



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:33 AM UTC

PDB ID : 3DYA / pdb_00003dya
Title : HIV-1 RT with non-nucleoside inhibitor annulated Pyrazole 1
Authors : Harris, S.F.; Villasenor, A.
Deposited on : 2008-07-25
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

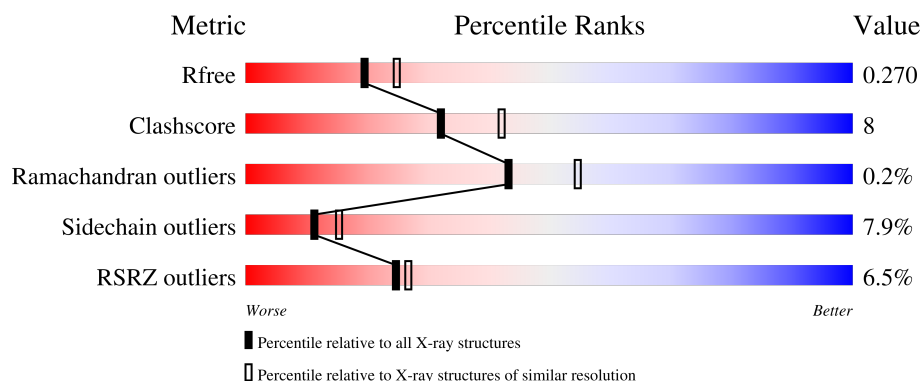
1 Overall quality at a glance

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	561	4% 78% 15% • •
2	B	440	9% 72% 16% • 9%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8161 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

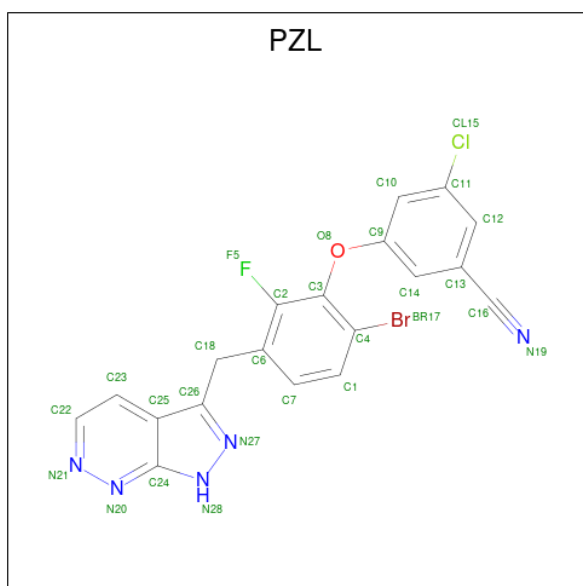
- Molecule 1 is a protein called REVERSE TRANSCRIPTASE/RIBONUCLEASE H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	551	Total	C	N	O	S	0	1	0
			4495	2906	751	830	8			

- Molecule 2 is a protein called p51 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	402	Total	C	N	O	S	0	0	0
			3327	2170	546	604	7			

- Molecule 3 is 3-[6-bromo-2-fluoro-3-(1H-pyrazolo[3,4-c]pyridazin-3-ylmethyl)phenoxy]-5-chlorobenzonitrile (CCD ID: PZL) (formula: C₁₉H₁₀BrClFN₅O).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	A	1	Total	Br	C	Cl	F	N	O	0	0
			28	1	19	1	1	5	1		

