



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 12:56 PM EDT

PDB ID : 8DX8 / pdb_00008dx8
Title : HIV-1 reverse transcriptase/rilpivirine with bound fragment 2-chloro-6-fluoro phenethylamine at the 415 site
Authors : Chopra, A.; Ruiz, F.X.; Bauman, J.D.; Arnold, E.
Deposited on : 2022-08-02
Resolution : 1.85 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

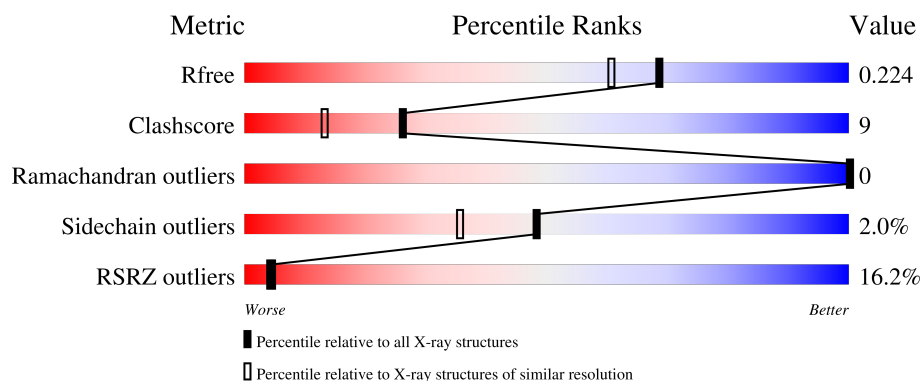
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	SO4	B	507	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 8703 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	556	Total	C	N	O	S	0	4	0
			4549	2942	759	840	8			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP P03366
A	0	VAL	-	expression tag	UNP P03366
A	172	ALA	LYS	engineered mutation	UNP P03366
A	173	ALA	LYS	engineered mutation	UNP P03366
A	280	SER	CYS	engineered mutation	UNP P03366

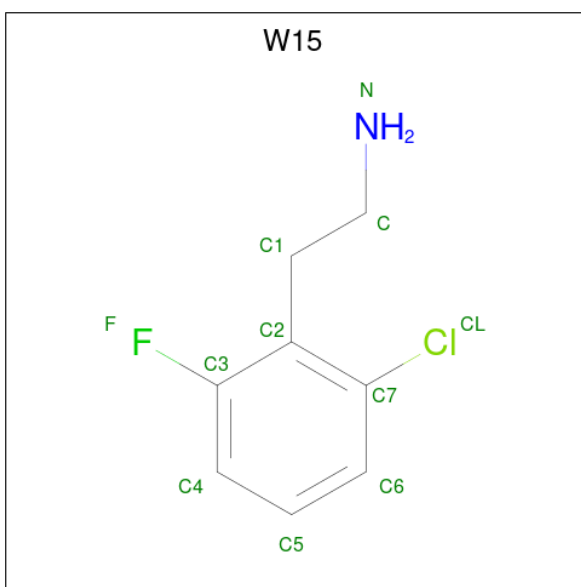
- Molecule 2 is a protein called p51 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	415	Total	C	N	O	S	4	5	0
			3466	2264	571	624	7			

There is a discrepancy between the modelled and reference sequences:

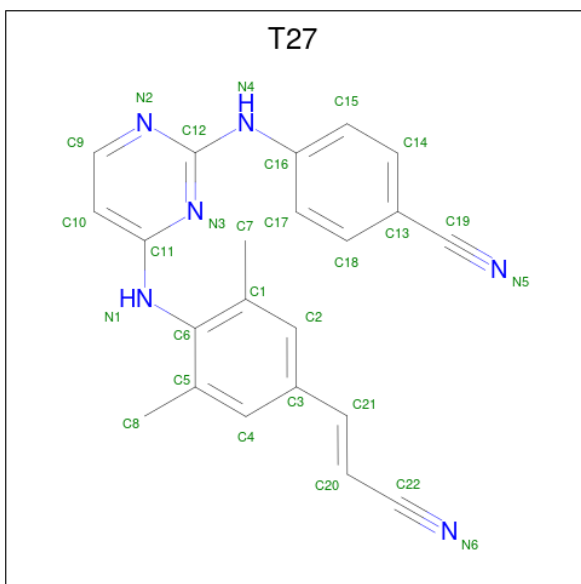
Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 3 is 2-(2-chloro-6-fluorophenyl)ethan-1-amine (CCD ID: W15) (formula: C₈H₉ClFN) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	F	N	0	0
			11	8	1	1	1		

- Molecule 4 is 4-{[4-({4-[(E)-2-cyanoethenyl]-2,6-dimethylphenyl}amino)pyrimidin-2-yl]amino}benzonitrile (CCD ID: T27) (formula: C₂₂H₁₈N₆).



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

- Molecule 5 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



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

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Mg	0	0
			1	1		

- Molecule 8 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

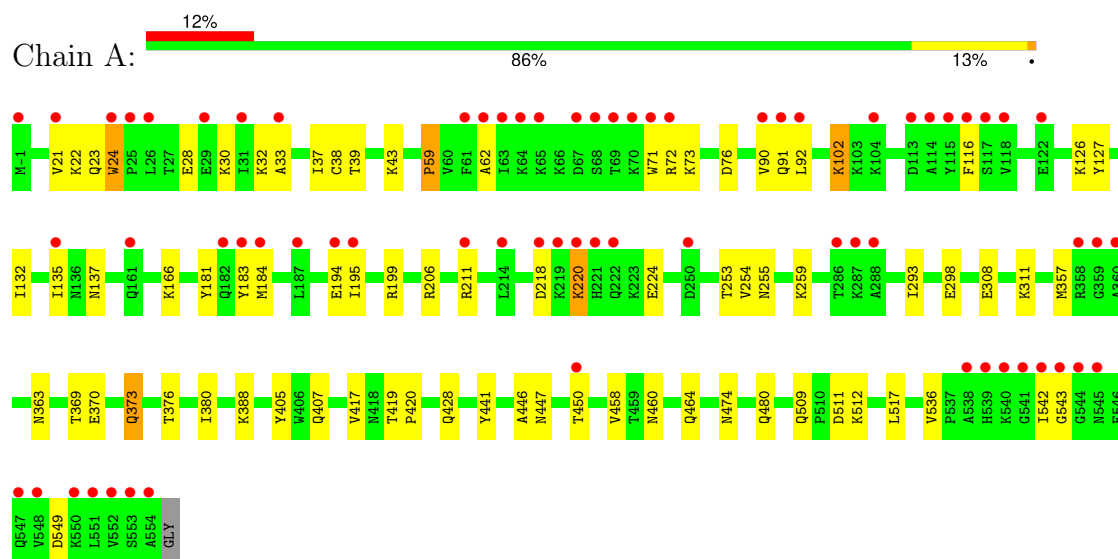
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	362	Total	O	0	0
			362	362		
9	B	221	Total	O	0	0
			221	221		

