



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 08:21 AM UTC

PDB ID : 9QHQ / pdb_00009qhq
EMDB ID : EMD-53177
Title : Cryo-EM structure of mouse TRPM3 alpha 2 in with agonists CIM-0216 and Pregnenolone sulfate (PregS)
Authors : Shkumatov, A.V.; Schenck, S.; Brunner, J.D.
Deposited on : 2025-03-16
Resolution : 3.07 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 : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

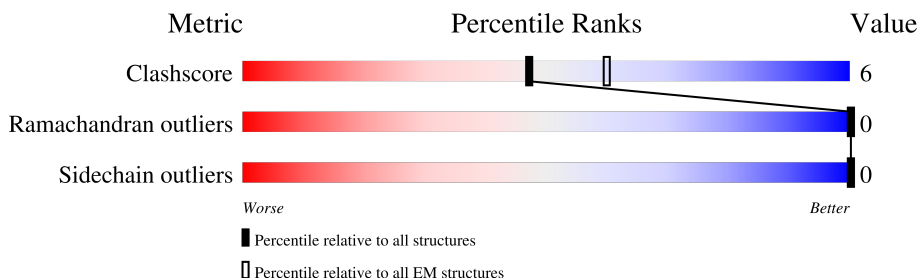
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.07 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	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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

Mol	Chain	Length	Quality of chain
1	A	1409	58% 10% 32%
1	B	1409	58% 9% 32%
1	C	1409	59% 9% 32%
1	D	1409	59% 9% 32%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 63184 atoms, of which 31876 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 MKIAA1616 protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	956	Total	C	H	N	O	S	0	0
			15617	5024	7871	1308	1355	59		
1	B	956	Total	C	H	N	O	S	0	0
			15617	5024	7871	1308	1355	59		
1	C	956	Total	C	H	N	O	S	0	0
			15617	5024	7871	1308	1355	59		
1	D	956	Total	C	H	N	O	S	0	0
			15617	5024	7871	1308	1355	59		

There are 264 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP Q69ZE8
A	1	SER	-	expression tag	UNP Q69ZE8
A	1345	ALA	-	expression tag	UNP Q69ZE8
A	1346	LEU	-	expression tag	UNP Q69ZE8
A	1347	GLU	-	expression tag	UNP Q69ZE8
A	1348	VAL	-	expression tag	UNP Q69ZE8
A	1349	LEU	-	expression tag	UNP Q69ZE8
A	1350	PHE	-	expression tag	UNP Q69ZE8
A	1351	GLN	-	expression tag	UNP Q69ZE8
A	1352	GLY	-	expression tag	UNP Q69ZE8
A	1353	PRO	-	expression tag	UNP Q69ZE8
A	1354	GLN	-	expression tag	UNP Q69ZE8
A	1355	GLY	-	expression tag	UNP Q69ZE8
A	1356	THR	-	expression tag	UNP Q69ZE8
A	1357	GLU	-	expression tag	UNP Q69ZE8
A	1358	GLN	-	expression tag	UNP Q69ZE8
A	1359	LYS	-	expression tag	UNP Q69ZE8
A	1360	LEU	-	expression tag	UNP Q69ZE8
A	1361	ILE	-	expression tag	UNP Q69ZE8
A	1362	SER	-	expression tag	UNP Q69ZE8
A	1363	GLU	-	expression tag	UNP Q69ZE8
A	1364	GLU	-	expression tag	UNP Q69ZE8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1365	ASP	-	expression tag	UNP Q69ZE8
A	1366	LEU	-	expression tag	UNP Q69ZE8
A	1367	ARG	-	expression tag	UNP Q69ZE8
A	1368	GLY	-	expression tag	UNP Q69ZE8
A	1369	ALA	-	expression tag	UNP Q69ZE8
A	1370	SER	-	expression tag	UNP Q69ZE8
A	1371	MET	-	expression tag	UNP Q69ZE8
A	1372	ASP	-	expression tag	UNP Q69ZE8
A	1373	GLU	-	expression tag	UNP Q69ZE8
A	1374	LYS	-	expression tag	UNP Q69ZE8
A	1375	THR	-	expression tag	UNP Q69ZE8
A	1376	THR	-	expression tag	UNP Q69ZE8
A	1377	GLY	-	expression tag	UNP Q69ZE8
A	1378	TRP	-	expression tag	UNP Q69ZE8
A	1379	ARG	-	expression tag	UNP Q69ZE8
A	1380	GLY	-	expression tag	UNP Q69ZE8
A	1381	GLY	-	expression tag	UNP Q69ZE8
A	1382	HIS	-	expression tag	UNP Q69ZE8
A	1383	VAL	-	expression tag	UNP Q69ZE8
A	1384	VAL	-	expression tag	UNP Q69ZE8
A	1385	GLU	-	expression tag	UNP Q69ZE8
A	1386	GLY	-	expression tag	UNP Q69ZE8
A	1387	LEU	-	expression tag	UNP Q69ZE8
A	1388	ALA	-	expression tag	UNP Q69ZE8
A	1389	GLY	-	expression tag	UNP Q69ZE8
A	1390	GLU	-	expression tag	UNP Q69ZE8
A	1391	LEU	-	expression tag	UNP Q69ZE8
A	1392	GLU	-	expression tag	UNP Q69ZE8
A	1393	GLN	-	expression tag	UNP Q69ZE8
A	1394	LEU	-	expression tag	UNP Q69ZE8
A	1395	ARG	-	expression tag	UNP Q69ZE8
A	1396	ALA	-	expression tag	UNP Q69ZE8
A	1397	ARG	-	expression tag	UNP Q69ZE8
A	1398	LEU	-	expression tag	UNP Q69ZE8
A	1399	GLU	-	expression tag	UNP Q69ZE8
A	1400	HIS	-	expression tag	UNP Q69ZE8
A	1401	HIS	-	expression tag	UNP Q69ZE8
A	1402	PRO	-	expression tag	UNP Q69ZE8
A	1403	GLN	-	expression tag	UNP Q69ZE8
A	1404	GLY	-	expression tag	UNP Q69ZE8
A	1405	GLN	-	expression tag	UNP Q69ZE8
A	1406	ARG	-	expression tag	UNP Q69ZE8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1407	GLU	-	expression tag	UNP Q69ZE8
A	1408	PRO	-	expression tag	UNP Q69ZE8
B	0	MET	-	initiating methionine	UNP Q69ZE8
B	1	SER	-	expression tag	UNP Q69ZE8
B	1345	ALA	-	expression tag	UNP Q69ZE8
B	1346	LEU	-	expression tag	UNP Q69ZE8
B	1347	GLU	-	expression tag	UNP Q69ZE8
B	1348	VAL	-	expression tag	UNP Q69ZE8
B	1349	LEU	-	expression tag	UNP Q69ZE8
B	1350	PHE	-	expression tag	UNP Q69ZE8
B	1351	GLN	-	expression tag	UNP Q69ZE8
B	1352	GLY	-	expression tag	UNP Q69ZE8
B	1353	PRO	-	expression tag	UNP Q69ZE8
B	1354	GLN	-	expression tag	UNP Q69ZE8
B	1355	GLY	-	expression tag	UNP Q69ZE8
B	1356	THR	-	expression tag	UNP Q69ZE8
B	1357	GLU	-	expression tag	UNP Q69ZE8
B	1358	GLN	-	expression tag	UNP Q69ZE8
B	1359	LYS	-	expression tag	UNP Q69ZE8
B	1360	LEU	-	expression tag	UNP Q69ZE8
B	1361	ILE	-	expression tag	UNP Q69ZE8
B	1362	SER	-	expression tag	UNP Q69ZE8
B	1363	GLU	-	expression tag	UNP Q69ZE8
B	1364	GLU	-	expression tag	UNP Q69ZE8
B	1365	ASP	-	expression tag	UNP Q69ZE8
B	1366	LEU	-	expression tag	UNP Q69ZE8
B	1367	ARG	-	expression tag	UNP Q69ZE8
B	1368	GLY	-	expression tag	UNP Q69ZE8
B	1369	ALA	-	expression tag	UNP Q69ZE8
B	1370	SER	-	expression tag	UNP Q69ZE8
B	1371	MET	-	expression tag	UNP Q69ZE8
B	1372	ASP	-	expression tag	UNP Q69ZE8
B	1373	GLU	-	expression tag	UNP Q69ZE8
B	1374	LYS	-	expression tag	UNP Q69ZE8
B	1375	THR	-	expression tag	UNP Q69ZE8
B	1376	THR	-	expression tag	UNP Q69ZE8
B	1377	GLY	-	expression tag	UNP Q69ZE8
B	1378	TRP	-	expression tag	UNP Q69ZE8
B	1379	ARG	-	expression tag	UNP Q69ZE8
B	1380	GLY	-	expression tag	UNP Q69ZE8
B	1381	GLY	-	expression tag	UNP Q69ZE8
B	1382	HIS	-	expression tag	UNP Q69ZE8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1383	VAL	-	expression tag	UNP Q69ZE8
B	1384	VAL	-	expression tag	UNP Q69ZE8
B	1385	GLU	-	expression tag	UNP Q69ZE8
B	1386	GLY	-	expression tag	UNP Q69ZE8
B	1387	LEU	-	expression tag	UNP Q69ZE8
B	1388	ALA	-	expression tag	UNP Q69ZE8
B	1389	GLY	-	expression tag	UNP Q69ZE8
B	1390	GLU	-	expression tag	UNP Q69ZE8
B	1391	LEU	-	expression tag	UNP Q69ZE8
B	1392	GLU	-	expression tag	UNP Q69ZE8
B	1393	GLN	-	expression tag	UNP Q69ZE8
B	1394	LEU	-	expression tag	UNP Q69ZE8
B	1395	ARG	-	expression tag	UNP Q69ZE8
B	1396	ALA	-	expression tag	UNP Q69ZE8
B	1397	ARG	-	expression tag	UNP Q69ZE8
B	1398	LEU	-	expression tag	UNP Q69ZE8
B	1399	GLU	-	expression tag	UNP Q69ZE8
B	1400	HIS	-	expression tag	UNP Q69ZE8
B	1401	HIS	-	expression tag	UNP Q69ZE8
B	1402	PRO	-	expression tag	UNP Q69ZE8
B	1403	GLN	-	expression tag	UNP Q69ZE8
B	1404	GLY	-	expression tag	UNP Q69ZE8
B	1405	GLN	-	expression tag	UNP Q69ZE8
B	1406	ARG	-	expression tag	UNP Q69ZE8
B	1407	GLU	-	expression tag	UNP Q69ZE8
B	1408	PRO	-	expression tag	UNP Q69ZE8
C	0	MET	-	initiating methionine	UNP Q69ZE8
C	1	SER	-	expression tag	UNP Q69ZE8
C	1345	ALA	-	expression tag	UNP Q69ZE8
C	1346	LEU	-	expression tag	UNP Q69ZE8
C	1347	GLU	-	expression tag	UNP Q69ZE8
C	1348	VAL	-	expression tag	UNP Q69ZE8
C	1349	LEU	-	expression tag	UNP Q69ZE8
C	1350	PHE	-	expression tag	UNP Q69ZE8
C	1351	GLN	-	expression tag	UNP Q69ZE8
C	1352	GLY	-	expression tag	UNP Q69ZE8
C	1353	PRO	-	expression tag	UNP Q69ZE8
C	1354	GLN	-	expression tag	UNP Q69ZE8
C	1355	GLY	-	expression tag	UNP Q69ZE8
C	1356	THR	-	expression tag	UNP Q69ZE8
C	1357	GLU	-	expression tag	UNP Q69ZE8
C	1358	GLN	-	expression tag	UNP Q69ZE8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1359	LYS	-	expression tag	UNP Q69ZE8
C	1360	LEU	-	expression tag	UNP Q69ZE8
C	1361	ILE	-	expression tag	UNP Q69ZE8
C	1362	SER	-	expression tag	UNP Q69ZE8
C	1363	GLU	-	expression tag	UNP Q69ZE8
C	1364	GLU	-	expression tag	UNP Q69ZE8
C	1365	ASP	-	expression tag	UNP Q69ZE8
C	1366	LEU	-	expression tag	UNP Q69ZE8
C	1367	ARG	-	expression tag	UNP Q69ZE8
C	1368	GLY	-	expression tag	UNP Q69ZE8
C	1369	ALA	-	expression tag	UNP Q69ZE8
C	1370	SER	-	expression tag	UNP Q69ZE8
C	1371	MET	-	expression tag	UNP Q69ZE8
C	1372	ASP	-	expression tag	UNP Q69ZE8
C	1373	GLU	-	expression tag	UNP Q69ZE8
C	1374	LYS	-	expression tag	UNP Q69ZE8
C	1375	THR	-	expression tag	UNP Q69ZE8
C	1376	THR	-	expression tag	UNP Q69ZE8
C	1377	GLY	-	expression tag	UNP Q69ZE8
C	1378	TRP	-	expression tag	UNP Q69ZE8
C	1379	ARG	-	expression tag	UNP Q69ZE8
C	1380	GLY	-	expression tag	UNP Q69ZE8
C	1381	GLY	-	expression tag	UNP Q69ZE8
C	1382	HIS	-	expression tag	UNP Q69ZE8
C	1383	VAL	-	expression tag	UNP Q69ZE8
C	1384	VAL	-	expression tag	UNP Q69ZE8
C	1385	GLU	-	expression tag	UNP Q69ZE8
C	1386	GLY	-	expression tag	UNP Q69ZE8
C	1387	LEU	-	expression tag	UNP Q69ZE8
C	1388	ALA	-	expression tag	UNP Q69ZE8
C	1389	GLY	-	expression tag	UNP Q69ZE8
C	1390	GLU	-	expression tag	UNP Q69ZE8
C	1391	LEU	-	expression tag	UNP Q69ZE8
C	1392	GLU	-	expression tag	UNP Q69ZE8
C	1393	GLN	-	expression tag	UNP Q69ZE8
C	1394	LEU	-	expression tag	UNP Q69ZE8
C	1395	ARG	-	expression tag	UNP Q69ZE8
C	1396	ALA	-	expression tag	UNP Q69ZE8
C	1397	ARG	-	expression tag	UNP Q69ZE8
C	1398	LEU	-	expression tag	UNP Q69ZE8
C	1399	GLU	-	expression tag	UNP Q69ZE8
C	1400	HIS	-	expression tag	UNP Q69ZE8

