Full wwPDB EM Validation Report ⓘ

Apr 6, 2025 – 01:43 AM JST

PDB ID	:	9J98 / pdb_00009j98
EMDB ID	:	EMD-61255
Title	:	Open structure of human XPR1
Authors	:	Wang, Y.; Wang, Y.; Yang, H.; Shen, H.
Deposited on	:	2024-08-22
Resolution	:	3.33 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:

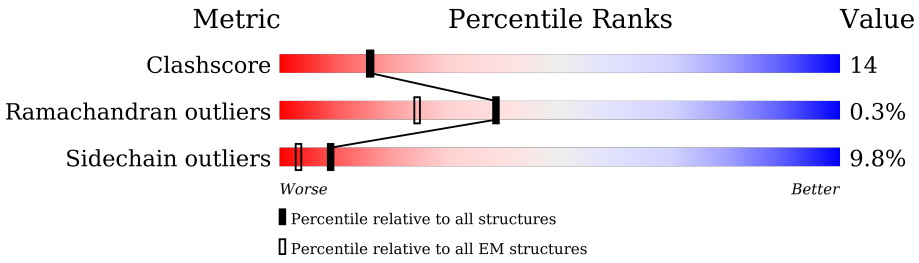
EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.33 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	969	28% 11% • 59%
1	B	969	28% 11% • 59%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6752 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,Green fluorescent protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	397	Total	C	N	O	S	0	0
			3301	2215	530	540	16		
1	B	397	Total	C	N	O	S	0	0
			3301	2215	530	540	16		

There are 82 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	697	GLY	-	linker	UNP Q9UBH6
A	698	GLY	-	linker	UNP Q9UBH6
A	699	ARG	-	linker	UNP Q9UBH6
A	700	LEU	-	linker	UNP Q9UBH6
A	701	GLU	-	linker	UNP Q9UBH6
A	702	VAL	-	linker	UNP Q9UBH6
A	703	LEU	-	linker	UNP Q9UBH6
A	704	PHE	-	linker	UNP Q9UBH6
A	705	GLN	-	linker	UNP Q9UBH6
A	706	GLY	-	linker	UNP Q9UBH6
A	707	PRO	-	linker	UNP Q9UBH6
A	708	ALA	-	linker	UNP Q9UBH6
A	709	ALA	-	linker	UNP Q9UBH6
A	710	ALA	-	linker	UNP Q9UBH6
A	711	ALA	-	linker	UNP Q9UBH6
A	712	VAL	-	linker	UNP Q9UBH6
A	775	LEU	PHE	conflict	UNP P42212
A	776	THR	SER	conflict	UNP P42212
A	818	THR	LYS	conflict	UNP P42212
A	917	LYS	ALA	conflict	UNP P42212
A	942	LEU	HIS	conflict	UNP P42212
A	950	SER	-	expression tag	UNP P42212
A	951	GLY	-	expression tag	UNP P42212
A	952	LEU	-	expression tag	UNP P42212
A	953	ARG	-	expression tag	UNP P42212
A	954	SER	-	expression tag	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
A	955	ASP	-	expression tag	UNP P42212
A	956	TYR	-	expression tag	UNP P42212
A	957	LYS	-	expression tag	UNP P42212
A	958	ASP	-	expression tag	UNP P42212
A	959	HIS	-	expression tag	UNP P42212
A	960	ASP	-	expression tag	UNP P42212
A	961	ILE	-	expression tag	UNP P42212
A	962	ASP	-	expression tag	UNP P42212
A	963	TYR	-	expression tag	UNP P42212
A	964	LYS	-	expression tag	UNP P42212
A	965	ASP	-	expression tag	UNP P42212
A	966	ASP	-	expression tag	UNP P42212
A	967	ASP	-	expression tag	UNP P42212
A	968	ASP	-	expression tag	UNP P42212
A	969	LYS	-	expression tag	UNP P42212
B	697	GLY	-	linker	UNP Q9UBH6
B	698	GLY	-	linker	UNP Q9UBH6
B	699	ARG	-	linker	UNP Q9UBH6
B	700	LEU	-	linker	UNP Q9UBH6
B	701	GLU	-	linker	UNP Q9UBH6
B	702	VAL	-	linker	UNP Q9UBH6
B	703	LEU	-	linker	UNP Q9UBH6
B	704	PHE	-	linker	UNP Q9UBH6
B	705	GLN	-	linker	UNP Q9UBH6
B	706	GLY	-	linker	UNP Q9UBH6
B	707	PRO	-	linker	UNP Q9UBH6
B	708	ALA	-	linker	UNP Q9UBH6
B	709	ALA	-	linker	UNP Q9UBH6
B	710	ALA	-	linker	UNP Q9UBH6
B	711	ALA	-	linker	UNP Q9UBH6
B	712	VAL	-	linker	UNP Q9UBH6
B	775	LEU	PHE	conflict	UNP P42212
B	776	THR	SER	conflict	UNP P42212
B	818	THR	LYS	conflict	UNP P42212
B	917	LYS	ALA	conflict	UNP P42212
B	942	LEU	HIS	conflict	UNP P42212
B	950	SER	-	expression tag	UNP P42212
B	951	GLY	-	expression tag	UNP P42212
B	952	LEU	-	expression tag	UNP P42212
B	953	ARG	-	expression tag	UNP P42212
B	954	SER	-	expression tag	UNP P42212
B	955	ASP	-	expression tag	UNP P42212