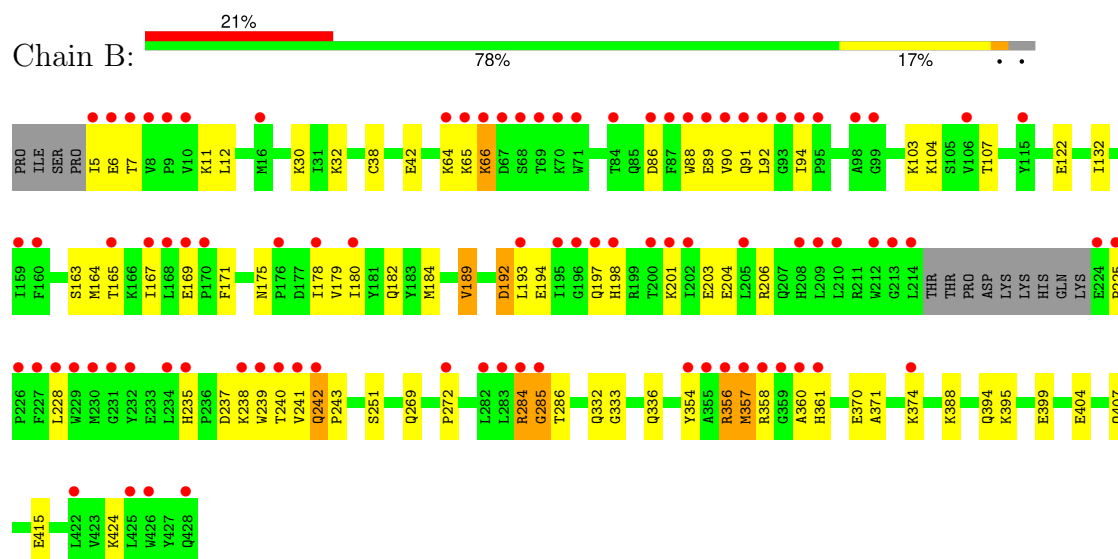
3 Residue-property plots [i](#)

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	161.67Å 73.12Å 109.35Å 90.00° 99.91° 90.00°	Depositor
Resolution (Å)	41.96 – 1.85 41.96 – 1.85	Depositor EDS
% Data completeness (in resolution range)	91.0 (41.96-1.85) 87.1 (41.96-1.85)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 1.86Å)	Xtriage
Refinement program	PHENIX dev_3051	Depositor
R, R_{free}	0.201 , 0.223 0.201 , 0.224	Depositor DCC
R_{free} test set	2000 reflections (1.87%)	wwPDB-VP
Wilson B-factor (Å ²)	28.7	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 45.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8703	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.27% 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, T27, W15, MG, EDO, 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	0.40	1/4670 (0.0%)	0.64	3/6345 (0.0%)
2	B	0.29	1/3581 (0.0%)	0.62	12/4867 (0.2%)
All	All	0.36	2/8251 (0.0%)	0.64	15/11212 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	32	LYS	C-N	-6.18	1.25	1.33
1	A	211	ARG	C-N	-5.63	1.25	1.33

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	59	PRO	CB-CA-C	-9.48	99.60	111.64
2	B	5	ILE	CA-C-N	-7.66	110.53	122.87
2	B	5	ILE	C-N-CA	-7.66	110.53	122.87
2	B	360	ALA	CA-C-O	-6.50	115.17	121.02
2	B	356	ARG	CA-C-N	-6.21	112.61	121.50
2	B	356	ARG	C-N-CA	-6.21	112.61	121.50
2	B	192	ASP	CA-C-N	-6.07	111.90	122.64
2	B	192	ASP	C-N-CA	-6.07	111.90	122.64
2	B	357	MET	O-C-N	5.78	129.80	123.04
2	B	360	ALA	N-CA-C	5.76	117.21	110.41
1	A	509	GLN	CA-C-O	-5.67	116.56	120.47
2	B	285	GLY	CA-C-O	-5.41	117.95	122.33
1	A	549	ASP	N-CA-C	-5.34	105.36	111.07
2	B	242	GLN	O-C-N	5.31	127.42	121.32
2	B	189	VAL	O-C-N	5.28	128.67	123.18

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	4549	0	4604	63	0
2	B	3466	0	3495	94	0
3	A	11	0	0	0	0
4	A	28	0	18	1	0
5	A	12	0	18	3	0
5	B	16	0	24	3	0
6	A	8	0	12	0	0
6	B	4	0	6	0	0
7	A	1	0	0	0	0
8	A	15	0	0	0	0
8	B	10	0	0	2	0
9	A	362	0	0	4	0
9	B	221	0	0	13	0
All	All	8703	0	8177	153	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 9.

