



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2022 – 01:11 pm BST

PDB ID : 7NBD
Title : Crystal structure of human serine racemase in complex with DSiP fragment Z235449082, XChem fragment screen.
Authors : Koulouris, C.R.; Roe, S.M.
Deposited on : 2021-01-26
Resolution : 1.86 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : **FAILED**
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) : 2.28

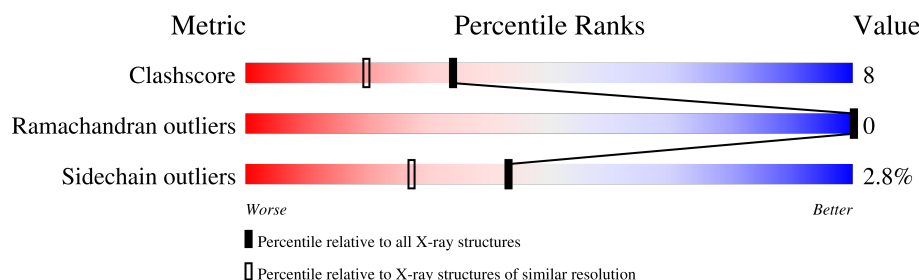
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.86 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	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)

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 failed to run properly.

Mol	Chain	Length	Quality of chain
1	AAA	346	79% 13% • 7%
1	BBB	346	80% 10% • 9%
1	CCC	346	83% 10% 7%
1	DDD	346	80% 11% • 8%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	AAA	403	-	-	X	-
3	GOL	AAA	404	-	-	X	-
3	GOL	AAA	409	-	-	X	-
3	GOL	BBB	402	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 11477 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 Serine racemase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	323	Total	C	N	O	S	0	35	0
			2688	1703	452	521	12			
1	BBB	315	Total	C	N	O	S	0	13	1
			2412	1535	400	466	11			
1	CCC	323	Total	C	N	O	S	5	22	1
			2573	1636	427	498	12			
1	DDD	318	Total	C	N	O	S	0	20	0
			2527	1603	434	477	13			

There are 32 discrepancies between the modelled and reference sequences:

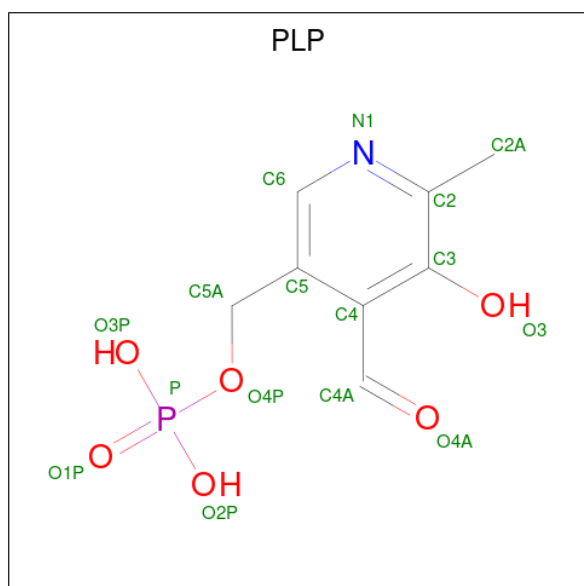
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	2	ASP	CYS	engineered mutation	UNP Q9GZT4
AAA	6	ASP	CYS	engineered mutation	UNP Q9GZT4
AAA	341	HIS	-	expression tag	UNP Q9GZT4
AAA	342	HIS	-	expression tag	UNP Q9GZT4
AAA	343	HIS	-	expression tag	UNP Q9GZT4
AAA	344	HIS	-	expression tag	UNP Q9GZT4
AAA	345	HIS	-	expression tag	UNP Q9GZT4
AAA	346	HIS	-	expression tag	UNP Q9GZT4
BBB	2	ASP	CYS	engineered mutation	UNP Q9GZT4
BBB	6	ASP	CYS	engineered mutation	UNP Q9GZT4
BBB	341	HIS	-	expression tag	UNP Q9GZT4
BBB	342	HIS	-	expression tag	UNP Q9GZT4
BBB	343	HIS	-	expression tag	UNP Q9GZT4
BBB	344	HIS	-	expression tag	UNP Q9GZT4
BBB	345	HIS	-	expression tag	UNP Q9GZT4
BBB	346	HIS	-	expression tag	UNP Q9GZT4
CCC	2	ASP	CYS	engineered mutation	UNP Q9GZT4
CCC	6	ASP	CYS	engineered mutation	UNP Q9GZT4
CCC	341	HIS	-	expression tag	UNP Q9GZT4
CCC	342	HIS	-	expression tag	UNP Q9GZT4
CCC	343	HIS	-	expression tag	UNP Q9GZT4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
CCC	344	HIS	-	expression tag	UNP Q9GZT4
CCC	345	HIS	-	expression tag	UNP Q9GZT4
CCC	346	HIS	-	expression tag	UNP Q9GZT4
DDD	2	ASP	CYS	engineered mutation	UNP Q9GZT4
DDD	6	ASP	CYS	engineered mutation	UNP Q9GZT4
DDD	362	HIS	-	expression tag	UNP Q9GZT4
DDD	363	HIS	-	expression tag	UNP Q9GZT4
DDD	364	HIS	-	expression tag	UNP Q9GZT4
DDD	365	HIS	-	expression tag	UNP Q9GZT4
DDD	366	HIS	-	expression tag	UNP Q9GZT4
DDD	367	HIS	-	expression tag	UNP Q9GZT4

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	AAA	1	Total	C	N	O	P	0	1
			30	16	2	10	2		
2	BBB	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	CCC	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	DDD	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	AAA	1	Total	C	O	0	0
			6	3	3		
3	AAA	1	Total	C	O	0	0
			6	3	3		
3	AAA	1	Total	C	O	0	0
			6	3	3		
3	AAA	1	Total	C	O	0	0
			6	3	3		
3	AAA	1	Total	C	O	0	0
			6	3	3		
3	BBB	1	Total	C	O	0	0
			6	3	3		
3	BBB	1	Total	C	O	0	0
			6	3	3		
3	CCC	1	Total	C	O	0	0
			6	3	3		