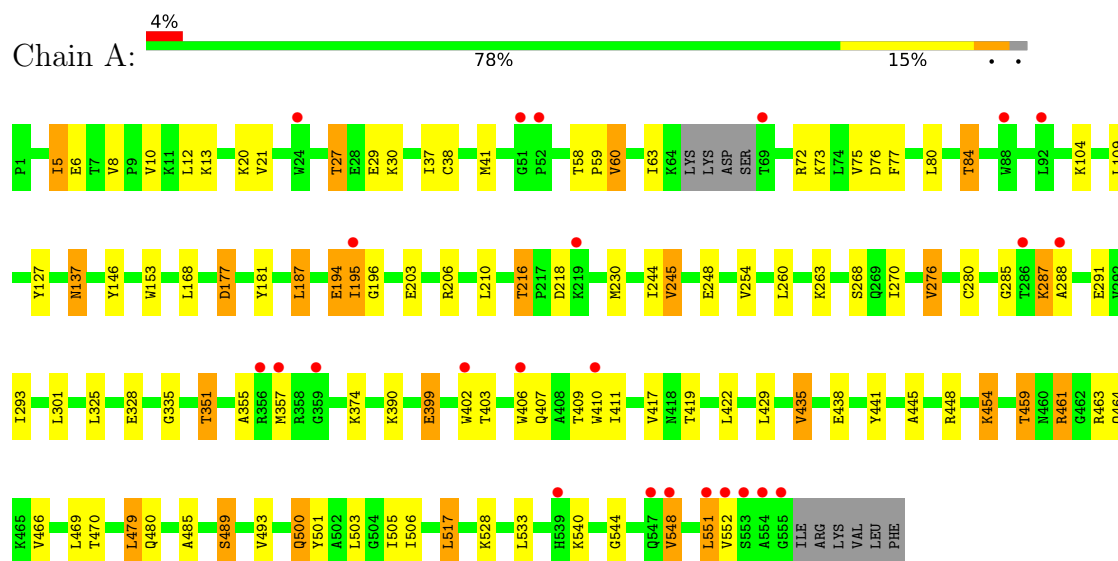
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	183	Total 183	O 183	0	0
4	B	128	Total 128	O 128	0	0

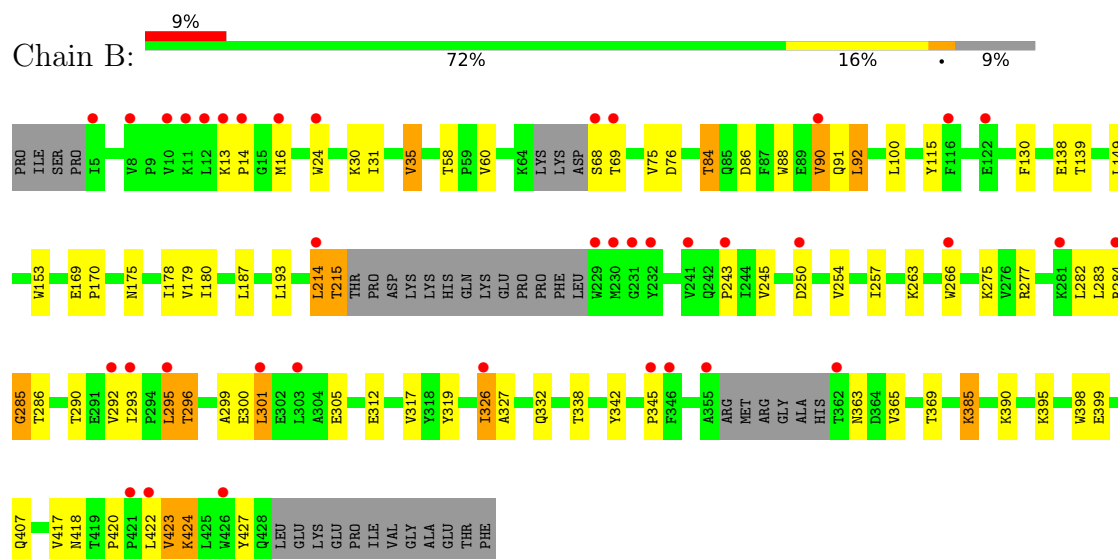
3 Residue-property plots [i](#)

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 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	117.66Å 153.67Å 155.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.98 – 2.30 46.98 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.6 (46.98-2.30) 96.5 (46.98-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.218 , 0.266 0.222 , 0.270	Depositor DCC
R_{free} test set	3093 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	52.5	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 40.6	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	8161	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% 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: PZL

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	0.74	0/4612	0.87	3/6267 (0.0%)
2	B	0.72	0/3421	0.85	1/4650 (0.0%)
All	All	0.73	0/8033	0.86	4/10917 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	493	VAL	N-CA-C	5.70	115.35	108.06
1	A	13	LYS	CA-C-N	5.28	126.44	119.84
1	A	13	LYS	C-N-CA	5.28	126.44	119.84
2	B	214	LEU	N-CA-C	5.16	114.95	108.45

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	4495	0	4536	74	0
2	B	3327	0	3348	63	0
3	A	28	0	10	0	0
4	A	183	0	0	5	0
4	B	128	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	8161	0	7894	126	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 8.

