



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:21 PM UTC

PDB ID : 3NBP / pdb_00003nbp
Title : HIV-1 reverse transcriptase with aminopyrimidine inhibitor 2
Authors : Harris, S.F.; Villasenor, A.G.
Deposited on : 2010-06-03
Resolution : 2.95 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

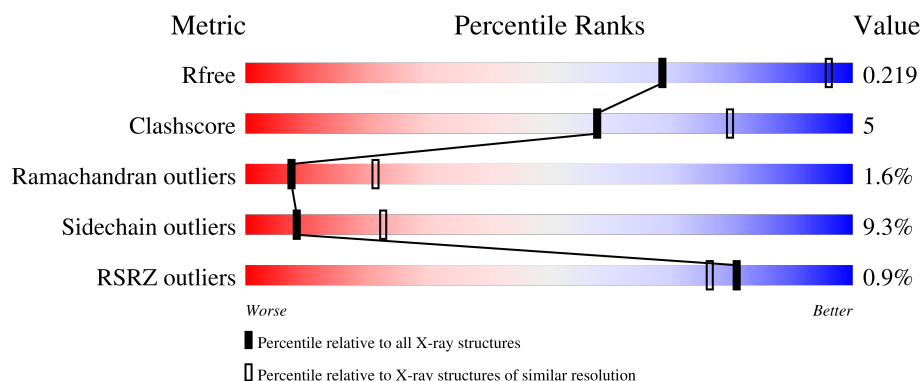
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	% 76% 20% ..
2	B	440	% 72% 17% .. 9%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7939 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	554	Total	C	N	O	S	0	0	0
			4501	2909	751	833	8			

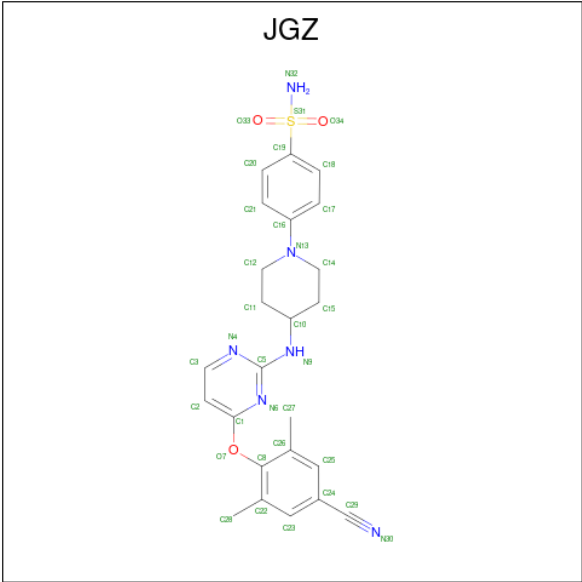
- Molecule 2 is a protein called p51 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	400	Total	C	N	O	S	0	0	0
			3311	2160	541	603	7			

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mn	0	0
			2	2		

- Molecule 4 is 4-(4-{[4-(4-cyano-2,6-dimethylphenoxy)pyrimidin-2-yl]amino}piperidin-1-yl)benzenesulfonamide (CCD ID: JGZ) (formula: C₂₄H₂₆N₆O₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			34	24	6	3	1		

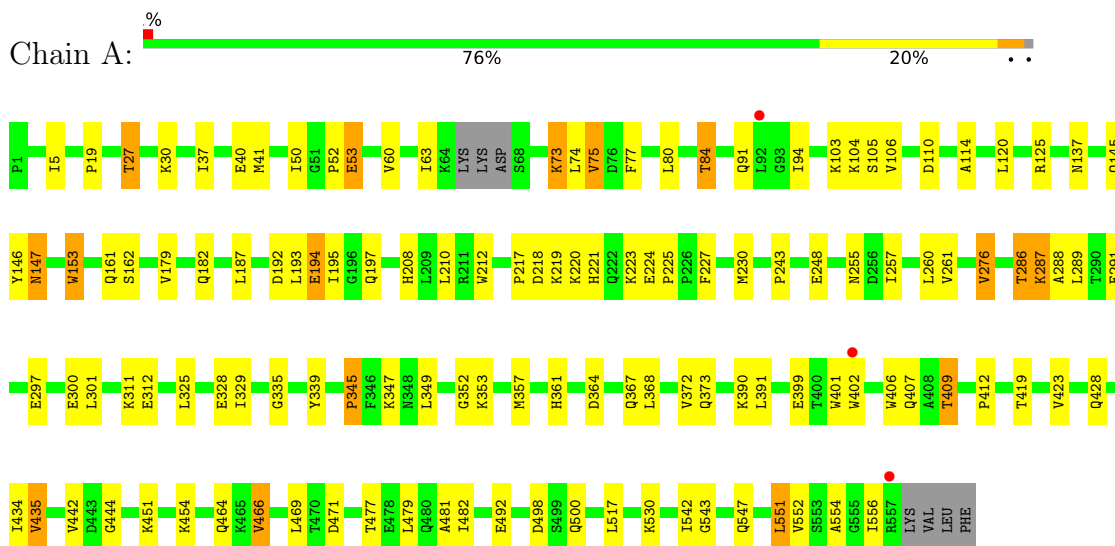
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	46	Total	O	0	0
			46	46		
5	B	45	Total	O	0	0
			45	45		