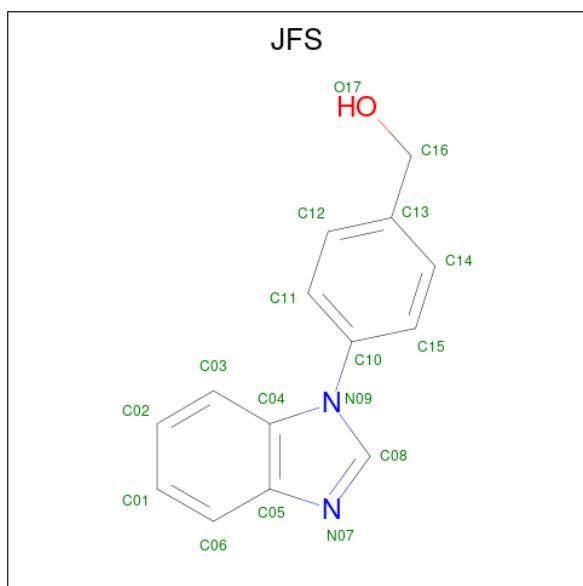
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	1	Total	Ca	0	0
			1	1		
4	BBB	2	Total	Ca	0	0
			2	2		
4	CCC	2	Total	Ca	0	1
			3	3		
4	DDD	2	Total	Ca	0	1
			3	3		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

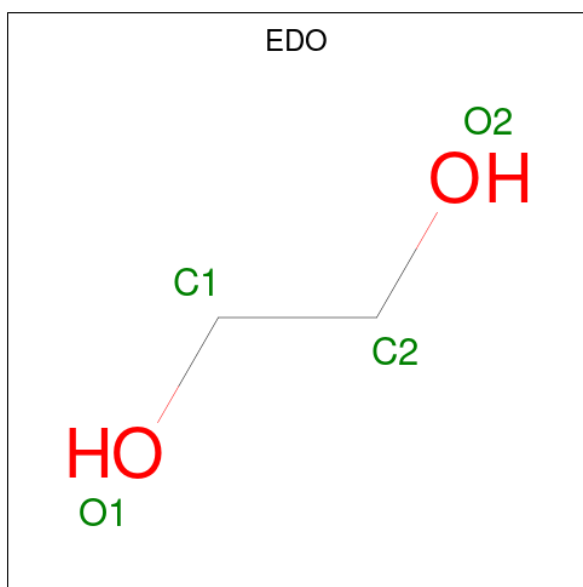
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AAA	1	Total	Mg	0	0
			1	1		
5	DDD	1	Total	Mg	0	0
			1	1		

- Molecule 6 is [4-(1H-benzimidazol-1-yl)phenyl]methanol (three-letter code: JFS) (formula: C₁₄H₁₂N₂O) (labeled as "Ligand of Interest" by depositor).



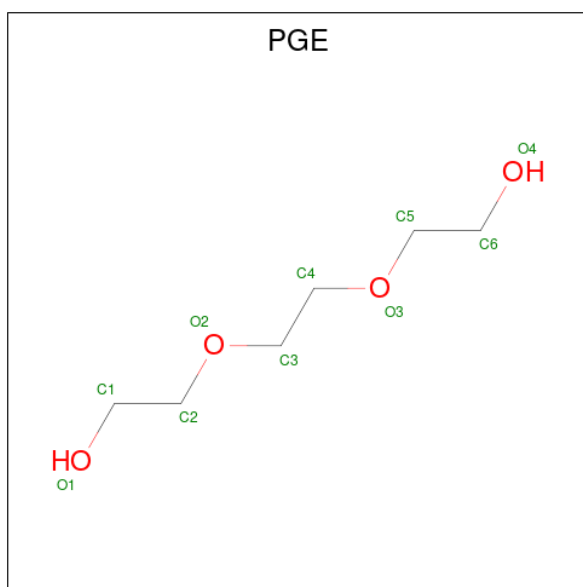
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	AAA	1	Total	C	N	O	0	1
			34	28	4	2		
6	BBB	1	Total	C	N	O	0	0
			17	14	2	1		

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	BBB	1	Total	C	O	0	0
			4	2	2		
7	CCC	1	Total	C	O	0	0
			4	2	2		
7	DDD	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	CCC	1	Total	C	O	0	0
			10	6	4		

- Molecule 9 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	DDD	1	Total	Na	0	0
			1	1		

- Molecule 10 is water.


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	AAA	323	Total	O	0	4
			327	327		
10	BBB	182	Total	O	0	2
			184	184		
10	CCC	262	Total	O	0	6
			268	268		
10	DDD	286	Total	O	0	4
			290	290		

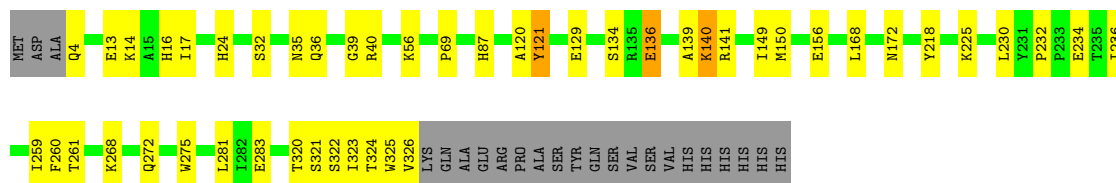
3 Residue-property plots

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 failed to run properly.

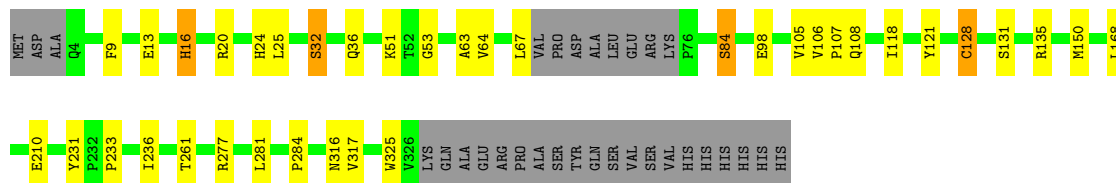
- Molecule 1: Serine racemase

Chain AAA: 




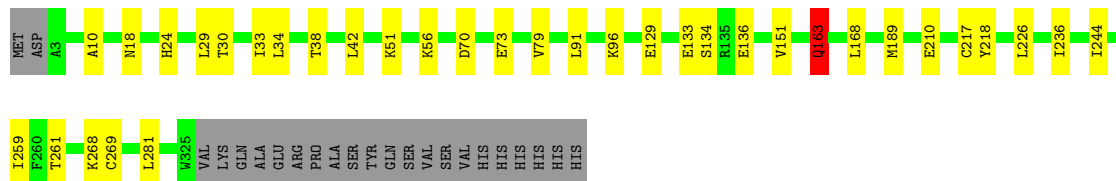
- Molecule 1: Serine racemase

Chain BBB: 