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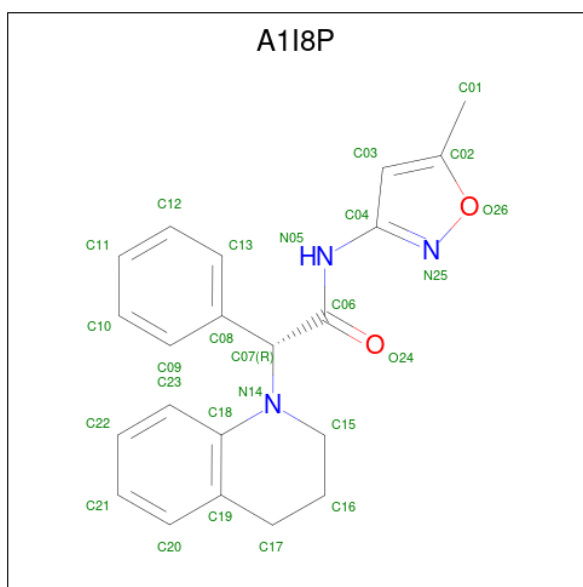
Chain	Residue	Modelled	Actual	Comment	Reference
C	1401	HIS	-	expression tag	UNP Q69ZE8
C	1402	PRO	-	expression tag	UNP Q69ZE8
C	1403	GLN	-	expression tag	UNP Q69ZE8
C	1404	GLY	-	expression tag	UNP Q69ZE8
C	1405	GLN	-	expression tag	UNP Q69ZE8
C	1406	ARG	-	expression tag	UNP Q69ZE8
C	1407	GLU	-	expression tag	UNP Q69ZE8
C	1408	PRO	-	expression tag	UNP Q69ZE8
D	0	MET	-	initiating methionine	UNP Q69ZE8
D	1	SER	-	expression tag	UNP Q69ZE8
D	1345	ALA	-	expression tag	UNP Q69ZE8
D	1346	LEU	-	expression tag	UNP Q69ZE8
D	1347	GLU	-	expression tag	UNP Q69ZE8
D	1348	VAL	-	expression tag	UNP Q69ZE8
D	1349	LEU	-	expression tag	UNP Q69ZE8
D	1350	PHE	-	expression tag	UNP Q69ZE8
D	1351	GLN	-	expression tag	UNP Q69ZE8
D	1352	GLY	-	expression tag	UNP Q69ZE8
D	1353	PRO	-	expression tag	UNP Q69ZE8
D	1354	GLN	-	expression tag	UNP Q69ZE8
D	1355	GLY	-	expression tag	UNP Q69ZE8
D	1356	THR	-	expression tag	UNP Q69ZE8
D	1357	GLU	-	expression tag	UNP Q69ZE8
D	1358	GLN	-	expression tag	UNP Q69ZE8
D	1359	LYS	-	expression tag	UNP Q69ZE8
D	1360	LEU	-	expression tag	UNP Q69ZE8
D	1361	ILE	-	expression tag	UNP Q69ZE8
D	1362	SER	-	expression tag	UNP Q69ZE8
D	1363	GLU	-	expression tag	UNP Q69ZE8
D	1364	GLU	-	expression tag	UNP Q69ZE8
D	1365	ASP	-	expression tag	UNP Q69ZE8
D	1366	LEU	-	expression tag	UNP Q69ZE8
D	1367	ARG	-	expression tag	UNP Q69ZE8
D	1368	GLY	-	expression tag	UNP Q69ZE8
D	1369	ALA	-	expression tag	UNP Q69ZE8
D	1370	SER	-	expression tag	UNP Q69ZE8
D	1371	MET	-	expression tag	UNP Q69ZE8
D	1372	ASP	-	expression tag	UNP Q69ZE8
D	1373	GLU	-	expression tag	UNP Q69ZE8
D	1374	LYS	-	expression tag	UNP Q69ZE8
D	1375	THR	-	expression tag	UNP Q69ZE8
D	1376	THR	-	expression tag	UNP Q69ZE8

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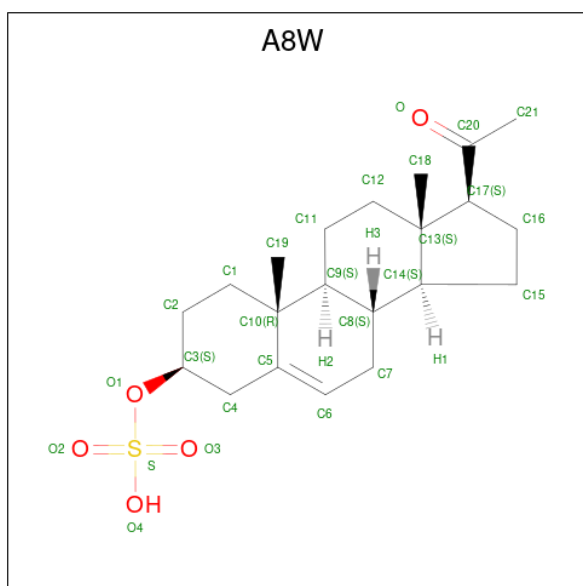
Chain	Residue	Modelled	Actual	Comment	Reference
D	1377	GLY	-	expression tag	UNP Q69ZE8
D	1378	TRP	-	expression tag	UNP Q69ZE8
D	1379	ARG	-	expression tag	UNP Q69ZE8
D	1380	GLY	-	expression tag	UNP Q69ZE8
D	1381	GLY	-	expression tag	UNP Q69ZE8
D	1382	HIS	-	expression tag	UNP Q69ZE8
D	1383	VAL	-	expression tag	UNP Q69ZE8
D	1384	VAL	-	expression tag	UNP Q69ZE8
D	1385	GLU	-	expression tag	UNP Q69ZE8
D	1386	GLY	-	expression tag	UNP Q69ZE8
D	1387	LEU	-	expression tag	UNP Q69ZE8
D	1388	ALA	-	expression tag	UNP Q69ZE8
D	1389	GLY	-	expression tag	UNP Q69ZE8
D	1390	GLU	-	expression tag	UNP Q69ZE8
D	1391	LEU	-	expression tag	UNP Q69ZE8
D	1392	GLU	-	expression tag	UNP Q69ZE8
D	1393	GLN	-	expression tag	UNP Q69ZE8
D	1394	LEU	-	expression tag	UNP Q69ZE8
D	1395	ARG	-	expression tag	UNP Q69ZE8
D	1396	ALA	-	expression tag	UNP Q69ZE8
D	1397	ARG	-	expression tag	UNP Q69ZE8
D	1398	LEU	-	expression tag	UNP Q69ZE8
D	1399	GLU	-	expression tag	UNP Q69ZE8
D	1400	HIS	-	expression tag	UNP Q69ZE8
D	1401	HIS	-	expression tag	UNP Q69ZE8
D	1402	PRO	-	expression tag	UNP Q69ZE8
D	1403	GLN	-	expression tag	UNP Q69ZE8
D	1404	GLY	-	expression tag	UNP Q69ZE8
D	1405	GLN	-	expression tag	UNP Q69ZE8
D	1406	ARG	-	expression tag	UNP Q69ZE8
D	1407	GLU	-	expression tag	UNP Q69ZE8
D	1408	PRO	-	expression tag	UNP Q69ZE8

- Molecule 2 is (2 {R})-2-(3,4-dihydro-2 {H}-quinolin-1-yl)- {N}-(5-methyl-1,2-oxazol-3-yl)-2-phenyl-ethanamide (CCD ID: A1I8P) (formula: C₂₁H₂₁N₃O₂) (labeled as "Ligand of Interest" by depositor).



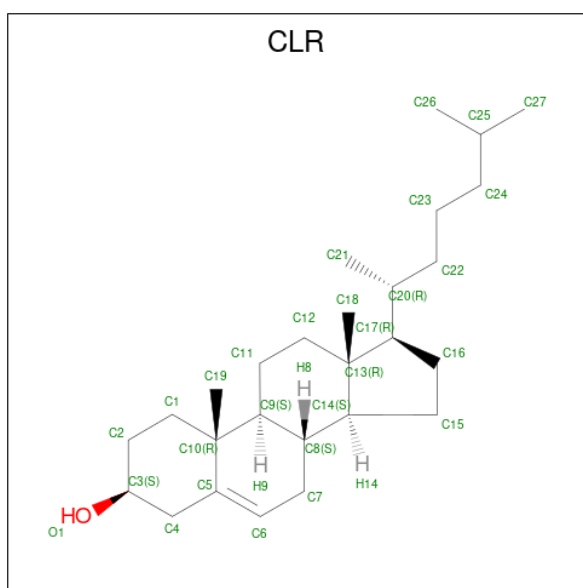
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	H	N	O	0
			47	21	21	3	2	
2	B	1	Total	C	H	N	O	0
			47	21	21	3	2	
2	C	1	Total	C	H	N	O	0
			47	21	21	3	2	
2	D	1	Total	C	H	N	O	0
			47	21	21	3	2	

- Molecule 3 is Pregnenolone sulfate (CCD ID: A8W) (formula: $C_{21}H_{32}O_5S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	H	O	S	0
			58	21	31	5	1	
3	B	1	Total	C	H	O	S	0
			58	21	31	5	1	
3	C	1	Total	C	H	O	S	0
			58	21	31	5	1	
3	D	1	Total	C	H	O	S	0
			58	21	31	5	1	

- Molecule 4 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$).

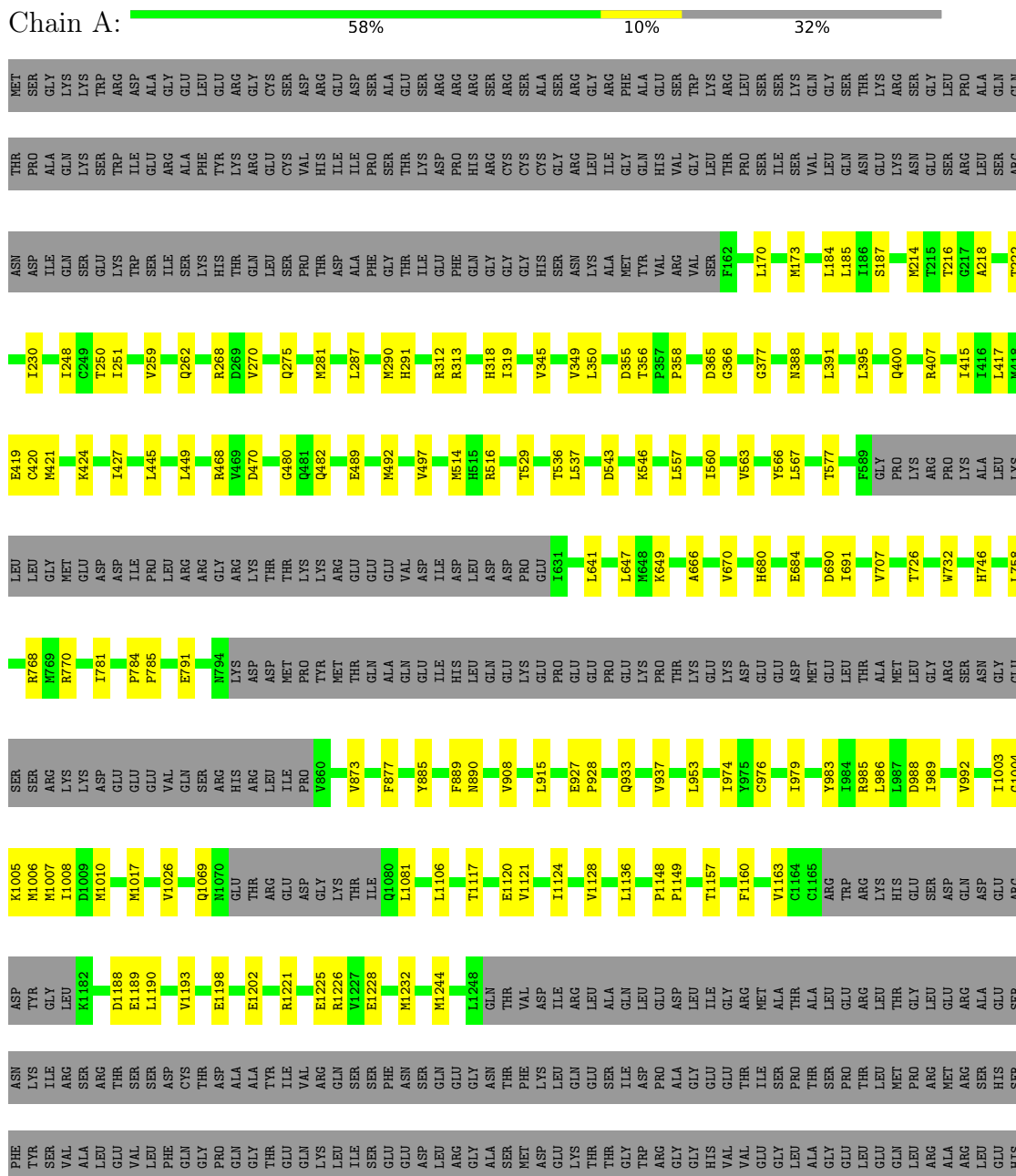


Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	H	O		0
			74	27	46	1		
4	A	1	Total	C	H	O		0
			74	27	46	1		
4	C	1	Total	C	H	O		0
			74	27	46	1		
4	D	1	Total	C	H	O		0
			74	27	46	1		

