



## Full wwPDB EM Validation Report ⓘ

Jul 15, 2025 – 08:46 PM JST

PDB ID : 8ZYU / pdb\_00008zyu  
EMDB ID : EMD-60579  
Title : Cryo-EM structure of neurotensin receptor 1 in complex with beta-arrestin1 and SBI-553 (complex 1)  
Authors : Sun, D.; Li, X.; Yuan, Q.; Yin, W.; Xu, H.E.; Tian, C.  
Deposited on : 2024-06-18  
Resolution : 2.65 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](mailto: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>.

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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 : 4-5-2 with Phenix2.0rc1  
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) : 2.44

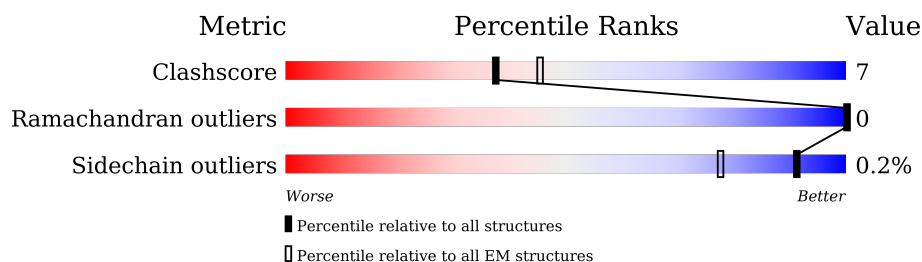
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.65 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  $\geq 3$ , 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	B	402	
2	D	260	
3	L	6	
4	Q	235	
5	R	557	

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8447 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 Beta-arrestin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	362	Total	C	N	O	S	0	0
			2734	1749	475	501	9		

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	MET	-	initiating methionine	UNP P49407
B	-19	GLY	-	expression tag	UNP P49407
B	-18	SER	-	expression tag	UNP P49407
B	-17	HIS	-	expression tag	UNP P49407
B	-16	HIS	-	expression tag	UNP P49407
B	-15	HIS	-	expression tag	UNP P49407
B	-14	HIS	-	expression tag	UNP P49407
B	-13	HIS	-	expression tag	UNP P49407
B	-12	HIS	-	expression tag	UNP P49407
B	-11	HIS	-	expression tag	UNP P49407
B	-10	HIS	-	expression tag	UNP P49407
B	-9	GLY	-	expression tag	UNP P49407
B	-8	SER	-	expression tag	UNP P49407
B	-7	LEU	-	expression tag	UNP P49407
B	-6	GLU	-	expression tag	UNP P49407
B	-5	VAL	-	expression tag	UNP P49407
B	-4	LEU	-	expression tag	UNP P49407
B	-3	PHE	-	expression tag	UNP P49407
B	-2	GLN	-	expression tag	UNP P49407
B	-1	GLY	-	expression tag	UNP P49407
B	0	PRO	-	expression tag	UNP P49407

- Molecule 2 is a protein called Fab30 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	221	Total	C	N	O	S	0	0
			1639	1038	276	320	5		

- Molecule 3 is a protein called neurotensin peptide 8-13.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	L	6	Total	C	N	O	0	0
			57	38	12	7		

- Molecule 4 is a protein called Fab30 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Q	216	Total	C	N	O	S	0	0
			1535	959	258	312	6		

- Molecule 5 is a protein called Soluble cytochrome b562,Neurotensin receptor type 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	R	313	Total	C	N	O	P	S	0	0
			2409	1574	399	416	4	16		

There are 37 discrepancies between the modelled and reference sequences:

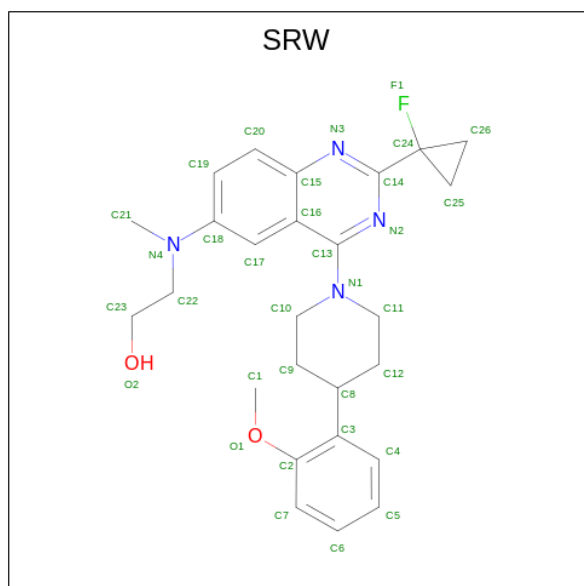
Chain	Residue	Modelled	Actual	Comment	Reference
R	-135	MET	-	initiating methionine	UNP P0ABE7
R	-134	LYS	-	expression tag	UNP P0ABE7
R	-133	THR	-	expression tag	UNP P0ABE7
R	-132	ILE	-	expression tag	UNP P0ABE7
R	-131	ILE	-	expression tag	UNP P0ABE7
R	-130	ALA	-	expression tag	UNP P0ABE7
R	-129	LEU	-	expression tag	UNP P0ABE7
R	-128	SER	-	expression tag	UNP P0ABE7
R	-127	TYR	-	expression tag	UNP P0ABE7
R	-126	ILE	-	expression tag	UNP P0ABE7
R	-125	PHE	-	expression tag	UNP P0ABE7
R	-124	CYS	-	expression tag	UNP P0ABE7
R	-123	LEU	-	expression tag	UNP P0ABE7
R	-122	VAL	-	expression tag	UNP P0ABE7
R	-121	PHE	-	expression tag	UNP P0ABE7
R	-120	ALA	-	expression tag	UNP P0ABE7
R	-119	GLY	-	expression tag	UNP P0ABE7
R	-118	SER	-	expression tag	UNP P0ABE7
R	-111	TRP	MET	conflict	UNP P0ABE7
R	-16	ILE	HIS	conflict	UNP P0ABE7
R	-12	LEU	-	linker	UNP P0ABE7
R	-11	ALA	-	linker	UNP P0ABE7
R	-10	SER	-	linker	UNP P0ABE7

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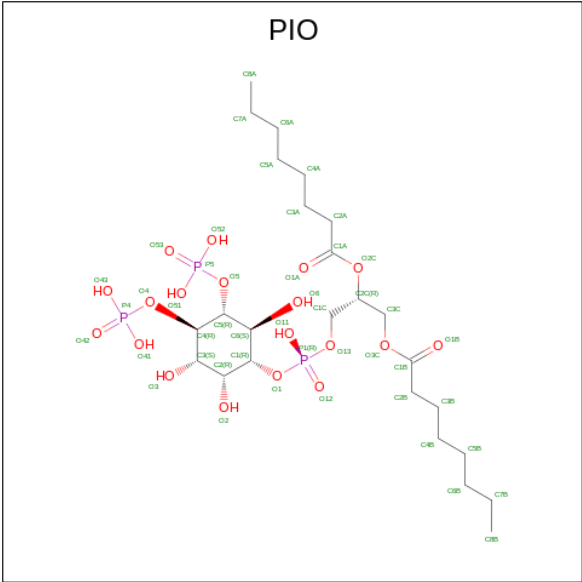
Chain	Residue	Modelled	Actual	Comment	Reference
R	-9	GLY	-	linker	UNP P0ABE7
R	-8	SER	-	linker	UNP P0ABE7
R	-7	LEU	-	linker	UNP P0ABE7
R	-6	GLU	-	linker	UNP P0ABE7
R	-5	VAL	-	linker	UNP P0ABE7
R	-4	LEU	-	linker	UNP P0ABE7
R	-3	PHE	-	linker	UNP P0ABE7
R	-2	GLN	-	linker	UNP P0ABE7
R	-1	GLY	-	linker	UNP P0ABE7
R	0	PRO	-	linker	UNP P0ABE7
R	382L	CYS	-	insertion	UNP P30989
R	382M	PHE	-	insertion	UNP P30989
R	382N	ASN	-	insertion	UNP P30989
R	382T	CYS	ALA	conflict	UNP P30989

- Molecule 6 is 2-[[2-(1-fluorocyclopropyl)-4-[4-(2-methoxyphenyl)piperidin-1-yl]quinazolin-6-yl](methyl)amino]ethan-1-ol (CCD ID: SRW) (formula: C<sub>26</sub>H<sub>31</sub>FN<sub>4</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
6	R	1	Total	C	F	N	O	0
			33	26	1	4	2	

