Full wwPDB EM Validation Report ⓘ

Oct 8, 2023 – 12:42 AM JST

PDB ID	:	8JD6
EMDB ID	:	EMD-36177
Title	:	Cryo-EM structure of Gi1-bound metabotropic glutamate receptor mGlu4
Authors	:	Wang, X.; Wang, M.; Xu, T.; Feng, Y.; Han, S.; Lin, S.; Zhao, Q.; Wu, B.
Deposited on	:	2023-05-12
Resolution	:	3.40 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:

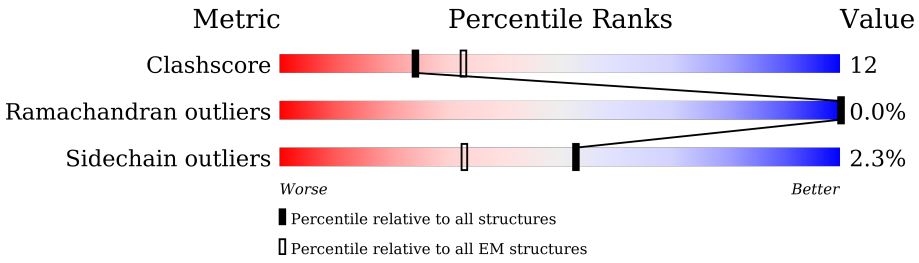
EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.40 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=5%

Mol	Chain	Length	Quality of chain
1	R	890	64% 22% 13%
1	S	890	65% 20% 14%
2	D	257	52% 37% • 10%
3	C	71	25% • 73%
4	B	351	60% 26% 14%
5	A	354	51% 12% 37%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 17192 atoms, of which 0 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 Metabotropic glutamate receptor 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	S	761	Total	C	N	O	S	0	0
			5700	3642	980	1039	39		
1	R	774	Total	C	N	O	S	0	0
			5779	3693	996	1053	37		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	23	ASP	-	expression tag	UNP Q14833
S	24	TYR	-	expression tag	UNP Q14833
S	25	LYS	-	expression tag	UNP Q14833
S	26	ASP	-	expression tag	UNP Q14833
S	27	ASP	-	expression tag	UNP Q14833
S	28	ASP	-	expression tag	UNP Q14833
S	29	ASP	-	expression tag	UNP Q14833
S	30	GLY	-	expression tag	UNP Q14833
S	31	ALA	-	expression tag	UNP Q14833
S	32	PRO	-	expression tag	UNP Q14833
R	23	ASP	-	expression tag	UNP Q14833
R	24	TYR	-	expression tag	UNP Q14833
R	25	LYS	-	expression tag	UNP Q14833
R	26	ASP	-	expression tag	UNP Q14833
R	27	ASP	-	expression tag	UNP Q14833
R	28	ASP	-	expression tag	UNP Q14833
R	29	ASP	-	expression tag	UNP Q14833
R	30	GLY	-	expression tag	UNP Q14833
R	31	ALA	-	expression tag	UNP Q14833
R	32	PRO	-	expression tag	UNP Q14833

- Molecule 2 is a protein called scFv.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	232	Total	C	N	O	S	0	0
			1730	1103	291	328	8		

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	19	Total	C	N	O	S	0	0
			114	69	19	25	1		

- Molecule 4 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	301	Total	C	N	O	S	0	0
			2188	1368	376	426	18		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-10	MET	-	initiating methionine	UNP P62873
B	-9	HIS	-	expression tag	UNP P62873
B	-8	HIS	-	expression tag	UNP P62873
B	-7	HIS	-	expression tag	UNP P62873
B	-6	HIS	-	expression tag	UNP P62873
B	-5	HIS	-	expression tag	UNP P62873
B	-4	HIS	-	expression tag	UNP P62873
B	-3	GLY	-	expression tag	UNP P62873
B	-2	SER	-	expression tag	UNP P62873
B	-1	LEU	-	expression tag	UNP P62873
B	0	LEU	-	expression tag	UNP P62873
B	1	GLN	-	expression tag	UNP P62873

- Molecule 5 is a protein called Guanine nucleotide-binding protein G(i) subunit alpha-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	223	Total	C	N	O	S	0	0
			1643	1048	272	312	11		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	47	ASN	SER	conflict	UNP P08754

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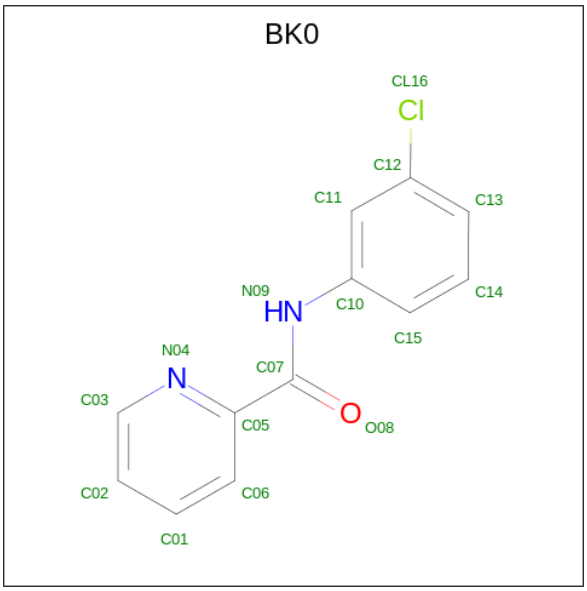
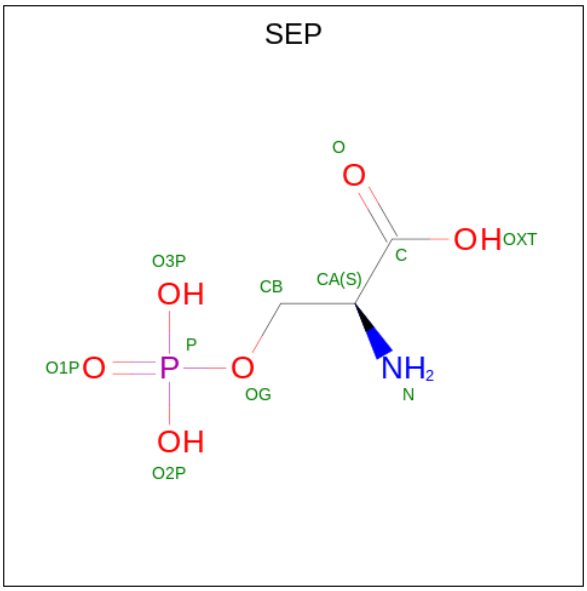
Chain	Residue	Modelled	Actual	Comment	Reference
A	191	ASP	PHE	conflict	UNP P08754
A	203	ALA	GLY	conflict	UNP P08754
A	245	ALA	GLU	conflict	UNP P08754
A	326	SER	ALA	conflict	UNP P08754

- Molecule 6 is N-(3-chlorophenyl)pyridine-2-carboxamide (three-letter code: BK0) (formula: $C_{12}H_9ClN_2O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
6	S	1	Total	C	Cl	N	O	0
			16	12	1	2	1	

- Molecule 7 is PHOSPHOSERINE (three-letter code: SEP) (formula: $C_3H_8NO_6P$) (labeled as "Ligand of Interest" by depositor).



