Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2024 – 10:22 AM EDT

PDB ID	:	3WCA
Title	:	The complex structure of TcSQS with ligand, FSPP
Authors	:	Shang, N.; Li, Q.; Ko, T.P.; Chan, H.C.; Huang, C.H.; Oldfield, E.; Guo, R.T.
Deposited on	:	2013-05-26
Resolution	:	2.24 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

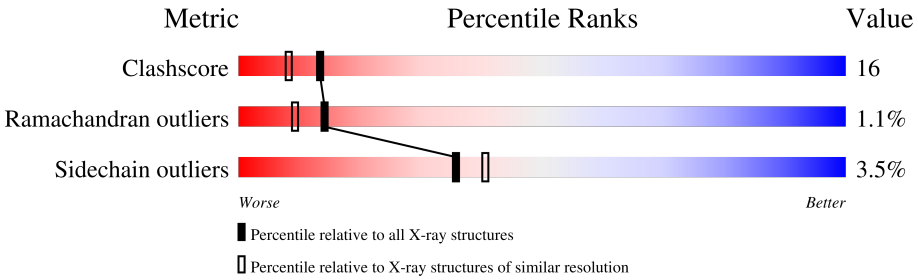
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.24 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	2539 (2.26-2.22)
Ramachandran outliers	138981	2489 (2.26-2.22)
Sidechain outliers	138945	2490 (2.26-2.22)

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

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	365	73% 20% · 7%
1	B	365	65% 24% · 7%
1	C	365	71% 21% · 7%
1	D	365	51% 39% · 7%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 11869 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 Farnesyltransferase, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	341	Total	C	N	O	S	0	0	0
			2751	1745	473	511	22			
1	B	341	Total	C	N	O	S	0	0	0
			2751	1745	473	511	22			
1	C	341	Total	C	N	O	S	0	0	0
			2751	1745	473	511	22			
1	D	341	Total	C	N	O	S	0	0	0
			2752	1745	473	512	22			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	MET	-	expression tag	UNP Q4CWB4
A	5	GLY	-	expression tag	UNP Q4CWB4
A	6	SER	-	expression tag	UNP Q4CWB4
A	7	SER	-	expression tag	UNP Q4CWB4
A	8	HIS	-	expression tag	UNP Q4CWB4
A	9	HIS	-	expression tag	UNP Q4CWB4
A	10	HIS	-	expression tag	UNP Q4CWB4
A	11	HIS	-	expression tag	UNP Q4CWB4
A	12	HIS	-	expression tag	UNP Q4CWB4
A	13	HIS	-	expression tag	UNP Q4CWB4
A	14	SER	-	expression tag	UNP Q4CWB4
A	15	SER	-	expression tag	UNP Q4CWB4
A	16	GLY	-	expression tag	UNP Q4CWB4
A	17	LEU	-	expression tag	UNP Q4CWB4
A	18	VAL	-	expression tag	UNP Q4CWB4
A	19	PRO	-	expression tag	UNP Q4CWB4
A	20	ARG	-	expression tag	UNP Q4CWB4
A	21	GLY	-	expression tag	UNP Q4CWB4
A	22	SER	-	expression tag	UNP Q4CWB4
A	23	HIS	-	expression tag	UNP Q4CWB4
A	24	MET	-	expression tag	UNP Q4CWB4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	82	GLU	ASP	engineered mutation	UNP Q4CWB4
B	4	MET	-	expression tag	UNP Q4CWB4
B	5	GLY	-	expression tag	UNP Q4CWB4
B	6	SER	-	expression tag	UNP Q4CWB4
B	7	SER	-	expression tag	UNP Q4CWB4
B	8	HIS	-	expression tag	UNP Q4CWB4
B	9	HIS	-	expression tag	UNP Q4CWB4
B	10	HIS	-	expression tag	UNP Q4CWB4
B	11	HIS	-	expression tag	UNP Q4CWB4
B	12	HIS	-	expression tag	UNP Q4CWB4
B	13	HIS	-	expression tag	UNP Q4CWB4
B	14	SER	-	expression tag	UNP Q4CWB4
B	15	SER	-	expression tag	UNP Q4CWB4
B	16	GLY	-	expression tag	UNP Q4CWB4
B	17	LEU	-	expression tag	UNP Q4CWB4
B	18	VAL	-	expression tag	UNP Q4CWB4
B	19	PRO	-	expression tag	UNP Q4CWB4
B	20	ARG	-	expression tag	UNP Q4CWB4
B	21	GLY	-	expression tag	UNP Q4CWB4
B	22	SER	-	expression tag	UNP Q4CWB4
B	23	HIS	-	expression tag	UNP Q4CWB4
B	24	MET	-	expression tag	UNP Q4CWB4
B	82	GLU	ASP	engineered mutation	UNP Q4CWB4
C	4	MET	-	expression tag	UNP Q4CWB4
C	5	GLY	-	expression tag	UNP Q4CWB4
C	6	SER	-	expression tag	UNP Q4CWB4
C	7	SER	-	expression tag	UNP Q4CWB4
C	8	HIS	-	expression tag	UNP Q4CWB4
C	9	HIS	-	expression tag	UNP Q4CWB4
C	10	HIS	-	expression tag	UNP Q4CWB4
C	11	HIS	-	expression tag	UNP Q4CWB4
C	12	HIS	-	expression tag	UNP Q4CWB4
C	13	HIS	-	expression tag	UNP Q4CWB4
C	14	SER	-	expression tag	UNP Q4CWB4
C	15	SER	-	expression tag	UNP Q4CWB4
C	16	GLY	-	expression tag	UNP Q4CWB4
C	17	LEU	-	expression tag	UNP Q4CWB4
C	18	VAL	-	expression tag	UNP Q4CWB4
C	19	PRO	-	expression tag	UNP Q4CWB4
C	20	ARG	-	expression tag	UNP Q4CWB4
C	21	GLY	-	expression tag	UNP Q4CWB4
C	22	SER	-	expression tag	UNP Q4CWB4

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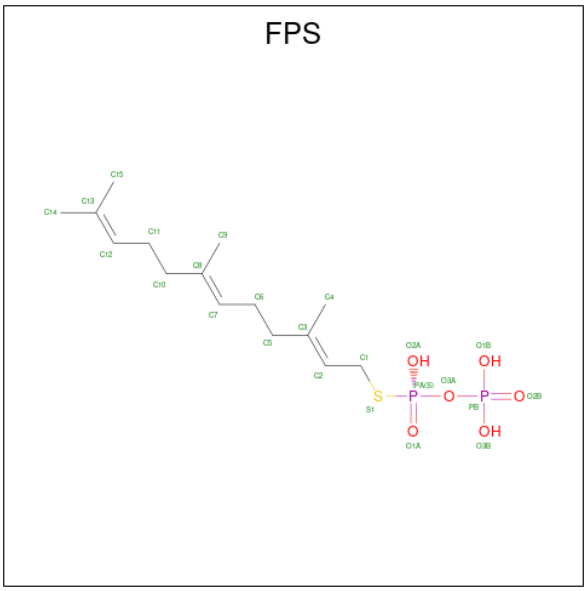
Chain	Residue	Modelled	Actual	Comment	Reference
C	23	HIS	-	expression tag	UNP Q4CWB4
C	24	MET	-	expression tag	UNP Q4CWB4
C	82	GLU	ASP	engineered mutation	UNP Q4CWB4
D	4	MET	-	expression tag	UNP Q4CWB4
D	5	GLY	-	expression tag	UNP Q4CWB4
D	6	SER	-	expression tag	UNP Q4CWB4
D	7	SER	-	expression tag	UNP Q4CWB4
D	8	HIS	-	expression tag	UNP Q4CWB4
D	9	HIS	-	expression tag	UNP Q4CWB4
D	10	HIS	-	expression tag	UNP Q4CWB4
D	11	HIS	-	expression tag	UNP Q4CWB4
D	12	HIS	-	expression tag	UNP Q4CWB4
D	13	HIS	-	expression tag	UNP Q4CWB4
D	14	SER	-	expression tag	UNP Q4CWB4
D	15	SER	-	expression tag	UNP Q4CWB4
D	16	GLY	-	expression tag	UNP Q4CWB4
D	17	LEU	-	expression tag	UNP Q4CWB4
D	18	VAL	-	expression tag	UNP Q4CWB4
D	19	PRO	-	expression tag	UNP Q4CWB4
D	20	ARG	-	expression tag	UNP Q4CWB4
D	21	GLY	-	expression tag	UNP Q4CWB4
D	22	SER	-	expression tag	UNP Q4CWB4
D	23	HIS	-	expression tag	UNP Q4CWB4
D	24	MET	-	expression tag	UNP Q4CWB4
D	82	GLU	ASP	engineered mutation	UNP Q4CWB4