3 Residue-property plots

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

• Molecule 1: MKIAA1616 protein



[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	58787	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	62	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: A8W, A1I8P, CLR

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	0.15	0/7923	0.33	0/10714
1	B	0.15	0/7923	0.33	0/10714
1	C	0.15	0/7923	0.32	0/10714
1	D	0.15	0/7923	0.32	0/10714
All	All	0.15	0/31692	0.32	0/42856

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7746	7871	7881	98	0
1	B	7746	7871	7881	99	0
1	C	7746	7871	7881	98	0
1	D	7746	7871	7881	100	0
2	A	26	21	0	3	0
2	B	26	21	0	3	0
2	C	26	21	0	3	0
2	D	26	21	0	3	0
3	A	27	31	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	27	31	0	0	0
3	C	27	31	0	0	0
3	D	27	31	0	0	0
4	A	56	92	92	0	0
4	C	28	46	46	0	0
4	D	28	46	46	0	0
All	All	31308	31876	31708	378	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 6.

All (378) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:985:ARG:NH1	1:A:988:ASP:OD2	2.07	0.88
1:D:976:CYS:O	1:D:979:ILE:HG22	1.79	0.83
1:C:976:CYS:O	1:C:979:ILE:HG22	1.78	0.83
1:A:976:CYS:O	1:A:979:ILE:HG22	1.78	0.81
1:B:976:CYS:O	1:B:979:ILE:HG22	1.79	0.81
1:D:890:ASN:OD1	1:D:979:ILE:HD11	1.87	0.74
1:C:568:MET:HE2	1:C:674:LEU:HD21	1.70	0.73
1:B:890:ASN:OD1	1:B:979:ILE:HD11	1.87	0.73
1:A:890:ASN:OD1	1:A:979:ILE:HD11	1.90	0.72
1:A:726:THR:CG2	1:A:758:LEU:HD11	2.21	0.71
1:D:718:GLU:N	1:D:718:GLU:OE2	2.25	0.68
1:C:1235:GLU:OE2	1:D:1233:ARG:NH1	2.26	0.68
1:A:1188:ASP:OD1	1:A:1189:GLU:N	2.28	0.67
1:B:889:PHE:HD1	1:B:908:VAL:HG11	1.61	0.65
1:C:781:ILE:HD12	1:C:877:PHE:CD1	2.31	0.65
1:A:1003:ILE:O	1:A:1007:MET:HG2	1.97	0.64
1:A:173:MET:HE1	1:A:251:ILE:HD12	1.80	0.63
1:A:726:THR:HG23	1:A:758:LEU:HD11	1.81	0.63
1:B:1003:ILE:O	1:B:1007:MET:HG2	1.99	0.63
1:D:885:TYR:HE1	1:D:908:VAL:HG13	1.63	0.63
1:B:718:GLU:OE2	1:B:718:GLU:N	2.30	0.63
1:C:568:MET:HE1	1:C:670:VAL:HG13	1.81	0.62
1:C:1157:THR:HA	1:C:1160:PHE:CE1	2.34	0.62
1:D:1003:ILE:O	1:D:1007:MET:HG2	1.99	0.62
1:A:222:THR:HG22	1:A:230:ILE:HD12	1.81	0.62
1:A:365:ASP:OD2	1:A:366:GLY:N	2.32	0.62
1:B:885:TYR:HE1	1:B:908:VAL:HG13	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1157:THR:HA	1:B:1160:PHE:CE1	2.34	0.62
1:C:214:MET:HA	1:C:214:MET:HE2	1.81	0.62
1:D:889:PHE:HD1	1:D:908:VAL:HG11	1.63	0.62
1:D:222:THR:HG22	1:D:230:ILE:HD12	1.82	0.61
1:B:680:HIS:NE2	1:B:684:GLU:OE2	2.33	0.61
1:A:1006:MET:N	1:A:1006:MET:HE2	2.15	0.61
1:B:214:MET:HE2	1:B:214:MET:HA	1.83	0.61
1:B:781:ILE:HD12	1:B:877:PHE:CD1	2.34	0.61
1:D:579:LYS:HE3	1:D:579:LYS:HA	1.81	0.61
1:B:222:THR:HG22	1:B:230:ILE:HD12	1.83	0.61
1:C:222:THR:HG22	1:C:230:ILE:HD12	1.83	0.61
1:C:579:LYS:HE3	1:C:579:LYS:HA	1.81	0.61
1:D:680:HIS:NE2	1:D:684:GLU:OE2	2.34	0.61
1:A:1157:THR:HA	1:A:1160:PHE:CE1	2.36	0.61
1:D:690:ASP:OD1	1:D:691:ILE:N	2.34	0.61
1:A:680:HIS:NE2	1:A:684:GLU:OE2	2.33	0.60
1:A:268:ARG:O	1:A:270:VAL:HG13	2.02	0.60
1:C:666:ALA:O	1:C:670:VAL:HG23	2.02	0.60
1:D:268:ARG:O	1:D:270:VAL:HG13	2.02	0.59
1:B:268:ARG:O	1:B:270:VAL:HG13	2.03	0.59
1:C:680:HIS:NE2	1:C:684:GLU:OE2	2.35	0.59
1:C:268:ARG:O	1:C:270:VAL:HG13	2.02	0.59
1:A:690:ASP:OD1	1:A:691:ILE:N	2.36	0.59
1:A:345:VAL:O	1:A:349:VAL:HG23	2.03	0.58
1:B:690:ASP:OD1	1:B:691:ILE:N	2.36	0.58
1:D:781:ILE:HD12	1:D:877:PHE:CD1	2.39	0.58
1:D:1005:LYS:HD3	1:D:1121:VAL:HG13	1.86	0.58
1:C:690:ASP:OD1	1:C:691:ILE:N	2.37	0.57
1:B:1005:LYS:HD3	1:B:1121:VAL:HG13	1.87	0.57
1:A:1005:LYS:HD3	1:A:1121:VAL:HG13	1.87	0.57
1:C:890:ASN:OD1	1:C:979:ILE:HD11	2.04	0.57
1:B:889:PHE:CD1	1:B:908:VAL:HG11	2.39	0.56
1:D:281:MET:SD	1:D:281:MET:N	2.78	0.56
1:B:281:MET:SD	1:B:281:MET:N	2.78	0.56
1:C:281:MET:SD	1:C:281:MET:N	2.78	0.56
1:A:560:ILE:HD11	1:A:647:LEU:HD13	1.87	0.55
1:C:1117:THR:O	1:C:1121:VAL:HG23	2.06	0.55
1:D:214:MET:HE2	1:D:214:MET:HA	1.88	0.55
1:D:889:PHE:CD1	1:D:908:VAL:HG11	2.40	0.55
1:A:281:MET:SD	1:A:281:MET:N	2.78	0.55
1:D:1006:MET:N	1:D:1006:MET:HE2	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1160:PHE:HA	1:A:1163:VAL:HG12	1.88	0.55
1:A:445:LEU:O	1:A:449:LEU:HD23	2.07	0.55
1:C:890:ASN:ND2	1:C:983:TYR:OH	2.37	0.55
1:B:1006:MET:N	1:B:1006:MET:HE2	2.22	0.55
1:C:214:MET:HE3	1:C:248:ILE:HG12	1.89	0.54
1:D:1159:ILE:O	1:D:1162:HIS:ND1	2.41	0.54
1:A:516:ARG:NH1	1:B:275:GLN:OE1	2.41	0.53
1:A:1120:GLU:O	1:A:1124:ILE:HD12	2.08	0.53
1:B:1004:GLY:O	1:B:1008:ILE:HD12	2.08	0.53
1:B:986:LEU:HD23	1:B:989:ILE:HD12	1.89	0.53
1:B:1160:PHE:HA	1:B:1163:VAL:HG12	1.91	0.53
1:C:1160:PHE:HA	1:C:1163:VAL:HG12	1.89	0.53
1:B:214:MET:HE3	1:B:248:ILE:HG12	1.92	0.52
1:C:986:LEU:HD23	1:C:989:ILE:HD12	1.90	0.52
1:A:889:PHE:CD1	1:A:908:VAL:HG11	2.45	0.52
1:A:781:ILE:HD12	1:A:877:PHE:CD1	2.44	0.52
1:A:1004:GLY:O	1:A:1008:ILE:HD12	2.09	0.52
1:C:1120:GLU:O	1:C:1124:ILE:HD12	2.10	0.52
1:D:497:VAL:HG13	1:D:529:THR:HG21	1.92	0.52
1:B:890:ASN:ND2	1:B:983:TYR:OH	2.36	0.52
1:A:214:MET:HA	1:A:214:MET:HE2	1.92	0.52
1:D:885:TYR:CE1	1:D:908:VAL:HG13	2.45	0.52
1:A:497:VAL:HG13	1:A:529:THR:HG21	1.92	0.52
1:C:497:VAL:HG13	1:C:529:THR:HG21	1.92	0.51
1:A:563:VAL:O	1:A:567:LEU:HD23	2.10	0.51
1:B:497:VAL:HG13	1:B:529:THR:HG21	1.92	0.51
1:A:187:SER:OG	1:A:312:ARG:NH2	2.41	0.51
1:A:889:PHE:HD1	1:A:908:VAL:HG11	1.74	0.51
1:B:1005:LYS:CD	1:B:1121:VAL:HG13	2.41	0.51
1:D:986:LEU:HD23	1:D:989:ILE:HD12	1.91	0.51
1:A:275:GLN:OE1	1:C:516:ARG:NH1	2.44	0.51
1:A:415:ILE:O	1:A:419:GLU:OE1	2.29	0.51
1:D:1005:LYS:CD	1:D:1121:VAL:HG13	2.41	0.51
1:B:415:ILE:O	1:B:419:GLU:OE1	2.29	0.51
1:A:1005:LYS:CD	1:A:1121:VAL:HG13	2.40	0.51
1:A:1017:MET:SD	1:A:1106:LEU:HD12	2.51	0.51
1:B:395:LEU:HD21	1:B:417:LEU:HD23	1.93	0.51
1:B:418:MET:HA	1:B:418:MET:HE2	1.92	0.50
1:B:356:THR:O	1:B:358:PRO:HD3	2.12	0.50
1:B:377:GLY:C	1:B:421:MET:HE3	2.37	0.50
1:B:885:TYR:CE1	1:B:908:VAL:HG13	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:415:ILE:O	1:D:419:GLU:OE1	2.29	0.50
1:A:536:THR:HG22	1:A:536:THR:O	2.12	0.50
1:B:514:MET:HE2	1:B:641:LEU:HD11	1.94	0.50
1:C:563:VAL:O	1:C:567:LEU:HD23	2.11	0.50
1:D:536:THR:HG22	1:D:536:THR:O	2.12	0.50
1:A:480:GLY:O	1:A:482:GLN:NE2	2.45	0.50
1:C:415:ILE:O	1:C:419:GLU:OE1	2.29	0.50
1:C:773:SER:O	1:C:777:VAL:HG23	2.11	0.50
1:D:356:THR:O	1:D:358:PRO:HD3	2.12	0.50
1:D:690:ASP:OD1	1:D:691:ILE:HG23	2.12	0.49
1:B:781:ILE:HD11	1:B:873:VAL:HG13	1.93	0.49
1:D:989:ILE:HG13	2:D:1503:A1I8P:C21	2.43	0.49
1:D:1188:ASP:OD2	1:D:1189:GLU:N	2.45	0.49
1:C:356:THR:O	1:C:358:PRO:HD3	2.12	0.49
1:B:536:THR:HG22	1:B:536:THR:O	2.11	0.49
1:C:992:VAL:HG22	1:C:1136:LEU:HD21	1.93	0.49
1:B:516:ARG:NH1	1:D:275:GLN:OE1	2.45	0.49
1:B:1188:ASP:OD2	1:B:1189:GLU:N	2.45	0.49
1:A:356:THR:O	1:A:358:PRO:HD3	2.12	0.49
1:B:1148:PRO:N	1:B:1149:PRO:HD2	2.28	0.49
1:B:563:VAL:O	1:B:567:LEU:HD23	2.13	0.49
1:B:989:ILE:HG13	2:B:1502:A1I8P:C21	2.43	0.49
1:C:781:ILE:HD12	1:C:877:PHE:HD1	1.74	0.49
1:A:514:MET:HE2	1:A:641:LEU:HD11	1.94	0.48
1:A:885:TYR:HE1	1:A:908:VAL:HG13	1.78	0.48
1:C:1232:MET:N	1:C:1232:MET:HE2	2.28	0.48
1:D:563:VAL:O	1:D:567:LEU:HD23	2.13	0.48
1:D:184:LEU:CD2	1:D:216:THR:HG21	2.43	0.48
1:D:1148:PRO:N	1:D:1149:PRO:HD2	2.29	0.48
1:A:1232:MET:N	1:A:1232:MET:HE2	2.28	0.48
1:D:992:VAL:HG22	1:D:1136:LEU:HD21	1.94	0.48
1:D:1159:ILE:HA	1:D:1162:HIS:HD1	1.79	0.48
1:C:1188:ASP:OD1	1:C:1189:GLU:N	2.45	0.48
1:B:972:ARG:NH1	1:D:1030:ALA:O	2.47	0.48
1:C:1148:PRO:N	1:C:1149:PRO:HD2	2.28	0.48
1:A:543:ASP:O	1:A:546:LYS:HE3	2.14	0.48
1:B:537:LEU:HD11	1:B:560:ILE:CD1	2.44	0.48
1:B:992:VAL:HG22	1:B:1136:LEU:HD21	1.94	0.48
1:C:537:LEU:HD11	1:C:560:ILE:CD1	2.44	0.48
1:B:1017:MET:CE	1:B:1106:LEU:HD12	2.43	0.47
1:C:989:ILE:HG13	2:C:1502:A1I8P:C21	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1017:MET:CE	1:D:1106:LEU:HD12	2.44	0.47
1:A:400:GLN:OE1	1:A:407:ARG:NH1	2.48	0.47
1:B:543:ASP:O	1:B:546:LYS:HE3	2.14	0.47
1:D:395:LEU:HD21	1:D:417:LEU:HD23	1.96	0.47
1:D:537:LEU:HD11	1:D:560:ILE:CD1	2.44	0.47
1:A:992:VAL:HG22	1:A:1136:LEU:HD21	1.96	0.47
1:D:890:ASN:ND2	1:D:983:TYR:OH	2.37	0.47
1:A:666:ALA:O	1:A:670:VAL:HG23	2.14	0.47
1:B:1232:MET:HE2	1:B:1232:MET:N	2.28	0.47
1:D:1232:MET:N	1:D:1232:MET:HE2	2.28	0.47
1:A:1148:PRO:N	1:A:1149:PRO:HD2	2.30	0.47
1:B:170:LEU:HD22	1:B:318:HIS:CD2	2.50	0.47
1:C:418:MET:HE2	1:C:418:MET:HA	1.97	0.47
1:D:418:MET:HE2	1:D:418:MET:HA	1.97	0.47
1:D:543:ASP:O	1:D:546:LYS:HE3	2.14	0.47
1:C:275:GLN:OE1	1:D:516:ARG:NH1	2.48	0.47
1:C:395:LEU:HD21	1:C:417:LEU:HD23	1.96	0.47
1:C:568:MET:HE1	1:C:670:VAL:CG1	2.45	0.47
1:C:649:LYS:HG3	1:C:649:LYS:O	2.16	0.47
1:D:965:GLN:OE1	1:D:969:SER:OG	2.33	0.46
1:B:649:LYS:O	1:B:649:LYS:HG3	2.15	0.46
1:C:543:ASP:O	1:C:546:LYS:HE3	2.15	0.46
1:C:726:THR:HG22	1:C:758:LEU:HD21	1.98	0.46
1:C:1002:MET:HG3	1:C:1121:VAL:HG12	1.96	0.46
1:D:170:LEU:HD22	1:D:318:HIS:CD2	2.51	0.46
1:C:480:GLY:O	1:C:482:GLN:NE2	2.49	0.46
1:A:250:THR:HG22	1:A:291:HIS:CD2	2.51	0.46
1:A:781:ILE:HD11	1:A:873:VAL:HG13	1.98	0.46
1:B:480:GLY:O	1:B:482:GLN:NE2	2.49	0.46
1:D:726:THR:HG22	1:D:758:LEU:HD21	1.98	0.46
1:D:468:ARG:HA	1:D:468:ARG:NE	2.31	0.46
1:D:726:THR:CG2	1:D:758:LEU:HD21	2.46	0.46
1:B:726:THR:HG22	1:B:758:LEU:HD21	1.98	0.46
1:D:187:SER:OG	1:D:312:ARG:NH2	2.42	0.46
1:A:989:ILE:HG13	2:A:1501:A1I8P:C21	2.46	0.46
1:C:170:LEU:HD22	1:C:318:HIS:CD2	2.51	0.46
