



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 6, 2025 – 12:20 PM JST

PDB ID : 9K0G / pdb_00009k0g
Title : Structure of Human HDAC2 in complex with inhibitor N-(2-aminophenyl)-4-(1-((phenylsulfonyl)methyl)-1H-1,2,3-triazol-4-yl)benzamide
Authors : Tojo, T.; Itoh, Y.; Kurohara, T.; Li, Y.; Singh, R.; Narozny, R.; Wiel, A.; Miyake, Y.; Yamashita, Y.; Kusakabe, K.; Uchida, S.; Suzuki, T.
Deposited on : 2024-10-15
Resolution : 1.62 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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
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)	:	2.46

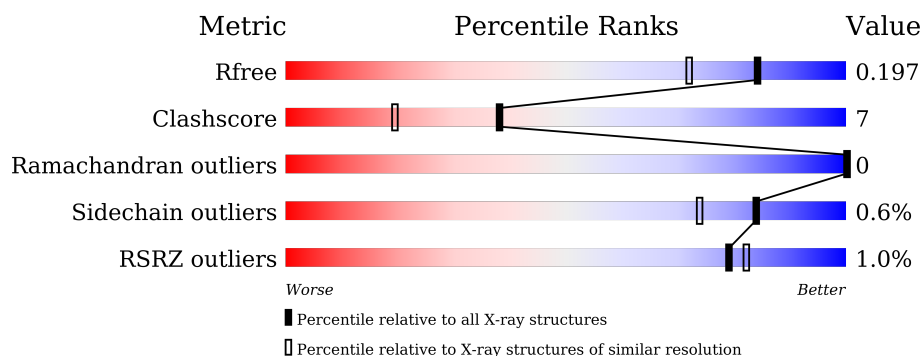
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.62 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}	164625	6077 (1.64-1.60)
Clashscore	180529	6617 (1.64-1.60)
Ramachandran outliers	177936	6498 (1.64-1.60)
Sidechain outliers	177891	6497 (1.64-1.60)
RSRZ outliers	164620	6075 (1.64-1.60)

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	404	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%;"></div> <div style="position: absolute; top: 10px; left: 0; width: 100%;"></div> <div style="position: absolute; left: 0; top: 0; width: 100%; height: 100%; background: linear-gradient(to right, red 0%, red 1%, orange 1%, orange 79%, yellow 79%, yellow 91%, grey 91%);"></div> <div style="position: absolute; left: 0; top: 0; width: 100%; height: 100%; background: linear-gradient(to right, red 0%, red 1%, orange 1%, orange 79%, yellow 79%, yellow 91%, grey 91%);"></div> </div> <div> 79% 12% 9% </div> </div>
1	B	404	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: 10px; left: 0; width: 100%;"></div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 100%; background: linear-gradient(to right, green 0%, green 77%, yellow 77%, yellow 91%, grey 91%);"></div> </div> <div> 77% 14% 9% </div> </div>
1	C	404	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%;"></div> <div style="position: absolute; top: 10px; left: 0; width: 100%;"></div> <div style="position: absolute; left: 0; top: 0; width: 100%; height: 100%; background: linear-gradient(to right, red 0%, red 1%, orange 1%, orange 81%, yellow 81%, yellow 90%, grey 90%);"></div> <div style="position: absolute; left: 0; top: 0; width: 100%; height: 100%; background: linear-gradient(to right, red 0%, red 1%, orange 1%, orange 81%, yellow 81%, yellow 90%, grey 90%);"></div> </div> <div> 81% 9% 9% </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	EDO	C	505	-	-	X	-
8	GOL	B	508	-	-	X	-

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 10361 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 Histone deacetylase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	369	Total	C	N	O	S	0	21	0
			3143	2005	532	576	30			
1	B	367	Total	C	N	O	S	0	21	0
			3137	1997	532	577	31			
1	C	367	Total	C	N	O	S	0	16	0
			3087	1970	525	563	29			

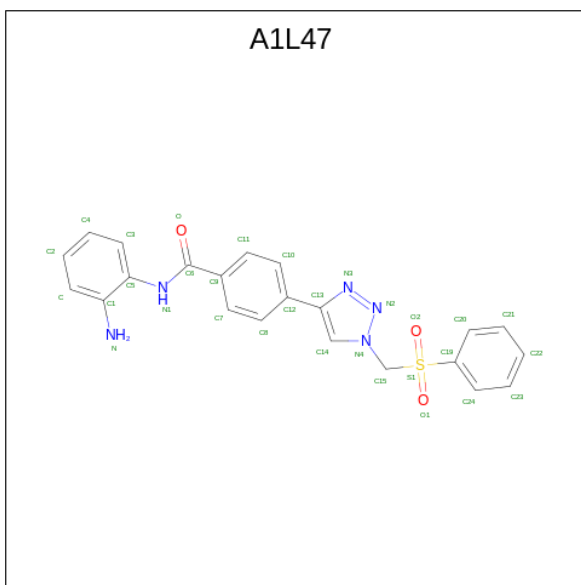
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

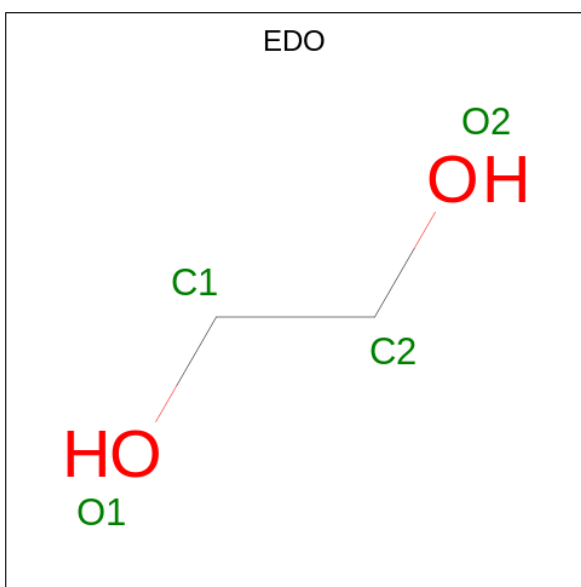
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Ca	0	0
			2	2		
3	B	2	Total	Ca	0	0
			2	2		
3	C	2	Total	Ca	0	0
			2	2		

- Molecule 4 is N-(2-aminophenyl)-4-(1-((phenylsulfonyl)methyl)-1H-1,2,3-triazol-4-yl)benzamide (CCD ID: A1L47) (formula: C₂₂H₁₉N₅O₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			21	15	5	1		
4	B	1	Total	C	N	O	0	0
			21	15	5	1		
4	C	1	Total	C	N	O	0	0
			21	15	5	1		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