All (126) 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:37:ILE:HG22	1:A:41:MET:HE2	1.19	1.09
1:A:500:GLN:NE2	2:B:422:LEU:HD12	1.66	1.08
1:A:268:SER:O	1:A:351:THR:HG22	1.71	0.89
2:B:84:THR:HG21	2:B:153:TRP:HE1	1.38	0.88
1:A:27:THR:HG21	4:A:660:HOH:O	1.75	0.85
1:A:80:LEU:O	1:A:84:THR:HG22	1.76	0.85
2:B:326:ILE:HD13	2:B:390:LYS:HD2	1.58	0.85
1:A:37:ILE:CG2	1:A:41:MET:HE2	2.08	0.79
1:A:84:THR:HG21	1:A:153:TRP:HE1	1.49	0.77
1:A:461:ARG:HG2	1:A:461:ARG:HH11	1.50	0.76
2:B:254:VAL:HG13	2:B:283:LEU:HD22	1.68	0.75
1:A:37:ILE:HG22	1:A:41:MET:CE	2.11	0.74
2:B:138:GLU:HG2	2:B:139:THR:HG23	1.71	0.73
1:A:406:TRP:CH2	2:B:418:ASN:HA	2.24	0.72
1:A:406:TRP:CZ3	1:A:407:GLN:HG2	2.25	0.71
2:B:365:VAL:O	2:B:369:THR:HG23	1.92	0.69
1:A:216:THR:HG22	4:A:563:HOH:O	1.92	0.68
1:A:466:VAL:CG2	1:A:551:LEU:HD12	2.24	0.68
2:B:24:TRP:HB2	4:B:443:HOH:O	1.94	0.67
1:A:485:ALA:O	1:A:489:SER:HB2	1.96	0.66
1:A:417:VAL:HG22	1:A:419:THR:HG23	1.77	0.66
1:A:435:VAL:HG23	2:B:290:THR:HG21	1.78	0.65
1:A:73:LYS:NZ	1:A:146:TYR:OH	2.30	0.65
2:B:296:THR:HG23	2:B:299:ALA:CB	2.27	0.64
1:A:27:THR:HG22	1:A:30:LYS:H	1.62	0.63
2:B:369:THR:HG22	2:B:398:TRP:CH2	2.35	0.61
2:B:91:GLN:HG2	2:B:92:LEU:HD13	1.82	0.61
2:B:295:LEU:HD12	2:B:300:GLU:OE1	1.99	0.61
2:B:326:ILE:HD12	2:B:327:ALA:N	2.15	0.60
1:A:409:THR:HG21	4:A:567:HOH:O	2.01	0.60
1:A:254:VAL:HG22	1:A:293:ILE:HD11	1.82	0.60
2:B:424:LYS:NZ	4:B:485:HOH:O	2.34	0.60
1:A:454:LYS:HE3	1:A:466:VAL:HG11	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:VAL:HG23	1:A:551:LEU:HD12	1.85	0.58
2:B:86:ASP:HA	2:B:90:VAL:HG13	1.85	0.58
2:B:254:VAL:HG13	2:B:283:LEU:CD2	2.33	0.58
2:B:301:LEU:HD22	4:B:482:HOH:O	2.02	0.58
2:B:58:THR:HG23	2:B:76:ASP:O	2.05	0.56
2:B:332:GLN:HG3	2:B:338:THR:HG23	1.88	0.56
1:A:12:LEU:HD11	1:A:127:TYR:CE1	2.41	0.56
1:A:503:LEU:HD12	1:A:533:LEU:CD2	2.36	0.55
2:B:266:TRP:HZ2	2:B:427:TYR:HH	1.54	0.55
1:A:406:TRP:CZ3	1:A:407:GLN:CG	2.90	0.54