1:C:935:VAL:HG13	1:C:939:LEU:HD23	1.98	0.46
1:D:935:VAL:HG13	1:D:939:LEU:HD23	1.98	0.46
1:A:1010:MET:HG3	1:B:1105:LEU:HD13	1.99	0.45
1:B:1017:MET:HE1	1:B:1106:LEU:HD12	1.98	0.45
1:D:649:LYS:O	1:D:649:LYS:HG3	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:666:ALA:O	1:D:670:VAL:HG23	2.15	0.45
1:B:468:ARG:NE	1:B:468:ARG:HA	2.31	0.45
1:B:666:ALA:O	1:B:670:VAL:HG23	2.16	0.45
1:C:1030:ALA:O	1:D:972:ARG:NH1	2.49	0.45
1:B:184:LEU:CD2	1:B:216:THR:HG21	2.45	0.45
1:A:170:LEU:HD22	1:A:318:HIS:CD2	2.51	0.45
1:B:184:LEU:HB3	1:B:218:ALA:HB2	1.98	0.45
1:C:468:ARG:HA	1:C:468:ARG:NE	2.31	0.45
1:D:480:GLY:O	1:D:482:GLN:NE2	2.48	0.45
1:D:670:VAL:HG21	1:D:732:TRP:CE3	2.52	0.45
1:A:395:LEU:HD21	1:A:417:LEU:HD23	1.99	0.45
1:D:337:LEU:HD11	1:D:440:ILE:HD11	1.99	0.45
1:C:915:LEU:HD13	2:C:1502:A1I8P:C03	2.47	0.45
1:D:184:LEU:HB3	1:D:218:ALA:HB2	1.97	0.45
1:C:184:LEU:CD2	1:C:216:THR:HG21	2.46	0.45
1:C:791:GLU:OE1	1:C:791:GLU:N	2.50	0.45
1:D:791:GLU:N	1:D:791:GLU:OE1	2.50	0.45
1:D:1017:MET:HE1	1:D:1106:LEU:HD12	1.98	0.45
1:A:791:GLU:N	1:A:791:GLU:OE1	2.49	0.45
1:A:768:ARG:O	1:A:770:ARG:NH1	2.50	0.45
1:B:935:VAL:HG13	1:B:939:LEU:HD23	1.99	0.45
1:C:726:THR:CG2	1:C:758:LEU:HD21	2.47	0.45
1:C:939:LEU:HD13	1:C:945:VAL:HG22	1.99	0.45
1:D:939:LEU:HD13	1:D:945:VAL:HG22	1.99	0.45
1:A:577:THR:O	1:A:577:THR:HG22	2.17	0.44
1:A:1124:ILE:O	1:A:1128:VAL:HG23	2.16	0.44
1:B:337:LEU:HD11	1:B:440:ILE:HD11	1.99	0.44
1:B:1124:ILE:O	1:B:1128:VAL:HG23	2.18	0.44
1:B:400:GLN:OE1	1:B:407:ARG:NH1	2.50	0.44
1:D:222:THR:CG2	1:D:230:ILE:HD12	2.47	0.44
1:D:400:GLN:OE1	1:D:407:ARG:NH1	2.50	0.44
1:A:468:ARG:HA	1:A:468:ARG:NE	2.31	0.44
1:A:1190:LEU:O	1:A:1193:VAL:HG12	2.17	0.44
1:B:577:THR:HG22	1:B:577:THR:O	2.18	0.44
1:C:337:LEU:HD11	1:C:440:ILE:HD11	1.99	0.44
1:B:939:LEU:HD13	1:B:945:VAL:HG22	1.99	0.44
1:C:400:GLN:OE1	1:C:407:ARG:NH1	2.50	0.44
1:C:867:PHE:O	1:C:873:VAL:HG21	2.18	0.44
1:A:184:LEU:CD2	1:A:216:THR:HG21	2.48	0.44
1:A:184:LEU:HB3	1:A:218:ALA:HB2	1.98	0.44
1:C:1100:LEU:CD1	1:D:1010:MET:HE1	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:915:LEU:HD13	2:A:1501:A1I8P:C03	2.48	0.44
1:B:726:THR:CG2	1:B:758:LEU:HD21	2.47	0.44
1:C:577:THR:HG22	1:C:577:THR:O	2.18	0.44
1:D:209:LEU:HD23	1:D:209:LEU:C	2.43	0.44
1:A:259:VAL:HG12	1:A:287:LEU:HD21	1.98	0.44
1:C:445:LEU:O	1:C:449:LEU:HD23	2.17	0.44
1:A:259:VAL:HG23	1:A:262:GLN:HB3	2.00	0.44
1:B:250:THR:HG22	1:B:291:HIS:CD2	2.53	0.44
1:A:313:ARG:NH2	1:A:355:ASP:OD2	2.50	0.43
1:B:791:GLU:N	1:B:791:GLU:OE1	2.50	0.43
1:C:933:GLN:O	1:C:937:VAL:HG12	2.18	0.43
1:A:537:LEU:HD11	1:A:560:ILE:CD1	2.48	0.43
1:B:201:LEU:HD13	1:B:432:MET:CE	2.48	0.43
1:B:445:LEU:O	1:B:449:LEU:HD23	2.18	0.43
1:C:222:THR:CG2	1:C:230:ILE:HD12	2.48	0.43
1:D:1124:ILE:O	1:D:1128:VAL:HG23	2.18	0.43
1:D:201:LEU:HD13	1:D:432:MET:CE	2.48	0.43
1:D:445:LEU:O	1:D:449:LEU:HD23	2.18	0.43
1:D:577:THR:O	1:D:577:THR:HG22	2.17	0.43
1:B:670:VAL:HG21	1:B:732:TRP:CE3	2.54	0.43
1:D:250:THR:HG22	1:D:291:HIS:CD2	2.53	0.43
1:D:313:ARG:NH2	1:D:355:ASP:OD2	2.49	0.43
1:D:933:GLN:O	1:D:937:VAL:HG12	2.18	0.43
1:A:185:LEU:HD11	1:A:319:ILE:CG2	2.49	0.43
1:B:209:LEU:HD23	1:B:209:LEU:C	2.43	0.43
1:A:1117:THR:O	1:A:1121:VAL:HG23	2.19	0.43
1:B:1155:HIS:O	1:B:1159:ILE:HG12	2.18	0.43
1:C:184:LEU:HB3	1:C:218:ALA:HB2	1.99	0.43
1:C:209:LEU:C	1:C:209:LEU:HD23	2.43	0.43
1:A:566:TYR:HD1	1:A:567:LEU:HD22	1.83	0.43
1:A:1244:MET:SD	1:A:1244:MET:C	3.01	0.43
1:B:260:GLU:O	1:B:274:TYR:OH	2.24	0.43
1:B:784:PRO:N	1:B:785:PRO:HD2	2.33	0.43
1:B:1010:MET:HE1	1:D:1100:LEU:CD1	2.49	0.43
1:B:989:ILE:HG13	2:B:1502:A1I8P:C20	2.49	0.43
1:D:784:PRO:N	1:D:785:PRO:HD2	2.33	0.43
1:D:989:ILE:HG13	2:D:1503:A1I8P:C20	2.49	0.43
1:D:1190:LEU:O	1:D:1193:VAL:HG12	2.19	0.43
1:A:784:PRO:N	1:A:785:PRO:HD2	2.34	0.43
1:B:781:ILE:HD12	1:B:877:PHE:HD1	1.81	0.43
1:B:933:GLN:O	1:B:937:VAL:HG12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:989:ILE:HG13	2:C:1502:A1I8P:C20	2.49	0.43
1:B:313:ARG:NH2	1:B:355:ASP:OD2	2.50	0.43
1:C:250:THR:HG22	1:C:291:HIS:CD2	2.54	0.43
1:C:313:ARG:NH2	1:C:355:ASP:OD2	2.49	0.43
1:C:784:PRO:N	1:C:785:PRO:HD2	2.34	0.43
1:C:1100:LEU:HD11	1:D:1010:MET:HE1	2.01	0.43
1:C:1124:ILE:O	1:C:1128:VAL:HG23	2.19	0.43
1:C:1190:LEU:O	1:C:1193:VAL:HG12	2.19	0.43
1:B:418:MET:HE2	1:B:418:MET:CA	2.49	0.42
1:B:489:GLU:O	1:B:492:MET:HG2	2.18	0.42
1:B:915:LEU:HD13	2:B:1502:A1I8P:C03	2.49	0.42
1:C:201:LEU:HD13	1:C:432:MET:CE	2.49	0.42
1:A:489:GLU:O	1:A:492:MET:HG2	2.18	0.42
1:B:557:LEU:O	1:B:560:ILE:HG22	2.20	0.42
1:B:986:LEU:CD2	1:B:989:ILE:HD12	2.49	0.42
1:C:927:GLU:N	1:C:928:PRO:CD	2.83	0.42
1:C:986:LEU:CD2	1:C:989:ILE:HD12	2.49	0.42
1:D:1117:THR:O	1:D:1121:VAL:HG23	2.20	0.42
1:A:1226:ARG:CZ	1:B:1228:GLU:OE2	2.67	0.42
1:B:222:THR:CG2	1:B:230:ILE:HD12	2.47	0.42
1:B:260:GLU:N	1:B:285:THR:O	2.51	0.42
1:C:895:VAL:O	1:C:896:LYS:HB3	2.20	0.42
1:D:290:MET:N	1:D:290:MET:SD	2.93	0.42
1:D:557:LEU:O	1:D:560:ILE:HG22	2.20	0.42
1:A:377:GLY:C	1:A:421:MET:HE3	2.44	0.42
1:C:557:LEU:O	1:C:560:ILE:HG22	2.20	0.42
1:A:350:LEU:HB2	1:A:420:CYS:SG	2.59	0.42
1:D:986:LEU:CD2	1:D:989:ILE:HD12	2.50	0.42
1:B:290:MET:N	1:B:290:MET:SD	2.93	0.42
1:C:568:MET:HG3	1:C:572:TYR:CD2	2.55	0.42
1:C:187:SER:OG	1:C:312:ARG:NH2	2.42	0.42
1:A:557:LEU:O	1:A:560:ILE:HG22	2.20	0.42
1:A:1148:PRO:HG2	1:A:1149:PRO:HD3	2.01	0.42
1:B:1190:LEU:O	1:B:1193:VAL:HG12	2.19	0.42
1:C:784:PRO:O	1:C:787:ILE:HD12	2.19	0.42
1:A:290:MET:N	1:A:290:MET:SD	2.93	0.42
1:A:985:ARG:O	1:A:985:ARG:HG3	2.19	0.42
1:B:927:GLU:N	1:B:928:PRO:CD	2.83	0.42
1:C:225:VAL:O	1:C:230:ILE:HG21	2.20	0.42
1:C:517:PHE:O	1:C:522:ARG:NH1	2.50	0.42
1:C:680:HIS:O	1:C:684:GLU:OE1	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1117:THR:O	1:B:1121:VAL:HG23	2.20	0.41
1:C:566:TYR:HD1	1:C:567:LEU:HD22	1.85	0.41
1:D:205:PHE:CZ	1:D:337:LEU:HD21	2.55	0.41
1:D:260:GLU:N	1:D:285:THR:O	2.51	0.41
1:D:915:LEU:HD13	2:D:1503:A1I8P:C03	2.50	0.41
1:A:670:VAL:HG21	1:A:732:TRP:CE3	2.56	0.41
1:A:986:LEU:HD23	1:A:989:ILE:HD12	2.01	0.41
1:B:395:LEU:HD23	1:B:414:PHE:CD1	2.55	0.41
1:B:1010:MET:HE1	1:D:1100:LEU:HD11	2.01	0.41
1:D:680:HIS:O	1:D:684:GLU:OE1	2.38	0.41
1:D:927:GLU:N	1:D:928:PRO:CD	2.83	0.41
1:A:933:GLN:O	1:A:937:VAL:HG12	2.19	0.41
1:A:1069:GLN:O	1:A:1081:LEU:HD12	2.20	0.41
1:A:388:ASN:OD1	1:A:391:LEU:HD13	2.21	0.41
1:A:649:LYS:O	1:A:649:LYS:HG3	2.19	0.41
1:A:707:VAL:HG23	1:A:746:HIS:NE2	2.35	0.41
1:A:1221:ARG:NH1	1:A:1225:GLU:OE1	2.53	0.41
1:A:1228:GLU:OE2	1:C:1226:ARG:CZ	2.68	0.41
1:C:290:MET:N	1:C:290:MET:SD	2.93	0.41
1:D:1148:PRO:HG2	1:D:1149:PRO:HD3	2.03	0.41
1:A:680:HIS:O	1:A:684:GLU:OE1	2.39	0.41
1:A:927:GLU:N	1:A:928:PRO:CD	2.84	0.41
1:C:690:ASP:OD1	1:C:691:ILE:HG23	2.21	0.41
1:C:707:VAL:HG23	1:C:746:HIS:NE2	2.36	0.41
1:C:889:PHE:HD2	1:C:979:ILE:HG13	1.86	0.41
1:B:225:VAL:O	1:B:230:ILE:HG21	2.20	0.41
1:D:536:THR:HG22	1:D:539:HIS:HB3	2.02	0.41
1:B:536:THR:HG22	1:B:539:HIS:HB3	2.02	0.41
1:C:424:LYS:HA	1:C:427:ILE:HD12	2.02	0.41
1:A:514:MET:CE	1:A:641:LEU:HD11	2.51	0.41
1:A:890:ASN:ND2	1:A:983:TYR:OH	2.40	0.41
1:B:388:ASN:OD1	1:B:391:LEU:HD13	2.21	0.41
1:B:566:TYR:HD1	1:B:567:LEU:HD22	1.85	0.41
1:C:678:MET:HE2	1:C:695:LEU:HD22	2.03	0.41
1:C:940:GLN:OE1	1:C:940:GLN:C	2.64	0.41
1:D:388:ASN:OD1	1:D:391:LEU:HD13	2.21	0.41
1:A:248:ILE:HD12	1:A:248:ILE:N	2.36	0.41
1:A:953:LEU:HG	1:A:974:ILE:HG23	2.02	0.41
1:A:989:ILE:HG13	2:A:1501:A1I8P:C20	2.51	0.41
1:A:1198:GLU:O	1:A:1202:GLU:HG3	2.21	0.41
1:B:205:PHE:CZ	1:B:337:LEU:HD21	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:680:HIS:O	1:B:684:GLU:OE1	2.39	0.41
1:C:781:ILE:HD11	1:C:873:VAL:HG13	2.03	0.41
1:C:1046:ILE:HD11	1:D:894:LEU:HD11	2.03	0.41
1:D:225:VAL:O	1:D:230:ILE:HG21	2.21	0.41
1:D:1069:GLN:HG3	1:D:1070:ASN:N	2.36	0.41
1:C:205:PHE:CZ	1:C:337:LEU:HD21	2.56	0.40
1:C:1069:GLN:HG3	1:C:1070:ASN:N	2.36	0.40
1:A:424:LYS:HA	1:A:427:ILE:HD12	2.03	0.40
1:B:514:MET:CE	1:B:641:LEU:HD11	2.51	0.40
1:D:424:LYS:HA	1:D:427:ILE:HD12	2.02	0.40
1:D:214:MET:HE3	1:D:248:ILE:HG13	2.03	0.40
1:D:566:TYR:HD1	1:D:567:LEU:HD22	1.85	0.40
1:A:1026:VAL:HG11	1:C:979:ILE:HD13	2.02	0.40
1:B:187:SER:OG	1:B:312:ARG:NH2	2.43	0.40
1:C:350:LEU:HB2	1:C:420:CYS:SG	2.62	0.40
1:C:1012:TYR:CD2	1:D:995:TYR:CE1	3.09	0.40
1:D:1198:GLU:O	1:D:1202:GLU:HG3	2.22	0.40
1:A:470:ASP:OD1	1:A:470:ASP:N	2.53	0.40
1:B:1069:GLN:HG3	1:B:1070:ASN:N	2.37	0.40
1:C:470:ASP:OD1	1:C:470:ASP:N	2.55	0.40
1:C:915:LEU:HD23	1:C:915:LEU:C	2.47	0.40
1:D:240:HIS:CE1	1:D:248:ILE:HD11	2.57	0.40
1:D:470:ASP:OD1	1:D:470:ASP:N	2.55	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	946/1409 (67%)	924 (98%)	22 (2%)	0	100	100
1	B	946/1409 (67%)	925 (98%)	21 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	946/1409 (67%)	925 (98%)	21 (2%)	0	100	100
1	D	946/1409 (67%)	927 (98%)	19 (2%)	0	100	100
All	All	3784/5636 (67%)	3701 (98%)	83 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	850/1247 (68%)	850 (100%)	0	100	100
1	B	850/1247 (68%)	850 (100%)	0	100	100
1	C	850/1247 (68%)	850 (100%)	0	100	100
1	D	850/1247 (68%)	850 (100%)	0	100	100
All	All	3400/4988 (68%)	3400 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	198	GLN
1	A	412	HIS
1	A	459	GLN
1	A	467	ASN
1	A	481	GLN
1	A	515	HIS
1	A	586	HIS
1	A	739	GLN
1	A	965	GLN
1	A	978	ASN
1	A	1115	ASN
1	B	412	HIS

