Full wwPDB X-ray Structure Validation Report (i)

Mar 24, 2022 – 12:51 pm GMT

PDB ID	:	6ELI
Title	:	Structure of HIV-1 reverse transcriptase (RT) in complex with rilpivirine and an RNase H inhibitor XZ462
Authors	:	Das, K.; Arnold, E.
Deposited on	:	2017-09-29
Resolution	:	2.20 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 (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

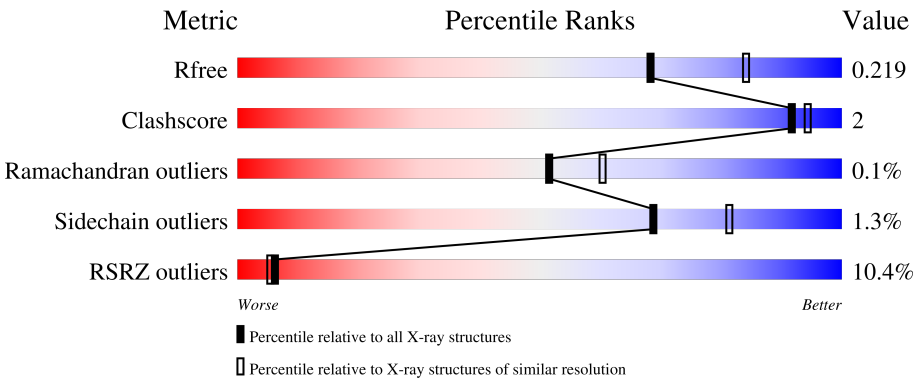
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.27
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 <=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	8% 95% 5%
2	B	428	14% 91% 6% •

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 8407 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	556	4524	2928	753	835	8	0	1	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP P03366
A	0	VAL	-	expression tag	UNP P03366
A	280	SER	CYS	engineered mutation	UNP P03366

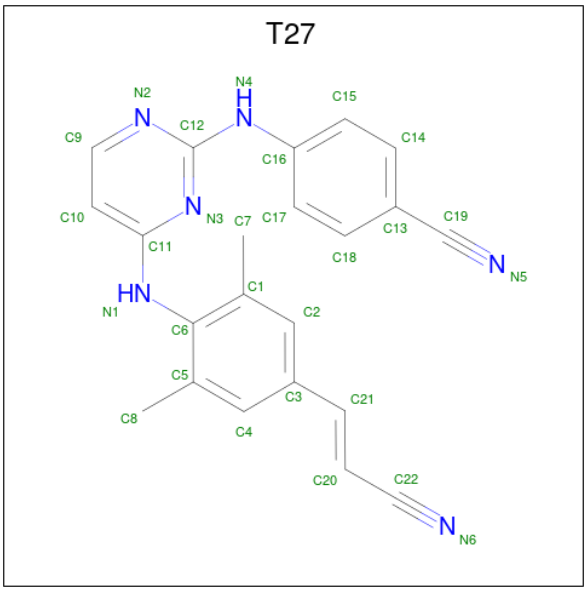
- Molecule 2 is a protein called Gag-Pol polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	416	3451	2249	569	626	7	0	2	0

There is a discrepancy between the modelled and reference sequences:

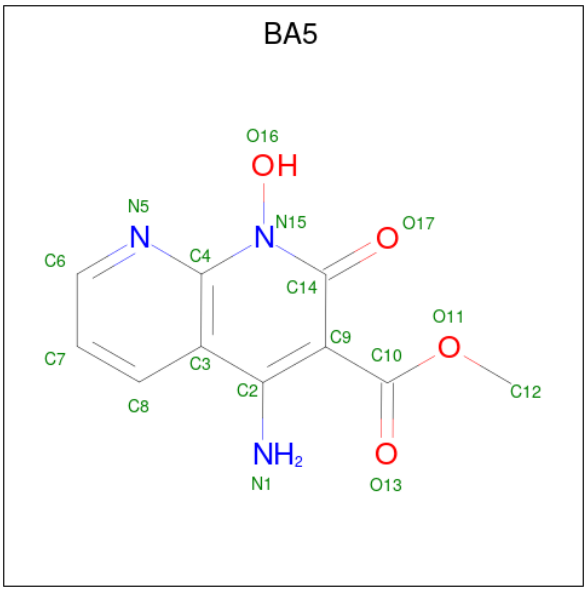
Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 3 is 4-{[4-({4-[(E)-2-cyanoethenyl]-2,6-dimethylphenyl}amino)pyrimidin-2-yl]amino}benzonitrile (three-letter code: T27) (formula: $C_{22}H_{18}N_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	N		
3	A	1	28	22	6	0	0

