



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2023 – 10:04 AM EDT

PDB ID : 8FFX
Title : Crystal structure of HIV-1 reverse transcriptase in complex with non-nucleoside inhibitor 19980
Authors : Rumrill, S.R.; Ruiz, F.X.; Arnold, E.
Deposited on : 2022-12-10
Resolution : 2.42 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.32.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.32.2

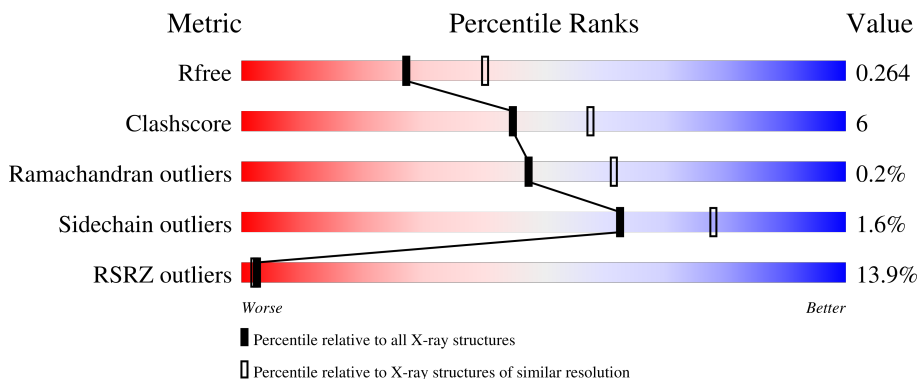
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.42 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}	130704	4647 (2.44-2.40)
Clashscore	141614	5161 (2.44-2.40)
Ramachandran outliers	138981	5073 (2.44-2.40)
Sidechain outliers	138945	5074 (2.44-2.40)
RSRZ outliers	127900	4543 (2.44-2.40)

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	
2	B	428	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 8124 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
			Total	C	N	O	S			
1	A	555	4508	2918	749	834	7	0	0	0

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
			Total	C	N	O	S			
2	B	416	3443	2244	568	624	7	0	0	0

There is a discrepancy between the modelled and reference sequences:

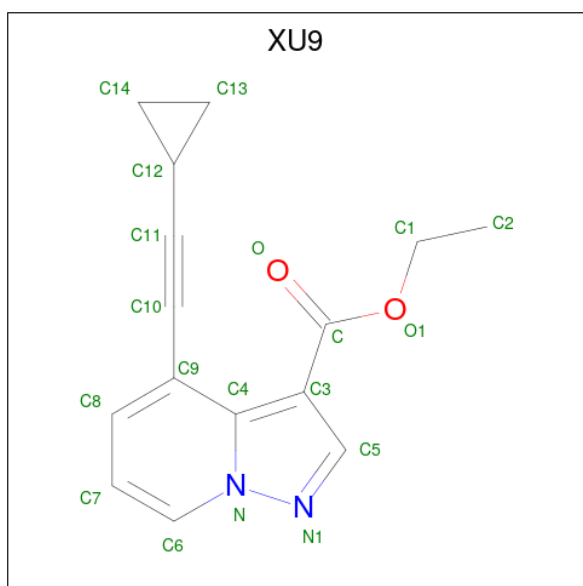
Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 3 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
3	A	1	4	2	1	1	0	0

- Molecule 4 is ethyl (8S)-4-(cyclopropylethynyl)pyrazolo[1,5-a]pyridine-3-carboxylate (three-letter code: XU9) (formula: $C_{15}H_{14}N_2O_2$) (labeled as "Ligand of Interest" by depositor).



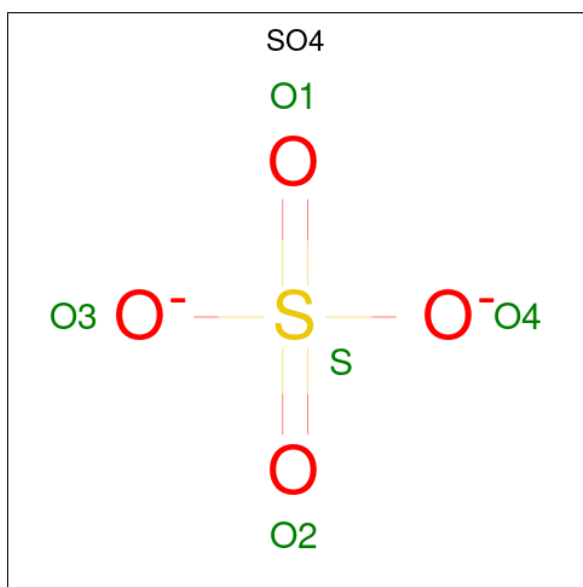
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	19	15	2	2	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		

