

Full wwPDB X-ray Structure Validation Report (i)

Oct 23, 2021 – 11:22 AM EDT

PDB ID	:	1FNP
Title	:	CRYSTAL STRUCTURE ANALYSIS OF THE MUTANT REACTION CEN-
		TER PRO L209-> PHE FROM THE PHOTOSYNTHETIC PURPLE BAC-
		TERIUM RHODOBACTER SPHAEROIDES
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Deposited on	:	2000-08-23
Resolution	:	2.60 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org* A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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.



Motria	Whole archive	Similar resolution				
wietric	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$				
Clashscore	141614	3518 (2.60-2.60)				
Ramachandran outliers	138981	3455 (2.60-2.60)				
Sidechain outliers	138945	3455 (2.60-2.60)				

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain		
1	L	281	74%	24%	•
2	М	307	73%	22%	••
3	Н	260	76%	14% •	8%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	BCL	L	304	Х	-	-	-
4	BCL	М	801	Х	-	-	-



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2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 7256 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

• Molecule 1 is a protein called REACTION CENTER PROTEIN L CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	281	Total 2236	C 1511	N 355	O 362	S 8	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	209	PHE	PRO	engineered mutation	UNP P02954

• Molecule 2 is a protein called REACTION CENTER PROTEIN M CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	М	301	Total 2399	C 1600	N 393	O 396	S 10	0	0	0

• Molecule 3 is a protein called REACTION CENTER PROTEIN H CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	Н	240	Total 1829	C 1169	N 314	0 337	S 9	0	0	0

• Molecule 4 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).





Mol	Chain	Residues		At	oms			ZeroOcc	AltConf
4	т	1	Total	С	Mg	Ν	Ο	0	0
4		1	66	55	1	4	6	0	0
4	т	1	Total	С	Mg	Ν	Ο	0	0
	1	66	55	1	4	6	0	0	
4	м	1	Total	С	Mg	Ν	0	0	0
4	111	1	66	55	1	4	6	0	0
	м	1	Total	С	Mg	Ν	Ο	0	0
4	111	1	66	55	1	4	6	0	0





Mol	Chain	Residues	A	ton	ns		ZeroOcc	AltConf
5	L	1	Total 65	C 55	N 4	O 6	0	0
5	М	1	Total 65	C 55	N 4	O 6	0	0

• Molecule 6 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	L	1	Total C O 48 44 4	0	0
6	М	1	Total C O 48 44 4	0	0

• Molecule 7 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $\rm C_{14}H_{31}NO).$





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	L	1	Total C N O 16 14 1 1	0	0
7	М	1	Total C N O 16 14 1 1	0	0
7	М	1	Total C N O 16 14 1 1	0	0
7	М	1	Total C N O 16 14 1 1	0	0
7	М	1	Total C N O 16 14 1 1	0	0
7	Н	1	Total C N O 16 14 1 1	0	0
7	Н	1	Total C N O 16 14 1 1	0	0

• Molecule 8 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	М	1	Total Fe 1 1	0	0

• Molecule 9 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).





Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
9	М	1	Total 5	0 4	Р 1	0	0

• Molecule 10 is SPHEROIDENE (three-letter code: SPO) (formula: $C_{41}H_{60}O$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
10	М	1	Total 42	C 41	0 1	0	0

• Molecule 11 is water.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	L	38	Total O 38 38	0	0
11	М	39	Total O 39 39	0	0
11	Н	65	Total O 65 65	0	0



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.

Note EDS was not executed.

• Molecule 1: REACTION CENTER PROTEIN L CHAIN





4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source	
Space group	P 31 2 1	Depositor	
Cell constants	141.75Å 141.75Å 187.41Å	Deperitor	
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor	
Resolution (Å)	50.00 - 2.60	Depositor	
% Data completeness	92.2 (50.00-2.60)	Depositor	
(in resolution range)	52.2 (50.00-2.00)		
R_{merge}	0.05	Depositor	
R_{sym}	(Not available)	Depositor	
Refinement program	CNS 0.3	Depositor	
R, R_{free}	0.216 , 0.248	Depositor	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	7256	wwPDB-VP	
Average B, all atoms $(Å^2)$	60.0	wwPDB-VP	



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: BCL, BPH, PO4, U10, SPO, FE, LDA

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).

Mal	Chain	Bond	lengths	Bond angles		
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	L	0.44	0/2324	0.48	0/3179	
2	М	0.43	0/2491	0.49	1/3400~(0.0%)	
3	Н	0.42	0/1877	0.53	0/2553	
All	All	0.43	0/6692	0.50	1/9132~(0.0%)	

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	L	0	1
2	М	0	3
All	All	0	4

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	М	213	LEU	CA-CB-CG	5.14	127.12	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	10	ARG	Sidechain
2	М	197	TYR	Sidechain
2	М	252	ARG	Sidechain
2	М	47	GLY	Peptide



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	L	2236	0	2189	53	0
2	М	2399	0	2306	59	0
3	Н	1829	0	1836	34	0
4	L	132	0	148	12	0
4	М	132	0	148	12	0
5	L	65	0	76	8	0
5	М	65	0	76	11	0
6	L	48	0	63	8	0
6	М	48	0	63	2	0
7	Н	32	0	62	2	0
7	L	16	0	31	0	0
7	М	64	0	124	1	0
8	М	1	0	0	0	0
9	М	5	0	0	1	0
10	М	42	0	60	1	0
11	Н	65	0	0	4	0
11	L	38	0	0	6	0
11	М	39	0	0	0	0
All	All	7256	0	7182	154	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 (154) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
4:L:304:BCL:HHC	4:L:304:BCL:HBB2	1.42	1.02
5:L:402:BPH:HHC	5:L:402:BPH:HBB3	1.48	0.95
4:M:801:BCL:HBB2	4:M:801:BCL:HHC	1.49	0.92
2:M:152:ALA:HB2	5:M:401:BPH:HAC1	1.54	0.90
3:H:194:GLN:HE21	3:H:194:GLN:H	1.21	0.85
4:L:302:BCL:CBB	4:L:302:BCL:HHC	2.10	0.82
11:L:731:HOH:O	2:M:217:MET:SD	2.39	0.81
11:L:706:HOH:O	2:M:252:ARG:HD3	1.82	0.79
4:M:802:BCL:HHC	4:M:802:BCL:CBB	2.15	0.77