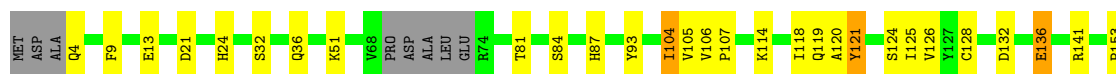
- Molecule 1: Serine racemase

Chain CCC: 



- Molecule 1: Serine racemase

Chain DDD: 



Q163	L168	K201	V204	E210	Y218	K223	Y231	I259	F260	T261	E266	L281	V317	V347	LYS	GLN	ALA	GLU	ARG	PRO	ALA	SER	TYR	GLN	SER	VAL	SER	VAL	HIS	HIS	HIS	HIS	HIS	HIS
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	48.01Å 154.85Å 85.45Å 90.00° 98.04° 90.00°	Depositor
Resolution (Å)	84.60 – 1.86	Depositor
% Data completeness (in resolution range)	93.9 (84.60-1.86)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 1.87Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.176 , 0.207	Depositor
Wilson B-factor (Å ²)	28.5	Xtriage
Anisotropy	0.038	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11477	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.26% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: MG, PGE, EDO, CA, NA, PLP, JFS, GOL

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	AAA	0.58	0/2735	0.82	2/3728 (0.1%)
1	BBB	0.48	0/2454	0.78	3/3352 (0.1%)
1	CCC	0.52	0/2619	0.80	1/3576 (0.0%)
1	DDD	0.57	1/2571 (0.0%)	0.85	1/3505 (0.0%)
All	All	0.54	1/10379 (0.0%)	0.81	7/14161 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	DDD	266	GLU	CD-OE2	-6.62	1.18	1.25

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	DDD	121	TYR	CB-CA-C	7.06	124.51	110.40
1	BBB	128	CYS	N-CA-CB	-5.90	99.98	110.60
1	AAA	283	GLU	CB-CA-C	5.84	122.08	110.40
1	BBB	121	TYR	CB-CA-C	5.72	121.85	110.40
1	BBB	277	ARG	CG-CD-NE	-5.66	99.91	111.80
1	AAA	121	TYR	CB-CA-C	5.61	121.62	110.40
1	CCC	163	GLN	CB-CG-CD	5.50	125.91	111.60

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	AAA	2688	0	2666	69	1
1	BBB	2412	0	2371	27	0
1	CCC	2573	0	2556	38	0
1	DDD	2527	0	2519	36	1
2	AAA	30	0	12	0	0
2	BBB	15	0	6	0	0
2	CCC	15	0	6	1	0
2	DDD	15	0	6	0	0
3	AAA	30	0	40	21	0
3	BBB	12	0	16	5	0
3	CCC	6	0	8	2	0
4	AAA	1	0	0	0	0
4	BBB	2	0	0	0	0
4	CCC	3	0	0	0	0
4	DDD	3	0	0	0	0
5	AAA	1	0	0	0	0
5	DDD	1	0	0	0	0
6	AAA	34	0	0	0	0
6	BBB	17	0	0	0	0
7	BBB	4	0	6	0	0
7	CCC	4	0	5	2	0
7	DDD	4	0	6	0	0
8	CCC	10	0	14	5	0
9	DDD	1	0	0	0	0
10	AAA	327	0	0	20	1
10	BBB	184	0	0	3	1
10	CCC	268	0	0	9	1
10	DDD	290	0	0	5	1
All	All	11477	0	10237	174	5

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 (174) 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)
3:AAA:403:GOL:H12	10:AAA:521:HOH:O	1.17	1.32
1:AAA:322[B]:SER:O	1:AAA:326[B]:VAL:HG12	1.39	1.18
1:AAA:261:THR:H	3:AAA:403:GOL:H32	1.13	1.08