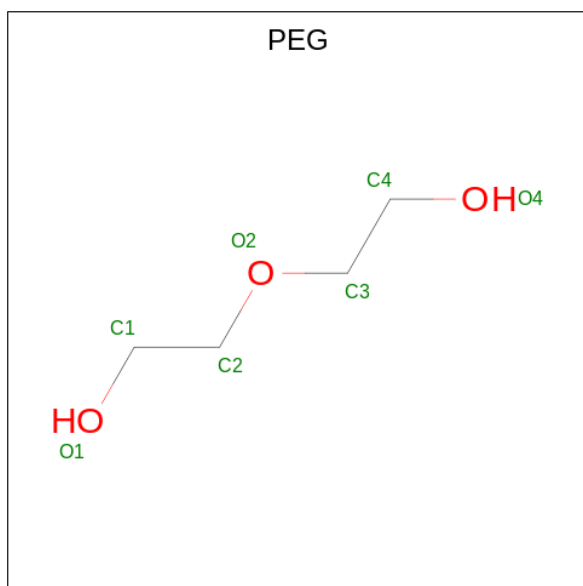
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		

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

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



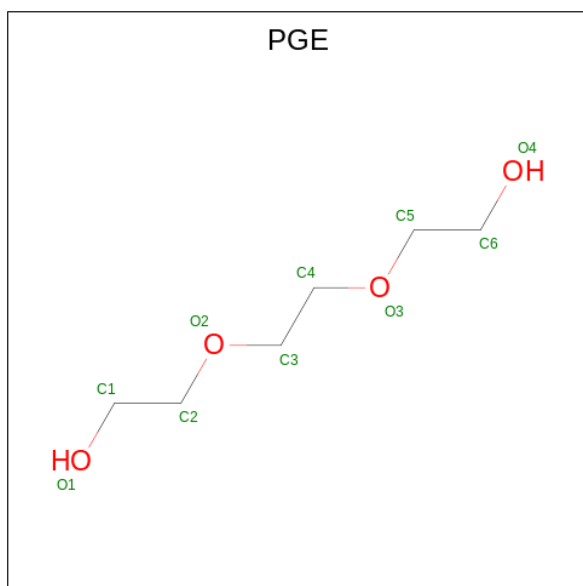
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	4	3		
6	A	1	Total	C	O	0	0
			7	4	3		
6	A	1	Total	C	O	0	0
			7	4	3		
6	B	1	Total	C	O	0	0
			7	4	3		

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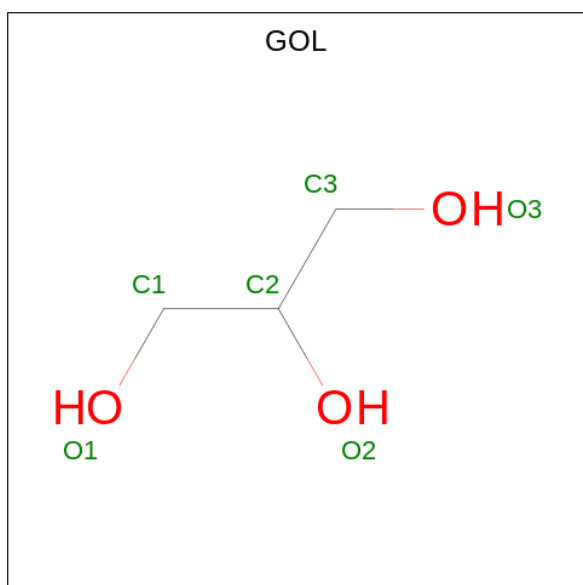
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



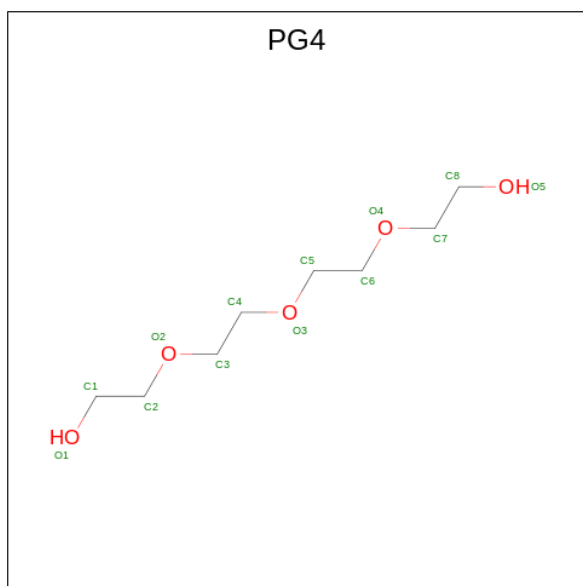
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			13	8	5		
9	C	1	Total	C	O	0	0
			13	8	5		

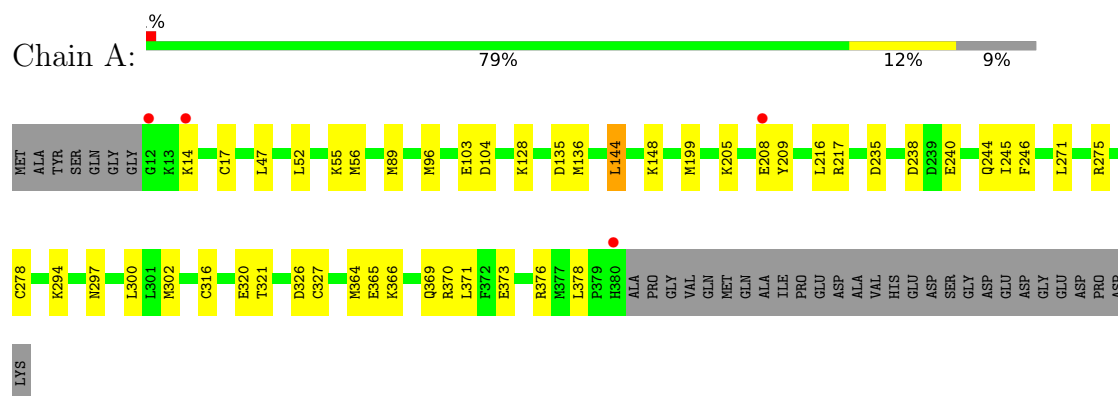
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	281	Total	O	0	0
			281	281		
10	B	305	Total	O	0	0
			305	305		
10	C	227	Total	O	0	0
			227	227		