	t i c	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
4:M:802:BCL:HHC	4:M:802:BCL:HBB3	1.67	0.77	
5:L:402:BPH:HBB2	2:M:209:TYR:HB3	1.68	0.76	
2:M:214:LEU:HA	2:M:217:MET:HE2	1.69	0.73	
4:M:801:BCL:HHC	4:M:801:BCL:CBB	2.17	0.73	
3:H:148:PRO:HA	3:H:151:LEU:HD22	1.71	0.72	
2:M:196:PHE:CZ	4:M:802:BCL:HBB2	2.26	0.71	
1:L:167:PHE:HB3	4:L:302:BCL:HMC3	1.72	0.71	
2:M:45:GLN:HE21	2:M:47:GLY:HA3	1.56	0.71	
1:L:241:VAL:HG21	5:L:402:BPH:HAC2	1.70	0.70	
2:M:196:PHE:HZ	4:M:802:BCL:HBB2	1.56	0.69	
4:L:304:BCL:HHC	4:L:304:BCL:CBB	2.20	0.68	
4:M:801:BCL:HBB3	4:M:802:BCL:H41	1.76	0.66	
1:L:30:TYR:O	1:L:103:ARG:NH2	2.29	0.66	
1:L:209:PHE:CE2	3:H:173:GLU:HG3	2.30	0.66	
4:L:302:BCL:HHC	4:L:302:BCL:HBB2	1.77	0.66	
3:H:94:GLU:HG3	11:H:744:HOH:O	1.95	0.65	
1:L:131:LEU:HD11	4:L:302:BCL:HED3	1.79	0.65	
2:M:242:THR:O	2:M:246:ARG:HG2	1.96	0.65	
1:L:190:HIS:HD1	6:L:502:U10:H4M1	1.62	0.64	
1:L:168:HIS:NE2	4:L:302:BCL:HBB2	2.14	0.63	
5:M:401:BPH:HBB3	5:M:401:BPH:HHC	1.80	0.62	
3:H:148:PRO:O	3:H:151:LEU:HB2	1.99	0.62	
2:M:118:SER:HB3	10:M:600:SPO:H311	1.82	0.62	
1:L:197:ALA:HB1	2:M:234:LEU:HD21	1.82	0.61	
1:L:7:ARG:HH21	3:H:98:HIS:CD2	2.18	0.61	
1:L:264:GLN:HA	1:L:267:VAL:HG12	1.82	0.60	
5:L:402:BPH:HBB3	5:L:402:BPH:CHC	2.28	0.60	
3:H:14:SER:HA	3:H:17:ILE:HG22	1.82	0.59	
4:L:302:BCL:H52	4:L:304:BCL:HBB3	1.83	0.59	
2:M:20:THR:HG23	2:M:25:LEU:HD21	1.84	0.58	
3:H:37:ARG:NH1	3:H:60:LYS:O	2.35	0.58	
1:L:69:PRO:HG2	1:L:142:TRP:HB2	1.86	0.58	
2:M:241:GLY:CA	3:H:117:ARG:HD2	2.34	0.58	
1:L:182:THR:HG22	1:L:236:LEU:HD13	1.86	0.58	
2:M:198:ASN:C	2:M:198:ASN:HD22	2.06	0.58	
4:L:302:BCL:HHC	4:L:302:BCL:HBB3	1.84	0.57	
2:M:228:PHE:HB2	2:M:243:ALA:HB2	1.86	0.57	
2:M:178:ILE:HG23	4:M:801:BCL:HED1	1.87	0.57	
1:L:103:ARG:HG3	11:L:711:HOH:O	2.04	0.57	
2:M:156:TRP:HB2	4:M:802:BCL:H62	1.85	0.57	
1:L:171:PRO:HA	1:L:174:MET:HG3	1.86	0.56	



		Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
6:M:501:U10:H202	7:H:702:LDA:H121	1.86	0.56	
1:L:7:ARG:NH2	3:H:98:HIS:CD2	2.74	0.56	
1:L:103:ARG:NH1	2:M:254:THR:O	2.39	0.56	
3:H:173:GLU:HG2	11:H:750:HOH:O	2.05	0.56	
2:M:242:THR:OG1	2:M:246:ARG:HD3	2.05	0.55	
4:M:801:BCL:HBB3	4:M:802:BCL:C4	2.37	0.55	
1:L:124:ALA:HB2	5:L:402:BPH:HAC1	1.89	0.54	
1:L:62:GLN:HE21	1:L:151:TRP:HE1	1.53	0.54	
2:M:10:GLN:HB2	3:H:144:ALA:HB3	1.90	0.53	
9:M:800:PO4:O3	7:M:704:LDA:HM23	2.08	0.53	
2:M:62:GLY:HA3	5:M:401:BPH:H6C1	1.91	0.53	
2:M:239:ASP:O	3:H:117:ARG:NH2	2.42	0.53	
1:L:181:PHE:CD2	5:M:401:BPH:HBB1	2.43	0.53	
1:L:197:ALA:CB	2:M:234:LEU:HD21	2.39	0.52	
1:L:117:ILE:HB	1:L:118:PRO:HD3	1.91	0.52	
2:M:147:TRP:HA	2:M:147:TRP:CE3	2.45	0.52	
3:H:206:ASN:HD21	3:H:248:ARG:HD2	1.74	0.52	
2:M:76:GLN:HE22	2:M:92:SER:H	1.58	0.51	
3:H:70:ARG:NH1	3:H:121:PRO:O	2.42	0.51	
2:M:107:PRO:HG2	2:M:110:GLU:HB2	1.92	0.51	
3:H:34:GLU:O	3:H:37:ARG:HG3	2.11	0.51	
2:M:84:PHE:HD2	2:M:85:LEU:HD12	1.76	0.50	
2:M:96:PRO:HG2	2:M:170:TRP:HB2	1.94	0.50	
3:H:32:GLN:NE2	7:H:702:LDA:H22	2.27	0.50	
1:L:135:ARG:HB3	1:L:136:PRO:HD3	1.94	0.50	
2:M:31:VAL:HG13	2:M:47:GLY:HA2	1.94	0.50	
2:M:147:TRP:HA	2:M:147:TRP:HE3	1.77	0.50	
1:L:69:PRO:HD3	1:L:83:GLY:O	2.12	0.49	
5:L:402:BPH:HMC3	2:M:212:ALA:HB3	1.93	0.49	
5:L:402:BPH:HMC3	2:M:212:ALA:CB	2.43	0.49	
2:M:198:ASN:HD22	2:M:200:PHE:H	1.60	0.49	
1:L:190:HIS:HA	6:L:502:U10:H4M1	1.95	0.49	
1:L:231:ARG:HD3	2:M:4:ASN:O	2.13	0.49	
1:L:227:LEU:O	1:L:231:ARG:HG3	2.13	0.48	
2:M:198:ASN:ND2	2:M:200:PHE:H	2.11	0.48	
2:M:241:GLY:HA2	3:H:117:ARG:HD2	1.94	0.48	
2:M:2:TYR:CZ	2:M:4:ASN:HA	2.49	0.48	
3:H:156:CYS:HB3	3:H:206:ASN:O	2.14	0.48	
5:M:401:BPH:H7C1	5:M:401:BPH:H4C1	1.96	0.47	
1:L:131:LEU:HD11	4:L:302:BCL:CED	2.44	0.47	
3:H:219:ILE:HG21	3:H:225:VAL:HG13	1.96	0.47	



		Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:L:223:SER:HA	6:L:502:U10:H1M2	1.96	0.47	
2:M:214:LEU:HD23	2:M:217:MET:CE	2.45	0.47	
2:M:234:LEU:HD12	2:M:234:LEU:HA	1.74	0.47	
2:M:214:LEU:HD23	2:M:217:MET:HE3	1.96	0.47	
1:L:181:PHE:HB3	5:M:401:BPH:CBB	2.44	0.46	
5:L:402:BPH:HHC	5:L:402:BPH:CBB	2.30	0.46	
1:L:129:LEU:O	1:L:133:LEU:HB3	2.15	0.46	
2:M:240:ARG:HD3	2:M:245:GLU:HG2	1.99	0.45	
1:L:18:GLY:O	1:L:21:LEU:HB2	2.16	0.45	
1:L:87:GLN:NE2	1:L:142:TRP:CD1	2.85	0.45	
2:M:45:GLN:HG2	2:M:47:GLY:H	1.82	0.45	
2:M:158:VAL:HA	2:M:162:ILE:HB	1.97	0.45	
2:M:15:ALA:HB1	2:M:31:VAL:HG21	1.99	0.45	
3:H:121:PRO:HB3	3:H:225:VAL:O	2.16	0.45	
3:H:70:ARG:HB3	3:H:118:ARG:HH12	1.80	0.45	
6:L:502:U10:H121	6:L:502:U10:H101	1.53	0.44	
1:L:104:GLU:HB3	1:L:118:PRO:HG3	1.99	0.44	
1:L:130:THR:HA	1:L:134:PHE:HB2	1.99	0.44	
3:H:241:LEU:HB2	11:H:707:HOH:O	2.17	0.44	
3:H:117:ARG:NH1	3:H:227:LEU:HD22	2.33	0.44	
1:L:173:HIS:CE1	1:L:177:ILE:HD11	2.53	0.44	
2:M:51:LEU:HD23	2:M:51:LEU:HA	1.85	0.43	
3:H:134:MET:HB2	3:H:167:ILE:O	2.18	0.43	
3:H:194:GLN:HE21	3:H:194:GLN:N	2.03	0.43	
1:L:60:ASN:O	1:L:64:ILE:HG13	2.17	0.43	
2:M:62:GLY:CA	5:M:401:BPH:H6C1	2.48	0.43	
1:L:225:GLY:H	6:L:502:U10:H3M2	1.84	0.43	
3:H:122:GLU:HB2	3:H:227:LEU:HD21	2.00	0.43	
1:L:58:THR:HG22	11:L:723:HOH:O	2.18	0.43	
1:L:183:ASN:ND2	1:L:237:SER:OG	2.51	0.43	
1:L:193:LEU:HD23	6:L:502:U10:H4M3	2.01	0.43	
1:L:84:GLY:O	1:L:88:ILE:HG13	2.19	0.43	
1:L:227:LEU:HD21	2:M:4:ASN:OD1	2.19	0.43	
2:M:52:GLY:O	2:M:56:VAL:HG23	2.19	0.43	
3:H:126:HIS:HB2	3:H:128:HIS:CD2	2.53	0.42	
1:L:7:ARG:HH21	3:H:98:HIS:CG	2.38	0.42	
1:L:224:ILE:HG13	2:M:42:GLY:HA3	2.02	0.42	
4:L:304:BCL:CBB	4:L:304:BCL:CHC	2.90	0.42	
2:M:163:ARG:O	2:M:167:MET:HG2	2.19	0.42	
5:M:401:BPH:H6C2	5:M:401:BPH:H102	1.88	0.42	
2:M:12:ARG:O	3:H:140:PHE:HA	2.20	0.42	



