



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:20 PM UTC

PDB ID : 8STV / pdb_00008stv
Title : Crystal Structure of HIV-1 Reverse Transcriptase (Y181C, V106A) variant in Complex with 5-(2-(2-(2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)ethoxy)phenoxy)-2-naphthonitrile (JLJ600), a non-nucleoside inhibitor
Authors : Hollander, K.; Jorgensen, W.L.; Anderson, K.S.
Deposited on : 2023-05-11
Resolution : 2.78 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

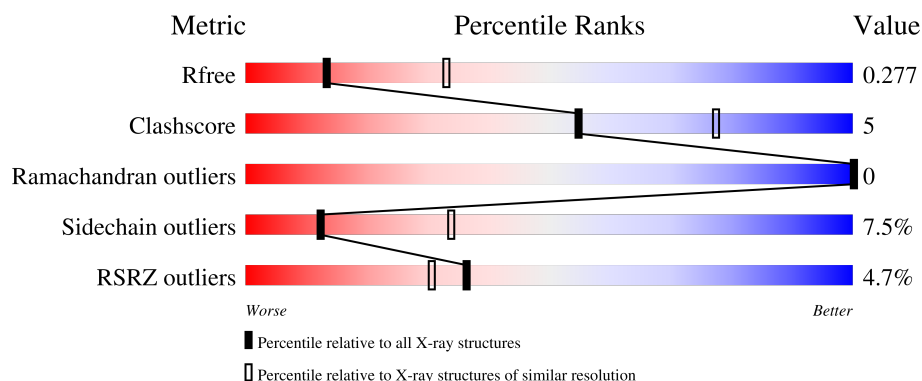
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.78 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	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (2.80-2.76)

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	558	3% 79% 17% ••
1	C	558	5% 78% 18% •
2	B	428	3% 82% 12% • 5%
2	D	428	7% 80% 13% • 6%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14571 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	544	Total	C	N	O	S	0	1	0
			4195	2703	695	790	7			
1	C	542	Total	C	N	O	S	0	2	0
			4072	2609	674	782	7			

There are 14 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	106	ALA	VAL	engineered mutation	UNP P03366
A	172	ALA	LYS	engineered mutation	UNP P03366
A	173	ALA	LYS	engineered mutation	UNP P03366
A	181	CYS	TYR	engineered mutation	UNP P03366
A	280	SER	CYS	engineered mutation	UNP P03366
C	-1	MET	-	expression tag	UNP P03366
C	0	VAL	-	expression tag	UNP P03366
C	106	ALA	VAL	engineered mutation	UNP P03366
C	172	ALA	LYS	engineered mutation	UNP P03366
C	173	ALA	LYS	engineered mutation	UNP P03366
C	181	CYS	TYR	engineered mutation	UNP P03366
C	280	SER	CYS	engineered mutation	UNP P03366

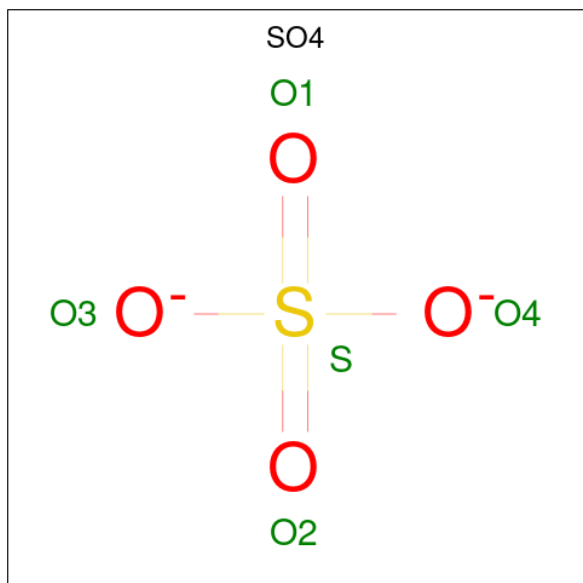
- Molecule 2 is a protein called p51 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	408	Total	C	N	O	S	19	1	0
			3285	2137	532	611	5			
2	D	401	Total	C	N	O	S	10	1	0
			2869	1838	488	540	3			

There are 2 discrepancies between the modelled and reference sequences:

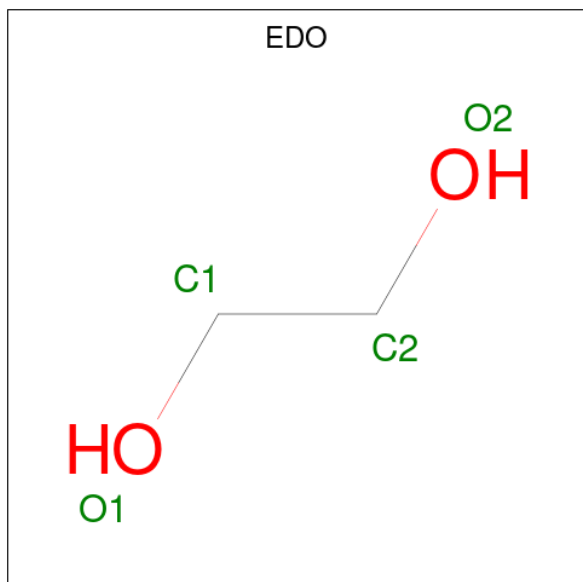
Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	engineered mutation	UNP P03366
D	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