All (153) 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:358:ARG:NH1	2:B:370[B]:GLU:HG2	1.70	1.05
2:B:11:LYS:HD3	2:B:12:LEU:O	1.59	1.01
2:B:370[B]:GLU:OE2	2:B:374:LYS:HE3	1.61	1.00
2:B:370[B]:GLU:CD	2:B:374:LYS:HE3	1.88	0.97
2:B:242:GLN:HG2	9:B:650:HOH:O	1.66	0.96
2:B:228:LEU:HB2	9:B:796:HOH:O	1.67	0.94
2:B:104:LYS:HG2	2:B:192:ASP:HA	1.57	0.86
2:B:104:LYS:HA	2:B:237:ASP:OD1	1.77	0.85
2:B:358:ARG:HH11	2:B:370[B]:GLU:HG2	1.39	0.84
2:B:272:PRO:HD2	9:B:788:HOH:O	1.76	0.84
2:B:180:ILE:HG12	2:B:189:VAL:HG13	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:GLN:H	5:A:604:DMS:H23	1.43	0.80
2:B:357:MET:HA	2:B:358:ARG:CZ	2.13	0.79
2:B:64:LYS:O	2:B:407:GLN:HG2	1.84	0.77
2:B:404:GLU:HG2	8:B:507:SO4:O2	1.84	0.76
2:B:404:GLU:CG	8:B:507:SO4:O2	2.36	0.74
1:A:23:GLN:NE2	9:A:701:HOH:O	2.21	0.72
2:B:357:MET:HA	2:B:358:ARG:NH1	2.04	0.72
2:B:333:GLY:O	2:B:336:GLN:HG2	1.91	0.71
2:B:370[B]:GLU:OE2	2:B:374:LYS:CE	2.38	0.71
1:A:72:ARG:CD	1:A:73:LYS:H	2.04	0.70
1:A:253:THR:HG22	1:A:255:ASN:H	1.58	0.69
2:B:356:ARG:HG2	2:B:358:ARG:HH21	1.58	0.68
2:B:424:LYS:HE3	9:B:690:HOH:O	1.94	0.67
2:B:358:ARG:HD2	2:B:358:ARG:H	1.60	0.67
1:A:32:LYS:HD2	1:A:33:ALA:N	2.09	0.67
1:A:194:GLU:HA	1:A:194:GLU:OE2	1.95	0.67
2:B:361:HIS:HB2	9:B:790:HOH:O	1.96	0.65
1:A:39:THR:HG22	1:A:43:LYS:HE3	1.77	0.65
2:B:358:ARG:H	2:B:358:ARG:CD	2.10	0.64
2:B:203:GLU:OE2	2:B:206:ARG:NH1	2.31	0.64
2:B:237:ASP:OD2	2:B:238:LYS:NZ	2.30	0.64
2:B:361:HIS:CB	9:B:790:HOH:O	2.45	0.64
2:B:370[B]:GLU:CD	2:B:374:LYS:CE	2.67	0.63
1:A:298:GLU:CD	1:A:298:GLU:H	2.07	0.63
2:B:104:LYS:HA	2:B:104:LYS:HE3	1.79	0.63
1:A:206:ARG:NH2	1:A:218:ASP:OD1	2.30	0.62
1:A:480[B]:GLN:NE2	9:A:703:HOH:O	2.29	0.62
2:B:193:LEU:HD12	2:B:193:LEU:N	2.14	0.62
1:A:308:GLU:OE1	1:A:311:LYS:HE2	1.99	0.61
2:B:356:ARG:HG2	2:B:358:ARG:NH2	2.15	0.61
2:B:399:GLU:HB3	5:B:503:DMS:H12	1.83	0.61
1:A:195:ILE:HG13	1:A:199:ARG:NH2	2.15	0.60
2:B:357:MET:CE	2:B:371:ALA:HB2	2.32	0.60
2:B:104:LYS:HD2	2:B:192:ASP:OD1	2.02	0.60
2:B:184:MET:HE3	9:B:608:HOH:O	2.01	0.60
1:A:30:LYS:HE2	1:A:71:TRP:CZ3	2.37	0.60
1:A:24:TRP:CZ3	1:A:59:PRO:HB3	2.36	0.59
1:A:357:MET:HE2	1:A:370:GLU:CD	2.27	0.59
1:A:28:GLU:HG3	1:A:135:ILE:HD12	1.85	0.58
1:A:428:GLN:N	5:A:604:DMS:H23	2.17	0.57
2:B:171:PHE:HE1	2:B:204:GLU:HG2	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:543:GLY:HA3	2:B:284:ARG:HA	1.86	0.56
1:A:298:GLU:CD	1:A:298:GLU:N	2.63	0.56
2:B:164:MET:HE3	2:B:182:GLN:OE1	2.04	0.56
2:B:171:PHE:CE1	2:B:204:GLU:HG2	2.40	0.56
1:A:253:THR:HG22	1:A:255:ASN:N	2.21	0.56
1:A:480[B]:GLN:HG3	1:A:517:LEU:HD21	1.86	0.56
2:B:104:LYS:HA	2:B:237:ASP:CG	2.31	0.55
2:B:104:LYS:HG2	2:B:192:ASP:CA	2.35	0.55
1:A:39:THR:O	1:A:43:LYS:HG3	2.06	0.54
2:B:107:THR:OG1	2:B:198:HIS:NE2	2.39	0.54
1:A:59:PRO:HG2	1:A:76:ASP:HB3	1.89	0.54
2:B:357:MET:HE3	2:B:371:ALA:HB2	1.90	0.53
2:B:104:LYS:CA	2:B:237:ASP:OD1	2.56	0.53
1:A:72:ARG:HD2	1:A:73:LYS:H	1.74	0.52
2:B:86:ASP:HB3	2:B:88:TRP:CE2	2.44	0.52
1:A:37:ILE:HD13	1:A:72:ARG:HD2	1.93	0.51
2:B:65:LYS:HE3	2:B:66:LYS:H	1.76	0.51
2:B:239:TRP:HE1	5:B:502:DMS:H23	1.75	0.51
2:B:235:HIS:H	5:B:502:DMS:H21	1.75	0.51
1:A:195:ILE:CG1	1:A:199:ARG:NH2	2.74	0.50
1:A:308:GLU:OE1	1:A:311:LYS:CE	2.59	0.50
1:A:543:GLY:HA3	2:B:285:GLY:H	1.77	0.50
2:B:203:GLU:OE2	2:B:206:ARG:HD2	2.11	0.49
1:A:369:THR:O	1:A:373[B]:GLN:HG2	2.12	0.49
1:A:135:ILE:HA	9:A:719:HOH:O	2.11	0.49
2:B:203:GLU:CD	2:B:206:ARG:HD2	2.38	0.49
2:B:94:ILE:O	2:B:94:ILE:HG13	2.13	0.49
