



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 02:10 am BST

PDB ID : 1JJC  
Title : Crystal structure at 2.6Å resolution of phenylalanyl-tRNA synthetase complexed with phenylalanyl-adenylate in the presence of manganese  
Authors : Safro, M.G.; Fishman, R.; Moor, N.; Ankilova, V.  
Deposited on : 2001-07-04  
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](mailto: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 ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) 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) : 2.11

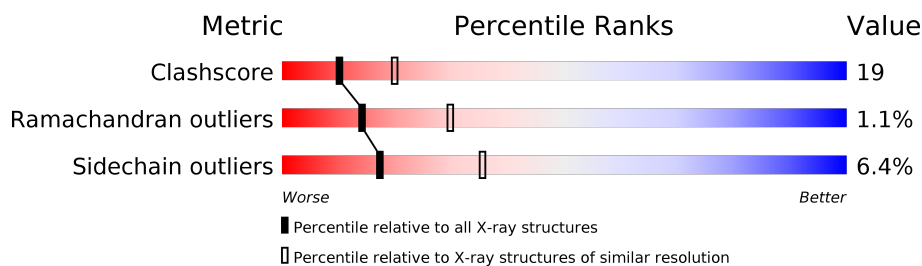
# 1 Overall quality at a glance

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.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	350	
2	B	785	

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
5	SO4	B	902	-	-	X	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8579 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.

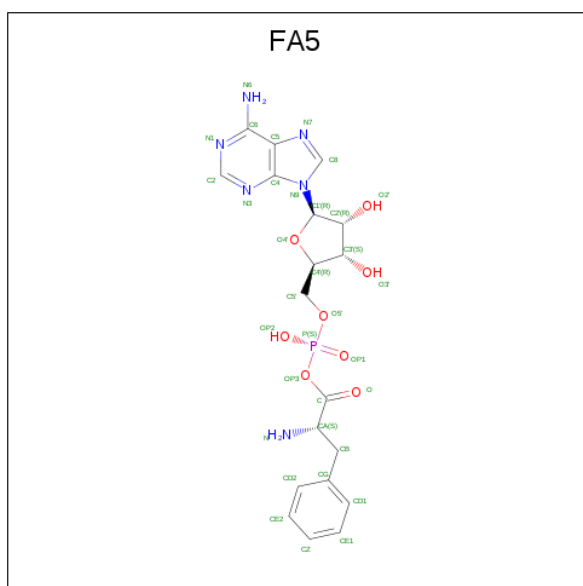
- Molecule 1 is a protein called PHENYLALANYL-TRNA SYNTHETASE ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	266	Total	C	N	O	S	0	0	0
			2123	1388	363	365	7			

- Molecule 2 is a protein called PHENYLALANYL-TRNA SYNTHETASE BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	785	Total	C	N	O	S	0	0	0
			6127	3925	1091	1101	10			

- Molecule 3 is ADENOSINE-5'-[PHENYLALANINYL-PHOSPHATE] (three-letter code: FA5) (formula:  $C_{19}H_{23}N_6O_8P$ ).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mn	0	0
			1	1		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	65	Total	O	0	0
			65	65		
6	B	224	Total	O	0	0
			224	224		





## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	173.40 Å   173.40 Å   138.40 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	50.00 – 2.60	Depositor
% Data completeness (in resolution range)	95.7 (50.00-2.60)	Depositor
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.216 , 0.258	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8579	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	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: MN, SO4, FA5

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	0.45	0/2191	0.75	3/2971 (0.1%)
2	B	0.46	2/6280 (0.0%)	0.67	9/8536 (0.1%)
All	All	0.45	2/8471 (0.0%)	0.69	12/11507 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	408	PRO	N-CD	-18.08	1.22	1.47
2	B	38	VAL	C-O	5.72	1.34	1.23

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	204	ARG	NE-CZ-NH1	10.43	125.52	120.30
1	A	263	PRO	CA-N-CD	-6.94	101.78	111.50
2	B	324	VAL	N-CA-C	-6.90	92.36	111.00
1	A	262	GLU	CA-C-N	6.80	136.13	117.10
2	B	324	VAL	N-CA-CB	6.72	126.29	111.50
2	B	38	VAL	CA-C-N	5.75	129.84	117.20
2	B	408	PRO	N-CD-CG	5.50	111.45	103.20
2	B	408	PRO	CA-C-N	-5.32	105.50	117.20
2	B	38	VAL	O-C-N	-5.24	114.31	122.70
2	B	331	ILE	CB-CA-C	-5.07	101.47	111.60
2	B	42	PRO	CA-N-CD	-5.04	104.44	111.50
2	B	405	PRO	C-N-CA	-5.04	109.09	121.70

There are no chirality outliers.

There are no planarity outliers.



## 5.2 Too-close contacts ⓘ

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	2123	0	2075	106	6
2	B	6127	0	6180	229	0
3	A	34	0	22	0	0
4	B	1	0	0	0	0
5	B	5	0	0	2	0
6	A	65	0	0	1	1
6	B	224	0	0	11	9
All	All	8579	0	8277	313	9

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 19.