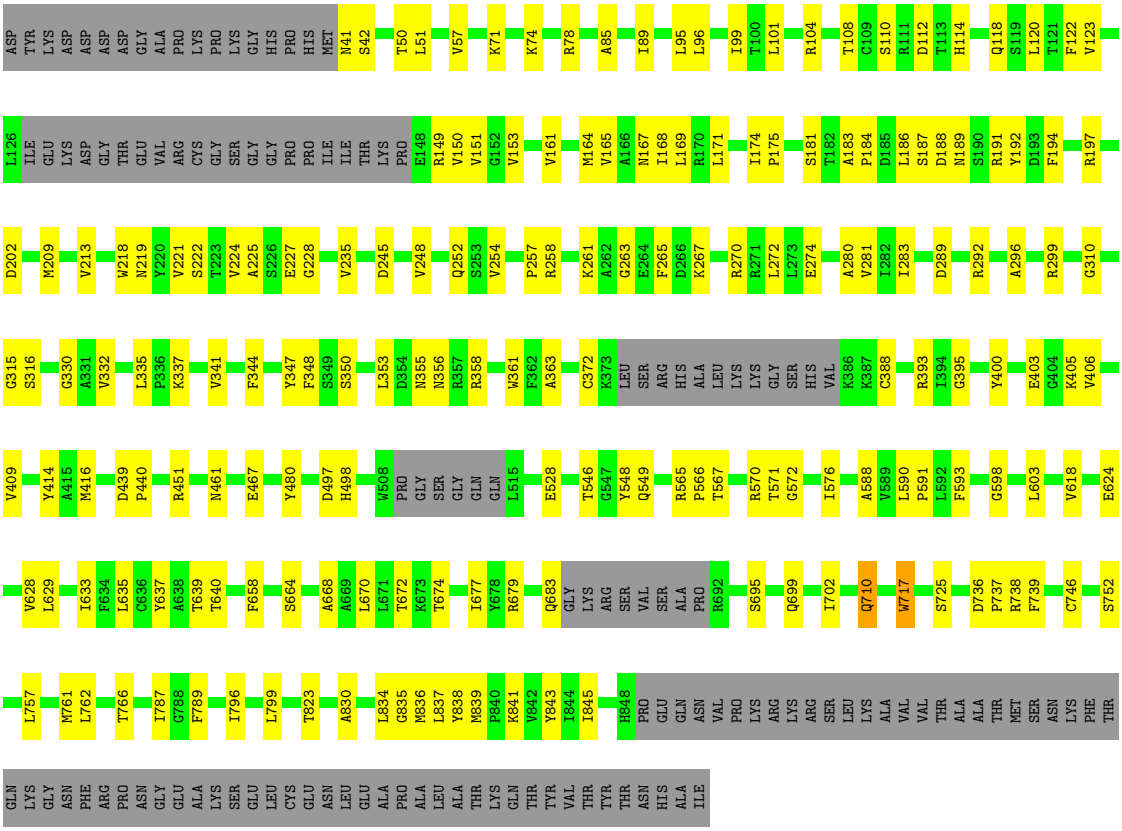
Mol	Chain	Residues	Atoms					AltConf
7	S	1	Total	C	N	O	P	0
			11	3	1	6	1	
7	R	1	Total	C	N	O	P	0
			11	3	1	6	1	

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.

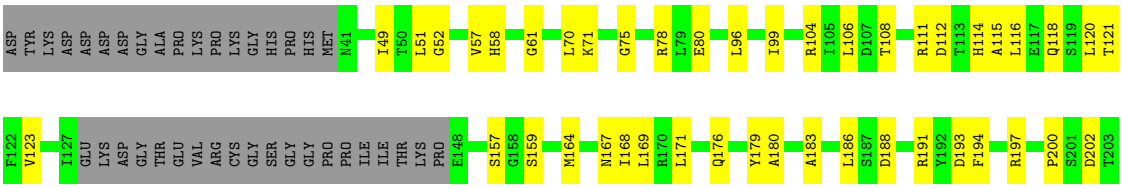
• Molecule 1: Metabotropic glutamate receptor 4

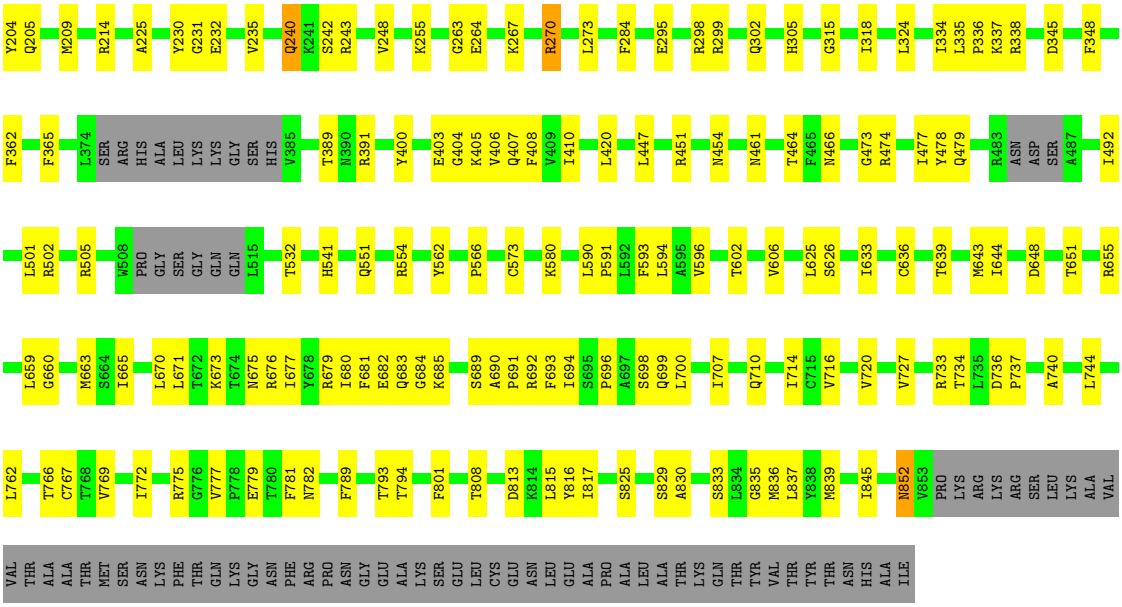
Chain S:



• Molecule 1: Metabotropic glutamate receptor 4

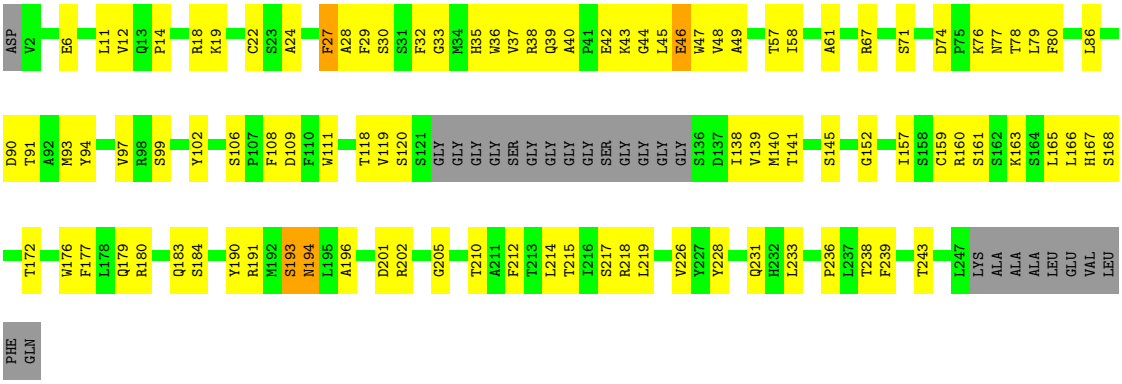
Chain R:





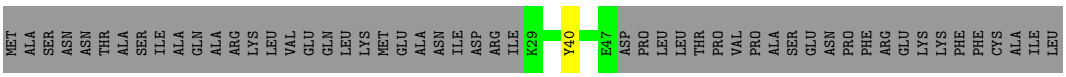
• Molecule 2: scFv

Chain D:



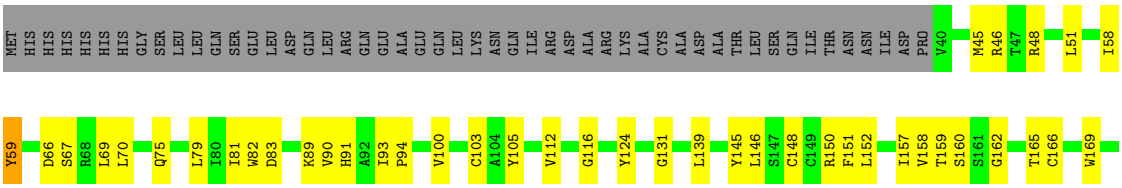
• Molecule 3: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2

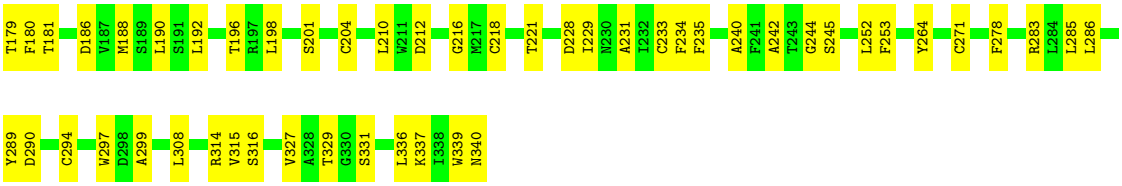
Chain C:



• Molecule 4: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1

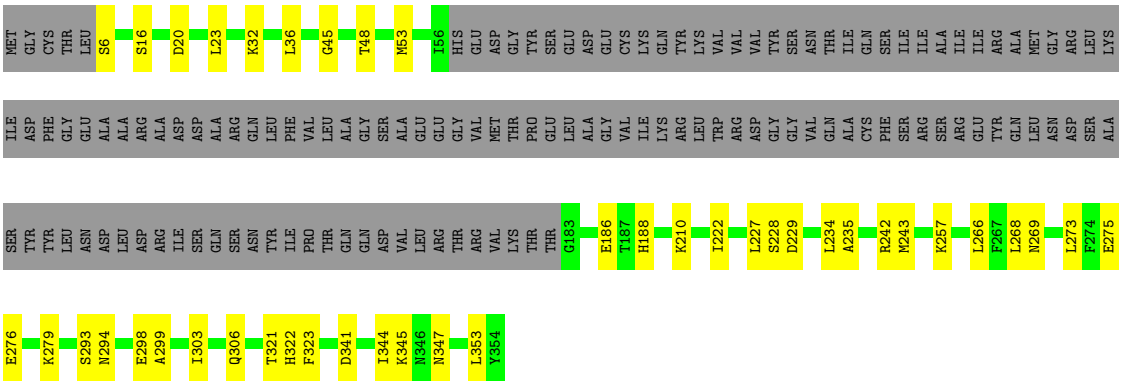
Chain B:





• Molecule 5: Guanine nucleotide-binding protein G(i) subunit alpha-3

Chain A:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	839200	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	70	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SEP, BK0

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	R	0.27	0/5908	0.49	0/8052
1	S	0.25	0/5828	0.48	0/7939
2	D	0.28	0/1773	0.53	0/2412
3	C	0.24	0/114	0.46	0/156
4	B	0.24	0/2233	0.49	0/3046
5	A	0.24	0/1671	0.45	0/2269
All	All	0.26	0/17527	0.49	0/23874

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

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	R	5779	0	5510	139	0
1	S	5700	0	5446	116	0
2	D	1730	0	1638	74	0
3	C	114	0	83	0	0
4	B	2188	0	2014	61	0
5	A	1643	0	1502	29	0
6	S	16	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	R	11	0	5	2	0
7	S	11	0	5	0	0
All	All	17192	0	16203	398	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 12.