A + a = 1	A + 2	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
3:H:11:ASP:HA	11:H:745:HOH:O	2.20	0.42	
1:L:128:TYR:HD1	4:L:304:BCL:HBB1	1.84	0.42	
2:M:188:PHE:O	2:M:192:HIS:HD2	2.02	0.42	
2:M:274:LEU:HD23	2:M:277:LEU:HD23	2.01	0.42	
1:L:100:TRP:CZ2	6:M:501:U10:H251	2.55	0.41	
1:L:189:LEU:HD13	1:L:216:PHE:HZ	1.84	0.41	
2:M:113:LEU:HD23	2:M:113:LEU:HA	1.93	0.41	
1:L:190:HIS:HD1	6:L:502:U10:C4M	2.32	0.41	
2:M:186:ASN:HA	4:M:802:BCL:HBC3	2.03	0.41	
5:M:401:BPH:H4C1	5:M:401:BPH:C7	2.48	0.41	
2:M:4:ASN:ND2	3:H:194:GLN:HG3	2.35	0.41	
2:M:198:ASN:HD22	2:M:199:PRO:N	2.19	0.41	
3:H:181:VAL:O	3:H:188:THR:HA	2.21	0.41	
1:L:8:LYS:HA	3:H:87:LEU:HD11	2.04	0.41	
2:M:67:PHE:O	2:M:71:ILE:HG12	2.21	0.41	
6:L:502:U10:H1M1	6:L:502:U10:H72	1.68	0.40	
1:L:269:LEU:HB2	1:L:272:TRP:NE1	2.37	0.40	
4:M:801:BCL:O2A	5:M:401:BPH:HBB2	2.21	0.40	
1:L:217:ARG:HD2	11:L:724:HOH:O	2.20	0.40	
1:L:219:LEU:HD12	2:M:131:ARG:NH2	2.36	0.40	
5:M:401:BPH:HBB3	5:M:401:BPH:CHC	2.50	0.40	
1:L:67:TYR:HE1	11:L:722:HOH:O	2.04	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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
1	L	279/281~(99%)	269~(96%)	10 (4%)	0	100	100
2	М	299/307~(97%)	283~(95%)	14~(5%)	2(1%)	22	43
3	Н	238/260~(92%)	229 (96%)	9~(4%)	0	100	100



Continued from previous page...

Mol	Chain	Analysed	Favoured Allowed		Outliers	Percentiles	
All	All	816/848~(96%)	781 (96%)	33 (4%)	2~(0%)	47 71	

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	М	4	ASN
2	М	300	HIS

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric Outliers		Percentiles		
1	L	220/220~(100%)	203~(92%)	17 (8%)	13 25		
2	М	235/240~(98%)	213~(91%)	22 (9%)	8 17		
3	Н	195/208~(94%)	179 (92%)	16 (8%)	11 22		
All	All	650/668~(97%)	595~(92%)	55~(8%)	10 21		

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	7	ARG
1	L	16	LEU
1	L	44	LEU
1	L	52	SER
1	L	58	THR
1	L	63	LEU
1	L	102	LEU
1	L	129	LEU
1	L	154	LEU
1	L	204	LYS
1	L	207	ARG
1	L	213	ASP
1	L	216	PHE
1	L	246	LEU



Mol	Chain	Res	Type
1	L	247	CYS
1	L	271	TRP
1	L	272	TRP
2	М	11	VAL
2	М	59	LEU
2	М	74	TRP
2	М	103	SER
2	М	110	GLU
2	М	115	LEU
2	М	135	ARG
2	М	155	LEU
2	М	181	HIS
2	М	190	LEU
2	М	195	LEU
2	М	198	ASN
2	М	203	LEU
2	М	213	LEU
2	М	214	LEU
2	М	215	PHE
2	М	234	LEU
2	М	246	ARG
2	М	249	LEU
2	М	284	LEU
2	М	299	ASN
2	М	300	HIS
3	Н	12	LEU
3	Н	70	ARG
3	Н	72	THR
3	Н	94	GLU
3	Н	115	VAL
3	Н	117	ARG
3	Н	118	ARG
3	Н	151	LEU
3	Н	185	ASP
3	Н	194	GLN
3	Н	200	SER
3	Н	221	SER
3	Н	223	THR
3	Н	225	VAL
3	Н	231	ASP
3	Н	249	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14)



such sidechains are listed below:MolChainResType1L62GLN

IVIOI	Unam	IUCS	Type		
1	L	62	GLN		
1	L	159	ASN		
1	L	173	HIS		
1	L	183	ASN		
2	М	24	ASN		
2	М	43	ASN		
2	М	45	GLN		
2	М	76	GLN		
2	М	192	HIS		
2	М	198	ASN		
3	Н	98	HIS		
3	Н	128	HIS		
3	Н	194	GLN		
3	Н	206	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 1 is monoatomic - leaving 17 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).



Mal	Turne	Chain	Dec	Tink	B	ond leng	gths	Bond angles		
	туре	Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
4	BCL	L	304	1	58,74,74	1.57	7 (12%)	69,115,115	2.11	12 (17%)
4	BCL	М	802	2	58,74,74	1.54	8 (13%)	69,115,115	2.03	12 (17%)
7	LDA	М	703	-	12,15,15	2.40	1 (8%)	14,17,17	0.58	0
4	BCL	L	302	1	58,74,74	1.49	9 (15%)	69,115,115	2.04	12 (17%)
6	U10	М	501	-	48,48,63	2.13	16 (33%)	58,61,79	1.05	4 (6%)
9	PO4	М	800	-	4,4,4	1.97	2 (50%)	6,6,6	0.92	0
5	BPH	М	401	-	64,70,70	1.18	5 (7%)	76,101,101	1.66	15 (19%)
7	LDA	М	701	-	12,15,15	2.49	1 (8%)	14,17,17	0.45	0
10	SPO	М	600	-	40,41,41	3.28	23 (57%)	47,50,50	1.97	12 (25%)
7	LDA	L	705	-	12,15,15	2.40	1 (8%)	14,17,17	0.50	0
7	LDA	М	707	-	12,15,15	2.21	1 (8%)	14,17,17	0.51	0
6	U10	L	502	-	48,48,63	1.92	14 (29%)	58,61,79	1.29	4 (6%)
7	LDA	Н	706	-	12,15,15	2.25	1 (8%)	14,17,17	0.53	0
5	BPH	L	402	-	64,70,70	1.12	4 (6%)	76,101,101	1.62	11 (14%)
4	BCL	М	801	2	58,74,74	1.49	7 (12%)	69,115,115	2.08	12 (17%)
7	LDA	М	704	-	12,15,15	2.33	1 (8%)	14,17,17	0.52	0
7	LDA	Н	702	-	12,15,15	2.40	1 (8%)	14,17,17	0.53	0