- Molecule 7 is [(2R)-2-octanoyloxy-3-[oxidanyl-[(1R,2R,3S,4R,5R,6S)-2,3,6-tris(oxidanyl)-4,5-diphosphonooxy-cyclohexyl]oxy-phosphoryl]oxy-propyl] octanoate (CCD ID: PIO) (formula: C<sub>25</sub>H<sub>49</sub>O<sub>19</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
7	R	1	40	18	19	3	0







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	359739	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (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: PIO, SEP, SRW, TPO

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	B	0.11	0/2796	0.29	0/3810
2	D	0.11	0/1681	0.29	0/2293
3	L	0.17	0/58	0.42	0/77
4	Q	0.12	0/1569	0.31	0/2145
5	R	0.18	0/2425	0.38	1/3311 (0.0%)
All	All	0.14	0/8529	0.32	1/11636 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	R	167	TYR	CB-CA-C	5.70	119.83	110.88

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	B	2734	0	2700	45	0
2	D	1639	0	1583	22	0
3	L	57	0	63	3	0
4	Q	1535	0	1392	21	0
5	R	2409	0	2369	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	R	33	0	0	0	0
7	R	40	0	24	2	0
All	All	8447	0	8131	121	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 (121) 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)
5:R:355:VAL:O	5:R:359:ILE:HG12	1.64	0.96
5:R:318:PRO:HA	5:R:321:VAL:HG12	1.63	0.78
5:R:351:ALA:O	5:R:355:VAL:HG23	1.85	0.76
2:D:28:VAL:HA	2:D:135:GLN:HE22	1.52	0.73
1:B:151:GLU:OE1	1:B:151:GLU:N	2.23	0.72
4:Q:157:LEU:HB2	4:Q:196:LEU:HB3	1.72	0.69
1:B:251:PRO:O	1:B:283:LYS:NZ	2.25	0.69
5:R:165:GLU:HG2	5:R:180:MET:HE1	1.74	0.68
4:Q:60:LYS:NZ	4:Q:102:GLU:O	2.28	0.67
2:D:123:ARG:HB2	2:D:127:TYR:HB3	1.77	0.66
3:L:9:ARG:HG3	3:L:10:PRO:HD2	1.77	0.66
2:D:146:THR:HG23	2:D:177:PRO:HG3	1.77	0.66
1:B:109:GLU:OE1	1:B:109:GLU:N	2.21	0.66
5:R:318:PRO:HA	5:R:321:VAL:CG1	2.26	0.65
5:R:159:VAL:HG11	5:R:312:PHE:CE2	2.32	0.64
1:B:203:ASP:OD1	1:B:207:TYR:OH	2.11	0.64
1:B:239:ASP:HB2	1:B:317:ILE:HB	1.81	0.61
1:B:84:GLN:NE2	1:B:87:PRO:O	2.31	0.60
4:Q:50:VAL:HA	4:Q:113:LYS:HD2	1.85	0.58
5:R:167:TYR:HB2	5:R:259:ILE:HD11	1.85	0.58
1:B:106:LYS:HD2	5:R:412:ALA:HA	1.85	0.57
2:D:180:VAL:HG23	2:D:230:HIS:HA	1.86	0.57
5:R:118:LEU:HD13	5:R:147:LEU:HD13	1.86	0.57
2:D:180:VAL:HG23	2:D:230:HIS:CA	2.35	0.57
1:B:291:LYS:NZ	1:B:297:THR:OG1	2.35	0.57
4:Q:69:ILE:HG22	4:Q:75:LEU:HD12	1.87	0.57
5:R:318:PRO:CA	5:R:321:VAL:HG12	2.35	0.57