All (398) 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:R:833:SER:O	1:R:837:LEU:HB2	1.81	0.80
4:B:204:CYS:HB2	4:B:228:ASP:HB3	1.64	0.80
1:S:184:PRO:HD3	1:S:202:ASP:HB2	1.66	0.78
4:B:315:VAL:HG22	4:B:331:SER:OG	1.85	0.77
2:D:39:GLN:HA	2:D:45:LEU:HA	1.69	0.73
1:R:643:MET:HA	1:R:655:ARG:HE	1.54	0.73
2:D:78:THR:HG22	2:D:79:LEU:H	1.53	0.73
2:D:157:ILE:HD13	2:D:243:THR:HG21	1.72	0.71
1:S:169:LEU:HD22	1:S:174:ILE:HD11	1.73	0.71
1:S:835:GLY:HA2	1:S:839:MET:HG2	1.71	0.71
2:D:145:SER:HB2	2:D:243:THR:HA	1.72	0.70
1:S:717:TRP:HH2	1:S:752:SER:HA	1.55	0.70
1:S:316:SER:H	1:S:335:LEU:HD22	1.59	0.67
4:B:160:SER:HB3	4:B:190:LEU:HD11	1.77	0.66
1:S:191:ARG:NH1	1:S:192:TYR:OH	2.28	0.65
1:R:159:SER:HB2	1:R:230:TYR:HB2	1.78	0.65
4:B:45:MET:HB2	4:B:339:TRP:HE1	1.61	0.64
1:S:171:LEU:HB3	1:R:120:LEU:HD22	1.78	0.64
5:A:276:GLU:N	5:A:276:GLU:OE1	2.30	0.64
1:R:263:GLY:O	1:R:267:LYS:NZ	2.30	0.64
2:D:190:TYR:HD2	2:D:196:ALA:HB2	1.62	0.64
1:S:670:LEU:HD21	1:S:787:ILE:HG23	1.80	0.63
2:D:71:SER:HB3	2:D:80:PHE:HB2	1.80	0.63
2:D:176:TRP:HE1	2:D:214:LEU:HG	1.64	0.63
2:D:11:LEU:HD13	2:D:118:THR:HB	1.80	0.63
2:D:38:ARG:N	2:D:46:GLU:O	2.29	0.63
1:S:187:SER:OG	1:S:197:ARG:NH2	2.31	0.62
1:R:479:GLN:HB2	1:R:492:ILE:HD13	1.81	0.62
1:R:447:LEU:O	1:R:451:ARG:HG2	1.98	0.62
1:R:671:LEU:HB2	1:R:767:CYS:SG	2.39	0.62
4:B:294:CYS:HB2	4:B:308:LEU:HB2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:834:LEU:HD12	1:S:838:TYR:HD2	1.65	0.61
1:S:757:LEU:O	1:S:761:MET:HG2	2.00	0.61
1:R:681:PHE:HA	5:A:344:ILE:HD12	1.83	0.61
1:S:96:LEU:HB3	1:S:99:ILE:HB	1.84	0.60
1:R:673:LYS:O	1:R:677:ILE:HG12	2.01	0.60
4:B:229:ILE:HA	4:B:245:SER:HA	1.83	0.60
1:R:405:LYS:NZ	7:R:1001:SEP:O2P	2.34	0.60
1:R:684:GLY:HA3	5:A:344:ILE:CD1	2.31	0.60
1:R:447:LEU:HD22	1:R:451:ARG:HE	1.67	0.60
1:S:635:LEU:O	1:S:639:THR:HG23	2.02	0.60
2:D:161:SER:HB3	2:D:210:THR:HA	1.83	0.60
1:S:225:ALA:HB2	1:S:235:VAL:HG11	1.82	0.60
1:R:551:GLN:HE21	1:R:554:ARG:HA	1.66	0.59
1:R:193:ASP:O	1:R:451:ARG:NH2	2.35	0.59
1:R:52:GLY:HA2	1:R:104:ARG:HB3	1.83	0.59
2:D:67:ARG:NH2	2:D:90:ASP:OD2	2.35	0.59
1:S:221:VAL:HG12	1:S:280:ALA:HB3	1.85	0.59
2:D:179:GLN:NE2	2:D:183:GLN:O	2.35	0.59
1:R:270:ARG:HA	1:R:273:LEU:HB2	1.84	0.59
1:R:684:GLY:HA3	5:A:344:ILE:HD13	1.83	0.59
2:D:6:GLU:HG2	2:D:22:CYS:HB3	1.85	0.59
2:D:91:THR:HG22	2:D:119:VAL:HB	1.84	0.59
1:S:350:SER:O	1:S:355:ASN:ND2	2.36	0.59
1:R:660:GLY:O	1:R:710:GLN:NE2	2.36	0.58
1:R:762:LEU:O	1:R:766:THR:HG23	2.03	0.58
5:A:228:SER:HB2	5:A:273:LEU:HD22	1.85	0.58
1:R:772:ILE:O	1:R:775:ARG:NH1	2.36	0.58
1:S:51:LEU:HD21	1:S:416:MET:HG2	1.85	0.58
4:B:233:CYS:SG	4:B:234:PHE:N	2.77	0.58
1:S:762:LEU:O	1:S:766:THR:HG23	2.04	0.57
1:R:58:HIS:HA	1:R:70:LEU:HA	1.86	0.57
1:R:202:ASP:OD1	1:R:205:GLN:NE2	2.38	0.57
1:R:675:ASN:O	1:R:679:ARG:HG3	2.05	0.57
1:S:717:TRP:CH2	1:S:752:SER:HA	2.40	0.56
1:S:78:ARG:HH21	1:S:405:LYS:HG3	1.70	0.56
1:R:362:PHE:O	1:R:365:PHE:HB3	2.05	0.56
1:R:665:ILE:HG13	1:R:707:ILE:HD11	1.87	0.56
1:R:693:PHE:HB3	1:R:698:SER:OG	2.04	0.56
4:B:58:ILE:O	4:B:316:SER:OG	2.23	0.56
2:D:14:PRO:HB3	2:D:120:SER:HB2	1.86	0.56
1:R:679:ARG:HB3	1:R:691:PRO:CB	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:86:LEU:HD13	2:D:119:VAL:HG13	1.87	0.56
1:S:330:GLY:HA2	1:S:480:TYR:O	2.05	0.56
2:D:193:SER:OG	2:D:205:GLY:O	2.22	0.56
1:S:51:LEU:HD13	1:S:101:LEU:HD23	1.87	0.56
5:A:48:THR:OG1	5:A:269:ASN:ND2	2.39	0.56
1:S:633:ILE:HG23	1:S:830:ALA:HB1	1.88	0.55
1:S:639:THR:HG22	1:S:658:PHE:HB3	1.88	0.55
1:R:502:ARG:HG3	1:R:505:ARG:HH21	1.70	0.55
2:D:42:GLU:HG2	2:D:43:LYS:H	1.71	0.55
1:R:682:GLU:HA	1:R:685:LYS:HD3	1.87	0.55
2:D:24:ALA:HB1	2:D:27:PHE:HE1	1.71	0.55
1:R:335:LEU:HB3	1:R:478:TYR:HE2	1.72	0.55
1:R:108:THR:HG23	1:R:115:ALA:HB2	1.89	0.55
2:D:48:VAL:HA	2:D:61:ALA:HB2	1.87	0.55
1:R:602:THR:O	1:R:606:VAL:HG22	2.07	0.55
4:B:283:ARG:HA	4:B:299:ALA:HB2	1.89	0.55
1:R:683:GLN:HB3	1:R:691:PRO:HG3	1.89	0.55
1:S:267:LYS:HA	1:S:270:ARG:NH1	2.22	0.54
4:B:145:TYR:OH	4:B:188:MET:SD	2.64	0.54
4:B:186:ASP:OD2	4:B:186:ASP:N	2.40	0.54
1:S:222:SER:HB3	1:S:281:VAL:HG22	1.90	0.54
1:R:677:ILE:HD12	5:A:353:LEU:HD21	1.88	0.54
2:D:180:ARG:NH2	2:D:184:SER:O	2.40	0.54
1:R:679:ARG:HH21	1:R:694:ILE:HG22	1.71	0.54
2:D:179:GLN:HB3	2:D:226:VAL:HG12	1.89	0.54
1:S:191:ARG:NH2	1:R:112:ASP:OD2	2.40	0.54
1:S:347:TYR:OH	1:S:358:ARG:NH2	2.40	0.54
1:S:837:LEU:O	1:S:841:LYS:NZ	2.37	0.54
1:R:205:GLN:O	1:R:209:MET:HG3	2.08	0.54
1:R:337:LYS:HG3	1:R:474:ARG:HB3	1.88	0.54
1:S:227:GLU:HB2	1:S:258:ARG:HG3	1.89	0.54
1:R:169:LEU:HD23	1:R:176:GLN:HB2	1.89	0.54
1:S:546:THR:HG22	1:S:549:GLN:HG2	1.90	0.53
2:D:39:GLN:HB2	2:D:45:LEU:HD13	1.90	0.53
1:R:267:LYS:HG3	1:R:270:ARG:NH2	2.23	0.53
1:R:336:PRO:HB2	1:R:408:PHE:CZ	2.44	0.53
4:B:59:TYR:HE1	4:B:75:GLN:HG3	1.74	0.53
4:B:289:TYR:HE1	4:B:297:TRP:HH2	1.56	0.53
1:R:114:HIS:O	1:R:118:GLN:HG2	2.08	0.53
1:R:562:TYR:HE1	1:R:733:ARG:HH21	1.56	0.53
1:R:625:LEU:O	1:R:673:LYS:HD3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:734:THR:OG1	1:R:740:ALA:O	2.27	0.53
2:D:38:ARG:O	2:D:46:GLU:N	2.35	0.52
5:A:266:LEU:HD23	5:A:321:THR:HG22	1.92	0.52
1:S:112:ASP:HA	1:S:161:VAL:HG22	1.91	0.52
1:S:175:PRO:HA	1:S:194:PHE:HB3	1.90	0.52
1:S:567:THR:HG22	1:S:572:GLY:H	1.74	0.52
1:R:696:PRO:O	1:R:700:LEU:HG	2.09	0.52
4:B:93:ILE:HD12	4:B:94:PRO:HD2	1.91	0.52
1:R:183:ALA:O	1:R:197:ARG:NH2	2.33	0.52
4:B:70:LEU:O	4:B:82:TRP:N	2.34	0.52
2:D:177:PHE:HB2	2:D:228:TYR:HB2	1.91	0.52
5:A:268:LEU:HB2	5:A:323:PHE:HA	1.91	0.52
4:B:242:ALA:HA	4:B:252:LEU:HA	1.92	0.52
4:B:51:LEU:N	4:B:336:LEU:O	2.36	0.52
1:R:680:ILE:HG23	5:A:347:ASN:HB2	1.91	0.52
5:A:186:GLU:OE2	5:A:188:HIS:NE2	2.43	0.51
1:S:588:ALA:C	1:S:591:PRO:HD2	2.31	0.51
4:B:83:ASP:N	4:B:83:ASP:OD1	2.44	0.51
4:B:46:ARG:H	4:B:339:TRP:HD1	1.59	0.51
1:R:643:MET:HG2	1:R:655:ARG:HD3	1.93	0.51
1:S:330:GLY:CA	1:S:480:TYR:O	2.58	0.51
1:R:49:ILE:HD13	1:R:420:LEU:HD13	1.93	0.51
4:B:218:CYS:SG	4:B:221:THR:OG1	2.69	0.51
2:D:28:ALA:O	2:D:29:PHE:HB3	2.11	0.50
1:S:618:VAL:HB	1:S:841:LYS:HD3	1.93	0.50
2:D:152:GLY:H	2:D:219:LEU:HB3	1.77	0.50
2:D:165:LEU:HA	2:D:233:LEU:HD11	1.93	0.50
4:B:148:CYS:SG	4:B:190:LEU:N	2.80	0.50
2:D:30:SER:HA	2:D:74:ASP:OD2	2.12	0.50
1:S:565:ARG:HG2	1:S:576:ILE:HG12	1.93	0.50
1:R:157:SER:HA	1:R:180:ALA:HB3	1.94	0.50
1:R:231:GLY:HA2	1:R:284:PHE:HB3	1.93	0.50
4:B:103:CYS:O	4:B:150:ARG:NH1	2.37	0.50
1:S:164:MET:HA	1:S:167:ASN:HD21	1.74	0.50
1:R:590:LEU:HD12	1:R:594:LEU:HD13	1.92	0.50
1:R:694:ILE:HA	1:R:699:GLN:NE2	2.27	0.50
1:R:727:VAL:HG13	1:R:744:LEU:HD13	1.93	0.50
1:R:676:ARG:HA	1:R:679:ARG:CZ	2.41	0.50
1:R:200:PRO:HB3	1:R:473:GLY:HA2	1.93	0.49
1:R:61:GLY:O	1:R:111:ARG:NH2	2.45	0.49
1:R:779:GLU:HA	1:R:782:ASN:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:341:VAL:HB	1:S:344:PHE:HB3	1.93	0.49
1:S:567:THR:HG22	1:S:571:THR:H	1.77	0.49
1:R:659:LEU:O	1:R:663:MET:HG2	2.12	0.49
1:R:78:ARG:HH11	1:R:179:TYR:HE1	1.60	0.49
1:S:668:ALA:O	1:S:672:THR:HG23	2.13	0.49
4:B:145:TYR:O	4:B:162:GLY:N	2.46	0.49
2:D:76:LYS:C	2:D:78:THR:H	2.16	0.49
1:S:149:ARG:HH12	1:S:151:VAL:HG12	1.78	0.49
2:D:40:ALA:N	2:D:44:GLY:O	2.30	0.49
4:B:190:LEU:HD22	4:B:201:SER:HA	1.95	0.49
1:S:219:ASN:HA	1:S:248:VAL:HG13	1.93	0.49
2:D:138:ILE:O	2:D:140:MET:N	2.46	0.49
1:S:261:LYS:O	1:S:263:GLY:N	2.42	0.48
1:S:679:ARG:O	1:S:683:GLN:NE2	2.43	0.48
4:B:166:CYS:HB2	4:B:180:PHE:HB2	1.94	0.48
1:R:295:GLU:HG2	1:R:299:ARG:HE	1.78	0.48
2:D:141:THR:H	2:D:160:ARG:HH21	1.61	0.48
1:R:116:LEU:HD13	1:R:164:MET:HG3	1.95	0.48
1:R:240:GLN:OE1	1:R:243:ARG:NH2	2.46	0.48
1:S:796:ILE:HG21	1:R:793:THR:HG23	1.95	0.48
1:S:629:LEU:O	1:S:633:ILE:HG12	2.13	0.48
1:R:845:ILE:HG23	1:R:852:ASN:HD21	1.79	0.48
1:S:96:LEU:HD12	1:S:101:LEU:HD11	1.96	0.48
5:A:229:ASP:HB2	5:A:242:ARG:HD2	1.95	0.48
5:A:293:SER:OG	5:A:294:ASN:N	2.47	0.48
1:R:345:ASP:OD1	1:R:400:TYR:OH	2.29	0.48
1:R:648:ASP:N	1:R:651:THR:OG1	2.47	0.48
4:B:51:LEU:HB2	4:B:336:LEU:HB2	1.94	0.48
5:A:227:LEU:HD11	5:A:303:ILE:HG21	1.96	0.48
1:R:532:THR:O	1:R:541:HIS:HB3	2.12	0.48
1:R:835:GLY:HA2	1:R:839:MET:HG2	1.96	0.48
1:S:843:TYR:OH	1:R:775:ARG:NH2	2.39	0.48
4:B:67:SER:O	4:B:67:SER:OG	2.31	0.48
5:A:293:SER:H	5:A:298:GLU:HG2	1.79	0.47
1:R:625:LEU:HD23	1:R:673:LYS:HG3	1.96	0.47
2:D:233:LEU:O	5:A:6:SER:N	2.48	0.47
4:B:81:ILE:HD12	4:B:91:HIS:HB2	1.96	0.47
4:B:89:LYS:H	5:A:16:SER:HB2	1.78	0.47
4:B:198:LEU:HD21	4:B:210:LEU:HD21	1.96	0.47
4:B:278:PHE:HE1	4:B:285:LEU:HD13	1.79	0.47
1:R:580:LYS:HA	1:R:815:LEU:HD21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:231:ALA:HB3	4:B:244:GLY:HA3	1.97	0.47
5:A:45:GLY:HA3	5:A:269:ASN:HD22	1.80	0.47
1:S:168:ILE:HD11	1:R:168:ILE:HG21	1.97	0.47
1:S:209:MET:O	1:S:213:VAL:HG22	2.14	0.47
1:R:106:LEU:HD12	1:R:118:GLN:HB3	1.95	0.47
1:R:676:ARG:O	1:R:680:ILE:HG13	2.14	0.47
2:D:35:HIS:HB2	2:D:97:VAL:HB	1.96	0.47
2:D:172:THR:HG21	2:D:212:PHE:CZ	2.50	0.47
2:D:190:TYR:CD2	2:D:196:ALA:HB2	2.47	0.47