- Molecule 2 is S-[(2E,6E)-3,7,11-TRIMETHYLDODECA-2,6,10-TRIENYL] TRIHYDROGEN THIODIPHOSPHATE (three-letter code: FPS) (formula: $C_{15}H_{28}O_6P_2S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O P S 24 15 6 2 1	0	0
2	B	1	Total C O P S 24 15 6 2 1	0	0
2	C	1	Total C O P S 24 15 6 2 1	0	0
2	C	1	Total C O P S 24 15 6 2 1	0	0
2	D	1	Total C O P S 24 15 6 2 1	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	B	2	Total Mg 2 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	233	Total O 233 233	0	0
4	B	208	Total O 208 208	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	195	Total O 195 195	0	0
4	D	105	Total O 105 105	0	0

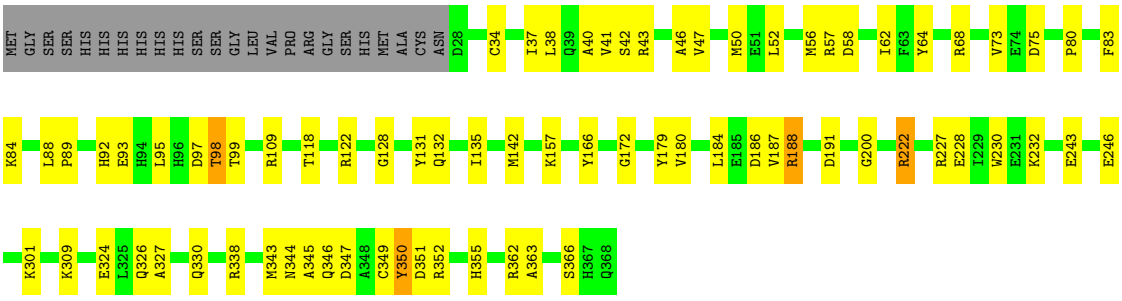
3 Residue-property plots (i)

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

Note EDS failed to run properly.

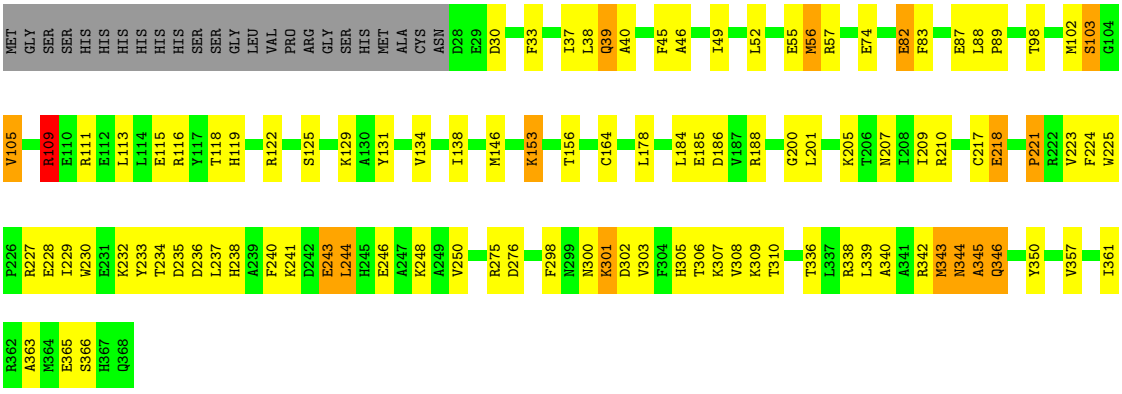
• Molecule 1: Farnesyltransferase, putative

Chain A:



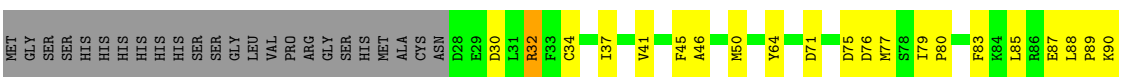
• Molecule 1: Farnesyltransferase, putative

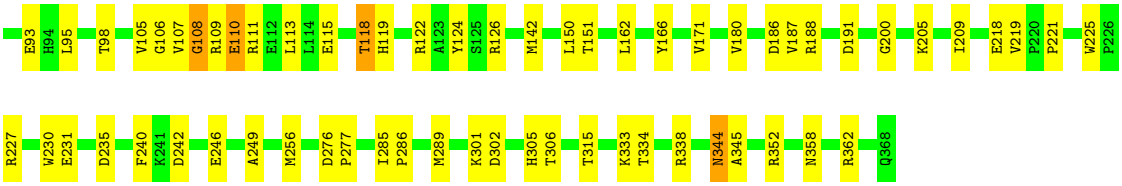
Chain B:



• Molecule 1: Farnesyltransferase, putative

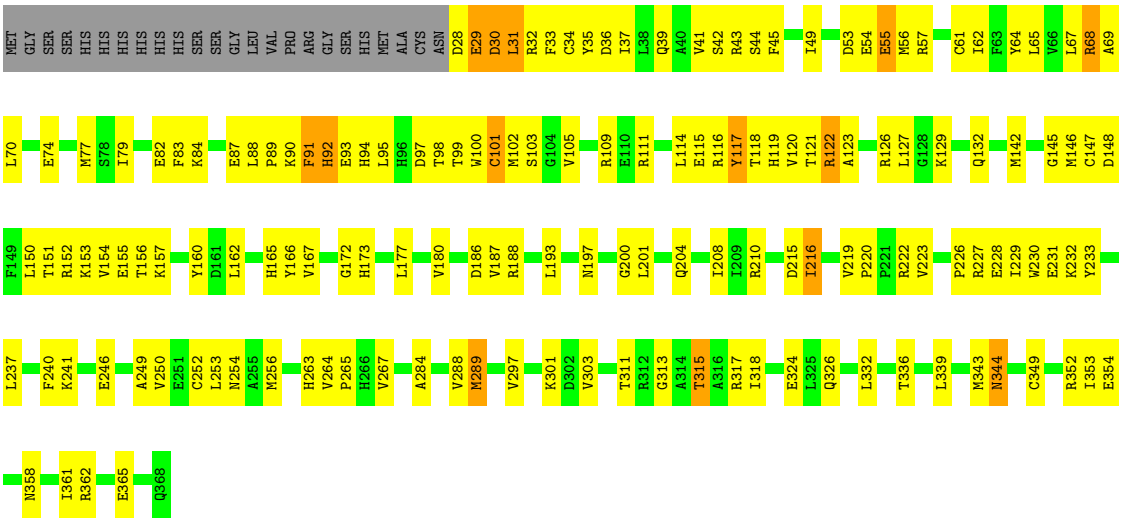
Chain C:





• Molecule 1: Farnesyltransferase, putative

Chain D:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	79.13Å 132.87Å 141.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.24	Depositor
% Data completeness (in resolution range)	(Not available) (25.00-2.24)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.99 (at 2.24Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.215 , 0.259	Depositor
Wilson B-factor (Å^2)	40.8	Xtriage
Anisotropy	0.197	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11869	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.37	0/2809	0.57	0/3806
1	B	0.35	0/2809	0.56	1/3806 (0.0%)
1	C	0.33	0/2809	0.53	0/3806
1	D	0.30	0/2810	0.52	0/3806
All	All	0.34	0/11237	0.55	1/15224 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	103	SER	N-CA-C	5.14	124.89	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2751	0	2698	51	0
1	B	2751	0	2698	96	0
1	C	2751	0	2698	63	0
1	D	2752	0	2698	144	0
2	A	24	0	25	3	0
2	B	24	0	25	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	48	0	50	6	0
2	D	24	0	25	3	0
3	A	1	0	0	0	0
3	B	2	0	0	0	0
4	A	233	0	0	2	0
4	B	208	0	0	3	0
4	C	195	0	0	0	0
4	D	105	0	0	0	0
All	All	11869	0	10917	355	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 16.