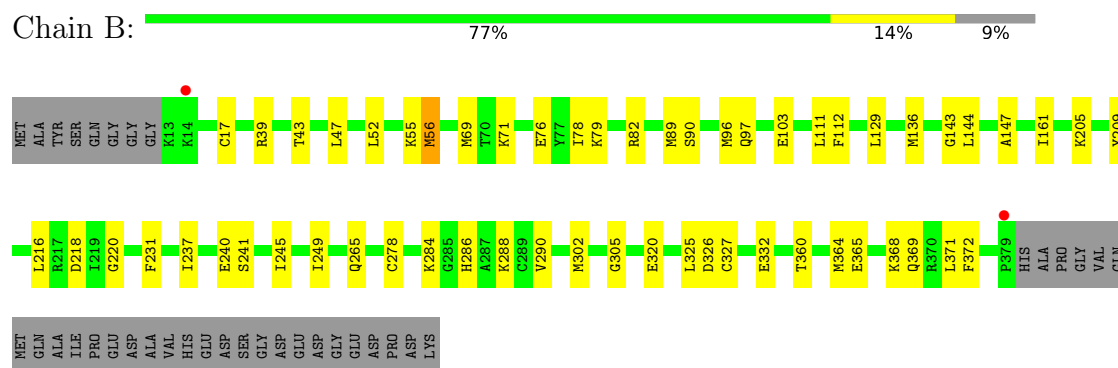
3 Residue-property plots [i](#)

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.

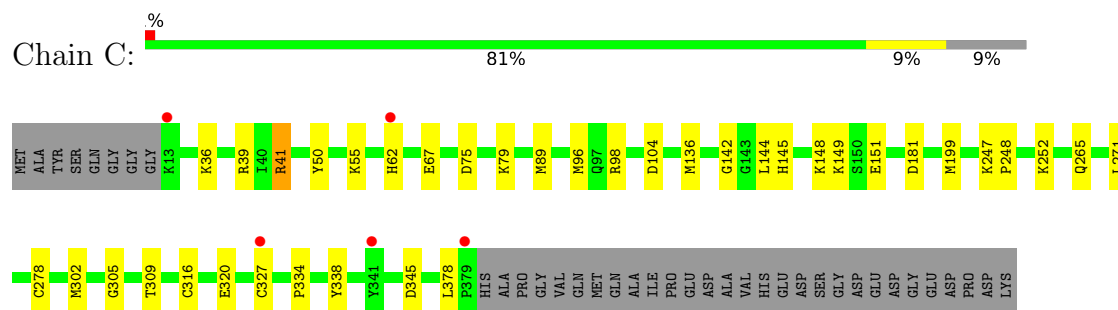
• Molecule 1: Histone deacetylase 2



• Molecule 1: Histone deacetylase 2



• Molecule 1: Histone deacetylase 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	92.14Å 98.48Å 139.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.62 50.00 – 1.62	Depositor EDS
% Data completeness (in resolution range)	99.1 (50.00-1.62) 99.1 (50.00-1.62)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.71 (at 1.62Å)	Xtriage
Refinement program	REFMAC 5.8.0218	Depositor
R, R_{free}	0.164 , 0.196 0.165 , 0.197	Depositor DCC
R_{free} test set	8173 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	19.7	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 36.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	10361	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% 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: PG4, A1L47, CA, GOL, PGE, PEG, ZN, 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	1.23	1/3233 (0.0%)	1.18	2/4361 (0.0%)
1	B	1.26	5/3217 (0.2%)	1.18	7/4340 (0.2%)
1	C	1.19	3/3170 (0.1%)	1.14	6/4273 (0.1%)
All	All	1.23	9/9620 (0.1%)	1.17	15/12974 (0.1%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	36	LYS	C-O	-6.93	1.18	1.24
1	A	217	ARG	CZ-NH1	6.09	1.41	1.32
1	B	220	GLY	N-CA	5.84	1.50	1.45
1	B	147	ALA	N-CA	5.68	1.53	1.46
1	B	69	MET	N-CA	5.51	1.53	1.46
1	C	309	THR	N-CA	5.32	1.53	1.46
1	B	265	GLN	N-CA	5.30	1.52	1.46
1	B	103	GLU	CA-C	5.26	1.55	1.52
1	C	142	GLY	N-CA	5.25	1.50	1.45

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	320	GLU	CA-CB-CG	-7.17	99.77	114.10
1	A	320	GLU	CA-CB-CG	-6.22	101.65	114.10
1	C	41	ARG	NE-CZ-NH1	-5.98	115.52	121.50
1	A	56	MET	CG-SD-CE	-5.62	88.54	100.90
1	B	305	GLY	N-CA-C	-5.27	103.47	110.58
1	B	43	THR	N-CA-C	-5.21	105.51	111.14
1	C	305	GLY	N-CA-C	-5.18	103.58	110.58
1	B	129	LEU	CA-C-O	-5.16	115.40	120.82
1	B	39	ARG	CG-CD-NE	-5.16	100.65	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	252	LYS	N-CA-C	-5.14	105.76	111.36
1	C	145	HIS	N-CA-C	5.09	119.12	113.01
1	C	320	GLU	CA-CB-CG	-5.07	103.97	114.10
1	C	39	ARG	CG-CD-NE	-5.06	100.88	112.00
1	B	56	MET	CG-SD-CE	-5.05	89.79	100.90
1	B	286	HIS	N-CA-C	-5.03	105.50	111.69

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	3143	0	3055	60	0
1	B	3137	0	3039	45	1
1	C	3087	0	3000	27	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
4	A	21	0	0	0	0
4	B	21	0	0	0	0
4	C	21	0	0	0	0
5	A	12	0	18	2	0
5	B	12	0	18	0	0
5	C	8	0	12	10	0
6	A	21	0	30	1	0
6	B	7	0	10	0	0
6	C	7	0	10	0	0
7	A	10	0	14	0	0
8	B	6	0	8	8	0
9	B	13	0	18	0	0
9	C	13	0	18	1	0
10	A	281	0	0	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	B	305	0	0	15	1
10	C	227	0	0	6	1
All	All	10361	0	9250	129	2