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	\mathbf{Res}	Link	Chirals	Torsions	Rings
4	BCL	L	304	1	1/1/21/25	7/37/137/137	-
4	BCL	М	802	2	-	10/37/137/137	-
7	LDA	М	703	-	-	6/13/13/13	-
4	BCL	L	302	1	-	7/37/137/137	-
6	U10	М	501	-	-	8/45/69/87	0/1/1/1
5	BPH	М	401	-	-	17/54/105/105	0/5/6/6
7	LDA	М	701	-	-	1/13/13/13	-
10	SPO	М	600	-	-	17/47/47/47	-
7	LDA	L	705	-	-	0/13/13/13	-
7	LDA	М	707	-	-	1/13/13/13	-
6	U10	L	502	-	-	17/45/69/87	0/1/1/1
7	LDA	Н	706	-	_	2/13/13/13	-



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BPH	L	402	-	-	12/54/105/105	0/5/6/6
4	BCL	М	801	2	1/1/21/25	12/37/137/137	-
7	LDA	М	704	-	-	2/13/13/13	-
7	LDA	Н	702	-	-	5/13/13/13	-

All (102) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	М	600	SPO	C6-C5	8.83	1.55	1.32
7	М	701	LDA	O1-N1	-8.53	1.22	1.42
7	М	703	LDA	O1-N1	-8.30	1.22	1.42
7	Н	702	LDA	O1-N1	-8.29	1.22	1.42
7	L	705	LDA	O1-N1	-8.25	1.22	1.42
7	М	704	LDA	O1-N1	-8.03	1.23	1.42
10	М	600	SPO	C10-C11	7.86	1.54	1.34
7	Н	706	LDA	O1-N1	-7.75	1.24	1.42
7	М	707	LDA	O1-N1	-7.63	1.24	1.42
10	М	600	SPO	C15-C16	7.44	1.53	1.34
4	L	304	BCL	O2D-CGD	7.14	1.50	1.33
6	М	501	U10	C7-C8	-6.65	1.41	1.50
10	М	600	SPO	C21-C20	5.32	1.49	1.36
10	М	600	SPO	C26-C25	5.15	1.47	1.34
4	L	304	BCL	O2A-CGA	4.87	1.47	1.33
4	М	802	BCL	MG-NA	4.84	2.17	2.06
6	L	502	U10	O3-C3	4.82	1.48	1.36
6	L	502	U10	C7-C8	-4.81	1.43	1.50
4	М	801	BCL	MG-NA	4.78	2.17	2.06
10	М	600	SPO	C27-C28	4.76	1.39	1.34
4	М	802	BCL	O2D-CGD	4.53	1.44	1.33
6	М	501	U10	O3-C3	4.39	1.47	1.36
4	L	302	BCL	MG-NA	4.36	2.16	2.06
4	L	302	BCL	O2D-CED	-4.28	1.35	1.45
4	М	801	BCL	O2A-CGA	4.21	1.45	1.33
5	L	402	BPH	O2D-CGD	4.07	1.43	1.33
5	М	401	BPH	O2A-CGA	4.06	1.45	1.33
4	М	802	BCL	C4B-NB	3.86	1.38	1.35
4	L	302	BCL	O2D-CGD	3.85	1.42	1.33
4	М	801	BCL	C1B-NB	3.82	1.38	1.35
4	L	302	BCL	C4B-NB	3.79	1.38	1.35
6	М	501	U10	O4-C4M	-3.77	1.36	1.45
4	М	801	BCL	O2D-CGD	3.76	1.42	1.33



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	М	802	BCL	C1B-NB	3.75	1.38	1.35
10	М	600	SPO	O1-CM1	3.57	1.54	1.43
4	М	801	BCL	C4B-NB	3.50	1.38	1.35
5	М	401	BPH	O2D-CED	-3.46	1.37	1.45
6	М	501	U10	O4-C4	3.45	1.45	1.36
4	М	802	BCL	O2A-CGA	3.35	1.43	1.33
6	М	501	U10	C27-C28	-3.35	1.39	1.50
6	L	502	U10	O4-C4	3.27	1.44	1.36
10	М	600	SPO	C9-C7	3.19	1.40	1.35
4	L	302	BCL	C1B-NB	3.15	1.38	1.35
4	М	801	BCL	O2D-CED	-3.14	1.37	1.45
4	L	304	BCL	C4B-NB	3.13	1.38	1.35
10	М	600	SPO	C11-C12	-3.12	1.39	1.45
5	М	401	BPH	O2D-CGD	3.11	1.40	1.33
6	М	501	U10	C33-C34	3.10	1.40	1.33
6	М	501	U10	C22-C23	-3.10	1.40	1.50
10	М	600	SPO	C25-C23	-3.10	1.39	1.45
10	М	600	SPO	C14-C12	3.07	1.39	1.35
4	М	802	BCL	O2D-CED	-3.01	1.38	1.45
10	М	600	SPO	C10-C9	3.00	1.52	1.43
6	L	502	U10	C33-C34	2.97	1.40	1.33
6	L	502	U10	C23-C24	2.96	1.40	1.33
10	М	600	SPO	C19-C17	2.95	1.39	1.35
5	L	402	BPH	O2D-CED	-2.92	1.38	1.45
6	L	502	U10	C28-C29	2.90	1.39	1.33
6	L	502	U10	C13-C14	2.89	1.39	1.33
4	L	304	BCL	MG-NA	2.89	2.13	2.06
4	L	304	BCL	C1B-NB	2.88	1.37	1.35
6	М	501	U10	O3-C3M	-2.87	1.38	1.45
5	М	401	BPH	C2-C3	2.84	1.39	1.33
5	L	402	BPH	C2-C3	2.83	1.39	1.33
10	М	600	SPO	C16-C17	-2.80	1.39	1.45
10	М	600	SPO	C32-C33	2.76	1.39	1.33
4	L	302	BCL	O2A-CGA	2.75	1.41	1.33
4	L	302	BCL	C2-C3	2.72	1.39	1.33
6	L	502	U10	C18-C19	2.71	1.39	1.33
6	L	502	U10	C8-C9	2.69	1.39	1.33
10	М	600	SPO	C37-C38	2.68	1.40	1.32
4	L	302	BCL	C1-C2	-2.67	1.41	1.49
4	М	801	BCL	C2-C3	2.66	1.39	1.33
10	М	600	SPO	C6-C7	-2.66	1.40	1.45
6	Μ	501	U10	C13-C14	2.65	1.39	1.33