All (355) 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:D:129:LYS:HA	1:D:132:GLN:HE21	1.20	1.00
1:A:362:ARG:HD3	1:D:111:ARG:HH12	1.30	0.97
1:B:340:ALA:HB2	1:B:357:VAL:HG21	1.50	0.93
1:B:234:THR:HG22	1:B:236:ASP:H	1.33	0.93
1:B:344:ASN:HD22	1:B:346:GLN:HG3	1.32	0.91
1:D:88:LEU:HB2	1:D:89:PRO:HD3	1.54	0.86
1:A:362:ARG:HD3	1:D:111:ARG:NH1	1.92	0.85
1:D:122:ARG:HH11	1:D:122:ARG:HB3	1.41	0.85
1:D:227:ARG:HG2	1:D:231:GLU:HG3	1.60	0.83
1:A:56:MET:HE1	1:A:179:TYR:HA	1.60	0.83
1:B:223:VAL:HG21	1:B:237:LEU:HD21	1.62	0.82
1:C:188:ARG:HG2	1:C:191:ASP:OD2	1.83	0.79
1:D:180:VAL:HG13	1:D:187:VAL:HA	1.65	0.78
1:A:97:ASP:OD1	1:A:99:THR:HG22	1.83	0.78
1:C:76:ASP:HB2	1:C:105:VAL:HG11	1.65	0.77
1:C:88:LEU:HB2	1:C:89:PRO:HD3	1.69	0.75
1:D:240:PHE:CE1	1:D:249:ALA:HA	2.22	0.75
1:A:41:VAL:HG11	1:A:68:ARG:HG2	1.70	0.73
1:D:358:ASN:HD22	1:D:362:ARG:HH22	1.35	0.73
1:C:46:ALA:O	1:C:50:MET:HG2	1.90	0.72
1:D:30:ASP:OD2	1:D:122:ARG:HB2	1.91	0.71
1:B:344:ASN:HD22	1:B:346:GLN:CG	2.03	0.71
1:A:98:THR:O	1:A:118:THR:HG23	1.91	0.70
1:D:361:ILE:O	1:D:365:GLU:HG3	1.91	0.70
1:B:306:THR:HG22	1:B:307:LYS:N	2.07	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:227:ARG:HA	1:D:230:TRP:NE1	2.08	0.69
1:C:90:LYS:HG2	1:C:93:GLU:OE1	1.93	0.68
1:D:237:LEU:HD12	1:D:240:PHE:CE2	2.28	0.68
1:B:164:CYS:HB3	1:B:201:LEU:HD22	1.76	0.68
1:B:344:ASN:ND2	1:B:346:GLN:HG3	2.07	0.67
1:D:204:GLN:O	1:D:208:ILE:HG12	1.95	0.67
1:A:343:MET:SD	1:A:350:TYR:HA	2.35	0.66
1:C:106:GLY:O	1:C:111:ARG:HB2	1.95	0.66
1:D:352:ARG:HH21	1:D:352:ARG:HG3	1.60	0.66
1:B:55:GLU:HG2	1:B:131:TYR:CE2	2.31	0.66
1:D:311:THR:O	1:D:315:THR:HG22	1.96	0.66
1:D:156:THR:HA	1:D:228:GLU:HB2	1.78	0.65
1:D:117:TYR:CD1	1:D:120:VAL:HG11	2.31	0.65
1:D:79:ILE:HG21	1:D:83:PHE:CD2	2.32	0.64
1:D:100:TRP:O	1:D:101:CYS:HB3	1.95	0.64
1:D:31:LEU:HD23	1:D:32:ARG:N	2.12	0.64
1:C:32:ARG:NH2	1:C:32:ARG:HB2	2.13	0.64
1:D:237:LEU:HD12	1:D:240:PHE:HE2	1.61	0.63
1:D:105:VAL:HG21	1:D:114:LEU:HD13	1.80	0.63
1:B:55:GLU:HG2	1:B:131:TYR:HE2	1.62	0.63
1:B:217:CYS:SG	1:B:241:LYS:HE3	2.38	0.63
1:B:306:THR:HG22	1:B:307:LYS:H	1.64	0.63
1:D:43:ARG:HG3	1:D:44:SER:H	1.61	0.63
1:B:223:VAL:HG21	1:B:237:LEU:CD2	2.28	0.63
1:B:234:THR:HG22	1:B:235:ASP:N	2.13	0.62
1:D:69:ALA:HB1	1:D:114:LEU:HD21	1.80	0.62
1:A:40:ALA:HB1	1:A:109:ARG:HG3	1.82	0.62
1:D:240:PHE:HE1	1:D:249:ALA:HA	1.62	0.62
1:D:230:TRP:HA	1:D:233:TYR:HD2	1.64	0.62
1:C:219:VAL:HA	1:C:221:PRO:HD3	1.81	0.61
1:D:142:MET:HG3	1:D:166:TYR:O	2.00	0.61
1:D:358:ASN:HD22	1:D:362:ARG:NH2	1.97	0.61
1:B:111:ARG:O	1:B:115:GLU:HG3	2.00	0.61
1:C:111:ARG:O	1:C:115:GLU:HG3	2.00	0.61
1:C:302:ASP:O	1:C:306:THR:HG22	1.99	0.61
1:B:246:GLU:CD	1:B:301:LYS:HG3	2.20	0.61
1:C:105:VAL:HG12	1:C:106:GLY:N	2.14	0.61
1:D:216:ILE:HG23	1:D:241:LYS:HE2	1.83	0.60
1:B:298:PHE:HZ	1:B:343:MET:HE3	1.65	0.60
1:B:363:ALA:O	1:B:366:SER:HB3	2.02	0.60
1:D:30:ASP:OD1	1:D:119:HIS:HA	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:334:THR:O	1:C:338:ARG:HG2	2.02	0.59
1:D:358:ASN:HB3	1:D:362:ARG:NH1	2.17	0.59
1:A:88:LEU:HB2	1:A:89:PRO:HD3	1.83	0.59
1:C:90:LYS:HG2	1:C:93:GLU:CD	2.23	0.59
1:D:67:LEU:HD22	1:D:142:MET:SD	2.43	0.59
1:C:344:ASN:HD22	1:C:344:ASN:C	2.06	0.59
1:D:28:ASP:O	1:D:29:GLU:C	2.41	0.58
1:D:30:ASP:CG	1:D:122:ARG:HB2	2.24	0.58
1:D:129:LYS:HA	1:D:132:GLN:NE2	2.05	0.58
1:A:188:ARG:HG3	1:A:191:ASP:OD2	2.04	0.58
1:C:105:VAL:CG1	1:C:106:GLY:N	2.66	0.58
1:C:32:ARG:HB2	1:C:32:ARG:HH21	1.68	0.57
1:D:142:MET:HE2	1:D:166:TYR:O	2.03	0.57
1:D:232:LYS:HG2	1:D:232:LYS:O	2.05	0.57
1:D:343:MET:SD	1:D:353:ILE:HG21	2.45	0.57
1:B:229:ILE:HA	1:B:232:LYS:NZ	2.20	0.56
1:B:233:TYR:O	1:B:248:LYS:HD3	2.05	0.56
1:D:157:LYS:HE2	1:D:229:ILE:HD11	1.87	0.56
1:B:244:LEU:O	1:B:244:LEU:HG	2.05	0.56
1:B:344:ASN:O	1:B:345:ALA:HB2	2.05	0.56
1:C:76:ASP:CB	1:C:105:VAL:HG11	2.35	0.56
1:B:207:ASN:HD22	2:B:401:FPS:H43	1.69	0.56
1:D:123:ALA:HA	1:D:126:ARG:HH11	1.71	0.56
1:D:227:ARG:HA	1:D:230:TRP:CE2	2.41	0.56
1:D:358:ASN:O	1:D:362:ARG:HG2	2.06	0.55
1:C:180:VAL:HG13	1:C:187:VAL:HA	1.88	0.55
1:D:153:LYS:HD2	1:D:154:VAL:H	1.72	0.55
1:B:52:LEU:O	1:B:57:ARG:HD3	2.07	0.55
1:B:116:ARG:HH21	1:B:119:HIS:HE1	1.55	0.55
1:D:42:SER:OG	1:D:45:PHE:HB3	2.06	0.55
1:D:358:ASN:HB3	1:D:362:ARG:HH12	1.71	0.55
1:D:95:LEU:O	1:D:121:THR:HG23	2.06	0.55
1:B:164:CYS:CB	1:B:201:LEU:HD22	2.36	0.55
2:C:401:FPS:H93	2:C:402:FPS:H152	1.89	0.55
1:C:118:THR:O	1:C:122:ARG:HB2	2.06	0.55
1:C:122:ARG:HG2	1:C:126:ARG:NH2	2.22	0.54
1:D:240:PHE:CD1	1:D:249:ALA:HA	2.42	0.54
1:D:97:ASP:HB3	1:D:100:TRP:HB2	1.89	0.54
1:D:92:HIS:CD2	1:D:93:GLU:HG3	2.43	0.54
1:D:264:VAL:HB	1:D:265:PRO:HD3	1.88	0.54
1:C:80:PRO:HG2	1:C:83:PHE:HB2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:232:LYS:NZ	1:D:232:LYS:HB3	2.23	0.54
1:B:46:ALA:O	1:B:49:ILE:HG22	2.08	0.54
1:B:246:GLU:OE2	1:B:301:LYS:HG3	2.08	0.54
1:C:64:TYR:HA	2:C:402:FPS:H142	1.90	0.54
1:D:70:LEU:HD12	1:D:91:PHE:HD1	1.73	0.54
1:C:30:ASP:HA	1:C:119:HIS:CD2	2.43	0.53
1:D:118:THR:O	1:D:122:ARG:HG2	2.08	0.53
1:C:186:ASP:OD2	1:C:188:ARG:HB3	2.08	0.53
1:B:83:PHE:CZ	1:B:87:GLU:HG3	2.43	0.53
1:C:110:GLU:O	1:C:113:LEU:HB3	2.08	0.53
1:D:68:ARG:HH21	1:D:68:ARG:HG3	1.74	0.53
1:C:45:PHE:HD2	2:C:401:FPS:O1A	1.92	0.53