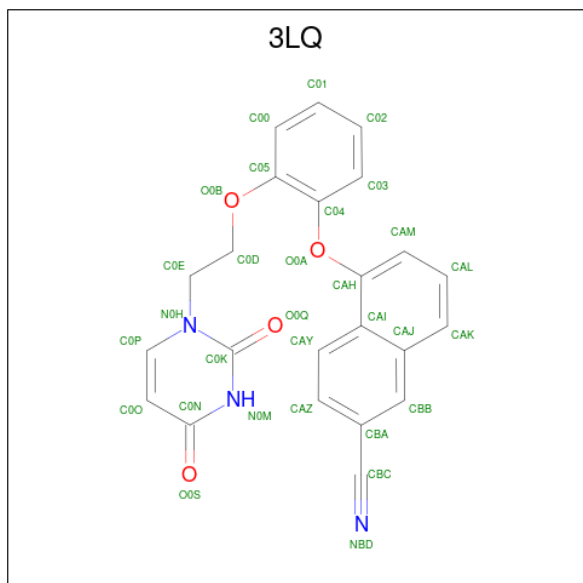
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

- Molecule 5 is 5-{2-[2-(2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)ethoxy]phenoxy}naphthalene-2-carbonitrile (CCD ID: 3LQ) (formula: C₂₃H₁₇N₃O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			30	23	3	4		
5	C	1	Total	C	N	O	0	0
			30	23	3	4		

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	1	Total	Mg	0	0
			1	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	31	Total	O	0	0
			31	31		

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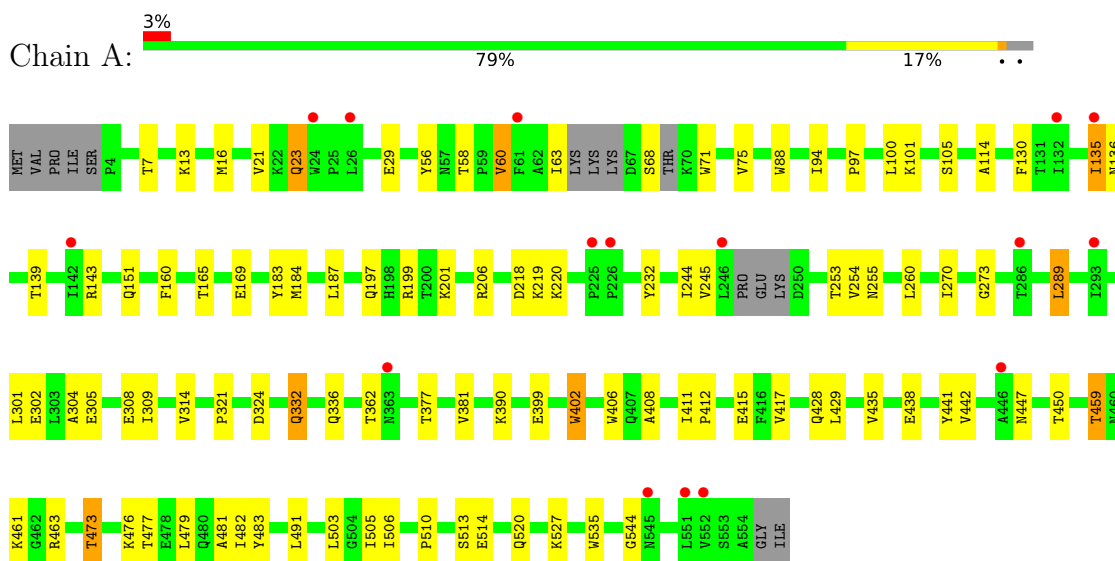
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	29	Total 29	O 29	0	0
7	C	3	Total 3	O 3	0	0
7	D	8	Total 8	O 8	0	0

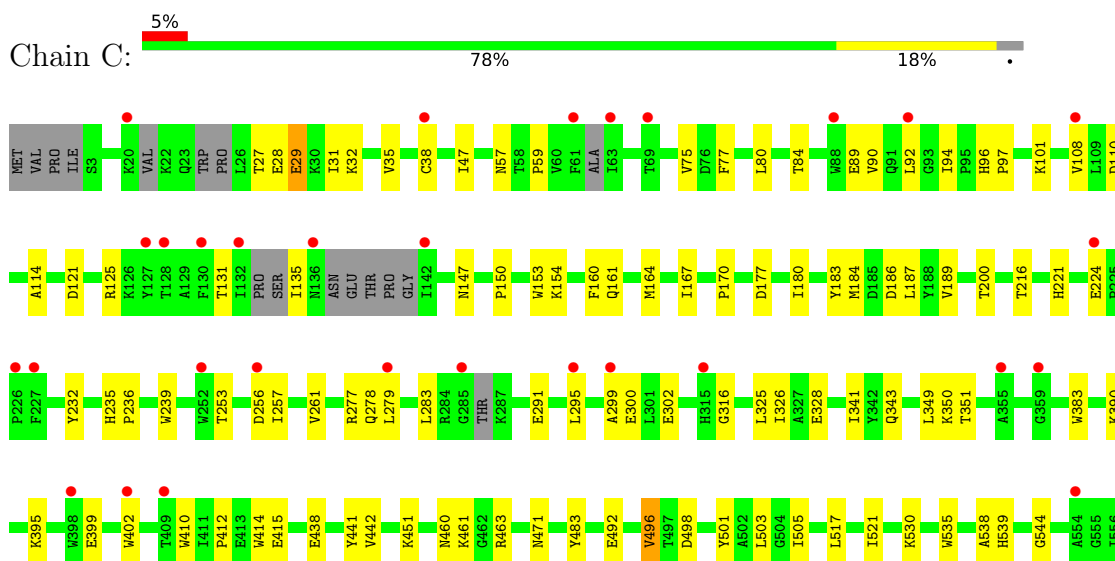
3 Residue-property plots [i](#)

