



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:34 PM UTC

PDB ID : 7R4E / pdb_00007r4e
Title : RVX-inhibited acetylcholinesterase in complex with 2-((hydroxyimino)methyl)-1-(5-(4-methyl-3-nitrobenzamido)pentyl)pyridinium
Authors : Forsgren, N.; Lindgren, C.; Edvinsson, L.; Linusson, A.; Ekstrom, F.
Deposited on : 2022-02-08
Resolution : 3.00 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

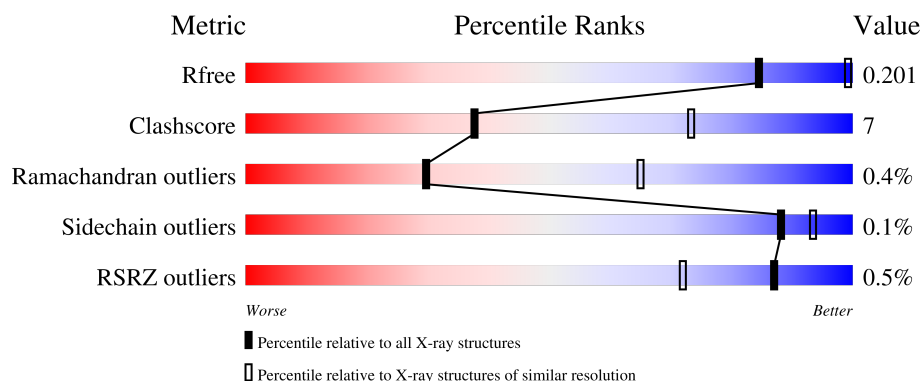
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	543	 81% 18% .
1	B	543	 % 82% 16% .

2 Entry composition [i](#)

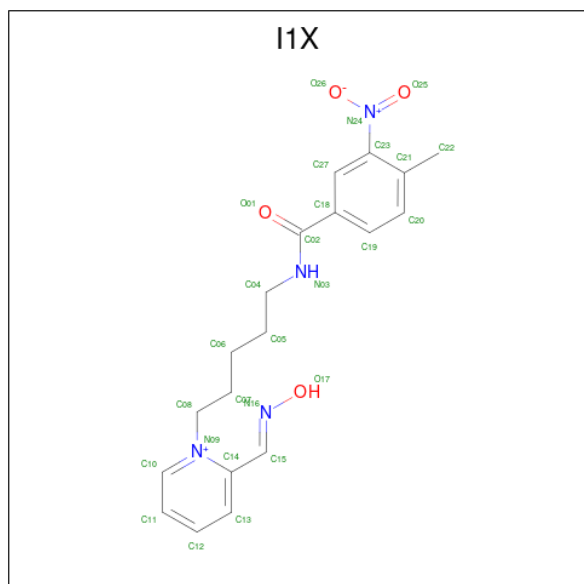
There are 7 unique types of molecules in this entry. The entry contains 8703 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Acetylcholinesterase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	537	Total	C	N	O	P	S	0	3	0
			4217	2703	735	764	1	14			
1	B	533	Total	C	N	O	P	S	0	3	0
			4186	2687	726	758	1	14			

- Molecule 2 is 4-methyl-3-nitro- {N}-[(2 {E},4 {E})-5-[2-[(oxidanylamino)methyl]pyridin-1-yl]penta-2,4-dienyl]benzamide (CCD ID: I1X) (formula: C₁₉H₂₃N₄O₄) (labeled as "Ligand of Interest" by depositor).



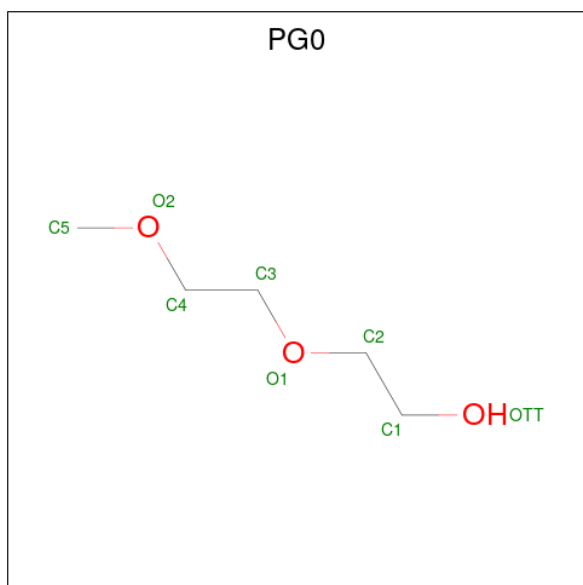
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			16	11	2	3		
2	B	1	Total	C	N	O	0	0
			14	9	2	3		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



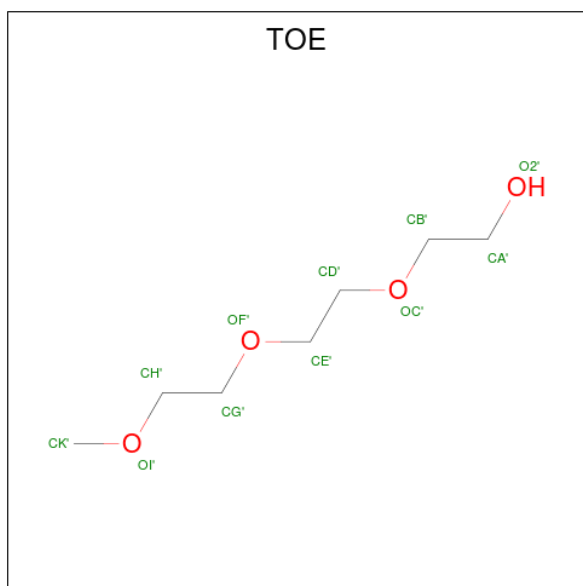
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is 2-(2-METHOXYETHOXY)ETHANOL (CCD ID: PG0) (formula: C₅H₁₂O₃).