1:D:79:ILE:HG21	1:D:83:PHE:HD2	1.74	0.53
1:C:83:PHE:CZ	1:C:87:GLU:HG3	2.44	0.53
1:D:91:PHE:HD2	1:D:91:PHE:O	1.92	0.53
1:D:226:PRO:HG2	1:D:229:ILE:CG1	2.39	0.53
1:B:118:THR:O	1:B:122:ARG:HG3	2.08	0.52
1:A:228:GLU:O	1:A:232:LYS:NZ	2.42	0.52
1:D:114:LEU:HA	1:D:117:TYR:HB2	1.91	0.52
1:D:62:ILE:HD12	1:D:127:LEU:HD11	1.90	0.52
1:D:102:MET:SD	1:D:105:VAL:HG21	2.49	0.52
1:D:35:TYR:OH	1:D:57:ARG:HG2	2.10	0.52
1:D:55:GLU:HG2	1:D:56:MET:N	2.25	0.52
1:D:232:LYS:HB3	1:D:232:LYS:HZ3	1.75	0.52
1:A:118:THR:HG22	1:A:122:ARG:HE	1.75	0.52
1:B:303:VAL:HG22	1:B:308:VAL:HG21	1.92	0.52
1:C:227:ARG:O	1:C:231:GLU:HB3	2.11	0.51
1:D:43:ARG:HG3	1:D:44:SER:N	2.24	0.51
1:C:358:ASN:HB3	1:C:362:ARG:HH12	1.76	0.51
1:B:237:LEU:HD12	1:B:240:PHE:CE2	2.44	0.51
1:D:349:CYS:HB2	1:D:353:ILE:HD13	1.93	0.51
1:D:324:GLU:OE1	1:D:326:GLN:HB2	2.11	0.51
1:D:142:MET:O	1:D:146:MET:HG3	2.10	0.51
1:B:40:ALA:HB1	1:B:109:ARG:HG2	1.93	0.51
1:D:230:TRP:HB3	1:D:252:CYS:SG	2.51	0.51
1:B:125:SER:HB3	4:B:694:HOH:O	2.11	0.51
1:D:227:ARG:O	1:D:231:GLU:HG3	2.11	0.50
1:D:263:HIS:O	1:D:267:VAL:HG23	2.11	0.50
1:A:343:MET:SD	1:A:350:TYR:HD1	2.35	0.50
1:C:302:ASP:HA	1:C:305:HIS:CE1	2.47	0.50
1:D:42:SER:HB2	1:D:64:TYR:OH	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:246:GLU:HA	1:C:249:ALA:HB3	1.93	0.50
1:D:28:ASP:O	1:D:30:ASP:N	2.44	0.50
1:D:162:LEU:O	1:D:165:HIS:HB3	2.12	0.50
1:B:56:MET:HE1	1:B:178:LEU:HB3	1.93	0.50
1:B:129:LYS:O	1:B:129:LYS:HD3	2.12	0.50
1:B:33:PHE:CZ	1:B:37:ILE:HG13	2.47	0.50
1:B:345:ALA:HA	1:B:350:TYR:CG	2.47	0.50
1:D:117:TYR:CE1	1:D:120:VAL:HG11	2.47	0.50
1:D:146:MET:O	1:D:150:LEU:HB2	2.12	0.50
1:B:234:THR:HG22	1:B:235:ASP:H	1.77	0.49
1:C:142:MET:HG3	1:C:166:TYR:O	2.12	0.49
1:D:352:ARG:HG3	1:D:352:ARG:NH2	2.24	0.49
1:C:107:VAL:O	1:C:108:GLY:C	2.51	0.49
1:D:103:SER:HA	1:D:115:GLU:HG2	1.93	0.49
1:B:153:LYS:NZ	1:B:153:LYS:HB3	2.28	0.49
1:D:172:GLY:HA2	2:D:401:FPS:H152	1.95	0.49
1:A:42:SER:HB2	1:A:64:TYR:OH	2.12	0.49
1:D:227:ARG:HG2	1:D:231:GLU:CG	2.36	0.49
1:A:58:ASP:O	1:A:62:ILE:HG12	2.13	0.49
1:D:252:CYS:O	1:D:256:MET:HG2	2.13	0.49
1:C:106:GLY:C	1:C:111:ARG:HB2	2.33	0.49
1:D:339:LEU:HD23	1:D:339:LEU:O	2.13	0.49
1:D:186:ASP:OD2	1:D:188:ARG:HB2	2.13	0.48
1:D:254:ASN:HB3	1:D:349:CYS:SG	2.53	0.48
1:D:313:GLY:O	1:D:317:ARG:HG3	2.12	0.48
1:B:238:HIS:O	1:B:241:LYS:HB3	2.13	0.48
1:A:42:SER:CB	1:A:64:TYR:OH	2.61	0.48
1:D:200:GLY:HA2	2:D:401:FPS:H102	1.95	0.48
1:A:346:GLN:HG3	1:A:347:ASP:H	1.79	0.48
1:C:200:GLY:HA2	2:C:401:FPS:H102	1.95	0.48
1:B:102:MET:HE2	1:B:105:VAL:CG2	2.43	0.48
1:B:103:SER:HA	1:B:115:GLU:HG2	1.96	0.48
1:B:306:THR:CG2	1:B:307:LYS:N	2.75	0.48
1:B:336:THR:HG22	1:B:357:VAL:HG13	1.95	0.48
1:B:243:GLU:O	1:B:246:GLU:HG3	2.13	0.48
1:D:197:ASN:O	1:D:201:LEU:HG	2.13	0.48
1:D:122:ARG:HH11	1:D:122:ARG:CB	2.20	0.48
1:D:148:ASP:O	1:D:152:ARG:HG2	2.13	0.48
1:A:118:THR:O	1:A:122:ARG:HG3	2.15	0.47
1:D:284:ALA:O	1:D:288:VAL:HG23	2.14	0.47
1:D:37:ILE:O	1:D:41:VAL:HG22	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:218:GLU:O	1:C:221:PRO:HA	2.15	0.47
1:C:285:ILE:HB	1:C:286:PRO:HD3	1.96	0.47
1:A:344:ASN:HB3	1:A:346:GLN:HG2	1.96	0.47
1:D:157:LYS:HE2	1:D:229:ILE:CD1	2.43	0.47
1:D:289:MET:HG2	1:D:318:ILE:HG21	1.96	0.47
1:B:82:GLU:CD	1:B:82:GLU:H	2.17	0.47
1:B:200:GLY:HA2	2:B:401:FPS:H102	1.95	0.47
1:B:227:ARG:HA	1:B:230:TRP:CE2	2.49	0.47
1:C:95:LEU:HB3	1:C:124:TYR:CE2	2.50	0.47
1:D:120:VAL:HG13	1:D:121:THR:N	2.28	0.47
1:D:210:ARG:HD2	1:D:210:ARG:O	2.15	0.47
1:D:246:GLU:O	1:D:250:VAL:HG23	2.15	0.47
1:A:324:GLU:OE1	1:A:326:GLN:HB2	2.15	0.47
1:D:35:TYR:O	1:D:39:GLN:HG3	2.15	0.47
1:D:157:LYS:O	1:D:160:TYR:HB3	2.15	0.47
1:D:353:ILE:HG22	1:D:354:GLU:N	2.30	0.46
1:B:227:ARG:HA	1:B:230:TRP:NE1	2.30	0.46
1:D:97:ASP:C	1:D:99:THR:H	2.19	0.46
1:A:346:GLN:HG3	1:A:347:ASP:N	2.30	0.46
1:D:33:PHE:HD2	1:D:119:HIS:HB2	1.81	0.46
1:D:129:LYS:O	1:D:129:LYS:HD3	2.16	0.46
1:B:210:ARG:HD3	1:B:307:LYS:HG3	1.97	0.46
1:B:237:LEU:HD12	1:B:240:PHE:CD2	2.51	0.46
1:B:309:LYS:HG2	1:B:310:THR:N	2.31	0.46
1:B:236:ASP:OD2	1:B:238:HIS:HB2	2.16	0.46
1:C:162:LEU:HD11	1:C:166:TYR:CZ	2.51	0.46
1:D:156:THR:HB	1:D:228:GLU:OE1	2.15	0.46
1:A:345:ALA:HA	1:A:350:TYR:CD2	2.51	0.46
1:D:92:HIS:NE2	1:D:93:GLU:HG3	2.31	0.46
1:A:128:GLY:O	1:A:132:GLN:HG3	2.15	0.46
1:B:343:MET:CE	1:B:350:TYR:HA	2.46	0.46
1:A:180:VAL:HG13	1:A:187:VAL:HA	1.97	0.46
1:D:68:ARG:HH21	1:D:68:ARG:CG	2.29	0.45
1:D:116:ARG:C	1:D:118:THR:H	2.19	0.45
1:B:40:ALA:CB	1:B:109:ARG:HG2	2.46	0.45
1:C:205:LYS:O	1:C:209:ILE:HG13	2.15	0.45
1:D:49:ILE:HG12	1:D:57:ARG:HG3	1.99	0.45
1:A:80:PRO:O	1:A:83:PHE:HB3	2.16	0.45
1:B:186:ASP:OD2	1:B:188:ARG:HG3	2.16	0.45
1:C:225:TRP:HA	1:C:256:MET:HE1	1.99	0.45
1:D:84:LYS:CD	1:D:150:LEU:HD21	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:ILE:O	1:C:41:VAL:HG22	2.17	0.45
1:D:232:LYS:NZ	1:D:232:LYS:CB	2.78	0.45
1:A:157:LYS:HG3	1:A:228:GLU:CD	2.37	0.45
1:B:234:THR:CG2	1:B:235:ASP:N	2.80	0.45
1:C:37:ILE:HD11	1:C:109:ARG:O	2.16	0.45
1:A:142:MET:HE2	1:A:166:TYR:O	2.17	0.45
1:A:186:ASP:OD2	1:A:188:ARG:HB2	2.17	0.45
1:B:38:LEU:HD21	1:B:49:ILE:HG21	1.99	0.45
1:D:297:VAL:HB	1:D:303:VAL:HG21	1.98	0.45
1:B:223:VAL:HG22	1:B:224:PHE:N	2.31	0.45