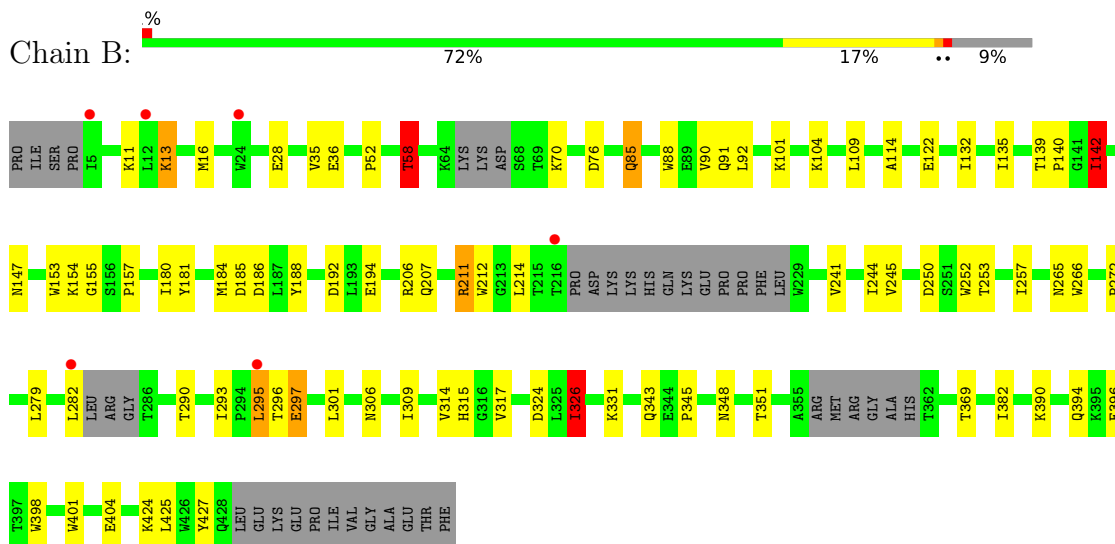
3 Residue-property plots [i](#)

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	118.69Å 152.87Å 154.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.14 – 2.95 25.14 – 2.95	Depositor EDS
% Data completeness (in resolution range)	95.7 (25.14-2.95) 95.6 (25.14-2.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 2.95Å)	Xtriage
Refinement program	BUSTER 2.9.2	Depositor
R, R_{free}	0.194 , 0.244 (Not available) , 0.219	Depositor DCC
R_{free} test set	1464 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	70.6	Xtriage
Anisotropy	0.630	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 61.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7939	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% 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: JGZ, MN

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	0.81	0/4617	1.35	20/6274 (0.3%)
2	B	0.82	0/3404	1.36	22/4627 (0.5%)
All	All	0.81	0/8021	1.36	42/10901 (0.4%)

There are no bond length outliers.