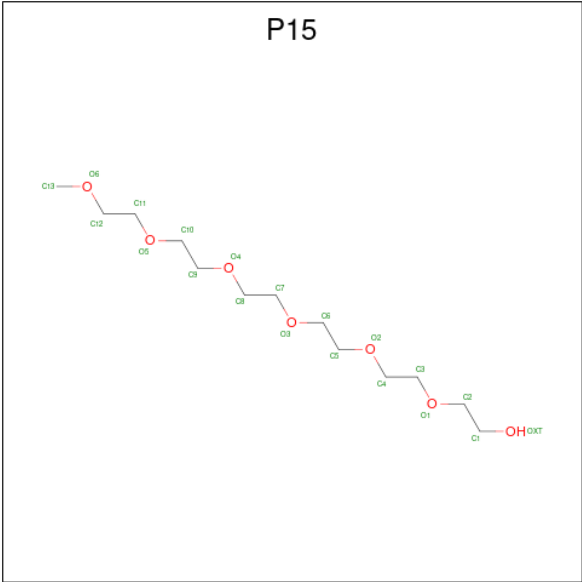
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			8	5	3		
4	A	1	Total	C	O	0	0
			8	5	3		
4	B	1	Total	C	O	0	0
			8	5	3		
4	B	1	Total	C	O	0	0
			8	5	3		
4	B	1	Total	C	O	0	0
			8	5	3		

- Molecule 5 is 2-[2-(2-METHOXY-ETHOXY)-ETHOXY]-ETHOXYL (CCD ID: TOE) (formula: $C_7H_{16}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			11	7	4		
5	A	1	Total	C	O	0	0
			11	7	4		
5	B	1	Total	C	O	0	0
			11	7	4		

- Molecule 6 is 2,5,8,11,14,17-HEXAOXANONADECAN-19-OL (CCD ID: P15) (formula: $C_{13}H_{28}O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			20	13	7		

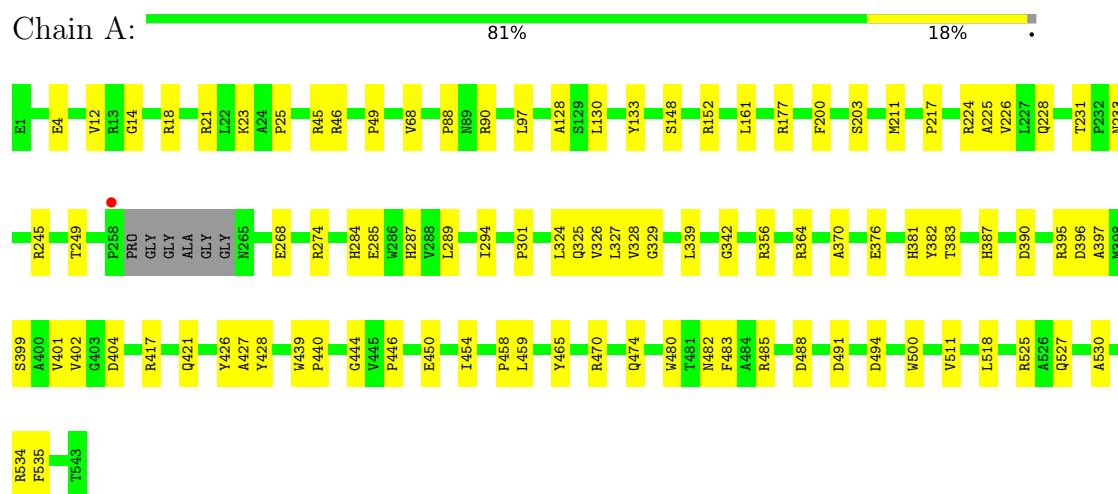
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	78	Total	O	0	0
			78	78		
7	B	43	Total	O	0	0
			43	43		

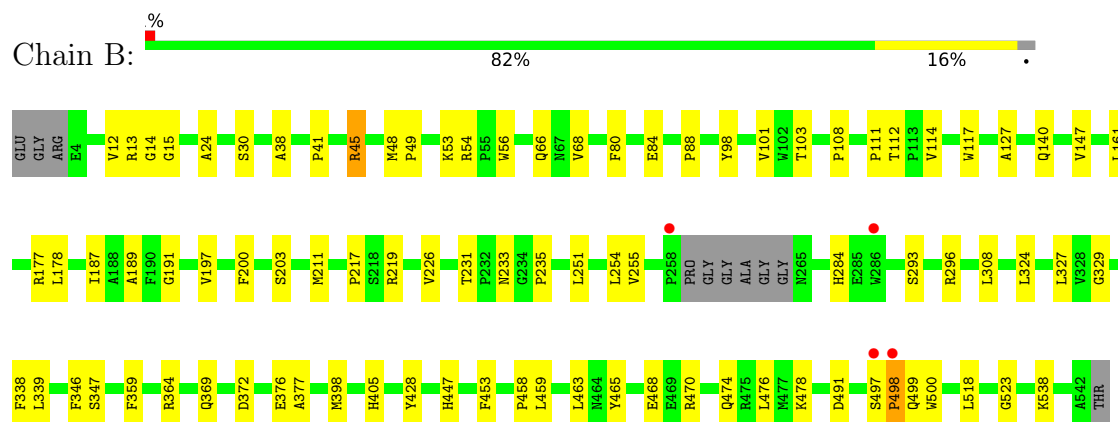
3 Residue-property plots [i](#)

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: Acetylcholinesterase



• Molecule 1: Acetylcholinesterase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.96Å 111.00Å 227.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.11 – 3.00 29.11 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (29.11-3.00) 99.8 (29.11-3.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.21 (at 3.00Å)	Xtriage
Refinement program	PHENIX 1.12_2829, PHENIX 1.12_2829	Depositor
R, R_{free}	0.164 , 0.205 0.168 , 0.201	Depositor DCC
R_{free} test set	800 reflections (0.80%)	wwPDB-VP
Wilson B-factor (Å ²)	50.2	Xtriage
Anisotropy	1.080	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 44.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8703	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% 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: PG0, P15, I1X, RVX, NAG, TOE

