



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 18, 2023 – 01:51 AM EDT

PDB ID : 1MZN
Title : CRYSTAL STRUCTURE at 1.9 ANGSTROEMS RESOLUTION OF THE HOMODIMER OF HUMAN RXR ALPHA LIGAND BINDING DOMAIN BOUND TO THE SYNTHETIC AGONIST COMPOUND BMS 649 AND A COACTIVATOR PEPTIDE
Authors : Egea, P.F.; Mitschler, A.; Moras, D.
Deposited on : 2002-10-09
Resolution : 1.90 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 ⓘ 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:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (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) : 2.36

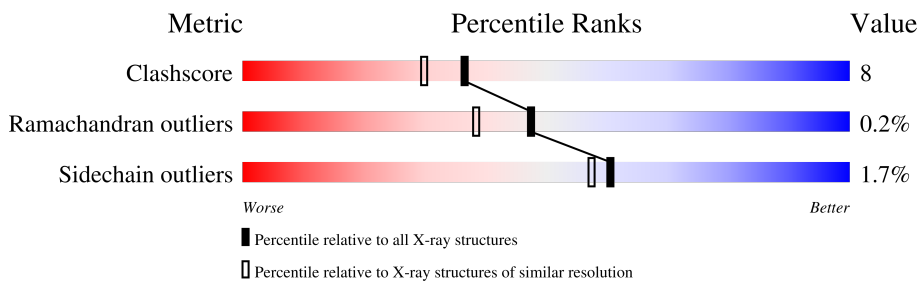
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	240	
1	C	240	
1	E	240	
1	G	240	
2	B	13	
2	D	13	
2	F	13	
2	H	13	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8177 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.

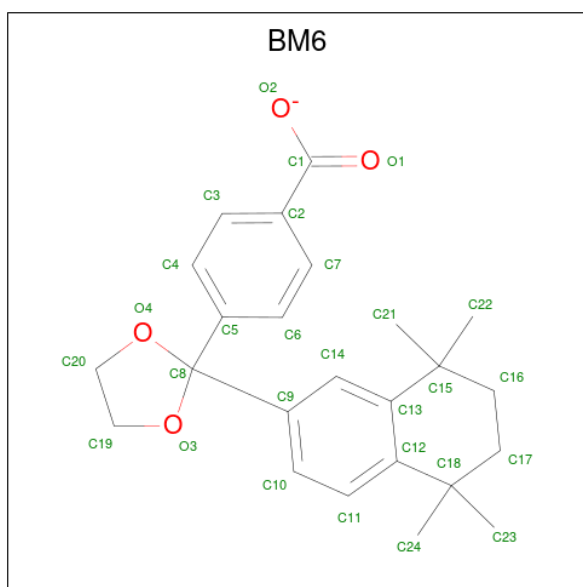
- Molecule 1 is a protein called RXR retinoid X receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	224	Total 1753	C 1126	N 299	O 318	S 10	0	0	0
1	C	212	Total 1672	C 1075	N 286	O 301	S 10	0	0	0
1	E	224	Total 1753	C 1126	N 299	O 318	S 10	0	0	0
1	G	212	Total 1672	C 1075	N 286	O 301	S 10	0	0	0

- Molecule 2 is a protein called Nuclear receptor coactivator 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	11	Total 98	C 63	N 21	O 14	0	0	0
2	D	11	Total 98	C 63	N 21	O 14	0	0	0
2	F	11	Total 98	C 63	N 21	O 14	0	0	0
2	H	11	Total 98	C 63	N 21	O 14	0	0	0

- Molecule 3 is 4-[2-(5,5,8,8-TETRAMETHYL-5,6,7,8-TETRAHYDRO-NAPHTHALEN-2-YL)-[1,3]DIOXOLAN-2-YL]-BENZOIC ACID (three-letter code: BM6) (formula: C₂₄H₂₇O₄).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	C O	0	0
			28	24 4		
3	C	1	Total	C O	0	0
			28	24 4		
3	E	1	Total	C O	0	0
			28	24 4		
3	G	1	Total	C O	0	0
			28	24 4		

- Molecule 4 is water.


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	222	Total	O	0	0
			222	222		
4	B	5	Total	O	0	0
			5	5		
4	C	180	Total	O	0	0
			180	180		
4	E	226	Total	O	0	0
			226	226		
4	F	10	Total	O	0	0
			10	10		
4	G	178	Total	O	0	0
			178	178		
4	H	2	Total	O	0	0
			2	2		

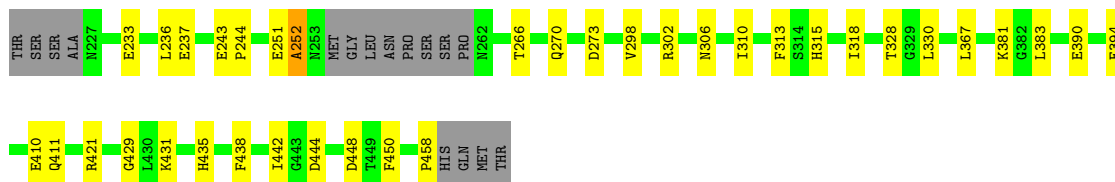
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