1:A:181:TYR:CE2	1:A:183:TYR:HB2	2.47	0.49
1:A:536:VAL:HB	1:A:542:ILE:HD13	1.95	0.48
2:B:354:TYR:HB2	2:B:357:MET:HE2	1.95	0.48
2:B:38:CYS:SG	2:B:132:ILE:HD11	2.52	0.48
2:B:356:ARG:O	2:B:358:ARG:NH2	2.46	0.48
1:A:30:LYS:HD3	1:A:62:ALA:HB3	1.94	0.48
2:B:361:HIS:HB3	9:B:790:HOH:O	2.13	0.48
2:B:104:LYS:HE3	2:B:237:ASP:CG	2.38	0.48
1:A:512:LYS:HE2	5:A:603:DMS:H13	1.95	0.48
2:B:242:GLN:O	2:B:242:GLN:OE1	2.32	0.47
2:B:92:LEU:C	2:B:92:LEU:HD12	2.39	0.47
1:A:195:ILE:HD11	1:A:199:ARG:HH22	1.80	0.47
1:A:126:LYS:HE3	1:A:127:TYR:CZ	2.50	0.47
2:B:88:TRP:HB3	2:B:92:LEU:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:193:LEU:HD21	2:B:201:LYS:NZ	2.29	0.47
2:B:269:GLN:NE2	9:B:603:HOH:O	2.27	0.47
1:A:446:ALA:H	1:A:474:ASN:ND2	2.13	0.46
1:A:183:TYR:CE2	1:A:184:MET:HE2	2.50	0.46
2:B:88:TRP:HA	2:B:91:GLN:O	2.15	0.46
1:A:255:ASN:OD1	1:A:259:LYS:HE3	2.15	0.46
2:B:193:LEU:HD21	2:B:201:LYS:HZ1	1.81	0.46
2:B:332:GLN:HB2	2:B:336:GLN:HG3	1.97	0.46
2:B:357:MET:HE1	2:B:371:ALA:HB2	1.97	0.45
1:A:420:PRO:HG3	9:A:829:HOH:O	2.16	0.45
2:B:6:GLU:CD	2:B:7:THR:H	2.25	0.45
1:A:72:ARG:HD2	1:A:72:ARG:HA	1.71	0.45
1:A:369:THR:HG22	1:A:373[A]:GLN:HE22	1.81	0.45
1:A:254:VAL:CG2	1:A:293:ILE:HD11	2.46	0.45
2:B:193:LEU:N	2:B:193:LEU:CD1	2.80	0.45
1:A:376:THR:O	1:A:380:ILE:HG12	2.16	0.44
4:A:602:T27:N3	4:A:602:T27:H17	2.33	0.44
2:B:284:ARG:HE	2:B:284:ARG:HB2	1.52	0.44
1:A:220:LYS:HB3	1:A:220:LYS:HE3	1.48	0.44
2:B:374:LYS:N	2:B:374:LYS:HD3	2.32	0.44
2:B:86:ASP:HB3	2:B:88:TRP:CZ2	2.52	0.43
2:B:175:ASN:HB3	2:B:178:ILE:HG13	2.00	0.43
2:B:240:THR:N	9:B:612:HOH:O	2.43	0.43
2:B:89:GLU:HG3	2:B:90:VAL:HG23	2.00	0.43
1:A:102:LYS:HB2	1:A:102:LYS:HE2	1.79	0.43
1:A:417:VAL:HG22	1:A:419:THR:HG23	2.00	0.43
2:B:103:LYS:HE2	2:B:179:VAL:CG2	2.48	0.43
2:B:42:GLU:OE1	9:B:601:HOH:O	2.21	0.43
2:B:66:LYS:HA	2:B:66:LYS:HD2	1.68	0.43
2:B:103:LYS:HE2	2:B:179:VAL:HG23	2.01	0.43
2:B:358:ARG:NH1	2:B:370[B]:GLU:CG	2.61	0.42
1:A:308:GLU:O	1:A:311:LYS:HB2	2.18	0.42
1:A:255:ASN:O	1:A:259:LYS:HG3	2.18	0.42
2:B:388:LYS:HE2	2:B:415:GLU:HG2	2.01	0.42
1:A:30:LYS:HB3	1:A:62:ALA:HB3	2.02	0.42
1:A:254:VAL:HG23	1:A:293:ILE:HD11	2.00	0.42
1:A:460:ASN:HA	2:B:286:THR:O	2.19	0.42
2:B:225:PRO:CB	9:B:796:HOH:O	2.67	0.42
1:A:38:CYS:SG	1:A:132:ILE:HD11	2.59	0.42
1:A:458:VAL:HG12	1:A:464:GLN:HG2	2.01	0.42
2:B:358:ARG:CD	2:B:358:ARG:N	2.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:ASN:HB3	1:A:450:THR:OG1	2.20	0.42
2:B:165:THR:O	2:B:169:GLU:HG2	2.19	0.42
1:A:72:ARG:NE	1:A:73:LYS:H	2.17	0.42
1:A:363:ASN:HA	1:A:511:ASP:OD1	2.20	0.41
2:B:242:GLN:HA	2:B:243:PRO:HD2	1.85	0.41
1:A:405:TYR:CE2	1:A:407:GLN:HB2	2.56	0.41
1:A:32:LYS:HD2	1:A:32:LYS:C	2.45	0.41
2:B:104:LYS:HE3	2:B:104:LYS:CA	2.48	0.41
2:B:241:VAL:HB	9:B:809:HOH:O	2.21	0.41
1:A:137:ASN:HD22	1:A:137:ASN:HA	1.74	0.41
1:A:407:GLN:OE1	2:B:394:GLN:HG2	2.20	0.41
2:B:395:LYS:HE2	2:B:399:GLU:OE1	2.20	0.41
2:B:194:GLU:HB3	2:B:197:GLN:HG3	2.03	0.41
1:A:441:TYR:CD1	2:B:286:THR:HG23	2.56	0.41
2:B:354:TYR:CB	2:B:357:MET:HE2	2.52	0.40
2:B:122:GLU:H	2:B:122:GLU:CD	2.29	0.40
2:B:163:SER:O	2:B:167:ILE:HG13	2.21	0.40
1:A:72:ARG:HD2	1:A:73:LYS:N	2.35	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	558/557 (100%)	544 (98%)	14 (2%)	0	100	100
2	B	416/428 (97%)	402 (97%)	14 (3%)	0	100	100
All	All	974/985 (99%)	946 (97%)	28 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	498/495 (101%)	483 (97%)	15 (3%)	36	21
2	B	381/390 (98%)	377 (99%)	4 (1%)	68	60
All	All	879/885 (99%)	860 (98%)	19 (2%)	48	32