All (313) 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)
2:B:239:MET:HE3	2:B:250:ASN:HB3	1.40	1.04
2:B:467:GLN:HE21	2:B:467:GLN:HA	1.21	1.03
2:B:282:ARG:HH11	2:B:282:ARG:HB3	1.25	0.99
1:A:348:GLY:O	1:A:350:LEU:HD12	1.63	0.98
2:B:408:PRO:HD2	6:B:944:HOH:O	1.63	0.96
2:B:734:PRO:HG2	2:B:735:PRO:HD3	1.46	0.96
2:B:141:PRO:O	2:B:144:THR:HG23	1.64	0.96
2:B:239:MET:CE	2:B:250:ASN:HB3	1.96	0.95
1:A:191:THR:HG22	2:B:484:ASP:OD2	1.66	0.92
2:B:736:LEU:HB3	2:B:737:PRO:HD2	1.52	0.90
2:B:680:LYS:HE2	2:B:681:PRO:HD2	1.56	0.85
1:A:255:PRO:HD3	2:B:469:TYR:CD2	2.12	0.85
2:B:286:LEU:CD2	2:B:323:GLU:OE2	2.25	0.84
2:B:286:LEU:HD23	2:B:323:GLU:OE2	1.78	0.83
2:B:516:MET:HE3	2:B:546:THR:H	1.44	0.83
2:B:602:ARG:HG3	2:B:602:ARG:HH11	1.43	0.83
1:A:155:THR:HB	2:B:534:LEU:HD21	1.63	0.80
1:A:262:GLU:O	1:A:263:PRO:C	2.06	0.80
1:A:262:GLU:HA	1:A:262:GLU:OE2	1.81	0.78
2:B:656:HIS:CE1	2:B:658:GLU:OE2	2.39	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:TRP:HZ3	1:A:276:LYS:HE2	1.51	0.75
2:B:192:LYS:H	2:B:381:GLN:HE22	1.33	0.74
2:B:163:ASN:ND2	2:B:164:ARG:HG2	2.03	0.74
2:B:344:ARG:CZ	6:B:1115:HOH:O	2.34	0.74
1:A:145:ALA:HA	1:A:148:MET:HE2	1.69	0.73
2:B:593:GLY:HA3	2:B:604:SER:HB3	1.71	0.73
2:B:649:VAL:HG23	2:B:673:LEU:HD22	1.70	0.73
2:B:344:ARG:NH2	6:B:1115:HOH:O	2.22	0.73
1:A:287:HIS:HE1	2:B:455:LEU:HD12	1.53	0.73
1:A:271:TRP:CZ3	1:A:276:LYS:HE2	2.24	0.72
2:B:255:GLU:OE2	2:B:375:ARG:HD2	1.90	0.72
2:B:701:VAL:HG23	2:B:777:PHE:CE1	2.24	0.72
2:B:489:GLU:HG3	2:B:493:ARG:HD2	1.71	0.72
2:B:775:ARG:NH1	2:B:775:ARG:HB3	2.04	0.72
2:B:583:THR:HG22	2:B:675:LEU:HD12	1.71	0.71
2:B:163:ASN:HD21	2:B:164:ARG:HG2	1.55	0.71
2:B:44:GLY:HA3	2:B:94:THR:OG1	1.90	0.70
2:B:256:ARG:NH2	2:B:375:ARG:HG3	2.07	0.70
2:B:736:LEU:HB3	2:B:737:PRO:CD	2.22	0.70
2:B:80:ASN:HD21	2:B:132:LEU:H	1.37	0.69
2:B:413:ARG:NH2	5:B:902:SO4:O4	2.26	0.68
1:A:128:GLU:OE2	1:A:185:ARG:HD2	1.94	0.68
1:A:279:GLU:HB3	6:A:1033:HOH:O	1.94	0.68
2:B:141:PRO:HD2	2:B:144:THR:HG21	1.74	0.68
1:A:115:ARG:CZ	2:B:493:ARG:HH21	2.07	0.68
2:B:488:VAL:HG22	6:B:1096:HOH:O	1.93	0.67
2:B:430:ARG:HB3	2:B:430:ARG:HH11	1.59	0.67
1:A:179:THR:OG1	1:A:220:GLU:HG3	1.93	0.67
2:B:467:GLN:NE2	2:B:467:GLN:HA	2.04	0.67
2:B:282:ARG:NH1	2:B:282:ARG:HB3	2.04	0.67
2:B:604:SER:HA	2:B:608:LEU:HD22	1.77	0.67
2:B:775:ARG:HH11	2:B:775:ARG:HB3	1.60	0.66
2:B:34:ARG:HD2	6:B:1026:HOH:O	1.94	0.66
1:A:262:GLU:HG3	2:B:457:GLU:HB3	1.78	0.66
2:B:399:LYS:H	2:B:399:LYS:NZ	1.94	0.66
2:B:710:VAL:HG11	2:B:743:LEU:HD12	1.78	0.65
2:B:399:LYS:H	2:B:399:LYS:HZ3	1.43	0.65
2:B:194:GLU:OE2	2:B:387:ARG:HD2	1.98	0.64
2:B:178:HIS:O	2:B:430:ARG:NH1	2.31	0.64
2:B:214:THR:HG22	2:B:394:GLU:HG3	1.79	0.63