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	304	BCL	C1-C2	-2.64	1.41	1.49
6	М	501	U10	C38-C39	2.64	1.39	1.32
6	L	502	U10	C38-C39	2.59	1.39	1.32
6	М	501	U10	C18-C19	2.58	1.39	1.33
4	L	304	BCL	C2-C3	2.57	1.39	1.33
10	М	600	SPO	C26-C27	2.55	1.51	1.43
9	М	800	PO4	P-O3	-2.53	1.47	1.54
10	М	600	SPO	C15-C14	2.51	1.51	1.43
6	М	501	U10	C23-C24	2.47	1.38	1.33
5	L	402	BPH	O2A-CGA	2.43	1.40	1.33
6	L	502	U10	O4-C4M	-2.41	1.39	1.45
10	М	600	SPO	O1-C1	2.39	1.55	1.41
4	М	802	BCL	C1-C2	-2.36	1.42	1.49
4	М	802	BCL	C2-C3	2.36	1.38	1.33
6	М	501	U10	C28-C29	2.32	1.38	1.33
10	М	600	SPO	C22-C23	2.32	1.38	1.35
6	М	501	U10	C8-C9	2.32	1.38	1.33
6	L	502	U10	O3-C3M	-2.27	1.40	1.45
10	М	600	SPO	C8-C7	2.26	1.55	1.50
6	М	501	U10	C17-C18	-2.19	1.43	1.50
5	М	401	BPH	C5-C3	2.15	1.55	1.51
6	L	502	U10	O2-C2	-2.14	1.18	1.23
6	М	501	U10	C36-C34	2.11	1.55	1.51
9	М	800	PO4	P-04	-2.10	1.48	1.54
4	L	302	BCL	MG-NC	2.10	2.11	2.06
6	L	502	U10	C7-C6	2.09	1.54	1.51
10	М	600	SPO	C24-C23	2.00	1.55	1.50

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All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	L	304	BCL	C4A-NA-C1A	8.18	110.38	106.71
4	М	801	BCL	C4A-NA-C1A	8.07	110.33	106.71
4	L	304	BCL	O2D-CGD-CBD	7.95	125.40	111.27
4	М	802	BCL	C4A-NA-C1A	7.88	110.25	106.71
4	L	302	BCL	C4A-NA-C1A	7.75	110.19	106.71
5	L	402	BPH	O2D-CGD-CBD	7.34	124.32	111.27
4	М	801	BCL	O2D-CGD-CBD	7.27	124.18	111.27
4	L	302	BCL	C1C-NC-C4C	7.09	109.89	106.71
5	М	401	BPH	O2D-CGD-CBD	7.06	123.82	111.27
4	М	802	BCL	C1C-NC-C4C	7.04	109.87	106.71
4	L	302	BCL	O2D-CGD-CBD	6.81	123.37	111.27



1	FNP

Mol	Chain	i previ	Unit Type	 Atoms	Z	Observed $(^{o})$	Ideal(°)
	M	901	DCI		6.64	100.60	106 71
4	M	802	BCI	0.00000000000000000000000000000000000	0.04 6.51	109.09	100.71
10	M	600	SPO	C15 C14 C12	6.17	118 50	111.27
10	IVI I	304	BCL	OID CCD CBD	5 50	113.05	127.51
5	M	401	BOL BPH	OID-CGD-CBD	5.20	113.05	124.40
	M	801	BCL	O1D-CGD-CBD	-5.25	113.00	124.40
5	IVI I	402	BOL BPH	OID-CGD-CBD	5 20	113.74	124.40
<u> </u>	L	402 502	U10	$\frac{\text{OID-OGD-ODD}}{\text{C3M-O3-C3}}$	5.14	134 69	116.47
	L	304	BCL	C1C-NC-C4C	$\frac{0.14}{4.74}$	104.05	106 71
4	M	802	BCL	O1D-CGD-CBD	-4.61	115.05	100.11
10	M	600	SPO	C20-C19-C17	-1.01	121.00	124.40
10	M	600	SPO	C20-C13-C17	-4.13	115.01	127.01 123.47
10	M	600	SPO	C25-C23-C22	-4.09	112.67	118.94
10	T.	302	BCL	01D-CGD-CBD	-4.06	112.07	124.48
6	L	502	U10	C7-C6-C5	3.98	123.27	118 48
5	L	402	RPH	OBD-CAD-CBD	-3 71	120.21	125.89
5	M	401	BPH	O2A-CGA-CBA	3.58	123.14	111 91
	L	304	BCL	CMB-C2B-C1B	-3.52	123.06	128.46
4	L	302	BCL	O2A-CGA-CBA	3 50	122.90	111 91
10	M	600	SPO	C15-C16-C17	-3.48	116.65	126.42
4	M	801	BCL	OBD-CAD-CBD	-3 42	121.01	125.89
5	M	401	BPH	OBD-CAD-CBD	-3.39	121.01	125.89
4	L	302	BCL	OBD-CAD-CBD	-3.39	121.06	125.89
4	M	802	BCL	O2A-CGA-CBA	3.38	122.50	111.91
4	L	304	BCL	C4D-C3D-CAD	-3.37	106.59	108.47
5	L	402	BPH	O2A-CGA-CBA	3.33	122.36	111.91
4	М	802	BCL	C4D-C3D-CAD	-3.31	106.62	108.47
4	М	801	BCL	C4D-C3D-CAD	-3.31	106.62	108.47
4	М	802	BCL	OBD-CAD-CBD	-3.23	121.27	125.89
10	М	600	SPO	C6-C7-C9	-3.08	114.21	118.94
4	L	304	BCL	O2A-CGA-CBA	3.01	121.37	111.91
4	М	801	BCL	O2A-CGA-CBA	2.98	121.27	111.91
4	L	302	BCL	C4D-C3D-CAD	-2.98	106.81	108.47
4	М	802	BCL	CMB-C2B-C1B	-2.94	123.94	128.46
4	L	304	BCL	CMD-C2D-C3D	2.88	130.06	124.68
5	L	402	BPH	C4A-NA-C1A	2.85	110.44	108.14
10	М	600	SPO	C8-C7-C6	2.85	122.57	118.08
4	L	304	BCL	OBD-CAD-CBD	-2.84	121.84	125.89
4	М	802	BCL	C1-C2-C3	2.83	130.93	126.04
4	М	801	BCL	C1-C2-C3	2.77	130.84	126.04
4	L	304	BCL	C4B-C3B-CAB	-2.77	121.78	127.13
5	М	401	BPH	C4A-NA-C1A	2.73	110.34	108.14