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	VAL
1	A	22	LYS
1	A	24	TRP
1	A	90	VAL
1	A	91	GLN
1	A	92	LEU
1	A	102	LYS
1	A	116	PHE
1	A	166	LYS
1	A	220	LYS
1	A	224	GLU
1	A	373[A]	GLN
1	A	373[B]	GLN
1	A	388[A]	LYS
1	A	388[B]	LYS
2	B	30	LYS
2	B	66	LYS
2	B	251	SER
2	B	284	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	ASN
1	A	151	GLN
1	A	520	GLN

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Mol	Chain	Res	Type
2	B	207	GLN
2	B	265	ASN
2	B	407	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 1 is monoatomic - leaving 17 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	$\# Z > 2$
8	SO4	B	507	-	4,4,4	0.36	0	6,6,6	0.07	0
6	EDO	A	606	-	3,3,3	0.41	0	2,2,2	0.42	0
8	SO4	B	506	-	4,4,4	0.40	0	6,6,6	0.05	0
5	DMS	B	501	-	3,3,3	2.68	1 (33%)	3,3,3	0.53	0
4	T27	A	602	-	30,30,30	1.20	3 (10%)	37,40,40	1.71	5 (13%)
5	DMS	A	603	-	3,3,3	2.73	1 (33%)	3,3,3	0.60	0
5	DMS	B	504	-	3,3,3	2.70	1 (33%)	3,3,3	0.53	0
6	EDO	B	505	-	3,3,3	0.40	0	2,2,2	0.36	0
8	SO4	A	609	-	4,4,4	0.47	0	6,6,6	0.11	0
8	SO4	A	610	-	4,4,4	0.37	0	6,6,6	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	A	605	-	3,3,3	2.75	1 (33%)	3,3,3	0.55	0
5	DMS	A	604	-	3,3,3	2.75	1 (33%)	3,3,3	0.62	0
5	DMS	B	502	-	3,3,3	2.72	1 (33%)	3,3,3	0.51	0
8	SO4	A	611	-	4,4,4	0.39	0	6,6,6	0.11	0
6	EDO	A	607	-	3,3,3	0.31	0	2,2,2	0.24	0
3	W15	A	601	-	11,11,11	0.37	0	13,14,14	0.74	1 (7%)
5	DMS	B	503	-	3,3,3	2.70	1 (33%)	3,3,3	0.53	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
6	EDO	A	606	-	-	0/1/1/1	-
4	T27	A	602	-	-	2/13/14/14	0/3/3/3
6	EDO	B	505	-	-	0/1/1/1	-
6	EDO	A	607	-	-	1/1/1/1	-
3	W15	A	601	-	-	0/3/3/3	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	605	DMS	O-S	4.62	1.80	1.50
5	A	604	DMS	O-S	4.61	1.80	1.50
5	A	603	DMS	O-S	4.58	1.80	1.50
5	B	502	DMS	O-S	4.57	1.80	1.50
5	B	501	DMS	O-S	4.54	1.80	1.50
5	B	504	DMS	O-S	4.54	1.80	1.50
5	B	503	DMS	O-S	4.53	1.80	1.50
4	A	602	T27	C12-N4	3.76	1.44	1.36
4	A	602	T27	C11-N1	3.23	1.44	1.38
4	A	602	T27	C13-C19	2.46	1.49	1.44

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	602	T27	C9-N2-C12	5.54	120.05	115.42
4	A	602	T27	N2-C12-N3	-4.95	121.63	126.42
4	A	602	T27	C10-C9-N2	-3.62	119.54	123.97
4	A	602	T27	C10-C11-N3	-3.13	117.91	123.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	602	T27	C6-N1-C11	-2.93	118.84	124.11
3	A	601	W15	C1-C-N	-2.55	105.73	112.71

There are no chirality outliers.

All (3) torsion outliers are listed below:

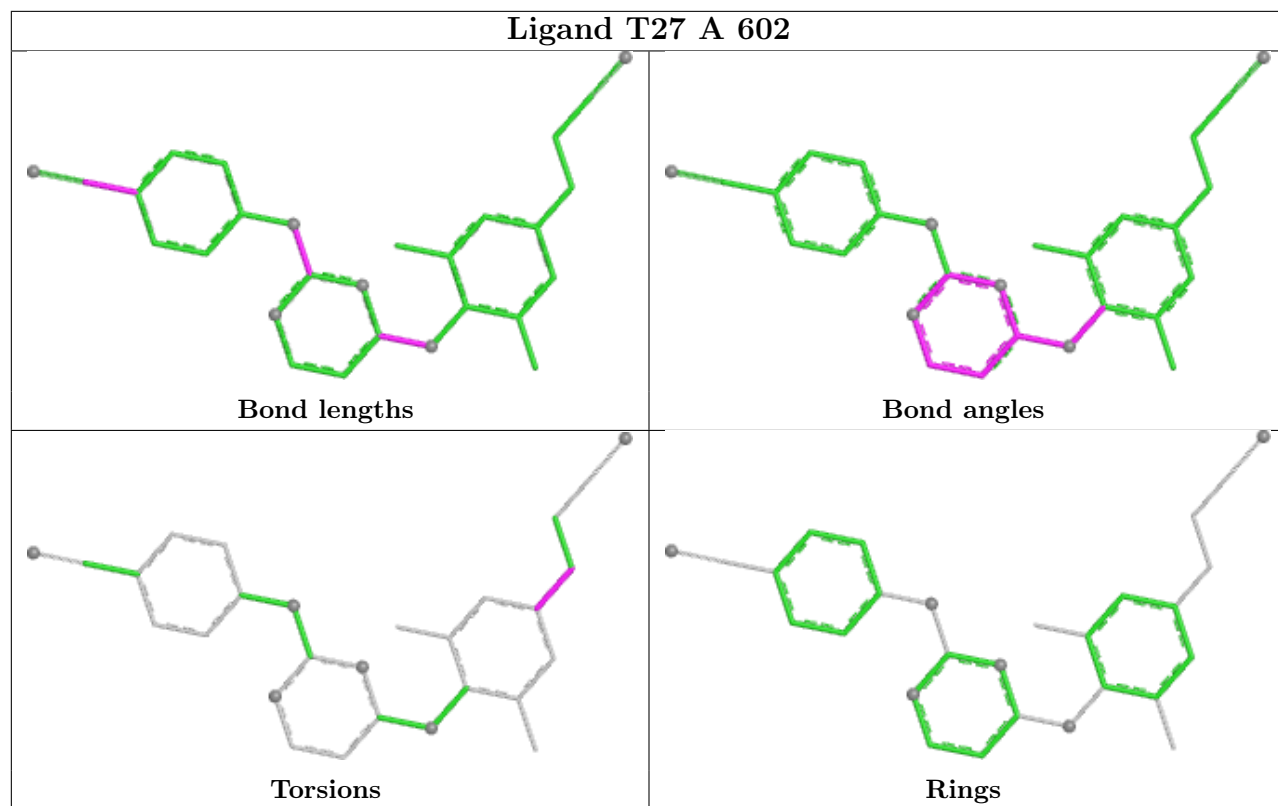
Mol	Chain	Res	Type	Atoms
4	A	602	T27	C20-C21-C3-C2
4	A	602	T27	C20-C21-C3-C4
6	A	607	EDO	O1-C1-C2-O2

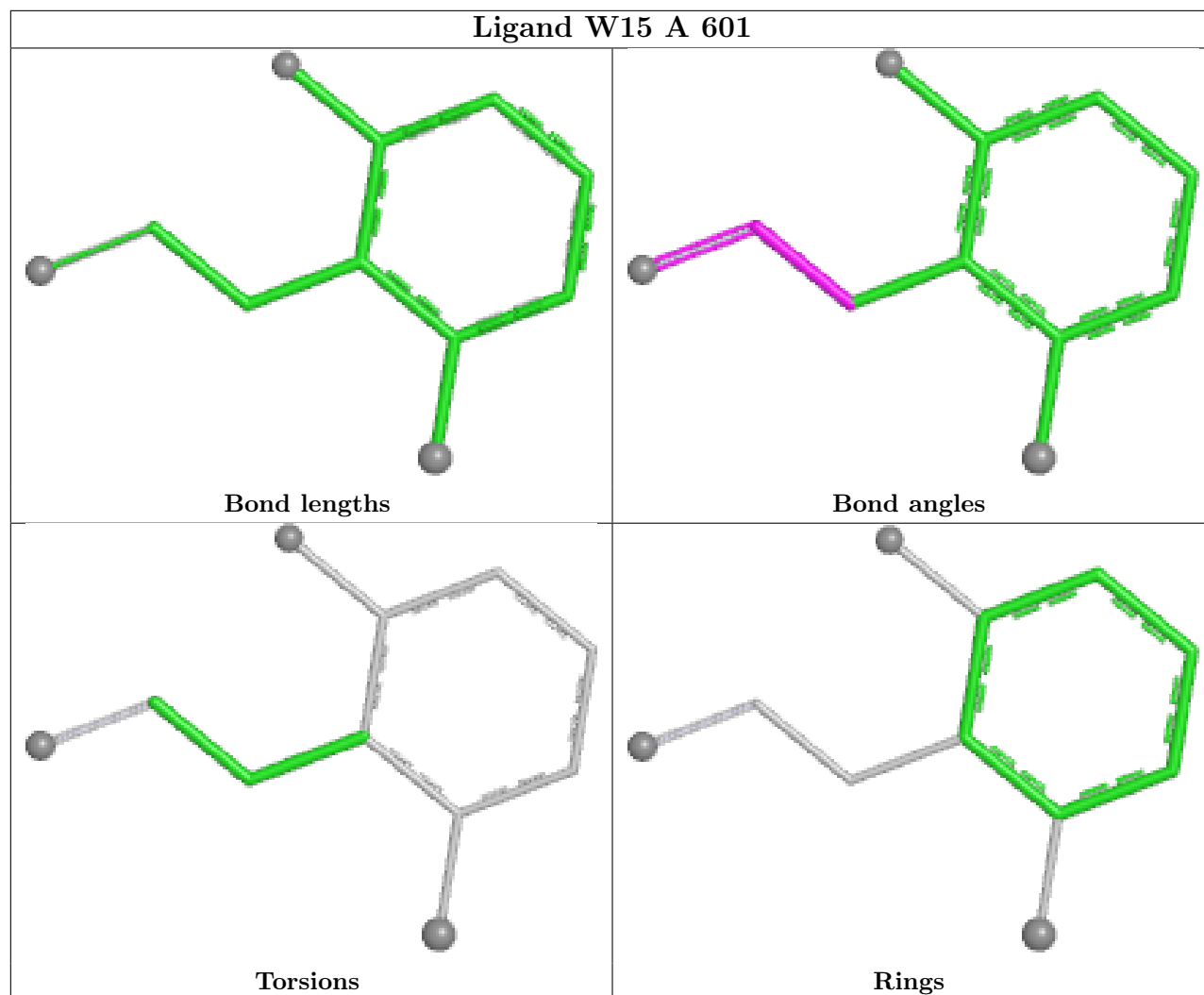
There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	507	SO4	2	0
4	A	602	T27	1	0
5	A	603	DMS	1	0
5	A	604	DMS	2	0
5	B	502	DMS	2	0
5	B	503	DMS	1	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	556/557 (99%)	0.65	68 (12%)	8 8	13, 39, 115, 234	4 (0%)
2	B	415/428 (96%)	0.97	89 (21%)	2 2	16, 43, 135, 247	5 (1%)
All	All	971/985 (98%)	0.79	157 (16%)	4 4	13, 40, 124, 247	9 (0%)