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	0/4329	0.59	0/5913
1	B	0.38	0/4298	0.59	0/5873
All	All	0.39	0/8627	0.59	0/11786

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	4217	0	4102	63	0
1	B	4186	0	4072	56	0
2	A	16	0	0	0	0
2	B	14	0	0	1	0
3	A	28	0	26	0	0
3	B	28	0	26	0	0
4	A	16	0	24	0	0
4	B	24	0	36	0	0
5	A	22	0	32	0	0
5	B	11	0	16	2	0
6	A	20	0	28	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	78	0	0	2	0
7	B	43	0	0	2	0
All	All	8703	0	8362	119	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 7.

All (119) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:ARG:O	1:A:274[A]:ARG:NH1	2.20	0.73
1:A:177:ARG:CZ	1:A:217:PRO:HB2	2.27	0.64
1:B:211:MET:HG2	1:B:308:LEU:HD21	1.77	0.64
1:B:200:PHE:HB2	1:B:226:VAL:HB	1.82	0.62
1:A:45[A]:ARG:NH1	1:A:49:PRO:O	2.32	0.61
1:A:21:ARG:HH22	1:A:23:LYS:NZ	1.98	0.60
1:A:327:LEU:HD12	1:A:426:TYR:HB2	1.83	0.60
1:A:459:LEU:HD23	1:A:470:ARG:HG2	1.83	0.59
1:A:224:ARG:HG2	1:A:325:GLN:HB2	1.84	0.59
1:B:68:VAL:HG11	1:B:88:PRO:HB3	1.85	0.59
1:A:328:VAL:O	1:A:427:ALA:HA	2.04	0.57
1:A:226:VAL:HG22	1:A:327:LEU:HB3	1.85	0.57
1:B:30:SER:HB2	1:B:103:THR:HG23	1.87	0.56
1:B:13:ARG:HA	5:B:607:TOE:H13	1.87	0.56
1:A:444:GLY:O	1:A:446:PRO:HD3	2.05	0.56
1:B:114:VAL:HB	1:B:197:VAL:HG22	1.87	0.56
1:B:66:GLN:HG3	1:B:98:TYR:CD2	2.41	0.55
1:B:219:ARG:NH2	7:B:702:HOH:O	2.39	0.55
1:B:478:LYS:NZ	1:B:491:ASP:OD2	2.29	0.55
1:A:211:MET:HE3	1:A:301:PRO:HG2	1.88	0.55
1:A:450:GLU:OE1	1:A:450:GLU:N	2.39	0.54
1:B:231:THR:HB	1:B:233:ASN:OD1	2.09	0.53
1:A:535:PHE:CE2	6:A:608:P15:H71	2.43	0.53
1:B:12:VAL:HG23	1:B:14:GLY:H	1.74	0.53
1:B:226:VAL:HG22	1:B:327:LEU:HB3	1.91	0.53
1:B:359:PHE:CD1	1:B:398:MET:HE2	2.45	0.52
1:A:417:ARG:O	1:A:421:GLN:HG3	2.10	0.51
1:A:294:ILE:HD11	1:A:402:VAL:HG21	1.91	0.51
1:A:327:LEU:HD11	1:A:500:TRP:CH2	2.45	0.51
1:B:48:MET:HE2	1:B:49:PRO:HD2	1.92	0.50
1:B:15:GLY:HA3	1:B:56:TRP:CE2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:ARG:HH22	1:A:23:LYS:HZ3	1.59	0.50
1:B:66:GLN:HG3	1:B:98:TYR:CG	2.47	0.49
1:B:200:PHE:CB	1:B:226:VAL:HB	2.42	0.49
1:B:498:PRO:HB3	1:B:518:LEU:HB2	1.94	0.49
1:A:25:PRO:HD3	7:A:765:HOH:O	2.13	0.49
1:A:68:VAL:HG23	1:A:90:ARG:HB2	1.94	0.49
1:A:245[B]:ARG:O	1:A:249:THR:HG23	2.12	0.48
1:A:381:HIS:HA	6:A:608:P15:H121	1.96	0.48
1:B:458:PRO:HA	1:B:465:TYR:CD2	2.49	0.48
1:B:101:VAL:HG22	1:B:147:VAL:HG22	1.94	0.48
1:B:428:TYR:HB3	1:B:500:TRP:CZ2	2.49	0.48
1:B:470:ARG:O	1:B:474:GLN:HG3	2.14	0.48
1:B:177:ARG:NH1	1:B:217:PRO:HG2	2.30	0.47
1:A:326:VAL:HG12	1:A:328:VAL:HG13	1.97	0.47
1:A:200:PHE:HB2	1:A:226:VAL:HB	1.97	0.47
1:A:491:ASP:HB3	1:A:494:ASP:HB3	1.96	0.47
1:B:369:GLN:HE22	1:B:405:HIS:CE1	2.32	0.47
1:A:454:ILE:HD12	1:A:480:TRP:CE2	2.51	0.46
1:B:189:ALA:HB2	5:B:607:TOE:H2	1.97	0.46
1:A:130:LEU:HD12	1:A:133:TYR:CE2	2.50	0.46
6:A:608:P15:H31	7:A:708:HOH:O	2.15	0.46
1:B:329:GLY:HA3	1:B:428:TYR:CZ	2.50	0.46
1:A:97:LEU:HD21	1:A:152:ARG:HG3	1.97	0.46
1:A:268:GLU:H	1:A:268:GLU:HG3	1.45	0.46
1:B:463:LEU:HA	1:B:463:LEU:HD23	1.74	0.46
1:B:111:PRO:HA	1:B:191:GLY:O	2.15	0.46
1:A:4:GLU:OE1	1:A:18:ARG:HD3	2.16	0.45
