



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2026 – 07:34 PM UTC

PDB ID : 6EEE / pdb_00006eee
Title : X-ray crystal structure of Pf-M17 in complex with inhibitor (6k) and regulatory zinc ion
Authors : Drinkwater, N.; McGowan, S.
Deposited on : 2018-08-13
Resolution : 2.30 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:

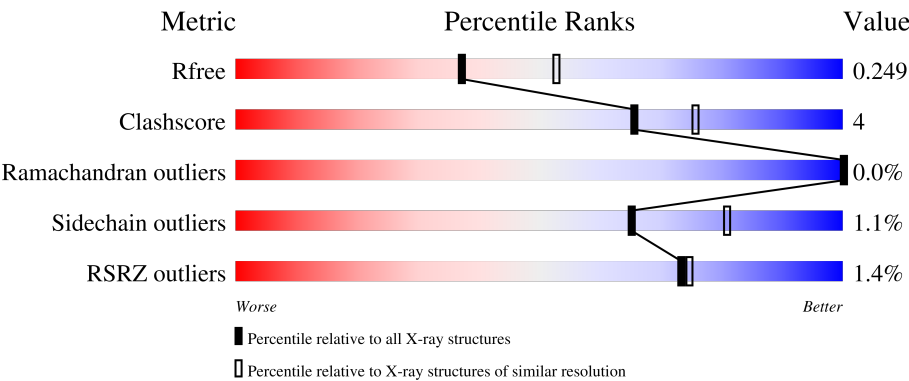
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.30 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))
R _{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	519	% 91%8%
1	B	519	3% 89%9%
1	C	519	% 92%8%
1	D	519	% 90%10%
1	E	519	% 89%9%

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Mol	Chain	Length	Quality of chain
1	F	519	
1	G	519	
1	H	519	
1	I	519	
1	J	519	
1	K	519	
1	L	519	

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
7	1PE	D	1007	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 50000 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 M17 LEUCYL-AMINOPEPTIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	514	Total	C	N	O	S	0	1	0
			3938	2525	634	760	19			
1	B	511	Total	C	N	O	S	0	0	0
			3859	2481	628	731	19			
1	C	518	Total	C	N	O	S	0	1	0
			3943	2537	639	748	19			
1	D	516	Total	C	N	O	S	0	1	0
			3933	2534	639	740	20			
1	E	510	Total	C	N	O	S	0	0	0
			3884	2504	626	735	19			
1	F	509	Total	C	N	O	S	0	0	0
			3847	2475	621	732	19			
1	G	517	Total	C	N	O	S	0	1	0
			3962	2544	637	761	20			
1	H	513	Total	C	N	O	S	0	1	0
			3865	2485	627	734	19			
1	I	518	Total	C	N	O	S	0	1	0
			3933	2526	638	750	19			
1	J	516	Total	C	N	O	S	0	1	0
			3951	2540	643	748	20			
1	K	510	Total	C	N	O	S	0	0	0
			3895	2508	628	740	19			
1	L	510	Total	C	N	O	S	0	0	0
			3831	2463	620	729	19			

There are 36 discrepancies between the modelled and reference sequences:

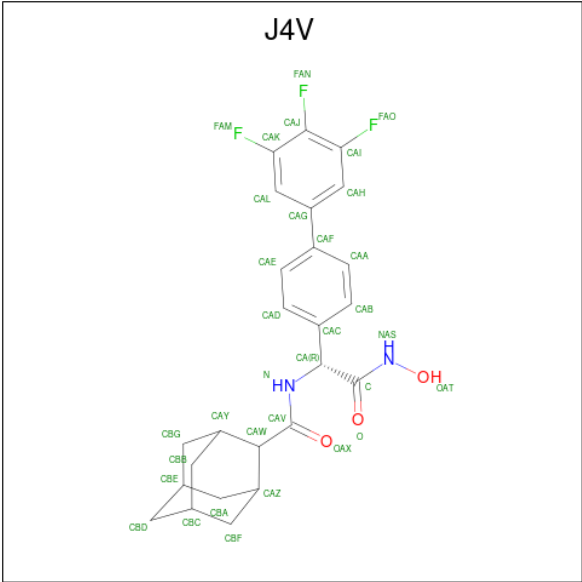
Chain	Residue	Modelled	Actual	Comment	Reference
A	152	GLN	ASN	engineered mutation	UNP A0A0L7KHE6
A	515	GLN	ASN	engineered mutation	UNP A0A0L7KHE6
A	546	GLN	ASN	engineered mutation	UNP A0A0L7KHE6
B	152	GLN	ASN	engineered mutation	UNP A0A0L7KHE6
B	515	GLN	ASN	engineered mutation	UNP A0A0L7KHE6

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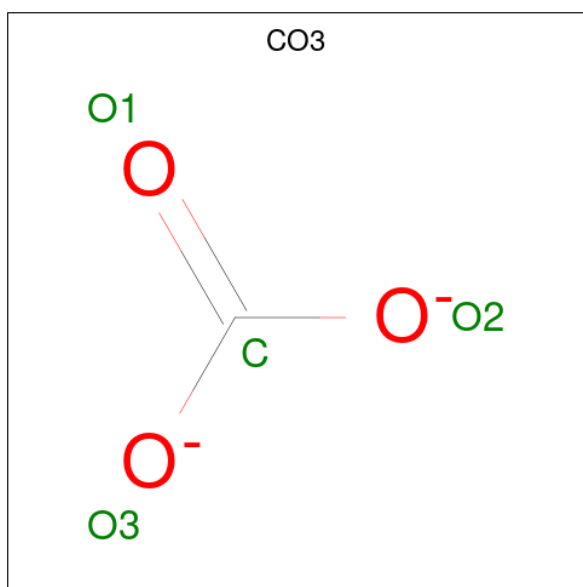
Chain	Residue	Modelled	Actual	Comment	Reference
B	546	GLN	ASN	engineered mutation	UNP A0A0L7KHE6
C	152	GLN	ASN	engineered mutation	UNP A0A0L7KHE6
C	515	GLN	ASN	engineered mutation	UNP A0A0L7KHE6
C	546	GLN	ASN	engineered mutation	UNP A0A0L7KHE6
D	152	GLN	ASN	engineered mutation	UNP A0A0L7KHE6
D	515	GLN	ASN	engineered mutation	UNP A0A0L7KHE6
D	546	GLN	ASN	engineered mutation	UNP A0A0L7KHE6
E	152	GLN	ASN	engineered mutation	UNP A0A0L7KHE6
E	515	GLN	ASN	engineered mutation	UNP A0A0L7KHE6
E	546	GLN	ASN	engineered mutation	UNP A0A0L7KHE6
F	152	GLN	ASN	engineered mutation	UNP A0A0L7KHE6
F	515	GLN	ASN	engineered mutation	UNP A0A0L7KHE6
F	546	GLN	ASN	engineered mutation	UNP A0A0L7KHE6
G	152	GLN	ASN	engineered mutation	UNP A0A0L7KHE6
G	515	GLN	ASN	engineered mutation	UNP A0A0L7KHE6
G	546	GLN	ASN	engineered mutation	UNP A0A0L7KHE6
H	152	GLN	ASN	engineered mutation	UNP A0A0L7KHE6
H	515	GLN	ASN	engineered mutation	UNP A0A0L7KHE6
H	546	GLN	ASN	engineered mutation	UNP A0A0L7KHE6
I	152	GLN	ASN	engineered mutation	UNP A0A0L7KHE6
I	515	GLN	ASN	engineered mutation	UNP A0A0L7KHE6
I	546	GLN	ASN	engineered mutation	UNP A0A0L7KHE6
J	152	GLN	ASN	engineered mutation	UNP A0A0L7KHE6
J	515	GLN	ASN	engineered mutation	UNP A0A0L7KHE6
J	546	GLN	ASN	engineered mutation	UNP A0A0L7KHE6
K	152	GLN	ASN	engineered mutation	UNP A0A0L7KHE6
K	515	GLN	ASN	engineered mutation	UNP A0A0L7KHE6
K	546	GLN	ASN	engineered mutation	UNP A0A0L7KHE6
L	152	GLN	ASN	engineered mutation	UNP A0A0L7KHE6
L	515	GLN	ASN	engineered mutation	UNP A0A0L7KHE6
L	546	GLN	ASN	engineered mutation	UNP A0A0L7KHE6