4:Q:154:VAL:HG12	4:Q:199:THR:HA	1.86	0.57
4:Q:134:PRO:HB3	4:Q:160:PHE:HB3	1.86	0.56
1:B:227:VAL:HG22	1:B:328:VAL:HG22	1.87	0.56
2:D:34:LEU:HD11	2:D:176:PHE:HE2	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:355:VAL:CG1	5:R:359:ILE:HD11	2.37	0.55
4:Q:27:GLN:O	4:Q:121:GLN:NE2	2.40	0.54
1:B:224:ASN:HA	1:B:263:PRO:HB3	1.89	0.53
2:D:35:VAL:HG11	2:D:109:LEU:HD12	1.90	0.53
1:B:250:CYS:HB2	5:R:94:LEU:HG	1.89	0.53
5:R:284:SER:HA	5:R:297:ALA:HB1	1.90	0.53
1:B:146:LYS:HE3	1:B:164:ARG:HH11	1.73	0.53
2:D:156:PRO:HG2	2:D:243:PRO:HB3	1.91	0.52
1:B:289:ASP:OD2	1:B:298:ASN:ND2	2.38	0.52
4:Q:112:TYR:HA	4:Q:117:VAL:HG12	1.91	0.52
5:R:252:ILE:HG22	5:R:309:VAL:HG22	1.92	0.52
5:R:322:ARG:HD3	5:R:349:THR:HG21	1.92	0.52
1:B:189:PHE:HB2	1:B:192:SER:HB2	1.92	0.51
3:L:10:PRO:HB3	5:R:342:TYR:CD1	2.45	0.51
5:R:233:VAL:HA	5:R:236:VAL:HG12	1.92	0.51
5:R:84:THR:HG23	5:R:371:PHE:HZ	1.76	0.51
1:B:43:ASP:HB3	1:B:46:TYR:HB3	1.92	0.50
5:R:126:ASN:HA	5:R:131:HIS:HB2	1.94	0.50
2:D:96:ASP:HB2	2:D:103:TYR:HE2	1.77	0.49
1:B:234:VAL:HG22	1:B:322:VAL:HG22	1.94	0.49
1:B:37:ASP:HB3	1:B:115:THR:HG23	1.94	0.49
5:R:325:MET:HE3	5:R:342:TYR:HD2	1.76	0.49
1:B:228:LYS:NZ	1:B:339:SER:OG	2.45	0.48
5:R:148:ARG:O	5:R:152:THR:HG23	2.13	0.48
2:D:198:ALA:HB1	2:D:206:TYR:HB3	1.94	0.48
2:D:55:SER:OG	2:D:121:ARG:NH1	2.47	0.48
5:R:189:ILE:O	5:R:192:ILE:HG12	2.14	0.48
1:B:253:ALA:HB1	1:B:273:LEU:HD22	1.96	0.48
5:R:290:ILE:HD12	5:R:291:GLU:HG3	1.96	0.47
1:B:146:LYS:HE3	1:B:164:ARG:NH1	2.29	0.47
1:B:203:ASP:OD1	1:B:203:ASP:N	2.48	0.47
4:Q:58:GLN:HB2	4:Q:68:LEU:HD11	1.97	0.47
4:Q:56:TRP:HD1	4:Q:69:ILE:HD11	1.81	0.46
5:R:245:PHE:O	5:R:249:MET:HB2	2.16	0.46
1:B:284:ARG:NH1	5:R:291:GLU:OE2	2.46	0.46
2:D:127:TYR:OH	4:Q:67:LEU:HD21	2.16	0.46
4:Q:56:TRP:HB2	4:Q:69:ILE:HG13	1.98	0.46
5:R:103:TYR:OH	7:R:501:PIO:O12	2.29	0.45
1:B:159:LYS:HE3	1:B:159:LYS:HB3	1.76	0.45
1:B:243:PHE:HD2	5:R:295:VAL:HG11	1.82	0.45
1:B:198:LEU:HD13	1:B:326:LEU:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:42:ILE:HG12	4:Q:123:THR:HG21	1.98	0.45
5:R:155:THR:O	5:R:159:VAL:HG23	2.16	0.45
1:B:97:THR:O	1:B:101:GLU:HG2	2.16	0.45
2:D:128:SER:HB2	4:Q:112:TYR:CD1	2.51	0.45
1:B:219:VAL:HB	1:B:267:PHE:HB3	1.99	0.44
1:B:362:ARG:NH2	4:Q:52:SER:H	2.16	0.44
5:R:71:LEU:O	5:R:75:VAL:HG13	2.17	0.44
2:D:182:VAL:HG22	2:D:228:VAL:HG22	1.99	0.44
5:R:318:PRO:C	5:R:321:VAL:HG12	2.42	0.44