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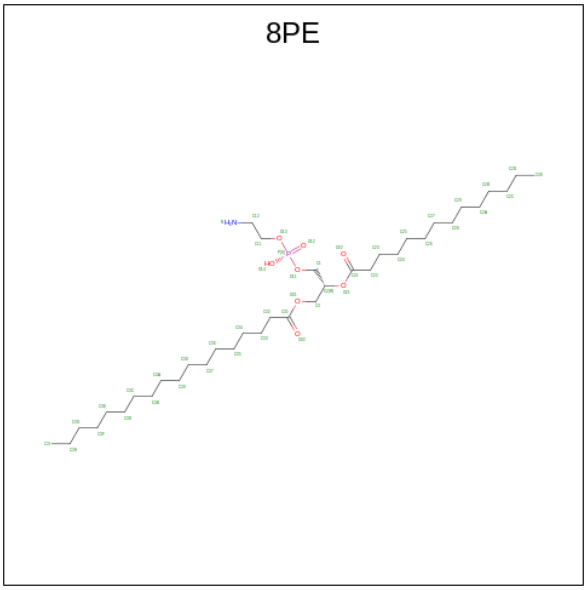
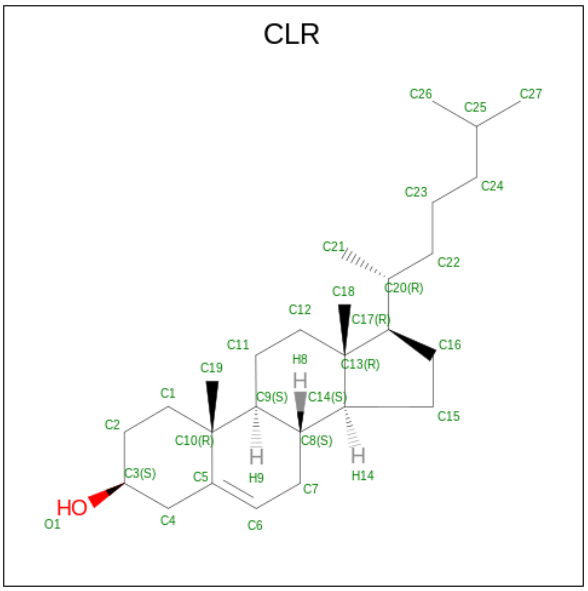
Chain	Residue	Modelled	Actual	Comment	Reference
B	956	TYR	-	expression tag	UNP P42212
B	957	LYS	-	expression tag	UNP P42212
B	958	ASP	-	expression tag	UNP P42212
B	959	HIS	-	expression tag	UNP P42212
B	960	ASP	-	expression tag	UNP P42212
B	961	ILE	-	expression tag	UNP P42212
B	962	ASP	-	expression tag	UNP P42212
B	963	TYR	-	expression tag	UNP P42212
B	964	LYS	-	expression tag	UNP P42212
B	965	ASP	-	expression tag	UNP P42212
B	966	ASP	-	expression tag	UNP P42212
B	967	ASP	-	expression tag	UNP P42212
B	968	ASP	-	expression tag	UNP P42212
B	969	LYS	-	expression tag	UNP P42212

- Molecule 2 is (2R)-3-{[(S)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-2-(tetradecanoyloxy) propyl octadecanoate (CCD ID: 8PE) (formula: $C_{37}H_{74}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			47	37	1	8	1	
2	B	1	Total	C	N	O	P	0
			47	37	1	8	1	

- Molecule 3 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$).



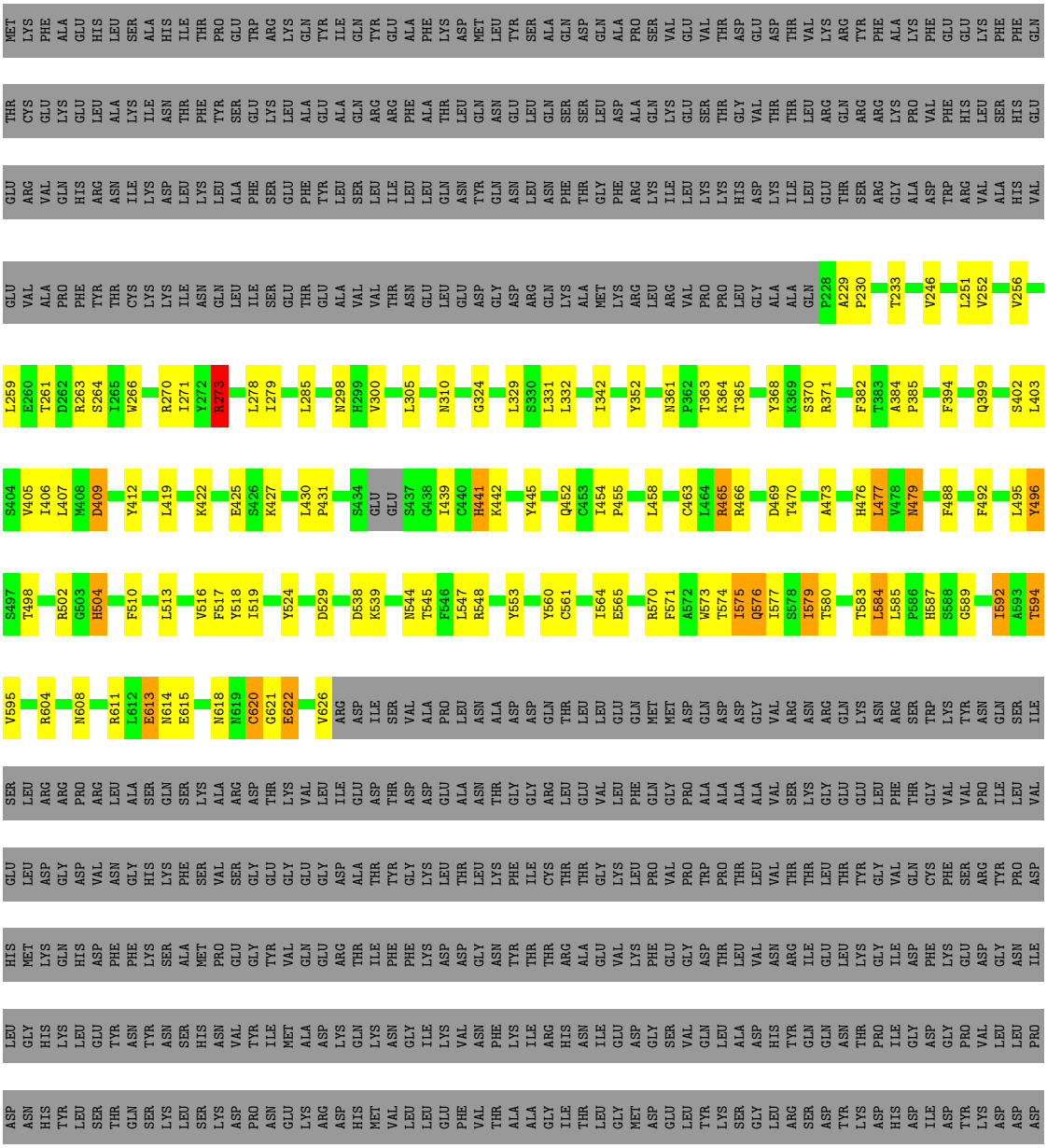
Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total	C	O	0
			28	27	1	
3	B	1	Total	C	O	0
			28	27	1	

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.