2:B:84:THR:HG23	2:B:88:TRP:HD1	1.73	0.54
2:B:243:PRO:O	2:B:245:VAL:HG13	2.07	0.54
2:B:296:THR:HG23	2:B:299:ALA:HB2	1.89	0.53
2:B:266:TRP:HZ2	2:B:427:TYR:OH	1.92	0.53
2:B:420:PRO:HB2	2:B:423:VAL:HG13	1.90	0.53
1:A:60:VAL:HG12	1:A:75:VAL:HG22	1.90	0.52
1:A:276:VAL:HG13	1:A:280:CYS:SG	2.50	0.52
1:A:8:VAL:O	1:A:10:VAL:HG23	2.10	0.52
1:A:459:THR:O	2:B:286:THR:HG21	2.09	0.52
2:B:266:TRP:CZ2	2:B:427:TYR:CZ	2.97	0.52
1:A:41:MET:HE1	1:A:73:LYS:HD3	1.90	0.52
1:A:429:LEU:HD11	1:A:506:ILE:HG22	1.91	0.51
2:B:84:THR:HG23	2:B:88:TRP:CD1	2.46	0.51
2:B:301:LEU:HD12	2:B:305:GLU:OE2	2.11	0.51
2:B:296:THR:HG23	2:B:299:ALA:HB3	1.93	0.50
1:A:84:THR:HG21	1:A:153:TRP:NE1	2.24	0.50
1:A:177:ASP:OD1	1:A:177:ASP:C	2.55	0.50
1:A:245:VAL:O	1:A:263:LYS:NZ	2.44	0.50
2:B:68:SER:OG	2:B:69:THR:N	2.44	0.50
1:A:41:MET:HE1	1:A:73:LYS:CD	2.42	0.49
1:A:438:GLU:HG3	1:A:461:ARG:HD3	1.94	0.48
2:B:395:LYS:NZ	2:B:399:GLU:OE1	2.46	0.48
1:A:435:VAL:CG2	2:B:290:THR:HG21	2.43	0.48
1:A:469:LEU:HD21	1:A:480:GLN:HG2	1.95	0.48
1:A:75:VAL:HG11	1:A:77:PHE:CZ	2.49	0.48
1:A:27:THR:CG2	1:A:30:LYS:H	2.25	0.47
1:A:137:ASN:ND2	4:A:585:HOH:O	2.46	0.47
2:B:326:ILE:CD1	2:B:390:LYS:HD2	2.38	0.47
1:A:445:ALA:HB3	1:A:552:VAL:HG12	1.96	0.47
2:B:60:VAL:HG12	2:B:75:VAL:HG22	1.97	0.46
1:A:287:LYS:HB3	1:A:291:GLU:OE1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:TRP:CE3	2:B:363:ASN:HB2	2.51	0.45
1:A:503:LEU:HD12	1:A:533:LEU:HD23	1.98	0.45
1:A:500:GLN:CD	2:B:422:LEU:HD12	2.38	0.45
1:A:181:TYR:CD1	2:B:138:GLU:HA	2.52	0.45
1:A:168:LEU:HD11	1:A:187:LEU:HD11	1.99	0.45
1:A:441:TYR:O	1:A:548:VAL:HG21	2.17	0.44
1:A:194:GLU:O	1:A:195:ILE:C	2.60	0.44
1:A:335:GLY:O	1:A:355:ALA:HA	2.17	0.44
2:B:282:LEU:HD11	2:B:296:THR:CG2	2.48	0.44
1:A:21:VAL:HB	1:A:59:PRO:HD3	1.99	0.44
1:A:328:GLU:HG2	1:A:390:LYS:HB2	2.00	0.44
2:B:115:TYR:HB3	2:B:149:LEU:HB2	1.99	0.44
1:A:195:ILE:CG2	1:A:196:GLY:N	2.80	0.44
1:A:406:TRP:HH2	2:B:418:ASN:HA	1.80	0.43