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	110	ASP	CA-CB-CG	8.02	120.62	112.60
2	B	211	ARG	N-CA-C	-7.97	98.68	110.48
1	A	276	VAL	CB-CA-C	7.19	117.81	110.70
2	B	401	TRP	N-CA-C	7.09	122.25	112.04
1	A	153	TRP	CA-C-N	7.03	131.36	120.82
1	A	153	TRP	C-N-CA	7.03	131.36	120.82
2	B	348	ASN	N-CA-C	6.91	119.74	109.59
2	B	296	THR	CA-C-N	6.87	129.81	120.54
2	B	296	THR	C-N-CA	6.87	129.81	120.54
1	A	345	PRO	CA-C-N	6.70	133.72	123.47
1	A	345	PRO	C-N-CA	6.70	133.72	123.47
1	A	94	ILE	CB-CA-C	6.56	116.49	110.13
1	A	225	PRO	N-CA-C	6.34	116.56	110.47
2	B	139	THR	CB-CA-C	6.33	118.38	108.63
1	A	419	THR	CB-CA-C	6.16	117.06	110.65
2	B	132	ILE	N-CA-C	-6.08	102.03	107.56
2	B	140	PRO	N-CA-C	5.86	121.19	113.86
2	B	206	ARG	CA-C-N	5.86	128.13	120.28
2	B	206	ARG	C-N-CA	5.86	128.13	120.28
2	B	142	ILE	N-CA-C	5.67	116.33	108.84
1	A	498	ASP	CA-CB-CG	5.57	118.17	112.60
1	A	221	HIS	CA-C-N	5.54	129.56	121.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	221	HIS	C-N-CA	5.54	129.56	121.31
2	B	58	THR	CB-CA-C	5.52	117.17	108.88
1	A	297	GLU	CB-CG-CD	5.51	121.96	112.60
2	B	343	GLN	N-CA-C	-5.50	105.61	112.93
2	B	250	ASP	N-CA-C	-5.47	106.96	113.97
2	B	35	VAL	N-CA-CB	5.44	117.27	110.47
1	A	347	LYS	CA-C-N	5.40	128.43	120.82
1	A	347	LYS	C-N-CA	5.40	128.43	120.82
2	B	185	ASP	CA-CB-CG	5.34	117.94	112.60
1	A	147	ASN	N-CA-C	-5.32	106.73	114.12
2	B	147	ASN	N-CA-C	-5.21	107.47	113.88
1	A	52	PRO	CA-C-N	5.17	128.18	120.31
1	A	52	PRO	C-N-CA	5.17	128.18	120.31
2	B	36	GLU	CA-C-N	5.13	127.22	120.60
2	B	36	GLU	C-N-CA	5.13	127.22	120.60
2	B	301	LEU	CA-C-N	5.07	127.38	120.54
2	B	301	LEU	C-N-CA	5.07	127.38	120.54
1	A	297	GLU	CA-C-N	5.03	127.02	120.28
1	A	297	GLU	C-N-CA	5.03	127.02	120.28
2	B	326	ILE	CB-CA-C	5.01	117.64	110.33

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	4501	0	4539	43	0
2	B	3311	0	3327	32	0
3	A	2	0	0	0	0
4	A	34	0	26	0	0
5	A	46	0	0	0	0
5	B	45	0	0	0	0
All	All	7939	0	7892	71	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 5.