5:R:355:VAL:HG12	5:R:359:ILE:HD11	2.00	0.44
5:R:167:TYR:O	5:R:168:LEU:C	2.58	0.44
2:D:90:ARG:HB3	2:D:107:ASN:O	2.18	0.43
2:D:95:ALA:HA	2:D:102:ALA:HA	1.99	0.43
5:R:318:PRO:O	5:R:321:VAL:HG12	2.18	0.43
4:Q:217:VAL:HG12	4:Q:219:HIS:H	1.83	0.43
4:Q:101:PRO:HA	4:Q:104:PHE:CE2	2.53	0.43
4:Q:159:ASN:HB3	4:Q:193:THR:HG21	2.00	0.43
1:B:24:ARG:NH1	5:R:407:TPO:O1P	2.48	0.43
3:L:11:TYR:HE1	5:R:223:VAL:HG13	1.83	0.43
1:B:9:LYS:HE3	5:R:408:LEU:HD12	1.99	0.43
1:B:249:LYS:HB2	5:R:97:LEU:HD11	2.01	0.42
2:D:27:LEU:HD11	2:D:132:TYR:HB3	2.00	0.42
5:R:212:ARG:NH2	5:R:225:THR:HG21	2.35	0.42
1:B:65:GLU:HG3	5:R:290:ILE:HD11	2.00	0.42
1:B:96:LEU:HD21	1:B:113:PRO:HG3	1.99	0.42
1:B:165:LEU:HD12	1:B:165:LEU:HA	1.87	0.42
2:D:166:ALA:N	2:D:214:VAL:O	2.53	0.42
2:D:173:LYS:NZ	2:D:201:GLN:OE1	2.51	0.42
5:R:74:PHE:O	5:R:78:THR:OG1	2.35	0.42
1:B:362:ARG:O	4:Q:113:LYS:HA	2.19	0.42
1:B:235:ARG:NH1	1:B:249:LYS:HD2	2.34	0.42
4:Q:196:LEU:HD13	4:Q:197:SER:N	2.35	0.42
1:B:323:LYS:NZ	7:R:501:PIO:O53	2.49	0.42
4:Q:163:ARG:O	4:Q:163:ARG:NH1	2.45	0.42
1:B:101:GLU:HG2	1:B:101:GLU:H	1.67	0.41
1:B:194:LYS:HD3	1:B:194:LYS:HA	1.95	0.41
5:R:201:VAL:HG23	5:R:202:PRO:HD3	2.02	0.41
1:B:28:ASP:O	1:B:171:GLN:HG2	2.21	0.41
5:R:115:THR:OG1	5:R:151:CYS:HB3	2.20	0.41
1:B:55:THR:OG1	1:B:82:ASN:OD1	2.28	0.41
1:B:21:LEU:HD12	1:B:165:LEU:HD23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:41:LEU:HD23	2:D:41:LEU:HA	1.96	0.40
2:D:135:GLN:CD	2:D:135:GLN:H	2.29	0.40
5:R:260:ALA:HA	5:R:302:VAL:HG12	2.02	0.40
2:D:29:GLU:HG2	2:D:119:CYS:SG	2.61	0.40
1:B:98:ARG:O	1:B:102:ARG:HG3	2.22	0.40
1:B:251:PRO:HB2	1:B:254:MET:HE2	2.04	0.40
5:R:370:ASN:O	5:R:374:ILE:HG13	2.21	0.40
1:B:42:VAL:HG21	1:B:86:PHE:CD1	2.57	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	B	360/402 (90%)	345 (96%)	15 (4%)	0	100	100
2	D	219/260 (84%)	209 (95%)	10 (5%)	0	100	100
3	L	4/6 (67%)	3 (75%)	1 (25%)	0	100	100
4	Q	214/235 (91%)	202 (94%)	12 (6%)	0	100	100
5	R	302/557 (54%)	294 (97%)	8 (3%)	0	100	100
All	All	1099/1460 (75%)	1053 (96%)	46 (4%)	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	B	288/357 (81%)	288 (100%)	0	100	100
2	D	178/213 (84%)	178 (100%)	0	100	100
3	L	6/6 (100%)	6 (100%)	0	100	100
4	Q	159/203 (78%)	158 (99%)	1 (1%)	84	92
5	R	245/459 (53%)	244 (100%)	1 (0%)	89	95
All	All	876/1238 (71%)	874 (100%)	2 (0%)	91	97