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Mol	Chain	Res	Type
1	B	586	HIS
1	B	739	GLN
1	B	965	GLN
1	C	412	HIS
1	C	586	HIS
1	C	739	GLN
1	C	1035	ASN
1	C	1115	ASN
1	D	412	HIS
1	D	586	HIS
1	D	739	GLN
1	D	1115	ASN
1	D	1132	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 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	A1I8P	D	1503	-	29,29,29	2.37	9 (31%)	36,40,40	3.03	17 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	CLR	A	1503	-	31,31,31	0.40	0	48,48,48	0.54	0
3	A8W	A	1502	-	30,30,30	3.91	18 (60%)	45,49,49	1.87	14 (31%)
2	A1I8P	C	1502	-	29,29,29	2.38	9 (31%)	36,40,40	3.07	17 (47%)
4	CLR	D	1501	-	31,31,31	0.40	0	48,48,48	0.53	0
2	A1I8P	B	1502	-	29,29,29	2.37	9 (31%)	36,40,40	3.03	17 (47%)
4	CLR	A	1504	-	31,31,31	0.39	0	48,48,48	0.53	0
2	A1I8P	A	1501	-	29,29,29	2.43	10 (34%)	36,40,40	3.04	17 (47%)
3	A8W	B	1501	-	30,30,30	3.91	18 (60%)	45,49,49	1.83	12 (26%)
3	A8W	D	1502	-	30,30,30	3.90	18 (60%)	45,49,49	1.83	14 (31%)
3	A8W	C	1503	-	30,30,30	3.90	18 (60%)	45,49,49	1.83	13 (28%)
4	CLR	C	1501	-	31,31,31	0.40	0	48,48,48	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	Res	Link	Chirals	Torsions	Rings
2	A1I8P	D	1503	-	-	4/16/26/26	0/4/4/4
4	CLR	A	1503	-	-	0/10/68/68	0/4/4/4
3	A8W	A	1502	-	-	0/9/67/67	0/4/4/4
2	A1I8P	C	1502	-	-	4/16/26/26	0/4/4/4
4	CLR	D	1501	-	-	0/10/68/68	0/4/4/4
2	A1I8P	B	1502	-	-	4/16/26/26	0/4/4/4
4	CLR	A	1504	-	-	0/10/68/68	0/4/4/4
2	A1I8P	A	1501	-	-	4/16/26/26	0/4/4/4
3	A8W	B	1501	-	-	2/9/67/67	0/4/4/4
3	A8W	D	1502	-	-	3/9/67/67	0/4/4/4
3	A8W	C	1503	-	-	2/9/67/67	0/4/4/4
4	CLR	C	1501	-	-	0/10/68/68	0/4/4/4