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 (129) 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:376:ARG:HD3	5:C:505:EDO:C2	1.74	1.16
1:C:148[A]:LYS:NZ	10:C:601:HOH:O	1.80	1.11
1:A:376:ARG:HD3	5:C:505:EDO:H22	1.36	1.02
1:B:288[B]:LYS:HE2	10:B:840:HOH:O	1.57	1.01
1:A:47[B]:LEU:HD23	1:A:52:LEU:HD12	1.43	1.00
1:B:284:LYS:NZ	8:B:508:GOL:H31	1.78	0.99
1:A:369:GLN:HG2	10:C:733:HOH:O	1.63	0.98
1:A:376:ARG:HD3	5:C:505:EDO:H21	1.45	0.96
1:A:376:ARG:CD	5:C:505:EDO:H22	1.95	0.95
1:A:148:LYS:NZ	10:A:601:HOH:O	1.97	0.95
1:C:89:MET:HE3	1:C:96:MET:HE1	1.49	0.91
1:A:376:ARG:CD	5:C:505:EDO:C2	2.50	0.90
1:A:366[A]:LYS:NZ	1:C:149[A]:LYS:HE2	1.87	0.89
1:A:47[B]:LEU:CD2	1:A:52:LEU:HD12	2.04	0.86
1:A:366[A]:LYS:HZ3	1:C:149[A]:LYS:HE2	1.42	0.82
1:B:284:LYS:HZ2	8:B:508:GOL:H31	1.45	0.79
1:C:41:ARG:HD3	1:C:338:TYR:OH	1.84	0.76
1:A:326:ASP:OD1	10:A:602:HOH:O	2.02	0.76
1:A:373[A]:GLU:HG2	5:C:505:EDO:H12	1.69	0.74
1:B:284:LYS:NZ	8:B:508:GOL:C3	2.53	0.71
1:A:55:LYS:HD3	1:A:327[B]:CYS:SG	2.31	0.71
1:A:366[B]:LYS:HE3	1:A:366[B]:LYS:HA	1.71	0.70
1:B:47[B]:LEU:HD23	1:B:52:LEU:HD12	1.71	0.70
1:C:151:GLU:HB3	5:C:505:EDO:H11	1.72	0.69
1:A:370:ARG:O	1:A:373[B]:GLU:HG2	1.94	0.68
1:C:144[B]:LEU:HD12	10:C:637:HOH:O	1.93	0.67
10:A:729:HOH:O	1:C:149[A]:LYS:HD2	1.93	0.66
1:B:360:THR:O	1:B:364[B]:MET:HG3	1.99	0.63
1:B:284:LYS:HZ1	8:B:508:GOL:H31	1.62	0.62
6:A:510:PEG:H42	10:A:833:HOH:O	1.99	0.62
1:B:218:ASP:OD2	10:B:601:HOH:O	2.16	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366[B]:LYS:HE3	10:A:622:HOH:O	2.00	0.61
1:B:332:GLU:CD	1:C:149[B]:LYS:HZ1	2.08	0.61
1:A:55:LYS:CD	1:A:327[B]:CYS:SG	2.89	0.60
1:C:149[A]:LYS:NZ	10:C:603:HOH:O	2.22	0.60
1:A:103:GLU:CD	1:A:104:ASP:H	2.09	0.60
1:A:14:LYS:HE2	1:A:297[A]:ASN:OD1	2.01	0.60
1:B:47[B]:LEU:CD2	1:B:52:LEU:HD12	2.32	0.59
1:C:62[B]:HIS:O	1:C:62[B]:HIS:CG	2.55	0.59
1:A:199:MET:HE1	1:A:378:LEU:HD21	1.85	0.59
1:A:47[A]:LEU:C	1:A:47[A]:LEU:HD12	2.28	0.59
1:B:55:LYS:NZ	1:B:327[A]:CYS:SG	2.76	0.58
1:A:244:GLN:HB2	5:A:507:EDO:H21	1.85	0.58
1:A:376:ARG:HD2	5:C:505:EDO:H22	1.83	0.58
1:B:284:LYS:HZ1	8:B:508:GOL:C3	2.17	0.58
1:B:369:GLN:HG3	10:B:616:HOH:O	2.04	0.58
1:A:205:LYS:CD	1:A:278[B]:CYS:SG	2.92	0.57
1:C:199:MET:HE1	1:C:378:LEU:HD21	1.86	0.57
1:B:78:ILE:O	1:B:82[B]:ARG:HG3	2.04	0.56
8:B:508:GOL:H32	1:C:67:GLU:HB3	1.86	0.56
1:B:284:LYS:HZ2	8:B:508:GOL:C3	2.15	0.56
1:B:288[B]:LYS:HD3	10:B:787:HOH:O	2.05	0.56
1:B:205:LYS:HD2	1:B:278[B]:CYS:SG	2.46	0.56
1:A:17[A]:CYS:SG	1:A:128:LYS:NZ	2.64	0.56
1:B:205:LYS:HE3	1:B:209:TYR:CD1	2.42	0.55
1:A:47[B]:LEU:HD21	1:A:321:THR:HB	1.89	0.55
1:B:249[A]:ILE:HD13	1:B:372:PHE:HE1	1.71	0.55
1:A:89:MET:HE3	1:A:96:MET:HE1	1.89	0.54
1:A:47[B]:LEU:CD2	1:A:52:LEU:CD1	2.84	0.54
1:A:366[A]:LYS:HE3	10:B:602:HOH:O	2.08	0.54
1:B:17[B]:CYS:SG	10:B:724:HOH:O	2.45	0.53
1:C:345:ASP:HA	10:C:788:HOH:O	2.07	0.53
1:B:56:MET:HB3	1:B:325:LEU:HD21	1.90	0.52
1:A:14:LYS:HB3	1:A:135:ASP:HB2	1.91	0.52
1:C:89:MET:HE3	1:C:96:MET:CE	2.31	0.52
1:A:376:ARG:CD	5:C:505:EDO:H21	2.28	0.51
