B	213	GLY	2.4
1	A	270	ILE	2.4
2	B	423	VAL	2.4
1	A	218	ASP	2.3
1	A	66	LYS	2.3
1	A	112	GLY	2.3
1	A	259	LYS	2.3
2	B	167	ILE	2.3
1	A	7	THR	2.3
1	A	187	LEU	2.3
1	A	301	LEU	2.3
1	A	224	GLU	2.3
1	A	184	MET	2.2
2	B	231	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	299	ALA	2.2
1	A	253	THR	2.2
1	A	144	TYR	2.2
2	B	209	LEU	2.2
1	A	65	LYS	2.2
1	A	274	ILE	2.2
1	A	277	ARG	2.2
1	A	108	VAL	2.2
1	A	25	PRO	2.2
1	A	298	GLU	2.2
1	A	202	ILE	2.1
1	A	111	VAL	2.1
1	A	118	VAL	2.1
1	A	168	LEU	2.1
2	B	283	LEU	2.1
1	A	0	VAL	2.1
2	B	314	VAL	2.1
2	B	163	SER	2.1
1	A	194	GLU	2.1
2	B	205	LEU	2.1
1	A	88	TRP	2.1
2	B	14	PRO	2.1
1	A	130	PHE	2.1
1	A	22	LYS	2.0
2	B	105	SER	2.0
1	A	127	TYR	2.0
2	B	104	LYS	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.

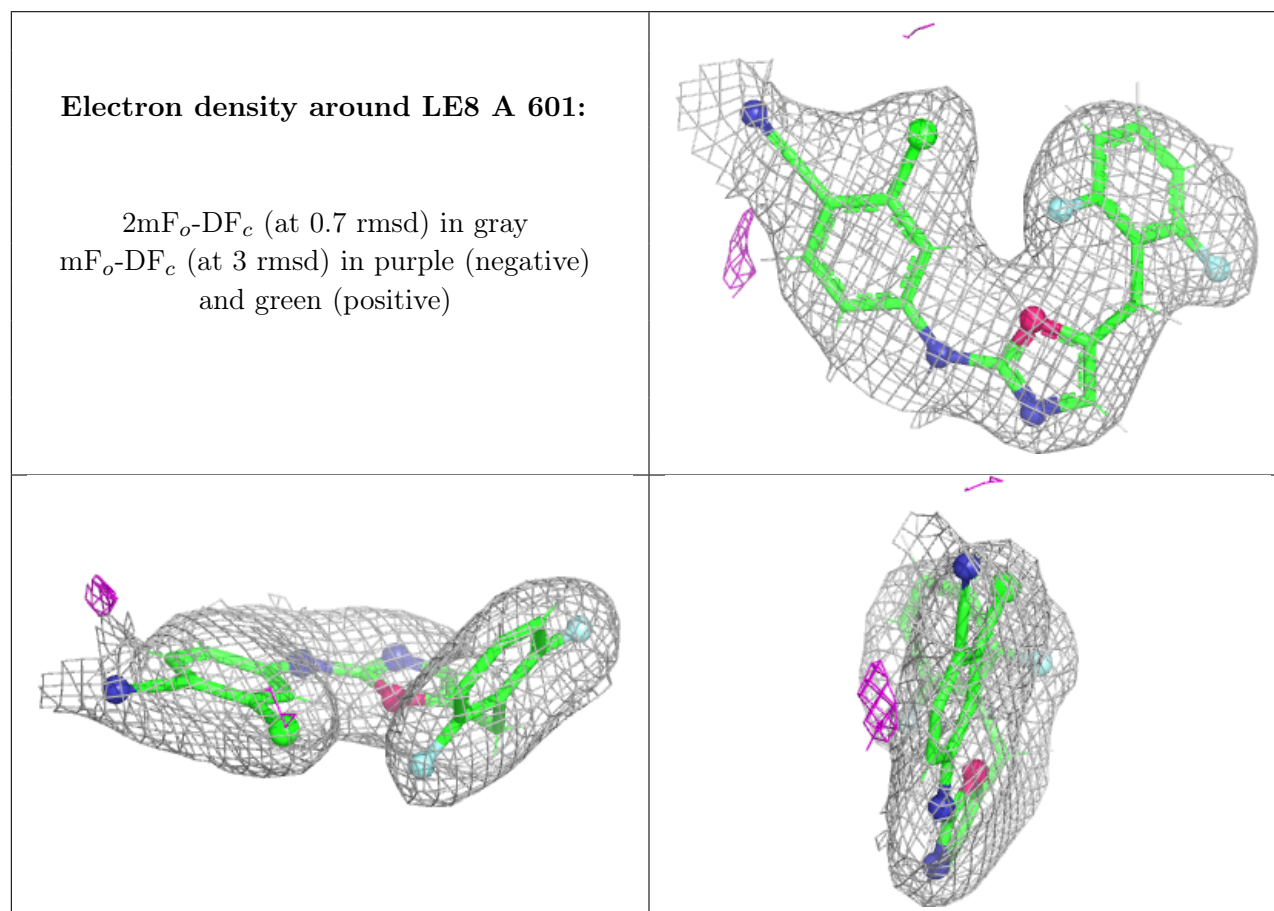
6.4 Ligands [i](#)

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(Å ²)	Q<0.9
3	LE8	A	601	24/24	0.94	0.08	54,65,80,108	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 ⓘ

There are no such residues in this entry.