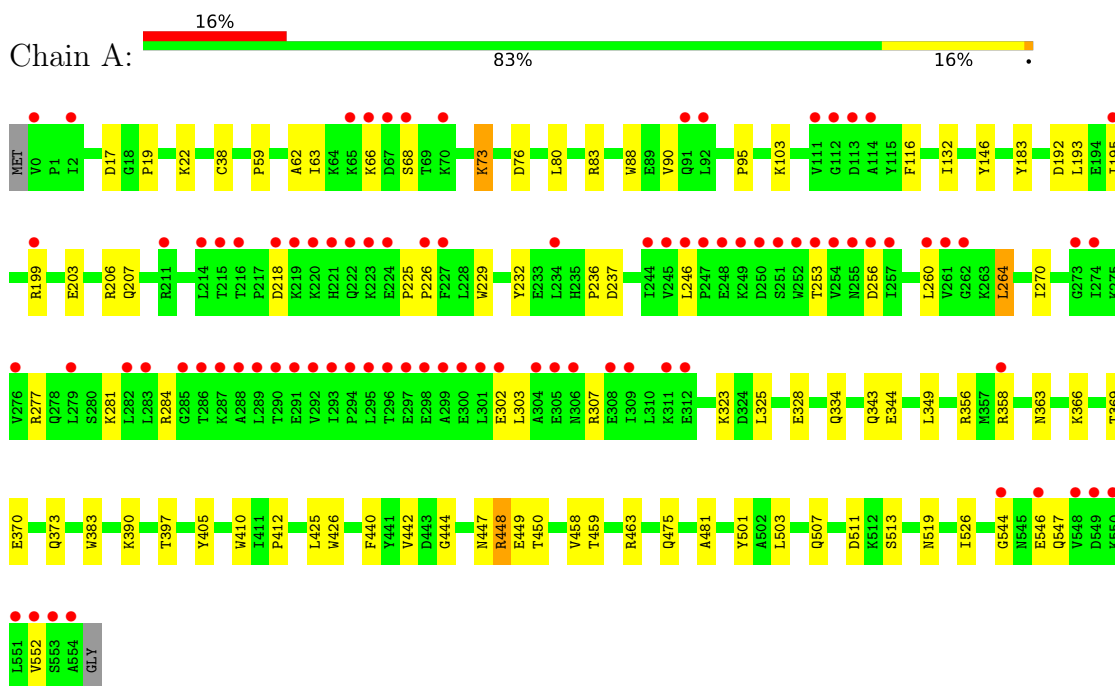
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	81	Total	O	0	0
			81	81		
7	B	42	Total	O	0	0
			42	42		

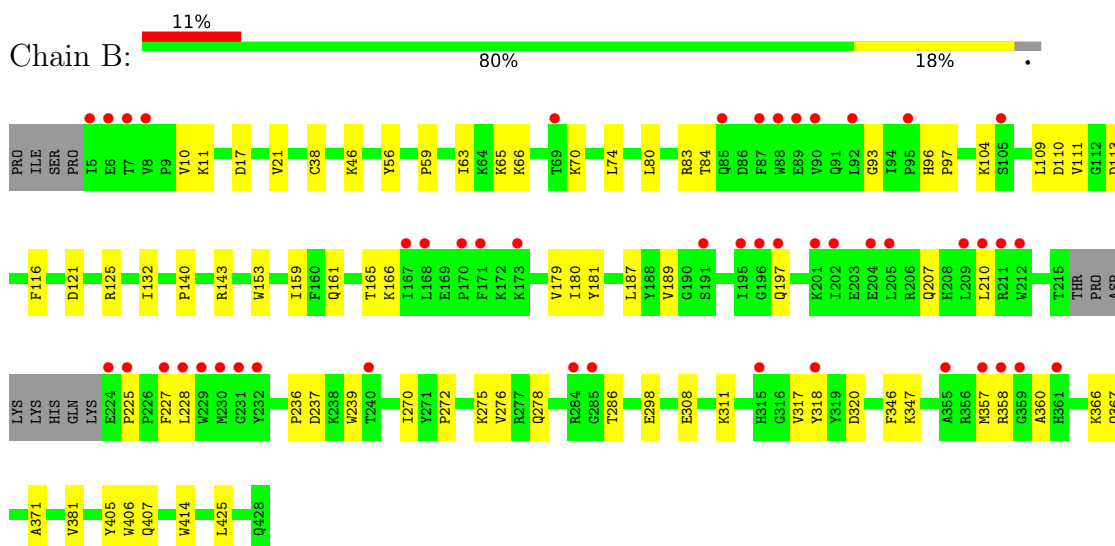
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Reverse transcriptase/ribonuclease H