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

Mol	Chain	Res	Type
4	Q	161	TYR
5	R	167	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	29	HIS
1	B	216	ASN
2	D	51	ASN
2	D	135	GLN
5	R	104	HIS
5	R	131	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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
5	SEP	R	409	5	8,9,10	1.53	1 (12%)	8,12,14	1.63	2 (25%)
5	SEP	R	410	5	8,9,10	1.54	1 (12%)	8,12,14	1.83	2 (25%)
5	SEP	R	404	5	8,9,10	1.55	1 (12%)	8,12,14	1.67	2 (25%)
5	TPO	R	407	5	8,10,11	1.06	0	10,14,16	1.88	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
5	SEP	R	409	5	-	0/5/8/10	-
5	SEP	R	410	5	-	3/5/8/10	-
5	SEP	R	404	5	-	4/5/8/10	-
5	TPO	R	407	5	-	0/9/11/13	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	R	404	SEP	P-O1P	3.38	1.61	1.50
5	R	410	SEP	P-O1P	3.37	1.61	1.50
5	R	409	SEP	P-O1P	3.35	1.61	1.50

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	R	407	TPO	P-OG1-CB	-5.30	107.19	123.21
5	R	410	SEP	OG-CB-CA	3.40	111.46	108.14
5	R	410	SEP	P-OG-CB	-3.39	108.95	118.30
5	R	409	SEP	OG-CB-CA	3.05	111.11	108.14
5	R	404	SEP	OG-CB-CA	3.04	111.11	108.14
5	R	404	SEP	P-OG-CB	-3.03	109.94	118.30
5	R	409	SEP	P-OG-CB	-2.85	110.45	118.30

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	R	410	SEP	CB-OG-P-O1P
5	R	410	SEP	CB-OG-P-O3P

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Mol	Chain	Res	Type	Atoms
5	R	404	SEP	CB-OG-P-O3P
5	R	404	SEP	N-CA-CB-OG
5	R	404	SEP	CB-OG-P-O1P
5	R	404	SEP	CB-OG-P-O2P
5	R	410	SEP	CB-OG-P-O2P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	R	407	TPO	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

2 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
7	PIO	R	501	-	40,40,47	1.64	9 (22%)	54,58,65	1.01	4 (7%)
6	SRW	R	500	-	37,37,37	2.57	12 (32%)	48,54,54	1.82	9 (18%)

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
7	PIO	R	501	-	-	16/37/61/68	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	SRW	R	500	-	-	5/17/37/37	1/5/5/5

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	R	500	SRW	C3-C8	6.64	1.63	1.52
6	R	500	SRW	C10-N1	5.97	1.56	1.46
6	R	500	SRW	C11-N1	5.32	1.55	1.46
6	R	500	SRW	O2-C23	-4.41	1.19	1.42
6	R	500	SRW	C13-N1	4.19	1.49	1.37
6	R	500	SRW	C26-C24	4.10	1.53	1.47
6	R	500	SRW	C25-C24	4.03	1.53	1.47
7	R	501	PIO	P5-O5	3.62	1.66	1.59
7	R	501	PIO	P1-O1	3.41	1.69	1.60
7	R	501	PIO	P4-O4	3.35	1.65	1.59
7	R	501	PIO	O2C-C1A	3.32	1.43	1.34
6	R	500	SRW	F1-C24	-3.26	1.37	1.42
6	R	500	SRW	C18-N4	3.16	1.48	1.39
7	R	501	PIO	O3C-C1B	3.16	1.42	1.33
6	R	500	SRW	O1-C2	3.15	1.42	1.37
6	R	500	SRW	C16-C15	-2.63	1.38	1.42
6	R	500	SRW	C9-C8	-2.39	1.46	1.53
7	R	501	PIO	P1-O13	2.34	1.68	1.59
7	R	501	PIO	O1-C1	-2.29	1.35	1.44
7	R	501	PIO	C2A-C1A	2.20	1.57	1.50
7	R	501	PIO	C6-C1	2.18	1.58	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	R	500	SRW	O1-C2-C3	5.76	121.34	115.83
6	R	500	SRW	N3-C14-N2	-5.52	121.41	129.29
6	R	500	SRW	C14-N3-C15	4.18	120.21	115.59
7	R	501	PIO	O2C-C1A-C2A	4.09	120.32	111.50
6	R	500	SRW	O1-C2-C7	-3.19	118.90	124.37
6	R	500	SRW	C14-N2-C13	2.61	122.05	114.53
7	R	501	PIO	O3C-C1B-C2B	2.60	120.08	111.91
7	R	501	PIO	C5-C6-C1	2.45	114.05	108.96
6	R	500	SRW	C1-O1-C2	-2.38	113.93	117.53
6	R	500	SRW	C24-C14-N3	2.33	119.68	115.32
6	R	500	SRW	C16-C15-N3	-2.32	120.34	122.81
6	R	500	SRW	O2-C23-C22	2.15	120.11	111.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	R	501	PIO	C6-C1-C2	-2.03	107.92	110.85