- Molecule 4 is methyl 4-azanyl-1-oxidanyl-2-oxidanylidene-1,8-naphthyridine-3-carbox ylate (three-letter code: BA5) (formula: $C_{10}H_9N_3O_4$) (labeled as "Ligand of Interest" by depositor).

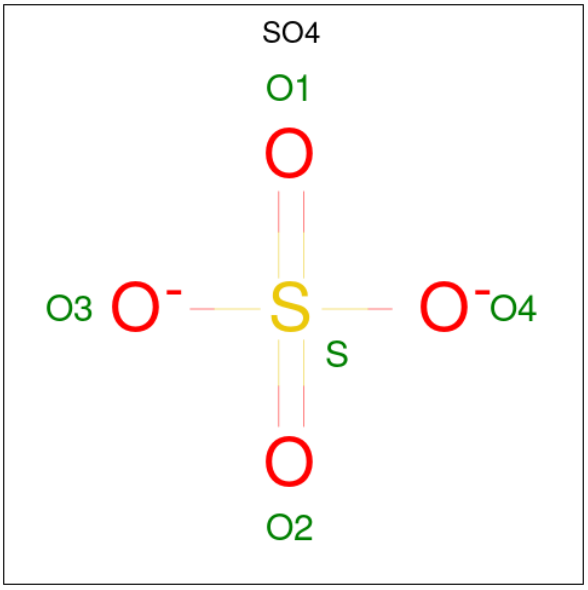


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	17	10	3	4	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

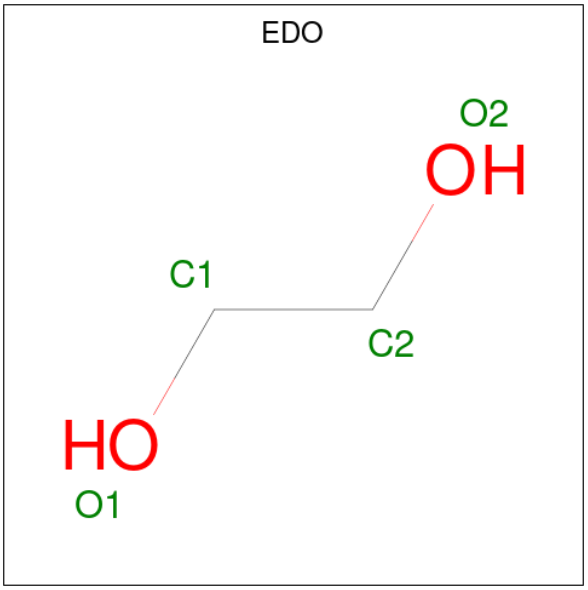
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
5	A	2	2	2	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 8 is water.

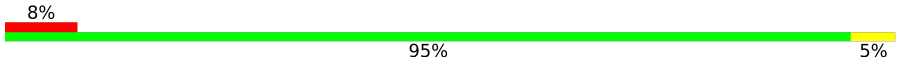
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	229	229	229	0	0
			Total	O		
8	B	142	142	142	0	0

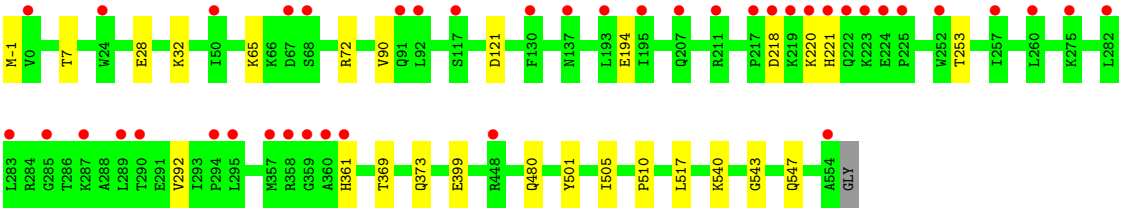
3 Residue-property plots (i)