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Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
10	М	600	SPO	C21-C22-C23	-2.70	123.45	127.31
5	М	401	BPH	OBB-CAB-C3B	2.70	125.39	120.41
4	L	302	BCL	CMB-C2B-C1B	-2.69	124.33	128.46
4	L	302	BCL	C1-C2-C3	2.69	130.69	126.04
6	М	501	U10	C7-C8-C9	2.68	131.26	126.79
5	М	401	BPH	C4D-CHA-C1A	-2.67	123.92	130.51
5	L	402	BPH	O2A-CGA-O1A	-2.61	117.02	123.59
10	М	600	SPO	C10-C9-C7	-2.60	123.60	127.31
5	L	402	BPH	C4D-CHA-C1A	-2.57	124.17	130.51
5	М	401	BPH	CMD-C2D-C3D	2.52	129.40	124.68
10	М	600	SPO	C24-C23-C25	2.52	122.05	118.08
4	L	302	BCL	O2A-CGA-O1A	-2.51	117.26	123.59
4	М	801	BCL	CMD-C2D-C3D	2.49	129.34	124.68
4	М	801	BCL	CMB-C2B-C1B	-2.47	124.67	128.46
6	М	501	U10	C4M-O4-C4	2.46	125.18	116.47
6	L	502	U10	C4M-O4-C4	2.44	125.11	116.47
5	М	401	BPH	CBB-CAB-C3B	-2.43	115.25	120.43
4	L	304	BCL	CMB-C2B-C3B	2.42	129.20	124.68
5	М	401	BPH	O2A-CGA-O1A	-2.42	117.49	123.59
5	М	401	BPH	CED-O2D-CGD	2.38	121.32	115.94
4	М	802	BCL	CED-O2D-CGD	2.34	121.24	115.94
5	М	401	BPH	C1-C2-C3	2.34	130.09	126.04
5	L	402	BPH	C3A-C4A-NA	-2.32	109.09	113.05
4	L	302	BCL	CED-O2D-CGD	2.32	121.18	115.94
5	L	402	BPH	C1-C2-C3	2.28	129.98	126.04
5	М	401	BPH	C3A-C4A-NA	-2.27	109.17	113.05
4	L	304	BCL	CED-O2D-CGD	2.22	120.95	115.94
4	М	802	BCL	C3A-C2A-C1A	2.19	104.62	101.34
4	L	302	BCL	CMD-C2D-C3D	2.15	128.71	124.68
5	М	401	BPH	C2A-C1A-NA	-2.15	109.39	111.86
5	L	402	BPH	C3A-C4A-CHB	2.13	125.50	121.83
5	М	401	BPH	C3A-C4A-CHB	2.11	125.47	121.83
4	М	801	BCL	C2A-C1A-CHA	2.09	127.51	123.86
4	М	801	BCL	C4B-C3B-CAB	-2.08	123.10	127.13
10	М	600	SPO	C18-C17-C19	-2.07	120.02	122.92
6	М	501	U10	O3-C3-C2	-2.06	109.59	116.56
6	М	501	U10	C3M-O3-C3	2.04	123.71	116.47
10	М	600	SPO	C13-C12-C11	2.03	121.28	118.08
4	М	802	BCL	O2A-CGA-O1A	-2.02	118.50	123.59
6	L	502	U10	C6-C1-C2	2.01	120.77	119.18
5	L	402	BPH	CMD-C2D-C3D	2.00	128.42	124.68

All (2) chirality outliers are listed below:



Mol	Chain	Res	Type	Atom
4	L	304	BCL	C13
4	М	801	BCL	C8

All (124) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	302	BCL	CBD-CGD-O2D-CED
4	L	302	BCL	O1D-CGD-O2D-CED
4	М	801	BCL	C4C-C3C-CAC-CBC
5	L	402	BPH	C4C-C3C-CAC-CBC
5	L	402	BPH	C2C-C3C-CAC-CBC
5	L	402	BPH	C2C-C1C-CHC-C4B
5	L	402	BPH	C4B-C3B-CAB-CBB
5	М	401	BPH	C4C-C3C-CAC-CBC
5	М	401	BPH	C2C-C3C-CAC-CBC
5	М	401	BPH	C4B-C3B-CAB-CBB
5	М	401	BPH	C4B-C3B-CAB-OBB
5	М	401	BPH	O2A-C1-C2-C3
5	М	401	BPH	C2-C3-C5-C6
5	М	401	BPH	C4-C3-C5-C6
6	L	502	U10	C1-C6-C7-C8
6	L	502	U10	C5-C6-C7-C8
6	L	502	U10	C12-C11-C9-C8
6	L	502	U10	C12-C11-C9-C10
6	L	502	U10	C13-C14-C16-C17
6	L	502	U10	C15-C14-C16-C17
6	М	501	U10	C29-C31-C32-C33
7	М	703	LDA	C2-C1-N1-O1
7	М	703	LDA	C2-C1-N1-CM1
7	Н	702	LDA	C2-C1-N1-O1
7	Н	702	LDA	C2-C1-N1-CM1
7	Н	702	LDA	N1-C1-C2-C3
10	М	600	SPO	C4-C1-O1-CM1
10	М	600	SPO	C36-C37-C38-C40
10	М	600	SPO	C36-C37-C38-C39
4	М	802	BCL	C3-C5-C6-C7
5	М	401	BPH	O1A-CGA-O2A-C1
5	М	401	BPH	CBA-CGA-O2A-C1
6	L	502	U10	C4-C3-O3-C3M
4	М	802	BCL	C13-C15-C16-C17
6	L	502	U10	C9-C11-C12-C13
6	L	502	U10	C29-C31-C32-C33
4	М	801	BCL	C15-C16-C17-C18



