



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:30 PM UTC

PDB ID : 8S75 / pdb_00008s75
Title : Soluble epoxide hydrolase in complex with PROTAC FL412
Authors : Kumar, A.; Schoenfeld, J.; Hiesinger, K.; Lillich, F.; Proschak, E.; Knapp, S.;
Structural Genomics Consortium (SGC)
Deposited on : 2024-02-29
Resolution : 1.42 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

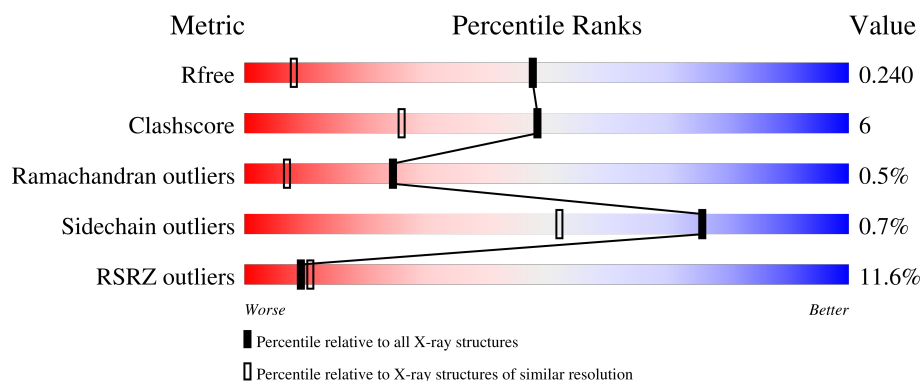
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.42 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	4041 (1.44-1.40)
Clashscore	190562	4154 (1.44-1.40)
Ramachandran outliers	187476	4083 (1.44-1.40)
Sidechain outliers	187428	4082 (1.44-1.40)
RSRZ outliers	180081	4039 (1.44-1.40)

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	367	4% 76% 11% 13%
1	B	367	16% 81% 5% 13%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PG4	A	601	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5765 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 Bifunctional epoxide hydrolase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	320	Total	C	N	O	S	0	9	0
			2610	1676	441	469	24			
1	B	320	Total	C	N	O	S	0	6	0
			2575	1653	434	465	23			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	198	MET	-	initiating methionine	UNP P34913
A	199	GLY	-	expression tag	UNP P34913
A	200	SER	-	expression tag	UNP P34913
A	201	SER	-	expression tag	UNP P34913
A	202	HIS	-	expression tag	UNP P34913
A	203	HIS	-	expression tag	UNP P34913
A	204	HIS	-	expression tag	UNP P34913
A	205	HIS	-	expression tag	UNP P34913
A	206	HIS	-	expression tag	UNP P34913
A	207	HIS	-	expression tag	UNP P34913
A	208	SER	-	expression tag	UNP P34913
A	209	SER	-	expression tag	UNP P34913
A	210	GLY	-	expression tag	UNP P34913
A	211	LEU	-	expression tag	UNP P34913
A	212	VAL	-	expression tag	UNP P34913
A	213	PRO	-	expression tag	UNP P34913
A	214	ARG	-	expression tag	UNP P34913
A	215	GLY	-	expression tag	UNP P34913
A	216	SER	-	expression tag	UNP P34913
A	217	HIS	-	expression tag	UNP P34913
A	218	MET	-	expression tag	UNP P34913
A	219	ALA	-	expression tag	UNP P34913
A	220	SER	-	expression tag	UNP P34913
A	221	MET	-	expression tag	UNP P34913
A	556	LEU	-	expression tag	UNP P34913

