



Full wwPDB EM Validation Report ⓘ

Oct 28, 2024 – 12:34 PM JST

PDB ID : 8JUN
EMDB ID : EMD-36662
Title : Cryo-EM structure of SIDT1 E555Q mutant
Authors : Sun, C.R.; Xu, D.; Li, Q.; Zhou, C.Z.; Chen, Y.
Deposited on : 2023-06-26
Resolution : 2.38 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>

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:

EMDB validation analysis : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

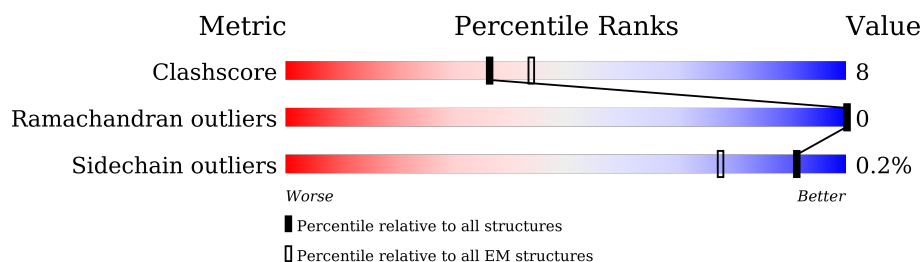
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY



The reported resolution of this entry is 2.38 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	827	
1	B	827	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11098 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 SID1 transmembrane family member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	678	Total	C	N	O	S	0	0
			5496	3627	881	955	33		
1	B	678	Total	C	N	O	S	0	0
			5496	3627	881	955	33		

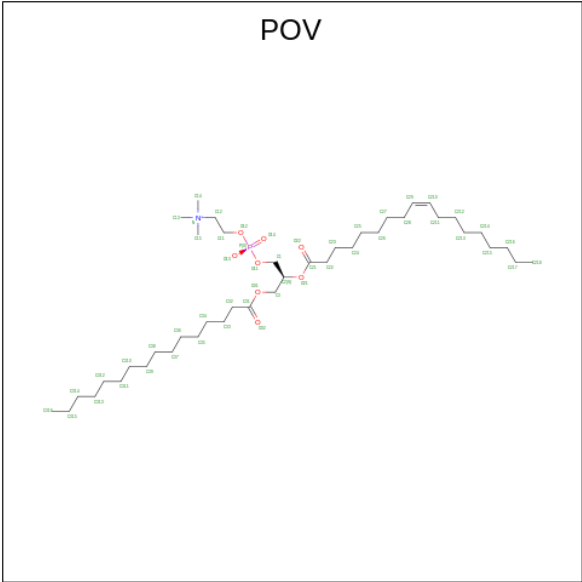
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	555	GLN	GLU	engineered mutation	UNP Q9NXL6
B	555	GLN	GLU	engineered mutation	UNP Q9NXL6

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 3 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (three-letter code: POV) (formula: C₄₂H₈₂NO₈P) (labeled as "Ligand of Interest" by depositor).