1:B:302:ASP:HA	1:B:305:HIS:CE1	2.52	0.45
1:B:361:ILE:O	1:B:365:GLU:HG3	2.17	0.45
1:C:227:ARG:HA	1:C:230:TRP:NE1	2.32	0.45
1:C:240:PHE:CE1	1:C:249:ALA:HA	2.52	0.45
1:D:339:LEU:HD23	1:D:339:LEU:C	2.37	0.45
1:C:289:MET:CE	1:C:315:THR:HG22	2.47	0.45
1:D:145:GLY:HA3	1:D:166:TYR:CD1	2.52	0.45
1:D:253:LEU:HD21	1:D:297:VAL:O	2.16	0.45
1:A:52:LEU:O	1:A:57:ARG:HD3	2.17	0.45
1:B:102:MET:HE1	1:B:105:VAL:HG21	1.99	0.45
1:D:61:CYS:O	1:D:65:LEU:HG	2.17	0.45
1:D:332:LEU:O	1:D:336:THR:HG23	2.17	0.45
1:D:74:GLU:HG3	1:D:146:MET:HB3	1.98	0.44
1:D:147:CYS:O	1:D:151:THR:HG23	2.17	0.44
1:A:172:GLY:HA2	2:A:501:FPS:H152	1.99	0.44
1:D:70:LEU:HD12	1:D:91:PHE:CD1	2.52	0.44
1:A:227:ARG:HA	1:A:230:TRP:CE2	2.52	0.44
1:A:352:ARG:O	1:A:355:HIS:CD2	2.71	0.44
1:B:74:GLU:HG3	1:B:146:MET:SD	2.58	0.44
1:B:306:THR:CG2	1:B:307:LYS:H	2.29	0.44
1:A:131:TYR:O	1:A:135:ILE:HG13	2.18	0.44
1:D:142:MET:HE1	1:D:167:VAL:O	2.16	0.44
1:D:344:ASN:C	1:D:344:ASN:HD22	2.20	0.44
2:A:501:FPS:H112	2:A:501:FPS:H91	1.79	0.44
2:D:401:FPS:H91	2:D:401:FPS:H112	1.79	0.44
1:D:28:ASP:CA	1:D:32:ARG:HG2	2.48	0.44
1:D:215:ASP:HB3	1:D:222:ARG:O	2.18	0.44
1:B:156:THR:HA	1:B:228:GLU:HB2	2.00	0.44
1:D:30:ASP:O	1:D:33:PHE:HB3	2.18	0.44
1:B:102:MET:CE	1:B:105:VAL:HG21	2.48	0.43
1:C:122:ARG:HG2	1:C:126:ARG:HH21	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:ILE:HG21	1:B:113:LEU:HD13	2.00	0.43
1:D:91:PHE:HA	1:D:94:HIS:CD2	2.52	0.43
1:B:134:VAL:O	1:B:138:ILE:HG12	2.18	0.43
1:D:223:VAL:CG2	1:D:237:LEU:HD23	2.48	0.43
1:B:205:LYS:O	1:B:209:ILE:HG13	2.18	0.43
1:C:98:THR:HG22	1:C:122:ARG:HH21	1.84	0.43
1:D:87:GLU:O	1:D:90:LYS:N	2.45	0.43
1:D:155:GLU:OE1	1:D:227:ARG:NE	2.49	0.43
1:B:300:ASN:HB2	1:B:342:ARG:HH22	1.83	0.43
1:D:173:HIS:O	1:D:177:LEU:HG	2.18	0.43
1:D:344:ASN:HD22	1:D:344:ASN:H	1.65	0.43
1:A:73:VAL:O	1:A:84:LYS:HE2	2.18	0.43
1:D:117:TYR:O	1:D:120:VAL:HG12	2.18	0.43
1:D:88:LEU:CB	1:D:89:PRO:HD3	2.35	0.43
1:D:173:HIS:ND1	1:D:193:LEU:HD13	2.34	0.43
1:B:344:ASN:OD1	1:B:344:ASN:N	2.52	0.43
1:C:79:ILE:HG13	1:C:105:VAL:HG21	2.01	0.43
1:C:218:GLU:O	1:C:221:PRO:N	2.51	0.43
1:C:171:VAL:HG21	2:C:402:FPS:H101	2.00	0.42
1:D:84:LYS:HD3	1:D:150:LEU:HD21	2.01	0.42
1:B:156:THR:HB	4:B:703:HOH:O	2.19	0.42
1:C:338:ARG:NH1	1:C:338:ARG:HG3	2.34	0.42
1:A:50:MET:HA	1:A:57:ARG:HD2	2.00	0.42
1:A:349:CYS:O	1:A:351:ASP:N	2.51	0.42
1:B:116:ARG:NH2	1:B:119:HIS:HE1	2.18	0.42
1:B:184:LEU:HD22	1:B:276:ASP:OD2	2.20	0.42
1:B:207:ASN:ND2	2:B:401:FPS:H43	2.35	0.42
1:B:345:ALA:HA	1:B:350:TYR:CD1	2.54	0.42
1:C:85:LEU:HD11	1:C:151:THR:HG21	2.01	0.42
1:B:229:ILE:HA	1:B:232:LYS:HZ1	1.84	0.42
1:D:30:ASP:OD1	1:D:122:ARG:HB2	2.20	0.42
1:B:339:LEU:HD23	1:B:339:LEU:C	2.40	0.42
1:C:34:CYS:O	1:C:37:ILE:HG22	2.19	0.42
1:D:219:VAL:HA	1:D:220:PRO:HA	1.91	0.42
1:D:250:VAL:O	1:D:253:LEU:HB3	2.20	0.42
1:A:34:CYS:O	1:A:37:ILE:HG22	2.20	0.42
1:B:336:THR:CG2	1:B:357:VAL:HG13	2.50	0.42
1:D:126:ARG:H	1:D:126:ARG:HD2	1.85	0.42
1:A:363:ALA:O	1:A:366:SER:HB3	2.19	0.42
1:D:226:PRO:HG2	1:D:229:ILE:HG13	2.02	0.42
1:A:43:ARG:O	1:A:47:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:PHE:CE2	1:B:37:ILE:HG13	2.54	0.42
1:C:289:MET:HE1	1:C:315:THR:HG22	2.01	0.42
1:D:28:ASP:N	1:D:31:LEU:HD22	2.35	0.42
1:A:309:LYS:HE3	4:A:833:HOH:O	2.20	0.42
1:B:102:MET:HE2	1:B:105:VAL:HG22	2.00	0.42
1:B:185:GLU:OE1	1:B:275:ARG:HG2	2.20	0.42
1:C:30:ASP:HA	1:C:119:HIS:HD2	1.84	0.42
1:B:346:GLN:H	1:B:346:GLN:HG2	1.66	0.41
1:B:30:ASP:OD1	1:B:119:HIS:HD2	2.03	0.41
1:B:223:VAL:HG22	1:B:225:TRP:H	1.84	0.41
1:C:71:ASP:O	1:C:75:ASP:HB2	2.20	0.41
1:C:358:ASN:HB3	1:C:362:ARG:NH1	2.35	0.41
1:A:200:GLY:HA2	2:A:501:FPS:H102	2.02	0.41
1:B:343:MET:SD	1:B:350:TYR:HA	2.61	0.41
1:C:289:MET:HE2	1:C:289:MET:HB3	1.79	0.41
1:A:75:ASP:CB	1:A:222:ARG:HH22	2.34	0.41
1:B:338:ARG:O	1:B:342:ARG:HG3	2.20	0.41
1:D:232:LYS:O	1:D:232:LYS:CG	2.67	0.41
1:A:243:GLU:O	1:A:246:GLU:HB2	2.21	0.41
1:D:129:LYS:HD3	1:D:129:LYS:C	2.40	0.41
1:B:300:ASN:OD1	1:B:302:ASP:N	2.51	0.41
1:B:39:GLN:HE21	1:B:39:GLN:HB3	1.62	0.41
1:C:85:LEU:HD11	1:C:151:THR:CG2	2.50	0.41
1:D:88:LEU:C	1:D:90:LYS:H	2.24	0.41
1:A:38:LEU:HG	1:A:46:ALA:HB2	2.02	0.41
1:A:92:HIS:CE1	1:A:93:GLU:HG3	2.56	0.41
1:B:218:GLU:O	1:B:221:PRO:HG3	2.20	0.41
1:C:79:ILE:CD1	1:C:105:VAL:HG21	2.51	0.41
1:A:327:ALA:HA	1:A:330:GLN:HG2	2.03	0.41
1:C:85:LEU:HD23	1:C:150:LEU:HD23	2.03	0.41
2:C:401:FPS:H91	2:C:401:FPS:H112	1.82	0.41
1:A:366:SER:O	1:D:109:ARG:HD2	2.21	0.41
1:B:344:ASN:O	1:B:345:ALA:CB	2.69	0.41
1:A:56:MET:HE2	1:A:184:LEU:HD12	2.03	0.40
1:A:349:CYS:O	1:A:350:TYR:C	2.59	0.40
1:B:234:THR:HG21	1:B:236:ASP:O	2.21	0.40
1:B:365:GLU:HB2	4:B:566:HOH:O	2.20	0.40
1:A:93:GLU:HG2	4:A:813:HOH:O	2.21	0.40
1:B:88:LEU:N	1:B:89:PRO:CD	2.85	0.40
1:C:276:ASP:HA	1:C:277:PRO:HD3	1.87	0.40
1:A:338:ARG:HD2	1:A:338:ARG:HA	1.97	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:GLU:O	1:B:250:VAL:HG23	2.21	0.40
1:D:34:CYS:HB3	1:D:65:LEU:HD11	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	339/365 (93%)	329 (97%)	8 (2%)	2 (1%)	25 23
1	B	339/365 (93%)	325 (96%)	10 (3%)	4 (1%)	13 8
1	C	339/365 (93%)	320 (94%)	17 (5%)	2 (1%)	25 23
1	D	339/365 (93%)	301 (89%)	31 (9%)	7 (2%)	7 2
All	All	1356/1460 (93%)	1275 (94%)	66 (5%)	15 (1%)	14 9