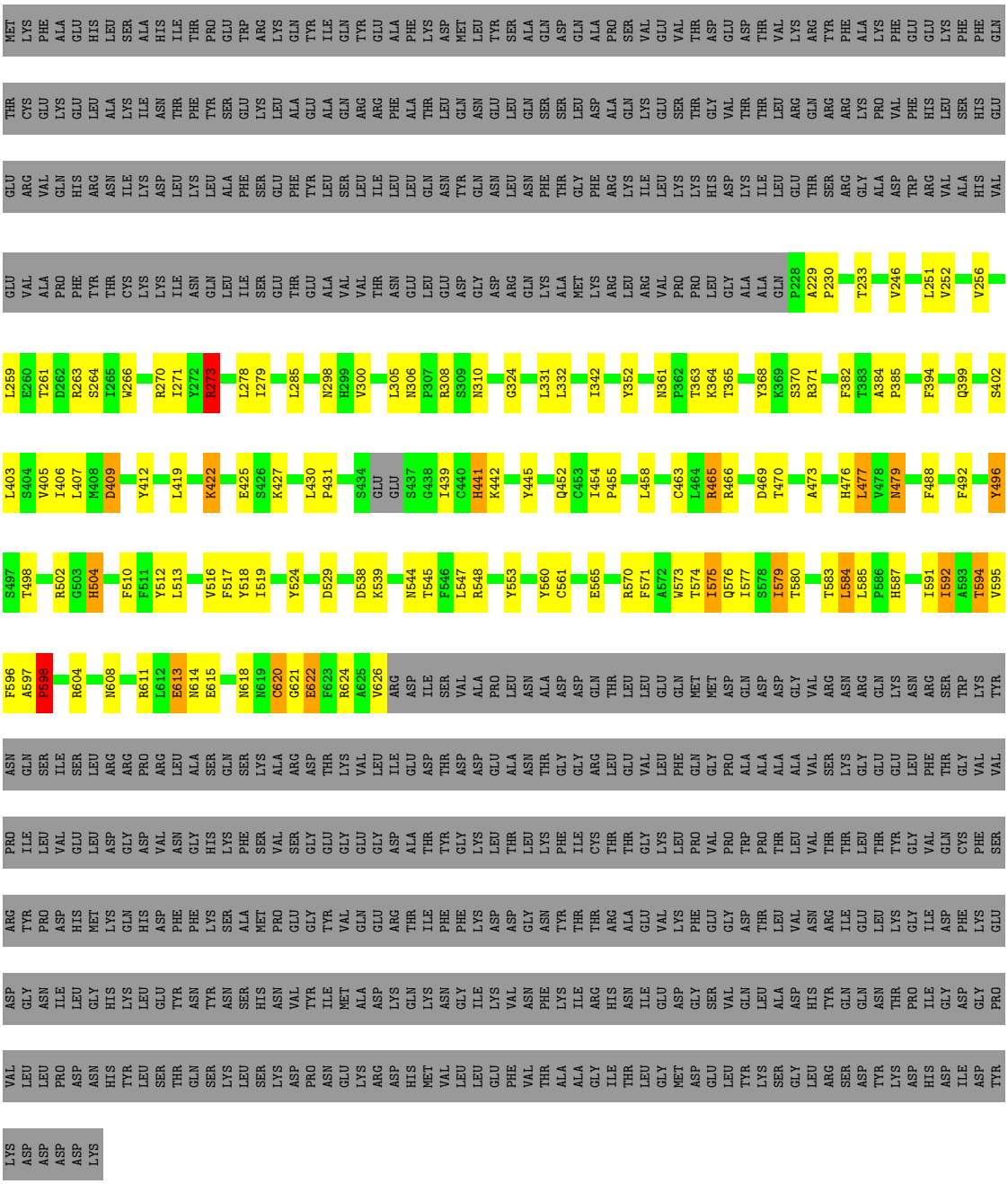
- Molecule 1: Solute carrier family 53 member 1,Green fluorescent protein

Chain A:



• Molecule 1: Solute carrier family 53 member 1,Green fluorescent protein

Chain B:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	46087	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CLR, 8PE

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	0.42	0/3411	0.54	3/4641 (0.1%)
1	B	0.46	1/3411 (0.0%)	0.55	4/4641 (0.1%)
All	All	0.44	1/6822 (0.0%)	0.55	7/9282 (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	B	598	PRO	C-O	-5.01	1.13	1.23

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	620	CYS	CB-CA-C	-5.72	98.95	110.40
1	A	620	CYS	CB-CA-C	-5.72	98.97	110.40
1	A	620	CYS	CA-CB-SG	-5.63	103.86	114.00
1	B	620	CYS	CA-CB-SG	-5.60	103.91	114.00
1	B	574	THR	CA-CB-OG1	-5.45	97.56	109.00
1	A	574	THR	CA-CB-OG1	-5.43	97.59	109.00
1	B	622	GLU	CB-CA-C	5.00	120.40	110.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	273	ARG	Sidechain
1	B	273	ARG	Sidechain

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	3301	0	3294	92	0
1	B	3301	0	3294	92	0
2	A	47	0	73	5	0
2	B	47	0	73	6	0
3	A	28	0	46	7	0
3	B	28	0	46	4	0
All	All	6752	0	6826	191	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 14.