2:D:37:VAL:HA	2:D:47:TRP:HA	1.97	0.47
2:D:58:ILE:O	2:D:58:ILE:HG22	2.15	0.47
5:A:36:LEU:HD12	5:A:222:ILE:HG13	1.97	0.47
1:S:393:ARG:HG3	1:S:395:GLY:H	1.80	0.47
4:B:235:PHE:HB2	4:B:240:ALA:HB3	1.96	0.47
1:R:336:PRO:HB2	1:R:408:PHE:HZ	1.80	0.47
4:B:66:ASP:OD1	4:B:66:ASP:N	2.47	0.47
1:S:618:VAL:HG21	1:S:845:ILE:HD11	1.98	0.46
1:R:242:SER:HB2	1:R:248:VAL:HB	1.96	0.46
1:R:590:LEU:HB3	1:R:591:PRO:HD3	1.98	0.46
1:S:228:GLY:HA2	1:S:258:ARG:HH21	1.81	0.46
1:S:672:THR:HB	1:S:699:GLN:HB3	1.96	0.46
1:S:315:GLY:HA3	1:S:335:LEU:HD13	1.96	0.46
1:S:737:PRO:HB2	1:S:739:PHE:CD1	2.50	0.46
2:D:29:PHE:HA	2:D:32:PHE:HB2	1.98	0.46
2:D:47:TRP:NE1	2:D:49:ALA:O	2.49	0.46
4:B:158:VAL:HG11	4:B:192:LEU:HD21	1.96	0.46
4:B:235:PHE:HA	4:B:278:PHE:HD2	1.81	0.46
1:S:171:LEU:HD21	1:R:116:LEU:HD23	1.97	0.46
1:R:232:GLU:HG2	1:R:255:LYS:HD2	1.98	0.46
2:D:190:TYR:CE2	2:D:194:ASN:HB2	2.50	0.46
1:R:813:ASP:HB3	1:R:816:TYR:HB2	1.97	0.46
4:B:290:ASP:OD2	4:B:314:ARG:NH1	2.49	0.46
4:B:180:PHE:HE1	4:B:216:GLY:HA2	1.81	0.46
5:A:275:GLU:O	5:A:279:LYS:HE3	2.16	0.45
1:S:497:ASP:OD1	1:S:498:HIS:ND1	2.44	0.45
2:D:141:THR:H	2:D:160:ARG:NH2	2.14	0.45
1:R:461:ASN:HD22	1:R:474:ARG:NH2	2.14	0.45
1:R:225:ALA:HB2	1:R:235:VAL:HG11	1.99	0.45
1:R:670:LEU:HD12	1:R:837:LEU:HD11	1.98	0.45
1:R:681:PHE:O	1:R:685:LYS:HG3	2.17	0.45
5:A:341:ASP:OD1	5:A:345:LYS:NZ	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:406:VAL:O	1:R:410:ILE:HG12	2.17	0.45
1:R:302:GLN:HG3	1:R:305:HIS:HB3	1.99	0.45
4:B:327:VAL:N	4:B:339:TRP:O	2.41	0.45
1:S:296:ALA:HA	1:S:299:ARG:HE	1.81	0.45
1:S:674:THR:HA	1:S:677:ILE:HG12	1.99	0.45
1:S:695:SER:O	1:S:699:GLN:HG2	2.16	0.45
1:R:188:ASP:HB3	1:R:191:ARG:HB2	1.98	0.45
1:S:164:MET:HA	1:S:167:ASN:ND2	2.32	0.45
1:R:777:VAL:HG11	1:R:781:PHE:HB2	1.99	0.45
4:B:89:LYS:NZ	5:A:20:ASP:OD1	2.49	0.45
1:R:167:ASN:OD1	1:R:168:ILE:N	2.50	0.45
1:R:298:ARG:HE	1:R:324:LEU:HD23	1.82	0.45
2:D:29:PHE:CE1	2:D:74:ASP:HA	2.52	0.45
4:B:89:LYS:HE2	5:A:23:LEU:HD22	1.98	0.45
2:D:86:LEU:HD23	2:D:86:LEU:HA	1.88	0.45
1:S:356:ASN:OD1	1:S:356:ASN:N	2.50	0.44
1:S:640:THR:HA	1:S:823:THR:HG23	1.99	0.44
1:S:789:PHE:HB3	1:R:789:PHE:HZ	1.81	0.44
1:R:405:LYS:HD3	1:R:408:PHE:HD2	1.82	0.44
1:S:114:HIS:O	1:S:118:GLN:HG2	2.17	0.44
1:R:794:THR:HG23	1:R:829:SER:HB2	1.99	0.44
2:D:152:GLY:H	2:D:219:LEU:HD23	1.82	0.44
4:B:152:LEU:HD22	4:B:196:THR:HG23	1.98	0.44
1:S:725:SER:HA	1:S:746:CYS:HA	1.98	0.44
1:R:766:THR:HA	1:R:769:VAL:HG12	1.99	0.44
2:D:33:GLY:N	2:D:99:SER:O	2.50	0.44
2:D:102:TYR:HB2	4:B:90:VAL:HG23	1.99	0.44
2:D:191:ARG:O	2:D:194:ASN:ND2	2.51	0.44
1:S:50:THR:O	1:S:150:VAL:HA	2.17	0.44
1:S:89:ILE:HD11	1:S:101:LEU:HD22	1.98	0.44
1:R:57:VAL:O	1:R:71:LYS:N	2.44	0.44
1:R:193:ASP:OD1	1:R:193:ASP:N	2.50	0.44
1:S:171:LEU:HD11	1:R:116:LEU:HG	1.99	0.44
1:R:80:GLU:HG3	1:R:348:PHE:CE1	2.52	0.44
2:D:36:TRP:HZ3	2:D:94:TYR:HB3	1.82	0.44
1:S:245:ASP:OD1	1:S:245:ASP:N	2.49	0.44
1:S:461:ASN:OD1	1:S:461:ASN:N	2.51	0.44
1:R:51:LEU:O	1:R:104:ARG:HB3	2.17	0.44
2:D:24:ALA:HB1	2:D:27:PHE:CE1	2.50	0.44
1:S:598:GLY:HA3	1:S:637:TYR:CZ	2.52	0.44
1:R:636:CYS:O	1:R:639:THR:HG22	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:217:SER:HB3	2:D:218:ARG:NH2	2.33	0.44
1:S:213:VAL:HG12	1:S:218:TRP:HE3	1.83	0.44
1:S:439:ASP:HB3	1:S:440:PRO:HD3	2.00	0.44
2:D:231:GLN:NE2	2:D:236:PRO:O	2.51	0.44
5:A:299:ALA:O	5:A:303:ILE:HG12	2.18	0.44
1:R:389:THR:HG23	1:R:391:ARG:H	1.82	0.43
1:R:403:GLU:HB3	1:R:406:VAL:HG23	2.00	0.43
1:R:801:PHE:HB2	1:R:825:SER:OG	2.18	0.43
2:D:138:ILE:HD11	2:D:163:LYS:HE2	2.00	0.43
1:R:318:ILE:HD13	1:R:318:ILE:HA	1.90	0.43
1:R:736:ASP:HB2	1:R:737:PRO:HD3	2.00	0.43
2:D:57:THR:O	2:D:58:ILE:HD13	2.18	0.43
2:D:166:LEU:HD23	2:D:168:SER:H	1.83	0.43
2:D:176:TRP:NE1	2:D:214:LEU:HG	2.30	0.43
1:S:108:THR:HG22	1:S:110:SER:H	1.84	0.43
2:D:205:GLY:HA2	2:D:215:THR:HG23	2.00	0.43
2:D:76:LYS:HG3	2:D:78:THR:OG1	2.19	0.43
2:D:106:SER:OG	2:D:109:ASP:OD1	2.28	0.43
4:B:329:THR:HB	4:B:339:TRP:CZ3	2.53	0.43
1:S:224:VAL:HG22	1:S:254:VAL:HB	2.01	0.43
1:R:808:THR:HG21	1:R:817:ILE:HD13	2.01	0.43
2:D:29:PHE:H	2:D:32:PHE:HD1	1.66	0.43
5:A:53:MET:SD	5:A:53:MET:N	2.76	0.43
1:S:664:SER:HB3	1:S:710:GLN:CD	2.39	0.43
1:R:264:GLU:HA	1:R:267:LYS:HE2	2.00	0.43
1:R:644:ILE:HD13	1:R:644:ILE:HA	1.88	0.43
4:B:139:LEU:HD13	4:B:169:TRP:CG	2.54	0.43
4:B:159:THR:HB	4:B:169:TRP:CD1	2.54	0.43
1:S:89:ILE:HB	1:S:95:LEU:HD23	2.01	0.42
1:S:181:SER:O	1:S:197:ARG:NH1	2.52	0.42
1:R:334:ILE:HD12	1:R:477:ILE:HG13	2.01	0.42
1:S:403:GLU:HB3	1:S:406:VAL:HG13	2.02	0.42
2:D:215:THR:O	2:D:215:THR:OG1	2.33	0.42
5:A:268:LEU:HD13	5:A:268:LEU:HA	1.86	0.42
1:S:189:ASN:ND2	1:S:467:GLU:O	2.52	0.42
1:S:672:THR:HG22	1:S:702:ILE:HD11	2.01	0.42
1:R:633:ILE:HG23	1:R:830:ALA:HB1	2.00	0.42
2:D:39:GLN:HB3	2:D:93:MET:HB3	2.01	0.42
1:S:799:LEU:HD23	1:S:799:LEU:HA	1.89	0.42
1:R:194:PHE:HA	1:R:447:LEU:HD11	2.01	0.42
1:R:689:SER:O	1:R:690:ALA:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:42:GLU:HG2	2:D:43:LYS:N	2.33	0.42
1:S:153:VAL:HG11	1:S:169:LEU:HD13	2.01	0.42
1:S:252:GLN:NE2	1:S:274:GLU:OE2	2.41	0.42
1:R:651:THR:O	1:R:655:ARG:HG3	2.19	0.42
5:A:303:ILE:HD13	5:A:306:GLN:HE22	1.85	0.42
1:S:224:VAL:HB	1:S:283:ILE:HD13	2.00	0.42
4:B:100:VAL:HA	4:B:116:GLY:HA3	2.00	0.42
1:S:71:LYS:CD	1:S:74:LYS:HZ3	2.33	0.42
1:R:57:VAL:HA	1:R:75:GLY:HA3	2.02	0.42
1:R:684:GLY:HA3	5:A:344:ILE:HD11	2.02	0.42
4:B:152:LEU:HD23	4:B:152:LEU:HA	1.90	0.42
1:S:272:LEU:HD13	1:S:281:VAL:HG21	2.02	0.42
1:S:372:CYS:HB3	1:S:388:CYS:HB3	1.96	0.42
4:B:146:LEU:HD23	4:B:146:LEU:HA	1.94	0.42
1:S:188:ASP:OD1	1:S:188:ASP:N	2.49	0.41
1:R:78:ARG:NH1	1:R:157:SER:OG	2.53	0.41
1:R:593:PHE:HA	1:R:596:VAL:HG12	2.01	0.41
2:D:12:VAL:HG11	2:D:18:ARG:HD3	2.02	0.41
4:B:271:CYS:HB2	4:B:290:ASP:HB3	2.02	0.41
1:S:120:LEU:HD12	1:R:171:LEU:HD23	2.02	0.41
1:R:789:PHE:HB3	1:R:836:MET:CE	2.50	0.41
2:D:28:ALA:C	2:D:30:SER:H	2.23	0.41
2:D:139:VAL:N	2:D:238:THR:HG21	2.35	0.41
4:B:69:LEU:HD23	4:B:83:ASP:HB3	2.01	0.41
1:S:183:ALA:HB3	1:S:186:LEU:HD13	2.01	0.41
1:S:738:ARG:HA	1:S:738:ARG:HD2	1.78	0.41
1:R:566:PRO:HA	1:R:573:CYS:HB3	2.01	0.41
5:A:234:LEU:HB3	5:A:235:ALA:H	1.64	0.41
1:S:120:LEU:HA	1:S:123:VAL:HG22	2.02	0.41
1:S:104:ARG:HG3	1:S:122:PHE:HE1	1.85	0.41
1:S:566:PRO:HA	1:S:572:GLY:O	2.20	0.41
1:R:501:LEU:HD12	1:R:501:LEU:HA	1.94	0.41
1:S:227:GLU:HG2	1:S:257:PRO:HA	2.03	0.41
1:S:265:PHE:CE2	1:S:292:ARG:HB2	2.55	0.41
1:S:337:LYS:HE2	1:S:337:LYS:HB2	1.90	0.41
1:R:96:LEU:HB3	1:R:99:ILE:HB	2.02	0.41
4:B:157:ILE:HB	4:B:169:TRP:HB2	2.03	0.41
1:R:118:GLN:O	1:R:121:THR:OG1	2.28	0.41
1:R:454:ASN:HA	1:R:464:THR:HG22	2.02	0.41
1:R:676:ARG:HB2	1:R:699:GLN:OE1	2.20	0.41
4:B:179:THR:O	4:B:179:THR:OG1	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:165:VAL:O	1:S:169:LEU:HG	2.20	0.41
1:S:189:ASN:HD21	1:S:451:ARG:HH12	1.68	0.41
1:S:310:GLY:N	1:S:332:VAL:O	2.52	0.41
1:R:186:LEU:HB2	1:R:197:ARG:NH2	2.35	0.41
1:R:315:GLY:HA3	1:R:335:LEU:HD13	2.02	0.41
1:R:625:LEU:HD12	1:R:625:LEU:HA	1.91	0.41
1:R:693:PHE:HB3	1:R:698:SER:CB	2.50	0.41
2:D:32:PHE:CZ	4:B:131:GLY:HA3	2.55	0.41
4:B:48:ARG:HG3	4:B:340:ASN:HB3	2.03	0.41
4:B:165:THR:HG22	4:B:181:THR:HG23	2.02	0.41
1:S:353:LEU:HD11	1:S:363:ALA:HA	2.03	0.41
1:S:546:THR:HG23	1:S:548:TYR:H	1.86	0.41
1:S:590:LEU:HB3	1:S:591:PRO:HD3	2.02	0.41
1:R:714:ILE:HD13	1:R:714:ILE:HA	1.88	0.41
4:B:337:LYS:HB2	4:B:339:TRP:CZ3	2.56	0.41
1:S:528:GLU:HA	1:S:570:ARG:HB2	2.03	0.40
1:R:120:LEU:HA	1:R:123:VAL:HG22	2.04	0.40
2:D:42:GLU:O	2:D:43:LYS:HD3	2.21	0.40
2:D:172:THR:HG21	2:D:212:PHE:HZ	1.84	0.40
4:B:315:VAL:CG2	4:B:331:SER:OG	2.64	0.40
4:B:329:THR:HB	4:B:339:TRP:HZ3	1.85	0.40
1:R:716:VAL:O	1:R:720:VAL:HG22	2.21	0.40
2:D:97:VAL:HG11	2:D:108:PHE:CD2	2.56	0.40
1:S:57:VAL:HG11	1:S:361:TRP:CD1	2.57	0.40
1:R:338:ARG:NH1	1:R:404:GLY:HA2	2.37	0.40
1:R:789:PHE:HB3	1:R:836:MET:HE1	2.02	0.40
1:S:41:ASN:HB3	1:S:42:SER:H	1.65	0.40
1:S:85:ALA:O	1:S:89:ILE:HG23	2.22	0.40
1:S:167:ASN:OD1	1:S:168:ILE:N	2.54	0.40
1:S:603:LEU:HD13	1:S:603:LEU:HA	1.97	0.40
1:S:624:GLU:O	1:S:628:VAL:HG13	2.22	0.40
2:D:111:TRP:CZ2	2:D:177:PHE:HE2	2.39	0.40
2:D:201:ASP:O	2:D:202:ARG:HG2	2.21	0.40
1:S:405:LYS:O	1:S:409:VAL:HG23	2.22	0.40
1:R:157:SER:HB3	7:R:1001:SEP:O1P	2.21	0.40
1:R:679:ARG:HB3	1:R:691:PRO:HB3	2.02	0.40
2:D:45:LEU:HD21	2:D:111:TRP:CZ3	2.57	0.40
4:B:112:VAL:HG13	4:B:124:TYR:HD2	1.87	0.40
4:B:289:TYR:CE1	4:B:297:TRP:HH2	2.38	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	R	764/890 (86%)	736 (96%)	27 (4%)	1 (0%)	51 82
1	S	751/890 (84%)	711 (95%)	40 (5%)	0	100 100
2	D	228/257 (89%)	207 (91%)	21 (9%)	0	100 100
3	C	17/71 (24%)	15 (88%)	2 (12%)	0	100 100
4	B	299/351 (85%)	273 (91%)	26 (9%)	0	100 100
5	A	219/354 (62%)	200 (91%)	19 (9%)	0	100 100
All	All	2278/2813 (81%)	2142 (94%)	135 (6%)	1 (0%)	100 100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	R	692	ARG