All (71) 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:84:THR:HG21	1:A:153:TRP:HE1	1.38	0.87
1:A:255:ASN:HB2	1:A:289:LEU:HG	1.77	0.67
2:B:252:TRP:HD1	2:B:295:LEU:HD22	1.62	0.65
1:A:451:LYS:HB3	1:A:471:ASP:HA	1.80	0.63
1:A:162:SER:HB2	2:B:52:PRO:HG3	1.81	0.63
1:A:84:THR:HG21	1:A:153:TRP:NE1	2.11	0.62
1:A:364:ASP:HB3	1:A:423:VAL:HG13	1.79	0.62
2:B:295:LEU:H	2:B:295:LEU:HD23	1.66	0.61
1:A:401:TRP:HD1	1:A:402:TRP:CD1	2.18	0.60
1:A:339:TYR:CZ	1:A:352:GLY:HA3	2.37	0.59
2:B:394:GLN:HE21	2:B:396:GLU:HB2	1.66	0.59
1:A:80:LEU:O	1:A:84:THR:HG22	2.03	0.58
1:A:161:GLN:HE21	1:A:182:GLN:HE21	1.50	0.58
1:A:328:GLU:HG2	1:A:390:LYS:HB2	1.85	0.57
2:B:314:VAL:HB	2:B:317:VAL:HG12	1.87	0.55
1:A:19:PRO:HG3	1:A:80:LEU:HB2	1.90	0.54
2:B:266:TRP:HH2	2:B:427:TYR:CZ	2.25	0.54
1:A:193:LEU:HB3	1:A:197:GLN:HB2	1.90	0.52
1:A:335:GLY:HA2	1:A:367:GLN:HE22	1.75	0.52
1:A:75:VAL:HB	1:A:77:PHE:CE1	2.45	0.52
2:B:157:PRO:HG3	2:B:184:MET:HA	1.93	0.51
1:A:406:TRP:CD1	1:A:407:GLN:HE21	2.29	0.50
1:A:37:ILE:HG21	1:A:73:LYS:HB2	1.92	0.50
2:B:114:ALA:HB2	2:B:214:LEU:HD11	1.94	0.50
2:B:154:LYS:HE2	2:B:184:MET:HE2	1.94	0.50
1:A:27:THR:HG22	1:A:30:LYS:HG3	1.94	0.50
1:A:73:LYS:NZ	1:A:146:TYR:OH	2.45	0.50
1:A:125:ARG:HD3	1:A:147:ASN:HA	1.93	0.49
1:A:402:TRP:O	2:B:331:LYS:NZ	2.43	0.49
2:B:266:TRP:CH2	2:B:427:TYR:CZ	3.01	0.49
1:A:402:TRP:CZ3	1:A:409:THR:HB	2.48	0.49
2:B:28:GLU:HA	2:B:135:ILE:HD11	1.94	0.48
2:B:241:VAL:HG12	2:B:351:THR:H	1.77	0.48
2:B:101:LYS:HD3	2:B:382:ILE:HG23	1.95	0.47
1:A:466:VAL:HG22	1:A:551:LEU:HD13	1.97	0.47
1:A:442:VAL:HB	1:A:481:ALA:HB1	1.96	0.46
1:A:442:VAL:HG21	1:A:482:ILE:HG13	1.98	0.46
2:B:326:ILE:HD11	2:B:390:LYS:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:VAL:HA	2:B:290:THR:HG21	1.99	0.45
2:B:207:GLN:O	2:B:211:ARG:HD3	2.15	0.45
2:B:180:ILE:HA	2:B:188:TYR:O	2.15	0.45
2:B:153:TRP:CZ2	2:B:155:GLY:HA3	2.51	0.45
1:A:368:LEU:O	1:A:372:VAL:HG23	2.17	0.44
2:B:58:THR:HG23	2:B:76:ASP:O	2.16	0.44
2:B:306:ASN:HA	2:B:309:ILE:HD12	1.99	0.44
1:A:208:HIS:O	1:A:212:TRP:HD1	2.01	0.44
1:A:37:ILE:HG22	1:A:41:MET:HE2	1.99	0.44
1:A:469:LEU:HD13	1:A:477:THR:HG22	1.99	0.43
2:B:253:THR:O	2:B:257:ILE:HD12	2.17	0.43
2:B:314:VAL:HB	2:B:317:VAL:CG1	2.48	0.43
1:A:257:ILE:O	1:A:261:VAL:HG23	2.19	0.43
1:A:492:GLU:HG2	1:A:530:LYS:HB2	2.00	0.43
1:A:53:GLU:H	1:A:53:GLU:HG3	1.54	0.42
1:A:162:SER:CB	2:B:52:PRO:HG3	2.49	0.42
2:B:85:GLN:HA	2:B:88:TRP:CE2	2.53	0.42
1:A:288:ALA:HB3	1:A:291:GLU:HB2	2.02	0.42
2:B:211:ARG:O	2:B:212:TRP:HB2	2.18	0.42
2:B:272:PRO:HG2	2:B:315:HIS:HB3	2.00	0.42
2:B:104:LYS:HB2	2:B:192:ASP:HA	2.02	0.42
1:A:401:TRP:CD1	1:A:402:TRP:CD1	3.03	0.41
2:B:297:GLU:H	2:B:297:GLU:HG3	1.63	0.41
1:A:194:GLU:H	1:A:197:GLN:NE2	2.18	0.41
1:A:27:THR:HG22	1:A:30:LYS:H	1.85	0.41
1:A:104:LYS:HB2	1:A:192:ASP:HA	2.02	0.41
2:B:369:THR:HG22	2:B:398:TRP:CH2	2.55	0.41
2:B:181:TYR:HB3	2:B:188:TYR:HB2	2.02	0.41
1:A:223:LYS:HE3	1:A:227:PHE:HA	2.03	0.41
2:B:142:ILE:H	2:B:142:ILE:HG13	1.67	0.41
1:A:329:ILE:HD12	1:A:391:LEU:CD2	2.51	0.40
1:A:120:LEU:HD23	1:A:125:ARG:HG2	2.02	0.40
1:A:311:LYS:HG3	1:A:312:GLU:HG2	2.03	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	550/561 (98%)	508 (92%)	30 (6%)	12 (2%)	5	15
2	B	390/440 (89%)	361 (93%)	26 (7%)	3 (1%)	16	37
All	All	940/1001 (94%)	869 (92%)	56 (6%)	15 (2%)	7	21