2:B:703:ALA:N	2:B:704:PRO:HD2	2.12	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:LEU:HD21	1:A:322:LEU:HD11	1.80	0.63
2:B:286:LEU:HD21	2:B:323:GLU:OE2	1.98	0.63
1:A:119:TYR:HB3	1:A:197:VAL:HG22	1.81	0.63
1:A:179:THR:HG1	1:A:220:GLU:HG3	1.64	0.63
1:A:257:TYR:CZ	1:A:259:PRO:HD3	2.33	0.62
2:B:407:ARG:HD3	2:B:456:GLU:OE2	1.99	0.62
2:B:258:GLN:HE22	2:B:369:GLN:NE2	1.98	0.62
2:B:697:LEU:O	2:B:697:LEU:HD12	1.99	0.61
2:B:656:HIS:HE1	2:B:658:GLU:OE2	1.82	0.61
2:B:578:ARG:O	2:B:579:GLU:HB3	1.99	0.61
1:A:211:THR:HG23	1:A:212:HIS:CE1	2.36	0.61
1:A:162:GLU:O	1:A:185:ARG:NH2	2.34	0.60
2:B:323:GLU:HG2	6:B:1070:HOH:O	2.00	0.60
1:A:278:LEU:HD13	1:A:325:LEU:HD13	1.83	0.60
1:A:348:GLY:O	1:A:350:LEU:CD1	2.46	0.60
1:A:350:LEU:N	1:A:350:LEU:HD12	2.16	0.60
2:B:101:GLN:CD	2:B:101:GLN:H	2.05	0.60
1:A:252:ARG:HB2	1:A:277:TRP:CZ3	2.37	0.59
1:A:271:TRP:NE1	1:A:273:GLU:HB3	2.17	0.59
1:A:262:GLU:CB	2:B:457:GLU:HB3	2.33	0.59
1:A:347:LYS:HD3	6:B:1028:HOH:O	2.03	0.59
2:B:732:GLN:HG3	2:B:740:HIS:O	2.03	0.59
2:B:582:GLU:OE2	2:B:584:HIS:HE1	1.85	0.59
2:B:596:LEU:HB2	2:B:599:ALA:HB3	1.83	0.58
2:B:680:LYS:HE2	2:B:680:LYS:HA	1.85	0.58
2:B:769:ALA:O	2:B:773:ARG:HG3	2.03	0.58
2:B:282:ARG:HH12	2:B:290:GLU:HG3	1.68	0.58
1:A:262:GLU:CG	2:B:457:GLU:HB3	2.34	0.58
2:B:551:GLY:O	2:B:555:VAL:HG23	2.03	0.58
2:B:496:GLN:O	2:B:500:GLU:HG3	2.03	0.58
2:B:695:ARG:HH11	2:B:695:ARG:HG3	1.69	0.57
2:B:609:LEU:HD13	2:B:652:LEU:HD11	1.86	0.57
2:B:696:ASP:OD1	2:B:746:HIS:HD2	1.87	0.57
1:A:145:ALA:HA	1:A:148:MET:CE	2.35	0.57
1:A:255:PRO:HD3	2:B:469:TYR:CE2	2.39	0.57
2:B:695:ARG:HE	2:B:761:VAL:HG11	1.70	0.57
2:B:239:MET:HE3	2:B:250:ASN:CB	2.26	0.56
1:A:257:TYR:OH	1:A:259:PRO:HG3	2.06	0.56
1:A:165:LEU:HD11	1:A:303:LEU:HD11	1.87	0.56
2:B:602:ARG:NH1	2:B:602:ARG:HG3	2.16	0.56
2:B:258:GLN:HE22	2:B:369:GLN:HE21	1.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:PRO:HG3	1:A:308:ARG:HH12	1.69	0.56
2:B:718:ALA:CB	2:B:722:LEU:HD22	2.36	0.56
1:A:287:HIS:HE1	2:B:455:LEU:CD1	2.19	0.56
2:B:239:MET:HE1	2:B:250:ASN:HB3	1.85	0.55
1:A:165:LEU:HD12	1:A:301:LEU:HD23	1.87	0.55
2:B:695:ARG:HA	2:B:784:THR:HB	1.88	0.55
2:B:768:VAL:O	2:B:772:LEU:HB2	2.06	0.55
2:B:601:GLU:O	2:B:602:ARG:HG3	2.07	0.55
2:B:680:LYS:NZ	2:B:681:PRO:HG2	2.22	0.55
2:B:278:ARG:HH22	2:B:308:SER:HB3	1.72	0.54
2:B:610:LYS:O	2:B:614:GLU:HG3	2.07	0.54
2:B:701:VAL:HG23	2:B:702:PRO:HD2	1.89	0.54
1:A:340:LEU:O	1:A:344:GLU:HG3	2.07	0.54
1:A:164:PRO:CB	1:A:188:VAL:CG2	2.86	0.54
2:B:761:VAL:O	2:B:765:VAL:HG13	2.08	0.54
2:B:701:VAL:HG23	2:B:777:PHE:HE1	1.71	0.54
1:A:161:LEU:O	1:A:169:VAL:HG12	2.08	0.54
1:A:287:HIS:ND1	1:A:288:PRO:N	2.56	0.54
2:B:695:ARG:HE	2:B:761:VAL:CG1	2.21	0.54
2:B:20:VAL:O	2:B:24:ARG:HG2	2.08	0.53
2:B:734:PRO:CG	2:B:735:PRO:HD3	2.28	0.53
2:B:702:PRO:C	2:B:704:PRO:HD2	2.29	0.53