All (191) 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:B:597:ALA:HB3	1:B:598:PRO:HD3	1.24	1.09
3:A:1002:CLR:H242	3:A:1002:CLR:H211	1.41	1.02
3:B:1002:CLR:H242	3:B:1002:CLR:H211	1.41	0.99
1:B:576:GLN:NE2	1:B:596:PHE:CD1	2.33	0.96
1:B:571:PHE:O	1:B:573:TRP:CD1	2.24	0.91
1:A:571:PHE:O	1:A:573:TRP:CD1	2.24	0.91
1:B:571:PHE:O	1:B:573:TRP:HD1	1.59	0.85
1:A:571:PHE:O	1:A:573:TRP:HD1	1.59	0.83
1:B:597:ALA:HB3	1:B:598:PRO:CD	2.07	0.82
1:A:553:TYR:CD2	3:A:1002:CLR:H6	2.15	0.80
1:B:553:TYR:CD2	3:B:1002:CLR:H6	2.16	0.80
1:B:259:LEU:HD13	1:B:261:THR:H	1.48	0.78
1:B:576:GLN:NE2	1:B:596:PHE:CG	2.52	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:TRP:NE1	1:A:587:HIS:CD2	2.51	0.78
1:A:259:LEU:HD13	1:A:261:THR:H	1.48	0.76
1:A:266:TRP:CD1	1:A:587:HIS:CD2	2.74	0.76
1:B:591:ILE:O	1:B:595:VAL:HG23	1.86	0.75
3:B:1002:CLR:H211	3:B:1002:CLR:C24	2.16	0.75
1:B:622:GLU:HG2	1:B:622:GLU:O	1.86	0.74
1:B:473:ALA:O	1:B:477:LEU:HB2	1.88	0.74
1:B:576:GLN:HE22	1:B:596:PHE:HB2	1.53	0.73
1:B:273:ARG:CZ	1:B:594:THR:OG1	2.36	0.73
1:A:473:ALA:O	1:A:477:LEU:HB2	1.88	0.72
1:A:615:GLU:OE1	1:A:620:CYS:SG	2.47	0.71
1:A:399:GLN:HE22	1:A:608:ASN:HD21	1.38	0.71
1:B:615:GLU:OE1	1:B:620:CYS:SG	2.48	0.71
1:A:622:GLU:O	1:A:622:GLU:HG3	1.89	0.70
1:B:399:GLN:HE22	1:B:608:ASN:HD21	1.38	0.69
1:A:273:ARG:CZ	1:A:594:THR:OG1	2.42	0.68
1:A:576:GLN:H	1:A:576:GLN:NE2	1.94	0.65
1:A:575:ILE:HD13	1:A:575:ILE:N	2.11	0.65
1:B:465:ARG:NH1	1:B:469:ASP:OD2	2.31	0.64
1:A:370:SER:HB3	2:A:1001:8PE:O32	1.98	0.64
1:A:251:LEU:HD21	1:A:331:LEU:HD23	1.80	0.63
1:A:529:ASP:OD2	1:A:570:ARG:NH1	2.31	0.63
1:A:465:ARG:NH1	1:A:469:ASP:OD2	2.31	0.63
1:B:251:LEU:HD21	1:B:331:LEU:HD23	1.80	0.63
1:B:575:ILE:HD13	1:B:575:ILE:N	2.11	0.63
1:B:529:ASP:OD2	1:B:570:ARG:NH1	2.31	0.63
1:B:266:TRP:CD1	1:B:587:HIS:CD2	2.87	0.63
1:B:229:ALA:HB1	1:B:233:THR:HB	1.80	0.62
1:B:266:TRP:NE1	1:B:587:HIS:CD2	2.67	0.62
1:B:370:SER:HB3	2:B:1001:8PE:O32	1.99	0.62
1:B:279:ILE:HD13	1:B:324:GLY:HA2	1.83	0.61
1:A:266:TRP:HE1	1:A:587:HIS:CD2	2.17	0.61
1:A:229:ALA:HB1	1:A:233:THR:HB	1.81	0.61
1:B:583:THR:O	1:B:583:THR:HG23	2.01	0.60
1:A:583:THR:HG23	1:A:583:THR:O	2.02	0.60
1:A:279:ILE:HD13	1:A:324:GLY:HA2	1.83	0.60
1:A:576:GLN:HB2	1:A:592:ILE:HD12	1.82	0.60
3:A:1002:CLR:H211	3:A:1002:CLR:C24	2.16	0.59
1:B:597:ALA:N	1:B:598:PRO:CD	2.64	0.59
1:B:597:ALA:CB	1:B:598:PRO:HD3	2.10	0.59
1:A:573:TRP:HA	1:A:576:GLN:HE22	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:576:GLN:H	1:A:576:GLN:HE21	1.52	0.58
1:A:580:THR:HG22	1:A:580:THR:O	2.04	0.58
1:A:614:ASN:HD21	1:A:620:CYS:HB3	1.69	0.57
1:B:580:THR:HG22	1:B:580:THR:O	2.04	0.57
1:B:595:VAL:HG12	1:B:595:VAL:O	2.04	0.57
1:B:614:ASN:HD21	1:B:620:CYS:HB3	1.69	0.57
1:A:553:TYR:CE2	3:A:1002:CLR:H6	2.41	0.56
1:A:270:ARG:O	1:A:409:ASP:OD1	2.25	0.55
1:A:266:TRP:HE1	1:A:587:HIS:HD2	1.55	0.55
1:B:576:GLN:NE2	1:B:596:PHE:HB2	2.19	0.55
3:A:1002:CLR:C24	3:A:1002:CLR:C21	2.84	0.54
1:B:300:VAL:HG23	1:B:305:LEU:HB2	1.88	0.54
1:B:553:TYR:CE2	3:B:1002:CLR:H6	2.42	0.54
1:A:273:ARG:NH1	1:A:594:THR:OG1	2.40	0.54
1:B:455:PRO:HA	1:B:458:LEU:HD12	1.88	0.54
1:A:363:THR:OG1	1:A:365:THR:OG1	2.26	0.54
1:A:300:VAL:HG23	1:A:305:LEU:HB2	1.88	0.54
1:A:246:VAL:HG11	1:B:246:VAL:HG11	1.89	0.53
1:A:455:PRO:HA	1:A:458:LEU:HD12	1.88	0.53
1:A:266:TRP:NE1	1:A:587:HIS:HD2	2.05	0.53
1:A:595:VAL:HG12	1:A:595:VAL:O	2.08	0.53
1:B:270:ARG:O	1:B:409:ASP:OD1	2.26	0.53
1:B:579:ILE:O	1:B:584:LEU:HD21	2.08	0.53
1:B:615:GLU:O	1:B:624:ARG:NH2	2.43	0.52
3:A:1002:CLR:H242	3:A:1002:CLR:C21	2.28	0.52
1:B:575:ILE:N	1:B:575:ILE:CD1	2.73	0.52
1:A:575:ILE:N	1:A:575:ILE:CD1	2.73	0.52
1:B:285:LEU:HD21	2:B:1001:8PE:H23A	1.91	0.52
1:A:285:LEU:HD21	2:A:1001:8PE:H23A	1.92	0.52
1:A:385:PRO:O	1:A:465:ARG:NE	2.28	0.51
1:B:361:ASN:ND2	1:B:363:THR:OG1	2.40	0.51
1:A:402:SER:HB3	1:A:604:ARG:HH21	1.76	0.51
1:B:402:SER:HB3	1:B:604:ARG:HH21	1.76	0.50
1:B:385:PRO:O	1:B:465:ARG:NE	2.28	0.50
1:B:399:GLN:HE22	1:B:608:ASN:ND2	2.09	0.50
1:B:273:ARG:NH2	1:B:594:THR:OG1	2.44	0.50
1:B:488:PHE:HB3	1:B:517:PHE:CD2	2.47	0.50
1:B:575:ILE:O	1:B:579:ILE:N	2.38	0.50
1:A:571:PHE:O	1:A:573:TRP:N	2.43	0.50
1:B:363:THR:OG1	1:B:365:THR:OG1	2.26	0.49
1:A:488:PHE:HB3	1:A:517:PHE:CD2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:620:CYS:SG	1:A:621:GLY:N	2.85	0.49