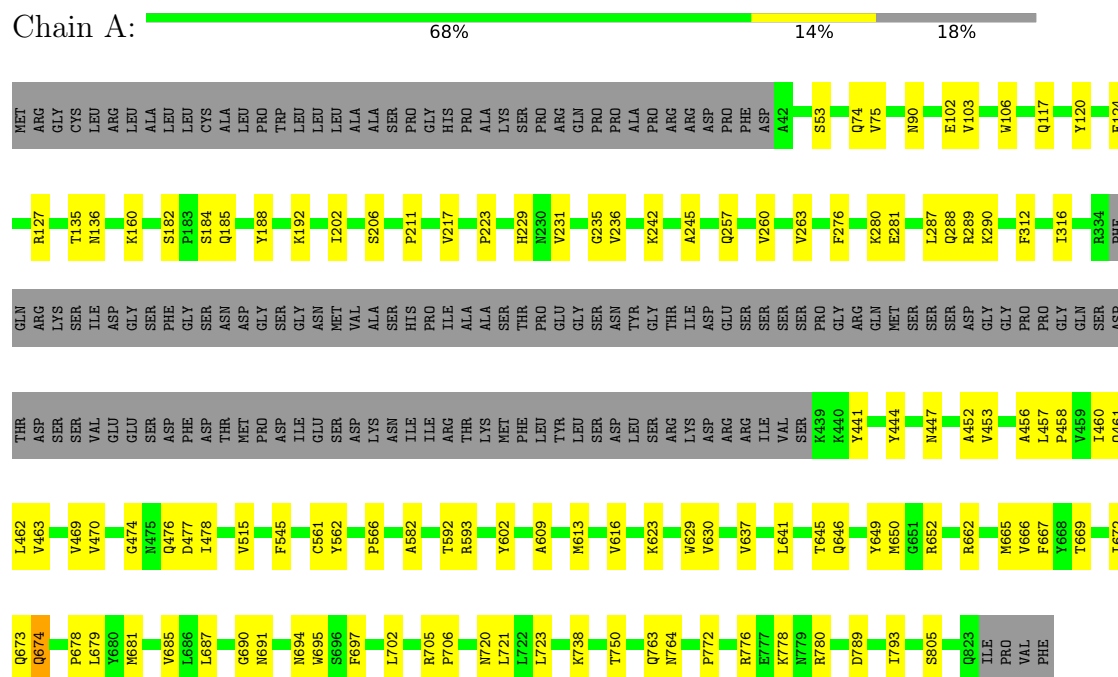


Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	B	1	Total	C	N	O	P	0
			52	42	1	8	1	

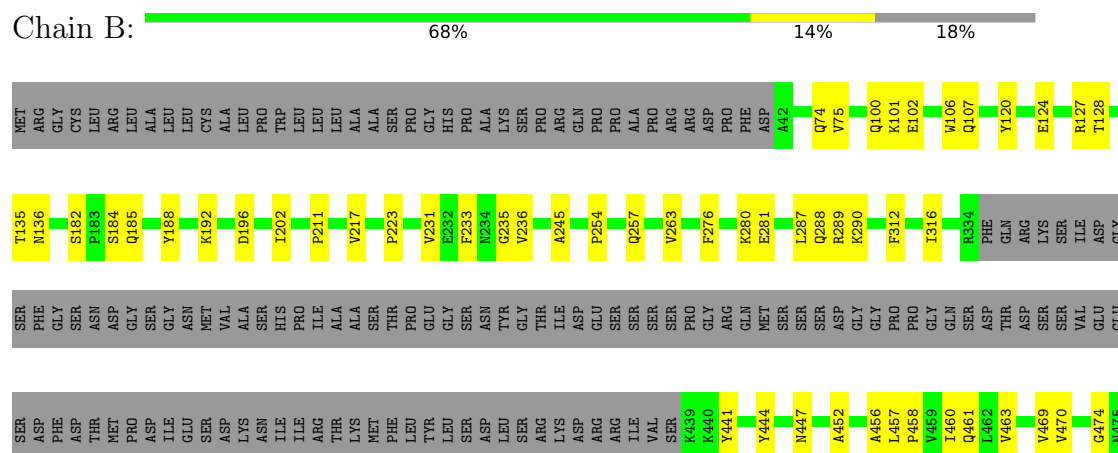
3 Residue-property plots [i](#)

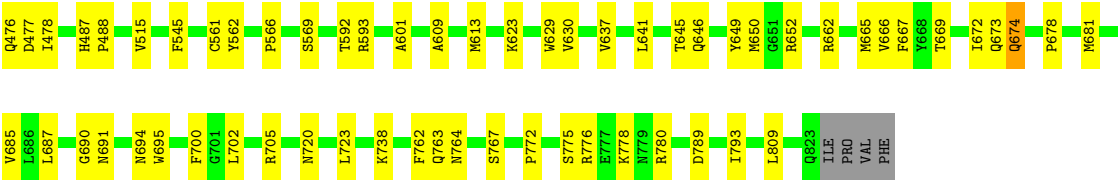
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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: SID1 transmembrane family member 1



- Molecule 1: SID1 transmembrane family member 1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1098736	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: POV, ZN

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	0.37	0/5646	0.49	2/7677 (0.0%)
1	B	0.37	0/5646	0.49	2/7677 (0.0%)
All	All	0.37	0/11292	0.49	4/15354 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	674	GLN	CA-CB-CG	5.56	125.64	113.40
1	A	674	GLN	CA-CB-CG	5.56	125.63	113.40
1	A	738	LYS	CD-CE-NZ	5.33	123.95	111.70
1	B	738	LYS	CD-CE-NZ	5.32	123.94	111.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5496	0	5488	94	0
1	B	5496	0	5488	88	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	52	0	82	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	52	0	82	5	0
All	All	11098	0	11140	167	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 8.