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

- Molecule 1: Reverse transcriptase/ribonuclease H

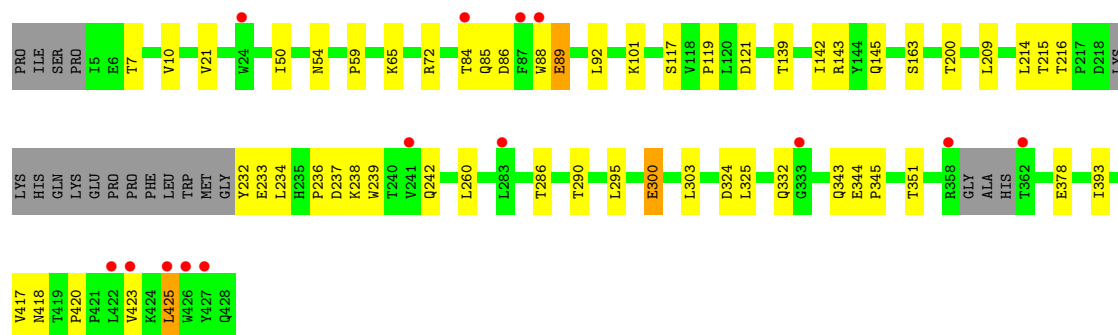


- Molecule 1: Reverse transcriptase/ribonuclease H



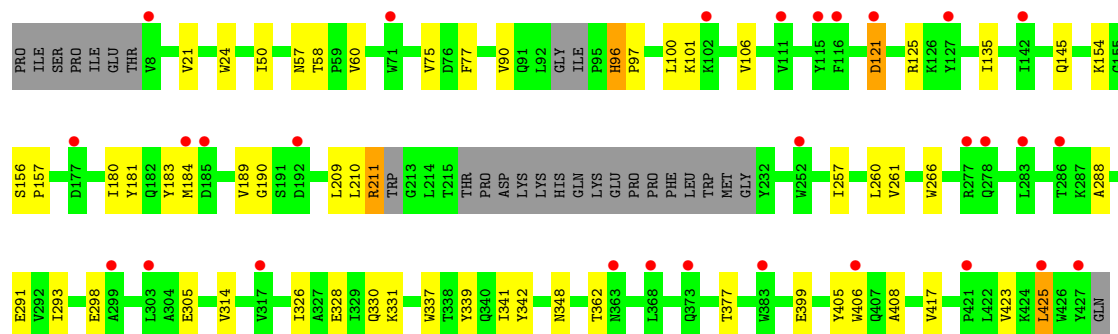
- Molecule 2: p51 RT

Chain B: 



• Molecule 2: p51 RT

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	111.59Å 73.22Å 170.66Å 90.00° 97.73° 90.00°	Depositor
Resolution (Å)	37.83 – 2.78 37.83 – 2.78	Depositor EDS
% Data completeness (in resolution range)	99.8 (37.83-2.78) 99.8 (37.83-2.78)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 2.77Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.232 , 0.276 0.231 , 0.277	Depositor DCC
R_{free} test set	3393 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	86.8	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 76.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14571	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 3LQ, MG, SO4, EDO

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	0.13	0/4306	0.30	0/5884
1	C	0.14	0/4175	0.29	0/5710
2	B	0.12	0/3381	0.31	0/4617
2	D	0.16	0/2949	0.33	1/4065 (0.0%)
All	All	0.14	0/14811	0.31	1/20276 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	210	LEU	N-CA-C	-5.43	105.28	112.34