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	345	ALA
1	D	29	GLU
1	D	54	GLU
1	D	101	CYS
1	A	350	TYR
1	B	98	THR
1	C	108	GLY
1	C	345	ALA
1	D	55	GLU
1	D	98	THR
1	A	98	THR
1	D	30	ASP
1	D	117	TYR

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Mol	Chain	Res	Type
1	B	109	ARG
1	B	221	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	298/318 (94%)	294 (99%)	4 (1%)	69	76
1	B	298/318 (94%)	284 (95%)	14 (5%)	26	27
1	C	298/318 (94%)	288 (97%)	10 (3%)	37	42
1	D	298/318 (94%)	284 (95%)	14 (5%)	26	27
All	All	1192/1272 (94%)	1150 (96%)	42 (4%)	36	40

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	LEU
1	A	188	ARG
1	A	222	ARG
1	A	301	LYS
1	B	39	GLN
1	B	45	PHE
1	B	56	MET
1	B	82	GLU
1	B	105	VAL
1	B	109	ARG
1	B	153	LYS
1	B	218	GLU
1	B	243	GLU
1	B	244	LEU
1	B	301	LYS
1	B	343	MET
1	B	344	ASN
1	B	346	GLN
1	C	32	ARG

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Mol	Chain	Res	Type
1	C	77	MET
1	C	110	GLU
1	C	118	THR
1	C	235	ASP
1	C	242	ASP
1	C	301	LYS
1	C	333	LYS
1	C	344	ASN
1	C	352	ARG
1	D	31	LEU
1	D	36	ASP
1	D	53	ASP
1	D	68	ARG
1	D	77	MET
1	D	82	GLU
1	D	91	PHE
1	D	92	HIS
1	D	122	ARG
1	D	216	ILE
1	D	289	MET
1	D	301	LYS
1	D	315	THR
1	D	344	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	HIS
1	A	144	ASN
1	A	238	HIS
1	A	245	HIS
1	A	320	HIS
1	B	39	GLN
1	B	119	HIS
1	B	144	ASN
1	B	207	ASN
1	B	344	ASN
1	B	358	ASN
1	C	94	HIS
1	C	119	HIS
1	C	144	ASN
1	C	204	GLN

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Mol	Chain	Res	Type
1	C	245	HIS
1	C	305	HIS
1	C	320	HIS
1	C	344	ASN
1	C	358	ASN
1	D	92	HIS
1	D	94	HIS
1	D	132	GLN
1	D	204	GLN
1	D	245	HIS
1	D	287	GLN
1	D	300	ASN
1	D	330	GLN
1	D	344	ASN
1	D	358	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 3 are monoatomic - leaving 5 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	$\#\|Z\|>2$
2	FPS	D	401	-	19,23,23	1.30	3 (15%)	23,31,31	1.72	6 (26%)
2	FPS	C	401	-	19,23,23	1.19	2 (10%)	23,31,31	1.40	5 (21%)
2	FPS	C	402	-	19,23,23	1.14	1 (5%)	23,31,31	1.82	8 (34%)
2	FPS	A	501	-	19,23,23	1.35	3 (15%)	23,31,31	1.36	3 (13%)
2	FPS	B	401	-	19,23,23	1.36	3 (15%)	23,31,31	1.78	7 (30%)

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	FPS	D	401	-	-	6/19/25/25	-
2	FPS	C	401	-	-	7/19/25/25	-
2	FPS	C	402	-	-	8/19/25/25	-
2	FPS	A	501	-	-	8/19/25/25	-
2	FPS	B	401	-	-	7/19/25/25	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	FPS	C2-C3	2.74	1.39	1.33
2	B	401	FPS	PB-O2B	2.64	1.59	1.50
2	C	401	FPS	C2-C3	2.62	1.39	1.33
2	B	401	FPS	C10-C8	2.53	1.56	1.51
2	B	401	FPS	C2-C3	2.52	1.39	1.33
2	D	401	FPS	C1-S1	2.44	1.87	1.84
2	D	401	FPS	C2-C3	2.39	1.38	1.33
2	C	402	FPS	PB-O2B	2.36	1.58	1.50
2	C	401	FPS	PB-O2B	2.19	1.57	1.50
2	A	501	FPS	PB-O2B	2.18	1.57	1.50
2	A	501	FPS	PA-O2A	-2.17	1.51	1.56
2	D	401	FPS	PB-O2B	2.12	1.57	1.50