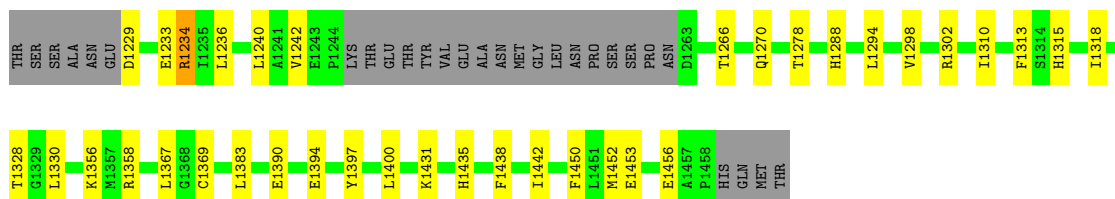
- Molecule 1: RXR retinoid X receptor

Chain A: 




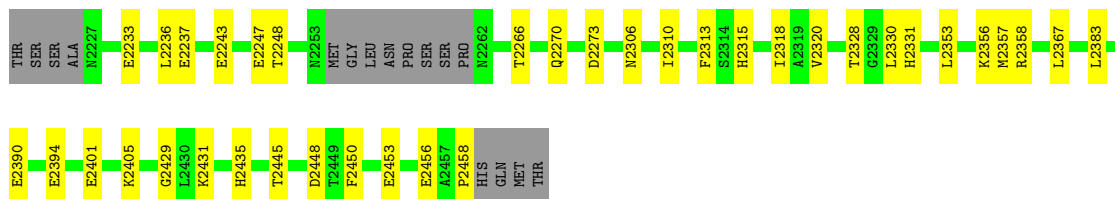
- Molecule 1: RXR retinoid X receptor

Chain C: 



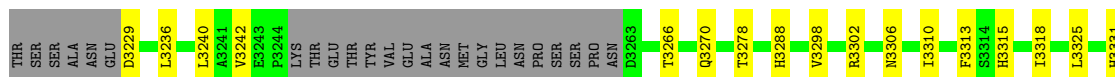
- Molecule 1: RXR retinoid X receptor

Chain E: 



- Molecule 1: RXR retinoid X receptor

Chain G: 

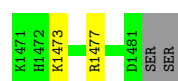




- Molecule 2: Nuclear receptor coactivator 2



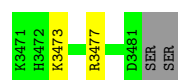
- Molecule 2: Nuclear receptor coactivator 2



- Molecule 2: Nuclear receptor coactivator 2



- Molecule 2: Nuclear receptor coactivator 2



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	47.12Å 64.69Å 94.78Å 109.97° 92.87° 89.99°	Depositor
Resolution (Å)	30.00 – 1.90	Depositor
% Data completeness (in resolution range)	98.7 (30.00-1.90)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.195 , 0.232	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8177	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BM6

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	0.33	0/1788	0.54	0/2421
1	C	0.30	0/1706	0.51	0/2308
1	E	0.33	0/1788	0.53	0/2421
1	G	0.30	0/1706	0.50	0/2308
2	B	0.31	0/99	0.48	0/130
2	D	0.28	0/99	0.42	0/130
2	F	0.29	0/99	0.48	0/130
2	H	0.28	0/99	0.42	0/130
All	All	0.31	0/7384	0.52	0/9978

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	G	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	3397	TYR	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	1753	0	1775	26	0
1	C	1672	0	1709	32	0
1	E	1753	0	1775	24	0
1	G	1672	0	1709	33	0
2	B	98	0	108	4	0
2	D	98	0	108	1	0
2	F	98	0	108	5	0
2	H	98	0	108	1	0
3	A	28	0	27	0	0
3	C	28	0	27	0	0
3	E	28	0	27	0	0
3	G	28	0	27	0	0
4	A	222	0	0	5	0
4	B	5	0	0	0	0
4	C	180	0	0	4	0
4	E	226	0	0	3	0
4	F	10	0	0	0	0
4	G	178	0	0	2	0
4	H	2	0	0	0	0
All	All	8177	0	7508	117	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 8.