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	4195	0	3982	48	0
1	C	4072	0	3724	44	0
2	B	3285	0	3200	23	0
2	D	2869	0	2419	24	0
3	A	10	0	0	0	0
4	A	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	4	0	6	1	0
5	A	30	0	17	1	0
5	C	30	0	17	0	0
6	C	1	0	0	0	0
7	A	31	0	0	2	0
7	B	29	0	0	0	0
7	C	3	0	0	0	0
7	D	8	0	0	0	0
All	All	14571	0	13371	134	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 (134) 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:C:451:LYS:HA	1:C:471:ASN:H	1.64	0.63
1:C:328:GLU:HG2	1:C:390:LYS:HB2	1.79	0.63
1:A:135:ILE:HD12	1:A:136:ASN:H	1.63	0.62
2:B:209:LEU:HB3	2:B:214:LEU:HB2	1.82	0.61
1:A:399:GLU:HA	1:A:402:TRP:CE3	2.39	0.57
1:A:438:GLU:OE2	1:A:459:THR:HG21	2.04	0.55
1:C:235:HIS:HB3	1:C:236:PRO:HD2	1.88	0.55
2:B:85:GLN:O	2:B:89:GLU:N	2.39	0.55
1:C:114:ALA:HB1	1:C:160:PHE:CE1	2.42	0.54
2:D:209:LEU:C	2:D:211:ARG:N	2.63	0.53
1:C:343:GLN:HG3	1:C:349:LEU:HD11	1.90	0.53
1:A:23:GLN:HE21	1:A:60:VAL:H	1.57	0.53
1:A:459:THR:HG23	1:A:461:LYS:H	1.73	0.53
1:A:429:LEU:HD11	1:A:506:ILE:HG22	1.92	0.52
1:A:402:TRP:C	1:A:402:TRP:CD1	2.87	0.52
2:B:10:VAL:HA	2:B:88:TRP:CH2	2.44	0.52
1:A:332:GLN:O	1:A:336:GLN:HB2	2.10	0.52
1:C:89:GLU:HG2	1:C:92:LEU:HG	1.92	0.52
2:D:50:ILE:HG21	2:D:145:GLN:HB3	1.92	0.52
1:C:460:ASN:HD22	2:D:288:ALA:HB2	1.74	0.51
1:A:60:VAL:HG13	1:A:75:VAL:HG22	1.93	0.51
1:A:56:TYR:O	1:A:143:ARG:NH2	2.44	0.51
2:B:7:THR:HG22	2:B:119:PRO:HG2	1.93	0.51
1:C:150:PRO:HB2	1:C:153:TRP:HB2	1.92	0.51
2:D:180:ILE:HD13	2:D:189:VAL:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:406:TRP:NE1	2:D:408:ALA:HB3	2.26	0.51
1:C:498:ASP:HB2	1:C:538:ALA:HB2	1.93	0.51
1:A:459:THR:HG22	1:A:463:ARG:H	1.76	0.50
1:C:438:GLU:OE2	1:C:463:ARG:HD3	2.12	0.50
1:C:441:TYR:CD2	1:C:544:GLY:HA3	2.46	0.50
2:D:156:SER:HB2	2:D:157:PRO:HD3	1.94	0.50
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.94	0.49
1:A:101:LYS:HE3	1:A:321:PRO:HG3	1.94	0.49
1:A:273:GLY:N	7:A:703:HOH:O	2.44	0.49
1:C:239:TRP:O	1:C:316:GLY:N	2.45	0.49
2:D:106:VAL:HA	2:D:190:GLY:HA2	1.94	0.49
1:A:114:ALA:HB1	1:A:160:PHE:CE1	2.47	0.49
1:A:206:ARG:CZ	1:A:218:ASP:HB2	2.43	0.49
1:C:278:GLN:H	1:C:302:GLU:CD	2.21	0.48
1:A:441:TYR:CD2	1:A:544:GLY:HA3	2.48	0.48
1:A:503:LEU:HD22	1:A:535:TRP:HB2	1.95	0.48
1:A:100:LEU:HB3	5:A:604:3LQ:H6	1.96	0.48
1:A:13:LYS:HD2	1:A:16:MET:HE3	1.95	0.47
1:C:57:ASN:HD21	1:C:131:THR:HB	1.79	0.47
2:D:60:VAL:HG12	2:D:75:VAL:HG22	1.96	0.47
1:A:447:ASN:HB3	1:A:450:THR:OG1	2.14	0.47
2:B:54:ASN:O	2:B:143:ARG:NH2	2.47	0.47
1:C:253:THR:HG23	1:C:256:ASP:H	1.80	0.47
1:C:59:PRO:O	1:C:75:VAL:HG13	2.15	0.47
1:C:77:PHE:HB3	1:C:80:LEU:HB3	1.97	0.47
1:C:89:GLU:OE1	1:C:90:VAL:N	2.47	0.47
2:D:96:HIS:N	2:D:97:PRO:HD2	2.30	0.47
2:D:266:TRP:CD2	2:D:425:LEU:HD13	2.50	0.46
1:A:114:ALA:HB1	1:A:160:PHE:CZ	2.50	0.46
2:B:295:LEU:HB3	2:B:300:GLU:HG2	1.97	0.46
2:B:332:GLN:HE22	2:B:425:LEU:HB2	1.80	0.46
1:C:164:MET:SD	1:C:187:LEU:HD21	2.55	0.46
2:D:209:LEU:C	2:D:211:ARG:H	2.24	0.46
1:A:505:ILE:O	1:A:510:PRO:HD3	2.16	0.46
2:D:154:LYS:O	2:D:157:PRO:HD2	2.17	0.45
1:C:295:LEU:HB3	1:C:300:GLU:CD	2.42	0.45
1:A:428:GLN:HE21	1:A:428:GLN:HB3	1.63	0.44
1:C:517:LEU:H	4:C:602:EDO:H22	1.81	0.44
2:D:58:THR:HG21	2:D:77:PHE:CD1	2.53	0.44
2:B:50:ILE:HG21	2:B:145:GLN:HB3	2.00	0.44
1:C:257:ILE:O	1:C:261:VAL:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:325:LEU:HD21	1:C:383:TRP:CE3	2.53	0.44