- Molecule 2: p51 RT



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	161.95Å 73.38Å 107.97Å 90.00° 100.05° 90.00°	Depositor
Resolution (Å)	48.29 – 2.42 48.29 – 2.42	Depositor EDS
% Data completeness (in resolution range)	99.0 (48.29-2.42) 94.8 (48.29-2.42)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 2.42Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.214 , 0.266 0.213 , 0.264	Depositor DCC
R_{free} test set	2000 reflections (4.20%)	wwPDB-VP
Wilson B-factor (Å ²)	52.6	Xtrriage
Anisotropy	0.267	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 49.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	8124	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.61% 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: DMS, EDO, XU9, SO4

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	0.32	0/4626	0.51	0/6289
2	B	0.31	0/3543	0.51	0/4814
All	All	0.32	0/8169	0.51	0/11103

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	4508	0	4563	60	0
2	B	3443	0	3470	47	0
3	A	4	0	6	0	0
4	A	19	0	0	0	0
5	A	4	0	6	3	0
5	B	8	0	12	0	0
6	A	10	0	0	0	0
6	B	5	0	0	0	0
7	A	81	0	0	4	0
7	B	42	0	0	2	0
All	All	8124	0	8057	104	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 6.

All (104) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:84:THR:HG21	2:B:153:TRP:HE1	1.36	0.90
2:B:425:LEU:HD13	7:B:641:HOH:O	1.81	0.78
1:A:328:GLU:HG3	1:A:390:LYS:HB2	1.65	0.78
2:B:56:TYR:O	2:B:143:ARG:NH2	2.21	0.73
2:B:360:ALA:HB2	2:B:366:LYS:HD2	1.74	0.70
1:A:343:GLN:HG3	1:A:349:LEU:HD11	1.73	0.69
1:A:426:TRP:H	5:A:603:EDO:HO2	1.39	0.66
1:A:458:VAL:HG12	2:B:286:THR:HG21	1.79	0.65
2:B:63:ILE:HG13	2:B:74:LEU:HD12	1.79	0.64
1:A:225:PRO:HB2	1:A:236:PRO:HD3	1.81	0.63
2:B:10:VAL:HG21	2:B:159:ILE:HD11	1.79	0.63
1:A:440:PHE:HA	1:A:459:THR:HG22	1.81	0.63
1:A:90:VAL:HG21	2:B:140:PRO:HB3	1.80	0.62
2:B:317:VAL:HG23	2:B:347:LYS:HB3	1.80	0.62
1:A:303:LEU:HD13	1:A:307:ARG:HD3	1.82	0.61
2:B:270:ILE:HG12	2:B:346:PHE:HB3	1.81	0.61
1:A:366:LYS:HE2	1:A:405:TYR:OH	2.02	0.60
1:A:195:ILE:HD11	1:A:199:ARG:HH21	1.65	0.59
1:A:203:GLU:HA	1:A:206:ARG:HG3	1.86	0.58
1:A:448:ARG:HD3	1:A:448:ARG:H	1.70	0.57
2:B:278:GLN:HE21	2:B:298:GLU:HB2	1.70	0.57
2:B:80:LEU:O	2:B:84:THR:HG23	2.05	0.56
1:A:88:TRP:CD1	2:B:143:ARG:HD2	2.41	0.56
1:A:426:TRP:N	5:A:603:EDO:O2	2.23	0.55
2:B:46:LYS:HE2	2:B:116:PHE:CD2	2.42	0.55
1:A:246:LEU:HD22	1:A:260:LEU:HD12	1.88	0.54
1:A:95:PRO:HD2	1:A:229:TRP:HH2	1.72	0.53
1:A:307:ARG:HD2	1:A:307:ARG:N	2.24	0.53
2:B:318:TYR:HE1	2:B:320:ASP:HB2	1.74	0.53
1:A:59:PRO:HG2	1:A:76:ASP:HB3	1.91	0.53
1:A:442:VAL:HB	1:A:481:ALA:HB1	1.90	0.52
2:B:425:LEU:CD1	7:B:641:HOH:O	2.49	0.50
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.94	0.49
2:B:207:GLN:HA	2:B:207:GLN:OE1	2.12	0.49
1:A:323:LYS:NZ	1:A:344:GLU:OE1	2.35	0.49
1:A:38:CYS:SG	1:A:132:ILE:HD11	2.52	0.49
1:A:302:GLU:N	1:A:302:GLU:OE1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:17:ASP:O	2:B:83:ARG:HD3	2.13	0.48
1:A:459:THR:OG1	1:A:463:ARG:HB3	2.13	0.48