- Molecule 2 is (1R,2r,3S,5R,7R)-N-[(1R)-2-(hydroxyamino)-2-oxo-1-(3',4',5'-trifluoro[1,1'-biphenyl]-4-yl)ethyl]tricyclo[3.3.1.1 3,7]decane-2-carboxamide (CCD ID: J4V) (formula: C₂₅H₂₅F₃N₂O₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 33	C 25	F 3	N 2	O 3	0	0
2	B	1	Total 33	C 25	F 3	N 2	O 3	0	0
2	C	1	Total 33	C 25	F 3	N 2	O 3	0	0
2	D	1	Total 33	C 25	F 3	N 2	O 3	0	0
2	E	1	Total 33	C 25	F 3	N 2	O 3	0	0
2	F	1	Total 33	C 25	F 3	N 2	O 3	0	0
2	G	1	Total 33	C 25	F 3	N 2	O 3	0	0
2	H	1	Total 33	C 25	F 3	N 2	O 3	0	0
2	I	1	Total 33	C 25	F 3	N 2	O 3	0	0
2	J	1	Total 33	C 25	F 3	N 2	O 3	0	0
2	K	1	Total 33	C 25	F 3	N 2	O 3	0	0
2	L	1	Total 33	C 25	F 3	N 2	O 3	0	0

- Molecule 3 is CARBONATE ION (CCD ID: CO3) (formula: CO₃).

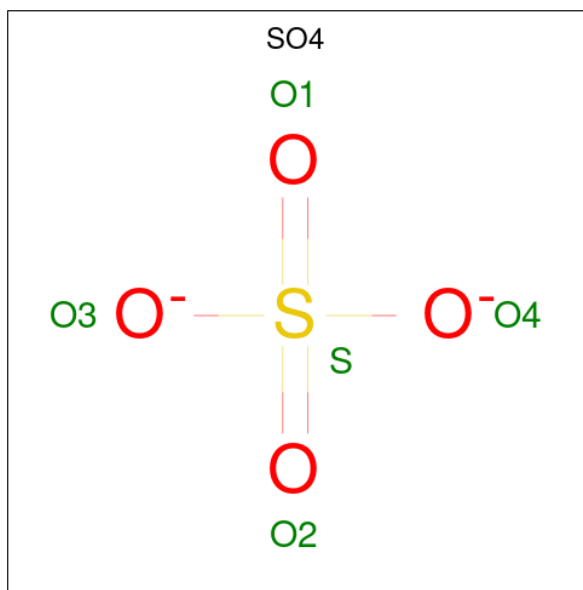


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	1	3		
3	B	1	Total	C	O	0	0
			4	1	3		
3	C	1	Total	C	O	0	0
			4	1	3		
3	D	1	Total	C	O	0	0
			4	1	3		
3	E	1	Total	C	O	0	0
			4	1	3		
3	F	1	Total	C	O	0	0
			4	1	3		
3	G	1	Total	C	O	0	0
			4	1	3		
3	H	1	Total	C	O	0	0
			4	1	3		
3	I	1	Total	C	O	0	0
			4	1	3		
3	J	1	Total	C	O	0	0
			4	1	3		
3	K	1	Total	C	O	0	0
			4	1	3		
3	L	1	Total	C	O	0	0
			4	1	3		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Zn 1 1	0	0
4	B	1	Total Zn 1 1	0	0
4	C	1	Total Zn 1 1	0	0
4	D	1	Total Zn 1 1	0	0
4	E	1	Total Zn 1 1	0	0
4	F	1	Total Zn 1 1	0	0
4	G	1	Total Zn 1 1	0	0
4	H	1	Total Zn 1 1	0	0
4	I	1	Total Zn 1 1	0	0
4	J	1	Total Zn 1 1	0	0
4	K	1	Total Zn 1 1	0	0
4	L	1	Total Zn 1 1	0	0

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



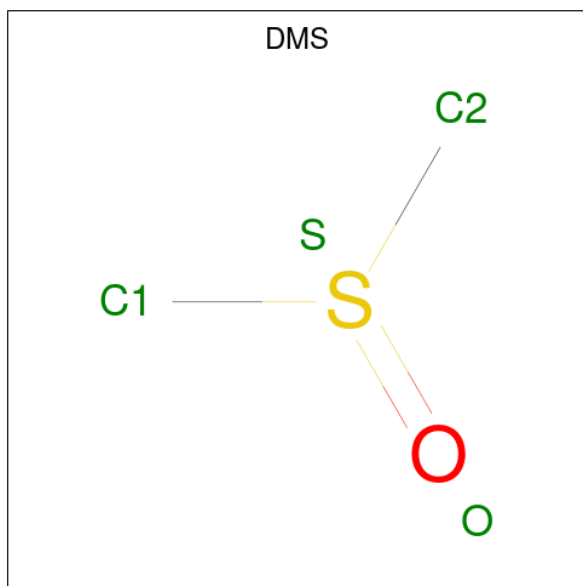
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0
5	E	1	Total O S 5 4 1	0	0
5	E	1	Total O S 5 4 1	0	0
5	F	1	Total O S 5 4 1	0	0
5	F	1	Total O S 5 4 1	0	0
5	G	1	Total O S 5 4 1	0	0
5	G	1	Total O S 5 4 1	0	0
5	H	1	Total O S 5 4 1	0	0
5	H	1	Total O S 5 4 1	0	0
5	H	1	Total O S 5 4 1	0	0
5	I	1	Total O S 5 4 1	0	0
5	I	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	I	1	Total	O	S	0	0
			5	4	1		
5	J	1	Total	O	S	0	0
			5	4	1		
5	J	1	Total	O	S	0	0
			5	4	1		
5	K	1	Total	O	S	0	0
			5	4	1		
5	K	1	Total	O	S	0	0
			5	4	1		
5	K	1	Total	O	S	0	0
			5	4	1		
5	L	1	Total	O	S	0	0
			5	4	1		
5	L	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