1:A:305:GLU:O	1:A:309:ILE:HG13	2.18	0.44
1:A:473:THR:O	1:A:477:THR:HG23	2.18	0.44
1:C:501:TYR:CZ	1:C:505:ILE:HD11	2.53	0.44
1:C:503:LEU:HD22	1:C:535:TRP:HB2	1.99	0.44
1:A:88:TRP:CZ2	2:B:143:ARG:HD3	2.53	0.44
1:A:408:ALA:O	2:B:393:ILE:HG13	2.18	0.44
1:A:60:VAL:HG22	1:A:130:PHE:HB2	2.00	0.43
1:A:304:ALA:O	1:A:308[A]:GLU:HG2	2.16	0.43
1:A:411:ILE:HG22	1:A:412:PRO:O	2.18	0.43
1:A:442:VAL:HB	1:A:481:ALA:HB1	2.01	0.43
2:B:260:LEU:HD21	2:B:303:LEU:HD13	1.99	0.43
2:B:324:ASP:O	2:B:343:GLN:HG2	2.18	0.43
1:C:97:PRO:HG2	1:C:232:TYR:CD1	2.53	0.43
2:B:344:GLU:HB3	2:B:345:PRO:HD2	2.01	0.43
1:C:180:ILE:HG12	1:C:189:VAL:HG22	1.99	0.43
1:C:483:TYR:HB2	1:C:521:ILE:HG12	2.00	0.43
2:D:24:TRP:CH2	2:D:399:GLU:HG2	2.54	0.43
1:C:492:GLU:OE2	1:C:530:LYS:HD3	2.19	0.43
2:D:331:LYS:HB2	2:D:337:TRP:CZ3	2.53	0.43
1:A:218:ASP:C	1:A:220:LYS:H	2.27	0.43
1:C:38:CYS:HA	1:C:47:ILE:HD11	2.01	0.43
1:C:183:TYR:CZ	1:C:184:MET:HE2	2.54	0.43
2:B:101:LYS:O	2:B:236:PRO:HB2	2.19	0.42
1:A:301:LEU:O	1:A:305:GLU:HG3	2.18	0.42
1:C:96:HIS:CE1	1:C:350:LYS:HD2	2.54	0.42
1:A:165:THR:O	1:A:169:GLU:HG3	2.20	0.42
1:C:29:GLU:H	1:C:29:GLU:HG3	1.43	0.42
1:A:255:ASN:HB2	1:A:289:LEU:HB3	2.01	0.42
1:A:406:TRP:NE1	2:B:420:PRO:HG3	2.35	0.42
2:B:325:LEU:HD23	2:B:343:GLN:HG3	2.00	0.42
1:C:501:TYR:CE2	1:C:505:ILE:HD11	2.54	0.42
1:A:270:ILE:HG13	1:A:314:VAL:HG12	2.02	0.42
1:C:167:ILE:O	1:C:170:PRO:HD2	2.19	0.42
2:D:135:ILE:HD13	2:D:135:ILE:HA	1.84	0.42
1:C:410:TRP:CZ2	1:C:412:PRO:HA	2.55	0.42
2:D:342:TYR:HB3	2:D:348:ASN:HA	2.02	0.42
1:A:97:PRO:HG2	1:A:232:TYR:CD1	2.55	0.41
2:B:232:TYR:CG	2:B:233:GLU:N	2.78	0.41
2:D:157:PRO:HG2	2:D:184:MET:HA	2.01	0.41
1:A:135:ILE:H	1:A:135:ILE:HG13	1.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:THR:HB	1:C:154:LYS:HD3	2.02	0.41
1:C:121:ASP:O	1:C:125:ARG:HG3	2.21	0.41
1:A:197:GLN:O	1:A:201:LYS:HG2	2.20	0.41
2:D:181:TYR:CZ	2:D:183:TYR:HB2	2.55	0.41
1:A:94:ILE:HG22	1:A:183:TYR:CE1	2.55	0.41
1:A:390:LYS:HB3	1:A:417:VAL:HG21	2.02	0.41
1:A:476:LYS:HE3	1:A:476:LYS:HB2	1.82	0.41
1:A:483:TYR:CE1	1:A:520:GLN:HB3	2.56	0.41
2:B:237:ASP:OD1	2:B:238:LYS:N	2.54	0.41
1:A:377:THR:O	1:A:381:VAL:HG23	2.21	0.41
2:B:65:LYS:HD2	2:B:72:ARG:HD2	2.03	0.41
2:B:239:TRP:CH2	2:B:378:GLU:HG2	2.56	0.41
1:C:279:LEU:HD13	1:C:299:ALA:HB1	2.02	0.41
1:C:438:GLU:HG3	1:C:461:LYS:HG2	2.03	0.41
1:C:441:TYR:HA	1:C:496:VAL:HG22	2.02	0.41
2:D:328:GLU:O	2:D:339:TYR:HA	2.21	0.41
2:D:121:ASP:O	2:D:125:ARG:HG3	2.21	0.40
2:D:326:ILE:O	2:D:341:ILE:HA	2.22	0.40
1:A:60:VAL:CG2	1:A:130:PHE:HB2	2.51	0.40
2:D:21:VAL:O	2:D:57:ASN:ND2	2.54	0.40
2:D:257:ILE:O	2:D:261:VAL:HG23	2.21	0.40
1:C:295:LEU:HB3	1:C:300:GLU:OE1	2.22	0.40
1:A:88:TRP:NE1	7:A:705:HOH:O	2.49	0.40
1:A:435:VAL:HA	2:B:290:THR:HG21	2.04	0.40
2:B:142:ILE:HD12	2:B:142:ILE:H	1.86	0.40
1:C:326:ILE:O	1:C:341:ILE:HA	2.22	0.40
1:C:395:LYS:HD3	1:C:414:TRP:CZ2	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	537/558 (96%)	530 (99%)	7 (1%)	0	100	100
1	C	530/558 (95%)	524 (99%)	6 (1%)	0	100	100
2	B	403/428 (94%)	397 (98%)	6 (2%)	0	100	100
2	D	394/428 (92%)	386 (98%)	8 (2%)	0	100	100
All	All	1864/1972 (94%)	1837 (99%)	27 (1%)	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	425/495 (86%)	388 (91%)	37 (9%)	9	27
1	C	393/495 (79%)	363 (92%)	30 (8%)	12	33
2	B	350/390 (90%)	330 (94%)	20 (6%)	18	46
2	D	242/390 (62%)	223 (92%)	19 (8%)	11	31
All	All	1410/1770 (80%)	1304 (92%)	106 (8%)	12	34