1:A:449:GLU:OE1	1:A:449:GLU:N	2.44	0.48
2:B:166:LYS:HD2	2:B:166:LYS:HA	1.75	0.48
1:A:426:TRP:HB3	1:A:526:ILE:HG12	1.95	0.47
1:A:444:GLY:HA2	1:A:552:VAL:HG11	1.96	0.47
2:B:236:PRO:HA	2:B:239:TRP:CD2	2.49	0.47
2:B:66:LYS:HZ3	2:B:358:ARG:HH11	1.62	0.47
1:A:62:ALA:C	1:A:63:ILE:HD12	2.35	0.47
1:A:19:PRO:HG3	1:A:80:LEU:HB2	1.96	0.47
2:B:109:LEU:HD12	2:B:228:LEU:HD22	1.97	0.47
1:A:410:TRP:CH2	1:A:412:PRO:HA	2.50	0.46
1:A:232:TYR:HB2	7:A:701:HOH:O	2.13	0.46
1:A:237:ASP:OD1	1:A:237:ASP:N	2.46	0.46
2:B:360:ALA:O	2:B:367:GLN:NE2	2.47	0.46
2:B:308:GLU:HA	2:B:311:LYS:HG3	1.98	0.46
1:A:511:ASP:HB3	5:A:603:EDO:H21	1.98	0.46
2:B:275:LYS:HE3	2:B:276:VAL:H	1.80	0.46
1:A:366:LYS:O	1:A:370:GLU:HG3	2.16	0.46
2:B:187:LEU:HD12	2:B:187:LEU:HA	1.81	0.45
1:A:229:TRP:HE3	7:A:701:HOH:O	1.99	0.45
2:B:121:ASP:O	2:B:125:ARG:HG3	2.17	0.45
1:A:363:ASN:HA	1:A:511:ASP:OD1	2.17	0.45
1:A:397:THR:HG23	1:A:425:LEU:HG	1.98	0.45
2:B:110:ASP:H	2:B:228:LEU:HD21	1.81	0.45
1:A:513:SER:N	1:A:519:ASN:OD1	2.48	0.45
2:B:161:GLN:O	2:B:165:THR:HG23	2.17	0.45
1:A:246:LEU:HB2	1:A:307:ARG:NH2	2.31	0.44
2:B:97:PRO:HG2	2:B:181:TYR:HB2	1.99	0.44
2:B:180:ILE:HD12	2:B:189:VAL:HG22	1.98	0.44
2:B:65:LYS:HA	2:B:407:GLN:OE1	2.17	0.44
1:A:203:GLU:O	1:A:207:GLN:HG2	2.17	0.44
2:B:63:ILE:HD11	2:B:406:TRP:HB3	1.99	0.44
2:B:111:VAL:HG11	2:B:187:LEU:HD22	1.99	0.44
1:A:17:ASP:O	1:A:83:ARG:NE	2.50	0.44
1:A:475:GLN:HB3	1:A:501:TYR:CE2	2.52	0.44
1:A:260:LEU:O	1:A:264:LEU:HD12	2.18	0.44
1:A:325:LEU:HD21	1:A:383:TRP:CE3	2.53	0.44
1:A:444:GLY:CA	1:A:552:VAL:HG11	2.48	0.44
1:A:206:ARG:HH22	1:A:218:ASP:HB3	1.83	0.44
2:B:366:LYS:HG3	2:B:405:TYR:CD1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:LYS:NZ	7:A:711:HOH:O	2.51	0.43
1:A:66:LYS:O	1:A:68:SER:N	2.50	0.43
1:A:73:LYS:HE2	1:A:146:TYR:OH	2.19	0.43
2:B:357:MET:HE3	2:B:371:ALA:HB2	2.00	0.43
1:A:253:THR:H	1:A:256:ASP:HB2	1.84	0.43
2:B:278:GLN:NE2	2:B:298:GLU:HB2	2.31	0.43
1:A:447:ASN:OD1	1:A:450:THR:HG22	2.18	0.43
2:B:11:LYS:HE2	2:B:11:LYS:HB3	1.79	0.43
1:A:440:PHE:CG	1:A:459:THR:HG22	2.53	0.42
1:A:225:PRO:HA	1:A:226:PRO:HA	1.63	0.42
2:B:104:LYS:HA	2:B:237:ASP:HB2	2.00	0.42
2:B:210:LEU:HD11	2:B:227:PHE:CD1	2.54	0.42
2:B:225:PRO:HB2	2:B:227:PHE:CE2	2.54	0.42
2:B:66:LYS:HZ3	2:B:358:ARG:NH1	2.17	0.42
1:A:356:ARG:NH1	7:A:713:HOH:O	2.54	0.41
1:A:103:LYS:HA	1:A:192:ASP:OD1	2.21	0.41
2:B:110:ASP:N	2:B:228:LEU:HD21	2.34	0.41
1:A:369:THR:O	1:A:373:GLN:HG2	2.20	0.41
1:A:544:GLY:H	1:A:547:GLN:HG3	1.85	0.41
1:A:260:LEU:HG	1:A:264:LEU:CD1	2.50	0.41
1:A:503:LEU:HD12	1:A:507:GLN:NE2	2.36	0.41
2:B:96:HIS:NE2	2:B:381:VAL:O	2.45	0.41
1:A:284:ARG:NH1	1:A:358:ARG:HH12	2.19	0.40
2:B:38:CYS:SG	2:B:132:ILE:HD11	2.60	0.40
2:B:179:VAL:O	2:B:180:ILE:HD13	2.21	0.40
1:A:277:ARG:O	1:A:281:LYS:N	2.52	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	553/557 (99%)	535 (97%)	18 (3%)	0	100	100
2	B	412/428 (96%)	392 (95%)	18 (4%)	2 (0%)	29	40
All	All	965/985 (98%)	927 (96%)	36 (4%)	2 (0%)	47	61