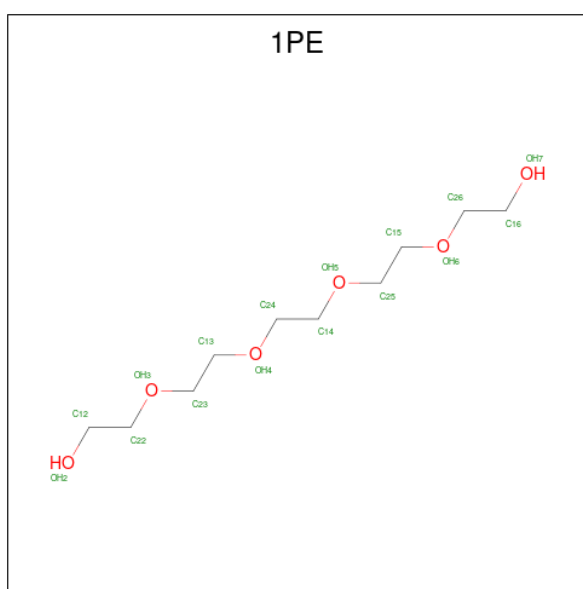
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	O	S	0	0
			4	2	1	1		
6	B	1	Total	C	O	S	0	0
			4	2	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	O	S	0	0
			4	2	1	1		
6	B	1	Total	C	O	S	0	0
			4	2	1	1		
6	G	1	Total	C	O	S	0	0
			4	2	1	1		
6	H	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 7 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



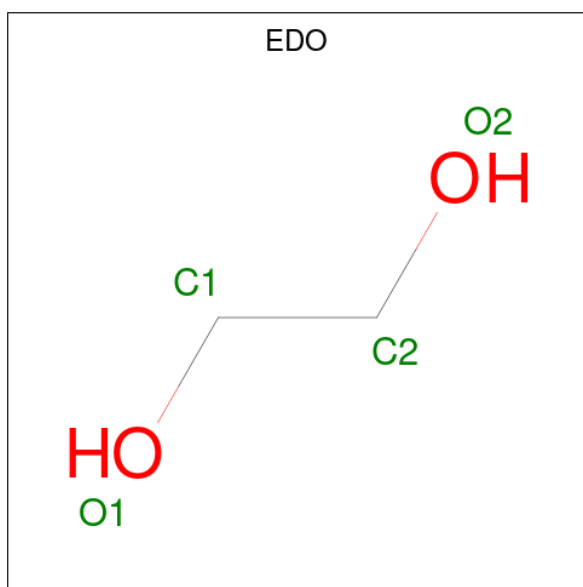
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	O		0	0
			15	10	5			
7	A	1	Total	C	O		0	0
			12	8	4			
7	B	1	Total	C	O		0	0
			9	6	3			
7	C	1	Total	C	O		0	0
			15	10	5			
7	C	1	Total	C	O		0	0
			12	8	4			
7	D	1	Total	C	O		0	0
			12	8	4			
7	D	1	Total	C	O		0	0
			7	4	3			

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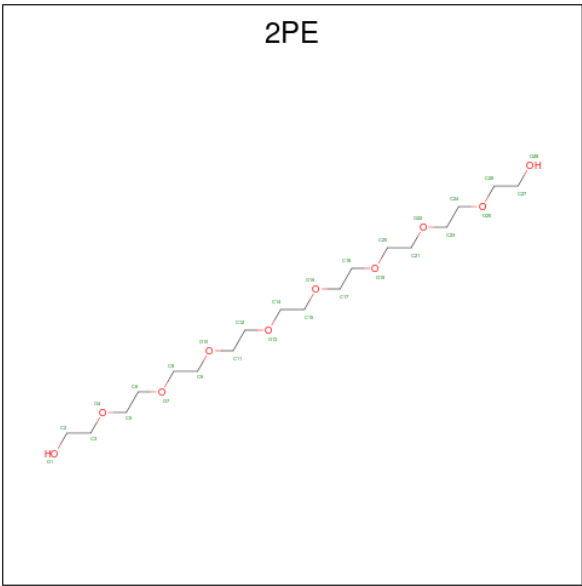
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	F	1	Total	C	O	0	0
			9	6	3		
7	F	1	Total	C	O	0	0
			9	6	3		
7	G	1	Total	C	O	0	0
			9	6	3		
7	G	1	Total	C	O	0	0
			9	6	3		
7	H	1	Total	C	O	0	0
			9	6	3		
7	I	1	Total	C	O	0	0
			12	8	4		
7	I	1	Total	C	O	0	0
			9	6	3		
7	J	1	Total	C	O	0	0
			9	6	3		
7	J	1	Total	C	O	0	0
			9	6	3		
7	J	1	Total	C	O	0	0
			13	9	4		
7	K	1	Total	C	O	0	0
			13	9	4		
7	K	1	Total	C	O	0	0
			15	10	5		
7	L	1	Total	C	O	0	0
			13	8	5		
7	L	1	Total	C	O	0	0
			12	8	4		
7	L	1	Total	C	O	0	0
			7	4	3		
7	L	1	Total	C	O	0	0
			5	3	2		

- Molecule 8 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	E	1	Total	C	O	0	0
			4	2	2		
8	F	1	Total	C	O	0	0
			4	2	2		
8	F	1	Total	C	O	0	0
			4	2	2		
8	G	1	Total	C	O	0	0
			4	2	2		
8	H	1	Total	C	O	0	0
			4	2	2		
8	I	1	Total	C	O	0	0
			4	2	2		
8	J	1	Total	C	O	0	0
			4	2	2		
8	J	1	Total	C	O	0	0
			4	2	2		
8	J	1	Total	C	O	0	0
			4	2	2		
8	K	1	Total	C	O	0	0
			4	2	2		
8	K	1	Total	C	O	0	0
			4	2	2		
8	K	1	Total	C	O	0	0
			4	2	2		
8	K	1	Total	C	O	0	0
			4	2	2		
8	L	1	Total	C	O	0	0
			4	2	2		

- Molecule 9 is NONAETHYLENE GLYCOL (CCD ID: 2PE) (formula: C₁₈H₃₈O₁₀).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	H	1	Total	C	O	0	0
			25	16	9		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	209	Total	O	0	0
			209	209		
10	B	158	Total	O	0	0
			158	158		
10	C	209	Total	O	0	0
			209	209		
10	D	198	Total	O	0	0
			198	198		
10	E	219	Total	O	0	0
			219	219		
10	F	155	Total	O	0	0
			155	155		
10	G	172	Total	O	0	0
			172	172		
10	H	152	Total	O	0	0
			152	152		
10	I	207	Total	O	0	0
			207	207		
10	J	180	Total	O	0	0
			180	180		

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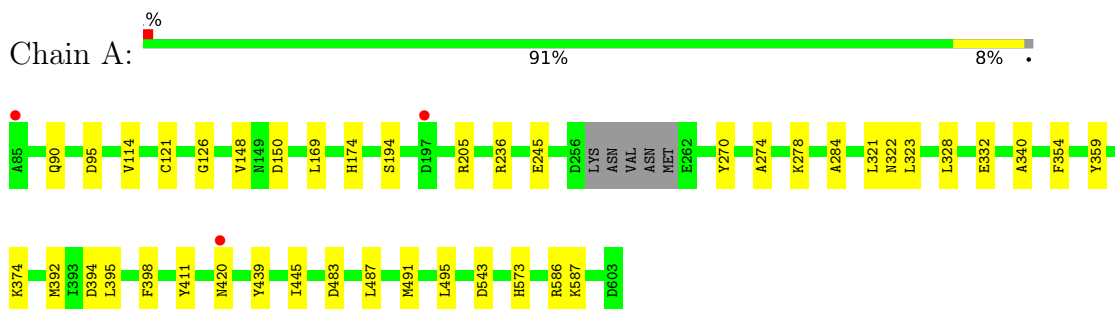
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	K	205	Total 205	O 205	0	0
10	L	135	Total 135	O 135	0	0