1:A:397:ALA:O	1:A:401:VAL:HG23	2.16	0.45
1:A:231:THR:HB	1:A:233:ASN:OD1	2.16	0.45
1:B:293:SER:HB3	1:B:296:ARG:HB2	1.98	0.45
2:B:601:I1X:O01	7:B:701:HOH:O	2.21	0.45
1:A:527:GLN:OE1	6:A:608:P15:H11	2.17	0.45
1:A:364:ARG:NH1	1:A:370:ALA:O	2.50	0.45
1:B:24:ALA:HB3	1:B:140:GLN:HG3	1.98	0.45
1:B:161:LEU:HA	1:B:161:LEU:HD23	1.68	0.45
1:B:117:TRP:HA	1:B:200:PHE:O	2.17	0.44
1:A:511:VAL:HG11	1:A:518:LEU:HD13	1.99	0.44
1:A:228:GLN:HG2	1:A:428:TYR:OH	2.16	0.44
1:A:356:ARG:NH1	1:A:383:THR:OG1	2.44	0.44
1:A:458:PRO:HA	1:A:465:TYR:CD1	2.52	0.44
1:B:15:GLY:HA3	1:B:56:TRP:NE1	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:GLY:HA3	1:A:428:TYR:CE2	2.52	0.44
1:A:161:LEU:HA	1:A:161:LEU:HD23	1.65	0.44
1:A:225:ALA:O	1:A:326:VAL:HA	2.18	0.44
1:B:468:GLU:CD	1:B:468:GLU:H	2.25	0.44
1:B:497:SER:O	1:B:499:GLN:N	2.50	0.44
1:A:289:LEU:HD23	1:A:289:LEU:HA	1.84	0.43
1:A:387:HIS:HB3	1:A:390:ASP:HB2	2.01	0.43
1:A:12:VAL:HG23	1:A:14:GLY:H	1.84	0.43
1:A:376:GLU:OE1	1:B:538:LYS:HE3	2.18	0.43
1:A:404:ASP:OD1	1:A:525:ARG:NH2	2.51	0.43
1:A:128:ALA:HB1	1:A:148:SER:OG	2.19	0.43
1:B:235:PRO:HB2	1:B:296:ARG:NH2	2.34	0.43
1:A:470:ARG:O	1:A:474:GLN:HG3	2.19	0.43
1:B:453:PHE:HB3	1:B:476:LEU:HD12	2.00	0.43
1:A:417:ARG:HD3	1:A:417:ARG:HA	1.90	0.43
1:B:38:ALA:HB2	1:B:178:LEU:HD23	2.00	0.43
1:B:251:LEU:O	1:B:255:VAL:HG22	2.19	0.42
1:B:254:LEU:HB3	1:B:284:HIS:ND1	2.34	0.42
1:B:339:LEU:HD13	1:B:346:PHE:CE2	2.54	0.42
1:A:395:ARG:HD2	1:A:396:ASP:OD1	2.19	0.42
1:A:90:ARG:HH21	1:A:90:ARG:HD2	1.73	0.42
1:A:483:PHE:HA	1:A:488:ASP:H	1.84	0.42
1:A:339:LEU:HD11	1:A:399:SER:HA	2.01	0.42
1:A:245[A]:ARG:O	1:A:249:THR:HG23	2.18	0.42
1:B:364:ARG:HA	1:B:364:ARG:HD2	1.89	0.42
1:A:324:LEU:HD12	1:A:324:LEU:HA	1.63	0.42
1:A:382:TYR:CD2	1:A:401:VAL:HG22	2.54	0.42
1:A:284:HIS:O	1:A:287:HIS:HB2	2.20	0.41
1:B:80:PHE:O	1:B:84:GLU:HG2	2.20	0.41
1:A:482:ASN:OD1	1:A:485:ARG:NH2	2.53	0.41
1:A:90:ARG:HD3	1:A:90:ARG:HA	1.89	0.41
1:B:41:PRO:HA	1:B:45[A]:ARG:HB3	2.02	0.41
1:B:68:VAL:HG13	1:B:127:ALA:HB2	2.02	0.41
1:A:530:ALA:O	1:A:534:ARG:HB2	2.20	0.41
1:B:187:ILE:HD12	1:B:187:ILE:HA	1.87	0.41
1:B:329:GLY:HA3	1:B:428:TYR:CE2	2.56	0.41
1:B:518:LEU:HD23	1:B:518:LEU:HA	1.81	0.41
1:B:108:PRO:HG3	1:B:112:THR:HG21	2.02	0.41
1:B:324:LEU:HD12	1:B:324:LEU:HA	1.87	0.41
1:A:68:VAL:HG11	1:A:88:PRO:HB3	2.01	0.41
1:A:439:TRP:HB3	1:A:440:PRO:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:GLU:C	1:A:287:HIS:H	2.29	0.41
1:B:372:ASP:O	1:B:376:GLU:HG3	2.21	0.40
1:B:338:PHE:HZ	1:B:447:HIS:CD2	2.39	0.40
1:A:535:PHE:CE1	1:B:377:ALA:HB2	2.56	0.40
1:B:53:LYS:HG3	1:B:54:ARG:O	2.21	0.40
1:B:459:LEU:HD12	1:B:459:LEU:N	2.37	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	535/543 (98%)	503 (94%)	31 (6%)	1 (0%)	43 76
1	B	531/543 (98%)	505 (95%)	23 (4%)	3 (1%)	21 56
All	All	1066/1086 (98%)	1008 (95%)	54 (5%)	4 (0%)	30 65

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	523	GLY
1	B	498	PRO
1	B	347	SER
1	A	342	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	440/442 (100%)	440 (100%)	0	100	100
1	B	438/442 (99%)	436 (100%)	2 (0%)	81	89
All	All	878/884 (99%)	876 (100%)	2 (0%)	88	92