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	THR
1	A	21	VAL
1	A	23	GLN
1	A	29	GLU
1	A	58	THR
1	A	60	VAL
1	A	63	ILE
1	A	68	SER
1	A	71	TRP
1	A	105	SER
1	A	135	ILE
1	A	139	THR
1	A	151	GLN

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Mol	Chain	Res	Type
1	A	184	MET
1	A	187	LEU
1	A	199	ARG
1	A	219	LYS
1	A	244	ILE
1	A	245	VAL
1	A	253	THR
1	A	254	VAL
1	A	260	LEU
1	A	289	LEU
1	A	302	GLU
1	A	324	ASP
1	A	332	GLN
1	A	362	THR
1	A	402	TRP
1	A	415	GLU
1	A	459	THR
1	A	473	THR
1	A	479	LEU
1	A	482	ILE
1	A	491	LEU
1	A	513	SER
1	A	514	GLU
1	A	527	LYS
2	B	84	THR
2	B	86	ASP
2	B	89	GLU
2	B	92	LEU
2	B	117	SER
2	B	121	ASP
2	B	139	THR
2	B	163	SER
2	B	200	THR
2	B	215	THR
2	B	216	THR
2	B	234	LEU
2	B	242	GLN
2	B	286	THR
2	B	300	GLU
2	B	351	THR
2	B	417	VAL
2	B	418	ASN

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Mol	Chain	Res	Type
2	B	423	VAL
2	B	425	LEU
1	C	27	THR
1	C	28	GLU
1	C	29	GLU
1	C	31	ILE
1	C	32	LYS
1	C	35	VAL
1	C	94	ILE
1	C	101	LYS
1	C	108	VAL
1	C	110[A]	ASP
1	C	110[B]	ASP
1	C	135	ILE
1	C	147	ASN
1	C	161	GLN
1	C	177	ASP
1	C	186	ASP
1	C	200	THR
1	C	216	THR
1	C	221	HIS
1	C	224	GLU
1	C	277	ARG
1	C	283	LEU
1	C	291	GLU
1	C	351	THR
1	C	399	GLU
1	C	402	TRP
1	C	415	GLU
1	C	442	VAL
1	C	496	VAL
1	C	539	HIS
2	D	90	VAL
2	D	96	HIS
2	D	100	LEU
2	D	101	LYS
2	D	121	ASP
2	D	211	ARG
2	D	260	LEU
2	D	291	GLU
2	D	293	ILE
2	D	298	GLU

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Mol	Chain	Res	Type
2	D	305	GLU
2	D	314	VAL
2	D	330	GLN
2	D	362	THR
2	D	377	THR
2	D	405	TYR
2	D	417	VAL
2	D	423	VAL
2	D	425	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	GLN
1	A	474	ASN
1	A	547	GLN
2	B	330	GLN
2	B	334	GLN
2	B	340	GLN
1	C	147	ASN
1	C	161	GLN
1	C	363	ASN
1	C	373	GLN
1	C	487	GLN
1	C	520	GLN
2	D	269	GLN
2	D	332	GLN
2	D	373	GLN
2	D	394	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 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	$\# Z > 2$
5	3LQ	A	604	-	33,33,33	0.48	0	45,45,45	0.52	0
3	SO4	A	602	-	4,4,4	0.24	0	6,6,6	0.07	0
5	3LQ	C	603	-	33,33,33	0.51	0	45,45,45	0.68	1 (2%)
4	EDO	C	602	-	3,3,3	0.40	0	2,2,2	0.43	0
3	SO4	A	601	-	4,4,4	0.23	0	6,6,6	0.08	0
4	EDO	A	603	-	3,3,3	0.44	0	2,2,2	0.30	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
4	EDO	A	603	-	-	1/1/1/1	-
5	3LQ	C	603	-	-	4/12/12/12	0/4/4/4
5	3LQ	A	604	-	-	0/12/12/12	0/4/4/4
4	EDO	C	602	-	-	1/1/1/1	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	603	3LQ	CAH-O0A-C04	-2.05	113.47	119.10

There are no chirality outliers.

All (6) torsion outliers are listed below:

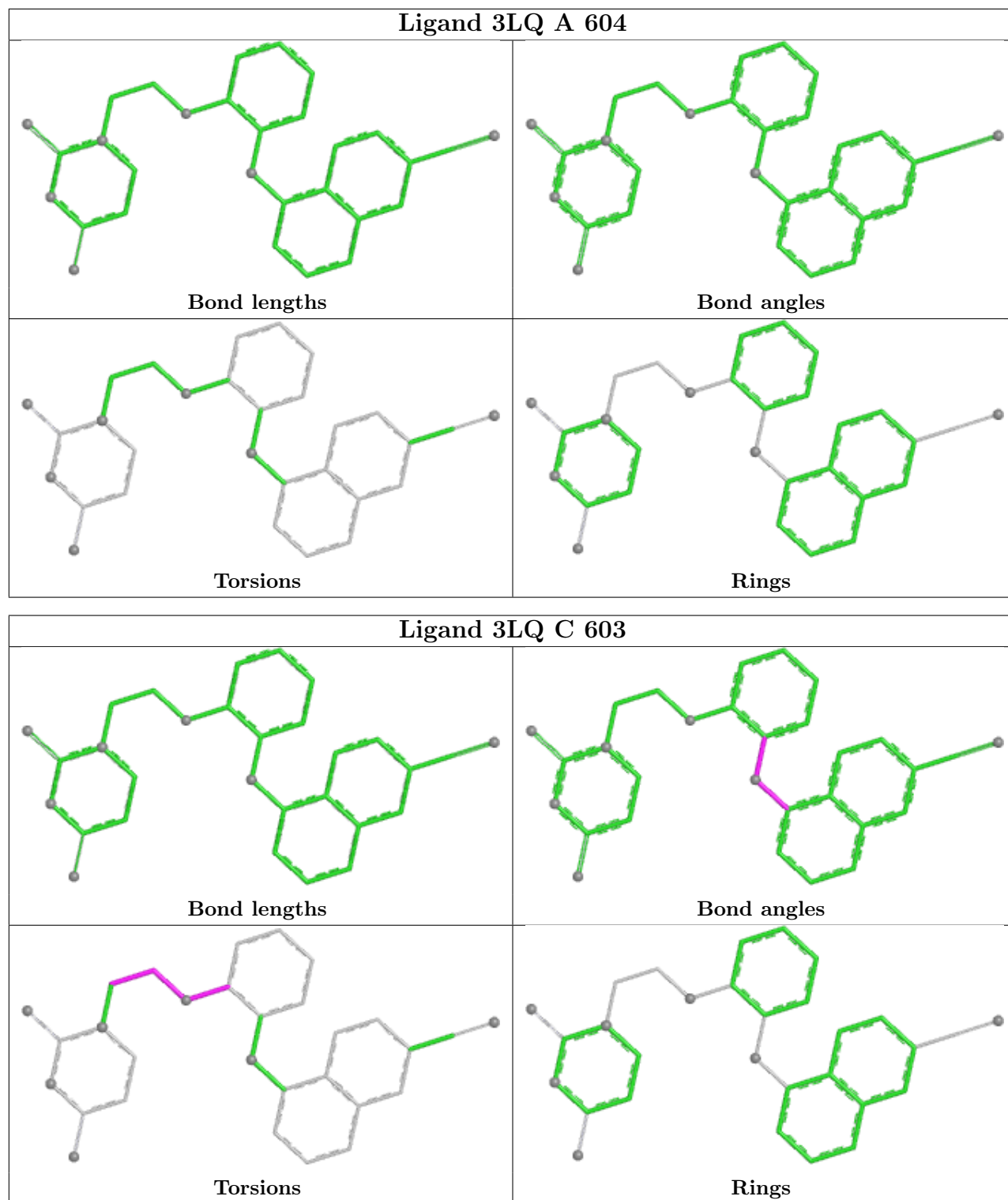
Mol	Chain	Res	Type	Atoms
5	C	603	3LQ	O0B-C0D-C0E-N0H
5	C	603	3LQ	C0E-C0D-O0B-C05
5	C	603	3LQ	C00-C05-O0B-C0D
5	C	603	3LQ	C04-C05-O0B-C0D
4	A	603	EDO	O1-C1-C2-O2
4	C	602	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	604	3LQ	1	0
4	C	602	EDO	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 ⓘ

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	544/558 (97%)	0.33	16 (2%)	53 46	47, 84, 134, 161	1 (0%)
1	C	542/558 (97%)	0.65	30 (5%)	30 25	65, 111, 148, 171	2 (0%)
2	B	408/428 (95%)	0.28	14 (3%)	48 41	38, 77, 121, 139	7 (1%)
2	D	401/428 (93%)	0.81	29 (7%)	21 17	72, 125, 159, 170	5 (1%)
All	All	1895/1972 (96%)	0.51	89 (4%)	36 31	38, 100, 150, 171	15 (0%)

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	130	PHE	4.5
2	D	299	ALA	4.1
1	A	246	LEU	4.0
2	B	427	TYR	4.0
2	D	184	MET	3.6
2	D	421	PRO	3.5
2	D	142	ILE	3.5
1	C	252	TRP	3.5
1	A	551	LEU	3.5
2	B	426	TRP	3.4
2	D	115	TYR	3.4
1	C	224	GLU	3.4
2	B	425	LEU	3.4
1	C	88	TRP	3.2
1	A	552	VAL	3.2
1	C	128	THR	3.1
2	D	177	ASP	3.0
1	C	409	THR	3.0
2	B	88	TRP	3.0
2	D	363	ASN	3.0
2	D	427	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
2	D	317	VAL	3.0
2	B	423	VAL	2.9
2	B	87	PHE	2.9
2	B	362	THR	2.9
1	C	61	PHE	2.8
2	D	127	TYR	2.8
2	D	252	TRP	2.7
1	C	355	ALA	2.7
1	C	63	ILE	2.7
1	C	256	ASP	2.7
2	D	373	GLN	2.7
1	C	142	ILE	2.7
1	C	402	TRP	2.7
2	D	406	TRP	2.6
1	C	295	LEU	2.6
2	D	116	PHE	2.6
2	D	185	ASP	2.5
2	B	241	VAL	2.5
1	C	20	LYS	2.5
1	C	398	TRP	2.5
1	A	135	ILE	2.5
1	C	554	ALA	2.4
1	C	132	ILE	2.4
2	D	383	TRP	2.4
1	C	285	GLY	2.4
1	A	446	ALA	2.4
1	A	226	PRO	2.4
1	C	226	PRO	2.4
1	C	227	PHE	2.4
2	D	368	LEU	2.3
2	D	286	THR	2.3
1	A	24	TRP	2.3
2	D	425	LEU	2.3
1	A	142	ILE	2.3
1	C	315	HIS	2.3
2	D	71	TRP	2.3
1	C	359	GLY	2.3
2	D	278	GLN	2.3
2	B	333	GLY	2.3
2	D	303	LEU	2.3
2	D	121	ASP	2.2
2	B	24	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	8	VAL	2.2
1	C	136	ASN	2.2
1	A	225	PRO	2.2
2	B	422	LEU	2.2
1	A	61	PHE	2.2
2	B	358	ARG	2.2
2	D	277	ARG	2.2
1	A	363	ASN	2.2
1	C	92	LEU	2.2
2	B	283	LEU	2.2
1	A	132	ILE	2.2
2	D	111	VAL	2.2
1	C	299	ALA	2.1
1	C	279	LEU	2.1
1	C	38	CYS	2.1
1	A	26	LEU	2.1
1	C	127	TYR	2.1
2	D	102	LYS	2.1
1	C	69	THR	2.1
2	B	84	THR	2.1
1	A	293	ILE	2.1
2	D	283	LEU	2.0
1	A	545	ASN	2.0
2	D	192	ASP	2.0
1	A	286	THR	2.0
1	C	108	VAL	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](#)