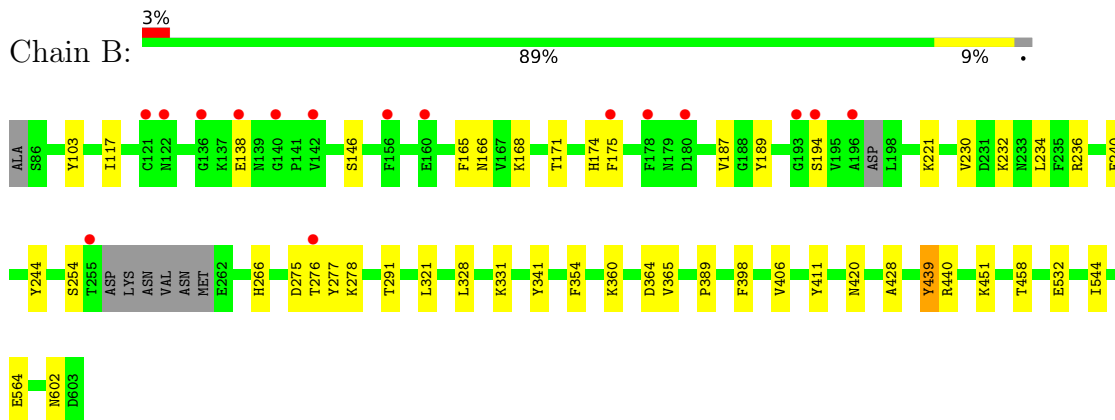
3 Residue-property plots [i](#)

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

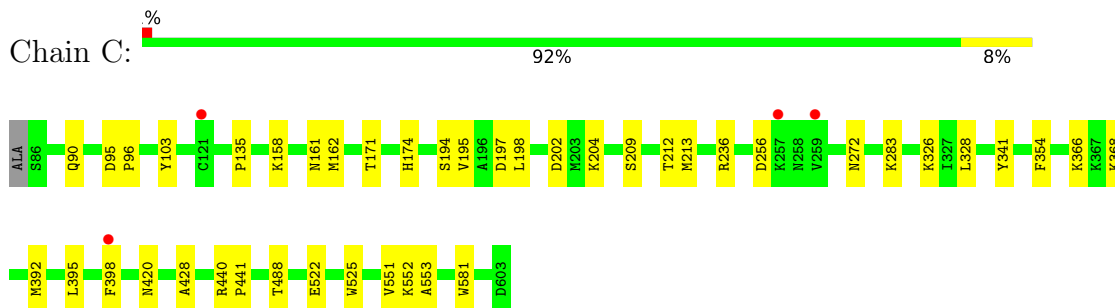
- Molecule 1: M17 LEUCYL-AMINOPEPTIDASE



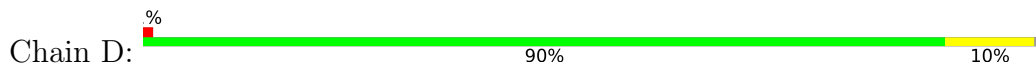
- Molecule 1: M17 LEUCYL-AMINOPEPTIDASE

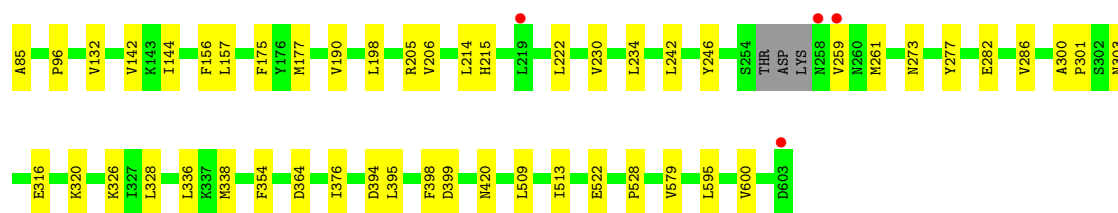


- Molecule 1: M17 LEUCYL-AMINOPEPTIDASE

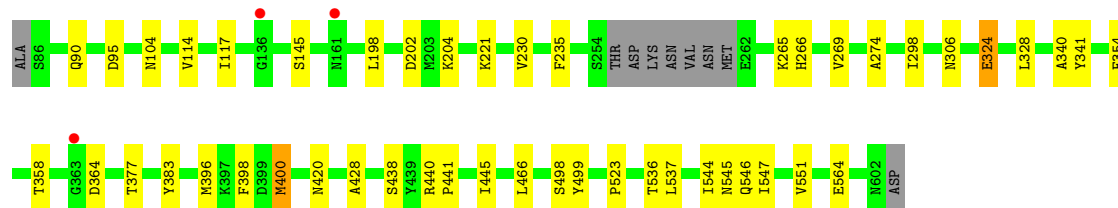
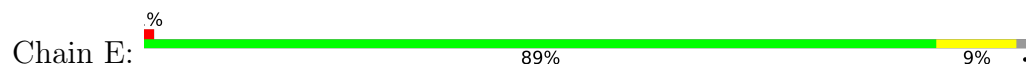


- Molecule 1: M17 LEUCYL-AMINOPEPTIDASE

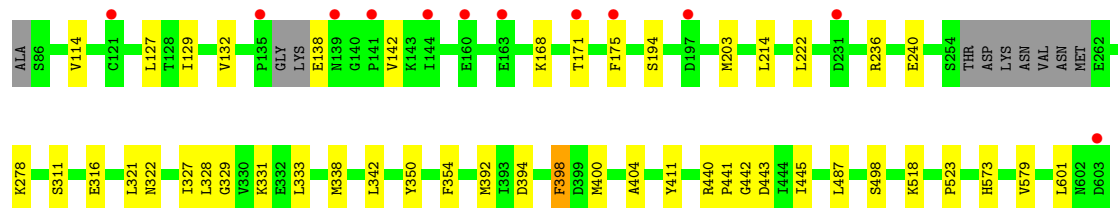
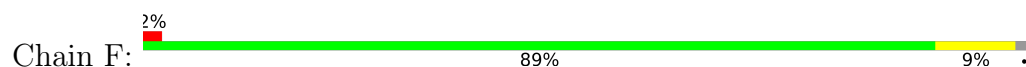




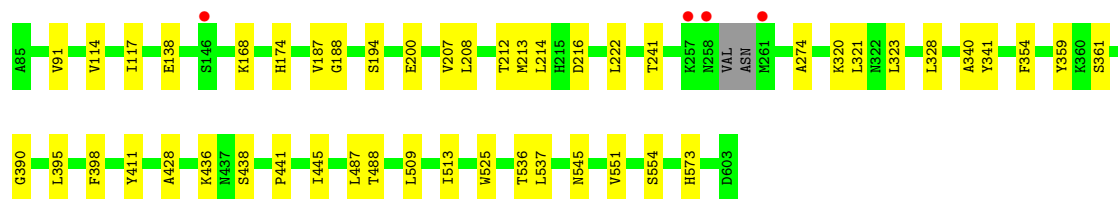
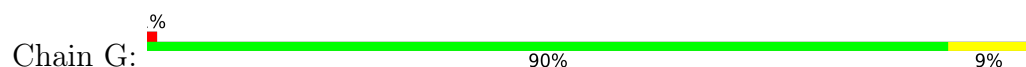
• Molecule 1: M17 LEUCYL-AMINOPEPTIDASE