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	93	GLY
2	B	272	PRO

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	494/495 (100%)	484 (98%)	10 (2%)	55	72
2	B	378/390 (97%)	374 (99%)	4 (1%)	73	86
All	All	872/885 (98%)	858 (98%)	14 (2%)	62	78

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	LYS
1	A	73	LYS
1	A	116	PHE
1	A	183	TYR
1	A	193	LEU
1	A	264	LEU
1	A	270	ILE
1	A	334	GLN
1	A	448	ARG
1	A	546	GLU
2	B	70	LYS
2	B	113	ASP
2	B	197	GLN
2	B	414	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	278	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 ligands are 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	$\# Z > 2$
4	XU9	A	602	-	18,21,21	0.72	1 (5%)	20,29,29	0.85	1 (5%)
6	SO4	B	503	-	4,4,4	0.14	0	6,6,6	0.06	0
5	EDO	B	502	-	3,3,3	0.44	0	2,2,2	0.65	0
6	SO4	A	604	-	4,4,4	0.14	0	6,6,6	0.06	0
5	EDO	A	603	-	3,3,3	0.40	0	2,2,2	0.45	0
3	DMS	A	601	-	3,3,3	0.74	0	3,3,3	0.51	0
6	SO4	A	605	-	4,4,4	0.13	0	6,6,6	0.12	0
5	EDO	B	501	-	3,3,3	0.44	0	2,2,2	0.45	0

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
5	EDO	B	502	-	-	0/1/1/1	-
4	XU9	A	602	-	-	3/10/14/14	0/3/3/3
5	EDO	B	501	-	-	0/1/1/1	-
5	EDO	A	603	-	-	1/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	602	XU9	C4-N	-2.44	1.37	1.40

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	602	XU9	C9-C4-N	-2.33	118.81	122.64

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	602	XU9	O-C-C3-C5
4	A	602	XU9	O1-C-C3-C5
4	A	602	XU9	C9-C10-C11-C12
5	A	603	EDO	O1-C1-C2-O2