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	R	501	PIO	C1C-O13-P1-O11
7	R	501	PIO	C1C-O13-P1-O12
7	R	501	PIO	O1A-C1A-O2C-C2C
7	R	501	PIO	C2A-C1A-O2C-C2C
7	R	501	PIO	O1B-C1B-O3C-C3C
7	R	501	PIO	C2B-C1B-O3C-C3C
7	R	501	PIO	C1C-O13-P1-O1
6	R	500	SRW	C4-C3-C8-C9
6	R	500	SRW	C7-C2-O1-C1
7	R	501	PIO	O13-C1C-C2C-O2C
7	R	501	PIO	C2A-C3A-C4A-C5A
6	R	500	SRW	C3-C2-O1-C1
6	R	500	SRW	C2-C3-C8-C9
7	R	501	PIO	C1-O1-P1-O12
7	R	501	PIO	O13-C1C-C2C-C3C
6	R	500	SRW	C4-C3-C8-C12
7	R	501	PIO	C1-O1-P1-O13
7	R	501	PIO	C2C-C1C-O13-P1
7	R	501	PIO	C1-O1-P1-O11
7	R	501	PIO	C1A-C2A-C3A-C4A
7	R	501	PIO	C3C-C2C-O2C-C1A

All (1) ring outliers are listed below:

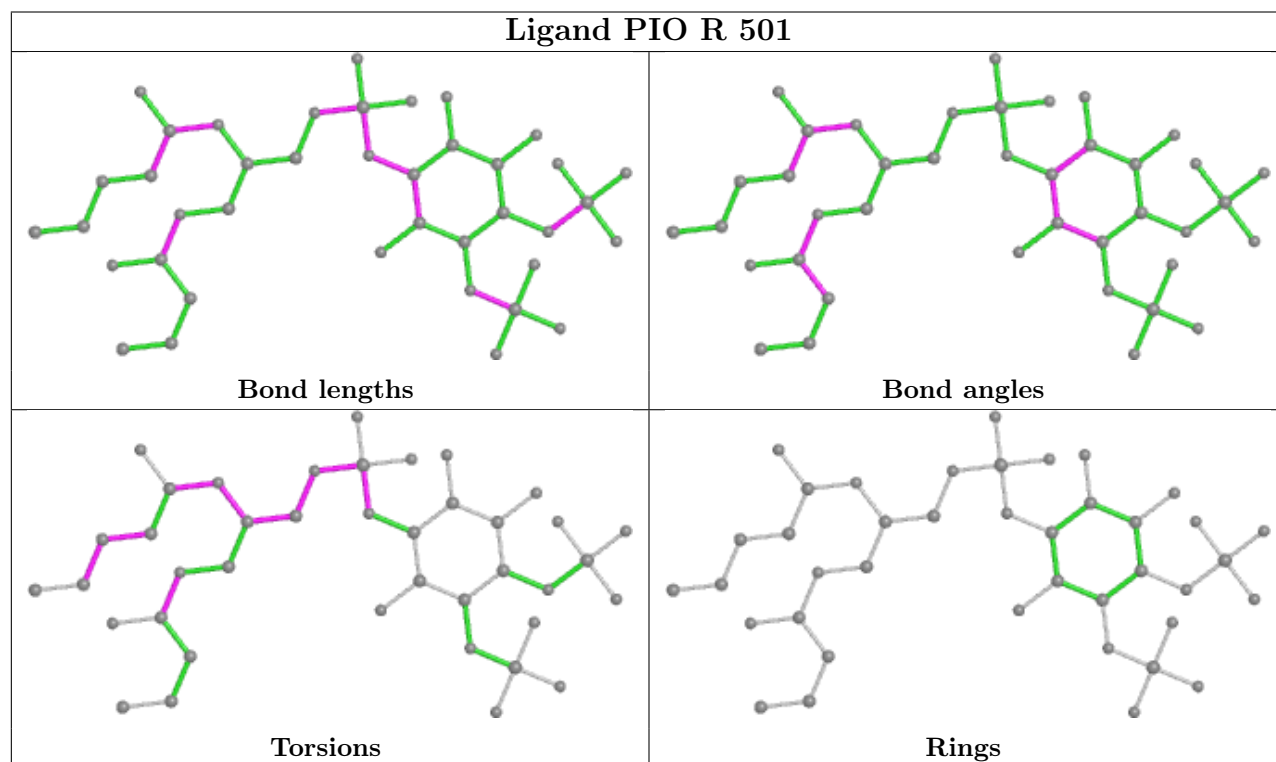
Mol	Chain	Res	Type	Atoms
6	R	500	SRW	C10-C11-C12-C8-C9-N1