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Chain	Residue	Modelled	Actual	Comment	Reference
A	557	LEU	-	expression tag	UNP P34913
A	558	GLU	-	expression tag	UNP P34913
A	559	HIS	-	expression tag	UNP P34913
A	560	HIS	-	expression tag	UNP P34913
A	561	HIS	-	expression tag	UNP P34913
A	562	HIS	-	expression tag	UNP P34913
A	563	HIS	-	expression tag	UNP P34913
A	564	HIS	-	expression tag	UNP P34913
B	198	MET	-	initiating methionine	UNP P34913
B	199	GLY	-	expression tag	UNP P34913
B	200	SER	-	expression tag	UNP P34913
B	201	SER	-	expression tag	UNP P34913
B	202	HIS	-	expression tag	UNP P34913
B	203	HIS	-	expression tag	UNP P34913
B	204	HIS	-	expression tag	UNP P34913
B	205	HIS	-	expression tag	UNP P34913
B	206	HIS	-	expression tag	UNP P34913
B	207	HIS	-	expression tag	UNP P34913
B	208	SER	-	expression tag	UNP P34913
B	209	SER	-	expression tag	UNP P34913
B	210	GLY	-	expression tag	UNP P34913
B	211	LEU	-	expression tag	UNP P34913
B	212	VAL	-	expression tag	UNP P34913
B	213	PRO	-	expression tag	UNP P34913
B	214	ARG	-	expression tag	UNP P34913
B	215	GLY	-	expression tag	UNP P34913
B	216	SER	-	expression tag	UNP P34913
B	217	HIS	-	expression tag	UNP P34913
B	218	MET	-	expression tag	UNP P34913
B	219	ALA	-	expression tag	UNP P34913
B	220	SER	-	expression tag	UNP P34913
B	221	MET	-	expression tag	UNP P34913
B	556	LEU	-	expression tag	UNP P34913
B	557	LEU	-	expression tag	UNP P34913
B	558	GLU	-	expression tag	UNP P34913
B	559	HIS	-	expression tag	UNP P34913
B	560	HIS	-	expression tag	UNP P34913
B	561	HIS	-	expression tag	UNP P34913
B	562	HIS	-	expression tag	UNP P34913
B	563	HIS	-	expression tag	UNP P34913
B	564	HIS	-	expression tag	UNP P34913

- Molecule 2 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	8	5		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



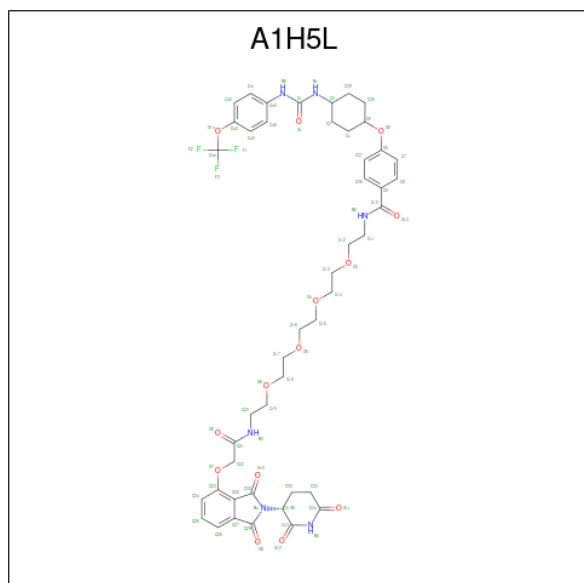
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		

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

- Molecule 4 is {N}-[2-[2-[2-[2-[2-[2-[2,6-bis(oxidanylidene)piperidin-3-yl]-1,3-bis(oxidanylidene)isoindol-4-yl]oxyethanoylamino]ethoxy]ethoxy]ethoxy]ethyl]-4-[4-[[4-(trifluoromethoxy)phenyl]carbamoylamino]cyclohexyl]oxy-benzamide (CCD ID: A1H5L) (formula: C₄₆H₅₃F₃N₆O₁₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	0	0
			31	21	3	3	4		
4	B	1	Total	C	F	N	O	0	0
			31	21	3	3	4		