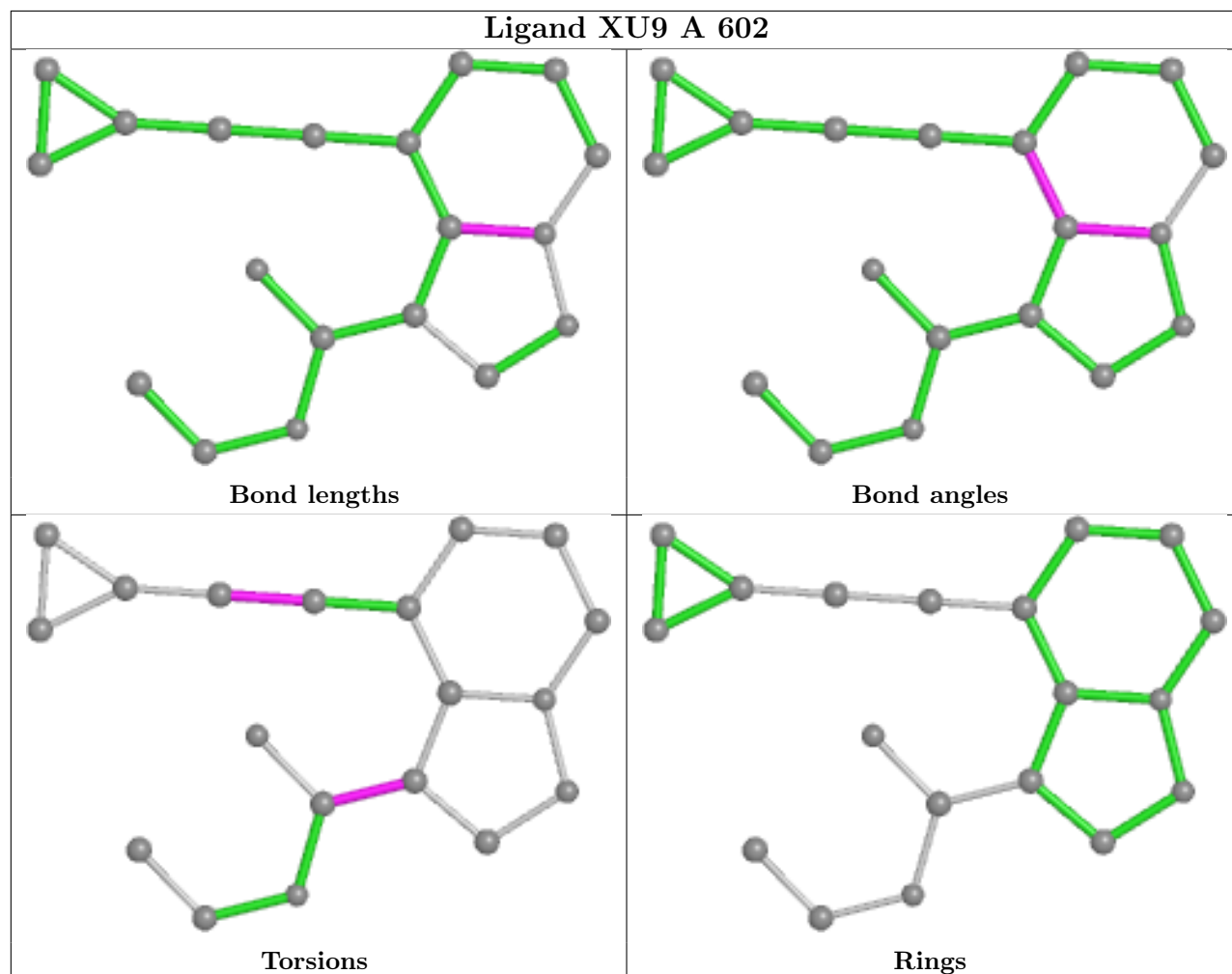
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	603	EDO	3	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	555/557 (99%)	0.80	87 (15%) 2 1	34, 75, 165, 234	0
2	B	416/428 (97%)	0.72	48 (11%) 4 4	37, 70, 158, 234	0
All	All	971/985 (98%)	0.77	135 (13%) 2 2	34, 73, 164, 234	0

All (135) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	227	PHE	14.1
1	A	246	LEU	11.1
1	A	290	THR	11.1
2	B	225	PRO	10.4
1	A	223	LYS	10.1
1	A	250	ASP	8.8
1	A	247	PRO	8.8
1	A	67	ASP	8.7
2	B	229	TRP	8.6
2	B	228	LEU	8.4
2	B	231	GLY	8.1
1	A	292	VAL	7.6
1	A	287	LYS	7.5
1	A	252	TRP	7.3
2	B	5	ILE	7.1
1	A	295	LEU	7.0
2	B	90	VAL	6.8
2	B	212	TRP	6.7
1	A	309	ILE	6.6
2	B	8	VAL	6.5
1	A	245	VAL	5.8
1	A	279	LEU	5.8
1	A	261	VAL	5.8
2	B	224	GLU	5.8