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	85	GLN
1	A	195	ILE
1	A	217	PRO
1	A	286	THR
1	A	287	LYS
1	A	543	GLY
1	A	243	PRO
1	A	554	ALA
1	A	114	ALA
1	A	412	PRO
2	B	13	LYS
1	A	345	PRO
1	A	556	ILE
2	B	345	PRO
1	A	444	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%)	438 (89%)	54 (11%)	6	17
2	B	365/400 (91%)	339 (93%)	26 (7%)	13	33
All	All	857/901 (95%)	777 (91%)	80 (9%)	8	23

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	27	THR
1	A	40	GLU
1	A	50	ILE
1	A	53	GLU
1	A	60	VAL
1	A	63	ILE
1	A	73	LYS
1	A	74	LEU
1	A	75	VAL
1	A	84	THR
1	A	91	GLN
1	A	103	LYS
1	A	105	SER
1	A	106	VAL
1	A	137	ASN
1	A	145	GLN
1	A	179	VAL
1	A	187	LEU
1	A	194	GLU
1	A	210	LEU
1	A	218	ASP
1	A	219	LYS
1	A	220	LYS
1	A	224	GLU
1	A	230	MET
1	A	248	GLU
1	A	260	LEU
1	A	276	VAL
1	A	286	THR
1	A	287	LYS
1	A	300	GLU
1	A	301	LEU
1	A	325	LEU
1	A	349	LEU

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Mol	Chain	Res	Type
1	A	353	LYS
1	A	357	MET
1	A	361	HIS
1	A	373	GLN
1	A	399	GLU
1	A	409	THR
1	A	428	GLN
1	A	434	ILE
1	A	435	VAL
1	A	454	LYS
1	A	464	GLN
1	A	466	VAL
1	A	479	LEU
1	A	500	GLN
1	A	517	LEU
1	A	542	ILE
1	A	547	GLN
1	A	551	LEU
1	A	552	VAL
2	B	11	LYS
2	B	13	LYS
2	B	16	MET
2	B	58	THR
2	B	70	LYS
2	B	90	VAL
2	B	91	GLN
2	B	92	LEU
2	B	109	LEU
2	B	122	GLU
2	B	142	ILE
2	B	186	ASP
2	B	194	GLU
2	B	244	ILE
2	B	245	VAL
2	B	265	ASN
2	B	279	LEU
2	B	282	LEU
2	B	293	ILE
2	B	295	LEU
2	B	297	GLU
2	B	324	ASP
2	B	326	ILE

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Mol	Chain	Res	Type
2	B	404	GLU
2	B	424	LYS
2	B	425	LEU

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	161	GLN
1	A	175	ASN
1	A	197	GLN
1	A	255	ASN
1	A	336	GLN
1	A	348	ASN
1	A	407	GLN
1	A	428	GLN
1	A	500	GLN
1	A	509	GLN
2	B	151	GLN
2	B	161	GLN
2	B	258	GLN
2	B	332	GLN
2	B	348	ASN
2	B	394	GLN
2	B	428	GLN

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

Of 3 ligands modelled in this entry, 2 are 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
4	JGZ	A	562	-	37,37,37	1.31	4 (10%)	53,53,53	2.73	16 (30%)

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
4	JGZ	A	562	-	-	6/20/30/30	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	562	JGZ	C5-N9	4.07	1.39	1.34
4	A	562	JGZ	S31-N32	3.11	1.66	1.60
4	A	562	JGZ	C1-N6	2.51	1.37	1.33
4	A	562	JGZ	C23-C22	-2.19	1.36	1.39