All (109) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1502	A8W	C12-C13	-8.06	1.40	1.54
3	B	1501	A8W	C12-C13	-8.03	1.40	1.54
3	C	1503	A8W	C12-C13	-7.98	1.40	1.54
3	D	1502	A8W	C12-C13	-7.98	1.40	1.54
3	B	1501	A8W	C11-C9	7.23	1.65	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1502	A8W	C11-C9	7.21	1.65	1.53
3	C	1503	A8W	C11-C9	7.19	1.65	1.53
3	D	1502	A8W	C11-C9	7.17	1.65	1.53
3	B	1501	A8W	C8-C14	-6.97	1.40	1.53
3	C	1503	A8W	C8-C14	-6.96	1.40	1.53
3	A	1502	A8W	C8-C14	-6.95	1.40	1.53
3	D	1502	A8W	C8-C14	-6.91	1.40	1.53
2	A	1501	A1I8P	C08-C07	6.72	1.60	1.52
2	C	1502	A1I8P	C08-C07	6.72	1.60	1.52
2	B	1502	A1I8P	C08-C07	6.68	1.60	1.52
2	D	1503	A1I8P	C08-C07	6.67	1.60	1.52
3	A	1502	A8W	C8-C9	5.87	1.64	1.53
3	D	1502	A8W	C8-C9	5.84	1.64	1.53
3	C	1503	A8W	C8-C9	5.81	1.64	1.53
3	B	1501	A8W	C8-C9	5.77	1.64	1.53
3	B	1501	A8W	C10-C9	-5.56	1.47	1.56
3	A	1502	A8W	O1-C3	-5.55	1.37	1.48
3	C	1503	A8W	O1-C3	-5.55	1.37	1.48
3	B	1501	A8W	C17-C20	-5.53	1.44	1.51
3	A	1502	A8W	C17-C20	-5.52	1.44	1.51
3	A	1502	A8W	C10-C9	-5.52	1.47	1.56
3	B	1501	A8W	O1-C3	-5.52	1.37	1.48
3	D	1502	A8W	C10-C9	-5.51	1.47	1.56
3	C	1503	A8W	C10-C9	-5.51	1.47	1.56
3	D	1502	A8W	O1-C3	-5.50	1.37	1.48
3	C	1503	A8W	C17-C20	-5.49	1.44	1.51
3	D	1502	A8W	C17-C20	-5.47	1.44	1.51
3	A	1502	A8W	C16-C15	5.26	1.68	1.54
3	B	1501	A8W	C16-C15	5.26	1.68	1.54
3	C	1503	A8W	C16-C15	5.26	1.68	1.54
3	D	1502	A8W	C16-C15	5.21	1.68	1.54
2	C	1502	A1I8P	C06-N05	5.07	1.45	1.36
2	A	1501	A1I8P	C06-N05	5.01	1.45	1.36
2	B	1502	A1I8P	C06-N05	5.00	1.45	1.36
2	D	1503	A1I8P	C06-N05	4.96	1.45	1.36
3	D	1502	A8W	C12-C11	4.61	1.62	1.53
3	B	1501	A8W	C12-C11	4.60	1.62	1.53
3	C	1503	A8W	C12-C11	4.56	1.62	1.53
3	A	1502	A8W	C12-C11	4.55	1.62	1.53
3	B	1501	A8W	C15-C14	4.45	1.63	1.54
3	D	1502	A8W	C15-C14	4.43	1.63	1.54
3	C	1503	A8W	C15-C14	4.42	1.63	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1502	A8W	C15-C14	4.37	1.63	1.54
2	A	1501	A1I8P	C07-N14	4.35	1.52	1.46
2	C	1502	A1I8P	C07-N14	4.19	1.51	1.46
2	B	1502	A1I8P	C07-N14	4.11	1.51	1.46
2	D	1503	A1I8P	C07-N14	4.10	1.51	1.46
3	B	1501	A8W	C6-C5	-3.99	1.24	1.33
3	C	1503	A8W	C6-C5	-3.98	1.24	1.33
3	D	1502	A8W	C6-C5	-3.96	1.24	1.33
3	A	1502	A8W	C6-C5	-3.93	1.24	1.33
3	B	1501	A8W	C1-C10	3.86	1.61	1.54
3	C	1503	A8W	C10-C5	-3.86	1.45	1.52
3	D	1502	A8W	C10-C5	-3.84	1.45	1.52
3	A	1502	A8W	C10-C5	-3.84	1.45	1.52
3	B	1501	A8W	C10-C5	-3.83	1.45	1.52
3	D	1502	A8W	C1-C10	3.83	1.61	1.54
3	C	1503	A8W	C1-C10	3.81	1.61	1.54
3	A	1502	A8W	C1-C10	3.81	1.61	1.54
2	D	1503	A1I8P	O26-N25	-3.47	1.36	1.42
2	A	1501	A1I8P	O26-N25	-3.44	1.36	1.42
2	B	1502	A1I8P	O26-N25	-3.41	1.36	1.42
2	C	1502	A1I8P	O26-N25	-3.39	1.36	1.42
2	A	1501	A1I8P	C03-C04	3.27	1.47	1.40
2	D	1503	A1I8P	C03-C04	3.26	1.47	1.40
2	B	1502	A1I8P	C03-C04	3.25	1.47	1.40
2	C	1502	A1I8P	C03-C04	3.24	1.47	1.40
2	A	1501	A1I8P	C04-N05	3.16	1.44	1.39
3	A	1502	A8W	C13-C14	-3.13	1.49	1.55
3	D	1502	A8W	C13-C14	-3.12	1.49	1.55
3	C	1503	A8W	C13-C14	-3.11	1.49	1.55
3	B	1501	A8W	C13-C14	-3.09	1.49	1.55
2	D	1503	A1I8P	C04-N05	3.05	1.44	1.39
2	C	1502	A1I8P	C04-N05	3.03	1.44	1.39
2	B	1502	A1I8P	C04-N05	3.02	1.44	1.39
2	A	1501	A1I8P	C18-N14	2.93	1.47	1.40
3	C	1503	A8W	C19-C10	2.87	1.59	1.54
3	A	1502	A8W	O1-S	2.85	1.65	1.57
3	C	1503	A8W	O1-S	2.85	1.65	1.57
3	B	1501	A8W	C19-C10	2.85	1.59	1.54
3	D	1502	A8W	O1-S	2.84	1.65	1.57
3	D	1502	A8W	C19-C10	2.83	1.59	1.54
3	B	1501	A8W	O1-S	2.83	1.65	1.57
3	A	1502	A8W	C19-C10	2.83	1.59	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1503	A8W	C4-C5	2.67	1.57	1.51
3	D	1502	A8W	C4-C5	2.66	1.57	1.51
3	D	1502	A8W	C1-C2	2.63	1.58	1.53
3	A	1502	A8W	C1-C2	2.61	1.58	1.53
3	A	1502	A8W	C4-C5	2.60	1.56	1.51
3	C	1503	A8W	C1-C2	2.60	1.58	1.53
3	B	1501	A8W	C4-C5	2.60	1.56	1.51
3	B	1501	A8W	C1-C2	2.58	1.58	1.53
2	B	1502	A1I8P	C18-N14	2.53	1.46	1.40
2	A	1501	A1I8P	C15-N14	2.52	1.50	1.46
2	D	1503	A1I8P	C18-N14	2.52	1.46	1.40
2	C	1502	A1I8P	C18-N14	2.50	1.46	1.40
2	A	1501	A1I8P	C04-N25	2.48	1.36	1.30
2	C	1502	A1I8P	C04-N25	2.47	1.36	1.30
2	B	1502	A1I8P	C04-N25	2.47	1.36	1.30
2	D	1503	A1I8P	C04-N25	2.45	1.36	1.30
2	B	1502	A1I8P	C15-N14	2.38	1.50	1.46
2	D	1503	A1I8P	C15-N14	2.35	1.50	1.46
2	C	1502	A1I8P	C15-N14	2.30	1.50	1.46
2	A	1501	A1I8P	C23-C18	2.10	1.42	1.39

All (121) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1502	A1I8P	C08-C07-N14	6.56	119.19	112.07
2	B	1502	A1I8P	C08-C07-N14	6.47	119.09	112.07
2	D	1503	A1I8P	C08-C07-N14	6.40	119.02	112.07
2	A	1501	A1I8P	C08-C07-N14	6.26	118.87	112.07
2	C	1502	A1I8P	O26-C02-C01	6.07	124.24	115.89
2	A	1501	A1I8P	C20-C19-C18	5.94	126.10	118.27
2	D	1503	A1I8P	O26-C02-C01	5.88	123.98	115.89
2	D	1503	A1I8P	C20-C19-C18	5.87	126.02	118.27
2	C	1502	A1I8P	C20-C19-C18	5.87	126.01	118.27
2	A	1501	A1I8P	O26-C02-C01	5.86	123.96	115.89
2	B	1502	A1I8P	O26-C02-C01	5.86	123.95	115.89
2	B	1502	A1I8P	C20-C19-C18	5.84	125.97	118.27
2	A	1501	A1I8P	C03-C04-N25	-5.33	103.52	112.20
2	D	1503	A1I8P	C03-C04-N25	-5.31	103.55	112.20
2	C	1502	A1I8P	C03-C04-N25	-5.31	103.55	112.20
2	B	1502	A1I8P	C03-C04-N25	-5.28	103.60	112.20
2	A	1501	A1I8P	O26-N25-C04	5.22	110.31	104.57
2	D	1503	A1I8P	O26-N25-C04	5.19	110.28	104.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1502	A1I8P	O26-N25-C04	5.15	110.23	104.57
2	C	1502	A1I8P	O26-N25-C04	5.13	110.22	104.57
2	A	1501	A1I8P	C23-C18-C19	-5.07	112.21	119.80
2	C	1502	A1I8P	C23-C18-C19	-4.93	112.43	119.80
2	D	1503	A1I8P	C23-C18-C19	-4.92	112.44	119.80
2	B	1502	A1I8P	C23-C18-C19	-4.91	112.46	119.80
2	C	1502	A1I8P	O24-C06-C07	-4.83	114.32	120.95
2	D	1503	A1I8P	O24-C06-C07	-4.76	114.43	120.95
2	B	1502	A1I8P	O24-C06-C07	-4.69	114.52	120.95
2	A	1501	A1I8P	O24-C06-C07	-4.69	114.53	120.95
3	A	1502	A8W	C15-C14-C8	-4.50	111.92	119.10
3	B	1501	A8W	C15-C14-C8	-4.49	111.94	119.10
3	C	1503	A8W	C15-C14-C8	-4.48	111.95	119.10
3	D	1502	A8W	C15-C14-C8	-4.45	112.00	119.10
3	A	1502	A8W	C12-C13-C17	-4.28	110.98	116.11
3	B	1501	A8W	C12-C13-C17	-4.14	111.15	116.11
3	C	1503	A8W	C12-C13-C17	-4.12	111.17	116.11
3	D	1502	A8W	C12-C13-C17	-4.05	111.26	116.11
3	A	1502	A8W	C7-C8-C9	-4.02	105.08	109.72
2	A	1501	A1I8P	C23-C18-N14	3.92	128.54	121.61
2	C	1502	A1I8P	C23-C18-N14	3.87	128.46	121.61
2	D	1503	A1I8P	C23-C18-N14	3.84	128.39	121.61
2	B	1502	A1I8P	C23-C18-N14	3.82	128.36	121.61
2	B	1502	A1I8P	O24-C06-N05	-3.63	116.65	122.61
2	C	1502	A1I8P	O24-C06-N05	-3.63	116.66	122.61
2	D	1503	A1I8P	O24-C06-N05	-3.63	116.66	122.61
2	A	1501	A1I8P	O24-C06-N05	-3.61	116.69	122.61
3	B	1501	A8W	C7-C8-C9	-3.60	105.56	109.72
2	C	1502	A1I8P	C04-C03-C02	3.54	109.49	104.79
3	C	1503	A8W	C7-C8-C9	-3.53	105.64	109.72
2	D	1503	A1I8P	C04-C03-C02	3.49	109.43	104.79
3	D	1502	A8W	C7-C8-C9	-3.48	105.70	109.72
2	A	1501	A1I8P	C04-C03-C02	3.46	109.39	104.79
2	B	1502	A1I8P	C04-C03-C02	3.45	109.37	104.79
3	A	1502	A8W	C8-C7-C6	-3.44	108.00	112.76
2	C	1502	A1I8P	O26-C02-C03	-3.35	106.11	109.88
2	D	1503	A1I8P	O26-C02-C03	-3.34	106.13	109.88
2	B	1502	A1I8P	O26-C02-C03	-3.28	106.20	109.88
3	B	1501	A8W	C8-C7-C6	-3.27	108.24	112.76
2	A	1501	A1I8P	O26-C02-C03	-3.27	106.21	109.88
3	C	1503	A8W	C8-C7-C6	-3.19	108.35	112.76
3	D	1502	A8W	C11-C9-C8	-3.18	107.35	111.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1502	A8W	C8-C7-C6	-3.08	108.49	112.76
3	C	1503	A8W	C11-C9-C8	-3.04	107.54	111.78
3	B	1501	A8W	C11-C9-C8	-2.98	107.62	111.78
3	C	1503	A8W	C4-C5-C6	-2.90	116.64	120.57
3	D	1502	A8W	C4-C5-C6	-2.89	116.65	120.57
2	C	1502	A1I8P	C13-C08-C07	2.87	124.90	120.69
2	B	1502	A1I8P	C13-C08-C07	2.87	124.89	120.69
2	D	1503	A1I8P	C13-C08-C07	2.85	124.86	120.69
3	B	1501	A8W	C4-C5-C6	-2.85	116.71	120.57
3	A	1502	A8W	C4-C5-C6	-2.84	116.72	120.57
2	A	1501	A1I8P	C13-C08-C07	2.72	124.67	120.69
3	A	1502	A8W	C11-C9-C8	-2.72	107.99	111.78
2	A	1501	A1I8P	C22-C21-C20	-2.72	116.89	120.24
2	B	1502	A1I8P	C22-C21-C20	-2.67	116.95	120.24
3	C	1503	A8W	C12-C13-C14	2.64	111.19	107.25
3	B	1501	A8W	C12-C13-C14	2.63	111.18	107.25
2	C	1502	A1I8P	C22-C21-C20	-2.62	117.01	120.24
3	A	1502	A8W	C12-C13-C14	2.60	111.14	107.25
2	D	1503	A1I8P	C22-C21-C20	-2.59	117.05	120.24
3	D	1502	A8W	C12-C13-C14	2.57	111.10	107.25
3	C	1503	A8W	C1-C10-C9	-2.56	105.35	108.74
3	D	1502	A8W	C1-C10-C9	-2.56	105.36	108.74
2	C	1502	A1I8P	C01-C02-C03	-2.55	129.64	134.05
3	B	1501	A8W	C1-C10-C9	-2.55	105.37	108.74
3	A	1502	A8W	C1-C10-C9	-2.49	105.44	108.74
2	B	1502	A1I8P	C09-C08-C13	-2.48	115.23	118.30
2	D	1503	A1I8P	C09-C08-C13	-2.47	115.24	118.30
2	A	1501	A1I8P	C09-C08-C13	-2.45	115.26	118.30
2	A	1501	A1I8P	C01-C02-C03	-2.44	129.83	134.05
2	C	1502	A1I8P	C09-C08-C13	-2.44	115.28	118.30
2	B	1502	A1I8P	C01-C02-C03	-2.43	129.85	134.05
2	D	1503	A1I8P	C01-C02-C03	-2.41	129.89	134.05
2	A	1501	A1I8P	C22-C23-C18	2.41	123.14	118.28
2	C	1502	A1I8P	C22-C23-C18	2.35	123.02	118.28
2	B	1502	A1I8P	C22-C23-C18	2.34	123.01	118.28
2	D	1503	A1I8P	C22-C23-C18	2.34	123.01	118.28
3	A	1502	A8W	O4-S-O1	2.31	111.67	106.37
3	C	1503	A8W	O4-S-O1	2.25	111.55	106.37
3	B	1501	A8W	O4-S-O1	2.25	111.54	106.37
3	D	1502	A8W	O4-S-O1	2.24	111.53	106.37
3	A	1502	A8W	C13-C17-C20	-2.20	111.90	114.95
3	D	1502	A8W	O4-S-O2	-2.15	101.04	108.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1501	A8W	O4-S-O2	-2.13	101.12	108.56
3	C	1503	A8W	O4-S-O2	-2.12	101.12	108.56
3	A	1502	A8W	O4-S-O2	-2.12	101.16	108.56
3	C	1503	A8W	C10-C5-C6	2.11	126.02	122.93
3	A	1502	A8W	C2-C1-C10	-2.11	108.29	112.78
2	C	1502	A1I8P	C02-O26-N25	2.11	110.61	108.47
2	D	1503	A1I8P	C02-O26-N25	2.10	110.61	108.47
2	B	1502	A1I8P	C02-O26-N25	2.09	110.59	108.47
3	A	1502	A8W	C17-C13-C14	2.08	101.90	99.72
3	D	1502	A8W	C10-C5-C6	2.07	125.96	122.93
3	D	1502	A8W	C16-C17-C20	-2.07	110.61	114.21
3	A	1502	A8W	C10-C5-C6	2.06	125.94	122.93
2	A	1501	A1I8P	C02-O26-N25	2.06	110.56	108.47
3	D	1502	A8W	C16-C15-C14	-2.06	101.12	105.14
3	B	1501	A8W	C2-C1-C10	-2.05	108.43	112.78
3	D	1502	A8W	C2-C1-C10	-2.04	108.43	112.78
3	C	1503	A8W	C2-C1-C10	-2.04	108.44	112.78
3	B	1501	A8W	C10-C5-C6	2.04	125.91	122.93
3	C	1503	A8W	C16-C15-C14	-2.02	101.19	105.14