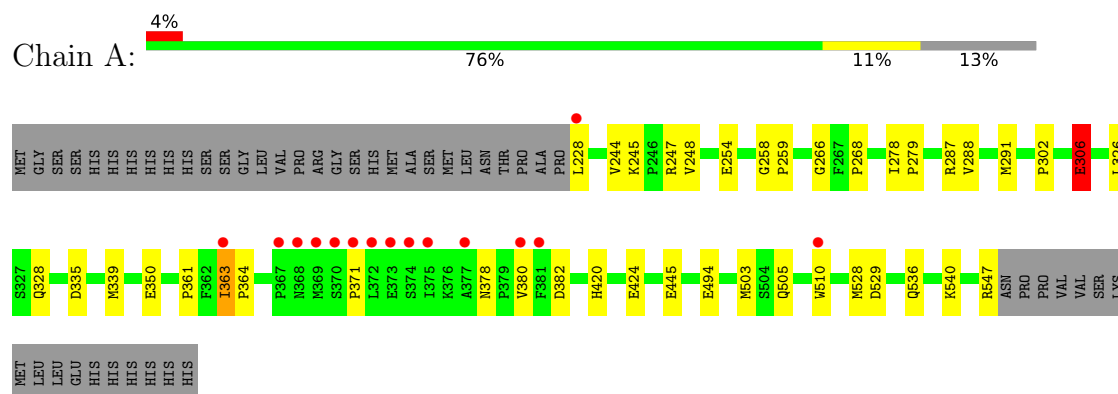
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	312	Total	O	0	0
			312	312		
5	B	165	Total	O	0	0
			165	165		

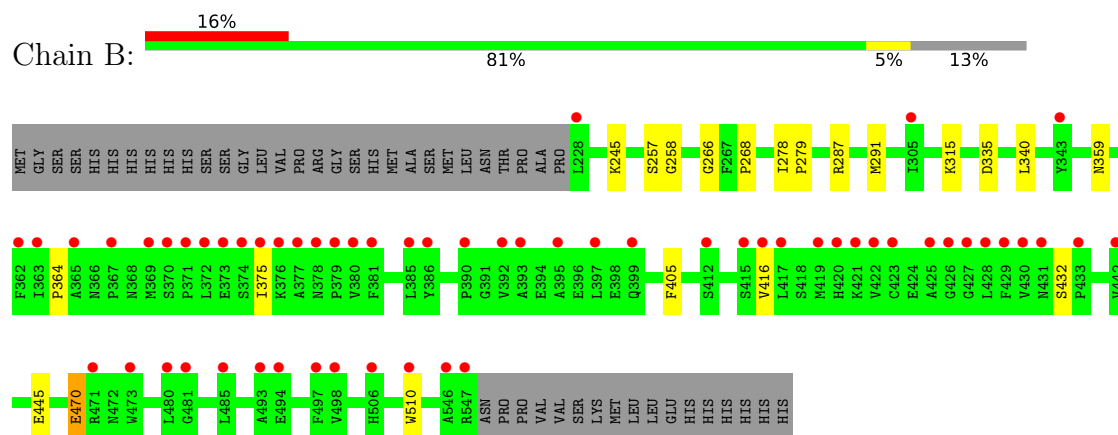
3 Residue-property plots

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: Bifunctional epoxide hydrolase 2



• Molecule 1: Bifunctional epoxide hydrolase 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	47.12Å 80.18Å 89.42Å 90.00° 91.54° 90.00°	Depositor
Resolution (Å)	47.15 – 1.42 47.15 – 1.42	Depositor EDS
% Data completeness (in resolution range)	99.2 (47.15-1.42) 99.3 (47.15-1.42)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 1.42Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.187 , 0.220 (Not available) , 0.240	Depositor DCC
R_{free} test set	6472 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å ²)	16.7	Xtriage
Anisotropy	0.450	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 33.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.059 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5765	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.73% 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: A1H5L, EDO, PG4

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	0.76	1/2690 (0.0%)	1.16	7/3654 (0.2%)
1	B	0.65	0/2651	1.03	2/3603 (0.1%)
All	All	0.71	1/5341 (0.0%)	1.09	9/7257 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	302	PRO	CA-CB	-7.95	1.46	1.53