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

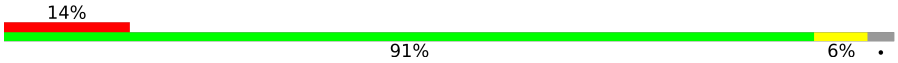
Chain A:

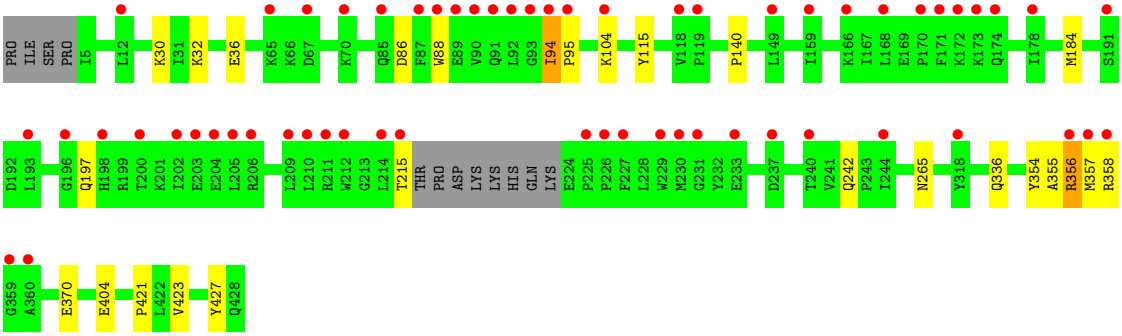




- Molecule 2: Gag-Pol polyprotein

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	163.12Å 72.92Å 109.25Å 90.00° 101.36° 90.00°	Depositor
Resolution (Å)	53.55 – 2.20 71.14 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (53.55-2.20) 100.0 (71.14-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.91 (at 2.20Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.184 , 0.221 0.184 , 0.219	Depositor DCC
R_{free} test set	1935 reflections (3.02%)	wwPDB-VP
Wilson B-factor (Å^2)	41.5	Xtriage
Anisotropy	0.168	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8407	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.49% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: SO4, T27, EDO, BA5, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.27	0/4645	0.51	0/6313
2	B	0.27	0/3554	0.52	0/4829
All	All	0.27	0/8199	0.51	0/11142

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 (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	4524	0	4579	11	0
2	B	3451	0	3476	16	0
3	A	28	0	18	1	0
4	A	17	0	0	0	0
5	A	2	0	0	0	0
6	A	10	0	0	0	0
7	B	4	0	6	0	0
8	A	229	0	0	0	0
8	B	142	0	0	1	0
All	All	8407	0	8079	26	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 2.