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Mol	Chain	Res	Type	RSRZ
1	A	293	ILE	5.7
1	A	221	HIS	5.6
1	A	254	VAL	5.5
1	A	256	ASP	5.4
1	A	257	ILE	5.4
2	B	7	THR	5.3
1	A	291	GLU	5.2
1	A	302	GLU	5.1
1	A	66	LYS	5.1
1	A	283	LEU	4.9
1	A	301	LEU	4.9
2	B	358	ARG	4.8
1	A	0	VAL	4.7
1	A	553	SER	4.7
1	A	294	PRO	4.7
1	A	224	GLU	4.6
1	A	282	LEU	4.6
1	A	298	GLU	4.6
1	A	304	ALA	4.6
1	A	216	THR	4.5
1	A	299	ALA	4.5
1	A	249	LYS	4.4
1	A	92	LEU	4.4
1	A	308	GLU	4.4
1	A	552	VAL	4.3
1	A	222	GLN	4.3
2	B	195	ILE	4.1
1	A	199	ARG	4.1
1	A	262	GLY	4.0
2	B	359	GLY	4.0
2	B	240	THR	4.0
2	B	357	MET	4.0
2	B	88	TRP	4.0
1	A	305	GLU	3.9
1	A	551	LEU	3.9
2	B	89	GLU	3.9
1	A	214	LEU	3.9
2	B	171	PHE	3.9
2	B	209	LEU	3.9
1	A	2	ILE	3.8
1	A	226	PRO	3.8
2	B	284	ARG	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	70	LYS	3.8
1	A	546	GLU	3.7
1	A	288	ALA	3.7
1	A	297	GLU	3.6
1	A	220	LYS	3.6
2	B	92	LEU	3.6
1	A	253	THR	3.5
1	A	227	PHE	3.5
1	A	286	THR	3.4
1	A	215	THR	3.4
2	B	210	LEU	3.3
2	B	202	ILE	3.3
2	B	211	ARG	3.3
1	A	114	ALA	3.3
2	B	205	LEU	3.2
1	A	312	GLU	3.2
1	A	251	SER	3.2
2	B	173	LYS	3.2
2	B	318	TYR	3.1
2	B	197	GLN	3.1
2	B	69	THR	3.1
1	A	234	LEU	3.0
2	B	315	HIS	3.0
2	B	168	LEU	3.0
2	B	191	SER	3.0
1	A	554	ALA	3.0
1	A	285	GLY	3.0
1	A	260	LEU	2.9
1	A	300	GLU	2.9
1	A	550	LYS	2.8
2	B	167	ILE	2.8
2	B	85	GLN	2.7
1	A	248	GLU	2.7
1	A	218	ASP	2.7
2	B	230	MET	2.7
2	B	87	PHE	2.6
1	A	311	LYS	2.6
1	A	91	GLN	2.6
2	B	105	SER	2.6
1	A	219	LYS	2.5
1	A	289	LEU	2.5
1	A	296	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	549	ASP	2.5
1	A	306	ASN	2.4
2	B	355	ALA	2.4
1	A	276	VAL	2.4
1	A	211	ARG	2.3
1	A	255	ASN	2.3
2	B	170	PRO	2.3
1	A	544	GLY	2.3
2	B	204	GLU	2.3
2	B	361	HIS	2.2
1	A	68	SER	2.2
2	B	285	GLY	2.2
1	A	244	ILE	2.2
2	B	6	GLU	2.2
1	A	274	ILE	2.1
2	B	232	TYR	2.1
1	A	111	VAL	2.1
2	B	95	PRO	2.1
2	B	201	LYS	2.1
1	A	358	ARG	2.1
1	A	112	GLY	2.1
2	B	196	GLY	2.1
1	A	548	VAL	2.1
1	A	195	ILE	2.1
1	A	273	GLY	2.1
1	A	113	ASP	2.0
1	A	65	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 monosaccharides in this entry.

