



Full wwPDB EM Validation Report ⓘ

Jul 8, 2025 – 03:33 PM JST

PDB ID : 9J53 / pdb_00009j53
EMDB ID : EMD-61141
Title : CryoEM structure of human XPR1 in complex with phosphate in state C
Authors : Zhang, W.H.; Chen, Y.K.; Guan, Z.Y.; Liu, Z.
Deposited on : 2024-08-11
Resolution : 3.30 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 : 4-5-2 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

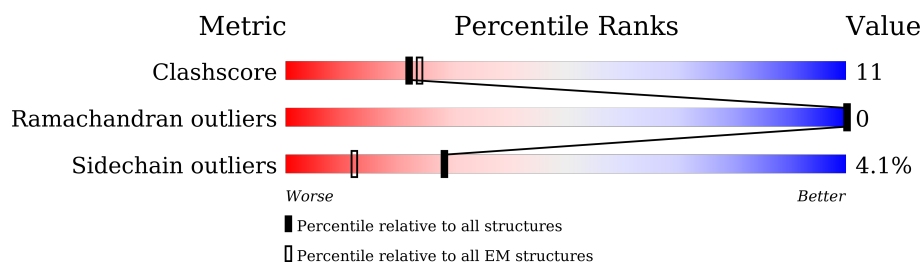
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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	720	
1	B	720	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6598 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 Solute carrier family 53 member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	382	Total	C	N	O	S	0	0
			3186	2143	510	518	15		
1	A	382	Total	C	N	O	S	0	0
			3186	2143	510	518	15		

There are 48 discrepancies between the modelled and reference sequences:

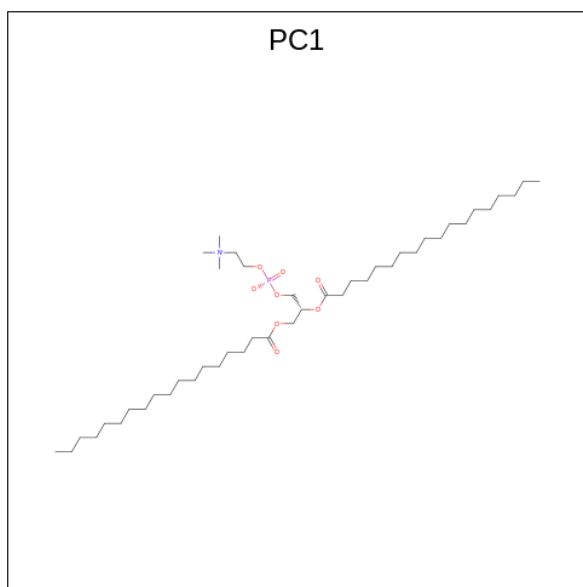
Chain	Residue	Modelled	Actual	Comment	Reference
B	697	LEU	-	expression tag	UNP Q9UBH6
B	698	GLU	-	expression tag	UNP Q9UBH6
B	699	ASP	-	expression tag	UNP Q9UBH6
B	700	TYR	-	expression tag	UNP Q9UBH6
B	701	LYS	-	expression tag	UNP Q9UBH6
B	702	ASP	-	expression tag	UNP Q9UBH6
B	703	HIS	-	expression tag	UNP Q9UBH6
B	704	ASP	-	expression tag	UNP Q9UBH6
B	705	GLY	-	expression tag	UNP Q9UBH6
B	706	ASP	-	expression tag	UNP Q9UBH6
B	707	TYR	-	expression tag	UNP Q9UBH6
B	708	LYS	-	expression tag	UNP Q9UBH6
B	709	ASP	-	expression tag	UNP Q9UBH6
B	710	HIS	-	expression tag	UNP Q9UBH6
B	711	ASP	-	expression tag	UNP Q9UBH6
B	712	ILE	-	expression tag	UNP Q9UBH6
B	713	ASP	-	expression tag	UNP Q9UBH6
B	714	TYR	-	expression tag	UNP Q9UBH6
B	715	LYS	-	expression tag	UNP Q9UBH6
B	716	ASP	-	expression tag	UNP Q9UBH6
B	717	ASP	-	expression tag	UNP Q9UBH6
B	718	ASP	-	expression tag	UNP Q9UBH6
B	719	ASP	-	expression tag	UNP Q9UBH6
B	720	LYS	-	expression tag	UNP Q9UBH6
A	697	LEU	-	expression tag	UNP Q9UBH6
A	698	GLU	-	expression tag	UNP Q9UBH6

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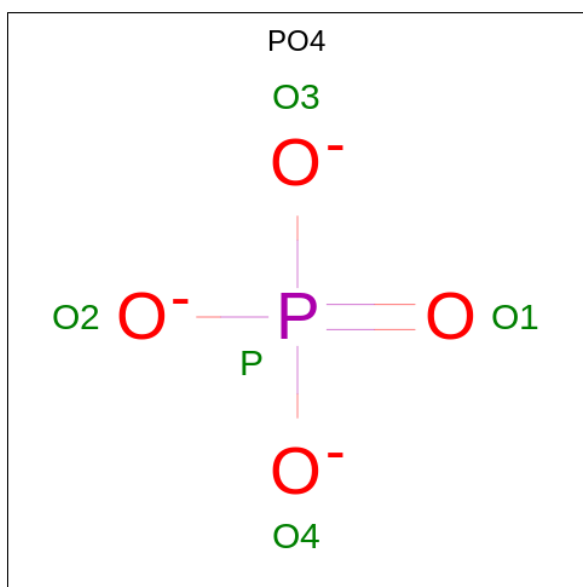
Chain	Residue	Modelled	Actual	Comment	Reference
A	699	ASP	-	expression tag	UNP Q9UBH6
A	700	TYR	-	expression tag	UNP Q9UBH6
A	701	LYS	-	expression tag	UNP Q9UBH6
A	702	ASP	-	expression tag	UNP Q9UBH6
A	703	HIS	-	expression tag	UNP Q9UBH6
A	704	ASP	-	expression tag	UNP Q9UBH6
A	705	GLY	-	expression tag	UNP Q9UBH6
A	706	ASP	-	expression tag	UNP Q9UBH6
A	707	TYR	-	expression tag	UNP Q9UBH6
A	708	LYS	-	expression tag	UNP Q9UBH6
A	709	ASP	-	expression tag	UNP Q9UBH6
A	710	HIS	-	expression tag	UNP Q9UBH6
A	711	ASP	-	expression tag	UNP Q9UBH6
A	712	ILE	-	expression tag	UNP Q9UBH6
A	713	ASP	-	expression tag	UNP Q9UBH6
A	714	TYR	-	expression tag	UNP Q9UBH6
A	715	LYS	-	expression tag	UNP Q9UBH6
A	716	ASP	-	expression tag	UNP Q9UBH6
A	717	ASP	-	expression tag	UNP Q9UBH6
A	718	ASP	-	expression tag	UNP Q9UBH6
A	719	ASP	-	expression tag	UNP Q9UBH6
A	720	LYS	-	expression tag	UNP Q9UBH6

- Molecule 2 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
2	B	1	Total	C	N	O	P	0
			54	44	1	8	1	
2	B	1	Total	C	N	O	P	0
			54	44	1	8	1	
2	A	1	Total	C	N	O	P	0
			54	44	1	8	1	
2	A	1	Total	C	N	O	P	0
			54	44	1	8	1	

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P) (labeled as "Ligand of Interest" by depositor).