2:B:530:ARG:HB2	2:B:530:ARG:NH1	2.24	0.53
2:B:413:ARG:NH2	5:B:902:SO4:S	2.82	0.53
2:B:516:MET:HE3	2:B:546:THR:N	2.19	0.53
1:A:198:VAL:HG13	1:A:220:GLU:HB2	1.89	0.53
2:B:140:LEU:HD21	2:B:149:ALA:HB2	1.91	0.53
2:B:321:GLU:O	2:B:325:ARG:NH2	2.42	0.53
2:B:635:HIS:ND1	2:B:637:GLY:N	2.51	0.53
1:A:211:THR:HG23	1:A:212:HIS:ND1	2.24	0.52
2:B:49:ARG:HG3	2:B:137:GLU:HG3	1.91	0.52
2:B:699:VAL:O	2:B:742:SER:HA	2.10	0.52
2:B:762:GLU:HA	2:B:765:VAL:HG22	1.91	0.52
2:B:768:VAL:HG12	2:B:768:VAL:O	2.09	0.52
2:B:283:LEU:HG	2:B:310:PRO:HB2	1.91	0.52
2:B:536:PRO:HB3	2:B:542:ALA:HA	1.91	0.52
2:B:281:GLU:HG2	2:B:310:PRO:HG2	1.92	0.52
2:B:297:ASP:OD2	2:B:350:HIS:HE1	1.93	0.52
2:B:370:VAL:HB	2:B:371:PRO:HD3	1.91	0.52
1:A:262:GLU:O	1:A:264:GLY:N	2.41	0.52
1:A:101:HIS:CG	1:A:102:PRO:HD2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:ARG:HG2	1:A:86:VAL:H	1.76	0.51
2:B:278:ARG:O	2:B:281:GLU:HB2	2.11	0.51
2:B:409:GLU:OE1	2:B:413:ARG:NH1	2.40	0.51
2:B:624:PHE:CE1	2:B:642:VAL:HG13	2.44	0.51
2:B:38:VAL:O	2:B:40:PRO:HD2	2.10	0.51
2:B:641:ARG:NH1	2:B:648:GLU:OE1	2.43	0.51
2:B:758:ASP:O	2:B:762:GLU:HG2	2.10	0.51
2:B:680:LYS:HE2	2:B:681:PRO:CD	2.32	0.51
2:B:764:ALA:HA	2:B:767:ARG:HE	1.76	0.51
1:A:169:VAL:HG22	1:A:170:GLU:N	2.25	0.51
2:B:624:PHE:HE1	2:B:642:VAL:HG13	1.76	0.51
2:B:326:GLU:CD	2:B:326:GLU:H	2.15	0.50
1:A:97:SER:OG	1:A:347:LYS:NZ	2.44	0.50
2:B:650:GLY:HA3	2:B:673:LEU:HD23	1.93	0.50
2:B:728:PHE:CZ	2:B:744:ALA:HB1	2.46	0.50
2:B:256:ARG:HD3	6:B:977:HOH:O	2.10	0.50
1:A:164:PRO:HG2	1:A:188:VAL:HG21	1.92	0.50
1:A:255:PRO:HG3	2:B:469:TYR:CZ	2.47	0.50
2:B:165:PRO:HB3	2:B:362:ARG:HB3	1.93	0.50
2:B:399:LYS:HZ2	2:B:399:LYS:HB3	1.76	0.50
2:B:530:ARG:HD2	2:B:579:GLU:H	1.77	0.50
2:B:772:LEU:HD23	2:B:779:LEU:HD22	1.94	0.49
1:A:271:TRP:CD2	1:A:325:LEU:HD21	2.47	0.49
2:B:198:LEU:HD12	2:B:393:LEU:HG	1.94	0.49
2:B:509:GLU:HB2	2:B:571:PHE:CE1	2.47	0.49
1:A:258:PHE:HB2	1:A:261:VAL:HG22	1.94	0.49
2:B:635:HIS:CE1	2:B:637:GLY:H	2.29	0.49
2:B:490:ALA:HB3	2:B:491:PRO:HD3	1.93	0.49
2:B:604:SER:HA	2:B:608:LEU:CD2	2.41	0.49
1:A:85:ARG:HG2	1:A:86:VAL:N	2.28	0.49
2:B:587:GLY:HA3	2:B:671:PHE:CE1	2.48	0.49
2:B:300:ILE:O	2:B:311:LEU:HB2	2.13	0.49
1:A:262:GLU:OE1	2:B:458:ASP:HA	2.12	0.49
2:B:560:LEU:HD21	2:B:590:PHE:CE2	2.48	0.48
1:A:325:LEU:HD23	1:A:325:LEU:O	2.13	0.48
2:B:588:LEU:HD23	2:B:588:LEU:C	2.34	0.48
2:B:633:PHE:CD1	2:B:634:LEU:HG	2.48	0.48
1:A:211:THR:OG1	1:A:321:ARG:NH2	2.46	0.48
1:A:326:ARG:HG3	1:A:326:ARG:HH11	1.77	0.48
2:B:282:ARG:NH1	2:B:290:GLU:HG3	2.27	0.48
2:B:554:ARG:HG2	2:B:554:ARG:HH11	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:703:ALA:N	2:B:704:PRO:CD	2.77	0.48
2:B:496:GLN:HB3	6:B:1027:HOH:O	2.14	0.47
1:A:237:ILE:HG13	1:A:253:PHE:HZ	1.79	0.47