1:A:270:ILE:HA	1:A:351:THR:HB	2.00	0.43
1:A:399:GLU:O	1:A:403:THR:HG23	2.18	0.43
1:A:500:GLN:HE21	2:B:422:LEU:HD12	1.71	0.43
1:A:5:ILE:HD13	1:A:6:GLU:O	2.18	0.43
1:A:58:THR:HG23	1:A:76:ASP:O	2.19	0.43
1:A:38:CYS:HA	1:A:41:MET:HE3	2.01	0.43
1:A:206:ARG:HG2	1:A:216:THR:HG21	2.01	0.43
1:A:459:THR:O	2:B:286:THR:CG2	2.67	0.43
2:B:257:ILE:HD12	2:B:293:ILE:HG21	2.01	0.42
2:B:31:ILE:O	2:B:35:VAL:HG13	2.18	0.42
1:A:109:LEU:HD22	1:A:216:THR:OG1	2.19	0.42
2:B:284:ARG:CG	2:B:285:GLY:N	2.83	0.42
2:B:169:GLU:HB3	2:B:170:PRO:HD3	2.01	0.42
2:B:342:TYR:CE1	2:B:345:PRO:HA	2.55	0.42
2:B:60:VAL:HG11	2:B:130:PHE:CD2	2.55	0.42
2:B:180:ILE:CG2	2:B:187:LEU:HD22	2.49	0.42
1:A:288:ALA:HB3	1:A:291:GLU:HB2	2.01	0.42
1:A:501:TYR:CZ	1:A:505:ILE:HD11	2.54	0.42
2:B:13:LYS:HG2	2:B:14:PRO:CD	2.48	0.42
1:A:27:THR:HG23	1:A:29:GLU:H	1.85	0.42
1:A:399:GLU:HA	1:A:402:TRP:CD1	2.55	0.41
1:A:463:ARG:C	1:A:464:GLN:HG2	2.45	0.41
2:B:30:LYS:NZ	4:B:536:HOH:O	2.52	0.41
2:B:100:LEU:CD1	2:B:179:VAL:HG23	2.50	0.41
2:B:295:LEU:H	2:B:295:LEU:HD23	1.85	0.41
1:A:479:LEU:HB3	1:A:517:LEU:HD13	2.02	0.41
2:B:214:LEU:O	2:B:215:THR:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:282:LEU:HB3	2:B:293:ILE:HD13	2.03	0.41
2:B:266:TRP:CH2	2:B:427:TYR:CZ	3.08	0.41
2:B:369:THR:HG22	2:B:398:TRP:CZ3	2.55	0.40
1:A:407:GLN:HE21	1:A:407:GLN:HB3	1.69	0.40
1:A:544:GLY:O	1:A:548:VAL:HG23	2.21	0.40
1:A:407:GLN:NE2	4:A:623:HOH:O	2.54	0.40
1:A:489:SER:HB3	1:A:528:LYS:NZ	2.37	0.40
2:B:175:ASN:HB3	2:B:178:ILE:HD12	2.04	0.40
2:B:266:TRP:HH2	2:B:427:TYR:CE1	2.40	0.40
2:B:282:LEU:HD11	2:B:296:THR:HG22	2.04	0.40
2:B:319:TYR:OH	2:B:385:LYS:HE3	2.22	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	548/561 (98%)	528 (96%)	19 (4%)	1 (0%)	43	55
2	B	394/440 (90%)	381 (97%)	12 (3%)	1 (0%)	36	46
All	All	942/1001 (94%)	909 (96%)	31 (3%)	2 (0%)	43	55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	285	GLY
2	B	285	GLY