All (26) 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:421:PRO:HB2	2:B:423:VAL:HG12	1.82	0.62
2:B:30:LYS:NZ	8:B:603:HOH:O	2.32	0.60
1:A:28:GLU:HG2	1:A:32:LYS:HE3	1.85	0.59
2:B:30:LYS:NZ	2:B:404:GLU:OE2	2.31	0.55
2:B:358:ARG:NH2	2:B:370[B]:GLU:OE1	2.41	0.54
2:B:356:ARG:H	2:B:356:ARG:CD	2.21	0.53
2:B:32:LYS:NZ	2:B:36:GLU:OE2	2.43	0.49
1:A:369:THR:O	1:A:373:GLN:HG2	2.12	0.49
2:B:86:ASP:HB3	2:B:88:TRP:CE2	2.47	0.49
1:A:361:HIS:HB3	1:A:510:PRO:HB3	1.95	0.48
2:B:356:ARG:H	2:B:356:ARG:HD2	1.79	0.47
3:A:701:T27:N3	3:A:701:T27:H17	2.32	0.45
1:A:7:THR:HG21	1:A:121:ASP:HA	2.00	0.44
1:A:540:LYS:HE3	2:B:265:ASN:OD1	2.16	0.44
1:A:480:GLN:HG3	1:A:517:LEU:HD21	2.00	0.44
1:A:501:TYR:CZ	1:A:505:ILE:HD11	2.54	0.43
2:B:104:LYS:HE2	2:B:104:LYS:HB3	1.87	0.43
1:A:90:VAL:HG11	2:B:140:PRO:HB3	2.01	0.43
1:A:253:THR:HG22	1:A:292:VAL:HG22	2.01	0.42
2:B:115:TYR:OH	2:B:184:MET:O	2.31	0.42
1:A:65:LYS:HE3	1:A:72:ARG:HD3	2.02	0.41
1:A:218:ASP:O	1:A:220:LYS:HD2	2.21	0.41
2:B:355:ALA:H	2:B:356:ARG:HE	1.67	0.41
2:B:94:ILE:HA	2:B:95:PRO:HD2	1.98	0.41
2:B:336:GLN:HA	2:B:354:TYR:O	2.21	0.40
2:B:423:VAL:HG22	2:B:427:TYR:CE2	2.56	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	555/557 (100%)	541 (98%)	13 (2%)	1 (0%)	47	55
2	B	414/428 (97%)	398 (96%)	16 (4%)	0	100	100
All	All	969/985 (98%)	939 (97%)	29 (3%)	1 (0%)	51	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	543	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	496/497 (100%)	491 (99%)	5 (1%)	76	86
2	B	379/390 (97%)	373 (98%)	6 (2%)	62	76
All	All	875/887 (99%)	864 (99%)	11 (1%)	69	81

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-1	MET
1	A	194	GLU
1	A	221	HIS
1	A	399	GLU
1	A	547	GLN
2	B	94	ILE
2	B	197	GLN
2	B	215	THR
2	B	242	GLN
2	B	356	ARG
2	B	357	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are

no such sidechains identified.

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)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	T27	A	701	-	30,30,30	1.24	3 (10%)	39,40,40	1.89	7 (17%)
6	SO4	A	705	-	4,4,4	0.15	0	6,6,6	0.06	0
7	EDO	B	501	-	3,3,3	0.46	0	2,2,2	0.34	0
4	BA5	A	702	5	18,18,18	3.55	8 (44%)	16,26,26	1.89	6 (37%)
6	SO4	A	706	-	4,4,4	0.14	0	6,6,6	0.06	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
3	T27	A	701	-	-	2/13/14/14	0/3/3/3
7	EDO	B	501	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BA5	A	702	5	-	3/6/6/6	0/2/2/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	702	BA5	O13-C10	6.58	1.40	1.22
4	A	702	BA5	C4-N15	-6.52	1.36	1.39
4	A	702	BA5	O11-C10	-6.35	1.19	1.33
4	A	702	BA5	O17-C14	6.30	1.40	1.24
4	A	702	BA5	C14-N15	-4.40	1.32	1.40
3	A	701	T27	C12-N4	4.06	1.44	1.36
4	A	702	BA5	C3-C4	-3.95	1.36	1.41
3	A	701	T27	C11-N1	3.40	1.44	1.38
4	A	702	BA5	C2-N1	3.27	1.45	1.36
3	A	701	T27	C13-C19	2.40	1.49	1.44
4	A	702	BA5	O11-C12	-2.08	1.40	1.45

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	701	T27	N2-C12-N3	-6.15	120.72	126.55
3	A	701	T27	C9-N2-C12	5.66	120.47	115.45
3	A	701	T27	C9-C10-C11	3.67	119.16	116.76
3	A	701	T27	C10-C9-N2	-3.38	119.75	123.96
4	A	702	BA5	O11-C10-C9	3.34	120.30	112.27
3	A	701	T27	C10-C11-N3	-3.22	117.72	123.16
4	A	702	BA5	C6-N5-C4	3.20	120.74	116.77
3	A	701	T27	C12-N3-C11	2.95	122.15	116.28
3	A	701	T27	C6-N1-C11	-2.91	118.92	124.18
4	A	702	BA5	C7-C8-C3	-2.76	117.06	120.89
4	A	702	BA5	O11-C10-O13	-2.52	118.52	123.45
4	A	702	BA5	C12-O11-C10	2.31	120.28	115.83
4	A	702	BA5	C7-C6-N5	-2.11	120.70	123.94