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	FPS	C9-C8-C10	4.28	122.47	115.27
2	C	402	FPS	C9-C8-C10	4.01	122.02	115.27
2	C	402	FPS	C10-C8-C7	-3.95	113.13	121.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	401	FPS	C9-C8-C10	3.87	121.78	115.27
2	D	401	FPS	C10-C8-C7	-3.59	113.85	121.12
2	B	401	FPS	C10-C8-C7	-3.57	113.90	121.12
2	D	401	FPS	C5-C3-C2	-3.29	114.45	121.12
2	C	402	FPS	C5-C6-C7	-3.18	101.42	111.88
2	A	501	FPS	C9-C8-C10	2.84	120.05	115.27
2	C	401	FPS	C9-C8-C10	2.74	119.87	115.27
2	D	401	FPS	C4-C3-C5	2.73	119.87	115.27
2	B	401	FPS	C6-C5-C3	2.49	121.17	112.98
2	B	401	FPS	O1B-PB-O3A	2.48	112.96	104.64
2	A	501	FPS	C10-C8-C7	-2.47	116.13	121.12
2	C	401	FPS	C10-C8-C7	-2.41	116.25	121.12
2	C	402	FPS	C5-C3-C2	-2.30	116.45	121.12
2	B	401	FPS	C5-C6-C7	-2.30	104.32	111.88
2	C	401	FPS	O1B-PB-O3A	2.28	112.29	104.64
2	D	401	FPS	O1B-PB-O3A	2.26	112.21	104.64
2	C	402	FPS	O1B-PB-O3A	2.20	112.01	104.64
2	C	401	FPS	C15-C13-C14	2.16	119.36	114.60
2	B	401	FPS	C4-C3-C5	2.12	118.83	115.27
2	C	402	FPS	C6-C5-C3	2.10	119.89	112.98
2	B	401	FPS	C5-C3-C2	-2.09	116.88	121.12
2	C	402	FPS	C4-C3-C5	2.09	118.79	115.27
2	C	401	FPS	C15-C13-C12	-2.07	116.67	122.65
2	C	402	FPS	C15-C13-C14	2.05	119.14	114.60
2	D	401	FPS	C15-C13-C14	2.03	119.09	114.60
2	A	501	FPS	C5-C3-C2	-2.02	117.04	121.12

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	FPS	C11-C10-C8-C7
2	A	501	FPS	C11-C10-C8-C9
2	A	501	FPS	PA-O3A-PB-O1B
2	A	501	FPS	PA-O3A-PB-O3B
2	B	401	FPS	PA-O3A-PB-O1B
2	C	402	FPS	C11-C10-C8-C9
2	D	401	FPS	C11-C10-C8-C7
2	D	401	FPS	C11-C10-C8-C9
2	B	401	FPS	C11-C10-C8-C9
2	B	401	FPS	C11-C10-C8-C7
2	C	402	FPS	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
2	C	402	FPS	C3-C5-C6-C7
2	C	402	FPS	C8-C10-C11-C12
2	A	501	FPS	C3-C5-C6-C7
2	C	401	FPS	C3-C5-C6-C7
2	C	401	FPS	C11-C10-C8-C9
2	B	401	FPS	C4-C3-C5-C6
2	D	401	FPS	C4-C3-C5-C6
2	D	401	FPS	C2-C3-C5-C6
2	B	401	FPS	C2-C3-C5-C6
2	C	401	FPS	C8-C10-C11-C12
2	D	401	FPS	C3-C5-C6-C7
2	C	401	FPS	PA-O3A-PB-O1B
2	C	402	FPS	C4-C3-C5-C6
2	C	402	FPS	C2-C3-C5-C6
2	C	401	FPS	C11-C10-C8-C7
2	B	401	FPS	PA-O3A-PB-O2B
2	B	401	FPS	C8-C10-C11-C12
2	D	401	FPS	C8-C10-C11-C12
2	C	401	FPS	C4-C3-C5-C6
2	C	401	FPS	C2-C3-C5-C6
2	A	501	FPS	C4-C3-C5-C6
2	C	402	FPS	PA-O3A-PB-O1B
2	C	402	FPS	PA-O3A-PB-O3B
2	A	501	FPS	PA-O3A-PB-O2B
2	A	501	FPS	C8-C10-C11-C12

There are no ring outliers.

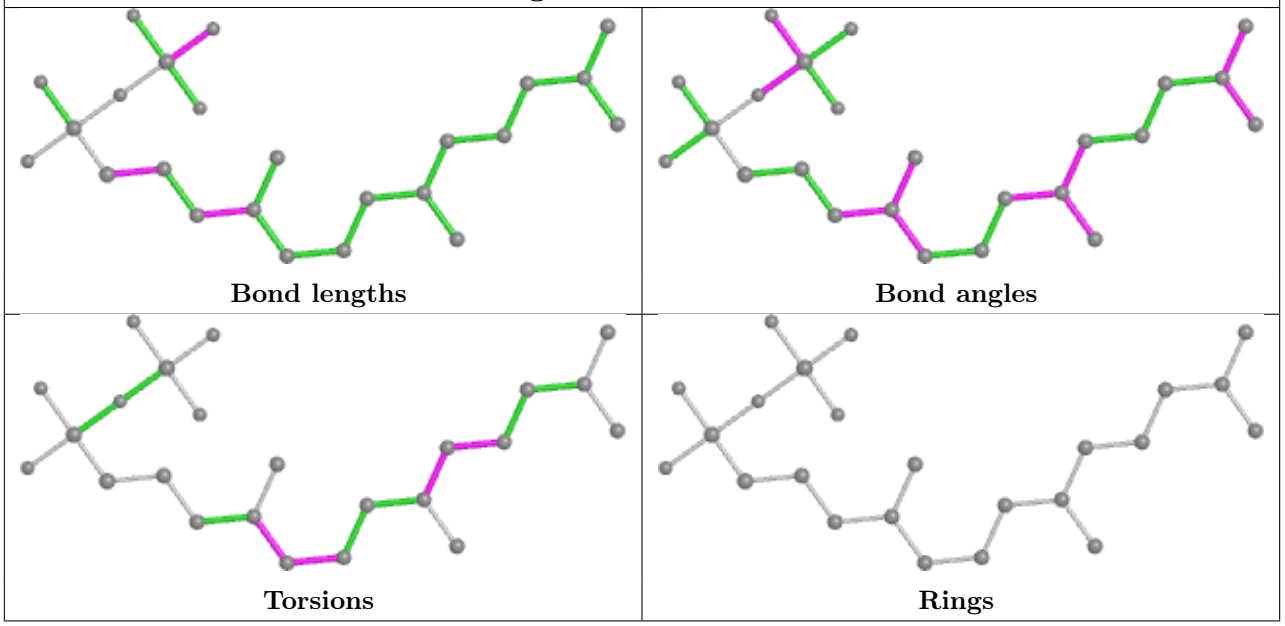
5 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	FPS	3	0
2	C	401	FPS	4	0
2	C	402	FPS	3	0
2	A	501	FPS	3	0
2	B	401	FPS	3	0

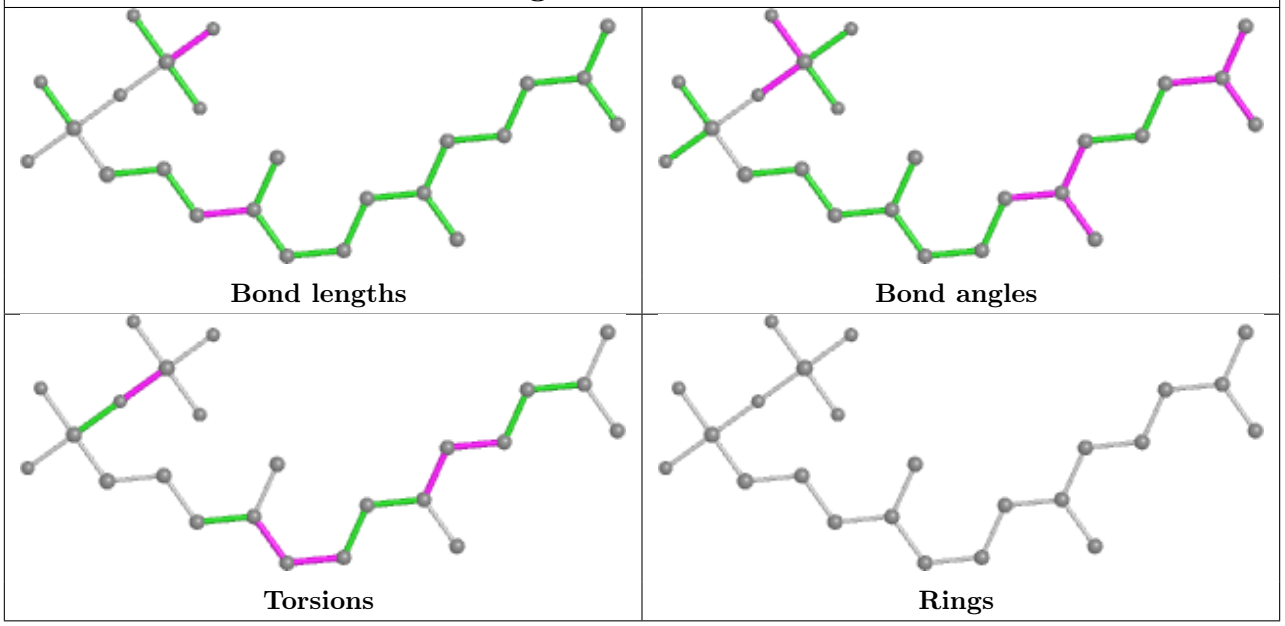
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