2:B:605:GLY:HA2	2:B:669:HIS:CD2	2.49	0.47
1:A:278:LEU:HD23	1:A:278:LEU:H	1.80	0.47
2:B:584:HIS:HD2	2:B:672:GLU:OE2	1.98	0.47
1:A:251:VAL:HG12	1:A:269:VAL:HG12	1.97	0.47
1:A:290:VAL:O	1:A:294:VAL:HG23	2.13	0.47
1:A:228:ILE:HG21	1:A:312:GLY:HA2	1.96	0.47
1:A:115:ARG:NH2	2:B:493:ARG:HH21	2.12	0.47
1:A:287:HIS:CE1	2:B:455:LEU:HD12	2.40	0.47
2:B:554:ARG:O	2:B:558:GLU:HG3	2.14	0.47
1:A:101:HIS:O	1:A:105:LEU:HD22	2.14	0.47
2:B:278:ARG:NH1	6:B:1079:HOH:O	2.41	0.47
2:B:588:LEU:HD23	2:B:589:LEU:N	2.30	0.47
1:A:187:MET:HB3	1:A:294:VAL:HG11	1.96	0.47
2:B:578:ARG:C	2:B:580:ARG:H	2.18	0.47
2:B:16:GLU:O	2:B:17:SER:HB3	2.14	0.47
2:B:533:LEU:O	2:B:536:PRO:HD3	2.15	0.47
2:B:622:LEU:CD2	2:B:680:LYS:HB2	2.46	0.47
2:B:729:ASP:HB3	2:B:744:ALA:CB	2.44	0.47
1:A:271:TRP:CE2	1:A:325:LEU:HD21	2.50	0.46
1:A:326:ARG:HG3	1:A:326:ARG:NH1	2.30	0.46
2:B:49:ARG:CG	2:B:137:GLU:HG3	2.45	0.46
1:A:141:GLU:HG2	1:A:142:HIS:CD2	2.50	0.46
2:B:623:ALA:O	2:B:644:VAL:HA	2.16	0.46
2:B:634:LEU:HD11	2:B:651:PHE:CD1	2.51	0.46
2:B:722:LEU:HD11	2:B:724:SER:O	2.15	0.46
2:B:762:GLU:O	2:B:765:VAL:HG22	2.15	0.46
1:A:321:ARG:HH11	1:A:321:ARG:HG2	1.80	0.46
2:B:567:ARG:O	2:B:568:ALA:HB2	2.15	0.46
1:A:185:ARG:O	1:A:188:VAL:HG22	2.16	0.45
2:B:724:SER:HB3	2:B:748:ARG:HB2	1.98	0.45
1:A:270:TRP:O	1:A:272:PRO:HD3	2.17	0.45
2:B:701:VAL:CG2	2:B:702:PRO:HD2	2.46	0.45
2:B:755:THR:HG22	2:B:756:LEU:N	2.32	0.45
2:B:563:ASP:C	2:B:565:PRO:HD3	2.37	0.45
1:A:258:PHE:HB2	1:A:261:VAL:CG2	2.47	0.44
2:B:38:VAL:HG23	2:B:39:PHE:CD2	2.52	0.44
1:A:262:GLU:HG3	2:B:457:GLU:CB	2.44	0.44
2:B:641:ARG:HD2	2:B:648:GLU:OE1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:710:VAL:O	2:B:714:VAL:HG23	2.17	0.44
1:A:289:LYS:HA	1:A:292:GLN:HE21	1.83	0.44
2:B:531:LEU:C	2:B:532:LEU:HD12	2.38	0.44
2:B:764:ALA:HA	2:B:767:ARG:HH21	1.82	0.44
1:A:203:PHE:CD1	1:A:203:PHE:N	2.86	0.44
2:B:215:LEU:HA	2:B:333:LEU:O	2.18	0.44
2:B:462:GLU:O	2:B:466:ILE:HG12	2.18	0.44
2:B:759:GLU:HG3	2:B:760:GLU:N	2.32	0.44
1:A:237:ILE:HG22	1:A:251:VAL:HG11	1.99	0.44
1:A:271:TRP:HE1	1:A:273:GLU:HB3	1.80	0.44
1:A:262:GLU:HB3	2:B:457:GLU:HB3	1.99	0.44
2:B:467:GLN:HE21	2:B:467:GLN:CA	2.04	0.44
2:B:567:ARG:HB3	2:B:591:GLY:HA3	2.00	0.44
1:A:179:THR:OG1	1:A:220:GLU:CG	2.63	0.43
1:A:298:ARG:NH1	1:A:304:PRO:O	2.49	0.43
2:B:192:LYS:N	2:B:381:GLN:HE22	2.08	0.43
2:B:554:ARG:HG2	2:B:554:ARG:NH1	2.32	0.43
2:B:505:LEU:HD22	2:B:612:TYR:HD1	1.82	0.43
2:B:224:ALA:N	2:B:244:ASN:ND2	2.66	0.43
2:B:362:ARG:HG2	2:B:362:ARG:HH11	1.82	0.43
2:B:697:LEU:HD12	2:B:697:LEU:C	2.39	0.43
2:B:736:LEU:CB	2:B:737:PRO:CD	2.92	0.43
2:B:695:ARG:HD2	2:B:765:VAL:HG11	2.00	0.43
2:B:549:PHE:CD2	2:B:550:PRO:HD3	2.54	0.43
2:B:567:ARG:CB	2:B:591:GLY:HA3	2.48	0.43