Mol	Chain	Res	Type	Atoms	
4	L	304	BCL	C10-C11-C12-C13	
10	М	600	SPO	C21-C22-C23-C24	
7	М	703	LDA	C3-C4-C5-C6	
5	М	401	BPH	C10-C11-C12-C13	
10	М	600	SPO	C34-C33-C35-C36	
7	М	701	LDA	C11-C10-C9-C8	
6	L	502	U10	C14-C16-C17-C18	
6	L	502	U10	C21-C22-C23-C24	
4	М	801	BCL	C1A-C2A-CAA-CBA	
10	М	600	SPO	C20-C21-C22-C23	
7	Н	702	LDA	C1-C2-C3-C4	
5	М	401	BPH	C2B-C3B-CAB-CBB	
5	L	402	BPH	C4-C3-C5-C6	
10	М	600	SPO	C2-C1-O1-CM1	
10	М	600	SPO	C3-C1-O1-CM1	
4	М	801	BCL	C11-C12-C13-C15	
4	М	802	BCL	C11-C12-C13-C15	
4	М	801	BCL	C11-C12-C13-C14	
5	L	402	BPH	C14-C13-C15-C16	
6	L	502	U10	C2-C3-O3-C3M	
4	L	302	BCL	C2A-CAA-CBA-CGA	
7	М	704	LDA	C4-C5-C6-C7	
4	М	801	BCL	CBA-CGA-O2A-C1	
5	L	402	BPH	C2-C3-C5-C6	
5	L	402	BPH	O2A-C1-C2-C3	
5	М	401	BPH	C3-C5-C6-C7	
4	L	304	BCL	C8-C10-C11-C12	
10	М	600	SPO	C24-C23-C25-C26	
10	М	600	SPO	C19-C20-C21-C22	
4	М	801	BCL	O1A-CGA-O2A-C1	
4	L	302	BCL	C12-C13-C15-C16	
4	М	801	BCL	C11-C10-C8-C7	
5	L	402	BPH	C4B-C3B-CAB-OBB	
7	М	707	LDA	C5-C6-C7-C8	
7	М	703	LDA	C2-C3-C4-C5	
7	Н	706	LDA	C2-C3-C4-C5	
5	М	401	BPH	C2B-C3B-CAB-OBB	
4	L	302	BCL	CAD-CBD-CGD-O2D	
4	L	304	BCL	CAD-CBD-CGD-O2D	
4	М	801	BCL	CAD-CBD-CGD-O2D	
4	М	802	BCL	C4-C3-C5-C6	
6	М	501	U10	C28-C29-C31-C32	

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Mol	Chain	Res	Type	Atoms	
7	М	703	LDA	C2-C1-N1-CM2	
7	Н	702	LDA	C2-C1-N1-CM2	
6	L	502	U10	C20-C19-C21-C22	
6	М	501	U10	C30-C29-C31-C32	
4	L	302	BCL	C14-C13-C15-C16	
4	L	302	BCL	C16-C17-C18-C20	
10	М	600	SPO	C29-C28-C30-C31	
4	L	304	BCL	CBA-CGA-O2A-C1	
4	L	304	BCL	O1A-CGA-O2A-C1	
10	М	600	SPO	C1-C4-C5-C6	
4	М	801	BCL	C3A-C2A-CAA-CBA	
4	М	802	BCL	C6-C7-C8-C10	
5	М	401	BPH	C11-C10-C8-C7	
4	М	802	BCL	C6-C7-C8-C9	
6	М	501	U10	C2-C3-O3-C3M	
4	М	802	BCL	C2-C3-C5-C6	
6	L	502	U10	C18-C19-C21-C22	
10	М	600	SPO	C27-C28-C30-C31	
10	М	600	SPO	C32-C33-C35-C36	
4	М	802	BCL	C11-C12-C13-C14	
10	М	600	SPO	C17-C19-C20-C21	
5	М	401	BPH	C2-C1-O2A-CGA	
7	М	703	LDA	C5-C6-C7-C8	
10	М	600	SPO	C18-C17-C19-C20	
4	М	802	BCL	C10-C11-C12-C13	
5	М	401	BPH	C8-C10-C11-C12	
7	Н	706	LDA	C6-C7-C8-C9	
6	М	501	U10	C25-C24-C26-C27	
10	М	600	SPO	C16-C17-C19-C20	
5	L	402	BPH	C8-C10-C11-C12	
6	L	502	U10	C25-C24-C26-C27	
4	М	801	BCL	C11-C10-C8-C9	
5	М	401	BPH	C11-C10-C8-C9	
4	L	304	BCL	C3A-C2A-CAA-CBA	
4	М	802	BCL	CAD-CBD-CGD-O2D	
5	L	402	BPH	CAD-CBD-CGD-O2D	
7	М	704	LDA	C7-C8-C9-C10	
6	М	501	U10	C23-C24-C26-C27	
6	М	501	U10	C24-C26-C27-C28	
6	L	502	U10	C11-C12-C13-C14	
4	М	801	BCL	C16-C17-C18-C20	
4	L	304	BCL	C1A-C2A-CAA-CBA	

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Mol	Chain	Res	Type	Atoms	
6	L	502	U10	C35-C34-C36-C37	
6	М	501	U10	C14-C16-C17-C18	
5	L	402	BPH	C11-C12-C13-C15	

There are no ring outliers.

12 monomers are involved in 55 short contacts:

Mol	Chain	\mathbf{Res}	Type	Clashes	Symm-Clashes
4	L	304	BCL	5	0
4	М	802	BCL	8	0
4	L	302	BCL	8	0
6	М	501	U10	2	0
9	М	800	PO4	1	0
5	М	401	BPH	11	0
10	М	600	SPO	1	0
6	L	502	U10	8	0
5	L	402	BPH	8	0
4	М	801	BCL	6	0
7	М	704	LDA	1	0
7	Н	702	LDA	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 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.

















5.7 Other polymers (i)

There are no such residues in this entry.



5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