All (167) 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:53:SER:OG	1:A:160:LYS:HD3	1.67	0.94
1:A:462:LEU:CD2	1:B:569:SER:HB2	2.01	0.90
1:B:678:PRO:HG2	1:B:681:MET:HB2	1.56	0.87
1:A:678:PRO:HG2	1:A:681:MET:HB2	1.56	0.87
1:A:462:LEU:HD23	1:B:569:SER:HB2	1.58	0.86
1:A:457:LEU:HD11	1:B:613:MET:HG2	1.64	0.79
1:B:135:THR:HG22	1:B:136:ASN:N	1.98	0.77
1:A:135:THR:HG22	1:A:136:ASN:H	1.49	0.77
1:B:135:THR:HG22	1:B:136:ASN:H	1.48	0.76
1:A:135:THR:HG22	1:A:136:ASN:N	1.98	0.76
1:B:694:ASN:HD21	1:B:720:ASN:HD21	1.36	0.74
1:A:616:VAL:HG21	1:B:457:LEU:HD21	1.70	0.74
1:A:694:ASN:HD21	1:A:720:ASN:HD21	1.36	0.73
1:B:762:PHE:HA	3:B:902:POV:H11A	1.78	0.65
1:A:457:LEU:CD1	1:B:613:MET:HG2	2.27	0.64
1:A:681:MET:HG2	1:A:685:VAL:HG23	1.81	0.63
1:B:681:MET:HG2	1:B:685:VAL:HG23	1.81	0.63
1:B:767:SER:HB2	1:B:775:SER:OG	1.98	0.63
1:A:462:LEU:HD21	1:B:569:SER:HB2	1.81	0.62
1:B:135:THR:CG2	1:B:136:ASN:H	2.12	0.62
1:B:288:GLN:HG2	1:B:290:LYS:HZ3	1.65	0.62
1:A:135:THR:CG2	1:A:136:ASN:H	2.12	0.62
1:A:697:PHE:CD2	3:A:902:POV:H37A	2.35	0.61
1:B:646:GLN:HE21	1:B:652:ARG:HB2	1.66	0.61
1:A:288:GLN:HG2	1:A:290:LYS:HZ3	1.66	0.61
1:A:706:PRO:HB3	3:A:902:POV:H1	1.82	0.60
1:A:646:GLN:HE21	1:A:652:ARG:HB2	1.66	0.60
1:A:453:VAL:HG13	1:A:457:LEU:HD11	1.83	0.60
1:A:673:GLN:HG3	1:A:674:GLN:H	1.68	0.59
1:B:673:GLN:HG3	1:B:674:GLN:H	1.68	0.59
1:A:53:SER:OG	1:A:160:LYS:CD	2.47	0.58
1:A:192:LYS:HG2	1:A:257:GLN:HG2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:THR:CG2	1:A:136:ASN:N	2.66	0.57
1:A:645:THR:HG22	1:A:687:LEU:HD21	1.87	0.57
1:B:645:THR:HG22	1:B:687:LEU:HD21	1.87	0.57
1:B:192:LYS:HG2	1:B:257:GLN:HG2	1.86	0.56
1:A:452:ALA:O	1:A:456:ALA:N	2.37	0.56
1:A:602:TYR:HE1	1:B:601:ALA:O	1.88	0.55
1:B:477:ASP:HB3	1:B:772:PRO:HG2	1.89	0.55
1:B:231:VAL:HG11	1:B:263:VAL:HG21	1.89	0.55
1:A:206:SER:OG	1:A:242:LYS:HA	2.07	0.55
1:A:616:VAL:CG2	1:B:457:LEU:HD21	2.37	0.55
1:A:231:VAL:HG11	1:A:263:VAL:HG21	1.89	0.55
1:A:477:ASP:HB3	1:A:772:PRO:HG2	1.89	0.54
1:A:476:GLN:O	1:A:776:ARG:NH2	2.41	0.54
1:B:452:ALA:O	1:B:456:ALA:N	2.37	0.54
1:B:690:GLY:HA2	1:B:723:LEU:HD21	1.89	0.54
1:B:476:GLN:O	1:B:776:ARG:NH2	2.41	0.54
1:B:592:THR:HG23	1:B:593:ARG:HG2	1.90	0.54
1:B:120:TYR:HB3	1:B:287:LEU:HD21	1.90	0.54
1:A:74:GLN:OE1	1:A:75:VAL:N	2.42	0.53
1:A:690:GLY:HA2	1:A:723:LEU:HD21	1.89	0.53
1:B:666:VAL:O	1:B:669:THR:OG1	2.25	0.53
1:A:120:TYR:HB3	1:A:287:LEU:HD21	1.90	0.53
1:A:629:TRP:CD1	1:A:705:ARG:HG2	2.43	0.53