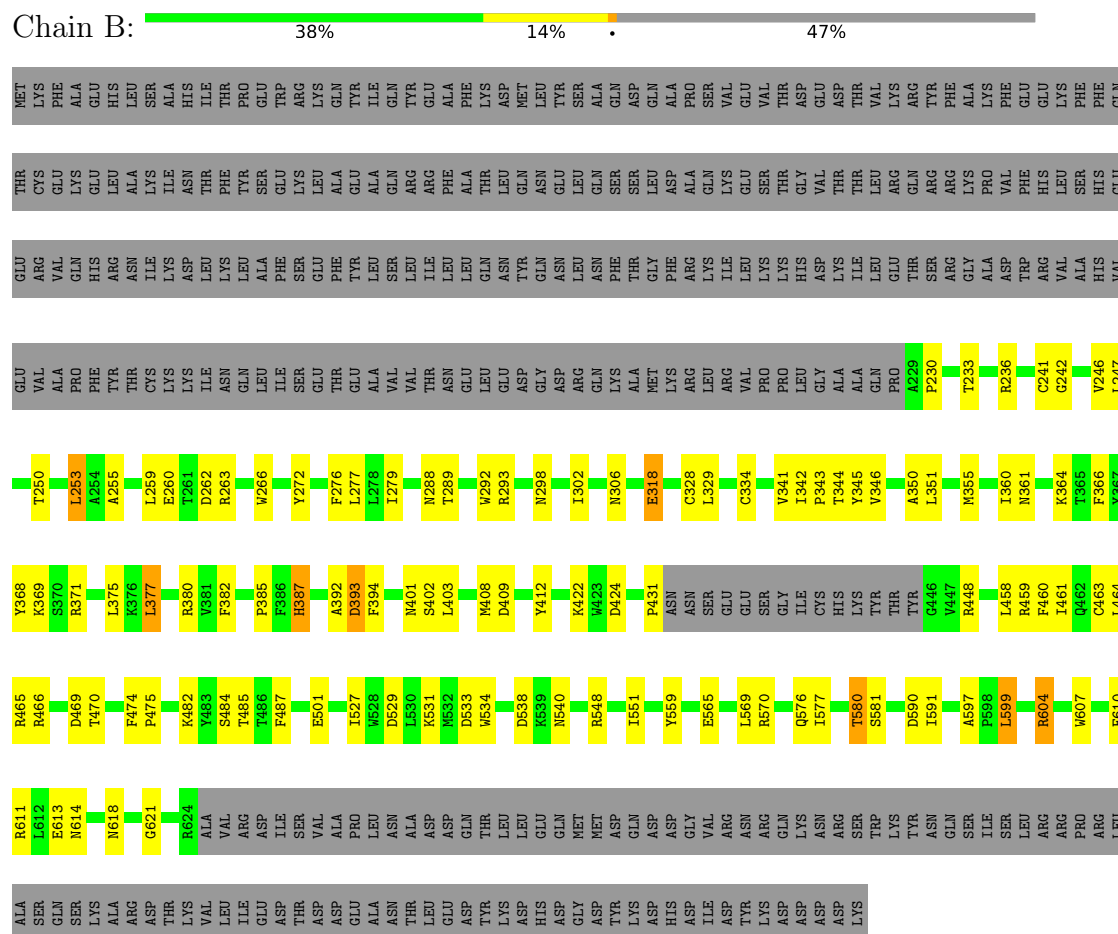


Mol	Chain	Residues	Atoms			AltConf
3	B	1	Total	O	P	0
			5	4	1	
3	A	1	Total	O	P	0
			5	4	1	

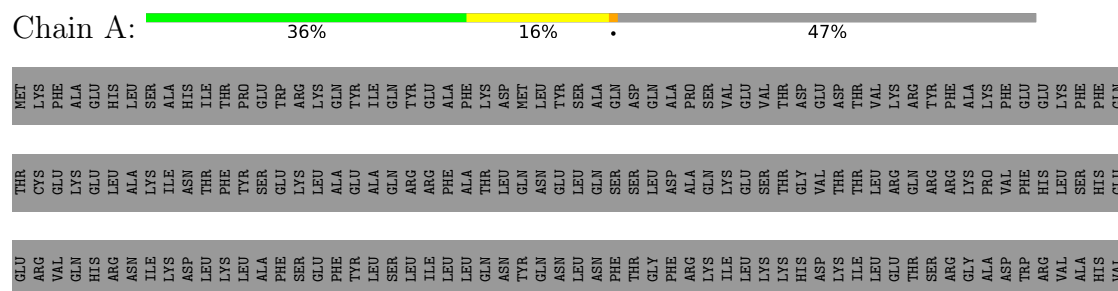
3 Residue-property plots

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. 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: Solute carrier family 53 member 1