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	45[A]	ARG
1	B	45[B]	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	140	GLN
1	A	413	GLN
1	A	509	GLN
1	B	66	GLN
1	B	184	GLN
1	B	533	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues 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
1	RVX	B	203	1	12,13,14	2.56	2 (16%)	10,17,19	1.06	1 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	RVX	A	203	1	12,13,14	2.33	2 (16%)	10,17,19	1.16	1 (10%)

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
1	RVX	B	203	1	-	3/12/14/16	-
1	RVX	A	203	1	-	2/12/14/16	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	203	RVX	P1-O2	6.51	1.65	1.58
1	A	203	RVX	P1-OG	5.30	1.64	1.58
1	B	203	RVX	P1-OG	4.95	1.64	1.58
1	A	203	RVX	P1-O2	4.89	1.63	1.58

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	203	RVX	OG-CB-CA	2.92	110.98	108.14
1	B	203	RVX	OG-P1-O1	-2.76	105.82	113.15

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	203	RVX	N-CA-CB-OG
1	B	203	RVX	N-CA-CB-OG
1	A	203	RVX	C2-O2-P1-C1
1	B	203	RVX	C2-O2-P1-C1
1	B	203	RVX	C3-C2-O2-P1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

15 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
3	NAG	B	603	1	14,14,15	0.56	0	17,19,21	0.68	0
5	TOE	B	607	-	10,10,10	0.50	0	9,9,9	0.88	0
2	I1X	B	601	-	14,14,28	3.65	3 (21%)	15,19,36	1.33	3 (20%)
3	NAG	B	602	1	14,14,15	1.35	2 (14%)	17,19,21	0.79	1 (5%)
5	TOE	A	606	-	10,10,10	0.64	0	9,9,9	0.83	0
2	I1X	A	601	-	16,16,28	2.19	2 (12%)	17,21,36	1.32	3 (17%)
4	PG0	B	604	-	7,7,7	0.53	0	6,6,6	0.88	0
4	PG0	B	605	-	7,7,7	0.61	0	6,6,6	0.70	0
4	PG0	A	604	-	7,7,7	0.58	0	6,6,6	0.96	0
4	PG0	A	605	-	7,7,7	0.56	0	6,6,6	0.66	0
6	P15	A	608	-	19,19,19	0.61	0	18,18,18	1.01	0
3	NAG	A	603	1	14,14,15	0.84	1 (7%)	17,19,21	0.64	1 (5%)
4	PG0	B	606	-	7,7,7	0.52	0	6,6,6	0.76	0
5	TOE	A	607	-	10,10,10	0.59	0	9,9,9	0.82	0
3	NAG	A	602	1	14,14,15	1.16	2 (14%)	17,19,21	0.80	1 (5%)

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	NAG	B	603	1	-	2/6/23/26	0/1/1/1
5	TOE	B	607	-	-	5/8/8/8	-
2	I1X	B	601	-	-	2/8/10/20	0/1/1/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	602	1	-	2/6/23/26	0/1/1/1
5	TOE	A	606	-	-	5/8/8/8	-
2	I1X	A	601	-	-	1/10/12/20	0/1/1/2
4	PG0	B	604	-	-	2/5/5/5	-
4	PG0	B	605	-	-	3/5/5/5	-
4	PG0	A	604	-	-	4/5/5/5	-
4	PG0	A	605	-	-	4/5/5/5	-
6	P15	A	608	-	-	9/17/17/17	-
3	NAG	A	603	1	-	0/6/23/26	0/1/1/1
4	PG0	B	606	-	-	3/5/5/5	-
5	TOE	A	607	-	-	4/8/8/8	-
3	NAG	A	602	1	-	2/6/23/26	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	I1X	C02-N03	12.19	1.49	1.33
2	A	601	I1X	C02-N03	6.48	1.48	1.33
2	B	601	I1X	O25-N24	4.89	1.31	1.22
2	A	601	I1X	O25-N24	4.87	1.31	1.22
3	B	602	NAG	O5-C1	4.34	1.51	1.43
3	A	602	NAG	O5-C1	3.39	1.49	1.43
3	A	603	NAG	C1-C2	2.50	1.55	1.52
2	B	601	I1X	C27-C23	2.44	1.44	1.39
3	A	602	NAG	C1-C2	2.44	1.55	1.52
3	B	602	NAG	C1-C2	2.20	1.55	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	I1X	O25-N24-C23	2.78	123.79	119.03
3	A	602	NAG	C1-O5-C5	2.50	115.54	112.19
2	B	601	I1X	C27-C23-C21	-2.38	118.42	121.43
3	B	602	NAG	C1-O5-C5	2.38	115.37	112.19
2	B	601	I1X	C18-C27-C23	2.27	121.95	119.06
2	B	601	I1X	O25-N24-C23	2.10	122.62	119.03
2	A	601	I1X	C27-C23-C21	-2.07	118.82	121.43
2	A	601	I1X	C18-C27-C23	2.06	121.68	119.06
3	A	603	NAG	C1-O5-C5	2.03	114.91	112.19