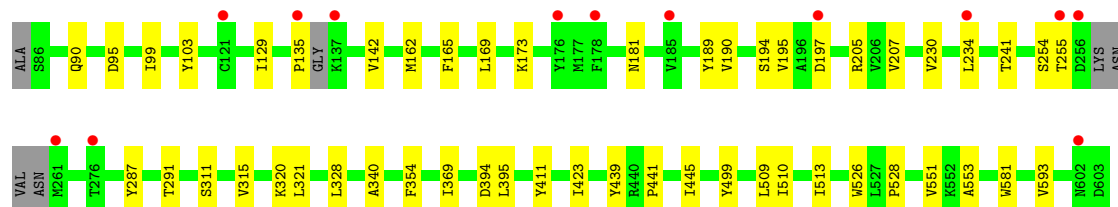
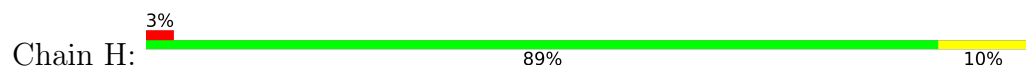
• Molecule 1: M17 LEUCYL-AMINOPEPTIDASE



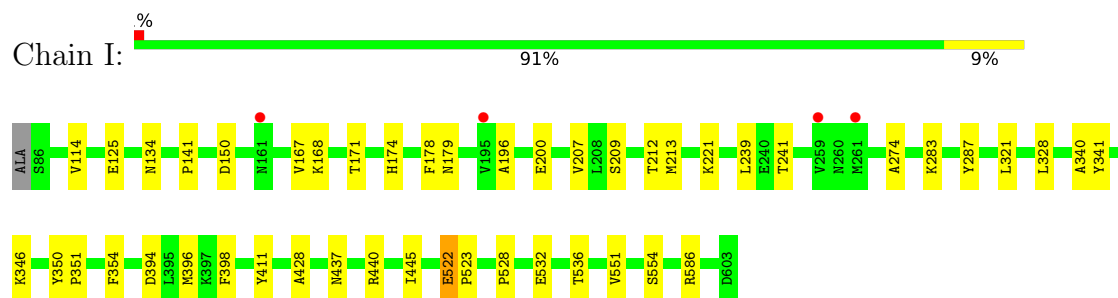
• Molecule 1: M17 LEUCYL-AMINOPEPTIDASE



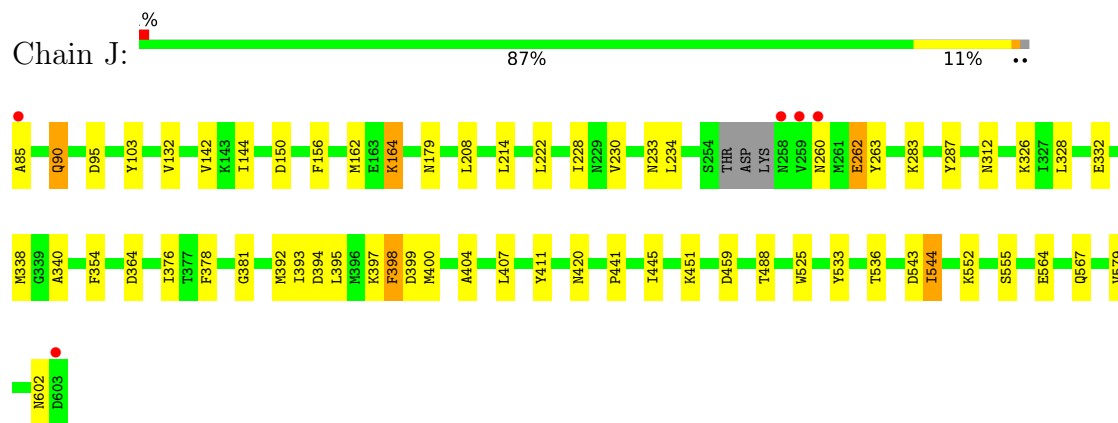
• Molecule 1: M17 LEUCYL-AMINOPEPTIDASE



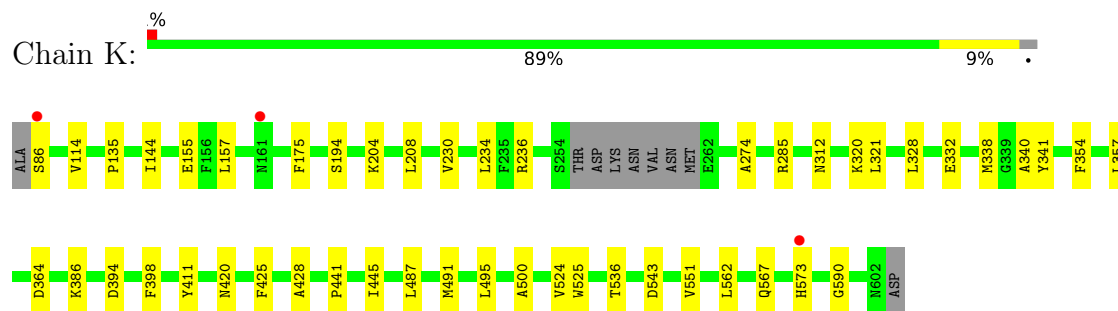
• Molecule 1: M17 LEUCYL-AMINOPEPTIDASE



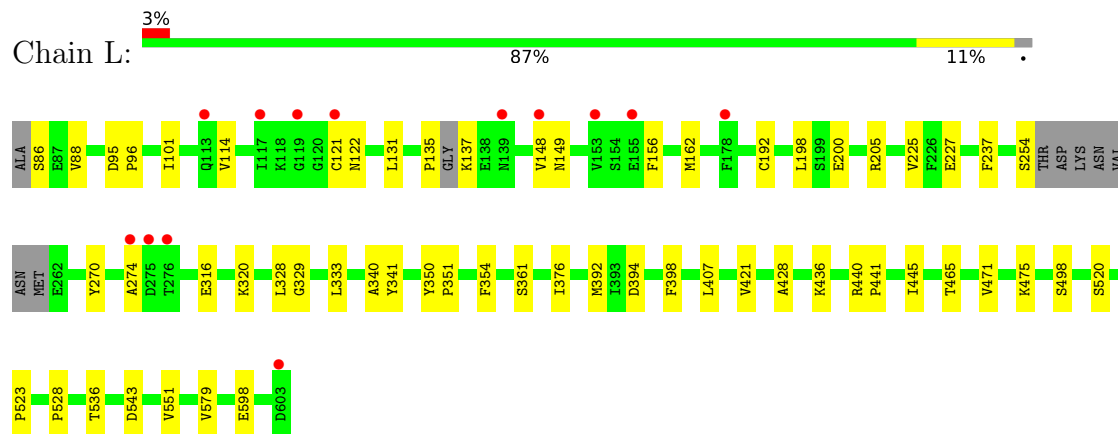
• Molecule 1: M17 LEUCYL-AMINOPEPTIDASE



• Molecule 1: M17 LEUCYL-AMINOPEPTIDASE



• Molecule 1: M17 LEUCYL-AMINOPEPTIDASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	173.68Å 177.40Å 229.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.17 – 2.30 48.17 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.17-2.30) 99.8 (48.17-2.30)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.193 , 0.246 0.199 , 0.249	Depositor DCC
R_{free} test set	15497 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	26.0	Xtriage
Anisotropy	0.779	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 49.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	50000	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.41 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.6342e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, ZN, CO3, SO4, 2PE, DMS, 1PE, J4V