1:A:136[B]:MET:HG2	1:A:300:LEU:HB3	1.92	0.51
1:B:245:ILE:HG22	1:B:368:LYS:HE2	1.93	0.50
1:B:332:GLU:OE2	10:B:602:HOH:O	2.18	0.50
1:B:82[A]:ARG:NH2	10:B:609:HOH:O	2.46	0.49
1:A:369:GLN:CD	10:A:622:HOH:O	2.54	0.49
1:B:290:VAL:HG13	1:B:302[B]:MET:HE1	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:GLY:HA2	1:B:161:ILE:HD11	1.94	0.49
1:A:205:LYS:HE2	1:A:235:ASP:OD1	2.13	0.49
1:B:111[B]:LEU:C	1:B:111[B]:LEU:HD23	2.38	0.49
1:A:244:GLN:OE1	10:A:603:HOH:O	2.20	0.48
1:B:89:MET:HE3	1:B:96:MET:HE1	1.96	0.48
1:B:249[A]:ILE:HD13	1:B:372:PHE:CE1	2.49	0.48
1:A:136[A]:MET:HE1	1:A:302[A]:MET:SD	2.53	0.47
1:A:245:ILE:HG12	1:A:364:MET:HE3	1.96	0.47
1:A:373[B]:GLU:HG3	1:C:98:ARG:NH1	2.29	0.47
1:C:271:LEU:HD11	1:C:316:CYS:HB2	1.95	0.47
1:A:271:LEU:HD11	1:A:316:CYS:HB2	1.97	0.47
1:A:205:LYS:HD2	1:A:278[B]:CYS:SG	2.55	0.46
1:A:365:GLU:OE2	5:A:507:EDO:C1	2.62	0.46
1:B:216:LEU:HD12	1:B:371:LEU:HD21	1.96	0.46
1:A:205:LYS:NZ	10:A:618:HOH:O	2.48	0.46
1:B:82[B]:ARG:HG2	1:B:112:PHE:CZ	2.50	0.46
1:B:332:GLU:OE1	1:C:149[B]:LYS:NZ	2.49	0.46
1:B:71:LYS:HE2	10:B:807:HOH:O	2.16	0.46
1:C:50:TYR:CZ	1:C:334:PRO:HD3	2.51	0.46
1:A:136[A]:MET:HB3	1:A:136[A]:MET:HE2	1.54	0.46
1:A:240[A]:GLU:O	1:A:244:GLN:HG3	2.16	0.45
1:A:373[A]:GLU:HG2	5:C:505:EDO:C1	2.41	0.45
1:B:136[B]:MET:HB3	1:B:136[B]:MET:HE2	1.40	0.45
1:A:238:ASP:OD1	1:A:240[B]:GLU:HG2	2.17	0.45
1:C:75:ASP:O	1:C:79[A]:LYS:HG3	2.16	0.45
1:C:55:LYS:NZ	1:C:327[A]:CYS:SG	2.90	0.44
9:C:508:PG4:H72	9:C:508:PG4:H52	1.72	0.44
1:B:205:LYS:CD	1:B:278[B]:CYS:SG	3.05	0.44
1:B:231:PHE:CE2	1:B:245:ILE:HD13	2.53	0.44
1:C:136[B]:MET:HE1	1:C:302[B]:MET:CE	2.48	0.44
1:B:240[A]:GLU:CD	1:B:240[A]:GLU:H	2.25	0.44
1:B:284:LYS:CE	8:B:508:GOL:H31	2.47	0.44
1:B:82[B]:ARG:CZ	10:B:698:HOH:O	2.65	0.43
1:A:14:LYS:HB3	1:A:135:ASP:CB	2.48	0.43
1:B:76:GLU:HG2	10:B:857:HOH:O	2.17	0.43
1:B:365:GLU:HG2	10:B:707:HOH:O	2.18	0.43
1:A:245:ILE:C	1:A:245:ILE:HD12	2.43	0.43
1:B:79:LYS:HD3	10:B:841:HOH:O	2.18	0.43
1:C:136[B]:MET:HE2	1:C:136[B]:MET:HB3	1.73	0.43
1:A:366[A]:LYS:NZ	10:B:602:HOH:O	2.52	0.43
1:B:237:ILE:HD11	1:B:364[B]:MET:HE1	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240[B]:GLU:O	1:A:244:GLN:HG3	2.18	0.42
1:C:104:ASP:HB2	10:C:804:HOH:O	2.20	0.42
1:A:275:ARG:HE	1:A:275:ARG:HB3	1.58	0.42
1:A:302[B]:MET:HE2	1:A:302[B]:MET:HB2	1.89	0.42
1:C:181:ASP:HB2	1:C:265:GLN:OE1	2.20	0.42
1:A:89:MET:CE	1:A:96:MET:HE1	2.50	0.41
1:C:62[B]:HIS:O	1:C:62[B]:HIS:CD2	2.73	0.41
1:A:366[A]:LYS:CE	10:B:602:HOH:O	2.66	0.41
1:B:89:MET:CE	1:B:96:MET:HE1	2.50	0.41
1:A:205:LYS:HE3	1:A:209:TYR:CD1	2.56	0.41
1:A:216[B]:LEU:HD12	1:A:371:LEU:HD21	2.02	0.41
1:B:241:SER:HB3	1:B:364[B]:MET:SD	2.60	0.41
1:A:144[B]:LEU:N	1:A:144[B]:LEU:HD23	2.36	0.41
1:A:245:ILE:HD12	1:A:246:PHE:N	2.36	0.41
1:C:247:LYS:HB3	1:C:248:PRO:HD3	2.03	0.40
1:A:366[B]:LYS:NZ	10:A:620:HOH:O	2.50	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:GLN:NE2	1:B:326[B]:ASP:OD1[3_654]	1.91	0.29
10:B:634:HOH:O	10:C:806:HOH:O[1_655]	2.15	0.05