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:14[B]:LYS:HE3	10:AAA:609:HOH:O	1.55	1.04
1:DDD:81[B]:THR:CG2	1:DDD:104[B]:ILE:CD1	2.37	1.02
1:AAA:140:LYS:HE3	1:AAA:150[B]:MET:HE3	1.47	0.96
1:DDD:81[B]:THR:CG2	1:DDD:104[B]:ILE:HD13	1.97	0.95
1:CCC:51[B]:LYS:NZ	10:CCC:501[B]:HOH:O	1.98	0.95
1:AAA:140:LYS:HE3	1:AAA:150[B]:MET:CE	1.98	0.94
1:DDD:223:LYS:HG2	10:DDD:506:HOH:O	1.68	0.94
1:AAA:136:GLU:HA	10:AAA:506:HOH:O	1.66	0.93
1:CCC:30:THR:OG1	8:CCC:402:PGE:H12	1.66	0.92
1:DDD:81[B]:THR:HG22	1:DDD:104[B]:ILE:HD13	1.51	0.92
1:DDD:51:LYS:NZ	10:DDD:502:HOH:O	2.03	0.91
1:AAA:172:ASN:ND2	10:AAA:501:HOH:O	2.06	0.87
1:CCC:51[A]:LYS:NZ	10:CCC:501[A]:HOH:O	2.05	0.87
1:CCC:79[A]:VAL:HG11	1:CCC:91:LEU:HG	1.56	0.87
1:AAA:149:ILE:HA	3:AAA:404:GOL:H32	1.57	0.86
1:DDD:81[B]:THR:HG23	1:DDD:104[B]:ILE:CD1	2.04	0.86
1:AAA:140:LYS:CE	1:AAA:150[B]:MET:HE1	2.05	0.86
1:AAA:272:GLN:HE21	1:AAA:325[B]:TRP:HE1	1.24	0.86
1:AAA:35[B]:ASN:O	1:AAA:39[B]:GLY:N	2.10	0.85
8:CCC:402:PGE:H32	10:CCC:718:HOH:O	1.76	0.84
1:CCC:30:THR:O	8:CCC:402:PGE:H42	1.78	0.84
1:AAA:140:LYS:CE	1:AAA:150[B]:MET:CE	2.55	0.83
1:CCC:24:HIS:NE2	1:CCC:51[B]:LYS:HE3	1.93	0.83
1:AAA:16[B]:HIS:CD2	3:AAA:409:GOL:HO2	1.95	0.83
1:DDD:21[B]:ASP:OD1	10:DDD:762[B]:HOH:O	1.96	0.83
1:AAA:322[B]:SER:O	1:AAA:326[B]:VAL:CG1	2.26	0.82
1:CCC:24:HIS:CE1	1:CCC:51[B]:LYS:HE3	2.15	0.81
1:AAA:16[B]:HIS:CD2	3:AAA:409:GOL:O2	2.34	0.81
1:DDD:81[B]:THR:HG23	1:DDD:104[B]:ILE:HD12	1.63	0.80
1:AAA:261:THR:H	3:AAA:403:GOL:C3	1.95	0.80
1:DDD:104[A]:ILE:HG21	1:DDD:118:ILE:HG21	1.62	0.80
1:AAA:261:THR:N	3:AAA:403:GOL:H32	1.96	0.79
1:AAA:322[B]:SER:C	1:AAA:326[B]:VAL:HG12	2.02	0.78
1:AAA:168:LEU:HD13	3:AAA:409:GOL:H31	1.65	0.76
1:CCC:18[A]:ASN:OD1	3:CCC:403:GOL:H11	1.85	0.76
3:AAA:402:GOL:H31	10:AAA:602:HOH:O	1.87	0.74
3:AAA:403:GOL:H31	10:AAA:718:HOH:O	1.88	0.74
1:AAA:322[A]:SER:O	1:AAA:324[A]:THR:N	2.20	0.74
1:CCC:129[A]:GLU:HG2	1:CCC:134:SER:CB	2.20	0.72
1:DDD:132:ASP:O	1:DDD:136:GLU:HG2	1.90	0.72
1:CCC:18[A]:ASN:OD1	3:CCC:403:GOL:C1	2.37	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:140:LYS:HE2	1:AAA:150[B]:MET:HE1	1.72	0.70
1:AAA:39[B]:GLY:O	1:AAA:40[B]:ARG:HG3	1.92	0.70
1:BBB:67[B]:LEU:CD1	1:BBB:67[B]:LEU:N	2.55	0.70
1:AAA:325[A]:TRP:O	1:AAA:325[A]:TRP:HE3	1.74	0.69
1:DDD:32:SER:O	1:DDD:36[A]:GLN:HG3	1.92	0.69
1:CCC:217[B]:CYS:HB2	1:CCC:244[B]:ILE:HD11	1.75	0.68
1:AAA:4[B]:GLN:CD	1:AAA:4[B]:GLN:N	2.49	0.67
1:BBB:281[B]:LEU:HD13	1:DDD:281[B]:LEU:HD21	1.77	0.66
1:BBB:107:PRO:HA	1:BBB:128:CYS:HB3	1.76	0.66
1:AAA:325[A]:TRP:O	1:AAA:325[A]:TRP:CE3	2.48	0.66
1:BBB:24:HIS:CE1	1:BBB:51:LYS:HE3	2.30	0.66
1:AAA:87:HIS:ND1	10:AAA:507:HOH:O	2.29	0.65
1:BBB:84:SER:HB3	1:BBB:118:ILE:HD11	1.78	0.65
1:AAA:69:PRO:O	10:AAA:503:HOH:O	2.14	0.65
1:AAA:234[B]:GLU:OE1	10:AAA:502:HOH:O	2.14	0.65
3:AAA:404:GOL:H31	10:AAA:639:HOH:O	1.96	0.65
1:DDD:223:LYS:HE3	10:DDD:506:HOH:O	1.96	0.64
1:CCC:236[B]:ILE:CD1	1:CCC:268:LYS:HG3	2.28	0.64
1:CCC:129[A]:GLU:HG2	1:CCC:134:SER:HB2	1.78	0.63
1:AAA:275:TRP:CH2	1:AAA:325[B]:TRP:CH2	2.87	0.62
1:AAA:149:ILE:CA	3:AAA:404:GOL:H32	2.29	0.62
1:AAA:232:PRO:HA	3:AAA:402:GOL:H32	1.82	0.62
1:CCC:236[B]:ILE:HD13	1:CCC:268:LYS:HG3	1.82	0.61
1:BBB:67[B]:LEU:N	1:BBB:67[B]:LEU:HD12	2.15	0.61
1:DDD:105:VAL:HG22	1:DDD:126[B]:VAL:CG2	2.31	0.60
1:AAA:156[B]:GLU:OE1	10:AAA:504:HOH:O	2.16	0.60
10:AAA:501:HOH:O	1:DDD:13:GLU:OE2	2.17	0.59
1:BBB:231[B]:TYR:N	3:BBB:402:GOL:O1	2.27	0.59
1:CCC:29:LEU:HB3	8:CCC:402:PGE:H5	1.85	0.59
1:BBB:105:VAL:HG12	1:BBB:128:CYS:HB2	1.86	0.58
1:BBB:231[A]:TYR:H	3:BBB:402:GOL:HO1	1.49	0.57
1:AAA:32:SER:O	1:AAA:36[A]:GLN:HG3	2.05	0.57
1:AAA:320[B]:THR:O	1:AAA:323[B]:ILE:CB	2.52	0.57
1:AAA:14[B]:LYS:HG3	10:AAA:631:HOH:O	2.05	0.57
1:AAA:56[B]:LYS:HD2	10:AAA:507:HOH:O	2.04	0.56
3:BBB:402:GOL:H11	10:BBB:621:HOH:O	2.04	0.56
1:DDD:104[A]:ILE:HD13	1:DDD:106:VAL:HG12	1.87	0.56
1:DDD:105:VAL:HG22	1:DDD:126[B]:VAL:HG21	1.87	0.56
1:BBB:281[B]:LEU:HG	1:BBB:317:VAL:HG11	1.88	0.55
1:BBB:32:SER:O	1:BBB:36:GLN:HG3	2.06	0.55
1:CCC:29:LEU:HD13	8:CCC:402:PGE:H5	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:139:ALA:HB1	1:AAA:150[A]:MET:CE	2.36	0.55
1:BBB:236[A]:ILE:HD12	1:BBB:284:PRO:HB3	1.88	0.55
3:AAA:404:GOL:O3	10:AAA:505:HOH:O	2.16	0.54