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	0.52	0/4015	0.80	0/5450
1	B	0.49	0/3935	0.79	0/5346
1	C	0.50	0/4024	0.82	3/5463 (0.1%)
1	D	0.52	0/4013	0.79	1/5443 (0.0%)
1	E	0.55	0/3961	0.80	0/5376
1	F	0.50	0/3923	0.80	0/5332
1	G	0.50	0/4039	0.79	1/5478 (0.0%)
1	H	0.51	0/3944	0.82	2/5363 (0.0%)
1	I	0.51	0/4014	0.80	3/5452 (0.1%)
1	J	0.52	0/4031	0.82	0/5466
1	K	0.53	0/3972	0.82	0/5390
1	L	0.48	0/3907	0.80	0/5313
All	All	0.51	0/47778	0.80	10/64872 (0.0%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	99	ILE	CA-C-N	-5.56	114.07	119.90
1	H	99	ILE	C-N-CA	-5.56	114.07	119.90
1	I	167	VAL	CB-CA-C	-5.49	105.88	112.19
1	C	522	GLU	CA-C-N	5.41	125.17	119.76
1	C	522	GLU	C-N-CA	5.41	125.17	119.76
1	G	91	VAL	N-CA-C	-5.25	106.56	111.45
1	I	522	GLU	CA-C-N	5.23	125.39	119.90
1	I	522	GLU	C-N-CA	5.23	125.39	119.90
1	C	488	THR	N-CA-C	5.12	117.42	108.76
1	D	259	VAL	N-CA-C	-5.07	107.52	112.29

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	3938	0	3854	27	0
1	B	3859	0	3741	30	0
1	C	3943	0	3867	27	0
1	D	3933	0	3874	39	0
1	E	3884	0	3812	33	0
1	F	3847	0	3733	30	0
1	G	3962	0	3890	28	0
1	H	3865	0	3730	30	0
1	I	3933	0	3834	25	0
1	J	3951	0	3900	44	0
1	K	3895	0	3827	32	0
1	L	3831	0	3689	35	0
2	A	33	0	0	1	0
2	B	33	0	0	0	0
2	C	33	0	0	0	0
2	D	33	0	0	0	0
2	E	33	0	0	0	0
2	F	33	0	0	0	0
2	G	33	0	0	1	0
2	H	33	0	0	0	0
2	I	33	0	0	0	0
2	J	33	0	0	1	0
2	K	33	0	0	0	0
2	L	33	0	0	0	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
3	C	4	0	0	0	0
3	D	4	0	0	0	0
3	E	4	0	0	0	0
3	F	4	0	0	0	0
3	G	4	0	0	0	0
3	H	4	0	0	0	0
3	I	4	0	0	0	0
3	J	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	K	4	0	0	0	0
3	L	4	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0
5	A	20	0	0	1	0
5	B	5	0	0	0	0
5	C	15	0	0	1	0
5	D	15	0	0	0	0
5	E	10	0	0	0	0
5	F	10	0	0	0	0
5	G	10	0	0	0	0
5	H	15	0	0	1	0
5	I	15	0	0	0	0
5	J	10	0	0	0	0
5	K	20	0	0	1	0
5	L	10	0	0	0	0
6	A	4	0	6	1	0
6	B	12	0	18	3	0
6	G	4	0	6	2	0
6	H	4	0	6	1	0
7	A	27	0	33	1	0
7	B	9	0	8	0	0
7	C	27	0	33	2	0
7	D	19	0	22	11	0
7	F	18	0	20	3	0
7	G	18	0	20	1	0
7	H	9	0	8	0	0
7	I	21	0	22	1	0
7	J	31	0	34	8	0
7	K	28	0	33	1	0
7	L	37	0	43	3	0
8	E	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	F	8	0	12	2	0
8	G	4	0	6	0	0
8	H	4	0	6	0	0
8	I	4	0	6	2	0
8	J	12	0	18	1	0
8	K	16	0	24	0	0
8	L	4	0	6	0	0
9	H	25	0	33	3	0
10	A	209	0	0	0	0
10	B	158	0	0	2	0
10	C	209	0	0	7	0
10	D	198	0	0	2	0
10	E	219	0	0	2	0
10	F	155	0	0	2	0
10	G	172	0	0	3	0
10	H	152	0	0	0	0
10	I	207	0	0	2	0
10	J	180	0	0	4	0
10	K	205	0	0	5	0
10	L	135	0	0	3	0
All	All	50000	0	46180	360	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 4.