1:B:629:TRP:CD1	1:B:705:ARG:HG2	2.43	0.52
1:A:666:VAL:O	1:A:669:THR:OG1	2.25	0.52
1:B:763:GLN:HE21	1:B:780:ARG:HH12	1.57	0.52
1:B:74:GLN:OE1	1:B:75:VAL:N	2.42	0.52
1:A:592:THR:HG23	1:A:593:ARG:HG2	1.90	0.52
1:A:669:THR:HB	1:A:672:ILE:HB	1.93	0.51
1:A:763:GLN:HE21	1:A:780:ARG:HH12	1.57	0.51
1:B:669:THR:HB	1:B:672:ILE:HB	1.93	0.51
1:A:469:VAL:HG13	1:A:470:VAL:HG23	1.93	0.51
1:B:469:VAL:HG13	1:B:470:VAL:HG23	1.93	0.50
1:A:217:VAL:O	1:A:235:GLY:HA3	2.11	0.50
1:A:281:GLU:OE2	1:A:287:LEU:HD12	2.12	0.50
1:B:217:VAL:O	1:B:235:GLY:HA3	2.11	0.50
1:A:453:VAL:HG11	1:B:609:ALA:HB1	1.93	0.50
1:B:641:LEU:HA	1:B:691:ASN:HD21	1.76	0.50
1:A:562:TYR:CZ	1:A:566:PRO:HB3	2.47	0.49
1:A:641:LEU:HA	1:A:691:ASN:HD21	1.76	0.49
1:B:562:TYR:CZ	1:B:566:PRO:HB3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:GLU:O	1:B:184:SER:OG	2.18	0.49
1:B:281:GLU:OE2	1:B:287:LEU:HD12	2.12	0.49
1:B:609:ALA:O	1:B:613:MET:HG3	2.13	0.48
1:A:673:GLN:HG3	1:A:674:GLN:N	2.28	0.48
1:B:667:PHE:O	1:B:669:THR:N	2.43	0.48
1:A:281:GLU:OE1	1:A:281:GLU:N	2.45	0.48
1:A:789:ASP:OD1	1:A:789:ASP:N	2.46	0.48
1:A:609:ALA:O	1:A:613:MET:HG3	2.13	0.48
1:B:281:GLU:N	1:B:281:GLU:OE1	2.45	0.48
1:A:637:VAL:HG13	1:A:695:TRP:NE1	2.29	0.48
1:B:637:VAL:HG13	1:B:695:TRP:NE1	2.29	0.48
1:A:124:GLU:O	1:A:184:SER:OG	2.18	0.48
1:A:276:PHE:CE1	1:A:289:ARG:HD2	2.49	0.48
1:A:453:VAL:HG13	1:A:457:LEU:CD1	2.44	0.48
1:A:697:PHE:HD2	3:A:902:POV:H37A	1.76	0.48
1:B:276:PHE:CE1	1:B:289:ARG:HD2	2.49	0.48
1:B:673:GLN:HG3	1:B:674:GLN:N	2.28	0.47
1:A:90:ASN:O	1:B:100:GLN:NE2	2.37	0.47
1:A:667:PHE:O	1:A:669:THR:N	2.43	0.47
1:B:630:VAL:HG12	1:B:702:LEU:HD11	1.97	0.47
1:A:616:VAL:HG11	1:B:457:LEU:HD11	1.96	0.46
1:B:135:THR:CG2	1:B:136:ASN:N	2.66	0.45
1:B:280:LYS:HB3	1:B:281:GLU:OE1	2.17	0.45
1:B:678:PRO:HG2	1:B:681:MET:CB	2.38	0.45
1:A:444:TYR:HA	1:A:447:ASN:OD1	2.16	0.45
1:B:700:PHE:CE2	3:B:902:POV:H38	2.51	0.45
1:B:789:ASP:O	1:B:793:ILE:HG12	2.17	0.45
1:A:280:LYS:HB3	1:A:281:GLU:OE1	2.17	0.45
1:B:444:TYR:HA	1:B:447:ASN:OD1	2.16	0.45
1:A:441:TYR:O	1:A:444:TYR:HB2	2.17	0.45
1:A:789:ASP:O	1:A:793:ILE:HG12	2.17	0.45
1:A:229:HIS:HA	1:B:233:PHE:CD1	2.52	0.45
3:B:902:POV:H26	3:B:902:POV:H29	1.30	0.45
1:A:630:VAL:HG12	1:A:702:LEU:HD11	1.97	0.45
1:B:470:VAL:HG11	1:B:478:ILE:HG13	1.99	0.45
1:A:202:ILE:O	1:A:245:ALA:HA	2.17	0.44
1:A:106:TRP:CZ3	1:A:127:ARG:HD2	2.52	0.44
1:B:441:TYR:O	1:B:444:TYR:HB2	2.17	0.44
1:A:457:LEU:N	1:A:458:PRO:HD2	2.33	0.44
1:A:457:LEU:HD11	1:B:613:MET:CG	2.41	0.44