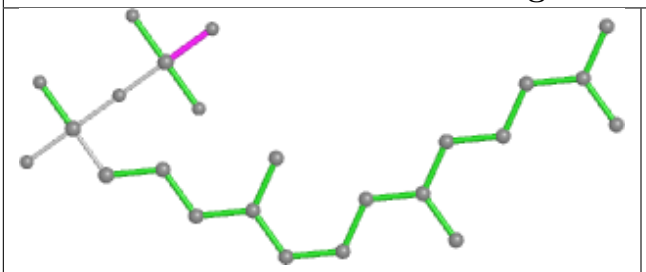
Ligand FPS D 401



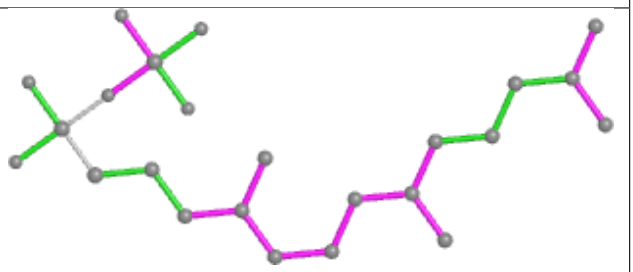
Ligand FPS C 401



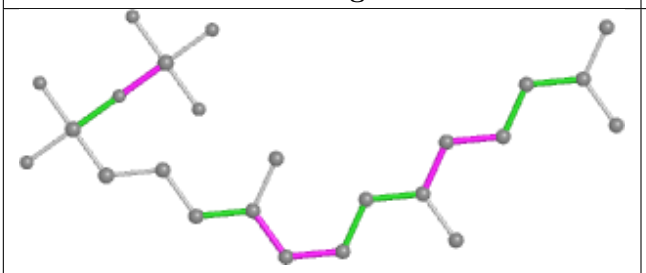
Ligand FPS C 402



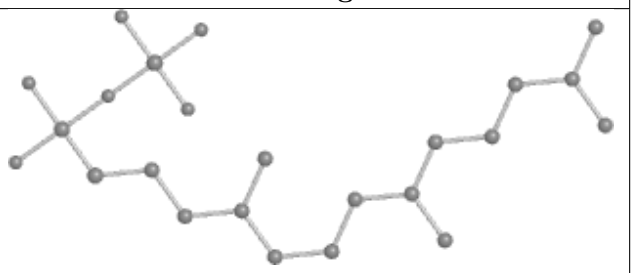
Bond lengths



Bond angles

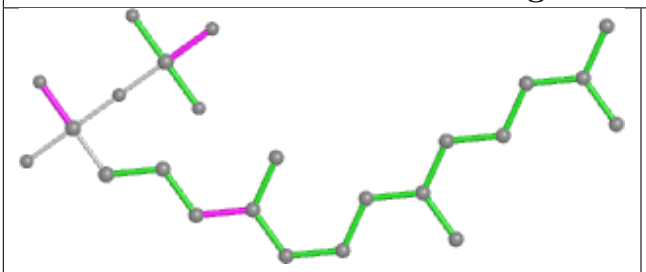


Torsions

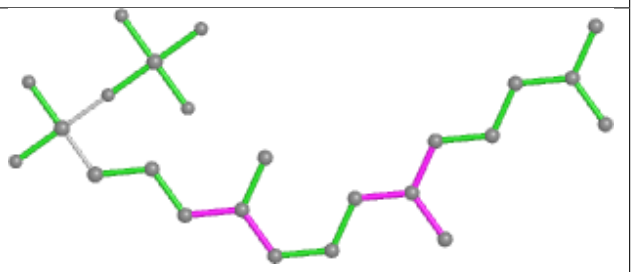


Rings

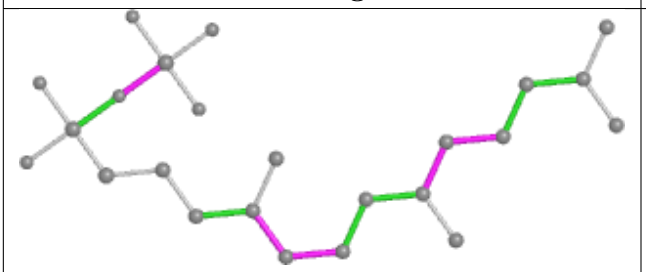
Ligand FPS A 501



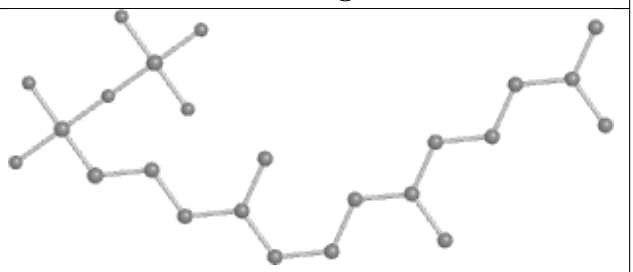
Bond lengths



Bond angles

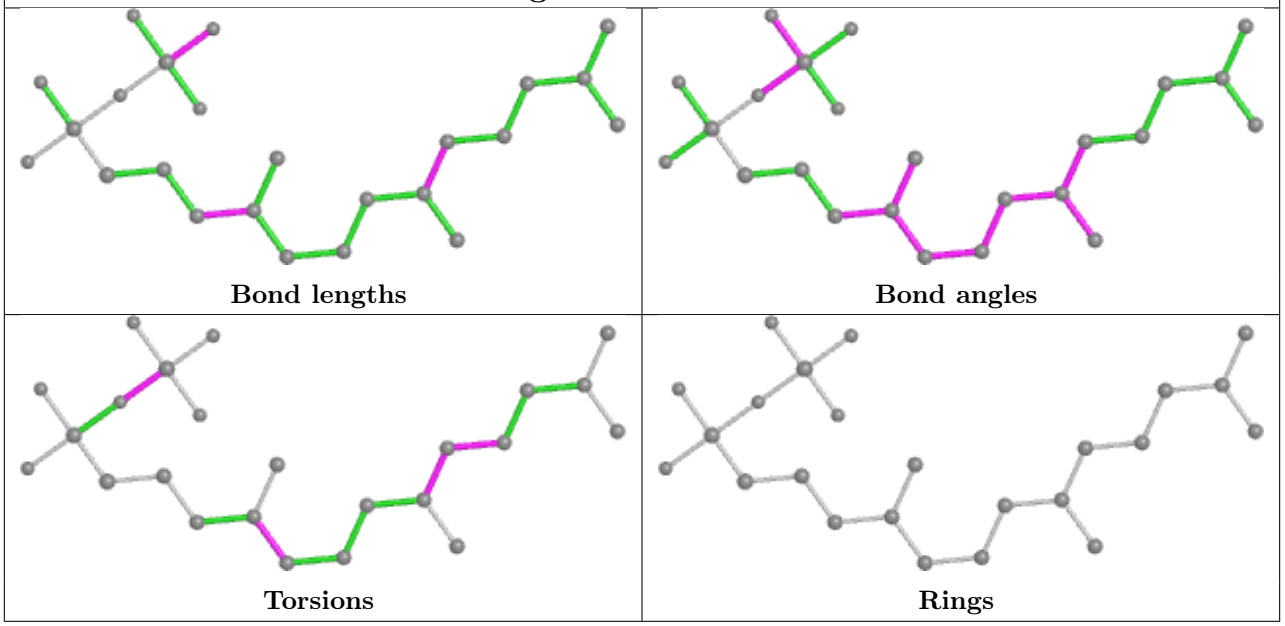


Torsions



Rings

Ligand FPS B 401



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

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

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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