1:A:502:ARG:HD2	1:A:504:HIS:CD2	2.48	0.49
1:A:576:GLN:NE2	1:A:576:GLN:N	2.60	0.49
1:B:620:CYS:SG	1:B:621:GLY:N	2.85	0.49
1:A:399:GLN:HE22	1:A:608:ASN:ND2	2.09	0.49
1:A:589:GLY:O	1:A:592:ILE:HG12	2.14	0.48
1:A:403:LEU:HG	1:A:406:ILE:HD12	1.96	0.48
1:A:545:THR:OG1	1:A:560:TYR:OH	2.28	0.48
1:B:266:TRP:HE1	1:B:587:HIS:CD2	2.31	0.48
1:B:576:GLN:NE2	1:B:596:PHE:CB	2.76	0.48
1:B:502:ARG:HD2	1:B:504:HIS:CD2	2.48	0.48
1:A:466:ARG:HE	1:A:476:HIS:HD2	1.62	0.47
1:B:403:LEU:HG	1:B:406:ILE:HD12	1.96	0.47
1:B:570:ARG:HD2	1:B:570:ARG:HA	1.67	0.47
1:B:496:TYR:HB2	1:B:510:PHE:HB3	1.96	0.47
1:B:545:THR:OG1	1:B:560:TYR:OH	2.28	0.47
1:A:496:TYR:HB2	1:A:510:PHE:HB3	1.96	0.47
1:A:364:LYS:HG3	1:A:368:TYR:CD2	2.50	0.47
1:A:570:ARG:HD2	1:A:570:ARG:HA	1.67	0.46
1:B:611:ARG:NH1	1:B:620:CYS:SG	2.89	0.46
1:B:584:LEU:H	1:B:584:LEU:HG	1.26	0.46
1:A:538:ASP:OD1	1:A:539:LYS:N	2.49	0.46
1:A:273:ARG:NH1	1:A:594:THR:HG1	2.13	0.46
1:B:538:ASP:OD1	1:B:539:LYS:N	2.49	0.46
1:A:251:LEU:HD13	1:A:332:LEU:HD13	1.98	0.46
1:B:364:LYS:HG3	1:B:368:TYR:CD2	2.50	0.46
1:B:466:ARG:HE	1:B:476:HIS:HD2	1.62	0.46
1:B:594:THR:O	1:B:594:THR:HG23	2.17	0.45
1:A:584:LEU:H	1:A:584:LEU:HG	1.30	0.45
1:A:594:THR:O	1:A:594:THR:HG23	2.17	0.45
1:A:611:ARG:NH1	1:A:620:CYS:SG	2.89	0.45
1:B:422:LYS:H	1:B:422:LYS:HG2	1.50	0.45
1:A:271:ILE:O	1:A:352:TYR:OH	2.34	0.44
1:A:361:ASN:ND2	1:A:363:THR:OG1	2.40	0.44
1:B:384:ALA:HB1	1:B:385:PRO:HD2	1.99	0.44
1:B:571:PHE:O	1:B:573:TRP:N	2.43	0.44
1:A:576:GLN:HE21	1:A:576:GLN:N	2.14	0.44
1:B:251:LEU:HD13	1:B:332:LEU:HD13	1.98	0.44
1:A:332:LEU:HD12	1:A:332:LEU:HA	1.85	0.44
1:A:405:VAL:O	1:A:409:ASP:HB2	2.17	0.44
2:B:1001:8PE:H38	2:B:1001:8PE:H3BA	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:405:VAL:O	1:B:409:ASP:HB2	2.18	0.44
1:A:454:ILE:N	1:A:455:PRO:HD2	2.33	0.43
1:B:454:ILE:N	1:B:455:PRO:HD2	2.33	0.43
1:B:466:ARG:HE	1:B:476:HIS:CD2	2.37	0.43
1:A:384:ALA:HB1	1:A:385:PRO:HD2	1.99	0.43
1:B:406:ILE:HG23	2:B:1001:8PE:H3HA	2.00	0.43
1:A:548:ARG:NH1	1:A:613:GLU:OE1	2.51	0.43
1:B:548:ARG:NH1	1:B:613:GLU:OE1	2.51	0.43
1:A:252:VAL:O	1:A:256:VAL:HG23	2.19	0.43
1:A:495:LEU:HD23	1:A:495:LEU:HA	1.89	0.42
1:B:252:VAL:O	1:B:256:VAL:HG23	2.19	0.42
3:A:1002:CLR:H273	3:A:1002:CLR:H232	1.75	0.42
1:A:361:ASN:HB3	1:A:371:ARG:NH1	2.35	0.42
1:A:575:ILE:O	1:A:579:ILE:N	2.49	0.42
1:B:264:SER:HB3	1:B:431:PRO:HD2	2.02	0.42
1:A:466:ARG:HE	1:A:476:HIS:CD2	2.36	0.42
1:A:573:TRP:O	1:A:577:ILE:HG22	2.19	0.42
1:B:278:LEU:HD21	2:B:1001:8PE:H3AB	2.00	0.42
1:B:463:CYS:SG	1:B:479:ASN:HB3	2.60	0.42
1:A:278:LEU:HD21	2:A:1001:8PE:H3AB	2.01	0.42
1:A:310:ASN:HA	2:A:1001:8PE:O14	2.20	0.42
1:B:516:VAL:O	1:B:519:ILE:HB	2.20	0.42
1:A:264:SER:HB3	1:A:431:PRO:HD2	2.02	0.42
1:A:463:CYS:SG	1:A:479:ASN:HB3	2.60	0.42
1:A:516:VAL:O	1:A:519:ILE:HB	2.20	0.42
1:A:573:TRP:HA	1:A:576:GLN:NE2	2.34	0.42
1:B:361:ASN:HB3	1:B:371:ARG:NH1	2.35	0.42
1:B:573:TRP:O	1:B:577:ILE:HG22	2.19	0.42
1:B:492:PHE:CE2	1:B:513:LEU:HB3	2.55	0.42
1:B:544:ASN:HB3	1:B:547:LEU:HB2	2.02	0.42
1:A:406:ILE:HG23	2:A:1001:8PE:H3HA	2.00	0.41
1:B:263:ARG:HG3	1:B:430:LEU:HB3	2.01	0.41
1:B:361:ASN:HB3	1:B:371:ARG:HH12	1.86	0.41
1:A:492:PHE:CE2	1:A:513:LEU:HB3	2.55	0.41
1:A:544:ASN:HB3	1:A:547:LEU:HB2	2.02	0.41
1:A:564:ILE:HD13	1:A:564:ILE:HA	1.96	0.41
1:A:263:ARG:HG3	1:A:430:LEU:HB3	2.01	0.41
1:A:442:LYS:HE3	1:A:442:LYS:HB2	1.84	0.41
1:B:306:ASN:HD21	1:B:308:ARG:HG3	1.86	0.41
1:A:594:THR:O	1:A:594:THR:CG2	2.69	0.41
1:B:271:ILE:O	1:B:352:TYR:OH	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:GLU:OE1	1:B:427:LYS:N	2.54	0.41
1:A:270:ARG:NH1	1:A:412:TYR:OH	2.54	0.41
1:A:441:HIS:CE1	1:A:442:LYS:HG3	2.55	0.41
1:A:595:VAL:O	1:A:595:VAL:CG1	2.67	0.41
1:B:270:ARG:NH1	1:B:412:TYR:OH	2.54	0.41
1:B:512:TYR:O	1:B:516:VAL:HG23	2.21	0.41
1:B:576:GLN:HG2	1:B:592:ILE:HB	2.03	0.41
1:A:329:LEU:HD23	1:A:329:LEU:HA	1.87	0.41
1:B:285:LEU:HD12	1:B:285:LEU:HA	1.91	0.41
1:B:441:HIS:CE1	1:B:442:LYS:HG3	2.55	0.41
1:B:594:THR:O	1:B:594:THR:CG2	2.69	0.41
1:A:361:ASN:HB3	1:A:371:ARG:HH12	1.86	0.40
1:B:310:ASN:HA	2:B:1001:8PE:O14	2.21	0.40
1:A:425:GLU:OE1	1:A:427:LYS:N	2.54	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	393/969 (41%)	351 (89%)	41 (10%)	1 (0%)	37	66
1	B	393/969 (41%)	352 (90%)	40 (10%)	1 (0%)	37	66
All	All	786/1938 (41%)	703 (89%)	81 (10%)	2 (0%)	38	66