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	390/404 (96%)	382 (98%)	8 (2%)	0	100	100
1	B	388/404 (96%)	382 (98%)	6 (2%)	0	100	100
1	C	381/404 (94%)	377 (99%)	4 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1159/1212 (96%)	1141 (98%)	18 (2%)	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	341/344 (99%)	337 (99%)	4 (1%)	67	49
1	B	340/344 (99%)	337 (99%)	3 (1%)	75	61
1	C	333/344 (97%)	331 (99%)	2 (1%)	84	74
All	All	1014/1032 (98%)	1005 (99%)	9 (1%)	84	61

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	144[A]	LEU
1	A	144[B]	LEU
1	A	208	GLU
1	A	294	LYS
1	B	90	SER
1	B	144[A]	LEU
1	B	144[B]	LEU
1	C	278[A]	CYS
1	C	278[B]	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	244	GLN
1	B	133	GLN
1	C	172	HIS
1	C	244	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 29 ligands modelled in this entry, 9 are monoatomic - leaving 20 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	EDO	A	507	-	3,3,3	0.48	0	2,2,2	0.80	0
5	EDO	B	506	-	3,3,3	0.57	0	2,2,2	0.06	0
5	EDO	B	505	-	3,3,3	0.56	0	2,2,2	0.16	0
5	EDO	A	505	-	3,3,3	0.53	0	2,2,2	0.51	0
6	PEG	A	510	-	6,6,6	0.35	0	5,5,5	0.58	0
9	PG4	C	508	-	12,12,12	0.47	0	11,11,11	0.57	0
5	EDO	A	506	-	3,3,3	0.45	0	2,2,2	0.39	0
9	PG4	B	510	-	12,12,12	0.62	0	11,11,11	0.64	0
6	PEG	B	509	-	6,6,6	0.64	0	5,5,5	0.33	0
4	A1L47	B	504	2	23,23,34	1.95	9 (39%)	29,31,48	1.82	7 (24%)
5	EDO	C	506	-	3,3,3	0.44	0	2,2,2	0.44	0
5	EDO	C	505	-	3,3,3	0.62	0	2,2,2	0.62	0
7	PGE	A	511	-	9,9,9	0.56	0	8,8,8	0.50	0
6	PEG	A	509	-	6,6,6	0.55	0	5,5,5	0.36	0
4	A1L47	A	504	2	23,23,34	1.82	4 (17%)	29,31,48	1.81	7 (24%)
5	EDO	B	507	-	3,3,3	0.51	0	2,2,2	0.24	0
4	A1L47	C	504	2	23,23,34	2.21	8 (34%)	29,31,48	2.35	12 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	PEG	A	508	-	6,6,6	0.55	0	5,5,5	0.53	0
6	PEG	C	507	-	6,6,6	0.46	0	5,5,5	0.51	0
8	GOL	B	508	-	5,5,5	0.36	0	5,5,5	0.49	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	A	507	-	-	0/1/1/1	-
5	EDO	B	506	-	-	1/1/1/1	-
5	EDO	B	505	-	-	1/1/1/1	-
5	EDO	A	505	-	-	1/1/1/1	-
6	PEG	A	510	-	-	3/4/4/4	-
9	PG4	C	508	-	-	6/10/10/10	-
5	EDO	A	506	-	-	1/1/1/1	-
9	PG4	B	510	-	-	2/10/10/10	-
6	PEG	B	509	-	-	2/4/4/4	-
4	A1L47	B	504	2	-	0/12/12/23	0/3/3/4
5	EDO	C	506	-	-	1/1/1/1	-
5	EDO	C	505	-	-	1/1/1/1	-
7	PGE	A	511	-	-	2/7/7/7	-
6	PEG	A	509	-	-	1/4/4/4	-
4	A1L47	A	504	2	-	0/12/12/23	0/3/3/4
5	EDO	B	507	-	-	1/1/1/1	-
4	A1L47	C	504	2	-	0/12/12/23	0/3/3/4
6	PEG	A	508	-	-	3/4/4/4	-
6	PEG	C	507	-	-	1/4/4/4	-
8	GOL	B	508	-	-	2/4/4/4	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	504	A1L47	C1-C5	6.58	1.49	1.40
4	B	504	A1L47	C1-C5	4.56	1.46	1.40
4	A	504	A1L47	N3-N2	4.56	1.41	1.34
4	B	504	A1L47	N3-N2	4.29	1.41	1.34
4	A	504	A1L47	C1-C5	4.27	1.46	1.40
4	C	504	A1L47	N3-N2	4.23	1.41	1.34
4	B	504	A1L47	C5-N1	-3.07	1.35	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	504	A1L47	C5-N1	-2.84	1.36	1.41
4	C	504	A1L47	C2-C	2.76	1.44	1.38
4	B	504	A1L47	C4-C2	2.75	1.45	1.38
4	B	504	A1L47	C2-C	2.56	1.44	1.38
4	B	504	A1L47	C11-C10	2.45	1.43	1.38
4	A	504	A1L47	N4-N2	2.41	1.41	1.33
4	B	504	A1L47	C4-C3	2.40	1.44	1.38
4	C	504	A1L47	N4-N2	2.38	1.41	1.33
4	C	504	A1L47	C6-N1	2.25	1.41	1.35
4	C	504	A1L47	C3-C5	2.23	1.43	1.39
4	B	504	A1L47	C8-C7	2.16	1.42	1.38
4	A	504	A1L47	C4-C2	2.15	1.43	1.38
4	B	504	A1L47	N4-N2	2.08	1.40	1.33
4	C	504	A1L47	C11-C9	2.04	1.42	1.39

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	504	A1L47	C3-C5-C1	-5.17	113.96	119.92
4	C	504	A1L47	C10-C11-C9	-4.79	115.21	120.78
4	C	504	A1L47	C7-C8-C12	-4.59	114.53	121.13
4	B	504	A1L47	C8-C7-C9	-4.13	115.97	120.78
4	A	504	A1L47	C8-C7-C9	-4.07	116.05	120.78
4	C	504	A1L47	C8-C7-C9	3.84	125.25	120.78
4	B	504	A1L47	C11-C9-C7	3.50	123.57	118.59
4	C	504	A1L47	O-C6-N1	-3.49	115.74	123.71
4	A	504	A1L47	C11-C10-C12	-3.46	116.16	121.13
4	A	504	A1L47	C8-C12-C10	3.26	124.09	117.59
4	A	504	A1L47	C-C1-C5	3.14	121.61	118.25
4	C	504	A1L47	C4-C3-C5	3.10	125.06	118.62
4	B	504	A1L47	C11-C10-C12	-3.07	116.72	121.13
4	A	504	A1L47	N3-N2-N4	-3.06	107.44	111.24
4	B	504	A1L47	C4-C2-C	-2.95	115.70	120.19
4	C	504	A1L47	C1-C5-N1	2.88	124.55	119.23
4	B	504	A1L47	C8-C12-C10	2.70	122.97	117.59
4	C	504	A1L47	C-C1-C5	2.63	121.06	118.25
4	C	504	A1L47	O-C6-C9	2.56	125.51	120.94
4	A	504	A1L47	C11-C9-C7	2.53	122.19	118.59
4	C	504	A1L47	C5-C1-N	-2.51	117.51	120.64
4	A	504	A1L47	C8-C12-C13	-2.46	117.40	121.28
4	B	504	A1L47	N3-N2-N4	-2.29	108.39	111.24
4	C	504	A1L47	C11-C10-C12	2.22	124.33	121.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	504	A1L47	C8-C12-C13	-2.20	117.81	121.28
4	B	504	A1L47	C10-C12-C13	-2.00	118.12	121.28

There are no chirality outliers.

All (29) torsion outliers are listed below:

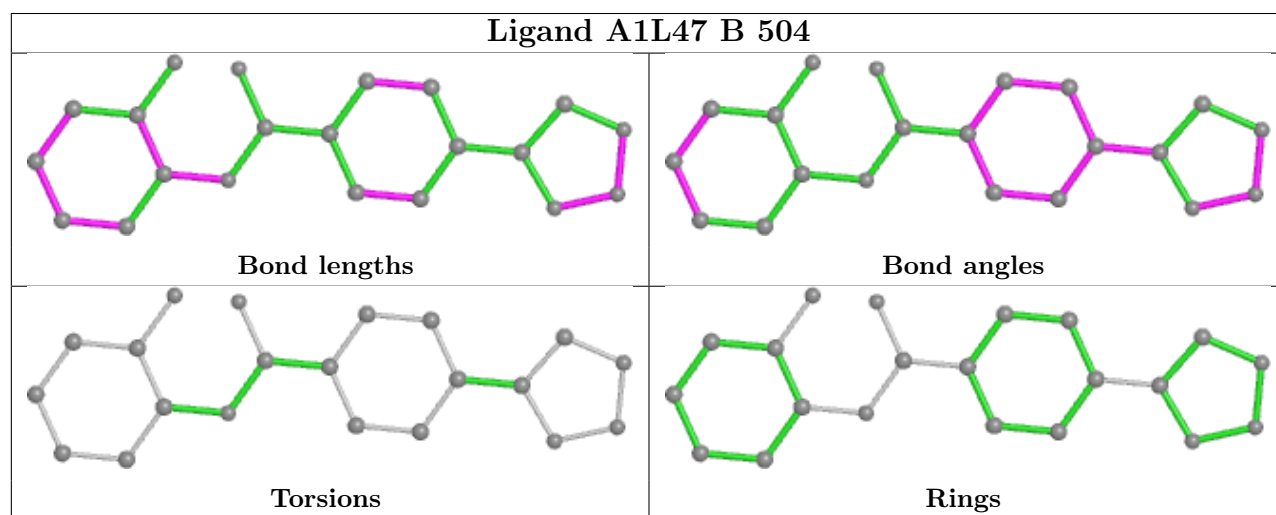
Mol	Chain	Res	Type	Atoms
9	C	508	PG4	C5-C6-O4-C7
9	C	508	PG4	O3-C5-C6-O4
9	C	508	PG4	O1-C1-C2-O2
5	B	507	EDO	O1-C1-C2-O2
6	A	508	PEG	O1-C1-C2-O2
6	A	510	PEG	O1-C1-C2-O2
6	B	509	PEG	O1-C1-C2-O2
7	A	511	PGE	O1-C1-C2-O2
5	A	505	EDO	O1-C1-C2-O2
6	A	510	PEG	O2-C3-C4-O4
9	C	508	PG4	O4-C7-C8-O5
5	B	505	EDO	O1-C1-C2-O2
5	C	506	EDO	O1-C1-C2-O2
5	A	506	EDO	O1-C1-C2-O2
5	B	506	EDO	O1-C1-C2-O2
6	A	510	PEG	C4-C3-O2-C2
6	B	509	PEG	O2-C3-C4-O4
7	A	511	PGE	C1-C2-O2-C3
9	B	510	PG4	C8-C7-O4-C6
6	A	508	PEG	C1-C2-O2-C3
9	B	510	PG4	O1-C1-C2-O2
5	C	505	EDO	O1-C1-C2-O2
9	C	508	PG4	C3-C4-O3-C5
6	A	509	PEG	C4-C3-O2-C2
6	A	508	PEG	O2-C3-C4-O4
6	C	507	PEG	O1-C1-C2-O2
9	C	508	PG4	C1-C2-O2-C3
8	B	508	GOL	C1-C2-C3-O3
8	B	508	GOL	O2-C2-C3-O3

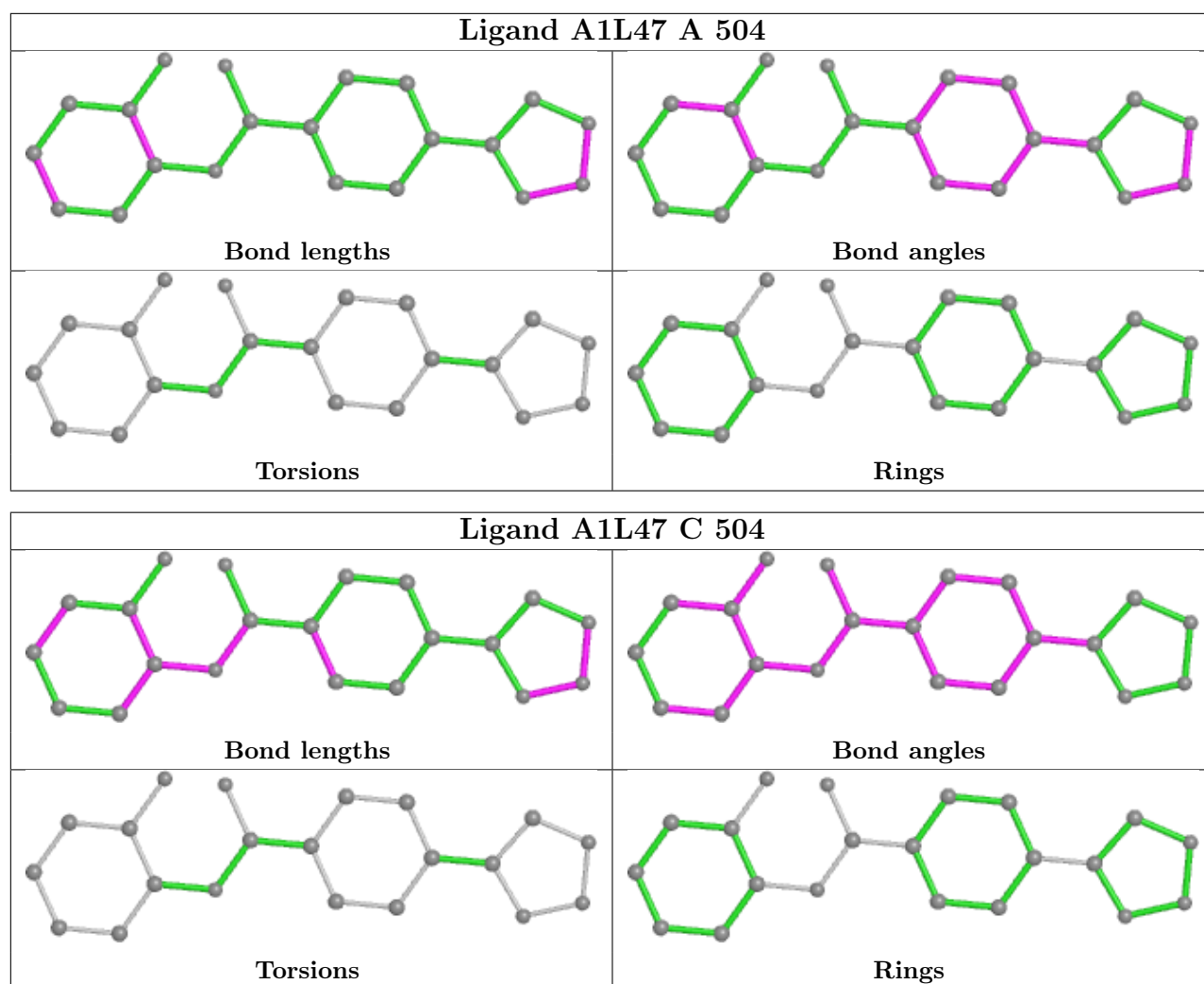
There are no ring outliers.