All (117) 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:C:1234:ARG:HH11	1:C:1234:ARG:HG3	1.15	1.05
1:E:2320:VAL:HG21	1:E:2331:HIS:CE1	2.09	0.87
1:G:3453:GLU:O	1:G:3456:GLU:HG2	1.80	0.81
2:F:2477:ARG:O	2:F:2481:ASP:CG	2.18	0.81
1:C:1234:ARG:HG3	1:C:1234:ARG:NH1	1.90	0.77
1:C:1240:LEU:HD12	1:G:3240:LEU:HD12	1.68	0.76
1:C:1242:VAL:HG13	1:C:1278:THR:HB	1.68	0.76
1:G:3242:VAL:HG13	1:G:3278:THR:HB	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1234:ARG:NH2	4:C:4743:HOH:O	2.16	0.72
2:B:477:ARG:O	2:B:481:ASP:CG	2.28	0.72
1:G:3356:LYS:HA	1:G:3356:LYS:HE2	1.69	0.71
1:E:2318:ILE:HD11	1:E:2357:MET:HB3	1.72	0.70
1:A:458:PRO:HA	2:B:472:HIS:HE1	1.57	0.69
1:E:2458:PRO:HA	2:F:2472:HIS:HE1	1.58	0.69
1:A:390:GLU:O	1:A:394:GLU:HG3	1.93	0.68
1:C:1236:LEU:HD12	1:G:3236:LEU:HD12	1.74	0.68
1:G:3266:THR:O	1:G:3270:GLN:HG3	1.94	0.67
1:C:1452:MET:O	1:C:1456:GLU:HG3	1.95	0.65
1:C:1356:LYS:HA	1:C:1356:LYS:HE2	1.80	0.64
1:E:2390:GLU:O	1:E:2394:GLU:HG3	1.96	0.64
1:G:3390:GLU:O	1:G:3394:GLU:HG3	1.99	0.63
1:E:2318:ILE:HD11	1:E:2357:MET:CB	2.29	0.62
1:E:2320:VAL:HG21	1:E:2331:HIS:HE1	1.65	0.62
1:E:2243:GLU:HG3	4:E:4232:HOH:O	1.99	0.62
1:G:3318:ILE:HG23	1:G:3358:ARG:HB2	1.82	0.61
1:C:1234:ARG:NH1	1:C:1234:ARG:CG	2.62	0.61
1:A:251:GLU:O	1:A:252:ALA:HB2	2.01	0.60
1:C:1390:GLU:O	1:C:1394:GLU:HG3	2.01	0.60
2:H:3473:LYS:O	2:H:3477:ARG:HG3	2.01	0.60
1:A:458:PRO:HA	2:B:472:HIS:CE1	2.38	0.59
2:D:1473:LYS:O	2:D:1477:ARG:HG3	2.04	0.58
1:C:1318:ILE:O	1:C:1358:ARG:HD3	2.04	0.57
1:A:243:GLU:HG3	4:A:4334:HOH:O	2.06	0.55
1:A:410:GLU:HG2	1:A:411:GLN:HG3	1.88	0.55
1:E:2431:LYS:O	1:E:2435:HIS:HD2	1.90	0.55
1:C:1233:GLU:OE2	1:G:3407:LYS:HE2	2.06	0.55
1:A:431:LYS:O	1:A:435:HIS:HD2	1.90	0.54
1:E:2273:ASP:CG	1:E:2448:ASP:HB2	2.28	0.54
1:A:315:HIS:CG	1:A:367:LEU:HD22	2.43	0.54
1:C:1438:PHE:CE2	1:C:1442:ILE:HD11	2.42	0.54
1:C:1328:THR:OG1	1:C:1330:LEU:HD23	2.08	0.53
1:G:3433:LEU:HD22	1:G:3437:PHE:CE1	2.42	0.53
1:G:3438:PHE:CZ	1:G:3442:ILE:HD11	2.44	0.53
1:C:1266:THR:O	1:C:1270:GLN:HG3	2.09	0.52
1:E:2318:ILE:HG23	1:E:2358:ARG:HB2	1.91	0.52
1:C:1242:VAL:CG1	1:C:1278:THR:HB	2.38	0.52
1:C:1310:ILE:HA	1:C:1313:PHE:CE2	2.44	0.52
1:A:438:PHE:O	1:A:442:ILE:HG12	2.10	0.51
1:E:2315:HIS:CG	1:E:2367:LEU:HD22	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3298:VAL:O	1:G:3302:ARG:HG3	2.11	0.51
2:B:477:ARG:O	2:B:481:ASP:OD1	2.28	0.51
1:A:266:THR:O	1:A:270:GLN:HG3	2.11	0.51
1:G:3318:ILE:O	1:G:3358:ARG:HD3	2.11	0.50
1:A:298:VAL:O	1:A:302:ARG:HG3	2.11	0.50
1:A:244:PRO:HG2	4:A:4204:HOH:O	2.11	0.50
1:C:1233:GLU:CD	1:G:3407:LYS:HE2	2.32	0.50
1:E:2266:THR:O	1:E:2270:GLN:HG3	2.12	0.50
1:E:2353:LEU:O	1:E:2357:MET:HG3	2.12	0.50
1:G:3388:GLU:HG2	4:G:4613:HOH:O	2.12	0.49
1:A:390:GLU:HG3	4:A:4291:HOH:O	2.13	0.49
1:C:1438:PHE:CZ	1:C:1442:ILE:HD11	2.48	0.49
2:F:2477:ARG:O	2:F:2481:ASP:OD1	2.29	0.49
1:C:1278:THR:HG21	4:C:4230:HOH:O	2.13	0.49
1:C:1298:VAL:O	1:C:1302:ARG:HG3	2.13	0.48