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1501	A1I8P	N05-C06-C07-N14
2	A	1501	A1I8P	C06-C07-N14-C15
2	B	1502	A1I8P	C06-C07-N14-C15
2	C	1502	A1I8P	C06-C07-N14-C15
2	D	1503	A1I8P	C06-C07-N14-C15
2	A	1501	A1I8P	O24-C06-C07-N14
2	B	1502	A1I8P	N05-C06-C07-N14
2	B	1502	A1I8P	O24-C06-C07-N14
2	C	1502	A1I8P	N05-C06-C07-N14
2	C	1502	A1I8P	O24-C06-C07-N14
2	D	1503	A1I8P	N05-C06-C07-N14
2	D	1503	A1I8P	O24-C06-C07-N14
3	C	1503	A8W	C3-O1-S-O4
3	D	1502	A8W	C3-O1-S-O4
2	A	1501	A1I8P	C08-C07-N14-C15
2	B	1502	A1I8P	C08-C07-N14-C15
2	C	1502	A1I8P	C08-C07-N14-C15
2	D	1503	A1I8P	C08-C07-N14-C15

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Mol	Chain	Res	Type	Atoms
3	B	1501	A8W	C3-O1-S-O4
3	D	1502	A8W	C3-O1-S-O3
3	B	1501	A8W	C3-O1-S-O3
3	C	1503	A8W	C3-O1-S-O3
3	D	1502	A8W	C13-C17-C20-C21

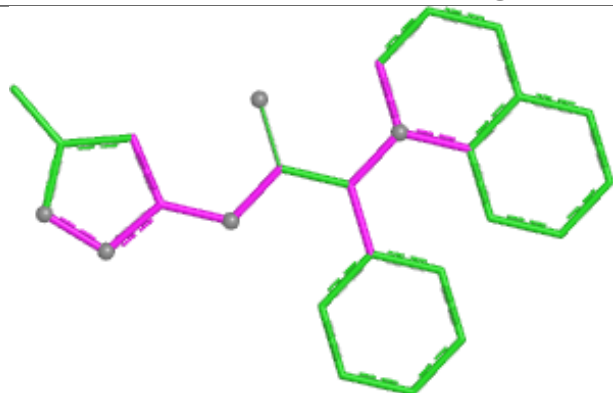
There are no ring outliers.

4 monomers are involved in 12 short contacts:

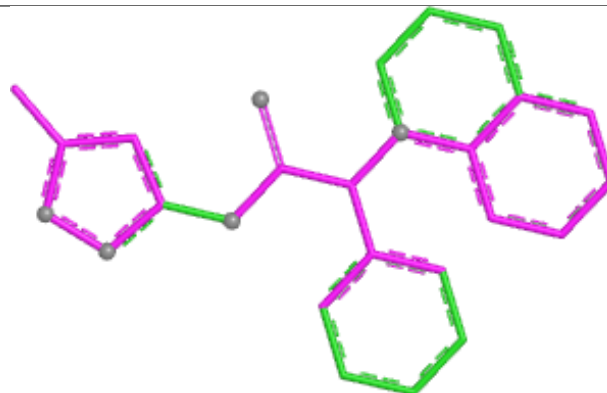
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1503	A1I8P	3	0
2	C	1502	A1I8P	3	0
2	B	1502	A1I8P	3	0
2	A	1501	A1I8P	3	0

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.