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	505	GLN	CA-C-N	-11.57	105.01	122.83
1	A	505	GLN	C-N-CA	-11.57	105.01	122.83
1	A	306	GLU	CB-CG-CD	6.50	123.65	112.60
1	A	494	GLU	CG-CD-OE1	-5.77	105.14	118.40
1	A	302	PRO	O-C-N	-5.55	118.76	121.31
1	A	350	GLU	CB-CG-CD	5.27	121.56	112.60
1	B	245	LYS	CB-CA-C	-5.26	101.81	109.97
1	A	529	ASP	CA-CB-CG	5.21	117.81	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	405	PHE	CA-CB-CG	-5.11	108.69	113.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	291	MET	Peptide
1	B	291	MET	Peptide

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	2610	0	2516	35	0
1	B	2575	0	2469	19	0
2	A	13	0	18	17	0
3	A	24	0	35	4	0
3	B	4	0	6	0	0
4	A	31	0	0	0	0
4	B	31	0	0	0	0
5	A	312	0	0	12	0
5	B	165	0	0	6	0
All	All	5765	0	5044	57	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 6.

All (57) 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:445:GLU:HG2	5:A:903:HOH:O	1.61	0.98
1:A:528:MET:HE2	5:A:705:HOH:O	1.61	0.97
1:A:245:LYS:HB2	1:A:248[B]:VAL:HG22	1.55	0.88
2:A:601:PG4:H62	1:B:287:ARG:HD2	1.60	0.83
1:A:378:ASN:CB	5:A:944:HOH:O	2.33	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:416:VAL:HG21	5:B:848:HOH:O	1.92	0.69
1:A:364:PRO:HG2	1:A:510:TRP:NE1	2.06	0.69
1:A:287:ARG:HD2	2:A:601:PG4:H61	1.76	0.67
2:A:601:PG4:H31	1:B:257:SER:HB2	1.78	0.66
1:A:536:GLN:NE2	5:A:701:HOH:O	2.01	0.66
1:B:364:PRO:HG2	1:B:510:TRP:CE2	2.30	0.66
2:A:601:PG4:H51	1:B:258:GLY:H	1.62	0.65
1:A:540:LYS:NZ	5:A:702:HOH:O	2.23	0.64
1:A:378:ASN:CB	5:A:1006:HOH:O	2.46	0.63
1:A:287:ARG:HD2	2:A:601:PG4:C6	2.30	0.61
2:A:601:PG4:H81	1:B:258:GLY:O	2.02	0.59
1:A:424:GLU:HG2	5:A:957:HOH:O	2.03	0.58
1:A:328:GLN:O	2:A:601:PG4:H11	2.04	0.57
1:A:244:VAL:HG23	1:A:248[B]:VAL:HG23	1.87	0.57
1:A:247:ARG:HB2	3:A:605:EDO:H11	1.86	0.57
1:A:258:GLY:O	2:A:601:PG4:H41	2.05	0.56
1:B:375:ILE:CB	5:B:796:HOH:O	2.53	0.56
1:A:380:VAL:HG22	1:A:420:HIS:CE1	2.42	0.55
1:B:445:GLU:HG2	5:B:841:HOH:O	2.06	0.54
1:B:340:LEU:C	1:B:340:LEU:HD23	2.32	0.54
2:A:601:PG4:H31	3:A:602:EDO:O1	2.08	0.53
1:A:266:GLY:HA3	1:A:335:ASP:HB3	1.91	0.52
1:A:244:VAL:CG2	1:A:248[B]:VAL:HG23	2.39	0.52
1:B:364:PRO:HG2	1:B:510:TRP:NE1	2.23	0.52
2:A:601:PG4:C3	3:A:602:EDO:O1	2.57	0.52
1:B:315:LYS:HG3	5:B:737:HOH:O	2.10	0.52
1:A:380:VAL:HG22	1:A:420:HIS:NE2	2.24	0.51
2:A:601:PG4:H72	1:B:287:ARG:HD3	1.92	0.50
1:B:266:GLY:HA3	1:B:335:ASP:HB3	1.93	0.49
1:A:536:GLN:HG3	5:A:802:HOH:O	2.11	0.49
1:A:244:VAL:HG23	1:A:248[B]:VAL:CG2	2.43	0.49
2:A:601:PG4:C5	1:B:258:GLY:H	2.26	0.48
1:A:278:ILE:HB	1:A:279:PRO:HD3	1.96	0.48
1:A:361:PRO:HG3	1:A:503:MET:HE2	1.95	0.47
1:A:547:ARG:HD3	5:A:715:HOH:O	2.13	0.47
1:A:306:GLU:H	1:A:306:GLU:CD	2.23	0.47
1:A:382:ASP:HB2	5:A:872:HOH:O	2.13	0.47
2:A:601:PG4:H72	1:B:287:ARG:CD	2.45	0.46
1:B:470:GLU:HB2	5:B:758:HOH:O	2.15	0.46
1:A:254:GLU:HA	1:A:288:VAL:O	2.15	0.46
1:A:339[A]:MET:HB2	1:A:339[A]:MET:HE2	1.63	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:ILE:N	1:A:363:ILE:HD13	2.32	0.44
1:B:416:VAL:HG11	5:B:848:HOH:O	2.17	0.44
1:A:228:LEU:N	5:A:711:HOH:O	2.50	0.43
1:A:259:PRO:HA	2:A:601:PG4:H32	2.00	0.43
1:A:364:PRO:HG2	1:A:510:TRP:CE2	2.54	0.42
1:B:278:ILE:HB	1:B:279:PRO:HD3	2.02	0.42
1:A:371:PRO:CB	5:A:763:HOH:O	2.69	0.41
1:A:326:LEU:HD22	2:A:601:PG4:H12	2.03	0.41
2:A:601:PG4:H52	3:A:602:EDO:O2	2.21	0.41
2:A:601:PG4:H51	1:B:258:GLY:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	327/367 (89%)	318 (97%)	8 (2%)	1 (0%)	36	17
1	B	324/367 (88%)	317 (98%)	5 (2%)	2 (1%)	21	5
All	All	651/734 (89%)	635 (98%)	13 (2%)	3 (0%)	24	7