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	230	PRO
1	B	230	PRO

5.3.2 Protein sidechains (i)

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	352/857 (41%)	317 (90%)	35 (10%)	6 25
1	B	352/857 (41%)	318 (90%)	34 (10%)	6 26
All	All	704/1714 (41%)	635 (90%)	69 (10%)	9 25

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	273	ARG
1	A	298	ASN
1	A	342	ILE
1	A	382	PHE
1	A	394	PHE
1	A	407	LEU
1	A	409	ASP
1	A	419	LEU
1	A	422	LYS
1	A	439	ILE
1	A	441	HIS
1	A	445	TYR
1	A	452	GLN
1	A	465	ARG
1	A	470	THR
1	A	477	LEU
1	A	479	ASN
1	A	496	TYR
1	A	498	THR
1	A	504	HIS
1	A	518	TYR
1	A	524	TYR
1	A	561	CYS
1	A	565	GLU
1	A	575	ILE
1	A	576	GLN
1	A	579	ILE

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Mol	Chain	Res	Type
1	A	584	LEU
1	A	585	LEU
1	A	592	ILE
1	A	594	THR
1	A	613	GLU
1	A	618	ASN
1	A	622	GLU
1	A	626	VAL
1	B	273	ARG
1	B	298	ASN
1	B	342	ILE
1	B	382	PHE
1	B	394	PHE
1	B	407	LEU
1	B	409	ASP
1	B	419	LEU
1	B	422	LYS
1	B	439	ILE
1	B	441	HIS
1	B	445	TYR
1	B	452	GLN
1	B	465	ARG
1	B	470	THR
1	B	477	LEU
1	B	479	ASN
1	B	496	TYR
1	B	498	THR
1	B	504	HIS
1	B	518	TYR
1	B	524	TYR
1	B	561	CYS
1	B	565	GLU
1	B	575	ILE
1	B	579	ILE
1	B	584	LEU
1	B	585	LEU
1	B	592	ILE
1	B	594	THR
1	B	598	PRO
1	B	613	GLU
1	B	618	ASN
1	B	626	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	294	GLN
1	A	298	ASN
1	A	315	HIS
1	A	399	GLN
1	A	499	HIS
1	A	576	GLN
1	A	587	HIS
1	A	608	ASN
1	A	614	ASN
1	B	294	GLN
1	B	298	ASN
1	B	315	HIS
1	B	399	GLN
1	B	499	HIS
1	B	576	GLN
1	B	587	HIS
1	B	608	ASN
1	B	614	ASN

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

4 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	8PE	A	1001	-	46,46,46	0.91	1 (2%)	49,51,51	0.82	0
3	CLR	B	1002	-	31,31,31	1.05	1 (3%)	48,48,48	1.80	11 (22%)
2	8PE	B	1001	-	46,46,46	0.91	1 (2%)	49,51,51	0.82	1 (2%)
3	CLR	A	1002	-	31,31,31	1.05	1 (3%)	48,48,48	1.80	11 (22%)

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	8PE	A	1001	-	-	28/50/50/50	-
3	CLR	B	1002	-	-	6/10/68/68	0/4/4/4
2	8PE	B	1001	-	-	28/50/50/50	-
3	CLR	A	1002	-	-	6/10/68/68	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	8PE	C32-C31	-2.22	1.44	1.50
2	B	1001	8PE	C32-C31	-2.19	1.44	1.50
3	B	1002	CLR	C20-C17	-2.19	1.50	1.54
3	A	1002	CLR	C20-C17	-2.18	1.50	1.54

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1002	CLR	C16-C17-C20	-4.98	104.44	112.15
3	A	1002	CLR	C16-C17-C20	-4.98	104.44	112.15
3	A	1002	CLR	C2-C3-C4	-4.46	104.18	110.31
3	B	1002	CLR	C2-C3-C4	-4.46	104.19	110.31
3	A	1002	CLR	C7-C8-C14	-3.88	105.28	110.91
3	B	1002	CLR	C7-C8-C14	-3.86	105.31	110.91
3	B	1002	CLR	C18-C13-C17	-3.46	105.25	111.71
3	A	1002	CLR	C18-C13-C17	-3.46	105.26	111.71
3	B	1002	CLR	C12-C13-C17	3.29	121.50	116.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1002	CLR	C12-C13-C17	3.26	121.45	116.57
3	A	1002	CLR	C11-C9-C8	-2.86	107.63	111.75
3	B	1002	CLR	C11-C9-C8	-2.82	107.69	111.75
3	B	1002	CLR	C15-C14-C13	-2.63	100.67	103.84
3	A	1002	CLR	C15-C14-C13	-2.61	100.70	103.84
3	A	1002	CLR	C15-C14-C8	-2.26	115.36	119.08
3	B	1002	CLR	C15-C14-C8	-2.19	115.48	119.08
3	A	1002	CLR	C1-C10-C9	2.16	111.74	108.73
3	B	1002	CLR	C1-C10-C9	2.16	111.74	108.73
3	A	1002	CLR	C13-C17-C20	-2.08	116.23	119.49
3	B	1002	CLR	C13-C17-C20	-2.05	116.28	119.49
3	A	1002	CLR	C19-C10-C1	-2.02	106.23	109.43
3	B	1002	CLR	C19-C10-C1	-2.01	106.26	109.43
2	B	1001	8PE	C2-O21-C21	2.00	122.72	117.79

There are no chirality outliers.