2:F:2477:ARG:O	2:F:2481:ASP:OD2	2.32	0.48
1:E:2401:GLU:O	1:E:2405:LYS:HG2	2.14	0.47
1:G:3406:HIS:O	1:G:3409:PRO:HD3	2.14	0.47
1:G:3369:CYS:HB2	1:G:3400:LEU:HD13	1.96	0.47
1:A:273:ASP:CG	1:A:448:ASP:HB2	2.35	0.47
1:A:315:HIS:O	1:A:318:ILE:HG12	2.14	0.47
1:A:442:ILE:HB	1:A:444:ASP:OD1	2.14	0.47
1:C:1236:LEU:C	1:C:1236:LEU:HD13	2.35	0.47
1:E:2453:GLU:O	1:E:2456:GLU:HG2	2.15	0.47
1:G:3315:HIS:CG	1:G:3367:LEU:HD22	2.49	0.47
1:A:328:THR:OG1	1:A:330:LEU:HD23	2.15	0.47
1:G:3394:GLU:HA	1:G:3397:TYR:CE2	2.50	0.46
1:A:251:GLU:O	1:A:252:ALA:CB	2.63	0.46
1:C:1236:LEU:HD12	1:G:3236:LEU:CD1	2.44	0.46
1:G:3229:ASP:O	1:G:3288:HIS:HE1	1.98	0.46
1:C:1394:GLU:HA	1:C:1397:TYR:CE2	2.50	0.46
1:G:3242:VAL:CG1	1:G:3278:THR:HB	2.41	0.46
1:G:3318:ILE:HG23	1:G:3358:ARG:CB	2.45	0.46
1:C:1229:ASP:O	1:C:1288:HIS:HE1	1.99	0.45
1:G:3310:ILE:HA	1:G:3313:PHE:CE2	2.52	0.45
1:C:1236:LEU:HD13	1:C:1236:LEU:O	2.17	0.45
1:C:1315:HIS:CG	1:C:1367:LEU:HD22	2.51	0.45
1:E:2247:GLU:HG3	1:E:2248:THR:N	2.32	0.44
1:E:2310:ILE:HA	1:E:2313:PHE:CE2	2.52	0.44
1:E:2318:ILE:HG23	1:E:2358:ARG:CB	2.47	0.44
1:G:3442:ILE:HG21	1:G:3444:ASP:OD2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3306:ASN:HB2	4:G:4075:HOH:O	2.18	0.44
1:A:302:ARG:NH1	1:A:458:PRO:HG3	2.33	0.43
1:E:2458:PRO:HA	2:F:2472:HIS:CE1	2.47	0.43
1:C:1356:LYS:HE3	4:C:4184:HOH:O	2.18	0.43
1:G:3306:ASN:ND2	1:G:3433:LEU:HG	2.33	0.43
4:E:4069:HOH:O	1:G:3381:LYS:HE3	2.18	0.43
1:G:3236:LEU:C	1:G:3236:LEU:HD13	2.39	0.43
1:A:315:HIS:CB	1:A:367:LEU:HD22	2.49	0.43
1:A:421:ARG:CD	4:A:4014:HOH:O	2.66	0.43
1:E:2328:THR:OG1	1:E:2330:LEU:HD23	2.18	0.43
1:E:2356:LYS:HE2	4:E:4109:HOH:O	2.19	0.42
1:C:1431:LYS:O	1:C:1435:HIS:HD2	2.03	0.42
1:C:1369:CYS:HB2	1:C:1400:LEU:HD13	2.02	0.42
1:G:3325:LEU:HD13	1:G:3331:HIS:CE1	2.54	0.42
1:A:233:GLU:O	1:A:237:GLU:HG3	2.20	0.42
1:A:306:ASN:OD1	1:A:429:GLY:O	2.37	0.42
1:A:310:ILE:HA	1:A:313:PHE:CE2	2.55	0.42
1:E:2315:HIS:CB	1:E:2367:LEU:HD22	2.50	0.42
1:G:3353:LEU:O	1:G:3357:MET:HG3	2.20	0.42
1:E:2233:GLU:O	1:E:2237:GLU:HG3	2.20	0.41
1:A:381:LYS:HE2	4:C:4410:HOH:O	2.20	0.41
1:A:421:ARG:HD2	4:A:4014:HOH:O	2.20	0.41
1:E:2306:ASN:OD1	1:E:2429:GLY:O	2.39	0.41
1:G:3438:PHE:CE2	1:G:3442:ILE:HD11	2.56	0.41
1:C:1453:GLU:HA	1:C:1456:GLU:CD	2.41	0.40
1:C:1318:ILE:HG23	1:C:1358:ARG:HB2	2.02	0.40
1:G:3431:LYS:O	1:G:3435:HIS:HD2	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	Percentiles	
1	A	220/240 (92%)	215 (98%)	4 (2%)	1 (0%)	29	18
1	C	208/240 (87%)	206 (99%)	2 (1%)	0	100	100
1	E	220/240 (92%)	214 (97%)	5 (2%)	1 (0%)	29	18
1	G	208/240 (87%)	206 (99%)	2 (1%)	0	100	100
2	B	9/13 (69%)	9 (100%)	0	0	100	100
2	D	9/13 (69%)	6 (67%)	3 (33%)	0	100	100
2	F	9/13 (69%)	7 (78%)	2 (22%)	0	100	100
2	H	9/13 (69%)	7 (78%)	2 (22%)	0	100	100
All	All	892/1012 (88%)	870 (98%)	20 (2%)	2 (0%)	47	38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	252	ALA
1	E	2445	THR