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	359	ASN
1	A	268	PRO
1	B	268	PRO

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	281/323 (87%)	279 (99%)	2 (1%)	76	52
1	B	275/323 (85%)	272 (99%)	3 (1%)	65	35
All	All	556/646 (86%)	551 (99%)	5 (1%)	76	43

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	306	GLU
1	A	363	ILE
1	B	432[A]	SER
1	B	432[B]	SER
1	B	470	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	328	GLN
1	A	452	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

10 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
4	A1H5L	B	602	-	33,33,74	0.43	0	46,46,100	1.10	5 (10%)
3	EDO	A	606	-	3,3,3	0.43	0	2,2,2	0.62	0
3	EDO	A	608	-	3,3,3	0.22	0	2,2,2	0.34	0
3	EDO	A	605	-	3,3,3	0.72	0	2,2,2	0.21	0
3	EDO	A	604	-	3,3,3	0.21	0	2,2,2	0.28	0
2	PG4	A	601	-	12,12,12	0.52	0	11,11,11	0.74	0
3	EDO	A	602	-	3,3,3	0.14	0	2,2,2	0.25	0
3	EDO	B	601	-	3,3,3	0.25	0	2,2,2	0.33	0
3	EDO	A	603	-	3,3,3	0.28	0	2,2,2	0.12	0
4	A1H5L	A	607	-	33,33,74	0.52	0	46,46,100	1.04	5 (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
4	A1H5L	B	602	-	-	3/21/31/88	0/3/3/6
3	EDO	A	606	-	-	0/1/1/1	-
3	EDO	A	608	-	-	0/1/1/1	-
3	EDO	A	605	-	-	0/1/1/1	-
3	EDO	A	604	-	-	0/1/1/1	-
2	PG4	A	601	-	-	6/10/10/10	-
3	EDO	A	602	-	-	1/1/1/1	-
3	EDO	B	601	-	-	0/1/1/1	-
3	EDO	A	603	-	-	0/1/1/1	-
4	A1H5L	A	607	-	-	0/21/31/88	0/3/3/6