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	701	T27	C20-C21-C3-C4
3	A	701	T27	C20-C21-C3-C2
7	B	501	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	A	702	BA5	O13-C10-C9-C14
4	A	702	BA5	O11-C10-C9-C2
4	A	702	BA5	O13-C10-C9-C2

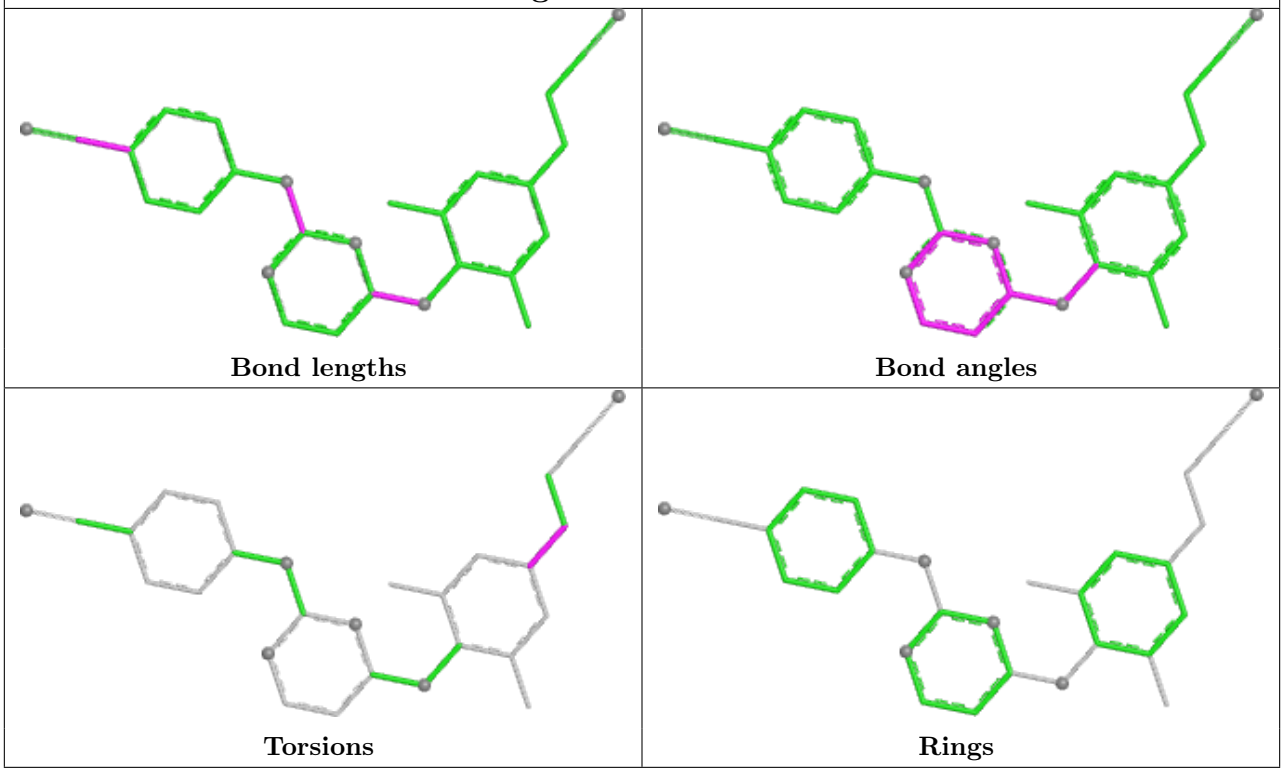
There are no ring outliers.