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 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	188/207 (91%)	185 (98%)	3 (2%)	62	60
1	C	182/207 (88%)	178 (98%)	4 (2%)	52	47
1	E	188/207 (91%)	185 (98%)	3 (2%)	62	60
1	G	182/207 (88%)	179 (98%)	3 (2%)	62	60
2	B	11/13 (85%)	11 (100%)	0	100	100
2	D	11/13 (85%)	11 (100%)	0	100	100
2	F	11/13 (85%)	11 (100%)	0	100	100
2	H	11/13 (85%)	11 (100%)	0	100	100
All	All	784/880 (89%)	771 (98%)	13 (2%)	60	57

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	236	LEU
1	A	383	LEU
1	A	450	PHE
1	C	1234	ARG
1	C	1294	LEU
1	C	1383	LEU
1	C	1450	PHE
1	E	2236	LEU
1	E	2383	LEU
1	E	2450	PHE
1	G	3383	LEU
1	G	3433	LEU
1	G	3450	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	435	HIS
2	B	472	HIS
1	C	1288	HIS
1	C	1406	HIS
1	C	1435	HIS
1	E	2435	HIS
2	F	2472	HIS
1	G	3288	HIS
1	G	3306	ASN
1	G	3331	HIS
1	G	3385	ASN
1	G	3435	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 monosaccharides 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
3	BM6	E	2200	-	31,31,31	0.99	1 (3%)	49,49,49	1.09	4 (8%)
3	BM6	A	200	-	31,31,31	1.08	1 (3%)	49,49,49	1.05	2 (4%)
3	BM6	C	1200	-	31,31,31	1.12	1 (3%)	49,49,49	1.20	5 (10%)
3	BM6	G	3200	-	31,31,31	1.06	1 (3%)	49,49,49	1.27	6 (12%)

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	BM6	E	2200	-	-	3/16/44/44	0/4/4/4
3	BM6	A	200	-	-	6/16/44/44	0/4/4/4
3	BM6	C	1200	-	-	5/16/44/44	0/4/4/4
3	BM6	G	3200	-	-	5/16/44/44	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1200	BM6	C11-C12	2.37	1.42	1.39
3	G	3200	BM6	C11-C12	2.29	1.42	1.39
3	A	200	BM6	C13-C12	2.25	1.44	1.40
3	E	2200	BM6	C14-C13	2.00	1.42	1.39

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1200	BM6	O4-C8-O3	-3.70	102.21	106.24
3	G	3200	BM6	O4-C8-O3	-3.13	102.84	106.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	3200	BM6	C17-C18-C12	3.12	115.19	110.16
3	G	3200	BM6	C19-O3-C8	3.04	111.48	106.69
3	C	1200	BM6	C19-O3-C8	2.84	111.16	106.69
3	A	200	BM6	C4-C5-C8	2.80	124.66	120.48
3	E	2200	BM6	C4-C5-C8	2.78	124.63	120.48
3	G	3200	BM6	C4-C5-C8	2.57	124.32	120.48
3	E	2200	BM6	C9-C8-C5	2.46	117.24	112.71
3	C	1200	BM6	C17-C18-C12	2.39	114.02	110.16
3	C	1200	BM6	C4-C5-C8	2.36	124.01	120.48
3	E	2200	BM6	C6-C5-C8	-2.35	116.98	120.48
3	G	3200	BM6	C16-C15-C13	2.10	113.55	110.16
3	A	200	BM6	C6-C5-C8	-2.10	117.36	120.48
3	G	3200	BM6	C6-C5-C8	-2.09	117.37	120.48
3	C	1200	BM6	C21-C15-C16	-2.01	101.14	109.20
3	E	2200	BM6	C16-C15-C13	2.00	113.39	110.16

There are no chirality outliers.