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	NAG	O5-C5-C6-O6
3	B	602	NAG	O5-C5-C6-O6
4	B	605	PG0	O1-C3-C4-O2
5	B	607	TOE	OC'-CD'-CE'-OF'
5	A	606	TOE	OC'-CD'-CE'-OF'
3	A	602	NAG	C4-C5-C6-O6
3	B	602	NAG	C4-C5-C6-O6
4	A	605	PG0	O1-C3-C4-O2
6	A	608	P15	O5-C10-C9-O4
4	B	606	PG0	O1-C3-C4-O2
4	B	606	PG0	OTT-C1-C2-O1
3	B	603	NAG	O5-C5-C6-O6
4	A	604	PG0	OTT-C1-C2-O1
5	B	607	TOE	OF'-CG'-CH'-OI'
5	A	607	TOE	OC'-CD'-CE'-OF'
4	A	605	PG0	OTT-C1-C2-O1
5	A	606	TOE	O2'-CA'-CB'-OC'
2	A	601	IIX	N03-C04-C05-C06
6	A	608	P15	O5-C11-C12-O6
5	A	606	TOE	OF'-CG'-CH'-OI'
5	A	607	TOE	O2'-CA'-CB'-OC'
5	B	607	TOE	O2'-CA'-CB'-OC'
5	A	607	TOE	OF'-CG'-CH'-OI'
5	B	607	TOE	CE'-CD'-OC'-CB'
4	B	605	PG0	OTT-C1-C2-O1
6	A	608	P15	O3-C7-C8-O4
6	A	608	P15	O1-C3-C4-O2
4	A	605	PG0	C3-C4-O2-C5
4	B	604	PG0	C1-C2-O1-C3
4	B	605	PG0	C4-C3-O1-C2
6	A	608	P15	C5-C6-O3-C7
5	B	607	TOE	CA'-CB'-OC'-CD'
6	A	608	P15	C3-C4-O2-C5
4	A	605	PG0	C4-C3-O1-C2
5	A	606	TOE	CD'-CE'-OF'-CG'
4	B	604	PG0	C4-C3-O1-C2
2	B	601	IIX	C27-C23-N24-O25
4	A	604	PG0	O1-C3-C4-O2
4	B	606	PG0	C1-C2-O1-C3
4	A	604	PG0	C1-C2-O1-C3

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Mol	Chain	Res	Type	Atoms
2	B	601	I1X	C21-C23-N24-O25
5	A	606	TOE	CH'-CG'-OF'-CE'
6	A	608	P15	C10-C9-O4-C8
5	A	607	TOE	CH'-CG'-OF'-CE'
3	B	603	NAG	C4-C5-C6-O6
6	A	608	P15	O2-C5-C6-O3
4	A	604	PG0	C4-C3-O1-C2
6	A	608	P15	C9-C10-O5-C11

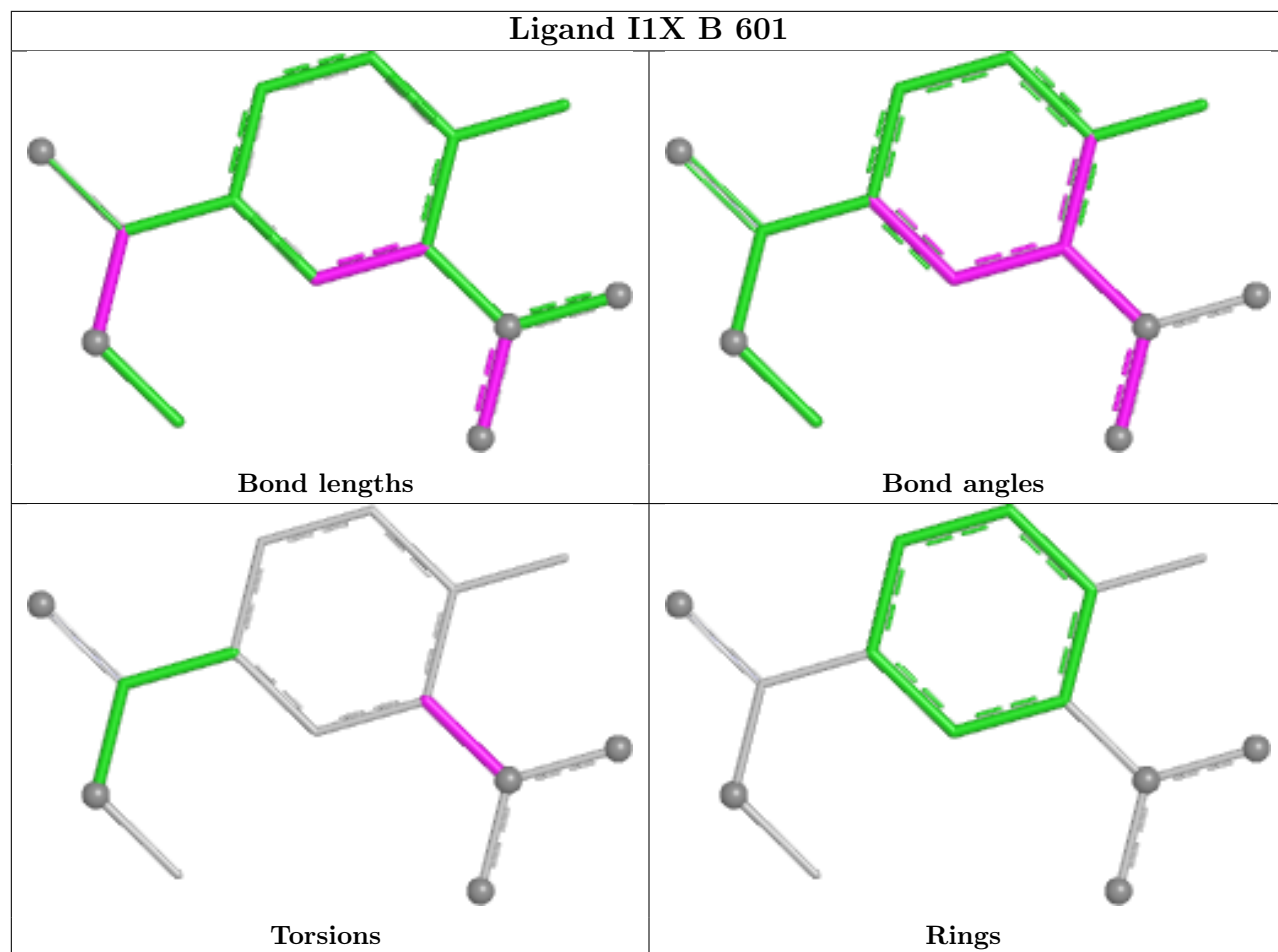
There are no ring outliers.