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	562	JGZ	N4-C5-N6	-9.93	116.82	126.42
4	A	562	JGZ	C5-N6-C1	9.66	126.05	115.00
4	A	562	JGZ	C15-C10-N9	-6.55	100.22	110.77
4	A	562	JGZ	C3-N4-C5	6.50	120.85	115.42
4	A	562	JGZ	N9-C5-N4	3.80	122.78	116.75
4	A	562	JGZ	C14-N13-C16	-3.32	109.06	118.11
4	A	562	JGZ	C5-N9-C10	-3.17	119.39	124.32
4	A	562	JGZ	C2-C1-N6	-2.72	117.83	123.48
4	A	562	JGZ	O34-S31-O33	2.44	122.54	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	562	JGZ	C25-C26-C8	2.40	121.41	117.94
4	A	562	JGZ	O33-S31-N32	2.13	110.42	107.35
4	A	562	JGZ	N9-C5-N6	2.11	120.40	117.09
4	A	562	JGZ	C26-C8-C22	-2.07	117.72	122.07
4	A	562	JGZ	O34-S31-N32	-2.05	104.39	107.35
4	A	562	JGZ	C17-C16-N13	-2.05	118.54	121.39
4	A	562	JGZ	O33-S31-C19	-2.03	105.06	107.35

There are no chirality outliers.

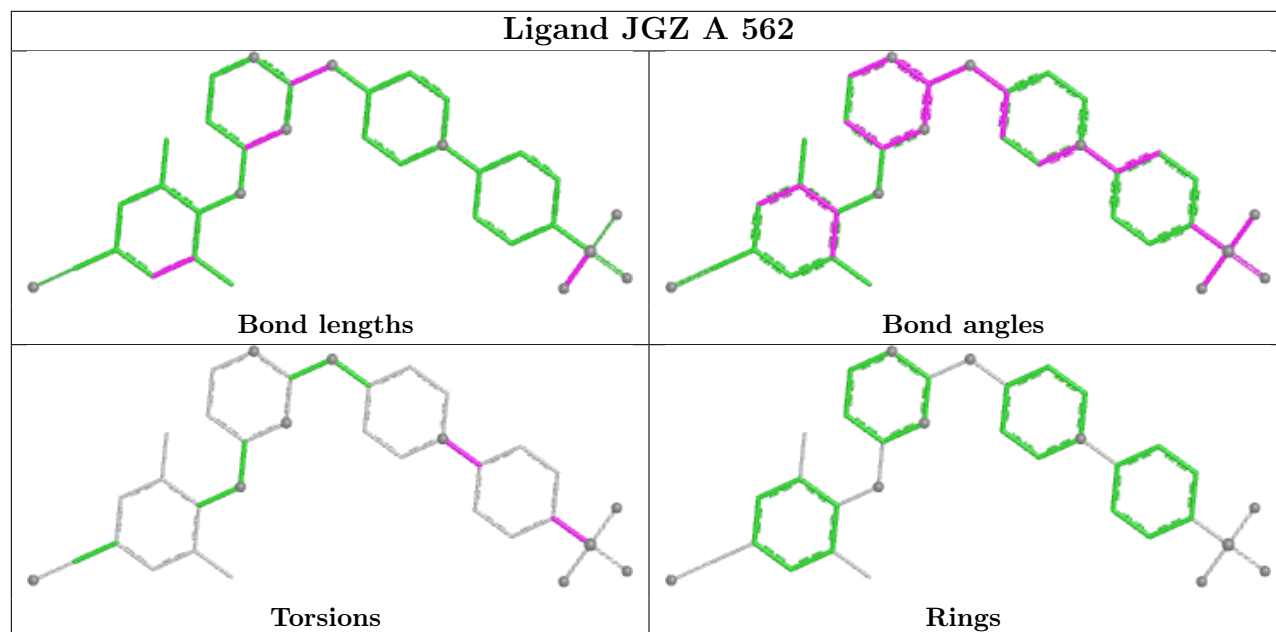
All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	562	JGZ	C21-C16-N13-C14
4	A	562	JGZ	C17-C16-N13-C14
4	A	562	JGZ	C18-C19-S31-O34
4	A	562	JGZ	C18-C19-S31-N32
4	A	562	JGZ	C20-C19-S31-O34
4	A	562	JGZ	C20-C19-S31-N32

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	554/561 (98%)	-0.17	3 (0%) 87 83	50, 77, 111, 138	0
2	B	400/440 (90%)	-0.21	6 (1%) 72 65	45, 76, 114, 133	0
All	All	954/1001 (95%)	-0.19	9 (0%) 81 76	45, 77, 112, 138	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	402	TRP	3.3
1	A	557	ARG	3.2
2	B	282	LEU	3.2
2	B	5	ILE	2.8
2	B	12	LEU	2.7
2	B	216	THR	2.6
2	B	295	LEU	2.4
2	B	24	TRP	2.3
1	A	92	LEU	2.1

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.