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 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	R	587/763 (77%)	579 (99%)	8 (1%)	67 83
1	S	582/763 (76%)	573 (98%)	9 (2%)	65 82
2	D	181/207 (87%)	172 (95%)	9 (5%)	24 54
3	C	6/58 (10%)	5 (83%)	1 (17%)	2 8
4	B	220/293 (75%)	212 (96%)	8 (4%)	35 63
5	A	158/310 (51%)	153 (97%)	5 (3%)	39 67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1734/2394 (72%)	1694 (98%)	40 (2%)	53 74

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	S	289	ASP
1	S	348	PHE
1	S	400	TYR
1	S	414	TYR
1	S	593	PHE
1	S	710	GLN
1	S	717	TRP
1	S	736	ASP
1	S	836	MET
1	R	204	TYR
1	R	214	ARG
1	R	240	GLN
1	R	270	ARG
1	R	407	GLN
1	R	466	ASN
1	R	626	SER
1	R	852	ASN
2	D	19	LYS
2	D	27	PHE
2	D	46	GLU
2	D	77	ASN
2	D	159	CYS
2	D	167	HIS
2	D	193	SER
2	D	194	ASN
2	D	239	PHE
3	C	40	TYR
4	B	59	TYR
4	B	79	LEU
4	B	105	TYR
4	B	151	PHE
4	B	212	ASP
4	B	253	PHE
4	B	264	TYR
4	B	286	LEU
5	A	32	LYS
5	A	210	LYS