1:B:202:ILE:O	1:B:245:ALA:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:650:MET:CE	1:A:662:ARG:HB3	2.48	0.43
1:A:678:PRO:HG2	1:A:681:MET:CB	2.38	0.43
1:B:650:MET:CE	1:B:662:ARG:HB3	2.48	0.43
1:A:211:PRO:HG2	1:A:289:ARG:O	2.18	0.43
1:B:106:TRP:CZ3	1:B:127:ARG:HD2	2.52	0.43
1:B:623:LYS:HD2	1:B:623:LYS:H	1.83	0.43
1:A:460:ILE:O	1:A:461:GLN:C	2.57	0.43
1:A:674:GLN:HE22	1:A:679:LEU:HD12	1.83	0.43
1:B:196:ASP:OD1	1:B:196:ASP:N	2.52	0.43
1:B:211:PRO:HG2	1:B:289:ARG:O	2.18	0.43
3:B:902:POV:H217	3:B:902:POV:H214	1.69	0.43
1:B:457:LEU:N	1:B:458:PRO:HD2	2.33	0.43
1:B:674:GLN:HB3	1:B:678:PRO:HB3	2.01	0.43
1:A:90:ASN:HA	1:B:101:LYS:HD3	2.00	0.42
1:A:470:VAL:HG11	1:A:478:ILE:HG13	1.99	0.42
1:A:623:LYS:H	1:A:623:LYS:HD2	1.83	0.42
1:A:649:TYR:O	1:A:650:MET:HB2	2.19	0.42
1:B:674:GLN:CB	1:B:678:PRO:HB3	2.50	0.42
1:A:463:VAL:HG11	1:A:561:CYS:O	2.19	0.42
1:A:674:GLN:CB	1:A:678:PRO:HB3	2.49	0.42
1:B:762:PHE:HE1	3:B:902:POV:H22	1.84	0.42
1:A:764:ASN:OD1	1:A:778:LYS:HD3	2.20	0.42
1:A:312:PHE:O	1:A:316:ILE:HG12	2.20	0.42
1:A:666:VAL:HG23	1:A:667:PHE:H	1.84	0.42
1:A:117:GLN:NE2	1:B:254:PRO:HG3	2.34	0.42
1:A:602:TYR:CD1	1:B:447:ASN:ND2	2.88	0.42
1:A:182:SER:HB3	1:A:185:GLN:HB2	2.02	0.41
1:B:236:VAL:HG12	1:B:474:GLY:HA2	2.02	0.41
1:B:649:TYR:O	1:B:650:MET:HB2	2.19	0.41
1:A:674:GLN:HB3	1:A:678:PRO:HB3	2.01	0.41
1:B:809:LEU:HD23	1:B:809:LEU:HA	1.91	0.41
1:A:102:GLU:OE2	1:A:223:PRO:HB3	2.21	0.41
1:B:312:PHE:O	1:B:316:ILE:HG12	2.20	0.41
1:A:674:GLN:OE1	1:A:679:LEU:HG	2.20	0.41
1:B:463:VAL:HG11	1:B:561:CYS:O	2.19	0.41
1:B:666:VAL:HG23	1:B:667:PHE:H	1.84	0.41
1:A:236:VAL:HG12	1:A:474:GLY:HA2	2.02	0.41
1:A:470:VAL:HG21	1:A:478:ILE:HG13	2.02	0.41
1:B:764:ASN:OD1	1:B:778:LYS:HD3	2.20	0.41
1:A:750:THR:HG23	1:A:805:SER:OG	2.21	0.41
1:B:102:GLU:OE2	1:B:223:PRO:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:SER:HB3	1:B:185:GLN:HB2	2.02	0.41
1:B:515:VAL:HG21	1:B:545:PHE:HB3	2.03	0.41
1:A:103:VAL:H	1:B:107:GLN:HE21	1.68	0.41
1:B:128:THR:HB	1:B:188:TYR:CE1	2.57	0.40
1:B:789:ASP:OD1	1:B:789:ASP:N	2.46	0.40
1:A:188:TYR:HA	1:A:260:VAL:O	2.22	0.40
1:B:487:HIS:HA	1:B:488:PRO:HD3	1.94	0.40
1:A:515:VAL:HG21	1:A:545:PHE:HB3	2.03	0.40
1:A:206:SER:O	1:A:242:LYS:HB2	2.22	0.40
1:B:460:ILE:O	1:B:461:GLN:C	2.60	0.40
1:B:470:VAL:HG21	1:B:478:ILE:HG13	2.02	0.40
1:A:582:ALA:HA	1:A:721:LEU:HD12	2.04	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 PDB entries followed by that with respect to all EM entries.