All (68) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	8PE	C11-O13-P-O11
2	A	1001	8PE	C11-O13-P-O12
2	A	1001	8PE	C22-C21-O21-C2
2	B	1001	8PE	C11-O13-P-O11
2	B	1001	8PE	C11-O13-P-O12
2	B	1001	8PE	C22-C21-O21-C2
2	A	1001	8PE	O22-C21-O21-C2
2	B	1001	8PE	O22-C21-O21-C2
3	A	1002	CLR	C21-C20-C22-C23
3	B	1002	CLR	C21-C20-C22-C23
2	A	1001	8PE	C3A-C3B-C3C-C3D
2	B	1001	8PE	C3A-C3B-C3C-C3D
2	A	1001	8PE	C38-C39-C3A-C3B
2	B	1001	8PE	C38-C39-C3A-C3B
2	A	1001	8PE	C21-C22-C23-C24
2	B	1001	8PE	C21-C22-C23-C24
2	A	1001	8PE	C1-O11-P-O13
2	B	1001	8PE	C1-O11-P-O13
2	A	1001	8PE	C29-C2A-C2B-C2C
2	B	1001	8PE	C29-C2A-C2B-C2C
2	A	1001	8PE	C3C-C3D-C3E-C3F
2	B	1001	8PE	C3C-C3D-C3E-C3F
3	A	1002	CLR	C17-C20-C22-C23

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Mol	Chain	Res	Type	Atoms
2	B	1001	8PE	C36-C37-C38-C39
3	B	1002	CLR	C17-C20-C22-C23
2	A	1001	8PE	C36-C37-C38-C39
2	A	1001	8PE	C33-C34-C35-C36
2	B	1001	8PE	C33-C34-C35-C36
2	B	1001	8PE	C37-C38-C39-C3A
2	A	1001	8PE	C37-C38-C39-C3A
2	A	1001	8PE	C35-C36-C37-C38
2	B	1001	8PE	C35-C36-C37-C38
2	A	1001	8PE	C31-C32-C33-C34
2	B	1001	8PE	C31-C32-C33-C34
2	A	1001	8PE	C3F-C3G-C3H-C3I
2	B	1001	8PE	C3F-C3G-C3H-C3I
3	A	1002	CLR	C23-C24-C25-C27
3	B	1002	CLR	C23-C24-C25-C27
2	B	1001	8PE	C2B-C2C-C2D-C2E
2	A	1001	8PE	C2B-C2C-C2D-C2E
2	A	1001	8PE	O11-C1-C2-O21
2	B	1001	8PE	O11-C1-C2-O21
3	A	1002	CLR	C23-C24-C25-C26
3	B	1002	CLR	C23-C24-C25-C26
2	A	1001	8PE	C26-C27-C28-C29
2	B	1001	8PE	C26-C27-C28-C29
3	A	1002	CLR	C13-C17-C20-C21
3	B	1002	CLR	C13-C17-C20-C21
2	A	1001	8PE	O21-C2-C3-O31
2	B	1001	8PE	O21-C2-C3-O31
2	A	1001	8PE	C1-O11-P-O12
2	B	1001	8PE	C1-O11-P-O12
2	A	1001	8PE	O11-C1-C2-C3
2	B	1001	8PE	O11-C1-C2-C3
2	A	1001	8PE	C28-C29-C2A-C2B
2	B	1001	8PE	C28-C29-C2A-C2B
2	A	1001	8PE	C1-C2-C3-O31
2	B	1001	8PE	C1-C2-C3-O31
3	A	1002	CLR	C13-C17-C20-C22
3	B	1002	CLR	C13-C17-C20-C22
2	A	1001	8PE	C39-C3A-C3B-C3C
2	B	1001	8PE	C39-C3A-C3B-C3C
2	A	1001	8PE	O21-C21-C22-C23
2	B	1001	8PE	O21-C21-C22-C23
2	B	1001	8PE	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
2	A	1001	8PE	C34-C35-C36-C37
2	A	1001	8PE	O22-C21-C22-C23
2	B	1001	8PE	O22-C21-C22-C23

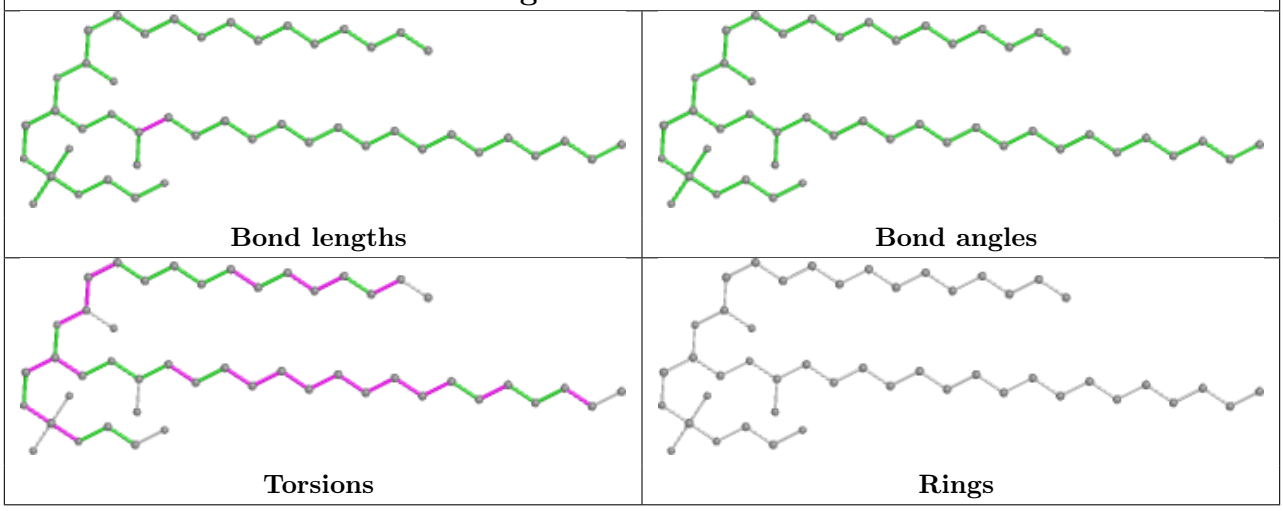
There are no ring outliers.