• Molecule 1: Solute carrier family 53 member 1



ASP	ASN	L375	F257	GLU
ASP	ARG	K376	K258	VAL
LYS	SER	L377	L259	ALA
	TRP	L378		PRO
	LYS	F379	R272	PHE
	ASN	R380	R273	TYR
	GLN	V381		THR
	ASN	F382	F276	CYS
	GLN	T383	L277	LYS
	SER	A384	L278	LYS
	ILE	P385	L279	ILE
	SER	P385		ILE
	LEU	H476		ASN
	LEU	L477	L285	GLN
	ARG			LEU
	ARG	R604		ILE
	PRO		Y290	
	ARG	N608		SER
	LEU	F609	Q294	GLU
	ALA	F610		THR
	SER	R611	H299	GLU
	GLN	L612		ALA
	SER	E613	F303	VAL
	LYS		E304	VAL
	ALA	N619	L305	THR
	ALA	C620	N306	ASN
	ARG	G621		GLU
	ASP		N310	LEU
	THR		H315	GLU
	LYS	R624	G324	GLY
	VAL	ALA		ASP
	VAL	VAL	C328	ARG
	ILE	ARG	L332	GLN
	ILE	ASP	A333	LYS
	GLU	PRO	C334	ARG
	GLU	LEU		LEU
	ALA	ALA	V341	LEU
	ASN	ASN	I342	ARG
	THR	ALA		ARG
	LEU	ASP	A350	VAL
	GLU	ASP	L351	PRO
	GLU	ASP	Y352	PRO
	ASP	GLN	G353	LEU
	ASP	THR	F354	GLY
	LYS	LEU	F355	ALA
	ASP	LEU	V356	ALA
	HIS	HIS	F357	GLN
	ASP	GLY		PRO
	GLY	MET	N361	
	TYR	E549	F366	
	ASP	E550	Y367	
	LYS	I551	Y368	
	TYR	V552	K369	
	ASP	Y553	S370	
	LYS	GLY	R371	
	ASP	GLY	F372	
	ASP	VAL	W373	
	ILE	ARG	L253	
	ASP	ARG		
	TYR	ASN		
	LYS	ARG		
	ASP	GLN		
	ASP	LYS		

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	132440	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	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: PC1, PO4

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	0.16	0/3292	0.34	0/4479
1	B	0.15	0/3292	0.34	0/4479
All	All	0.16	0/6584	0.34	0/8958

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	3186	0	3185	81	0
1	B	3186	0	3186	69	0
2	A	108	0	176	9	0
2	B	108	0	176	2	0
3	A	5	0	0	0	0
3	B	5	0	0	1	0
All	All	6598	0	6723	151	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 11.