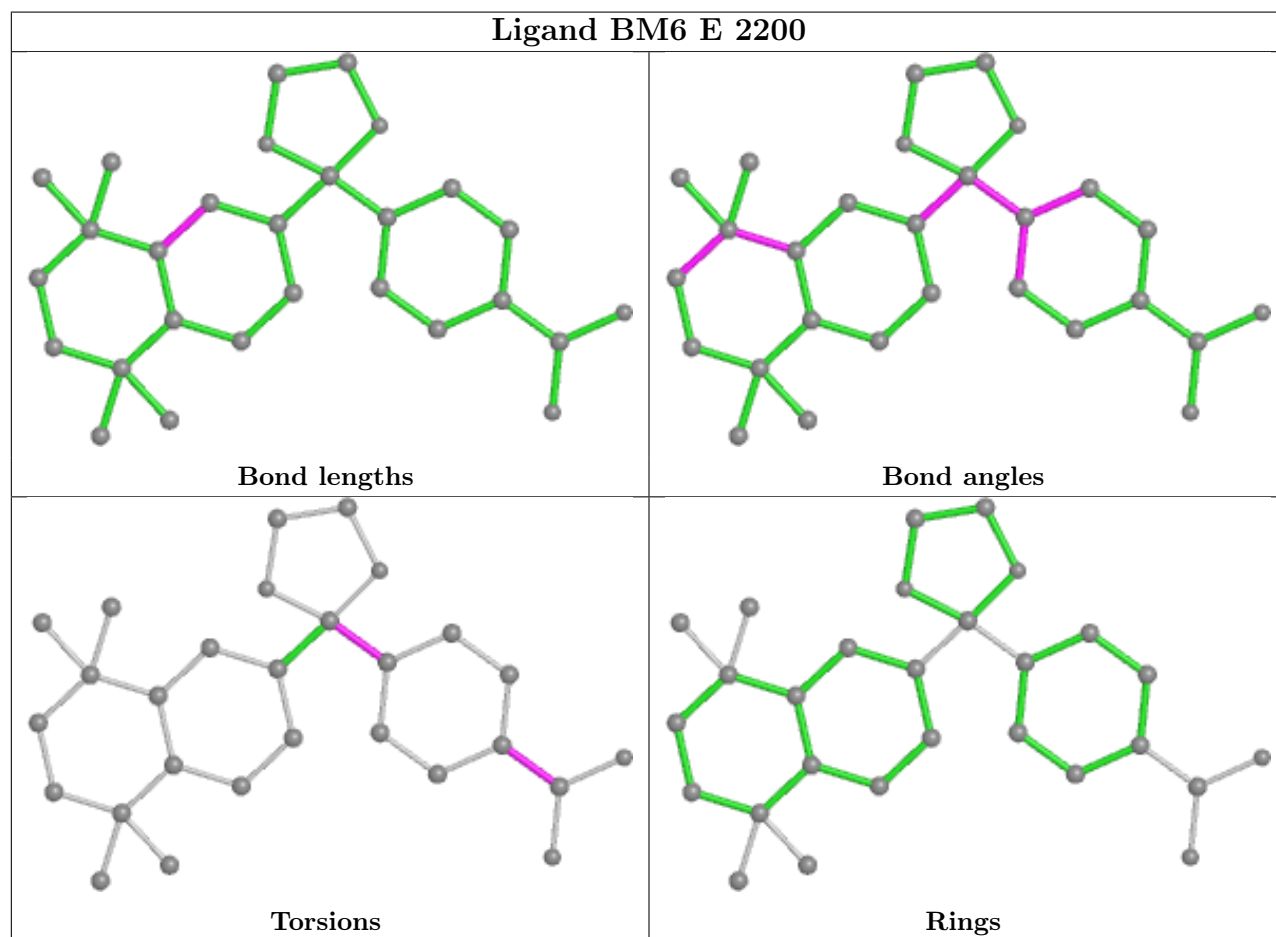
All (19) torsion outliers are listed below:

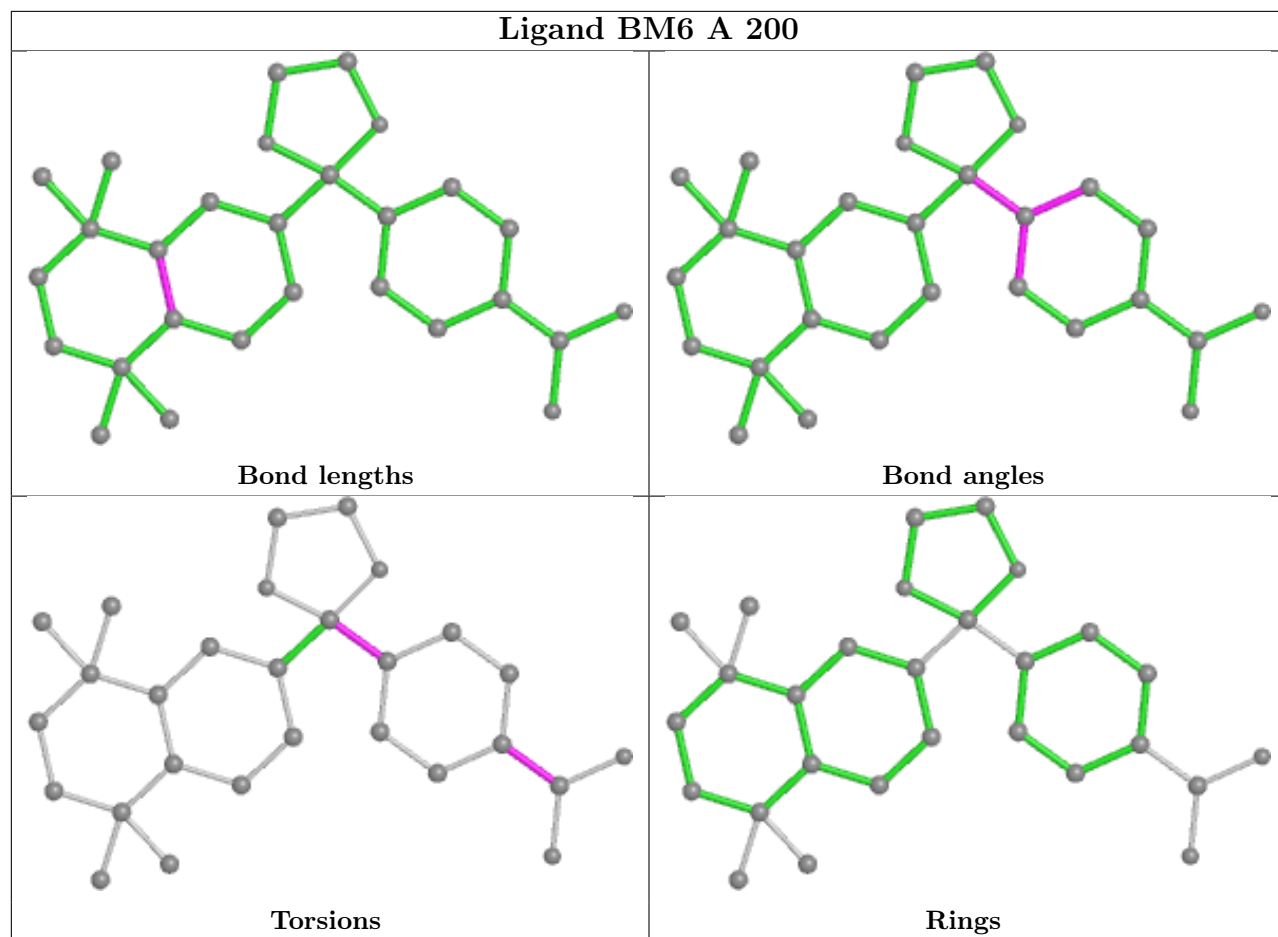
Mol	Chain	Res	Type	Atoms
3	C	1200	BM6	O2-C1-C2-C3
3	A	200	BM6	O2-C1-C2-C3
3	G	3200	BM6	O2-C1-C2-C3
3	C	1200	BM6	C6-C5-C8-C9
3	G	3200	BM6	C6-C5-C8-C9
3	A	200	BM6	O2-C1-C2-C7
3	A	200	BM6	O1-C1-C2-C3
3	A	200	BM6	O1-C1-C2-C7
3	C	1200	BM6	O1-C1-C2-C3
3	C	1200	BM6	C4-C5-C8-C9
3	G	3200	BM6	C4-C5-C8-C9
3	G	3200	BM6	O2-C1-C2-C7
3	A	200	BM6	C4-C5-C8-C9
3	E	2200	BM6	C4-C5-C8-C9
3	G	3200	BM6	O1-C1-C2-C3
3	A	200	BM6	C6-C5-C8-C9
3	E	2200	BM6	C6-C5-C8-C9
3	E	2200	BM6	O1-C1-C2-C3
3	C	1200	BM6	O2-C1-C2-C7