1:BBB:231[B]:TYR:H	3:BBB:402:GOL:HO1	1.53	0.54
1:AAA:13[B]:GLU:OE1	3:AAA:409:GOL:O3	2.24	0.54
1:CCC:24:HIS:NE2	1:CCC:51[B]:LYS:CE	2.67	0.54
1:DDD:201:LYS:HG2	1:DDD:204:VAL:HG23	1.88	0.54
1:DDD:259[A]:ILE:HG22	10:DDD:623:HOH:O	2.08	0.53
1:CCC:269[B]:CYS:SG	10:CCC:752:HOH:O	2.59	0.53
1:AAA:322[A]:SER:O	1:AAA:323[A]:ILE:C	2.45	0.53
1:DDD:104[B]:ILE:HG22	1:DDD:106:VAL:HG12	1.89	0.53
1:DDD:105:VAL:HA	1:DDD:126[B]:VAL:HG23	1.91	0.53
1:CCC:70:ASP:OD2	10:CCC:502:HOH:O	2.19	0.53
1:AAA:120:ALA:HB3	10:AAA:580:HOH:O	2.09	0.52
1:AAA:13[A]:GLU:OE2	1:DDD:13:GLU:HG2	2.11	0.51
1:AAA:136:GLU:O	10:AAA:506:HOH:O	2.19	0.51
1:AAA:322[A]:SER:C	1:AAA:324[A]:THR:N	2.62	0.51
1:BBB:233:PRO:O	10:BBB:501:HOH:O	2.19	0.51
1:AAA:139:ALA:HB3	10:AAA:506:HOH:O	2.10	0.51
10:BBB:584:HOH:O	1:DDD:24:HIS:HE1	1.94	0.51
1:BBB:281[A]:LEU:HD21	1:DDD:281[A]:LEU:HD13	1.92	0.50
1:AAA:272:GLN:NE2	1:AAA:325[B]:TRP:HE1	2.02	0.50
1:BBB:53:GLY:HA3	1:BBB:316:ASN:HD21	1.76	0.50
1:BBB:107:PRO:CA	1:BBB:128:CYS:HB3	2.42	0.50
1:DDD:218:TYR:N	1:DDD:259[A]:ILE:HD13	2.27	0.50
1:DDD:259[A]:ILE:O	1:DDD:259[A]:ILE:HG23	2.12	0.49
1:AAA:218:TYR:CE1	3:AAA:403:GOL:H11	2.47	0.49
1:AAA:281[B]:LEU:HD21	1:CCC:281[B]:LEU:HD13	1.95	0.49
1:AAA:39[B]:GLY:O	1:AAA:40[B]:ARG:CG	2.62	0.48
1:AAA:321[B]:SER:C	1:AAA:323[B]:ILE:N	2.67	0.48
1:DDD:107:PRO:HA	1:DDD:128[B]:CYS:O	2.14	0.48
1:AAA:236:ILE:HD11	1:AAA:325[A]:TRP:CD1	2.49	0.47
1:CCC:226:LEU:HD11	1:CCC:244[A]:ILE:HG13	1.96	0.47
1:DDD:9:PHE:CE1	1:DDD:168[B]:LEU:HD21	2.49	0.47
1:DDD:118:ILE:O	1:DDD:119:GLN:HB2	2.14	0.47
1:AAA:268:LYS:HE2	1:AAA:325[B]:TRP:HB2	1.96	0.47
1:CCC:79[A]:VAL:CG1	1:CCC:91:LEU:HG	2.38	0.47
1:DDD:118:ILE:C	1:DDD:120:ALA:H	2.17	0.47
1:BBB:16:HIS:O	1:BBB:20:ARG:HB3	2.16	0.46
1:BBB:236[B]:ILE:HD11	1:BBB:325:TRP:CE2	2.50	0.46
1:CCC:38:THR:HG21	1:CCC:42:LEU:HD11	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DDD:106:VAL:HG13	1:DDD:125:ILE:HG23	1.97	0.46
1:CCC:236[B]:ILE:HD11	1:CCC:268:LYS:HG3	1.97	0.46
1:BBB:13:GLU:HG3	1:CCC:10:ALA:HA	1.98	0.46
1:CCC:218:TYR:HA	1:CCC:259[B]:ILE:HG21	1.96	0.46
1:CCC:33[B]:ILE:HG23	10:CCC:575:HOH:O	2.16	0.46
1:AAA:139:ALA:HB1	1:AAA:150[A]:MET:HE1	1.97	0.46
1:BBB:63:ALA:O	1:BBB:67[A]:LEU:HB2	2.15	0.45
1:BBB:64:VAL:HG12	1:BBB:98:GLU:HG3	1.98	0.45
1:BBB:128:CYS:SG	1:BBB:135:ARG:HA	2.57	0.45
1:BBB:210:GLU:O	1:BBB:261:THR:HA	2.16	0.45
1:AAA:275:TRP:CH2	1:AAA:325[B]:TRP:HH2	2.32	0.45
1:CCC:226:LEU:CD1	1:CCC:244[A]:ILE:HG13	2.47	0.45
1:DDD:51:LYS:HD2	1:DDD:93:TYR:OH	2.16	0.45
1:DDD:87:HIS:CG	1:DDD:153:PRO:HB3	2.51	0.44
1:CCC:236[B]:ILE:HD13	1:CCC:268:LYS:CG	2.47	0.44
1:CCC:56:LYS:NZ	2:CCC:401:PLP:O3	2.50	0.44
1:BBB:67[B]:LEU:H	1:BBB:67[B]:LEU:HD13	1.82	0.44
1:CCC:210[A]:GLU:HB2	10:CCC:518[A]:HOH:O	2.17	0.44
1:AAA:322[A]:SER:O	1:AAA:325[A]:TRP:N	2.51	0.44
1:CCC:151:VAL:O	7:CCC:406:EDO:H21	2.17	0.44
1:AAA:39[B]:GLY:C	1:AAA:40[B]:ARG:HG3	2.37	0.44
1:DDD:84:SER:HA	1:DDD:121:TYR:OH	2.19	0.43
1:CCC:217[B]:CYS:HA	1:CCC:244[B]:ILE:HD12	2.01	0.43
1:BBB:231[B]:TYR:N	3:BBB:402:GOL:HO1	2.14	0.43
1:CCC:217[B]:CYS:CB	1:CCC:244[B]:ILE:HD11	2.47	0.43
1:AAA:129[B]:GLU:HB2	1:AAA:134:SER:CB	2.49	0.43
1:DDD:126[B]:VAL:HG23	1:DDD:126[B]:VAL:O	2.18	0.43
1:AAA:150[A]:MET:H	3:AAA:404:GOL:C3	2.31	0.43
1:AAA:14[B]:LYS:HD2	10:AAA:798:HOH:O	2.18	0.43
1:AAA:168:LEU:HD22	3:AAA:409:GOL:H31	2.01	0.43
1:AAA:259[B]:ILE:O	1:AAA:259[B]:ILE:HG23	2.18	0.42
1:CCC:236[B]:ILE:HG21	1:CCC:268:LYS:HE3	2.01	0.42
1:AAA:140:LYS:CE	1:AAA:150[B]:MET:HE3	2.27	0.42
1:AAA:150[B]:MET:H	3:AAA:404:GOL:C3	2.33	0.42
1:AAA:322[B]:SER:O	1:AAA:326[B]:VAL:N	2.49	0.42
1:AAA:230:LEU:HA	1:AAA:230:LEU:HD23	1.80	0.41
1:AAA:13[A]:GLU:O	1:AAA:17[A]:ILE:HG12	2.20	0.41
3:AAA:404:GOL:C3	10:AAA:639:HOH:O	2.64	0.41
1:BBB:9:PHE:HE1	1:BBB:168:LEU:HD21	1.84	0.41
1:CCC:217[B]:CYS:HB2	1:CCC:244[B]:ILE:CD1	2.47	0.41
1:AAA:321[B]:SER:C	1:AAA:323[B]:ILE:H	2.22	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:24:HIS:CE1	10:CCC:603:HOH:O	2.73	0.41
1:DDD:210:GLU:O	1:DDD:261:THR:HA	2.21	0.41
1:AAA:260:PHE:HA	3:AAA:403:GOL:O3	2.21	0.41
7:CCC:406:EDO:H12	10:CCC:727:HOH:O	2.20	0.41
1:CCC:163:GLN:HB3	1:CCC:189:MET:HA	2.03	0.40
1:AAA:14[B]:LYS:HE2	1:AAA:14[B]:LYS:HB2	1.78	0.40
1:CCC:210[A]:GLU:O	1:CCC:261:THR:HA	2.22	0.40