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Mol	Chain	Res	Type
5	A	243	MET
5	A	257	LYS
5	A	322	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	R	699	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

3 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	$\#\|Z\| > 2$
6	BK0	S	1001	-	17,17,17	1.39	3 (17%)	22,22,22	1.19	2 (9%)
7	SEP	S	1002	-	9,10,10	1.60	2 (22%)	12,14,14	1.74	4 (33%)
7	SEP	R	1001	-	9,10,10	1.59	2 (22%)	12,14,14	1.75	4 (33%)

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	BK0	S	1001	-	-	6/8/8/8	0/2/2/2
7	SEP	S	1002	-	-	6/10/10/10	-
7	SEP	R	1001	-	-	5/10/10/10	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	S	1001	BK0	C07-N09	3.81	1.45	1.35
7	S	1002	SEP	P-O1P	3.36	1.61	1.50
7	R	1001	SEP	P-O1P	3.33	1.61	1.50
6	S	1001	BK0	O08-C07	-2.18	1.18	1.23
7	R	1001	SEP	OXT-C	-2.14	1.23	1.30
7	S	1002	SEP	OXT-C	-2.13	1.23	1.30
6	S	1001	BK0	C10-N09	2.12	1.45	1.41

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	R	1001	SEP	OG-CB-CA	3.43	111.05	108.06
7	S	1002	SEP	OG-CB-CA	3.33	110.96	108.06
6	S	1001	BK0	C03-N04-C05	3.26	121.16	116.93
7	S	1002	SEP	P-OG-CB	-3.02	109.96	118.30
7	R	1001	SEP	P-OG-CB	-2.99	110.06	118.30
7	S	1002	SEP	OXT-C-O	-2.66	118.04	124.09
7	R	1001	SEP	OXT-C-O	-2.65	118.08	124.09
6	S	1001	BK0	C05-C07-N09	2.25	119.50	114.04
7	S	1002	SEP	OXT-C-CA	2.24	121.00	113.38
7	R	1001	SEP	OXT-C-CA	2.23	120.98	113.38

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	S	1002	SEP	O-C-CA-CB
7	S	1002	SEP	OXT-C-CA-CB
7	R	1001	SEP	N-CA-CB-OG
7	R	1001	SEP	OXT-C-CA-CB

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Mol	Chain	Res	Type	Atoms
6	S	1001	BK0	C06-C05-C07-O08
6	S	1001	BK0	N04-C05-C07-N09
6	S	1001	BK0	C06-C05-C07-N09
6	S	1001	BK0	N04-C05-C07-O08
7	R	1001	SEP	O-C-CA-CB
7	R	1001	SEP	CB-OG-P-O1P
7	S	1002	SEP	OXT-C-CA-N
7	S	1002	SEP	O-C-CA-N
7	S	1002	SEP	N-CA-CB-OG
7	S	1002	SEP	CB-OG-P-O1P
6	S	1001	BK0	C15-C10-N09-C07
6	S	1001	BK0	C11-C10-N09-C07
7	R	1001	SEP	CA-CB-OG-P

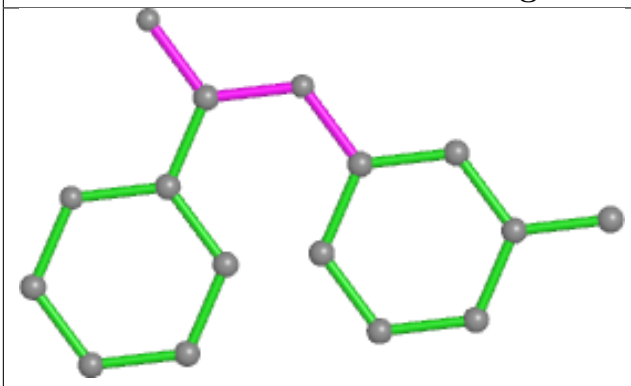
There are no ring outliers.