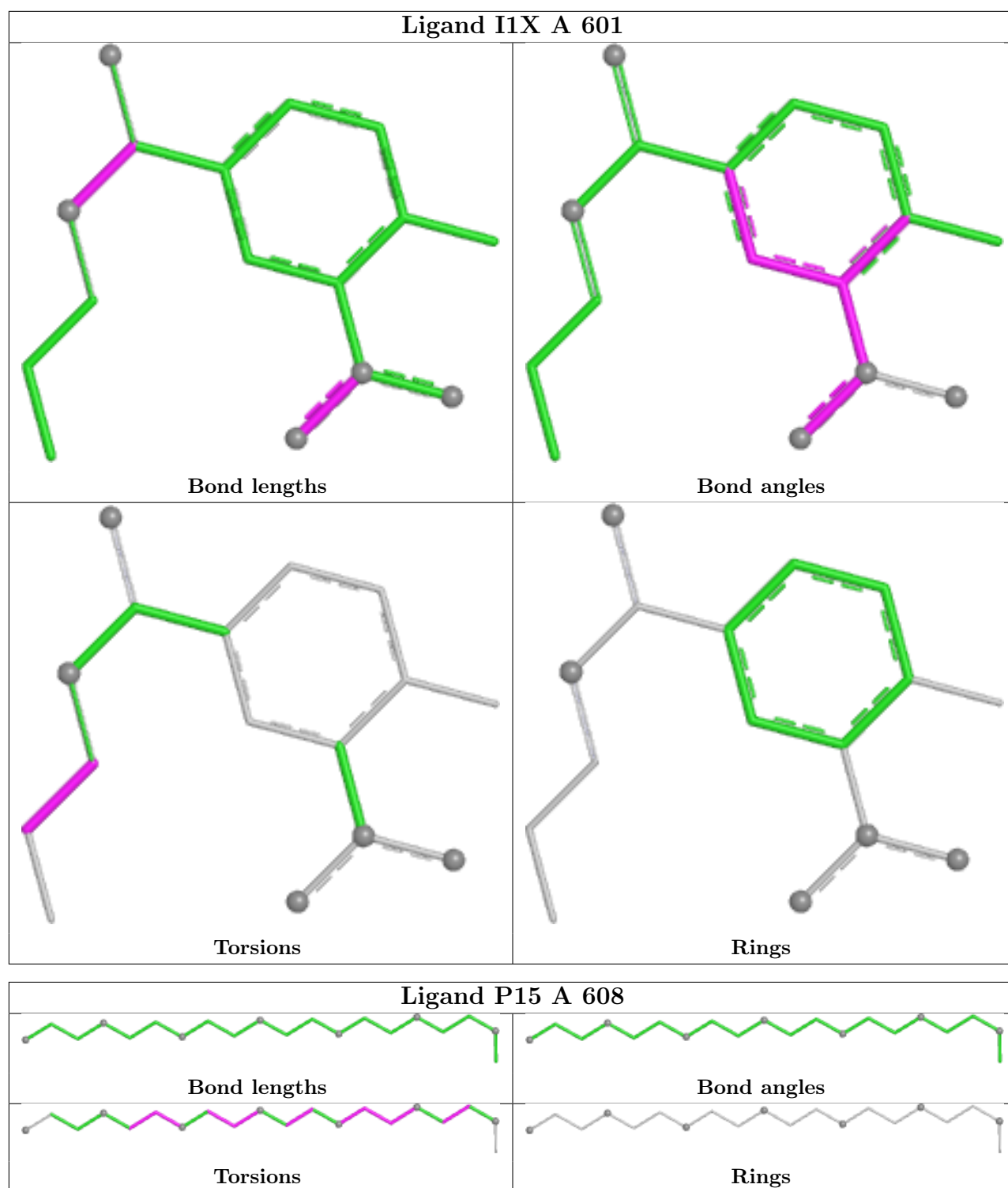
3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	607	TOE	2	0
2	B	601	I1X	1	0
6	A	608	P15	4	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.

Ligand I1X B 601





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 [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	536/543 (98%)	-0.55	1 (0%) 91 83	24, 49, 84, 143	3 (0%)
1	B	532/543 (97%)	-0.50	4 (0%) 82 64	22, 55, 89, 137	3 (0%)
All	All	1068/1086 (98%)	-0.53	5 (0%) 87 72	22, 52, 86, 143	6 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	497	SER	3.3
1	A	258	PRO	3.1
1	B	258	PRO	2.9
1	B	498	PRO	2.7
1	B	286	TRP	2.7

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	RVX	B	203	14/15	0.97	0.06	35,41,50,53	0
1	RVX	A	203	14/15	0.98	0.07	30,37,46,49	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