All (5) 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)
10:DDD:530:HOH:O	10:DDD:597:HOH:O[1_655]	1.82	0.38
10:AAA:693:HOH:O	10:AAA:764:HOH:O[1_455]	2.07	0.13
10:CCC:521:HOH:O	10:CCC:707:HOH:O[1_455]	2.07	0.13
1:AAA:129[B]:GLU:OE2	1:DDD:231:TYR:OH[1_554]	2.09	0.11
10:BBB:572:HOH:O	10:BBB:601:HOH:O[1_655]	2.16	0.04

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	AAA	355/346 (103%)	339 (96%)	16 (4%)	0	100	100
1	BBB	323/346 (93%)	314 (97%)	9 (3%)	0	100	100
1	CCC	343/346 (99%)	334 (97%)	9 (3%)	0	100	100
1	DDD	334/346 (96%)	326 (98%)	8 (2%)	0	100	100
All	All	1355/1384 (98%)	1313 (97%)	42 (3%)	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 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	AAA	293/291 (101%)	288 (98%)	5 (2%)	60	47
1	BBB	257/291 (88%)	249 (97%)	8 (3%)	40	23
1	CCC	279/291 (96%)	270 (97%)	9 (3%)	39	22
1	DDD	272/291 (94%)	262 (96%)	10 (4%)	34	17
All	All	1101/1164 (95%)	1069 (97%)	32 (3%)	43	26

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	121	TYR
1	AAA	136	GLU
1	AAA	140	LYS
1	AAA	141	ARG
1	AAA	225	LYS
1	BBB	16	HIS
1	BBB	25	LEU
1	BBB	32	SER
1	BBB	84	SER
1	BBB	106	VAL
1	BBB	108	GLN
1	BBB	131	SER
1	BBB	150	MET
1	CCC	34[A]	LEU
1	CCC	34[B]	LEU
1	CCC	73	GLU
1	CCC	96	LYS
1	CCC	133	GLU
1	CCC	136[A]	GLU
1	CCC	136[B]	GLU
1	CCC	163	GLN
1	CCC	168	LEU
1	DDD	4	GLN
1	DDD	104[A]	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	DDD	104[B]	ILE
1	DDD	114	LYS
1	DDD	124	SER
1	DDD	136	GLU
1	DDD	141[A]	ARG
1	DDD	141[B]	ARG
1	DDD	163	GLN
1	DDD	317	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 32 ligands modelled in this entry, 12 are monoatomic - leaving 20 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	$\# Z > 2$
6	JFS	AAA	407[A]	-	19,19,19	0.73	1 (5%)	21,26,26	0.75	0
7	EDO	BBB	406	-	3,3,3	0.06	0	2,2,2	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	JFS	BBB	407	-	19,19,19	0.77	0	21,26,26	0.86	0
2	PLP	DDD	401	1	15,15,16	0.76	1 (6%)	20,22,23	1.09	1 (5%)
2	PLP	BBB	401	1	15,15,16	0.78	1 (6%)	20,22,23	0.78	0
3	GOL	AAA	409	-	5,5,5	0.12	0	5,5,5	0.28	0
7	EDO	CCC	406	-	3,3,3	0.79	0	2,2,2	0.28	0
7	EDO	DDD	406	-	3,3,3	0.10	0	2,2,2	0.21	0
3	GOL	AAA	404	-	5,5,5	0.15	0	5,5,5	0.51	0
3	GOL	AAA	402	-	5,5,5	0.15	0	5,5,5	0.26	0
2	PLP	CCC	401	1	15,15,16	0.92	0	20,22,23	1.15	2 (10%)
3	GOL	CCC	403	-	5,5,5	0.08	0	5,5,5	0.31	0
3	GOL	BBB	402	-	5,5,5	0.14	0	5,5,5	0.14	0
2	PLP	AAA	401[B]	1	15,15,16	0.84	1 (6%)	20,22,23	0.83	0
3	GOL	BBB	403	-	5,5,5	0.10	0	5,5,5	0.32	0
6	JFS	AAA	407[B]	-	19,19,19	0.74	1 (5%)	21,26,26	0.77	0
3	GOL	AAA	403	-	5,5,5	0.19	0	5,5,5	0.60	0
2	PLP	AAA	401[A]	1	15,15,16	0.85	1 (6%)	20,22,23	1.33	2 (10%)
3	GOL	AAA	408	-	5,5,5	0.18	0	5,5,5	0.39	0
8	PGE	CCC	402	-	9,9,9	0.17	0	8,8,8	0.26	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
6	JFS	AAA	407[A]	-	-	0/6/6/6	0/3/3/3
7	EDO	BBB	406	-	-	0/1/1/1	-
6	JFS	BBB	407	-	-	2/6/6/6	0/3/3/3
2	PLP	DDD	401	1	-	0/6/6/8	0/1/1/1
2	PLP	BBB	401	1	-	0/6/6/8	0/1/1/1
3	GOL	AAA	409	-	-	0/4/4/4	-
7	EDO	CCC	406	-	-	1/1/1/1	-
7	EDO	DDD	406	-	-	1/1/1/1	-
3	GOL	AAA	404	-	-	2/4/4/4	-
3	GOL	AAA	402	-	-	2/4/4/4	-
2	PLP	CCC	401	1	-	0/6/6/8	0/1/1/1
3	GOL	CCC	403	-	-	0/4/4/4	-
3	GOL	BBB	402	-	-	2/4/4/4	-
2	PLP	AAA	401[B]	1	-	3/6/6/8	0/1/1/1
3	GOL	BBB	403	-	-	2/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	JFS	AAA	407[B]	-	-	1/6/6/6	0/3/3/3
3	GOL	AAA	403	-	-	1/4/4/4	-
2	PLP	AAA	401[A]	1	-	0/6/6/8	0/1/1/1
3	GOL	AAA	408	-	-	2/4/4/4	-
8	PGE	CCC	402	-	-	6/7/7/7	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AAA	401[B]	PLP	C4A-C4	-2.62	1.46	1.51
2	AAA	401[A]	PLP	C4A-C4	-2.55	1.46	1.51
2	DDD	401	PLP	C4A-C4	-2.51	1.46	1.51
2	BBB	401	PLP	C4A-C4	-2.24	1.47	1.51
6	AAA	407[B]	JFS	C08-N07	-2.11	1.30	1.34
6	AAA	407[A]	JFS	C08-N07	-2.08	1.31	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AAA	401[A]	PLP	O4P-C5A-C5	4.48	117.89	109.35
2	DDD	401	PLP	O4P-C5A-C5	3.35	115.73	109.35
2	CCC	401	PLP	C4A-C4-C5	3.08	124.11	120.94
2	AAA	401[A]	PLP	C4A-C4-C5	2.33	123.33	120.94
2	CCC	401	PLP	O4P-C5A-C5	2.17	113.48	109.35