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	674/827 (82%)	643 (95%)	31 (5%)	0	100	100
1	B	674/827 (82%)	642 (95%)	32 (5%)	0	100	100
All	All	1348/1654 (82%)	1285 (95%)	63 (5%)	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 PDB entries followed by that with respect to all EM entries.

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	604/732 (82%)	603 (100%)	1 (0%)	92	97
1	B	604/732 (82%)	603 (100%)	1 (0%)	92	97
All	All	1208/1464 (82%)	1206 (100%)	2 (0%)	91	97

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

Mol	Chain	Res	Type
1	A	665	MET
1	B	665	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	113	GLN
1	A	185	GLN
1	A	504	HIS
1	A	541	HIS
1	A	591	GLN
1	A	624	ASN
1	A	646	GLN
1	A	691	ASN
1	A	694	ASN
1	A	763	GLN
1	B	113	GLN
1	B	185	GLN
1	B	504	HIS
1	B	541	HIS
1	B	591	GLN
1	B	624	ASN
1	B	646	GLN
1	B	691	ASN
1	B	694	ASN
1	B	763	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\# Z > 2$
3	POV	B	902	-	51,51,51	0.92	2 (3%)	57,59,59	2.26	11 (19%)
3	POV	A	902	-	51,51,51	0.96	2 (3%)	57,59,59	2.23	9 (15%)

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	POV	B	902	-	-	31/55/55/55	-
3	POV	A	902	-	-	31/55/55/55	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	902	POV	O31-C31	4.64	1.46	1.33
3	B	902	POV	O21-C21	3.50	1.44	1.34
3	A	902	POV	O21-C21	3.29	1.43	1.34
3	B	902	POV	O31-C31	3.23	1.42	1.33