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	492/501 (98%)	447 (91%)	45 (9%)	9	11
2	B	366/400 (92%)	343 (94%)	23 (6%)	16	23
All	All	858/901 (95%)	790 (92%)	68 (8%)	11	15

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	20	LYS
1	A	27	THR
1	A	60	VAL
1	A	63	ILE
1	A	72	ARG
1	A	84	THR
1	A	104	LYS
1	A	137	ASN
1	A	177	ASP
1	A	187	LEU
1	A	194	GLU
1	A	195	ILE
1	A	203	GLU
1	A	210	LEU
1	A	216	THR
1	A	218	ASP
1	A	230	MET
1	A	244	ILE
1	A	245	VAL
1	A	248	GLU
1	A	260	LEU
1	A	276	VAL
1	A	287	LYS
1	A	301	LEU
1	A	325	LEU
1	A	351	THR

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Mol	Chain	Res	Type
1	A	357	MET
1	A	374	LYS
1	A	399	GLU
1	A	411	ILE
1	A	422	LEU
1	A	435	VAL
1	A	448	ARG
1	A	454	LYS
1	A	459	THR
1	A	461	ARG
1	A	470	THR
1	A	479	LEU
1	A	489	SER
1	A	500	GLN
1	A	517	LEU
1	A	540	LYS
1	A	548	VAL
1	A	551	LEU
2	B	16	MET
2	B	35	VAL
2	B	84	THR
2	B	90	VAL
2	B	92	LEU
2	B	193	LEU
2	B	215	THR
2	B	250	ASP
2	B	263	LYS
2	B	275	LYS
2	B	277	ARG
2	B	292	VAL
2	B	295	LEU
2	B	296	THR
2	B	301	LEU
2	B	312	GLU
2	B	317	VAL
2	B	326	ILE
2	B	385	LYS
2	B	407	GLN
2	B	417	VAL
2	B	423	VAL
2	B	424	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	ASN
1	A	145	GLN
1	A	198	HIS
1	A	278	GLN
1	A	332	GLN
1	A	336	GLN
1	A	407	GLN
1	A	428	GLN
1	A	500	GLN
1	A	507	GLN
1	A	524	GLN
2	B	147	ASN
2	B	197	GLN
2	B	208	HIS
2	B	255	ASN
2	B	258	GLN
2	B	265	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](#)

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	PZL	A	562	-	31,31,31	2.24	7 (22%)	39,44,44	2.88	17 (43%)

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	PZL	A	562	-	-	0/10/10/10	0/4/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	562	PZL	C13-C16	-7.87	1.27	1.44
3	A	562	PZL	N21-N20	5.61	1.42	1.34
3	A	562	PZL	C26-N27	3.29	1.35	1.29
3	A	562	PZL	C25-C24	-3.28	1.37	1.41
3	A	562	PZL	C25-C26	-3.12	1.38	1.45
3	A	562	PZL	C3-C4	-2.48	1.35	1.41
3	A	562	PZL	C24-N28	-2.22	1.33	1.35

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	562	PZL	C24-N28-N27	-9.63	105.84	111.18
3	A	562	PZL	C6-C18-C26	-6.34	101.37	113.16
3	A	562	PZL	C24-C25-C26	5.63	108.06	105.02
3	A	562	PZL	C25-C24-N20	-4.24	122.28	126.50
3	A	562	PZL	C7-C6-C2	4.22	119.56	116.46
3	A	562	PZL	F5-C2-C6	3.78	123.11	118.00
3	A	562	PZL	C22-N21-N20	3.55	121.63	118.91
3	A	562	PZL	BR17-C4-C1	3.48	124.46	117.82
3	A	562	PZL	O8-C3-C4	-3.37	115.83	120.61
3	A	562	PZL	C9-O8-C3	3.27	123.55	118.40
3	A	562	PZL	BR17-C4-C3	-3.00	114.19	118.50
3	A	562	PZL	C23-C22-N21	-2.82	119.84	123.66
3	A	562	PZL	C13-C16-N19	-2.71	171.17	177.87
3	A	562	PZL	C23-C25-C24	2.63	119.78	117.16
3	A	562	PZL	C14-C13-C16	2.30	122.66	119.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	562	PZL	N28-C24-N20	2.21	127.69	125.64
3	A	562	PZL	C26-N27-N28	2.20	109.69	105.03