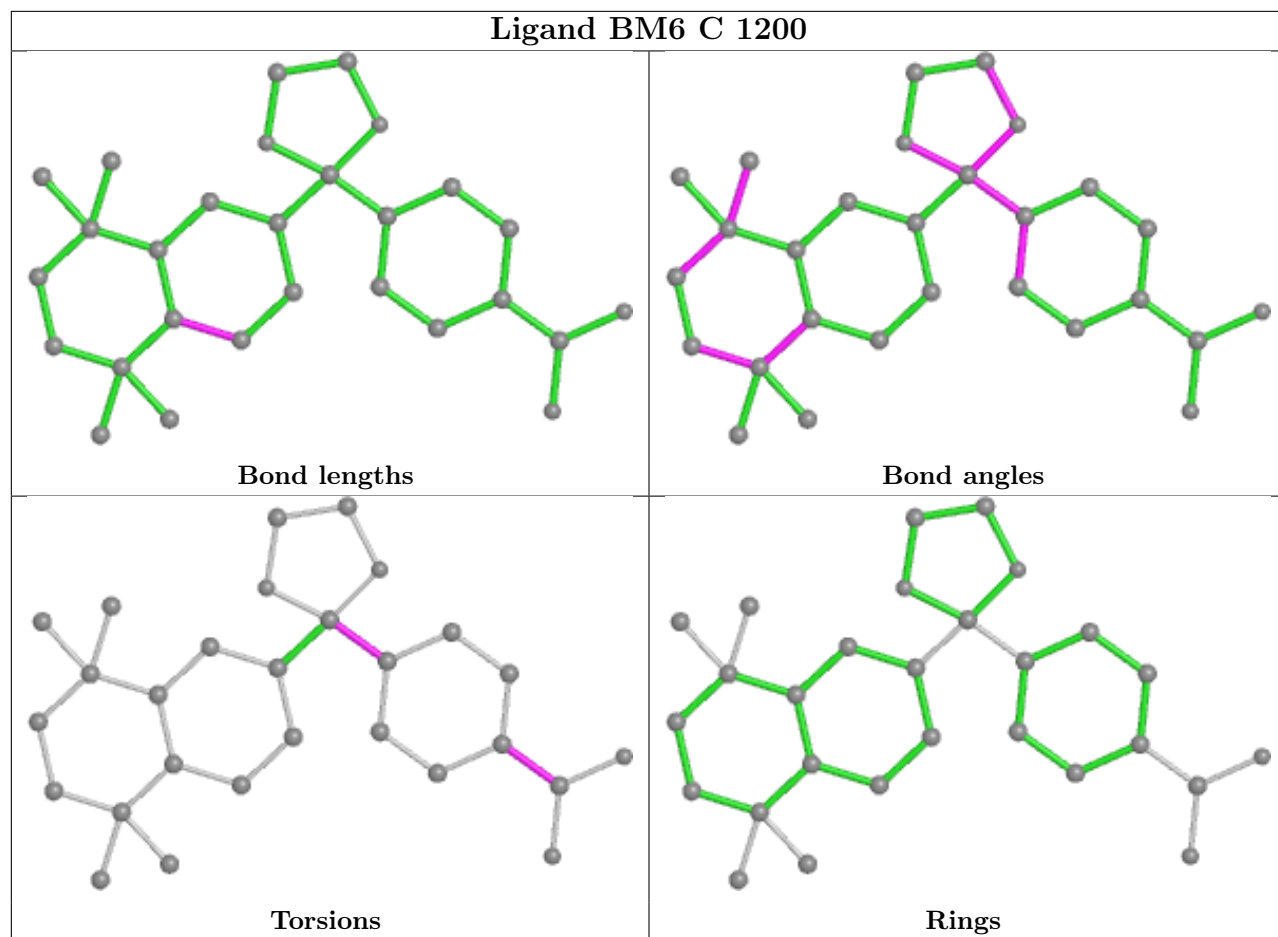
There are no ring outliers.