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	902	POV	C15-N-C14	-10.16	82.86	108.97
3	B	902	POV	C15-N-C14	-9.92	83.47	108.97
3	B	902	POV	C15-N-C13	-7.36	90.04	108.97
3	A	902	POV	C15-N-C12	-6.66	82.66	109.92
3	A	902	POV	C15-N-C13	-5.49	94.85	108.97
3	B	902	POV	C15-N-C12	-5.02	89.38	109.92
3	A	902	POV	C14-N-C13	4.78	121.26	108.97
3	B	902	POV	O21-C21-C22	4.02	120.17	111.50
3	A	902	POV	O21-C21-C22	3.90	119.92	111.50
3	B	902	POV	C14-N-C12	3.84	125.61	109.92
3	B	902	POV	C14-N-C13	3.49	117.96	108.97
3	B	902	POV	O31-C3-C2	-3.09	99.43	108.43
3	B	902	POV	C2-O21-C21	-2.93	110.58	117.79
3	A	902	POV	C14-N-C12	2.82	121.44	109.92
3	A	902	POV	O31-C31-C32	2.81	120.71	111.91
3	A	902	POV	C2-O21-C21	-2.78	110.96	117.79
3	B	902	POV	O31-C31-C32	2.70	120.39	111.91
3	A	902	POV	C3-C2-C1	-2.45	105.99	111.79
3	B	902	POV	C3-C2-C1	-2.39	106.13	111.79
3	B	902	POV	C11-C12-N	-2.27	108.18	115.78

There are no chirality outliers.

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	902	POV	C11-O12-P-O11
3	B	902	POV	C11-O12-P-O14
3	B	902	POV	O12-C11-C12-N
3	B	902	POV	C11-C12-N-C15
3	B	902	POV	C11-C12-N-C14
3	A	902	POV	C11-C12-N-C14
3	B	902	POV	C211-C212-C213-C214
3	B	902	POV	C35-C36-C37-C38
3	A	902	POV	C39-C310-C311-C312
3	B	902	POV	C32-C33-C34-C35
3	A	902	POV	C311-C312-C313-C314
3	B	902	POV	C212-C213-C214-C215
3	A	902	POV	C312-C313-C314-C315
3	A	902	POV	C35-C36-C37-C38
3	A	902	POV	C36-C37-C38-C39
3	A	902	POV	C32-C33-C34-C35
3	A	902	POV	C37-C38-C39-C310
3	B	902	POV	C39-C310-C311-C312

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Mol	Chain	Res	Type	Atoms
3	B	902	POV	C37-C38-C39-C310
3	A	902	POV	C31-C32-C33-C34
3	A	902	POV	C34-C35-C36-C37
3	A	902	POV	C214-C215-C216-C217
3	A	902	POV	C22-C21-O21-C2
3	A	902	POV	O22-C21-O21-C2
3	A	902	POV	C210-C211-C212-C213
3	B	902	POV	C26-C27-C28-C29
3	A	902	POV	C310-C311-C312-C313
3	A	902	POV	C1-C2-C3-O31
3	B	902	POV	C25-C26-C27-C28
3	A	902	POV	C26-C27-C28-C29
3	A	902	POV	C313-C314-C315-C316
3	A	902	POV	C211-C212-C213-C214
3	B	902	POV	C313-C314-C315-C316
3	B	902	POV	C1-C2-C3-O31
3	B	902	POV	C34-C35-C36-C37
3	A	902	POV	C24-C25-C26-C27
3	A	902	POV	O11-C1-C2-C3
3	A	902	POV	C311-C310-C39-C38
3	B	902	POV	C11-O12-P-O11
3	A	902	POV	C11-O12-P-O14
3	A	902	POV	O11-C1-C2-O21
3	A	902	POV	O21-C2-C3-O31
3	B	902	POV	O21-C2-C3-O31
3	B	902	POV	C310-C311-C312-C313
3	A	902	POV	C1-C2-O21-C21
3	B	902	POV	C27-C28-C29-C210
3	B	902	POV	C312-C313-C314-C315
3	B	902	POV	C215-C216-C217-C218
3	B	902	POV	O11-C1-C2-C3
3	A	902	POV	C22-C23-C24-C25
3	B	902	POV	O11-C1-C2-O21
3	A	902	POV	O31-C31-C32-C33
3	A	902	POV	C33-C34-C35-C36
3	B	902	POV	C210-C211-C212-C213
3	B	902	POV	C22-C23-C24-C25
3	B	902	POV	C29-C210-C211-C212
3	B	902	POV	O31-C31-C32-C33
3	B	902	POV	O22-C21-O21-C2
3	B	902	POV	C36-C37-C38-C39
3	A	902	POV	C3-C2-O21-C21