All (151) 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:611:ARG:NH1	1:A:620:CYS:SG	2.55	0.80
1:A:395:TRP:O	1:A:399:GLN:NE2	2.17	0.76
1:A:385:PRO:HB3	1:A:465:ARG:HB2	1.69	0.73
1:A:389:VAL:HG11	1:A:466:ARG:HG2	1.72	0.71
1:B:529:ASP:HA	1:B:533:ASP:HB3	1.72	0.71
1:A:368:TYR:HA	1:A:371:ARG:HH11	1.56	0.70
1:A:529:ASP:HA	1:A:533:ASP:HB2	1.73	0.69
1:B:465:ARG:NH1	1:B:469:ASP:OD2	2.26	0.68
1:A:399:GLN:OE1	1:A:608:ASN:ND2	2.26	0.68
1:A:482:LYS:O	1:A:485:THR:OG1	2.12	0.68
1:B:482:LYS:O	1:B:485:THR:OG1	2.12	0.67
1:A:582:THR:HG23	1:A:584:LEU:H	1.60	0.67
1:B:346:VAL:O	1:B:350:ALA:N	2.26	0.65
1:A:368:TYR:HA	1:A:371:ARG:HD3	1.78	0.65
1:B:277:LEU:HD21	1:B:597:ALA:HB1	1.79	0.65
1:A:551:ILE:O	1:A:559:TYR:OH	2.13	0.65
1:A:341:VAL:HG13	1:A:342:ILE:HG12	1.79	0.65
1:A:355:MET:HB3	2:A:801:PC1:H2A2	1.77	0.65
1:A:285:LEU:HD21	2:A:801:PC1:H332	1.78	0.64
1:A:357:PHE:O	1:A:361:ASN:ND2	2.30	0.64
1:A:619:ASN:HD22	1:A:624:ARG:HB2	1.62	0.64
1:A:306:ASN:O	1:A:310:ASN:ND2	2.31	0.64
1:B:385:PRO:HD3	1:B:461:ILE:HD12	1.79	0.63
1:B:533:ASP:O	1:B:614:ASN:ND2	2.30	0.63
1:A:551:ILE:O	1:A:553:TYR:N	2.34	0.60
1:A:466:ARG:NH2	1:A:621:GLY:O	2.33	0.60
1:A:276:PHE:HE1	2:A:802:PC1:H2I1	1.67	0.59
1:B:422:LYS:HE2	1:B:424:ASP:HB2	1.84	0.59
1:B:534:TRP:O	1:B:548:ARG:NH2	2.32	0.59
1:A:361:ASN:O	1:A:371:ARG:NH2	2.32	0.59
1:A:548:ARG:NH1	1:A:613:GLU:OE2	2.36	0.59
1:B:230:PRO:O	1:B:233:THR:OG1	2.20	0.59
1:B:360:ILE:HA	1:B:375:LEU:HD11	1.84	0.59
1:A:408:MET:HE2	1:A:452:GLN:HB2	1.84	0.58
1:A:534:TRP:O	1:A:548:ARG:NH2	2.35	0.58
1:B:266:TRP:HZ2	1:B:591:ILE:HG13	1.68	0.58
1:A:482:LYS:HD3	1:A:525:THR:HG22	1.84	0.58
1:A:393:ASP:N	1:A:393:ASP:OD1	2.26	0.58
1:B:466:ARG:NH2	1:B:621:GLY:O	2.37	0.58
1:A:374:LEU:HD21	2:A:801:PC1:H3A1	1.86	0.58
1:B:272:TYR:OH	1:B:334:CYS:SG	2.53	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:466:ARG:O	1:B:470:THR:OG1	2.16	0.57
1:B:614:ASN:OD1	1:B:618:ASN:ND2	2.36	0.57
1:A:465:ARG:NH1	1:A:469:ASP:OD1	2.36	0.57
1:B:369:LYS:HB3	2:B:801:PC1:H132	1.87	0.57
1:B:236:ARG:NE	1:B:318:GLU:OE2	2.32	0.56
1:B:402:SER:HB2	1:B:604:ARG:HG2	1.87	0.56
1:A:517:PHE:HA	1:A:520:ILE:HG22	1.87	0.56
1:B:576:GLN:O	1:B:580:THR:OG1	2.24	0.56
1:B:341:VAL:HG23	1:B:342:ILE:HG12	1.87	0.56
1:A:461:ILE:HD12	1:A:464:LEU:HD12	1.87	0.56
1:B:527:ILE:HG13	1:B:531:LYS:HD3	1.87	0.55
1:A:473:ALA:HA	1:A:477:LEU:HD23	1.88	0.55
1:B:298:ASN:HD22	1:B:302:ILE:HG13	1.71	0.55
1:A:377:LEU:HD21	1:A:392:ALA:HB1	1.88	0.55
1:A:475:PRO:HB2	1:A:528:TRP:HH2	1.71	0.55
1:B:402:SER:OG	1:B:604:ARG:NE	2.36	0.54
1:B:576:GLN:NE2	1:B:580:THR:OG1	2.40	0.54
1:B:366:PHE:O	1:B:371:ARG:NH2	2.31	0.54
1:B:380:ARG:NH2	1:B:393:ASP:OD2	2.41	0.54
1:B:401:ASN:ND2	3:B:803:PO4:O3	2.31	0.54
1:B:382:PHE:HA	1:B:458:LEU:HD21	1.89	0.54
1:A:299:HIS:HB2	1:A:303:PHE:HD2	1.74	0.53
1:B:247:LEU:HA	1:B:250:THR:HG22	1.92	0.52
1:B:298:ASN:HB3	1:B:302:ILE:HG13	1.91	0.52
1:A:451:VAL:HG23	1:A:454:ILE:HD12	1.91	0.52
1:A:369:LYS:HG2	2:A:801:PC1:H152	1.92	0.52
1:B:484:SER:HA	1:B:487:PHE:HD2	1.75	0.51
1:B:529:ASP:OD2	1:B:570:ARG:NH2	2.31	0.51
1:A:230:PRO:HB2	1:A:233:THR:HB	1.91	0.51
1:B:577:ILE:O	1:B:581:SER:OG	2.27	0.51
1:A:350:ALA:O	1:A:354:PHE:N	2.32	0.51
1:A:489:MET:HE2	1:A:574:THR:HG22	1.93	0.51
1:B:266:TRP:CZ2	1:B:591:ILE:HG13	2.46	0.51
1:A:279:ILE:HD13	1:A:324:GLY:HA2	1.92	0.50
1:B:393:ASP:N	1:B:393:ASP:OD1	2.45	0.50
1:A:258:LYS:HG3	1:A:259:LEU:H	1.77	0.50
1:A:588:SER:OG	1:A:589:GLY:N	2.40	0.50
1:A:406:ILE:HA	1:A:409:ASP:HB2	1.93	0.50
1:B:569:LEU:HD22	1:B:599:LEU:HB3	1.94	0.50
1:A:351:LEU:HD11	1:A:355:MET:HE3	1.95	0.49
1:A:385:PRO:HB3	1:A:465:ARG:HD3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:533:ASP:OD2	1:B:611:ARG:NH1	2.46	0.48
1:A:290:TYR:O	1:A:294:GLN:HG2	2.14	0.48
1:B:590:ASP:N	1:B:590:ASP:OD1	2.47	0.47
1:A:544:ASN:ND2	1:A:548:ARG:O	2.35	0.47
1:B:364:LYS:HA	1:B:368:TYR:HB3	1.96	0.47
1:B:289:THR:O	1:B:293:ARG:N	2.45	0.47
1:B:551:ILE:HD12	1:B:559:TYR:CE2	2.50	0.47
1:A:374:LEU:HD22	2:A:801:PC1:H252	1.98	0.46
1:A:381:VAL:HG21	1:A:396:LEU:HB2	1.98	0.46
1:A:353:GLY:O	1:A:357:PHE:N	2.38	0.46
1:A:379:PHE:O	1:A:383:THR:OG1	2.34	0.46
1:A:354:PHE:HA	1:A:357:PHE:HB2	1.98	0.46
1:B:377:LEU:HD11	1:B:392:ALA:HB1	1.98	0.45
1:A:366:PHE:O	1:A:371:ARG:HD2	2.15	0.45
1:B:361:ASN:HB3	1:B:371:ARG:HH11	1.81	0.45
1:B:351:LEU:O	1:B:355:MET:HG3	2.17	0.45
1:B:534:TRP:HE1	1:B:607:TRP:CD1	2.33	0.45
1:A:403:LEU:O	1:A:406:ILE:HG12	2.17	0.45
1:B:551:ILE:HG23	1:B:559:TYR:HE2	1.82	0.45
1:A:304:GLU:OE1	1:A:373:TRP:NE1	2.42	0.45
1:A:402:SER:OG	1:A:604:ARG:NE	2.35	0.45
1:A:247:LEU:HB3	1:A:328:CYS:HB3	1.99	0.44
1:B:255:ALA:HA	1:B:259:LEU:HD13	1.98	0.44
1:B:402:SER:CB	1:B:604:ARG:HG2	2.47	0.44
1:B:501:GLU:N	1:B:501:GLU:OE1	2.50	0.44
1:A:272:TYR:OH	1:A:334:CYS:SG	2.52	0.43
1:A:315:HIS:HD2	1:A:367:TYR:CE1	2.36	0.43
1:A:482:LYS:HE2	1:A:528:TRP:CG	2.53	0.43
1:B:242:GLY:O	1:B:246:VAL:HG23	2.19	0.43
1:A:369:LYS:HD3	2:A:801:PC1:H143	2.00	0.43
1:B:343:PRO:C	1:B:344:THR:HG1	2.26	0.43
1:B:408:MET:HE3	1:B:448:ARG:HH21	1.84	0.43
1:A:585:LEU:HB3	1:A:587:HIS:CE1	2.54	0.43
1:B:474:PHE:HB2	1:B:475:PRO:HD3	2.01	0.43
1:A:273:ARG:O	1:A:277:LEU:HG	2.19	0.42
1:A:273:ARG:HA	1:A:276:PHE:HB3	2.01	0.42
1:B:247:LEU:HB3	1:B:328:CYS:HB3	2.00	0.42
1:B:387:HIS:CD2	1:B:387:HIS:H	2.35	0.42
1:B:538:ASP:HB3	1:B:540:ASN:OD1	2.19	0.42
1:B:260:GLU:CB	1:B:263:ARG:HB2	2.48	0.42
1:B:262:ASP:O	1:B:431:PRO:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:ARG:HA	1:A:451:VAL:HG12	2.00	0.42
1:B:610:PHE:O	1:B:613:GLU:HG3	2.20	0.42
1:A:242:GLY:O	1:A:246:VAL:HG23	2.20	0.42
1:A:375:LEU:HD23	1:A:375:LEU:HA	1.77	0.42
1:B:288:ASN:HB3	1:B:292:TRP:CZ2	2.55	0.42
1:B:565:GLU:O	1:B:569:LEU:HG	2.19	0.41
1:B:276:PHE:HA	1:B:279:ILE:HD12	2.03	0.41
1:B:460:PHE:CZ	1:B:464:LEU:HD11	2.55	0.41
1:A:475:PRO:HB2	1:A:528:TRP:CH2	2.54	0.41
1:A:369:LYS:HE3	1:A:369:LYS:HB3	1.92	0.41
1:A:461:ILE:HD12	1:A:461:ILE:HA	1.87	0.41
1:A:541:ALA:HA	1:A:549:GLU:HG2	2.02	0.41
1:A:332:LEU:HD23	1:A:332:LEU:HA	1.92	0.41
1:B:306:ASN:HB2	2:B:801:PC1:H153	2.02	0.41
1:A:253:LEU:O	1:A:257:PHE:HB2	2.21	0.41
1:A:573:TRP:CZ2	1:A:577:ILE:HD11	2.56	0.41
1:A:370:SER:HB2	2:A:801:PC1:H12	2.03	0.41
1:A:452:GLN:OE1	1:A:581:SER:OG	2.39	0.41
1:A:492:PHE:HD1	1:A:510:PHE:HD1	1.68	0.41
1:A:497:SER:HB3	1:A:584:LEU:HB2	2.03	0.41
1:A:412:TYR:O	1:A:416:PHE:N	2.47	0.41
1:B:409:ASP:HA	1:B:412:TYR:HB3	2.02	0.40
1:A:520:ILE:O	1:A:524:TYR:HB2	2.20	0.40
2:A:802:PC1:H2B2	2:A:802:PC1:H282	1.81	0.40
1:A:515:ILE:O	1:A:519:ILE:HG12	2.21	0.40
1:B:253:LEU:HD13	1:B:253:LEU:HA	1.92	0.40
1:B:459:ARG:HD2	1:B:459:ARG:HA	1.86	0.40
1:B:570:ARG:HA	1:B:570:ARG:HD3	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	378/720 (52%)	348 (92%)	30 (8%)	0	100	100
1	B	378/720 (52%)	343 (91%)	35 (9%)	0	100	100
All	All	756/1440 (52%)	691 (91%)	65 (9%)	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	339/644 (53%)	325 (96%)	14 (4%)	26	54
1	B	339/644 (53%)	325 (96%)	14 (4%)	26	54
All	All	678/1288 (53%)	650 (96%)	28 (4%)	28	54