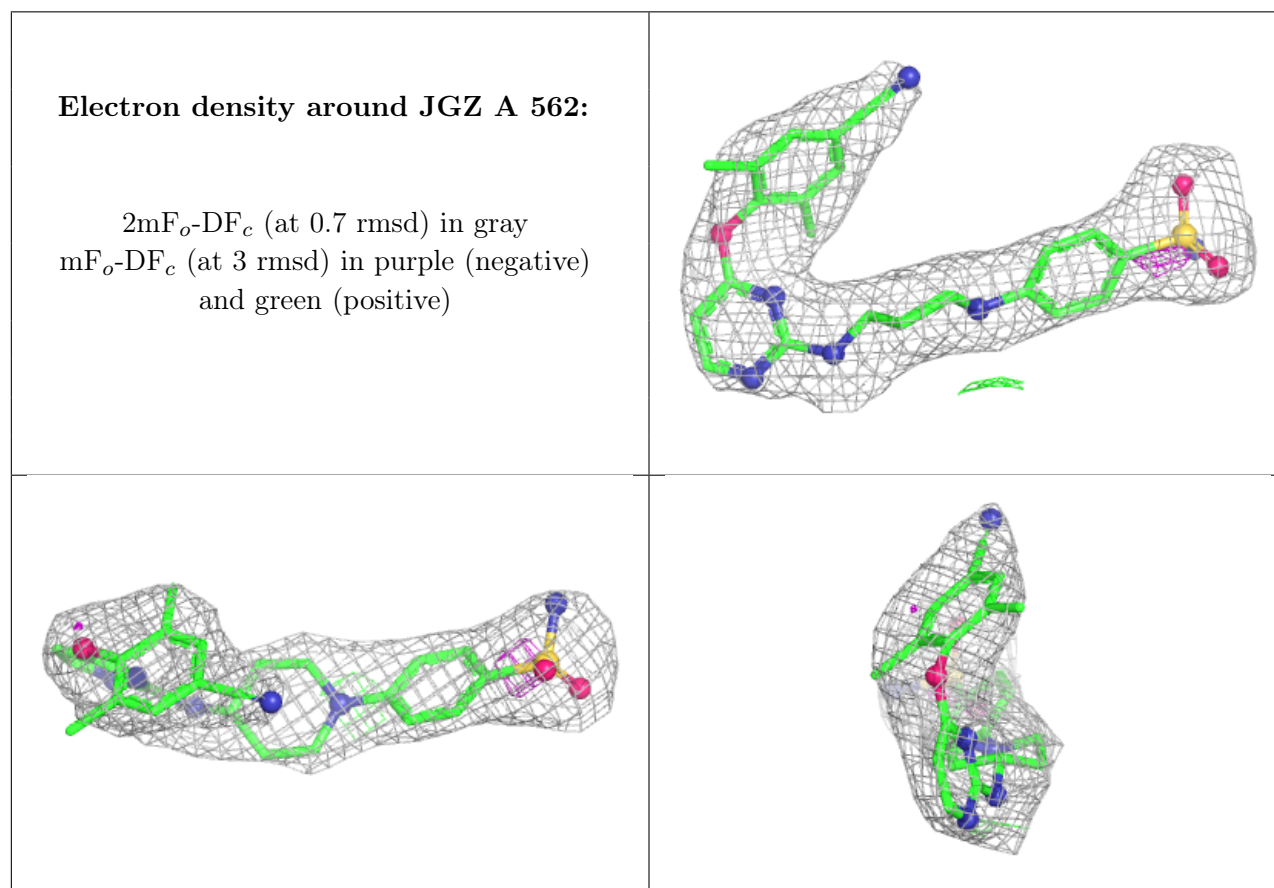
6.4 Ligands [i](#)

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	MN	A	602	1/1	0.82	0.07	157,157,157,157	0
3	MN	A	601	1/1	0.90	0.18	239,239,239,239	0
4	JGZ	A	562	34/34	0.94	0.09	60,67,93,94	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.