1 monomer is involved in 1 short contact:

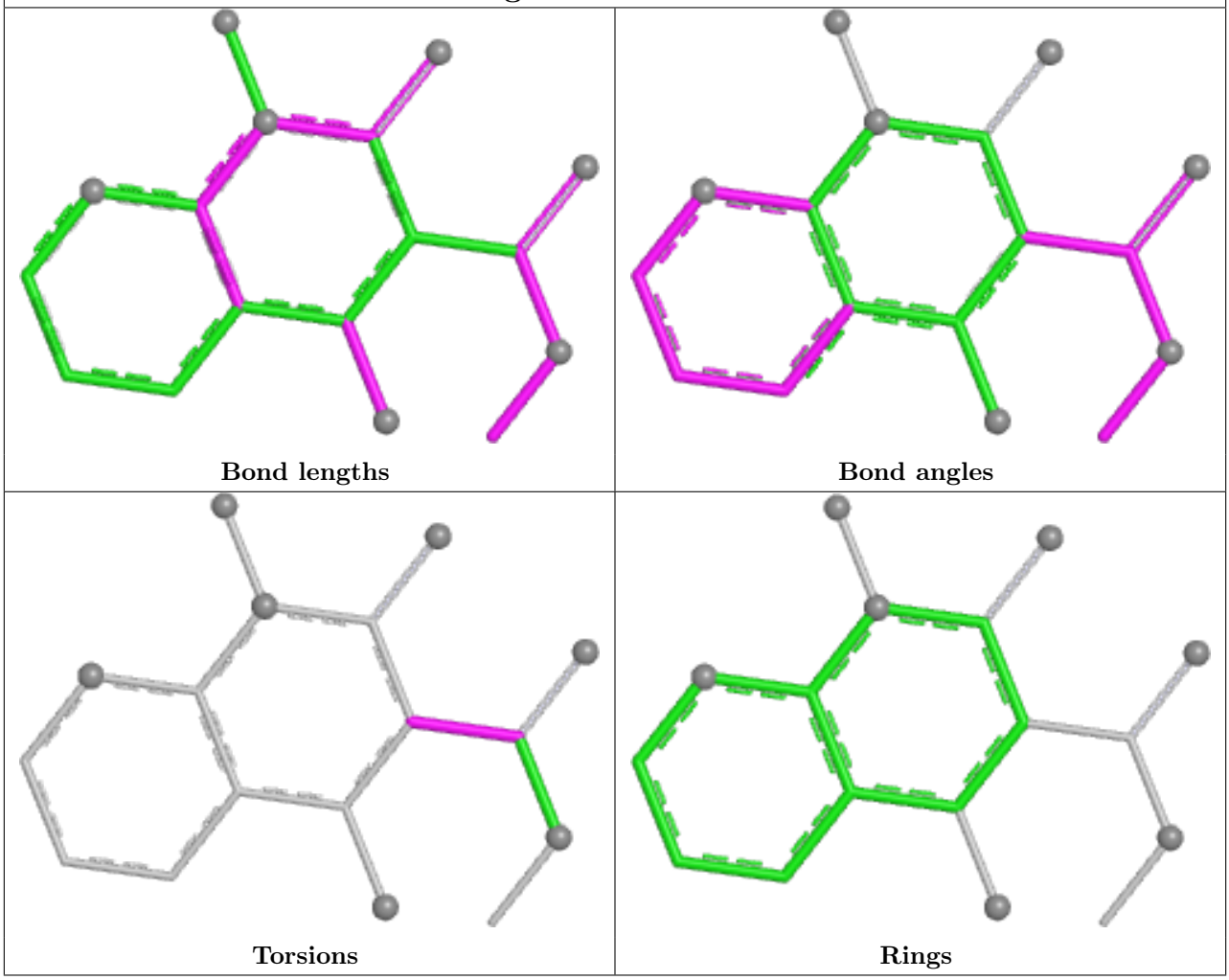
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	701	T27	1	0

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 then 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.