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	241	CYS
1	B	253	LEU
1	B	318	GLU
1	B	329	LEU
1	B	345	TYR
1	B	377	LEU
1	B	387	HIS
1	B	393	ASP
1	B	394	PHE
1	B	403	LEU
1	B	463	CYS
1	B	580	THR
1	B	599	LEU
1	B	604	ARG
1	A	369	LYS
1	A	377	LEU
1	A	379	PHE
1	A	393	ASP

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Mol	Chain	Res	Type
1	A	394	PHE
1	A	399	GLN
1	A	405	VAL
1	A	409	ASP
1	A	415	CYS
1	A	461	ILE
1	A	517	PHE
1	A	526	LEU
1	A	565	GLU
1	A	609	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	298	ASN
1	B	618	ASN
1	A	587	HIS
1	A	608	ASN
1	A	619	ASN

5.3.3 RNA [i](#)

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](#)

6 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
2	PC1	B	802	-	53,53,53	0.50	0	59,61,61	0.47	1 (1%)
2	PC1	A	802	-	53,53,53	0.51	0	59,61,61	0.49	1 (1%)
3	PO4	B	803	-	4,4,4	1.42	1 (25%)	6,6,6	0.47	0
2	PC1	A	801	-	53,53,53	0.49	0	59,61,61	0.48	1 (1%)
3	PO4	A	803	-	4,4,4	1.38	1 (25%)	6,6,6	0.55	0
2	PC1	B	801	-	53,53,53	0.49	0	59,61,61	0.48	1 (1%)

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
2	PC1	B	802	-	-	21/57/57/57	-
2	PC1	A	801	-	-	25/57/57/57	-
2	PC1	B	801	-	-	23/57/57/57	-
2	PC1	A	802	-	-	29/57/57/57	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	803	PO4	P-O1	2.48	1.56	1.50
3	A	803	PO4	P-O1	2.39	1.56	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	802	PC1	O12-P-O14	2.42	124.21	112.24
2	B	802	PC1	O12-P-O14	2.38	124.01	112.24
2	B	801	PC1	O12-P-O14	2.34	123.82	112.24
2	A	801	PC1	O12-P-O14	2.32	123.71	112.24

There are no chirality outliers.