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	AAA	401[B]	PLP	C4-C5-C5A-O4P
2	AAA	401[B]	PLP	C6-C5-C5A-O4P
3	AAA	404	GOL	C1-C2-C3-O3
3	AAA	404	GOL	O2-C2-C3-O3
3	AAA	408	GOL	O1-C1-C2-O2
3	AAA	408	GOL	O1-C1-C2-C3
8	CCC	402	PGE	O2-C3-C4-O3
8	CCC	402	PGE	O1-C1-C2-O2
6	BBB	407	JFS	C11-C10-N09-C08
3	AAA	402	GOL	C1-C2-C3-O3
3	BBB	403	GOL	C1-C2-C3-O3
3	BBB	403	GOL	O2-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	BBB	407	JFS	C15-C10-N09-C08
8	CCC	402	PGE	C3-C4-O3-C5
2	AAA	401[B]	PLP	C5A-O4P-P-O1P
6	AAA	407[B]	JFS	C15-C10-N09-C08
7	DDD	406	EDO	O1-C1-C2-O2
7	CCC	406	EDO	O1-C1-C2-O2
8	CCC	402	PGE	C6-C5-O3-C4
3	BBB	402	GOL	O1-C1-C2-C3
3	BBB	402	GOL	C1-C2-C3-O3
8	CCC	402	PGE	C4-C3-O2-C2
3	AAA	402	GOL	O2-C2-C3-O3
3	AAA	403	GOL	O2-C2-C3-O3
8	CCC	402	PGE	C1-C2-O2-C3

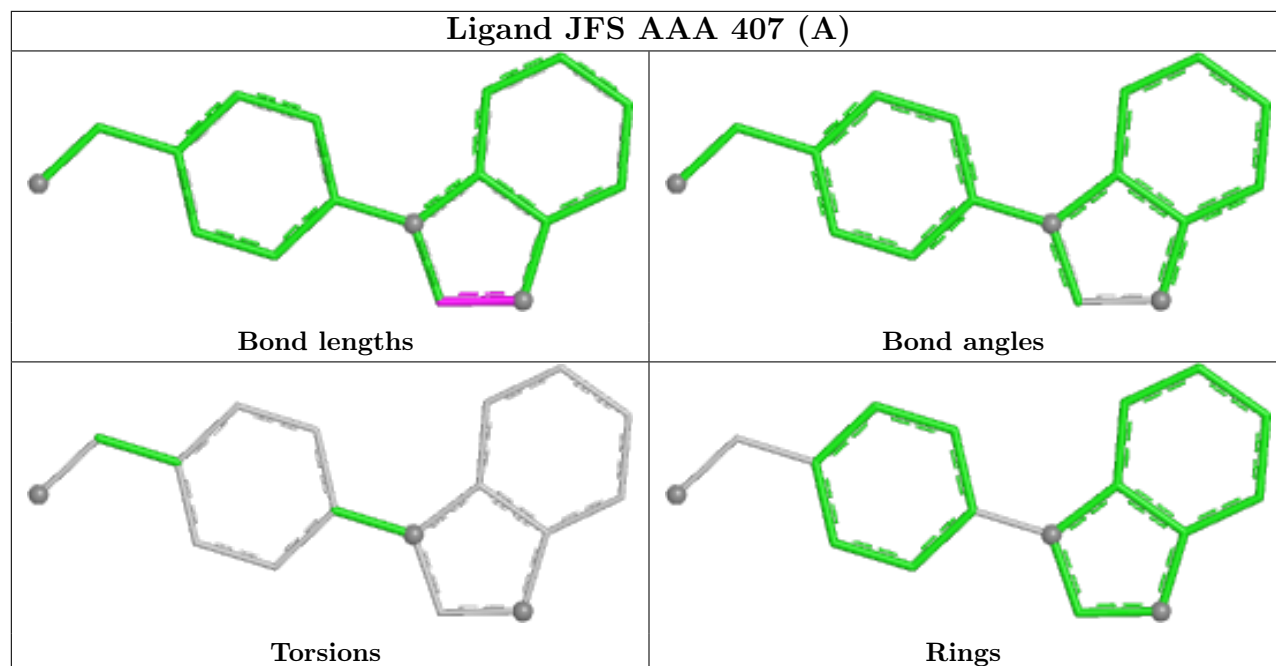
There are no ring outliers.