2:B:224:ALA:H	2:B:244:ASN:ND2	2.16	0.43
2:B:517:ASP:HB3	2:B:520:ASP:OD2	2.19	0.43
2:B:609:LEU:HD13	2:B:652:LEU:CD1	2.48	0.43
2:B:206:ASP:OD2	2:B:276:ARG:HD3	2.18	0.43
2:B:221:LEU:HD23	2:B:386:ALA:HB2	2.00	0.42
1:A:194:PHE:C	1:A:194:PHE:CD1	2.92	0.42
2:B:28:LEU:HD13	2:B:176:ASP:HB3	2.02	0.42
2:B:322:SER:C	2:B:323:GLU:O	2.54	0.42
2:B:344:ARG:NH1	6:B:1115:HOH:O	2.48	0.42
2:B:779:LEU:HD23	2:B:779:LEU:N	2.34	0.42
2:B:203:LYS:HE3	2:B:205:GLU:OE2	2.18	0.42
1:A:160:ARG:HG2	1:A:160:ARG:NH1	2.35	0.42
1:A:180:SER:N	1:A:181:PRO:HD2	2.34	0.42
1:A:245:PHE:HE2	1:A:269:VAL:HG21	1.84	0.42
1:A:237:ILE:HG13	1:A:253:PHE:CZ	2.55	0.42
1:A:269:VAL:HG23	1:A:278:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:GLN:OE1	1:A:247:PRO:HA	2.19	0.42
1:A:257:TYR:CE2	1:A:259:PRO:HD3	2.55	0.42
1:A:350:LEU:CD1	1:A:350:LEU:N	2.83	0.42
2:B:680:LYS:HZ1	2:B:681:PRO:HG2	1.85	0.42
2:B:775:ARG:HH11	2:B:775:ARG:CB	2.27	0.42
2:B:264:ASP:OD2	2:B:266:ARG:HD3	2.20	0.42
2:B:772:LEU:O	2:B:777:PHE:HB2	2.20	0.42
1:A:252:ARG:HB2	1:A:277:TRP:CH2	2.55	0.42
1:A:160:ARG:HG2	1:A:160:ARG:HH11	1.85	0.41
1:A:235:GLY:HA3	2:B:475:ALA:O	2.19	0.41
1:A:252:ARG:NH2	1:A:279:GLU:OE2	2.53	0.41
2:B:276:ARG:HG3	2:B:295:PRO:O	2.20	0.41
2:B:641:ARG:HG3	2:B:643:LEU:HD11	2.02	0.41
2:B:239:MET:HE2	2:B:254:LEU:HD11	2.02	0.41
1:A:159:PHE:N	2:B:530:ARG:HD3	2.34	0.41
2:B:728:PHE:CE1	2:B:744:ALA:HB1	2.55	0.41
2:B:773:ARG:HH11	2:B:773:ARG:HG2	1.84	0.41
1:A:160:ARG:HD3	2:B:580:ARG:NH2	2.35	0.41
1:A:350:LEU:H	1:A:350:LEU:HD12	1.82	0.41
2:B:259:PRO:HB2	2:B:360:PHE:CE2	2.56	0.41
2:B:163:ASN:ND2	2:B:163:ASN:C	2.74	0.41
2:B:698:ALA:HA	2:B:743:LEU:O	2.20	0.41
1:A:197:VAL:HA	1:A:220:GLU:O	2.20	0.41
1:A:237:ILE:CG1	1:A:253:PHE:HZ	2.33	0.41
2:B:622:LEU:HD23	2:B:680:LYS:HB2	2.02	0.41
2:B:222:ARG:O	2:B:244:ASN:ND2	2.53	0.41
2:B:696:ASP:O	2:B:697:LEU:HB3	2.20	0.41
2:B:701:VAL:HG22	2:B:705:THR:HB	2.01	0.41
1:A:160:ARG:HD2	2:B:579:GLU:OE2	2.21	0.41
2:B:718:ALA:HB3	2:B:722:LEU:HD22	2.01	0.41
1:A:113:ILE:CD1	1:A:244:LEU:HD13	2.51	0.41
2:B:223:VAL:HA	2:B:244:ASN:HD22	1.86	0.41
1:A:343:LEU:HD13	2:B:509:GLU:O	2.21	0.41
2:B:654:ALA:HB2	2:B:669:HIS:CE1	2.56	0.41
2:B:657:PRO:O	2:B:661:GLN:OE1	2.39	0.40
1:A:164:PRO:HB2	1:A:188:VAL:CG2	2.52	0.40
1:A:110:LEU:HB3	1:A:219:LEU:HD22	2.03	0.40
2:B:158:LEU:HD12	2:B:173:LEU:HD21	2.02	0.40
2:B:213:PHE:CD2	2:B:274:VAL:HG21	2.56	0.40
2:B:579:GLU:O	2:B:579:GLU:HG3	2.20	0.40
1:A:325:LEU:HD23	1:A:325:LEU:C	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:VAL:O	1:A:349:VAL:HG12	2.22	0.40
2:B:128:TYR:CB	2:B:240:ARG:HD2	2.51	0.40
2:B:309:PHE:HA	2:B:310:PRO:HD3	1.84	0.40
1:A:201:ARG:NH2	2:B:512:THR:O	2.54	0.40
2:B:80:ASN:N	2:B:80:ASN:HD22	2.18	0.40
2:B:96:LEU:HA	2:B:97:PRO:HD3	1.92	0.40