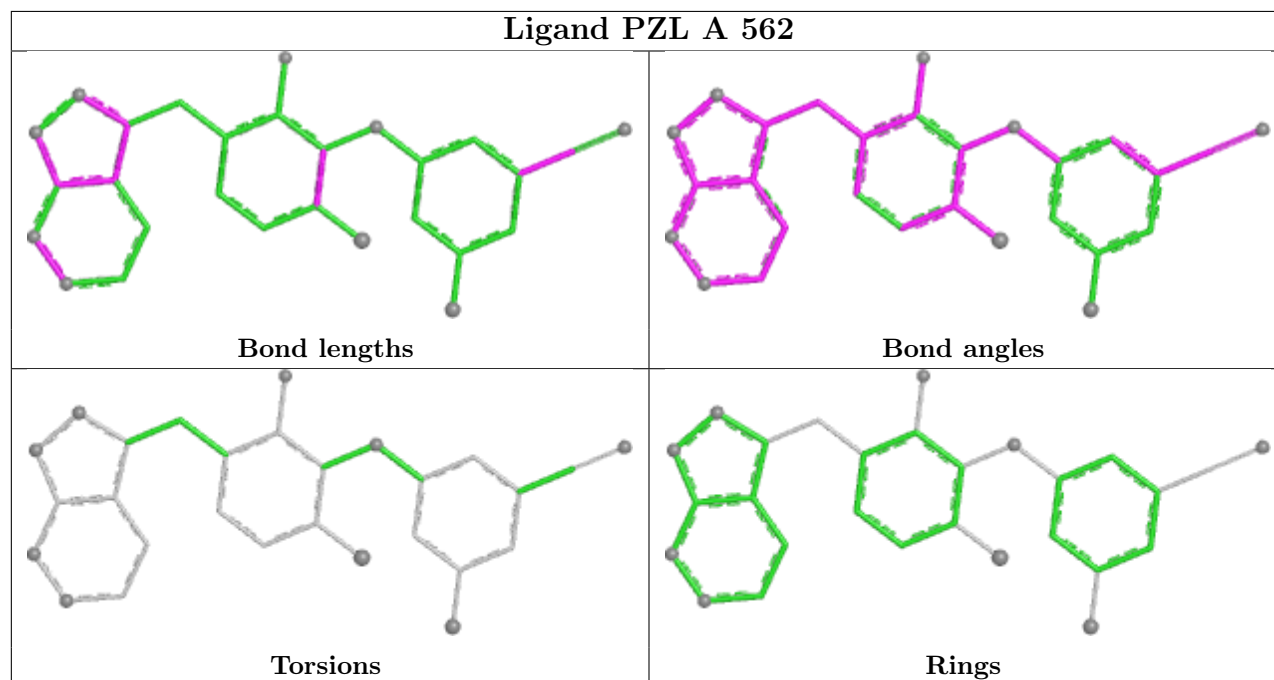
There are no chirality outliers.

There are no torsion outliers.

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	551/561 (98%)	0.60	24 (4%)	39 41	25, 56, 73, 95	1 (0%)
2	B	402/440 (91%)	0.68	38 (9%)	14 15	39, 54, 85, 90	0
All	All	953/1001 (95%)	0.63	62 (6%)	25 27	25, 55, 81, 95	1 (0%)