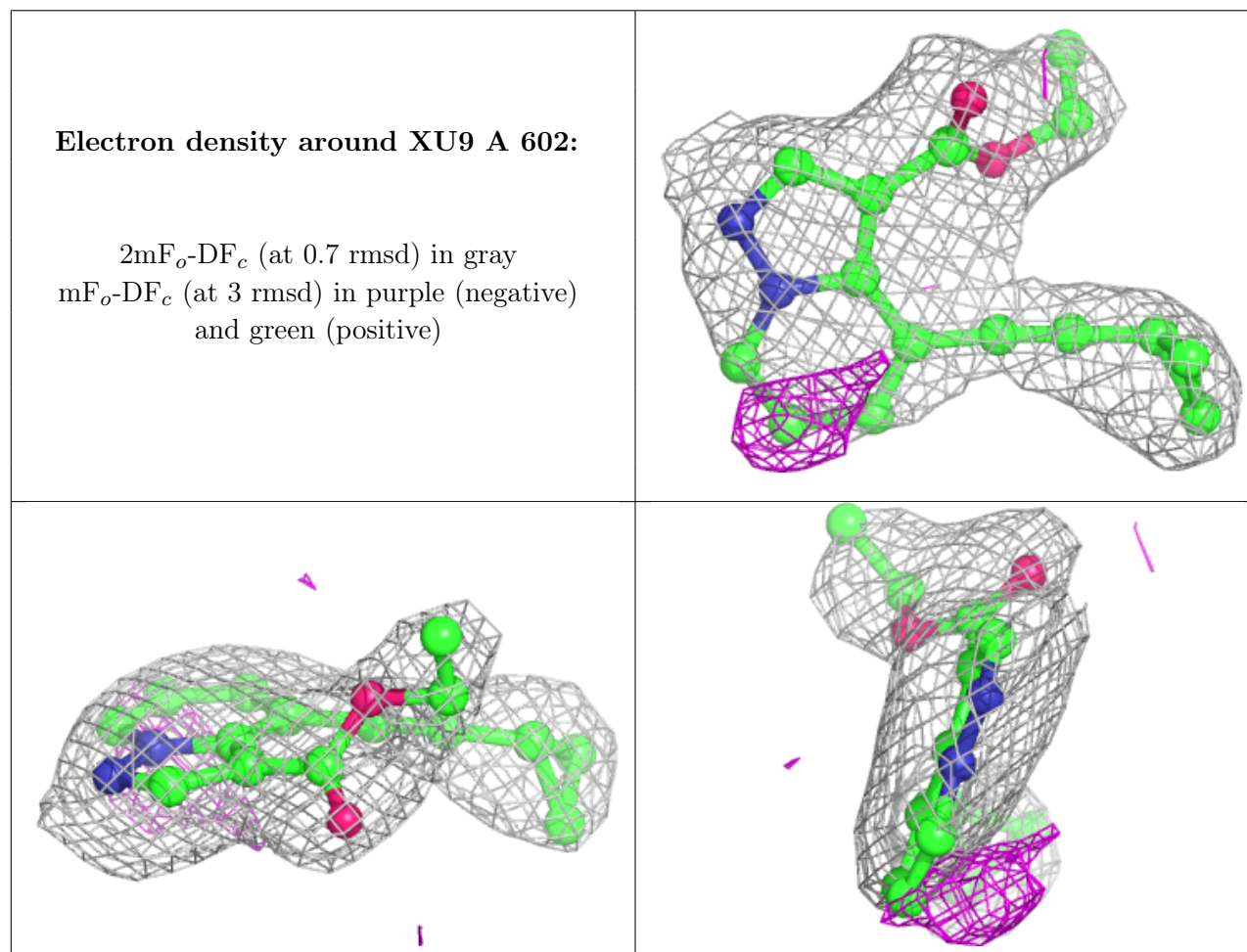
6.4 Ligands [i](#)

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
5	EDO	A	603	4/4	0.84	0.26	51,51,60,61	0
4	XU9	A	602	19/19	0.90	0.27	71,80,88,95	0
6	SO4	A	604	5/5	0.90	0.27	104,135,150,150	0
6	SO4	A	605	5/5	0.91	0.13	106,109,123,126	0
6	SO4	B	503	5/5	0.92	0.25	132,135,153,174	0
5	EDO	B	502	4/4	0.93	0.30	48,54,61,79	0
5	EDO	B	501	4/4	0.93	0.26	72,76,78,83	0
3	DMS	A	601	4/4	0.98	0.17	37,47,55,59	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.