All (360) 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)
2:J:1001:J4V:NAS	2:J:1001:J4V:OAT	1.58	1.33
1:E:298:ILE:HA	1:E:400:MET:HE1	1.20	1.10
1:E:298:ILE:HA	1:E:400:MET:CE	1.89	1.03
1:E:298:ILE:CA	1:E:400:MET:HE1	1.96	0.96
1:J:451:LYS:HG2	7:J:1011:1PE:H131	1.48	0.95
1:L:320:LYS:HZ2	7:L:1008:1PE:H151	1.42	0.84
1:D:316:GLU:HG3	7:D:1007:1PE:H152	1.65	0.79
1:B:103:TYR:HB2	6:B:1005:DMS:H12	1.66	0.77
1:E:324:GLU:HG3	1:E:358:THR:HB	1.71	0.73
1:F:411:TYR:HE1	7:F:1008:1PE:H141	1.51	0.73
1:K:567:GLN:NE2	10:K:1101:HOH:O	2.22	0.71
1:H:328:LEU:HB2	1:H:354:PHE:HB3	1.73	0.71
1:J:90:GLN:HB3	1:J:95:ASP:HB2	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:144:ILE:HG13	1:K:157:LEU:HD22	1.74	0.69
1:E:298:ILE:CG1	1:E:400:MET:HE1	2.22	0.69
1:E:298:ILE:HG12	1:E:400:MET:HE1	1.76	0.67
1:B:451:LYS:NZ	1:B:564:GLU:O	2.27	0.67
1:L:328:LEU:HB2	1:L:354:PHE:HB3	1.77	0.67
1:L:361:SER:HB2	1:L:421:VAL:O	1.95	0.67
1:D:320:LYS:HZ1	7:D:1007:1PE:H131	1.60	0.66
1:G:340:ALA:HA	1:G:445:ILE:HD12	1.78	0.66
1:I:532:GLU:H	8:I:1007:EDO:H21	1.61	0.65
1:H:195:VAL:HG12	1:H:197:ASP:H	1.61	0.65
1:H:340:ALA:HA	1:H:445:ILE:HD12	1.78	0.65
1:F:411:TYR:CE1	7:F:1008:1PE:H141	2.32	0.64
1:L:114:VAL:HG12	1:L:274:ALA:HB1	1.79	0.64
1:L:135:PRO:O	1:L:137:LYS:N	2.31	0.64
1:F:331:LYS:H	8:F:1006:EDO:H12	1.63	0.63
1:J:132:VAL:HG21	1:J:142:VAL:HG13	1.83	0.61
1:K:562:LEU:HD12	1:K:573:HIS:HD2	1.66	0.61
1:C:195:VAL:HG12	1:C:197:ASP:H	1.65	0.61
1:E:298:ILE:CB	1:E:400:MET:HE1	2.30	0.61
1:I:178:PHE:HZ	1:K:155:GLU:HG2	1.65	0.61
1:L:121:CYS:HB2	1:L:148:VAL:HG12	1.81	0.60
1:F:114:VAL:O	1:F:278:LYS:NZ	2.34	0.59
1:B:165:PHE:HB3	1:B:189:TYR:OH	2.03	0.58
1:I:340:ALA:HA	1:I:445:ILE:HD12	1.84	0.58
1:C:158:LYS:HB2	1:C:161[B]:ASN:ND2	2.19	0.58
1:A:394:ASP:HA	1:C:441:PRO:HB2	1.85	0.58
1:G:390:GLY:H	6:G:1006:DMS:H12	1.69	0.57
1:L:536:THR:HG21	1:L:551:VAL:HG23	1.86	0.57
1:E:328:LEU:HB2	1:E:354:PHE:HB3	1.87	0.57
1:L:86:SER:N	10:L:1106:HOH:O	2.37	0.57
1:C:368:LYS:NZ	10:C:1102:HOH:O	2.24	0.57
1:E:383:TYR:HE2	1:E:438:SER:HB2	1.70	0.57
1:G:321:LEU:HD11	1:G:411:TYR:HA	1.85	0.57
1:B:221:LYS:HB2	1:B:266:HIS:HB2	1.86	0.57
1:K:562:LEU:CD1	1:K:573:HIS:HD2	2.18	0.57
1:B:275:ASP:HA	1:B:278:LYS:HZ2	1.70	0.56
1:G:328:LEU:HB2	1:G:354:PHE:HB3	1.87	0.56
1:H:142:VAL:HG23	1:H:162:MET:HB3	1.87	0.56
1:G:214:LEU:HD21	1:G:222:LEU:HD22	1.87	0.56
1:E:536:THR:HG21	1:E:551:VAL:HG23	1.87	0.56
1:D:320:LYS:HZ1	7:D:1007:1PE:H142	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:544:ILE:HD12	1:J:564:GLU:HG3	1.88	0.55
1:J:552:LYS:HG2	8:J:1007:EDO:H11	1.88	0.55
1:I:328:LEU:HB2	1:I:354:PHE:HB3	1.87	0.55
1:K:320:LYS:HE2	7:K:1012:1PE:H252	1.87	0.55
1:B:440:ARG:NH2	10:B:1107:HOH:O	2.40	0.55
1:C:552:LYS:NZ	10:C:1109:HOH:O	2.37	0.55
1:A:328:LEU:HB2	1:A:354:PHE:HB3	1.89	0.54
1:D:394:ASP:HA	1:F:441:PRO:HB2	1.89	0.54
1:A:90:GLN:HB3	1:A:95:ASP:HB2	1.89	0.54
1:A:491:MET:HE1	1:A:495:LEU:HD12	1.90	0.54
1:G:487:LEU:HD22	1:G:573:HIS:CE1	2.42	0.54
1:H:291:THR:HG22	1:H:593:VAL:HB	1.88	0.54
1:E:298:ILE:HG12	1:E:400:MET:CE	2.37	0.54
1:D:215:HIS:O	1:D:261:MET:HB3	2.07	0.54
1:K:441:PRO:HB2	1:L:394:ASP:HA	1.90	0.54
1:C:328:LEU:HB2	1:C:354:PHE:HB3	1.90	0.54
1:D:205:ARG:HD3	10:D:1263:HOH:O	2.09	0.53
1:J:602:ASN:ND2	10:J:1103:HOH:O	2.30	0.53
1:G:536:THR:HG21	1:G:551:VAL:HG23	1.90	0.53
1:K:135:PRO:HA	1:K:194:SER:O	2.08	0.53
1:E:114:VAL:HG12	1:E:274:ALA:HB1	1.90	0.53
1:K:321:LEU:HD11	1:K:411:TYR:HA	1.91	0.53
1:B:364:ASP:O	1:B:420:ASN:HA	2.09	0.52
1:B:602:ASN:ND2	10:B:1101:HOH:O	2.27	0.52
8:I:1007:EDO:H22	10:I:1171:HOH:O	2.08	0.52
1:F:168:LYS:O	1:F:171:THR:HG22	2.10	0.52
1:H:254:SER:OG	1:H:255:THR:N	2.41	0.52
1:J:338:MET:HE2	10:J:1150:HOH:O	2.10	0.52
1:B:331:LYS:HB2	6:B:1007:DMS:H21	1.92	0.52
1:I:125:GLU:HG3	1:I:221:LYS:HD3	1.92	0.52
1:D:328:LEU:HB2	1:D:354:PHE:HB3	1.91	0.51
1:B:230:VAL:HG12	1:B:234:LEU:HD23	1.91	0.51
1:F:132:VAL:HG21	1:F:142:VAL:HG13	1.93	0.51
1:D:320:LYS:NZ	7:D:1007:1PE:H131	2.25	0.51
1:J:394:ASP:HA	1:L:441:PRO:HB2	1.92	0.51
1:L:156:PHE:O	1:L:162:MET:HE3	2.10	0.51
1:C:366:LYS:HG3	1:C:420:ASN:HB3	1.91	0.51
1:I:396:MET:SD	1:I:398:PHE:HE2	2.34	0.51
1:L:340:ALA:HA	1:L:445:ILE:HD12	1.93	0.51
1:K:340:ALA:HA	1:K:445:ILE:HD12	1.91	0.51
1:J:533:TYR:O	1:J:536:THR:HG22	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:144:ILE:HG13	1:D:157:LEU:HD22	1.92	0.50
1:F:311:SER:HB2	1:F:327:ILE:HD12	1.92	0.50
1:K:328:LEU:HB2	1:K:354:PHE:HB3	1.93	0.50
1:H:320:LYS:NZ	9:H:1007:2PE:H142	2.26	0.50
1:J:543:ASP:CG	7:J:1011:1PE:H132	2.36	0.50
1:F:487:LEU:HD22	1:F:573:HIS:CE1	2.47	0.50