All (157) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	24	TRP	8.0
2	B	241	VAL	7.5
1	A	544	GLY	7.2
1	A	548	VAL	7.2
1	A	542	ILE	7.0
1	A	116	PHE	7.0
1	A	543	GLY	6.7
2	B	92	LEU	6.3
1	A	551	LEU	6.0
1	A	115	TYR	6.0
1	A	90	VAL	5.8
1	A	552	VAL	5.8
2	B	5	ILE	5.7
2	B	229	TRP	5.6
1	A	554	ALA	5.5
1	A	71	TRP	5.4
2	B	94	ILE	5.4
2	B	90	VAL	5.3
1	A	545	ASN	5.2
2	B	95	PRO	5.1
1	A	92	LEU	5.0
2	B	93	GLY	4.8
2	B	357	MET	4.7
2	B	209	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	358[A]	ARG	4.5
2	B	240	THR	4.5
2	B	88	TRP	4.5
2	B	283	LEU	4.4
2	B	227	PHE	4.3
1	A	65	LYS	4.2
2	B	226	PRO	4.1
2	B	168	LEU	4.1
2	B	214	LEU	4.1
1	A	63	ILE	4.0
2	B	242	GLN	4.0
2	B	66	LYS	4.0
2	B	232	TYR	3.9
2	B	212	TRP	3.9
2	B	425	LEU	3.9
1	A	114	ALA	3.9
2	B	196	GLY	3.9
2	B	69	THR	3.8
1	A	135	ILE	3.8
1	A	117	SER	3.7
2	B	284	ARG	3.7
2	B	65	LYS	3.7
1	A	211	ARG	3.7
1	A	288	ALA	3.6
1	A	541	GLY	3.6
2	B	87	PHE	3.6
2	B	428	GLN	3.6
2	B	228	LEU	3.6
1	A	-1	MET	3.5
2	B	201	LYS	3.5
2	B	359	GLY	3.5
2	B	272	PRO	3.5
2	B	200	THR	3.4
1	A	69	THR	3.4
2	B	64	LYS	3.4
2	B	180	ILE	3.3
1	A	72	ARG	3.3
2	B	205	LEU	3.2
2	B	198	HIS	3.2
2	B	239	TRP	3.1
2	B	225	PRO	3.1
1	A	64	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	170	PRO	3.1
1	A	113	ASP	3.1
1	A	221	HIS	3.1
2	B	285	GLY	3.1
1	A	91	GLN	3.0
1	A	553	SER	3.0
1	A	550	LYS	3.0
2	B	360	ALA	3.0
2	B	356	ARG	3.0
1	A	286	THR	3.0
2	B	358	ARG	3.0
2	B	422	LEU	2.9
2	B	71	TRP	2.9
1	A	250	ASP	2.9
2	B	67	ASP	2.9
2	B	210	LEU	2.8
1	A	547	GLN	2.8
1	A	61	PHE	2.8
2	B	195	ILE	2.8
2	B	197	GLN	2.7
2	B	8	VAL	2.7
2	B	234	LEU	2.7
1	A	25	PRO	2.7
1	A	118	VAL	2.7
2	B	10	VAL	2.7
1	A	70	LYS	2.6
1	A	104	LYS	2.6
2	B	167	ILE	2.6
1	A	359	GLY	2.6
1	A	68	SER	2.6
2	B	9	PRO	2.5
2	B	354	TYR	2.5
2	B	176	PRO	2.5
2	B	160	PHE	2.5
2	B	355	ALA	2.5
2	B	115	TYR	2.5
2	B	91	GLN	2.5
1	A	62	ALA	2.5
2	B	165	THR	2.5
2	B	193	LEU	2.4
2	B	361	HIS	2.4
2	B	68	SER	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	89	GLU	2.4
2	B	106	VAL	2.4
1	A	26	LEU	2.4
1	A	220	LYS	2.4
2	B	235	HIS	2.4
1	A	183	TYR	2.3
2	B	202	ILE	2.3
2	B	99	GLY	2.3
2	B	169	GLU	2.3
2	B	70	LYS	2.3
2	B	213	GLY	2.3
1	A	122	GLU	2.3
1	A	187	LEU	2.3
1	A	214	LEU	2.3
2	B	84	THR	2.3
2	B	426[A]	TRP	2.2
2	B	224	GLU	2.2
2	B	178	ILE	2.2
1	A	219	LYS	2.2
1	A	218	ASP	2.2
1	A	540	LYS	2.2
2	B	7	THR	2.2
1	A	161	GLN	2.2
1	A	360	ALA	2.2
1	A	184	MET	2.2
1	A	539	HIS	2.2
2	B	230	MET	2.2
2	B	86	ASP	2.2
1	A	287	LYS	2.2
2	B	282	LEU	2.1
2	B	16	MET	2.1
1	A	33	ALA	2.1
1	A	538	ALA	2.1
2	B	159	ILE	2.1
1	A	450	THR	2.1
2	B	6	GLU	2.1
2	B	231	GLY	2.1
1	A	67	ASP	2.1
1	A	31	ILE	2.0
2	B	374	LYS	2.0
2	B	208	HIS	2.0
1	A	182	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	21	VAL	2.0
2	B	98	ALA	2.0
1	A	29	GLU	2.0
1	A	194	GLU	2.0
2	B	238	LYS	2.0
1	A	195	ILE	2.0
1	A	222	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	SO4	A	610	5/5	0.37	0.19	100,101,107,120	0
5	DMS	B	502	4/4	0.44	0.26	77,96,107,113	0
8	SO4	A	611	5/5	0.50	0.14	64,67,88,99	0
6	EDO	A	606	4/4	0.69	0.34	44,46,50,55	0
5	DMS	A	605	4/4	0.70	0.21	49,59,67,81	0
8	SO4	B	506	5/5	0.70	0.15	54,57,61,81	0
5	DMS	B	504	4/4	0.77	0.23	53,56,61,78	0
5	DMS	B	501	4/4	0.83	0.22	37,44,49,60	0
7	MG	A	608	1/1	0.84	0.12	82,82,82,82	0
3	W15	A	601	11/11	0.85	0.13	32,40,53,60	0
5	DMS	A	603	4/4	0.86	0.19	47,50,54,55	0
6	EDO	A	607	4/4	0.89	0.14	30,32,40,45	0
8	SO4	B	507	5/5	0.90	0.10	51,54,57,113	0
6	EDO	B	505	4/4	0.91	0.16	39,42,45,48	0
5	DMS	B	503	4/4	0.93	0.13	36,41,45,52	0
4	T27	A	602	28/28	0.95	0.07	23,27,32,36	0