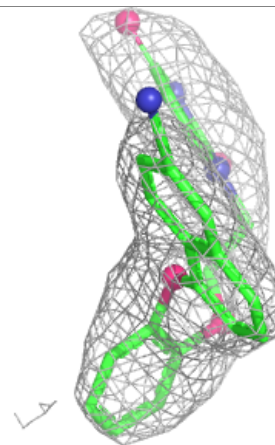
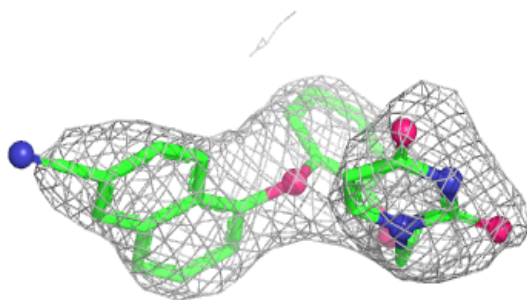
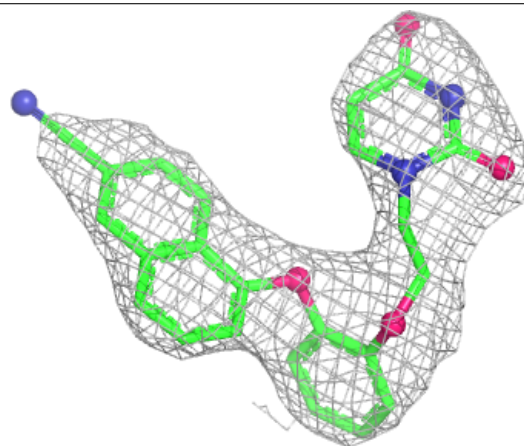
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	C	602	4/4	0.48	0.21	99,100,105,117	0
4	EDO	A	603	4/4	0.64	0.18	75,81,85,87	0
6	MG	C	601	1/1	0.73	0.18	100,100,100,100	0
3	SO4	A	602	5/5	0.81	0.08	107,119,130,140	0
3	SO4	A	601	5/5	0.90	0.13	106,107,115,130	0
5	3LQ	C	603	30/30	0.95	0.11	85,100,109,118	0
5	3LQ	A	604	30/30	0.96	0.10	51,64,77,86	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.

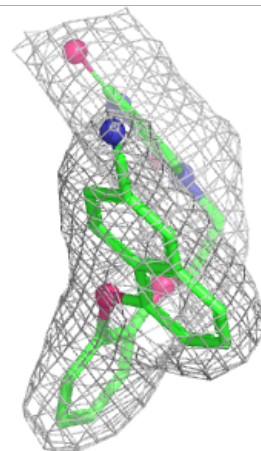
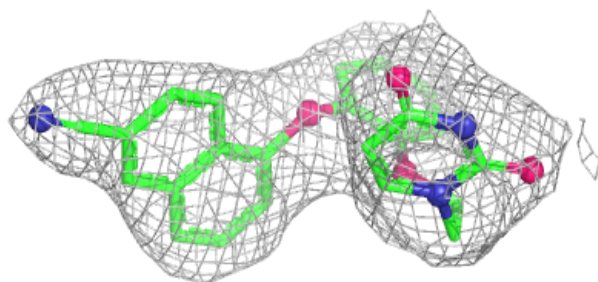
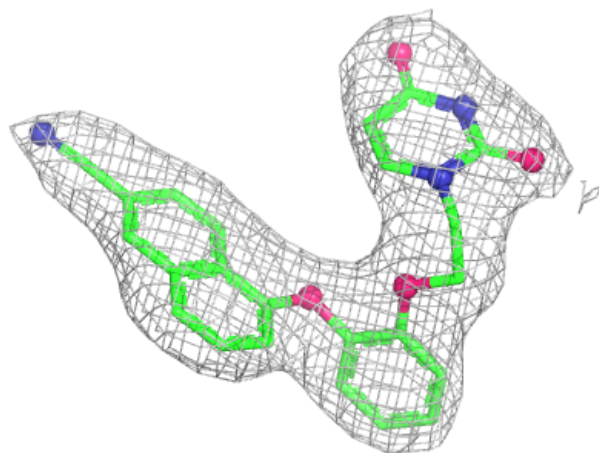
Electron density around 3LQ C 603:

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 3LQ A 604:

$2mF_o-DF_c$ (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.