All (9) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:1045:HOH:O	6:B:1110:HOH:O[2_664]	0.20	2.00
6:A:1043:HOH:O	6:B:950:HOH:O[5_665]	0.22	1.98
6:B:1018:HOH:O	6:B:1078:HOH:O[3_565]	0.59	1.61
1:A:350:LEU:O	6:B:1071:HOH:O[4_555]	1.46	0.74
1:A:350:LEU:N	6:B:1071:HOH:O[4_555]	1.63	0.57
1:A:349:VAL:C	6:B:1071:HOH:O[4_555]	1.84	0.36
1:A:350:LEU:C	6:B:1071:HOH:O[4_555]	1.85	0.35
1:A:350:LEU:CA	6:B:1071:HOH:O[4_555]	1.97	0.23
1:A:349:VAL:O	6:B:1071:HOH:O[4_555]	2.08	0.12

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	Percentiles	
1	A	264/350 (75%)	252 (96%)	10 (4%)	2 (1%)	19	39
2	B	783/785 (100%)	737 (94%)	37 (5%)	9 (1%)	14	30
All	All	1047/1135 (92%)	989 (94%)	47 (4%)	11 (1%)	14	30

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	349	VAL
2	B	244	ASN
2	B	323	GLU
2	B	439	GLY
2	B	725	LEU
2	B	737	PRO
1	A	262	GLU
2	B	279	GLU
2	B	697	LEU
2	B	606	TYR
2	B	40	PRO