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	602	A1H5L	C4-C3-C2	-3.46	107.70	111.49
4	B	602	A1H5L	C38-C39-C2	2.89	114.67	111.49
4	B	602	A1H5L	C2-N1-C1	2.70	128.72	122.92
4	A	607	A1H5L	C8-C9-C10	-2.63	113.88	121.06
4	B	602	A1H5L	C3-C2-N1	2.34	115.26	110.57
4	A	607	A1H5L	C36-C9-C10	2.30	127.32	121.06
4	B	602	A1H5L	C39-C38-C5	2.30	114.66	110.96
4	A	607	A1H5L	O2-C6-C7	-2.20	109.14	119.90
4	A	607	A1H5L	O2-C6-C37	2.04	129.88	119.90
4	A	607	A1H5L	O2-C5-C4	-2.02	103.61	108.31

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	602	A1H5L	C3-C2-N1-C1
2	A	601	PG4	O2-C3-C4-O3
2	A	601	PG4	O4-C7-C8-O5
3	A	602	EDO	O1-C1-C2-O2
2	A	601	PG4	C1-C2-O2-C3
4	B	602	A1H5L	C37-C6-O2-C5
2	A	601	PG4	C8-C7-O4-C6
4	B	602	A1H5L	C7-C6-O2-C5
2	A	601	PG4	C4-C3-O2-C2
2	A	601	PG4	O3-C5-C6-O4

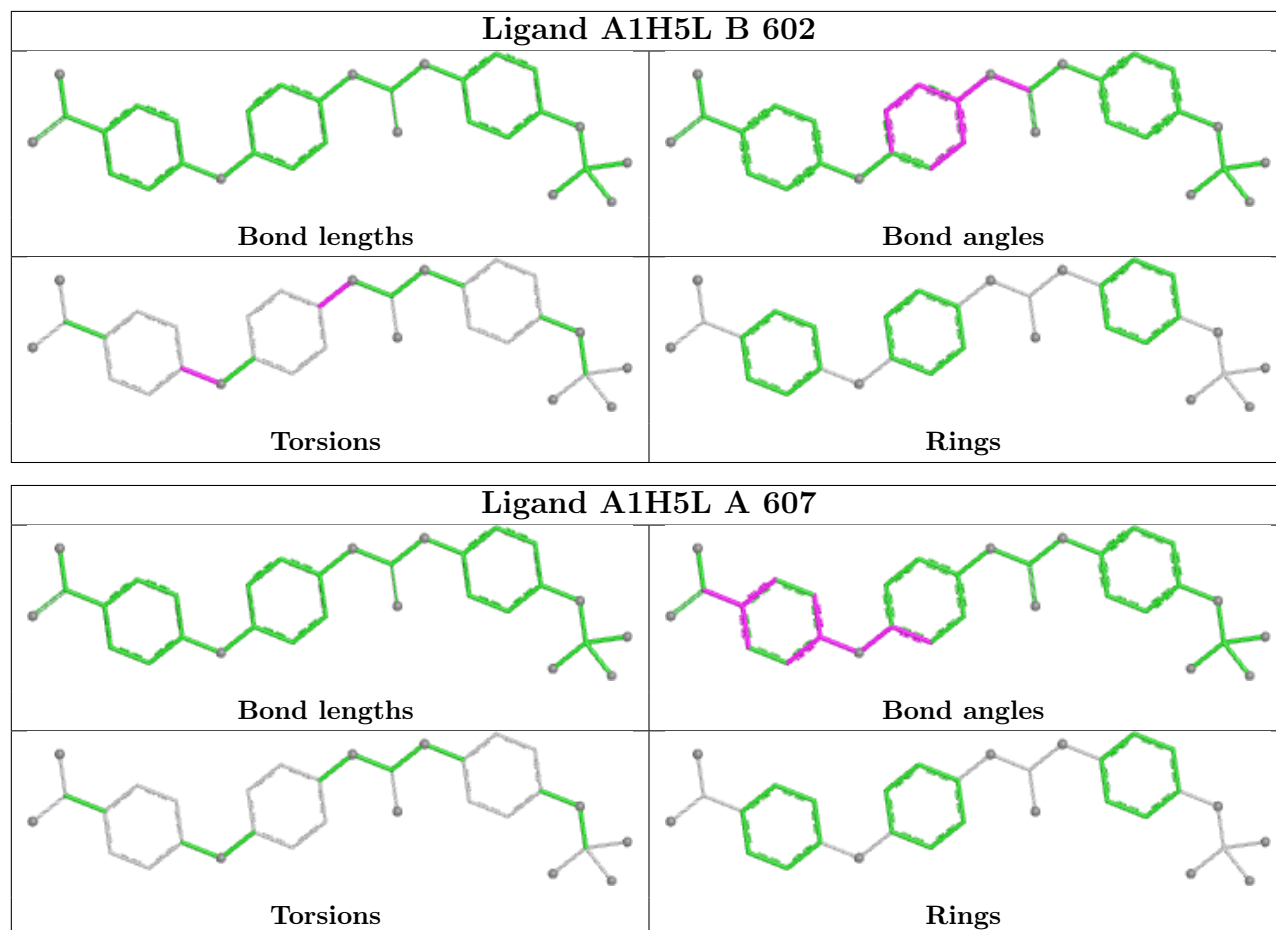
There are no ring outliers.