5 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	507	EDO	2	0
6	A	510	PEG	1	0
9	C	508	PG4	1	0
5	C	505	EDO	10	0
8	B	508	GOL	8	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 [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	369/404 (91%)	-0.31	4 (1%) 77 81	7, 22, 46, 122	21 (5%)
1	B	367/404 (90%)	-0.41	2 (0%) 87 90	6, 19, 41, 84	21 (5%)
1	C	367/404 (90%)	-0.08	5 (1%) 73 77	10, 26, 48, 100	16 (4%)
All	All	1103/1212 (91%)	-0.27	11 (0%) 79 82	6, 22, 46, 122	58 (5%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	380	HIS	3.2
1	C	62[A]	HIS	3.1
1	B	379	PRO	2.7
1	C	341	TYR	2.6
1	C	327[A]	CYS	2.5
1	A	12	GLY	2.5
1	C	379	PRO	2.4
1	B	14	LYS	2.1
1	A	208	GLU	2.1
1	A	14	LYS	2.1
1	C	13	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

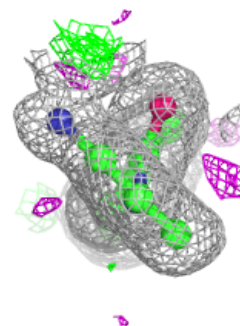
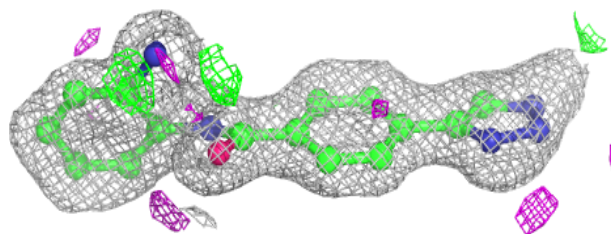
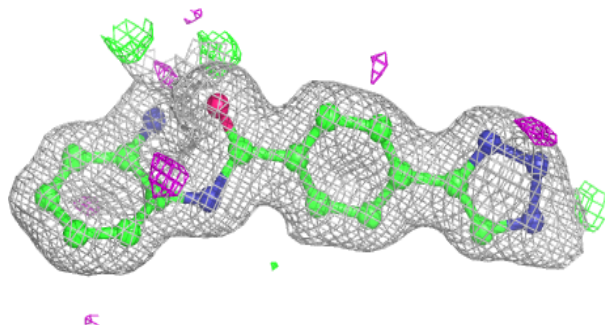
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	EDO	B	507	4/4	0.80	0.17	63,67,72,72	0
5	EDO	A	507	4/4	0.82	0.12	32,37,45,45	0
5	EDO	C	505	4/4	0.82	0.12	41,43,43,46	0
5	EDO	B	506	4/4	0.83	0.18	62,65,73,75	0
6	PEG	A	509	7/7	0.84	0.14	53,54,59,60	0
6	PEG	A	508	7/7	0.85	0.12	46,50,57,60	0
6	PEG	A	510	7/7	0.85	0.14	51,56,65,67	0
6	PEG	B	509	7/7	0.85	0.15	53,55,59,65	0
8	GOL	B	508	6/6	0.85	0.14	52,53,58,62	0
7	PGE	A	511	10/10	0.87	0.11	41,50,53,57	0
5	EDO	B	505	4/4	0.87	0.15	49,50,54,56	0
9	PG4	B	510	13/13	0.88	0.11	34,46,57,60	0
5	EDO	A	506	4/4	0.89	0.16	57,59,62,67	0
9	PG4	C	508	13/13	0.92	0.11	39,47,58,59	0
5	EDO	A	505	4/4	0.93	0.09	46,47,50,50	0
5	EDO	C	506	4/4	0.94	0.09	40,43,44,46	0
6	PEG	C	507	7/7	0.94	0.09	36,38,41,49	0
4	A1L47	C	504	21/31	0.97	0.05	13,17,37,40	0
4	A1L47	A	504	21/31	0.97	0.05	13,16,34,39	0
4	A1L47	B	504	21/31	0.98	0.05	12,15,35,40	0
2	ZN	C	501	1/1	0.99	0.02	17,17,17,17	0
3	CA	A	502	1/1	0.99	0.07	19,19,19,19	0
3	CA	A	503	1/1	0.99	0.04	24,24,24,24	0
3	CA	B	503	1/1	0.99	0.03	23,23,23,23	0
3	CA	C	503	1/1	0.99	0.09	22,22,22,22	0
3	CA	B	502	1/1	1.00	0.03	17,17,17,17	0
2	ZN	B	501	1/1	1.00	0.02	12,12,12,12	0
3	CA	C	502	1/1	1.00	0.05	21,21,21,21	0
2	ZN	A	501	1/1	1.00	0.01	14,14,14,14	0

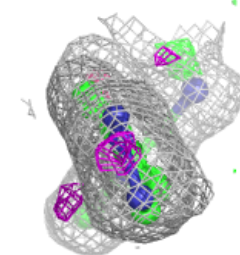
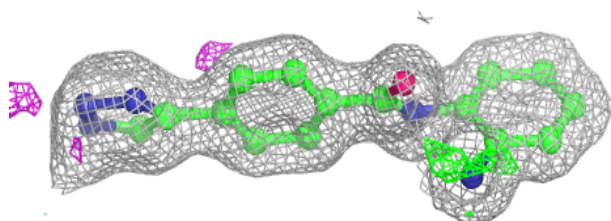
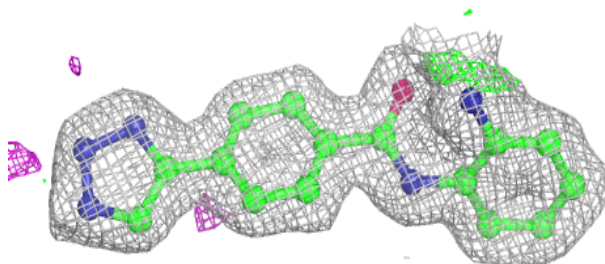
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1L47 C 504:

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

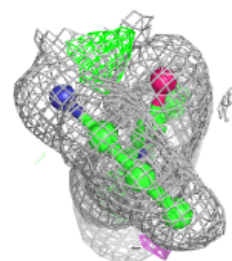
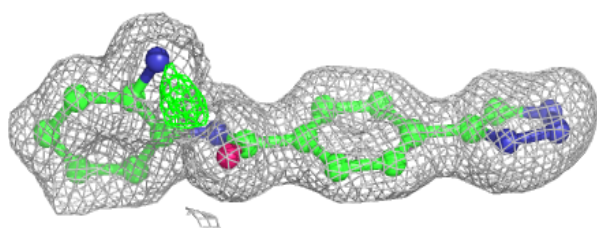
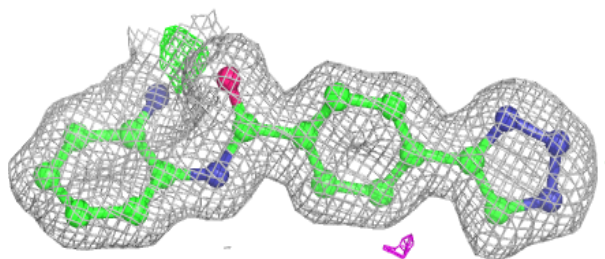
**Electron density around A1L47 A 504:**

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



Electron density around A1L47 B 504:

$2mF_o-DF_c$ (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.