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	5	ILE	4.7
2	B	232	TYR	4.5
2	B	346	PHE	4.3
2	B	266	TRP	4.3
1	A	554	ALA	4.2
2	B	116	PHE	4.1
2	B	295	LEU	4.0
1	A	555	GLY	3.8
2	B	24	TRP	3.8
2	B	362	THR	3.7
2	B	14	PRO	3.7
1	A	92	LEU	3.4
2	B	12	LEU	3.3
2	B	214	LEU	3.3
1	A	88	TRP	3.3
2	B	231	GLY	3.2
1	A	24	TRP	3.2
2	B	13	LYS	3.2
1	A	553	SER	3.2
1	A	288	ALA	3.1
2	B	230	MET	3.1
1	A	286	THR	3.1
2	B	68	SER	3.1
2	B	241	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	345	PRO	2.9
1	A	547	GLN	2.9
2	B	303	LEU	2.8
1	A	406	TRP	2.8
1	A	52	PRO	2.7
2	B	284	ARG	2.7
1	A	539	HIS	2.7
2	B	292	VAL	2.7
2	B	16	MET	2.6
2	B	281	LYS	2.6
2	B	229	TRP	2.6
2	B	10	VAL	2.6
2	B	422	LEU	2.6
1	A	548	VAL	2.6
1	A	356	ARG	2.4
2	B	426	TRP	2.4
1	A	195	ILE	2.4
1	A	357	MET	2.4
2	B	11	LYS	2.4
1	A	402	TRP	2.4
2	B	355	ALA	2.3
2	B	250	ASP	2.3
1	A	359	GLY	2.3
1	A	219	LYS	2.3
1	A	551	LEU	2.2
1	A	51	GLY	2.2
2	B	421	PRO	2.2
1	A	410	TRP	2.2
2	B	122	GLU	2.1
1	A	69	THR	2.1
2	B	69	THR	2.1
2	B	293	ILE	2.1
1	A	552	VAL	2.1
2	B	8	VAL	2.1
2	B	301	LEU	2.1
2	B	90	VAL	2.1
2	B	243	PRO	2.0
2	B	326	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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](#)

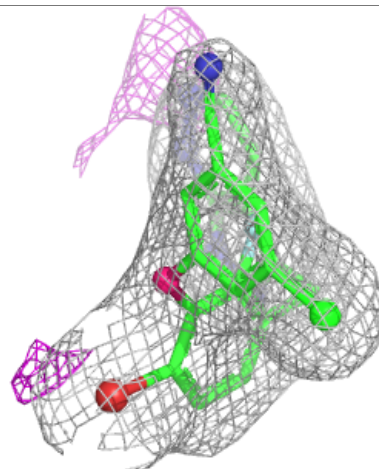
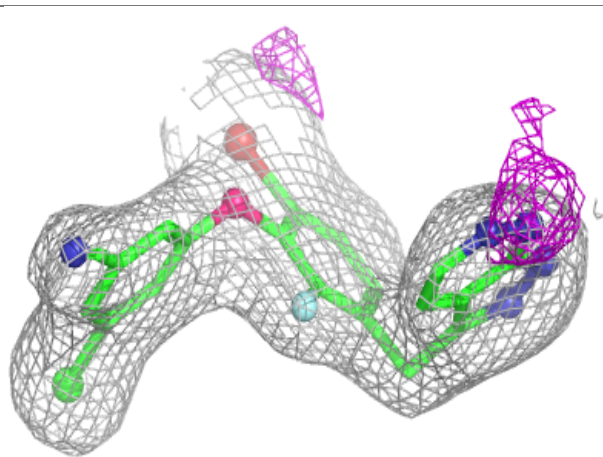
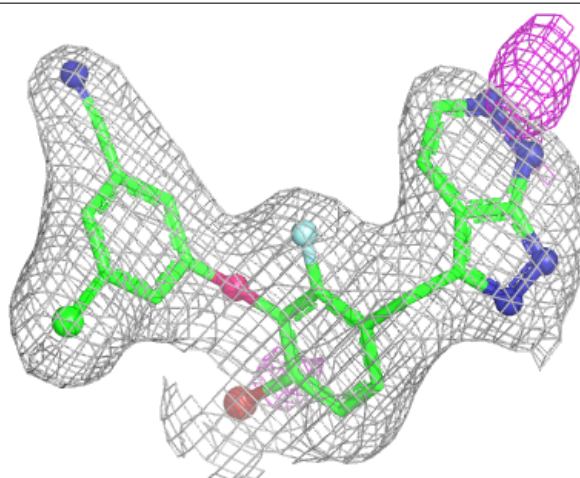
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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	PZL	A	562	28/28	0.97	0.08	46,48,52,53	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 PZL A 562:

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.