Ligand T27 A 701



Ligand BA5 A 702



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	556/557 (99%)	0.64	42 (7%) 13 12	26, 54, 108, 163	0
2	B	416/428 (97%)	1.01	59 (14%) 2 2	28, 52, 122, 171	0
All	All	972/985 (98%)	0.80	101 (10%) 6 5	26, 54, 118, 171	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	90	VAL	16.7
2	B	227	PHE	12.8
2	B	226	PRO	12.6
2	B	92	LEU	11.8
1	A	221	HIS	11.4
1	A	220	LYS	10.6
2	B	214	LEU	9.7
2	B	91	GLN	9.3
2	B	240	THR	9.0
2	B	230	MET	8.4
2	B	88	TRP	7.7
2	B	229	TRP	7.6
2	B	89	GLU	7.5
2	B	202	ILE	7.2
2	B	87	PHE	7.2
1	A	67	ASP	6.9
2	B	215	THR	6.7
2	B	198	HIS	6.6
2	B	93	GLY	6.5
1	A	222	GLN	6.4
1	A	287	LYS	6.2
1	A	219	LYS	6.0
2	B	94	ILE	5.0
2	B	212	TRP	4.9

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Mol	Chain	Res	Type	RSRZ
2	B	95	PRO	4.7
1	A	218	ASP	4.7
1	A	223	LYS	4.7
2	B	225	PRO	4.5
2	B	231	GLY	4.3
2	B	359	GLY	4.2
1	A	257	ILE	4.0
2	B	205	LEU	4.0
2	B	118	VAL	3.9
1	A	0	VAL	3.9
1	A	130	PHE	3.9
2	B	178	ILE	3.9
1	A	358	ARG	3.8
2	B	168	LEU	3.7
1	A	68	SER	3.7
1	A	290	THR	3.7
2	B	65	LYS	3.7
1	A	224	GLU	3.7
2	B	358	ARG	3.6
1	A	225	PRO	3.5
2	B	357	MET	3.4
2	B	211	ARG	3.4
1	A	275	LYS	3.4
1	A	260	LEU	3.4
2	B	360	ALA	3.4
1	A	289	LEU	3.3
2	B	356	ARG	3.3
1	A	24	TRP	3.3
2	B	171	PHE	3.2
2	B	200	THR	3.2
1	A	295	LEU	3.0
2	B	193	LEU	2.9
2	B	166	LYS	2.9
2	B	191	SER	2.9
2	B	206	ARG	2.9
2	B	173	LYS	2.9
1	A	217	PRO	2.9
2	B	233	GLU	2.9
1	A	357	MET	2.9
1	A	294	PRO	2.8
2	B	318	TYR	2.8
2	B	172	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	361	HIS	2.8
2	B	67	ASP	2.8
2	B	70	LYS	2.7
1	A	211[A]	ARG	2.7
1	A	195	ILE	2.7
2	B	104	LYS	2.7
1	A	448	ARG	2.7
1	A	252	TRP	2.7
1	A	207	GLN	2.6
2	B	85	GLN	2.6
2	B	210	LEU	2.6
2	B	209	LEU	2.5
2	B	159	ILE	2.5
1	A	193	LEU	2.5
2	B	196	GLY	2.5
1	A	92	LEU	2.5
1	A	282	LEU	2.5
1	A	554	ALA	2.4
2	B	170	PRO	2.3
2	B	174	GLN	2.3
2	B	119	PRO	2.3
2	B	204	GLU	2.2
2	B	12	LEU	2.2
2	B	244	ILE	2.2
1	A	91	GLN	2.2
1	A	117	SER	2.2
1	A	283	LEU	2.1
1	A	359	GLY	2.1
2	B	203	GLU	2.1
1	A	285	GLY	2.1
2	B	149	LEU	2.0
1	A	50	ILE	2.0
1	A	360	ALA	2.0
2	B	237	ASP	2.0
1	A	137	ASN	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)