4 monomers are involved in 22 short contacts:

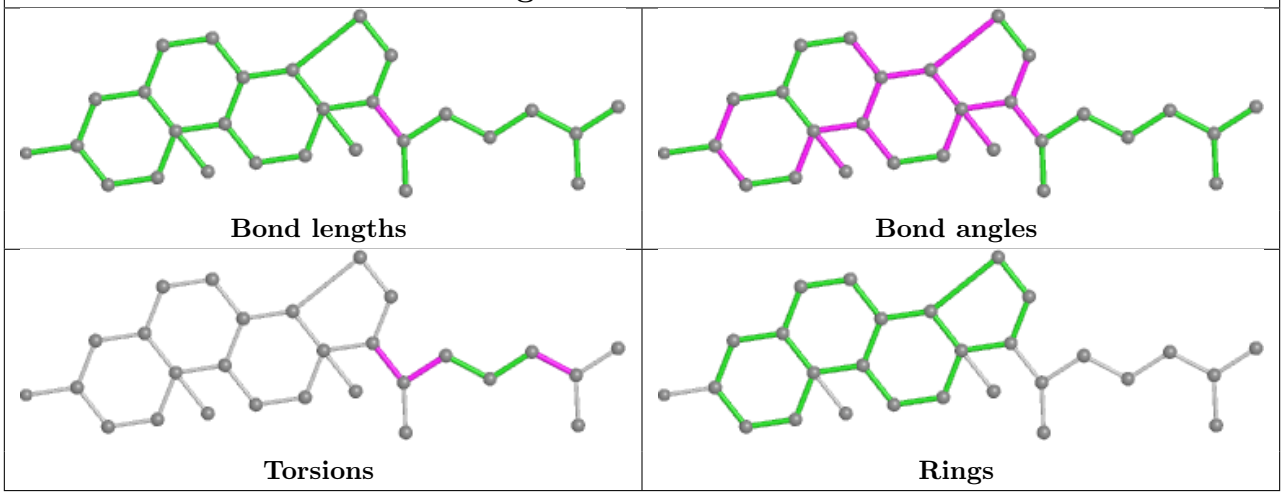
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	8PE	5	0
3	B	1002	CLR	4	0
2	B	1001	8PE	6	0
3	A	1002	CLR	7	0

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 then 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.

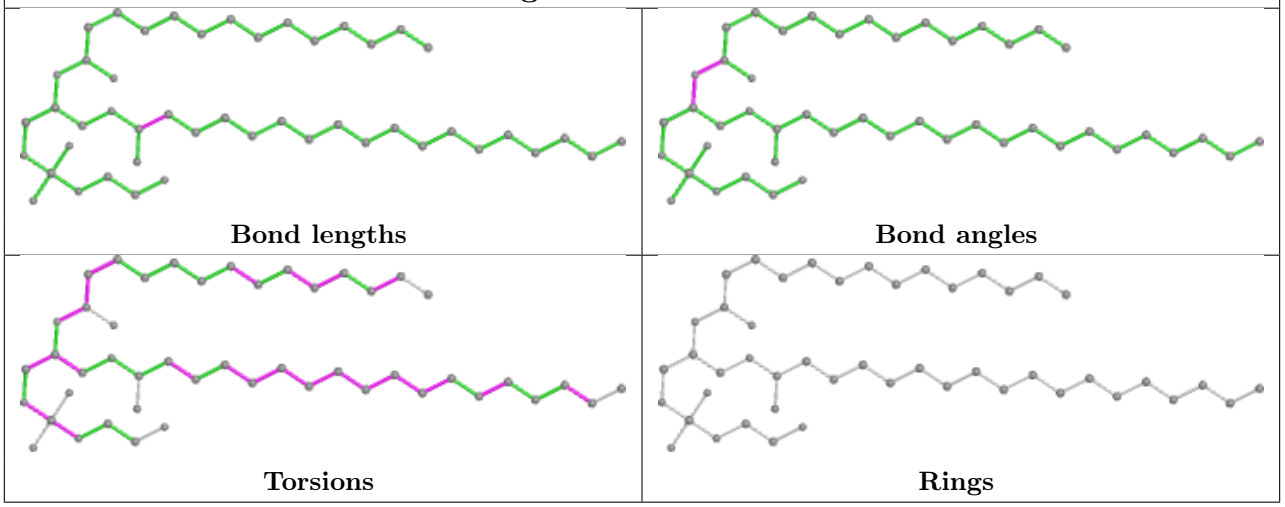
Ligand 8PE A 1001



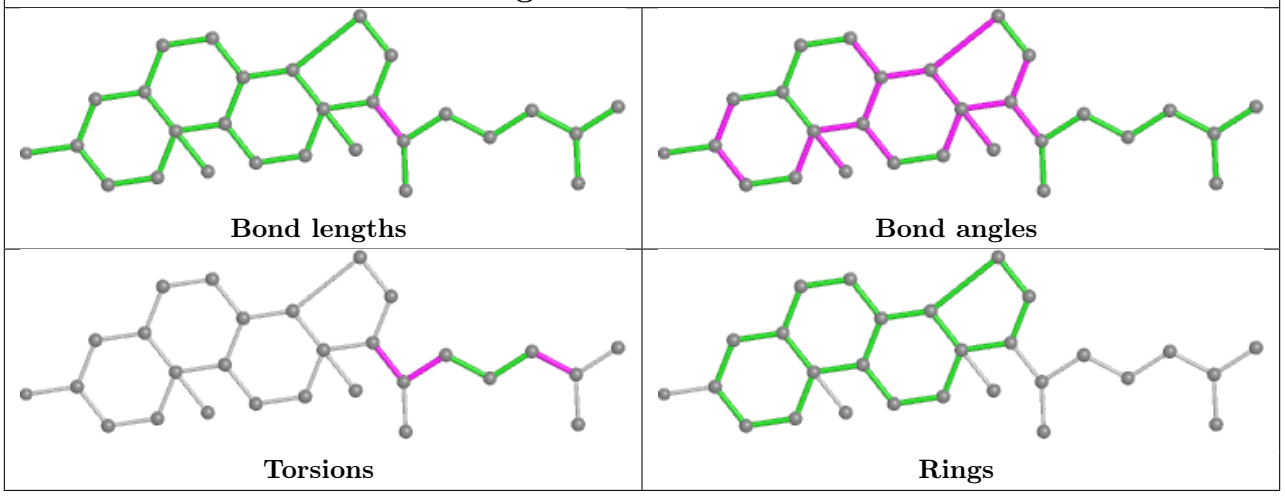
Ligand CLR B 1002



Ligand 8PE B 1001



Ligand CLR A 1002



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.