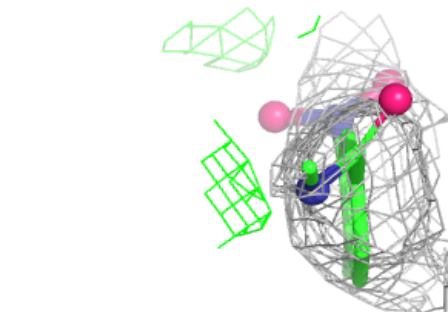
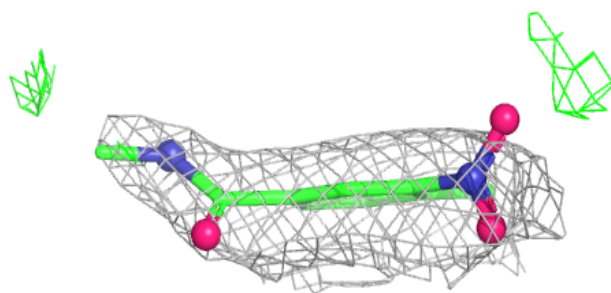
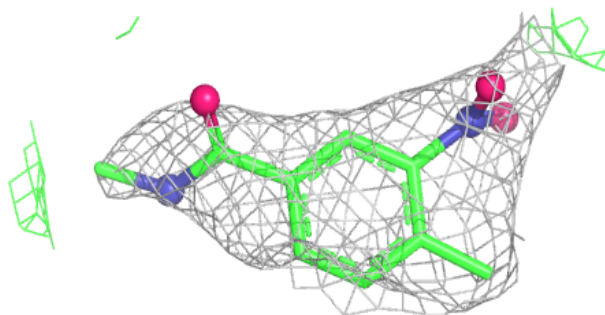
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	B	602	14/15	0.57	0.18	54,95,104,104	0
3	NAG	B	603	14/15	0.62	0.14	101,119,125,125	0
3	NAG	A	602	14/15	0.66	0.18	77,96,105,105	0
5	TOE	B	607	11/11	0.76	0.20	71,91,95,96	0
4	PG0	B	604	8/8	0.81	0.23	75,81,92,93	0
4	PG0	B	605	8/8	0.83	0.18	71,77,84,86	0
5	TOE	A	607	11/11	0.84	0.24	76,84,104,105	0
3	NAG	A	603	14/15	0.84	0.11	80,93,101,102	0
4	PG0	B	606	8/8	0.85	0.17	64,79,87,87	0
4	PG0	A	604	8/8	0.88	0.14	67,78,87,88	0
2	I1X	B	601	14/27	0.88	0.19	95,111,119,119	0
4	PG0	A	605	8/8	0.91	0.17	69,77,86,89	0
5	TOE	A	606	11/11	0.91	0.14	66,72,92,93	0
2	I1X	A	601	16/27	0.93	0.12	59,75,89,93	0
6	P15	A	608	20/20	0.93	0.14	35,63,93,96	0

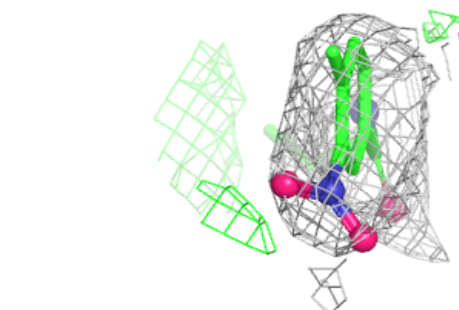
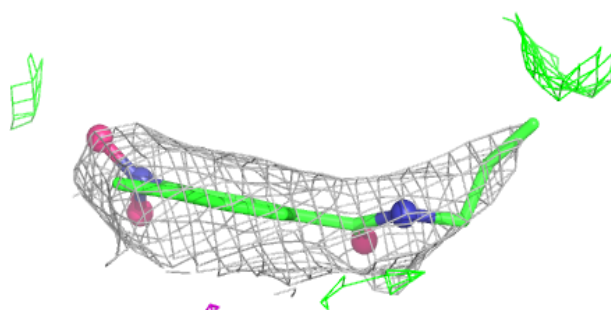
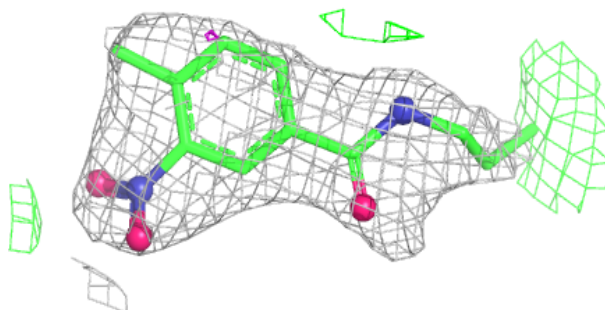
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around I1X B 601:

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

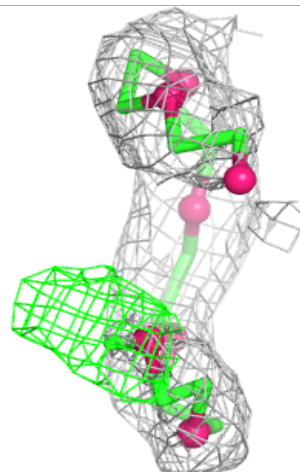
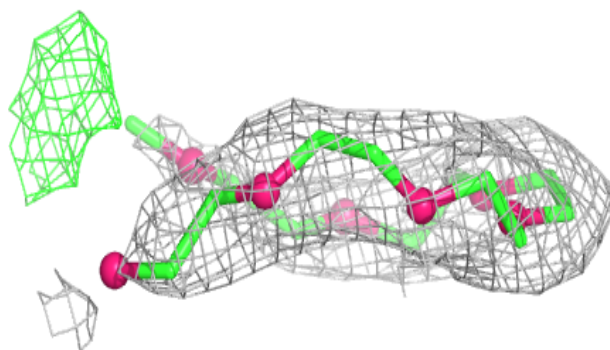
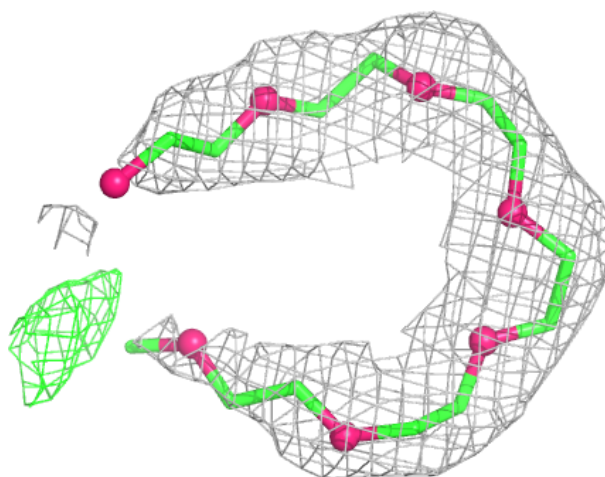
**Electron density around I1X A 601:**

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



Electron density around P15 A 608:

$2mF_o-DF_c$ (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.