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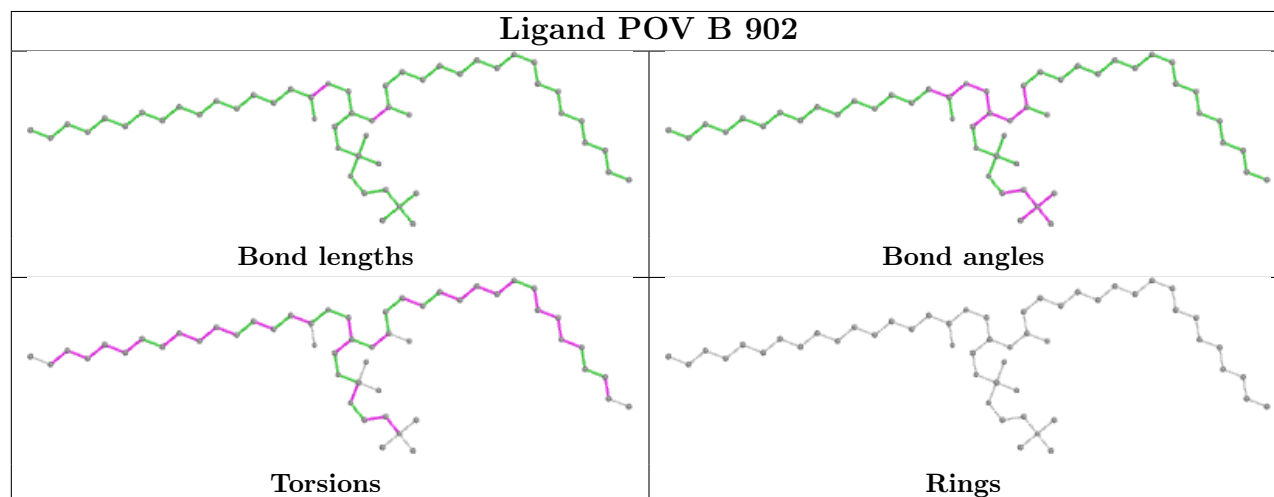
Mol	Chain	Res	Type	Atoms
3	B	902	POV	C24-C25-C26-C27
3	B	902	POV	C311-C312-C313-C314

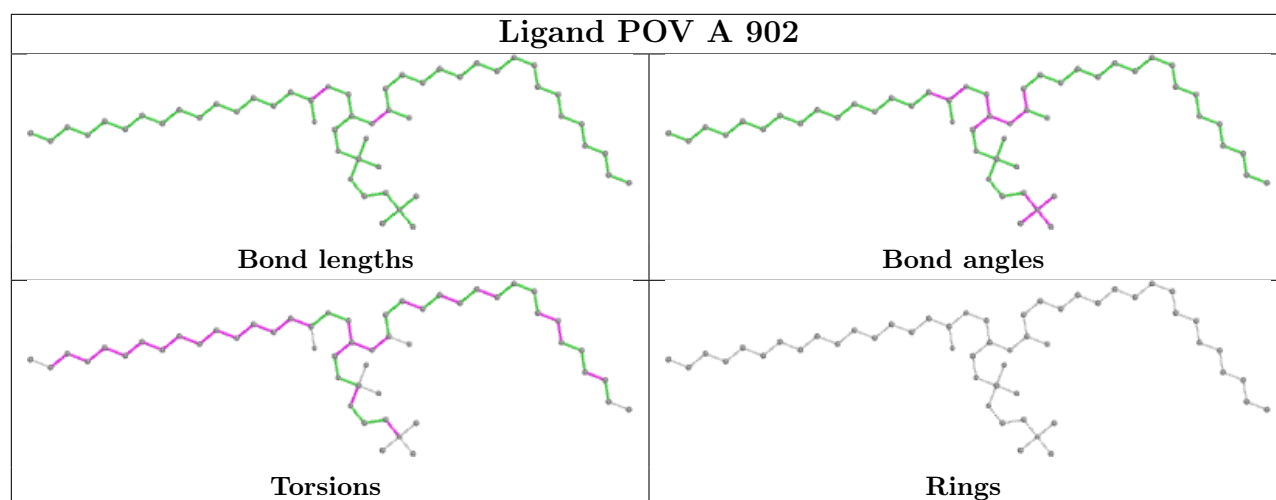
There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	902	POV	5	0
3	A	902	POV	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.