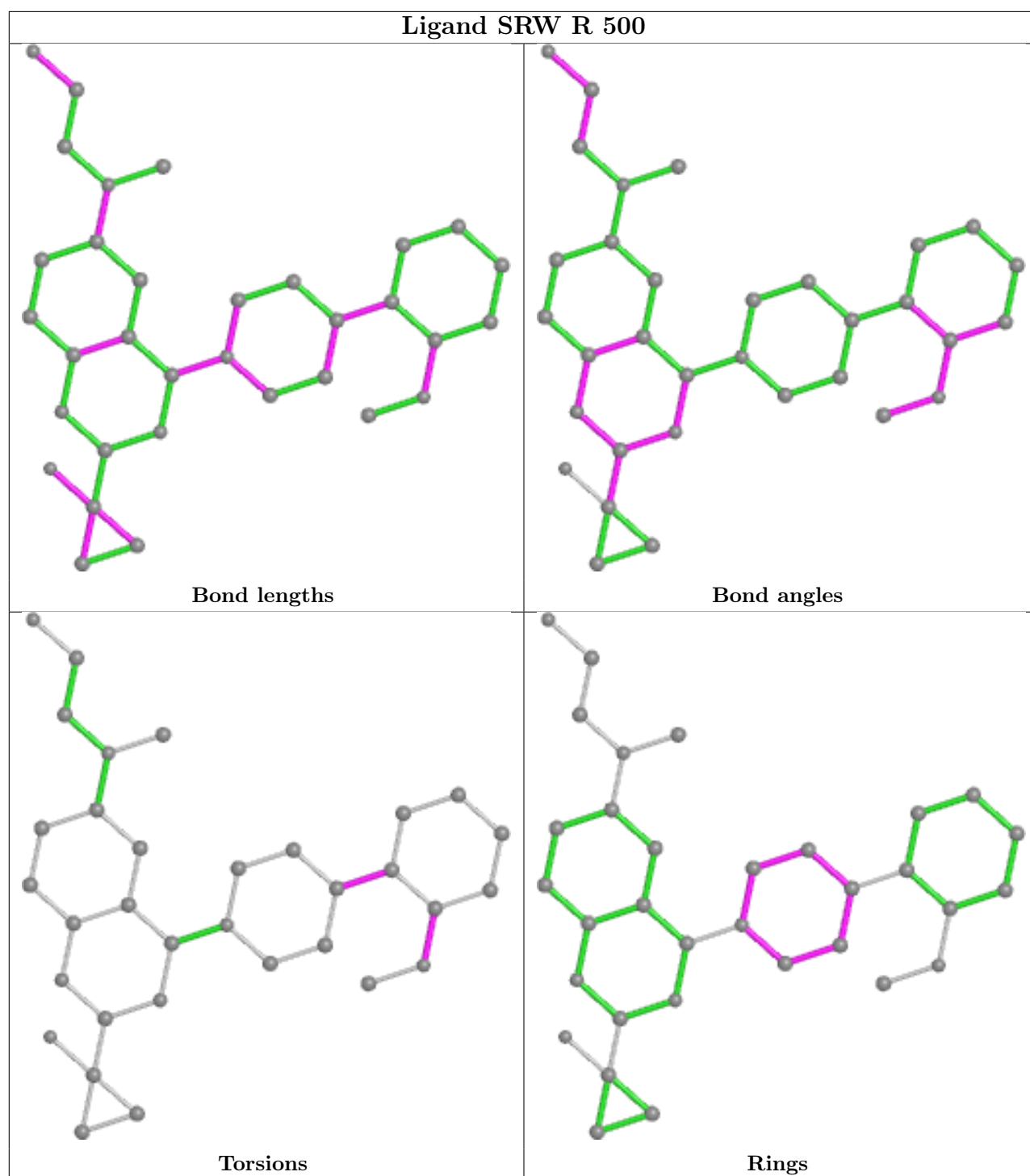
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	R	501	PIO	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.