3 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	605	EDO	1	0
2	A	601	PG4	17	0
3	A	602	EDO	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	320/367 (87%)	0.22	15 (4%) 36 39	6, 16, 36, 79	9 (2%)
1	B	320/367 (87%)	1.02	59 (18%) 3 4	8, 25, 61, 89	6 (1%)
All	All	640/734 (87%)	0.62	74 (11%) 9 11	6, 19, 56, 89	15 (2%)

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	372	LEU	6.2
1	B	380	VAL	6.1
1	B	510	TRP	5.8
1	B	430[A]	VAL	5.3
1	B	480	LEU	5.0
1	B	370	SER	4.9
1	B	372	LEU	4.8
1	B	375	ILE	4.7
1	B	377	ALA	4.6
1	B	371	PRO	4.5
1	B	379	PRO	4.3
1	B	416	VAL	4.2
1	B	381	PHE	4.2
1	B	422	VAL	4.2
1	B	417	LEU	3.8
1	B	385	LEU	3.7
1	A	380	VAL	3.7
1	B	374	SER	3.6
1	B	363	ILE	3.6
1	B	420	HIS	3.6
1	B	378	ASN	3.5
1	A	228	LEU	3.5
1	B	228	LEU	3.5
1	B	428	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	363	ILE	3.5
1	B	425	ALA	3.4
1	A	374	SER	3.3
1	B	412[A]	SER	3.3
1	A	510	TRP	3.3
1	B	373	GLU	3.3
1	B	423	CYS	3.2
1	B	547	ARG	3.2
1	B	305	ILE	3.1
1	B	421	LYS	3.1
1	A	377	ALA	3.1
1	B	426	GLY	3.1
1	B	546	ALA	3.1
1	B	395	ALA	3.0
1	B	392	VAL	3.0
1	A	381	PHE	2.9
1	A	371	PRO	2.8
1	B	429	PHE	2.7
1	A	373	GLU	2.7
1	B	481	GLY	2.6
1	B	442	VAL	2.6
1	B	365	ALA	2.5
1	B	427	GLY	2.5
1	B	399	GLN	2.5
1	B	431	ASN	2.5
1	B	390	PRO	2.4
1	B	362	PHE	2.4
1	B	369	MET	2.4
1	B	397	LEU	2.4
1	B	493	ALA	2.4
1	A	370	SER	2.4
1	B	415[A]	SER	2.4
1	B	393	ALA	2.3
1	B	473	TRP	2.3
1	B	494	GLU	2.3
1	A	368	ASN	2.3
1	B	497	PHE	2.3
1	B	343	TYR	2.3
1	A	367	PRO	2.2
1	A	375	ILE	2.2
1	B	367	PRO	2.2
1	B	376	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	433	PRO	2.2
1	B	471	ARG	2.1
1	B	506	HIS	2.1
1	A	369	MET	2.1
1	B	419	MET	2.1
1	B	485	LEU	2.0
1	B	498	VAL	2.0
1	B	386	TYR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