### 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 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	A	214/277 (77%)	202 (94%)	12 (6%)	21	42
2	B	630/630 (100%)	588 (93%)	42 (7%)	16	33
All	All	844/907 (93%)	790 (94%)	54 (6%)	17	35

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	178	HIS
1	A	191	THR
1	A	197	VAL
1	A	198	VAL
1	A	201	ARG
1	A	220	GLU
1	A	256	VAL
1	A	260	PHE
1	A	262	GLU
1	A	278	LEU
1	A	321	ARG
1	A	322	LEU
2	B	32	THR

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Mol	Chain	Res	Type
2	B	42	PRO
2	B	80	ASN
2	B	89	LEU
2	B	111	VAL
2	B	157	ASP
2	B	158	LEU
2	B	163	ASN
2	B	170	LEU
2	B	171	LEU
2	B	173	LEU
2	B	180	LEU
2	B	191	LEU
2	B	276	ARG
2	B	282	ARG
2	B	283	LEU
2	B	286	LEU
2	B	298	LEU
2	B	325	ARG
2	B	329	GLU
2	B	333	LEU
2	B	362	ARG
2	B	375	ARG
2	B	387	ARG
2	B	399	LYS
2	B	430	ARG
2	B	441	THR
2	B	445	THR
2	B	467	GLN
2	B	470	GLU
2	B	505	LEU
2	B	548	LEU
2	B	562	LEU
2	B	575	ARG
2	B	579	GLU
2	B	584	HIS
2	B	609	LEU
2	B	670	LEU
2	B	680	LYS
2	B	737	PRO
2	B	763	GLU
2	B	779	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	GLN
1	A	142	HIS
1	A	190	HIS
1	A	207	GLN
1	A	292	GLN
2	B	80	ASN
2	B	101	GLN
2	B	163	ASN
2	B	178	HIS
2	B	212	HIS
2	B	231	GLN
2	B	244	ASN
2	B	258	GLN
2	B	261	HIS
2	B	350	HIS
2	B	381	GLN
2	B	467	GLN
2	B	584	HIS
2	B	629	GLN
2	B	661	GLN
2	B	669	HIS
2	B	746	HIS

### 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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	SO4	B	902	-	4,4,4	1.16	0	6,6,6	3.13	2 (33%)
3	FA5	A	999	-	33,37,37	2.48	3 (9%)	37,54,54	1.39	1 (2%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FA5	A	999	-	-	2/17/39/39	0/4/4/4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	FA5	C2-N1	11.55	1.55	1.33
3	A	999	FA5	O4'-C1'	3.88	1.46	1.41
3	A	999	FA5	C8-N7	3.82	1.41	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	999	FA5	N3-C2-N1	-6.91	117.88	128.68
5	B	902	SO4	O4-S-O1	6.49	143.18	109.31
5	B	902	SO4	O4-S-O3	-2.93	96.56	109.06

There are no chirality outliers.

All (2) torsion outliers are listed below:

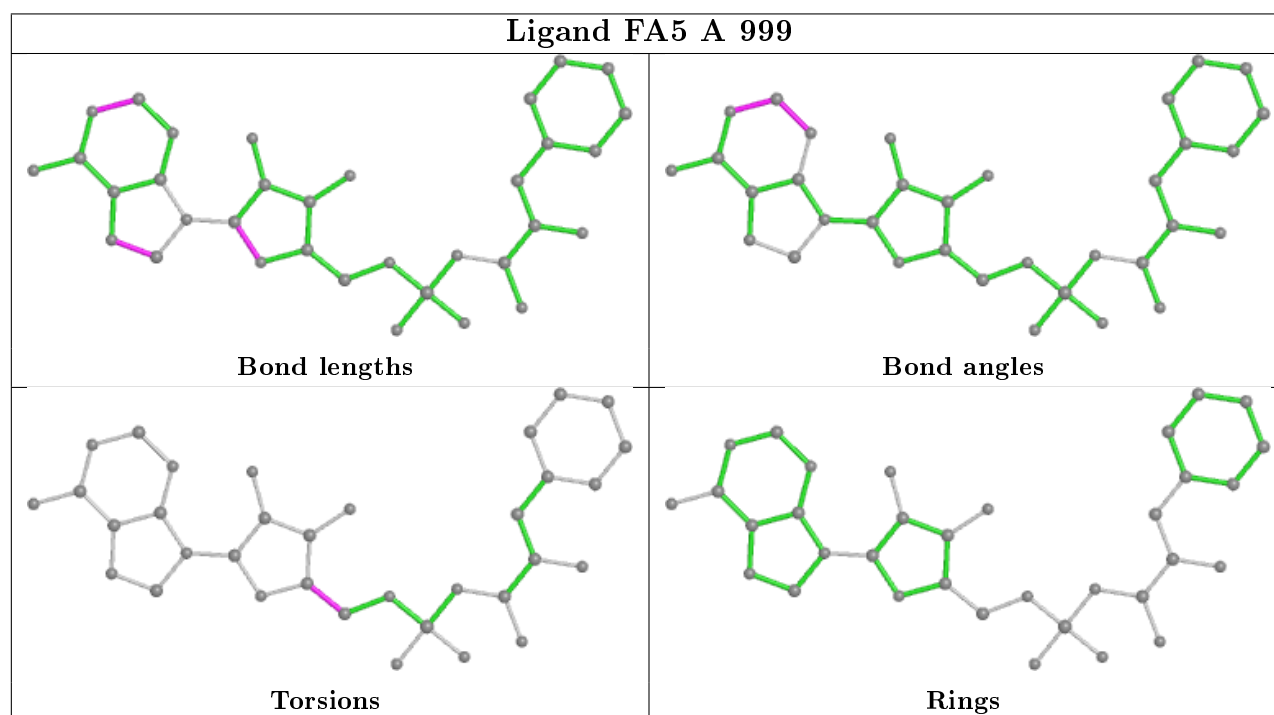
Mol	Chain	Res	Type	Atoms
3	A	999	FA5	O4'-C4'-C5'-O5'
3	A	999	FA5	C3'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	902	SO4	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.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.