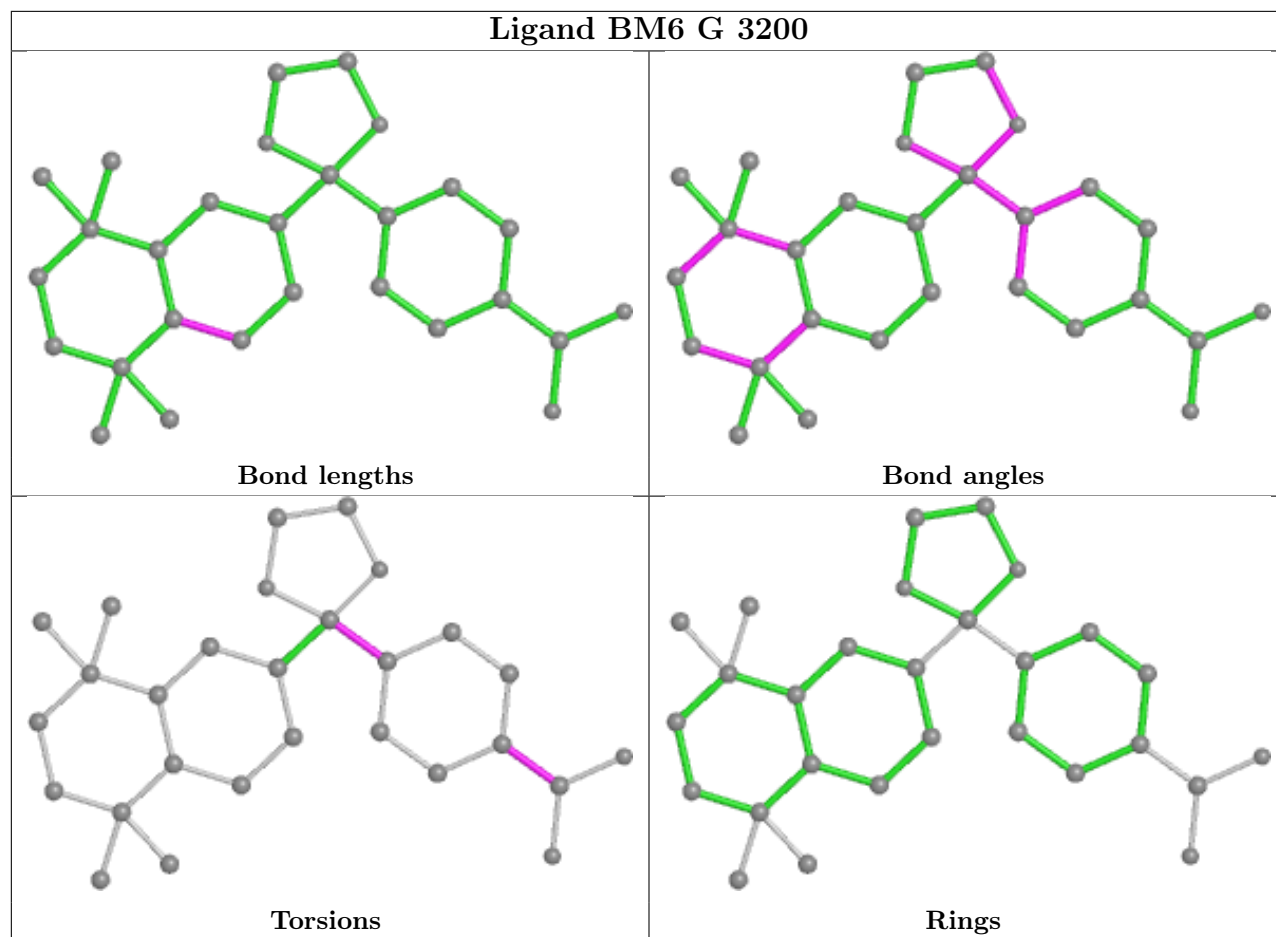
No monomer is involved in short contacts.

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.