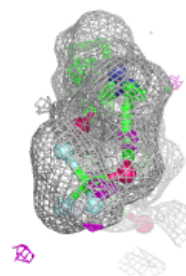
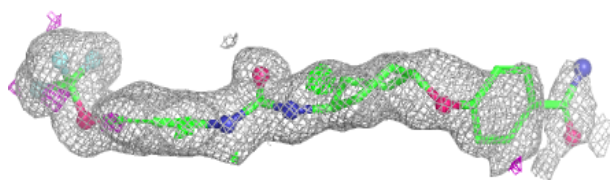
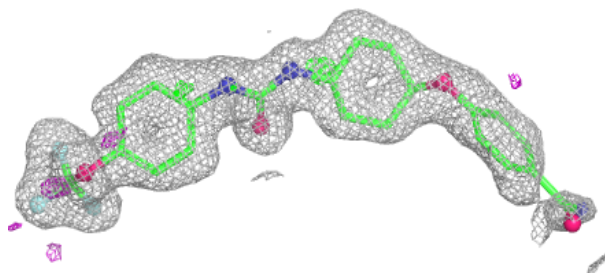
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	EDO	A	602	4/4	0.83	0.13	36,36,38,39	0
2	PG4	A	601	13/13	0.84	0.13	24,26,32,40	0
3	EDO	A	608	4/4	0.85	0.13	39,40,42,43	0
3	EDO	B	601	4/4	0.85	0.15	32,39,41,43	0
3	EDO	A	603	4/4	0.86	0.14	40,41,41,42	0
3	EDO	A	606	4/4	0.86	0.14	31,34,35,37	0
3	EDO	A	605	4/4	0.88	0.12	31,37,37,39	0
4	A1H5L	B	602	31/69	0.89	0.13	21,32,65,68	0
3	EDO	A	604	4/4	0.92	0.11	25,28,32,33	0
4	A1H5L	A	607	31/69	0.95	0.09	14,18,40,50	0

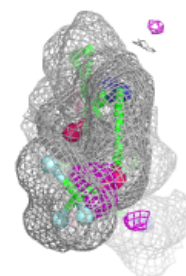
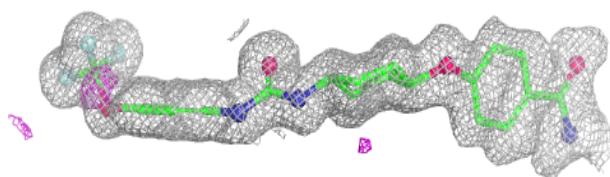
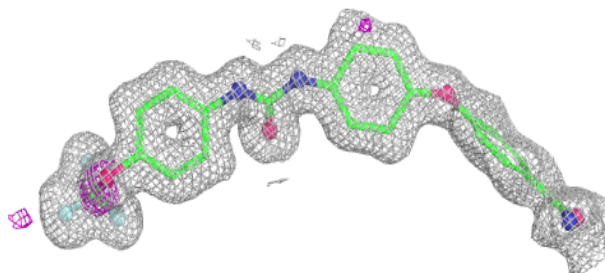
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1H5L B 602:

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

**Electron density around A1H5L A 607:**

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



6.5 Other polymers ⓘ

There are no such residues in this entry.