All (98) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	801	PC1	C11-O13-P-O12
2	B	801	PC1	C11-O13-P-O14
2	B	802	PC1	C11-O13-P-O12
2	B	802	PC1	C12-C11-O13-P
2	B	802	PC1	O13-C11-C12-N
2	B	802	PC1	O22-C21-O21-C2
2	A	801	PC1	C11-O13-P-O12
2	A	802	PC1	C11-O13-P-O12
2	A	802	PC1	C11-O13-P-O14
2	A	802	PC1	C11-O13-P-O11
2	A	802	PC1	C1-O11-P-O12
2	A	802	PC1	C1-O11-P-O14
2	A	802	PC1	C22-C21-O21-C2
2	A	802	PC1	O22-C21-O21-C2
2	B	802	PC1	C22-C21-O21-C2
2	A	801	PC1	O32-C31-O31-C3
2	A	801	PC1	C32-C31-O31-C3
2	B	802	PC1	C2C-C2D-C2E-C2F
2	B	801	PC1	C26-C27-C28-C29
2	B	802	PC1	C2A-C2B-C2C-C2D
2	A	801	PC1	C21-C22-C23-C24
2	A	802	PC1	C21-C22-C23-C24
2	B	801	PC1	C11-O13-P-O11
2	B	802	PC1	C11-O13-P-O11
2	A	801	PC1	C11-O13-P-O11
2	A	802	PC1	C1-O11-P-O13
2	B	801	PC1	C32-C31-O31-C3
2	B	801	PC1	C32-C33-C34-C35
2	A	802	PC1	C25-C26-C27-C28
2	A	801	PC1	C36-C37-C38-C39
2	A	802	PC1	C2B-C2C-C2D-C2E
2	B	802	PC1	C3A-C3B-C3C-C3D
2	B	801	PC1	C27-C28-C29-C2A
2	B	801	PC1	C2A-C2B-C2C-C2D
2	B	801	PC1	C21-C22-C23-C24
2	A	802	PC1	C3C-C3D-C3E-C3F
2	B	801	PC1	O32-C31-O31-C3
2	A	802	PC1	C11-C12-N-C15
2	B	801	PC1	C31-C32-C33-C34
2	A	802	PC1	C3A-C3B-C3C-C3D
2	A	801	PC1	C28-C29-C2A-C2B
2	A	802	PC1	C2C-C2D-C2E-C2F
2	A	801	PC1	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
2	B	801	PC1	C25-C26-C27-C28
2	B	801	PC1	C2C-C2D-C2E-C2F
2	A	801	PC1	C27-C28-C29-C2A
2	B	802	PC1	C24-C25-C26-C27
2	A	801	PC1	C38-C39-C3A-C3B
2	B	801	PC1	C2E-C2F-C2G-C2H
2	B	802	PC1	C2F-C2G-C2H-C2I
2	B	801	PC1	C35-C36-C37-C38
2	A	802	PC1	C3D-C3E-C3F-C3G
2	B	801	PC1	C1-C2-C3-O31
2	A	801	PC1	O11-C1-C2-O21
2	B	802	PC1	C2B-C2C-C2D-C2E
2	A	801	PC1	O11-C1-C2-C3
2	A	801	PC1	C37-C38-C39-C3A
2	A	802	PC1	C22-C23-C24-C25
2	B	801	PC1	C33-C34-C35-C36
2	B	801	PC1	C28-C29-C2A-C2B
2	B	802	PC1	C33-C34-C35-C36
2	A	801	PC1	C11-C12-N-C14
2	A	801	PC1	C2E-C2F-C2G-C2H
2	A	802	PC1	C11-C12-N-C13
2	B	801	PC1	O13-C11-C12-N
2	A	801	PC1	O13-C11-C12-N
2	A	802	PC1	C36-C37-C38-C39
2	A	802	PC1	C34-C35-C36-C37
2	A	801	PC1	C11-C12-N-C15
2	A	802	PC1	C11-C12-N-C14
2	B	802	PC1	C35-C36-C37-C38
2	B	802	PC1	C1-C2-C3-O31
2	A	801	PC1	C11-C12-N-C13
2	B	802	PC1	C3B-C3C-C3D-C3E
2	B	802	PC1	C2D-C2E-C2F-C2G
2	B	802	PC1	C31-C32-C33-C34
2	A	802	PC1	C29-C2A-C2B-C2C
2	B	801	PC1	C37-C38-C39-C3A
2	A	802	PC1	C2-C1-O11-P
2	B	801	PC1	C34-C35-C36-C37
2	A	801	PC1	C32-C33-C34-C35
2	A	802	PC1	C28-C29-C2A-C2B
2	A	801	PC1	C26-C27-C28-C29
2	A	801	PC1	O21-C21-C22-C23
2	A	801	PC1	O31-C31-C32-C33

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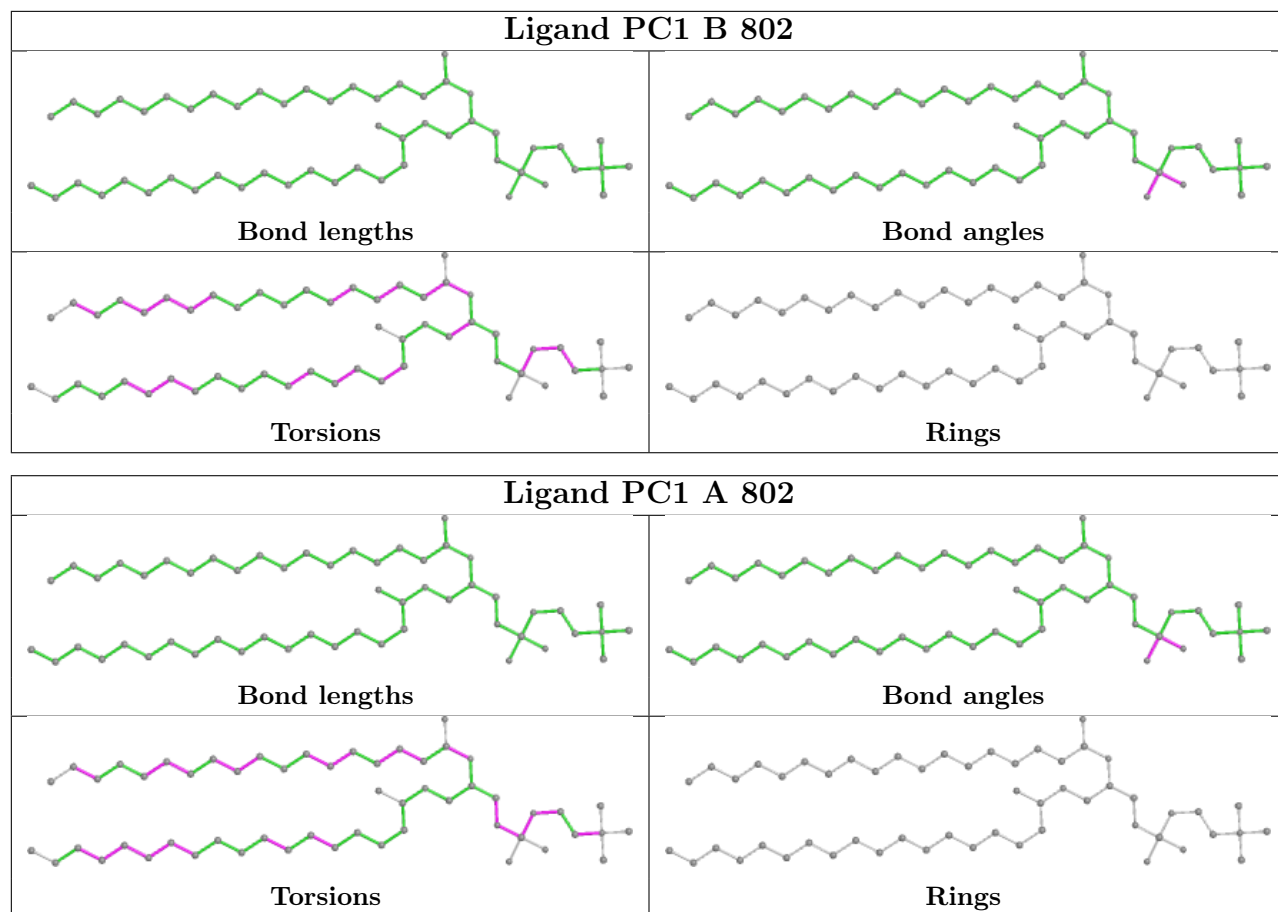
Mol	Chain	Res	Type	Atoms
2	A	802	PC1	C2F-C2G-C2H-C2I
2	B	802	PC1	C3C-C3D-C3E-C3F
2	B	801	PC1	C3B-C3C-C3D-C3E
2	A	802	PC1	C3B-C3C-C3D-C3E
2	A	802	PC1	C3E-C3F-C3G-C3H
2	A	801	PC1	O22-C21-C22-C23
2	A	802	PC1	C24-C25-C26-C27
2	B	802	PC1	C22-C23-C24-C25
2	B	801	PC1	C22-C23-C24-C25
2	A	801	PC1	C22-C23-C24-C25
2	A	802	PC1	C12-C11-O13-P
2	A	801	PC1	O32-C31-C32-C33
2	B	802	PC1	O21-C21-C22-C23