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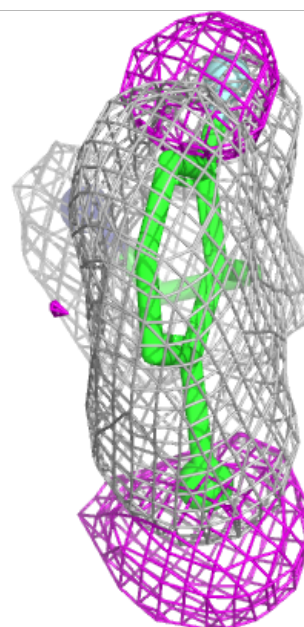
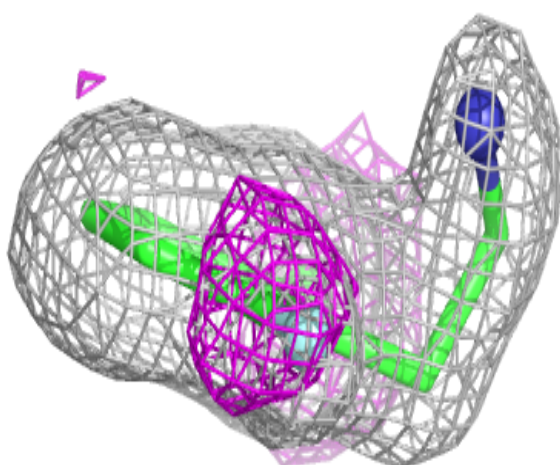
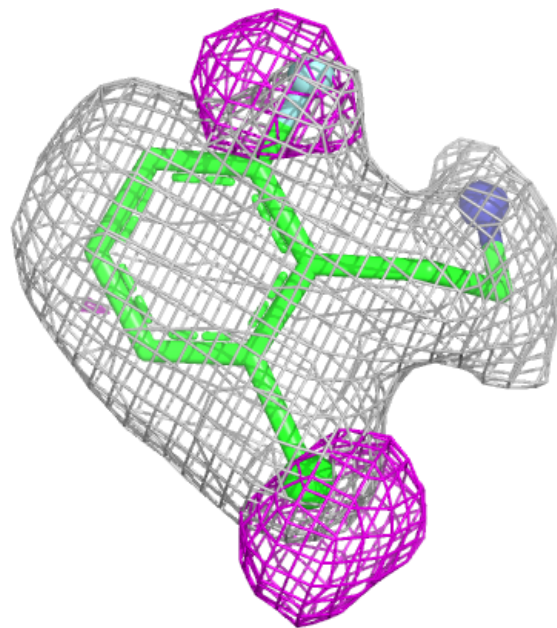
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	SO4	A	609	5/5	0.95	0.06	50,53,57,59	0
5	DMS	A	604	4/4	0.96	0.10	38,44,46,46	0

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.

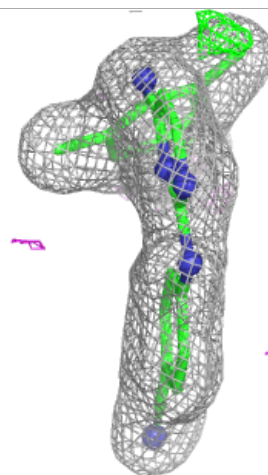
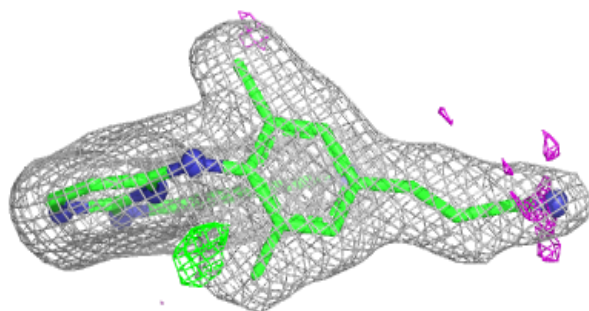
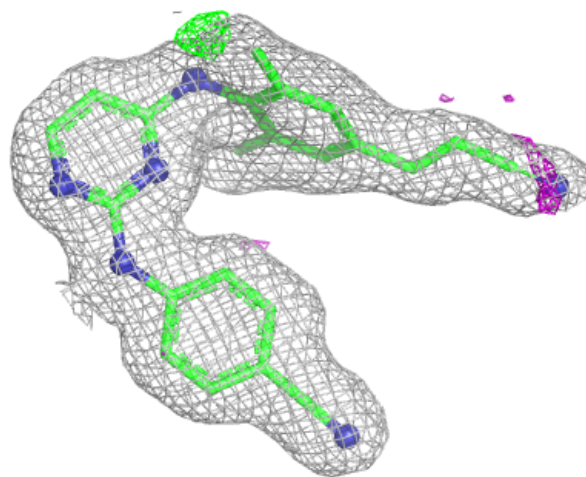
Electron density around W15 A 601:

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 T27 A 602:

$2mF_o-DF_c$ (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.