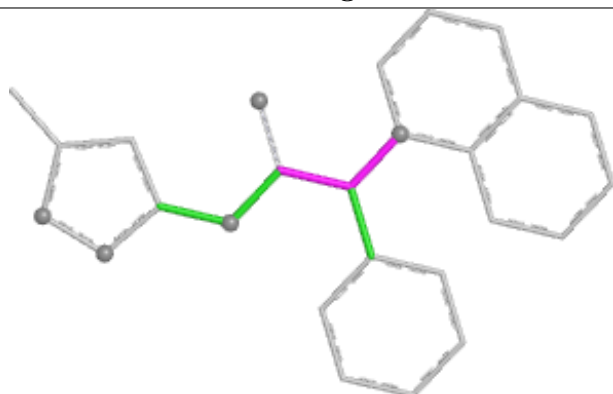
Ligand A1I8P D 1503



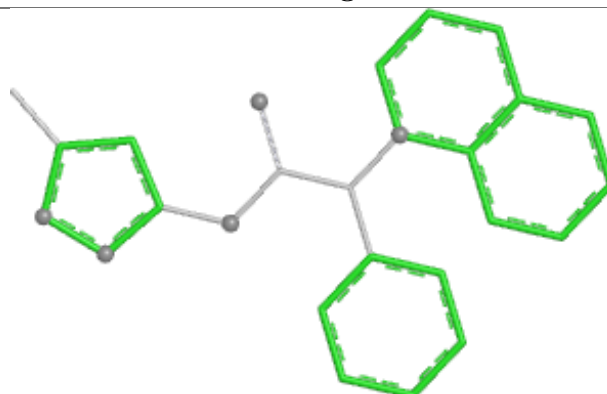
Bond lengths



Bond angles

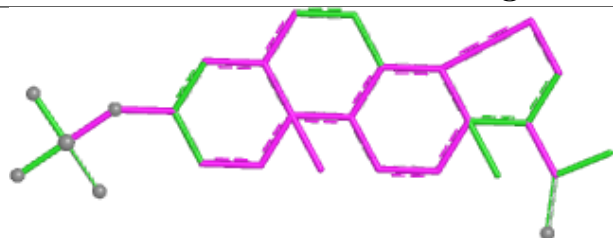


Torsions

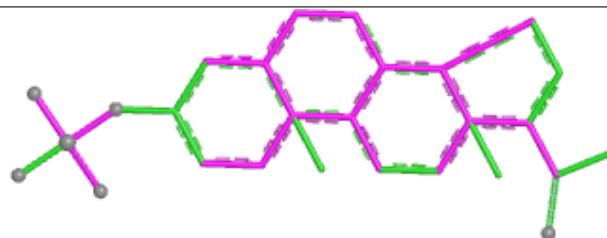


Rings

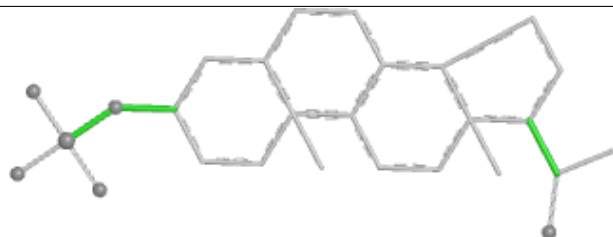
Ligand A8W A 1502



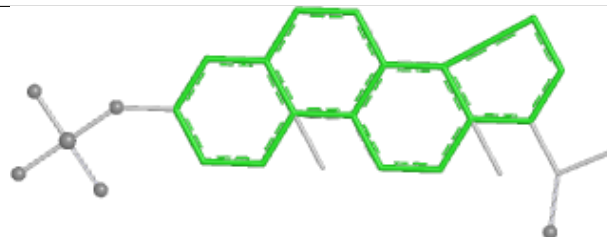
Bond lengths



Bond angles

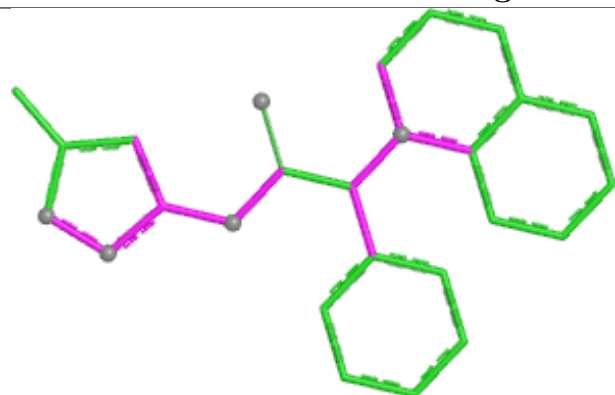


Torsions

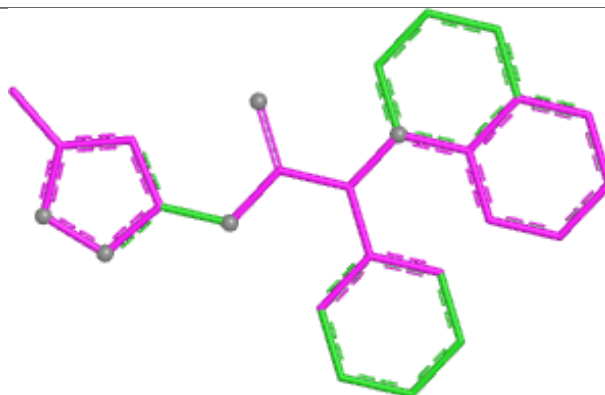


Rings

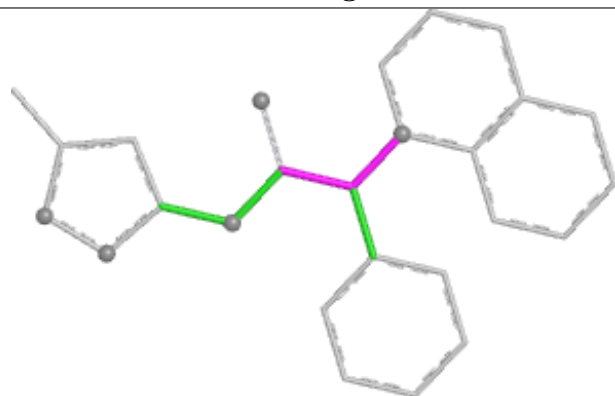
Ligand A1I8P C 1502



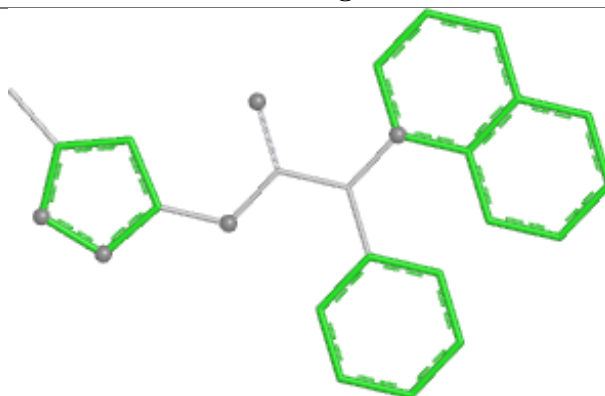
Bond lengths



Bond angles

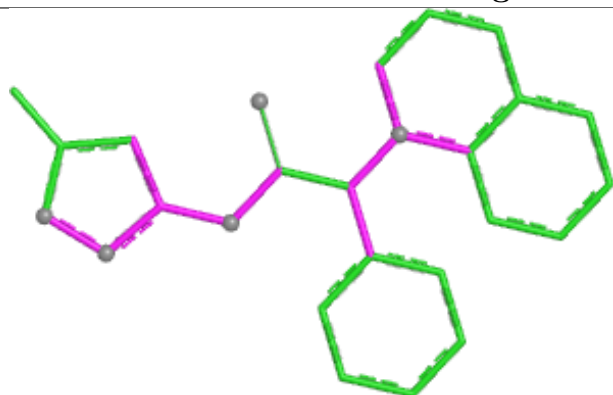


Torsions

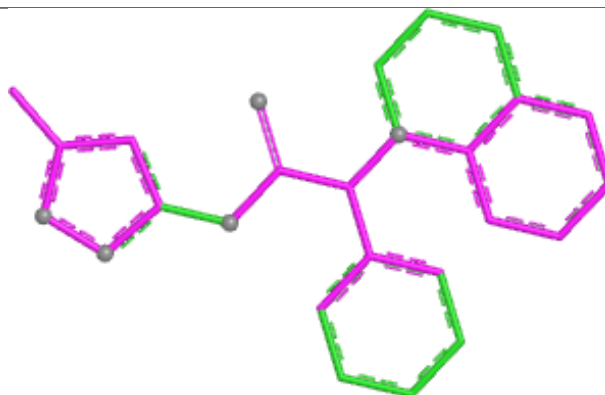


Rings

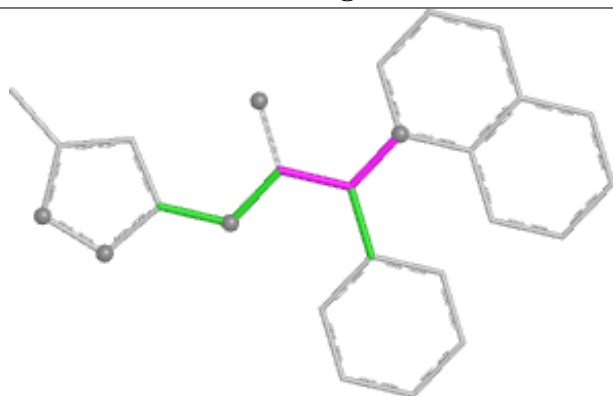
Ligand A1I8P B 1502



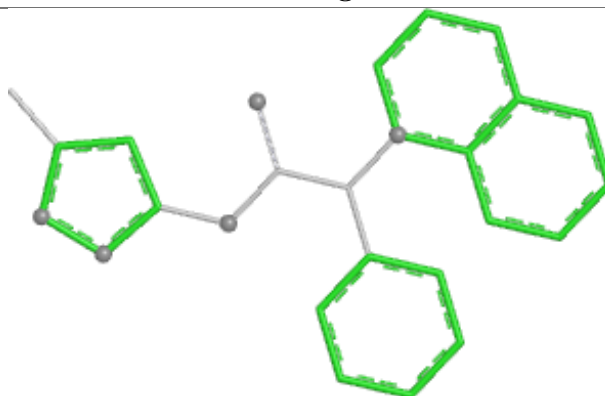
Bond lengths



Bond angles

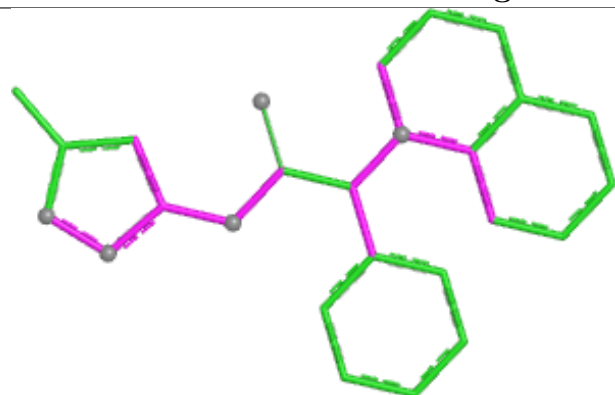


Torsions

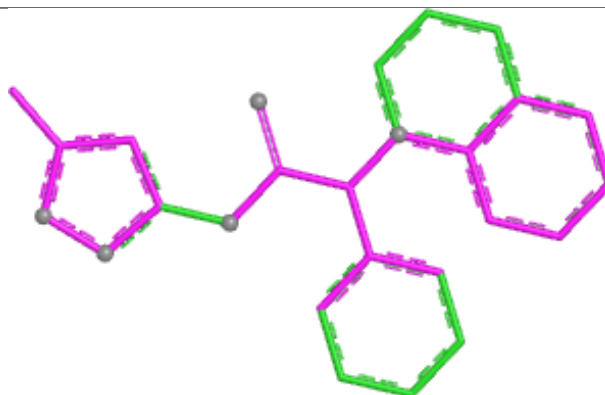


Rings

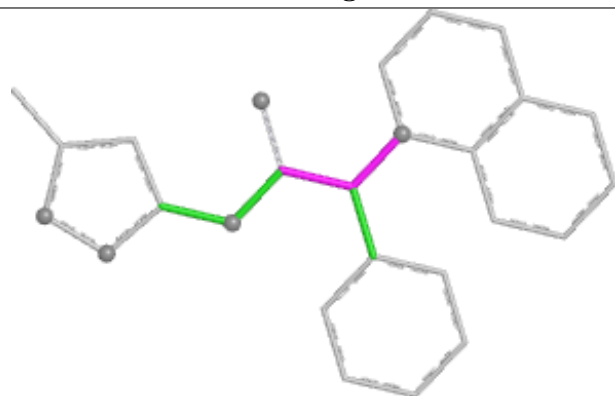
Ligand A1I8P A 1501



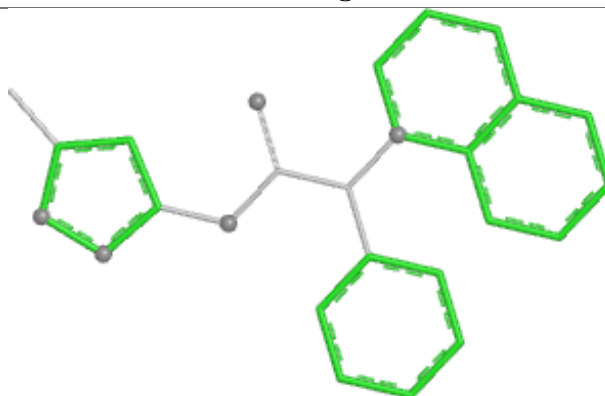
Bond lengths



Bond angles

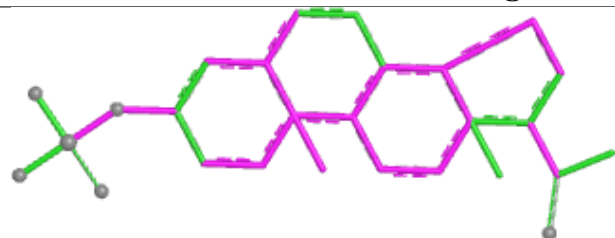


Torsions

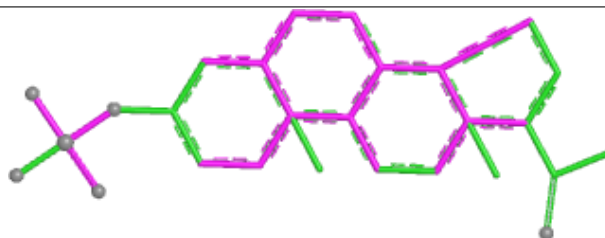


Rings

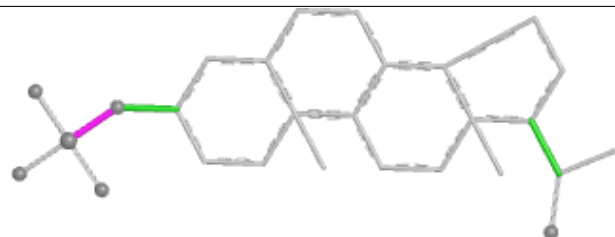
Ligand A8W B 1501



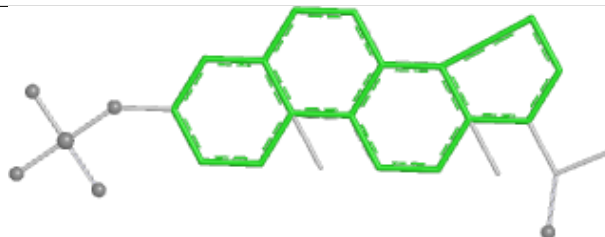
Bond lengths



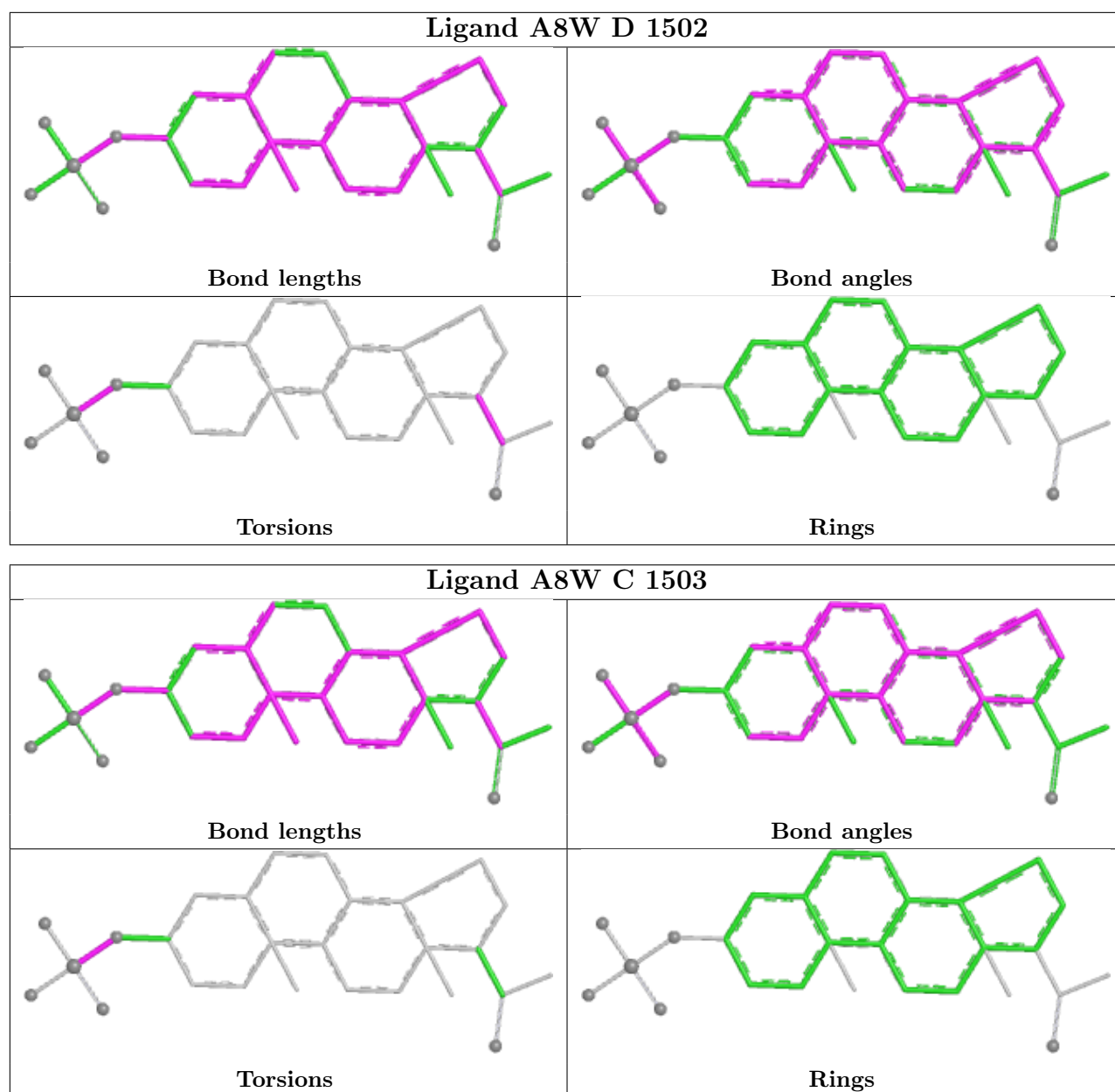
Bond angles



Torsions



Rings



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 Map visualisation

This section contains visualisations of the EMDB entry EMD-53177. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis ⓘ

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.