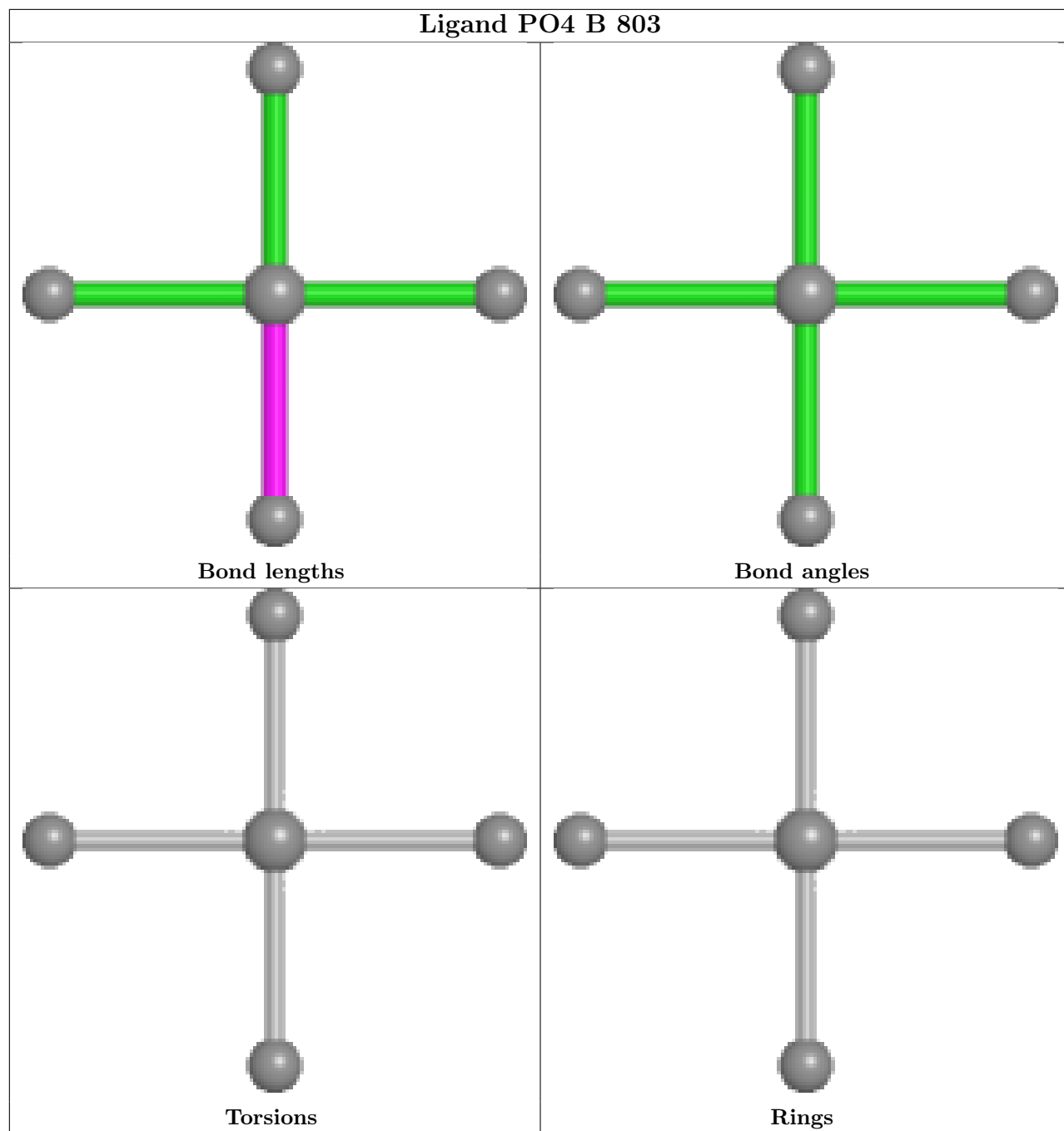
There are no ring outliers.

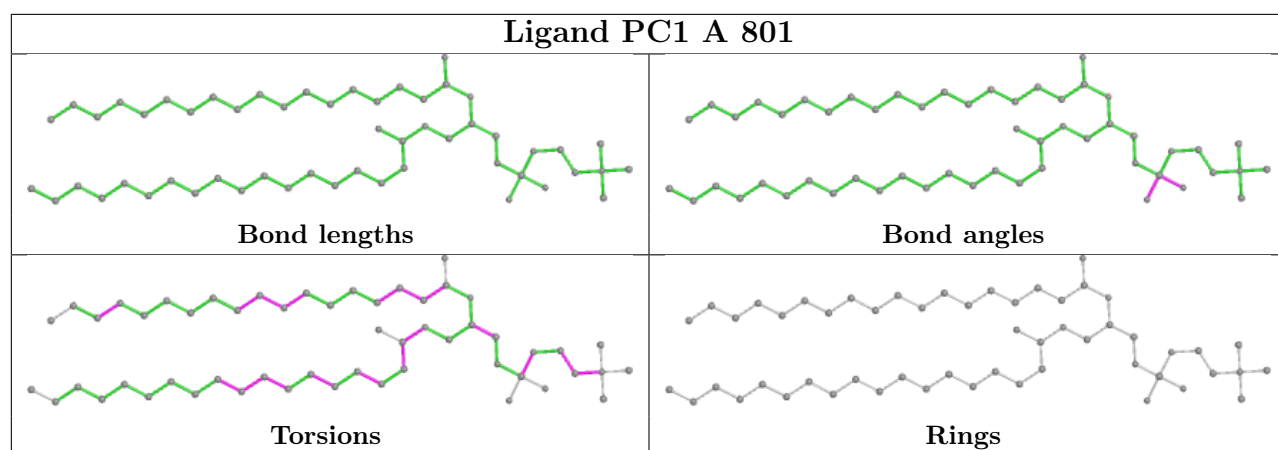
4 monomers are involved in 12 short contacts:

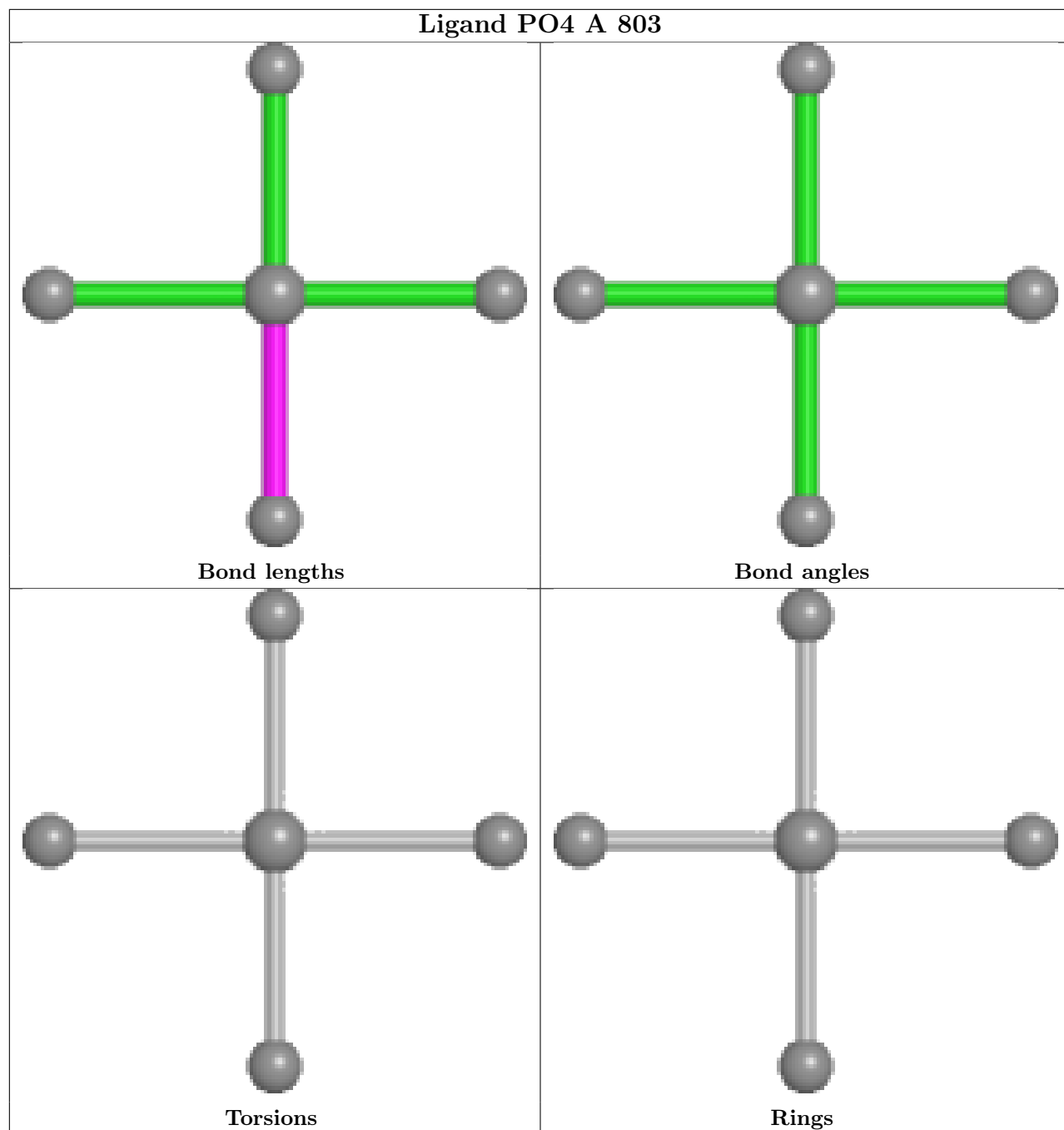
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	802	PC1	2	0
3	B	803	PO4	1	0
2	A	801	PC1	7	0
2	B	801	PC1	2	0

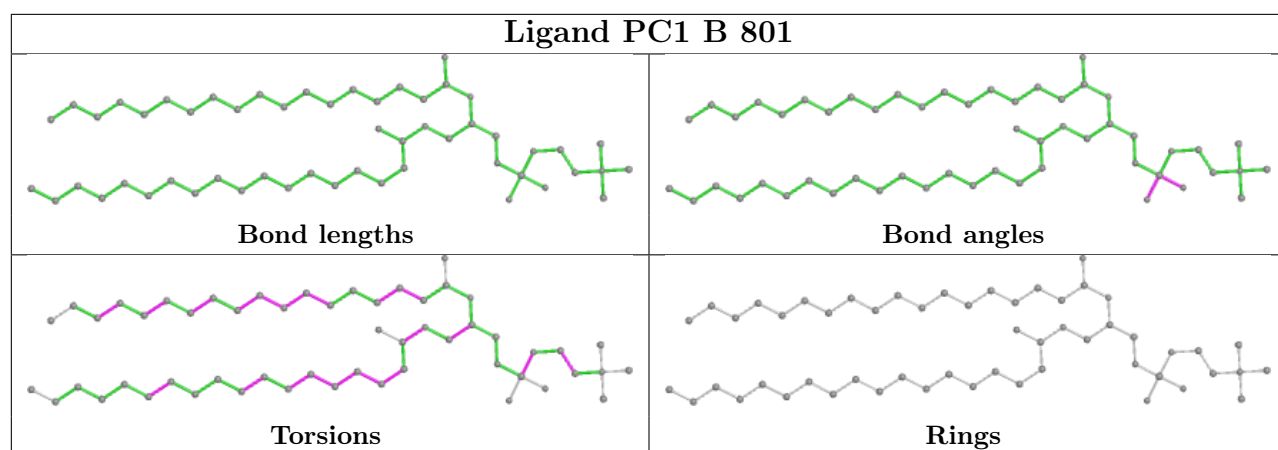
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 [i](#)

There are no chain breaks in this entry.