1 monomer is involved in 2 short contacts:

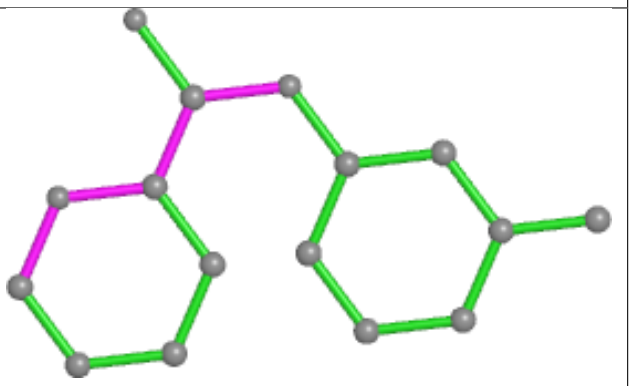
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	R	1001	SEP	2	0

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

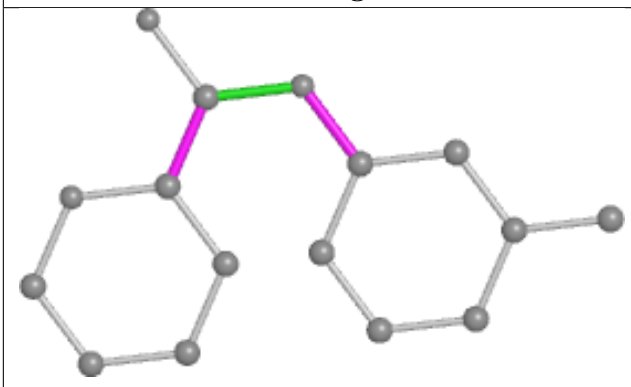
Ligand BK0 S 1001



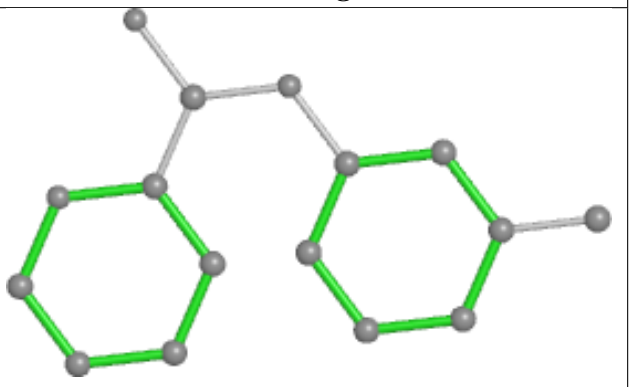
Bond lengths



Bond angles

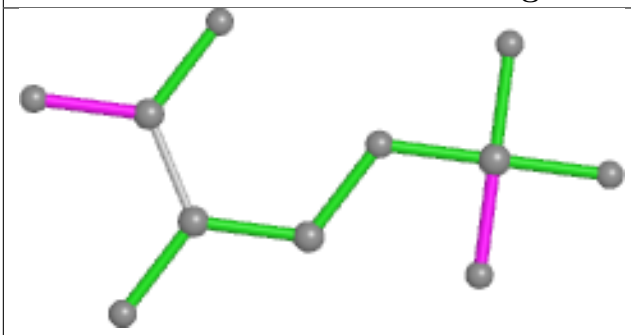


Torsions

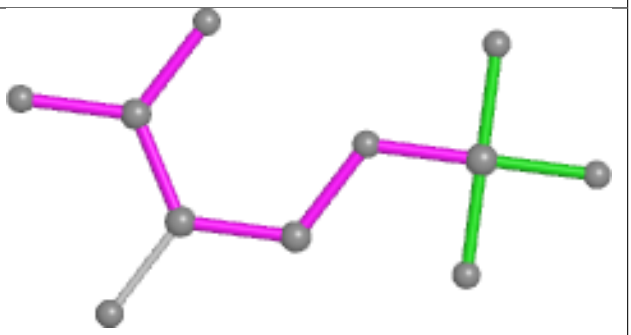


Rings

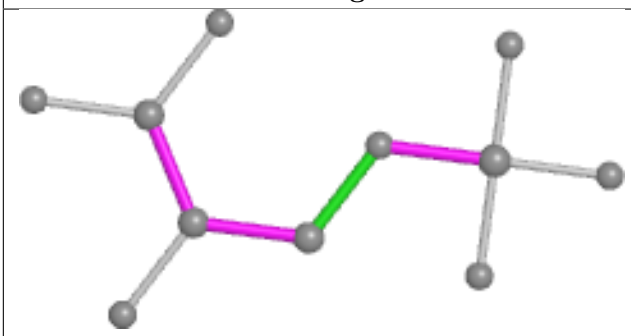
Ligand SEP S 1002



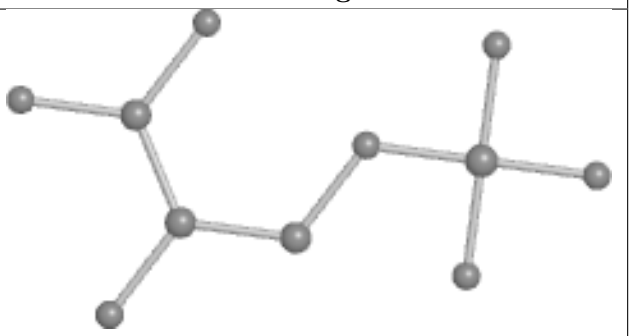
Bond lengths



Bond angles



Torsions



Rings

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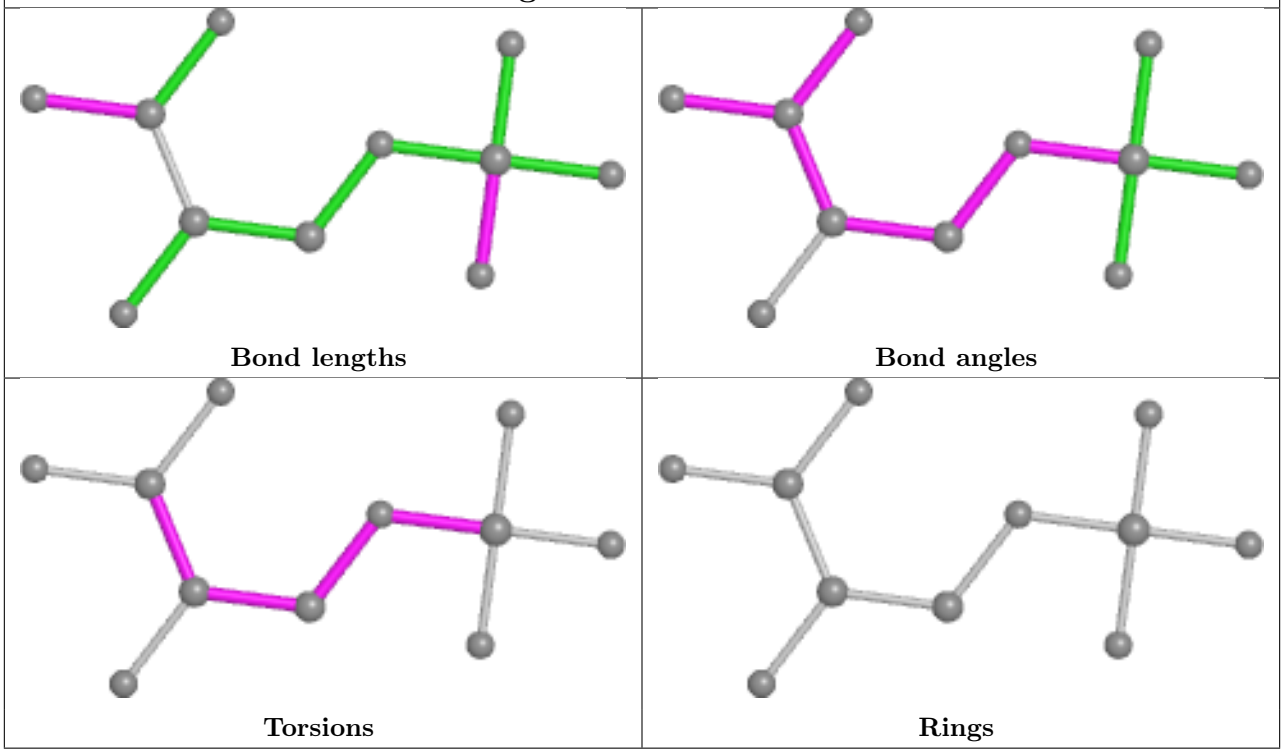

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.