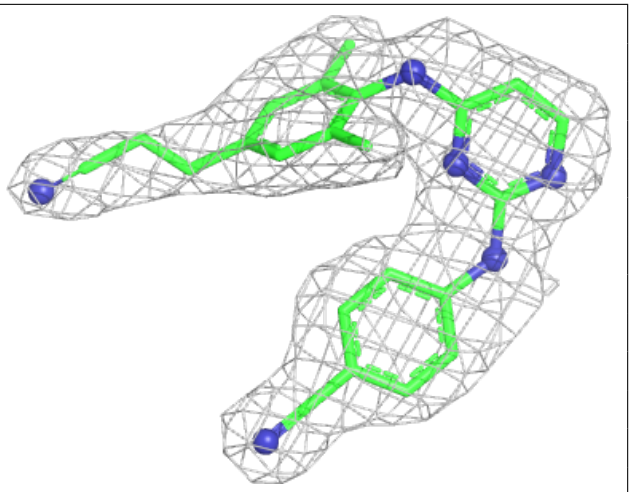
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

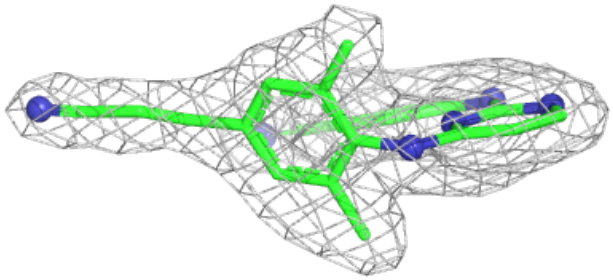
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	EDO	B	501	4/4	0.83	0.24	58,62,65,67	0
5	MG	A	703	1/1	0.84	0.08	31,31,31,31	0
6	SO4	A	706	5/5	0.86	0.16	87,94,103,107	0
6	SO4	A	705	5/5	0.90	0.27	98,102,106,111	0
5	MG	A	704	1/1	0.93	0.08	36,36,36,36	0
3	T27	A	701	28/28	0.94	0.16	36,44,55,59	0
4	BA5	A	702	17/17	0.95	0.14	32,43,50,53	0

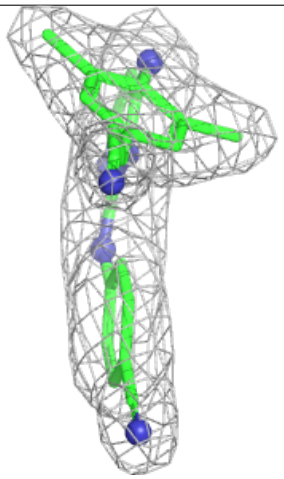
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around T27 A 701:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

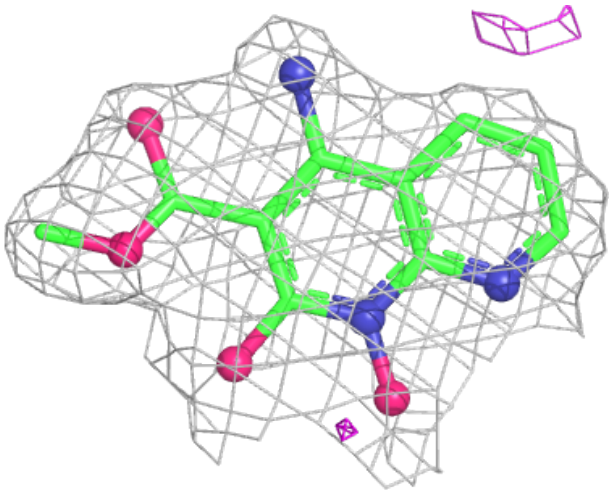


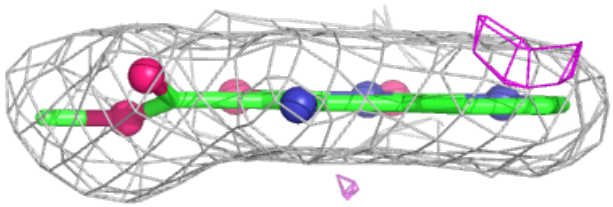


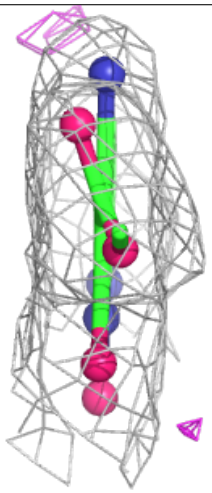


Electron density around BA5 A 702:

$2mF_o$-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.