9 monomers are involved in 36 short contacts:

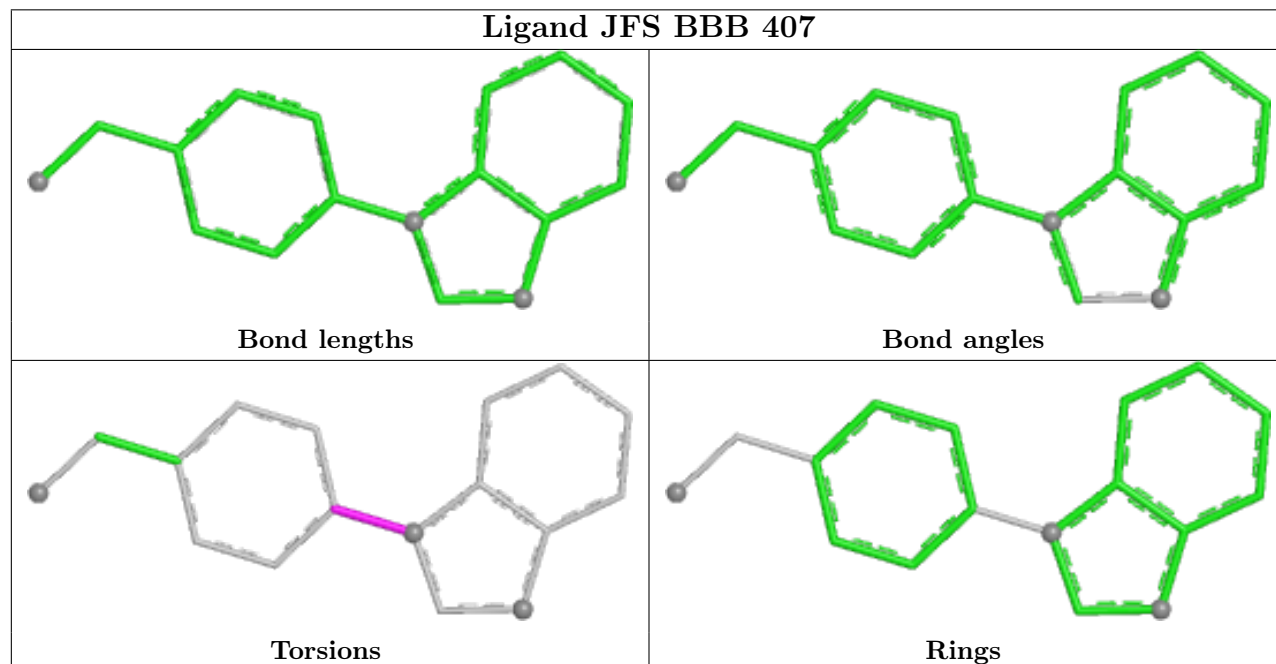
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	AAA	409	GOL	5	0
7	CCC	406	EDO	2	0
3	AAA	404	GOL	7	0
3	AAA	402	GOL	2	0
2	CCC	401	PLP	1	0
3	CCC	403	GOL	2	0
3	BBB	402	GOL	5	0
3	AAA	403	GOL	7	0
8	CCC	402	PGE	5	0

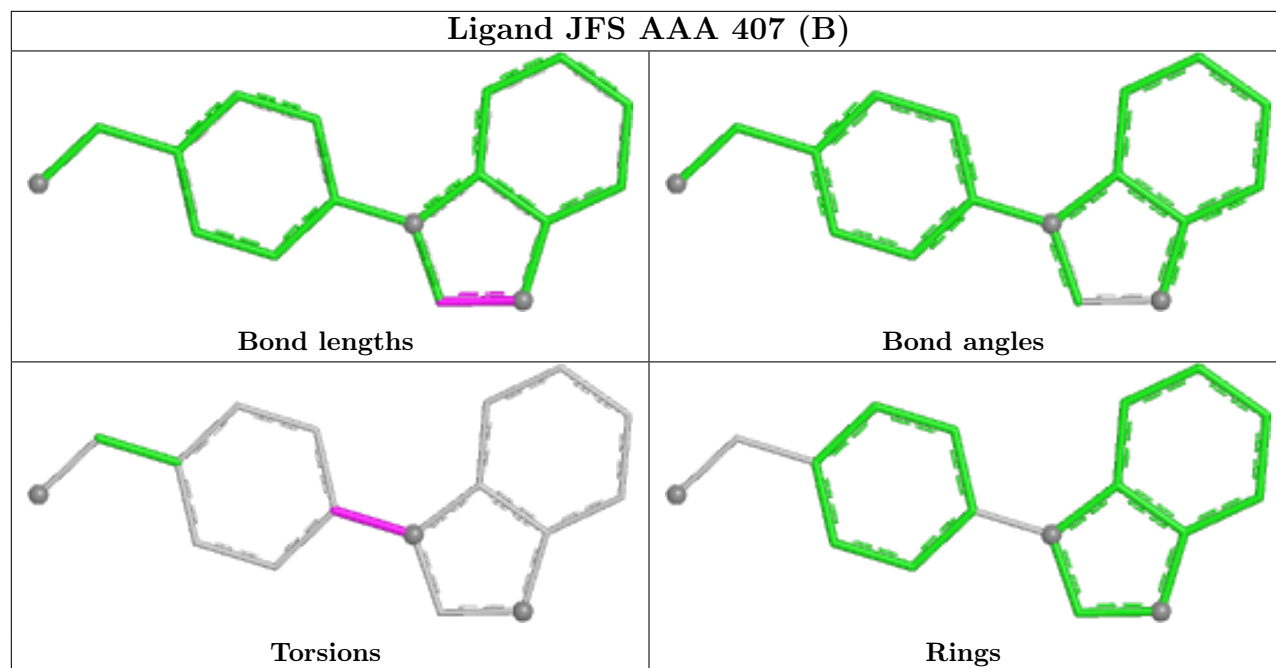
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 JFS AAA 407 (A)



Ligand JFS BBB 407





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS failed to run properly - this section is therefore empty.

6.4 Ligands [i](#)

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers [i](#)

EDS failed to run properly - this section is therefore empty.