1:G:168:LYS:NZ	10:G:1109:HOH:O	2.45	0.50
1:G:208:LEU:O	1:G:212:THR:HG23	2.12	0.50
1:I:528:PRO:HB3	1:J:525:TRP:CZ3	2.47	0.50
1:J:328:LEU:HB2	1:J:354:PHE:HB3	1.92	0.50
1:H:90:GLN:HB3	1:H:95:ASP:HB2	1.93	0.50
1:D:326[B]:LYS:HD2	1:D:328:LEU:HD11	1.94	0.49
1:D:214:LEU:HD21	1:D:222:LEU:HD22	1.95	0.49
1:K:543:ASP:OD2	1:L:254:SER:HB3	2.13	0.49
1:F:329:GLY:HA3	8:F:1006:EDO:H21	1.95	0.49
1:D:326[A]:LYS:HD2	1:D:328:LEU:HD11	1.93	0.49
1:I:536:THR:HG21	1:I:551:VAL:HG23	1.94	0.49
1:B:328:LEU:HB2	1:B:354:PHE:HB3	1.94	0.49
1:C:368:LYS:NZ	10:C:1114:HOH:O	2.45	0.49
1:B:532:GLU:OE2	1:E:498:SER:OG	2.29	0.49
1:G:207:VAL:HG11	1:G:241:THR:HG22	1.95	0.49
1:J:156:PHE:O	1:J:162:MET:HE3	2.12	0.49
1:G:488:THR:HA	2:G:1001:J4V:OAX	2.12	0.49
1:K:491:MET:HE1	1:K:495:LEU:HD12	1.95	0.49
1:G:174:HIS:NE2	1:G:213:MET:HE2	2.28	0.48
1:J:400:MET:CE	1:J:404:ALA:HB2	2.42	0.48
1:E:221:LYS:HG3	1:E:266:HIS:HB2	1.94	0.48
1:J:326:LYS:HE3	1:J:328:LEU:HD11	1.95	0.48
1:B:389:PRO:HA	6:B:1006:DMS:H23	1.95	0.48
1:K:536:THR:HG21	1:K:551:VAL:HG23	1.94	0.48
1:L:520:SER:HB3	1:L:598:GLU:HG3	1.95	0.48
1:C:198:LEU:HD22	1:C:202:ASP:HB3	1.95	0.48
1:E:383:TYR:CE2	1:E:438:SER:HB2	2.49	0.48
1:L:237:PHE:HB2	10:L:1173:HOH:O	2.12	0.48
1:A:374:LYS:NZ	2:A:1001:J4V:OAT	2.46	0.48
1:A:586:ARG:HD2	5:C:1004:SO4:O2	2.14	0.48
1:C:440:ARG:NH2	10:C:1116:HOH:O	2.47	0.48
7:C:1007:1PE:H241	7:C:1007:1PE:H222	1.94	0.48
1:J:150:ASP:OD1	1:J:179:ASN:HB2	2.13	0.48
1:A:245:GLU:OE1	1:A:587:LYS:NZ	2.43	0.48
1:K:500:ALA:HB3	1:K:524:VAL:HG22	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:236:ARG:HD2	1:C:283:LYS:HG2	1.96	0.47
1:D:320:LYS:NZ	7:D:1007:1PE:H251	2.30	0.47
1:B:175:PHE:N	1:B:187:VAL:O	2.40	0.47
1:J:340:ALA:HA	1:J:445:ILE:HD12	1.96	0.47
1:H:441:PRO:HB2	1:I:394:ASP:HA	1.95	0.47
1:G:114:VAL:HG12	1:G:274:ALA:HB1	1.96	0.47
1:G:320:LYS:HD3	7:G:1009:1PE:H132	1.96	0.47
1:G:390:GLY:H	6:G:1006:DMS:C1	2.27	0.47
1:B:275:ASP:HA	1:B:278:LYS:NZ	2.29	0.47
1:E:537:LEU:HA	1:E:545:ASN:HB2	1.97	0.47
1:H:509:LEU:O	1:H:513:ILE:HG12	2.15	0.47
1:H:551:VAL:HG12	1:H:553:ALA:H	1.78	0.47
1:K:285:ARG:HG2	10:K:1288:HOH:O	2.14	0.47
1:L:192:CYS:HB3	1:L:198:LEU:HD11	1.97	0.47
1:F:236:ARG:NH1	10:F:1101:HOH:O	2.43	0.47
1:H:395:LEU:HD21	1:H:581:TRP:CD1	2.49	0.47
1:B:166:ASN:OD1	1:B:168:LYS:HB2	2.15	0.47
1:B:138:GLU:O	1:B:194:SER:OG	2.32	0.46
1:E:340:ALA:HA	1:E:445:ILE:HD12	1.97	0.46
1:A:323:LEU:HD22	1:A:359:TYR:HB2	1.96	0.46
1:K:114:VAL:HG12	1:K:274:ALA:HB1	1.97	0.46
1:A:487:LEU:HD12	1:A:487:LEU:HA	1.74	0.46
1:F:138:GLU:HA	1:F:194:SER:OG	2.16	0.46
5:H:1006:SO4:O3	1:I:586:ARG:HD2	2.15	0.46
1:I:321:LEU:HD11	1:I:411:TYR:HA	1.98	0.46
1:K:357:LEU:HB2	1:K:425:PHE:HB2	1.96	0.46
1:G:436:LYS:HB3	1:G:436:LYS:HE2	1.77	0.46
1:J:103:TYR:HB3	7:J:1009:1PE:H142	1.98	0.46
1:J:378:PHE:CZ	1:L:441:PRO:HD2	2.50	0.46
1:C:272:ASN:ND2	10:C:1115:HOH:O	2.46	0.46
1:B:244:TYR:CE1	1:B:291:THR:HG22	2.51	0.46
1:H:320:LYS:HG2	9:H:1007:2PE:H121	1.97	0.46
1:J:262:GLU:OE1	1:J:263:TYR:N	2.49	0.46
1:J:397:LYS:O	1:J:400:MET:HG2	2.16	0.46
1:K:86:SER:O	1:K:312:ASN:ND2	2.38	0.46
1:C:392:MET:HE2	1:C:395:LEU:HB2	1.98	0.46
1:D:132:VAL:HG21	1:D:142:VAL:HG13	1.98	0.46
1:H:165:PHE:CD2	1:H:173:LYS:HG3	2.51	0.45
1:G:441:PRO:HB2	1:H:394:ASP:HA	1.98	0.45
1:A:420:ASN:N	1:A:420:ASN:HD22	2.14	0.45
1:C:341:TYR:CE1	1:C:428:ALA:HB1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:567:GLN:OE1	7:J:1011:1PE:H262	2.16	0.45
1:A:340:ALA:HA	1:A:445:ILE:HD12	1.98	0.45
1:B:232:LYS:NZ	1:B:276:THR:O	2.47	0.45
1:C:204:LYS:HD3	10:C:1293:HOH:O	2.17	0.45
1:E:265:LYS:HB3	10:E:1222:HOH:O	2.17	0.45
1:J:392:MET:HE3	1:J:395:LEU:HD22	1.98	0.45
1:L:329:GLY:O	1:L:333:LEU:HG	2.16	0.45
1:L:471:VAL:O	1:L:475:LYS:HG3	2.16	0.45
1:D:509:LEU:O	1:D:513:ILE:HG12	2.16	0.45
1:G:341:TYR:CE1	1:G:428:ALA:HB1	2.52	0.45
1:L:122:ASN:OD1	1:L:149:ASN:ND2	2.36	0.45
1:A:114:VAL:HG12	1:A:274:ALA:HB1	1.98	0.45
1:C:209:SER:O	1:C:212:THR:OG1	2.32	0.45
1:L:316:GLU:O	1:L:320:LYS:HG3	2.16	0.45
1:B:174:HIS:HB3	1:F:175:PHE:CD1	2.51	0.45
1:L:341:TYR:CE1	1:L:428:ALA:HB1	2.51	0.45
1:A:236:ARG:HG3	1:A:284:ALA:HB2	1.99	0.45
1:D:198:LEU:HD23	1:D:198:LEU:HA	1.76	0.45
1:D:320:LYS:NZ	7:D:1007:1PE:H142	2.31	0.45
1:K:341:TYR:CE1	1:K:428:ALA:HB1	2.52	0.45
1:K:364:ASP:O	1:K:420:ASN:HA	2.17	0.45
1:E:544:ILE:HD12	1:E:564:GLU:HG3	1.99	0.45
1:E:499:TYR:CD2	1:E:523:PRO:HB2	2.53	0.44
1:E:546:GLN:HG2	1:E:547:ILE:HG23	2.00	0.44
1:I:114:VAL:HG12	1:I:274:ALA:HB1	1.98	0.44
1:K:230:VAL:HG13	1:K:234:LEU:HB3	1.99	0.44
1:K:562:LEU:HD12	1:K:573:HIS:CD2	2.50	0.44
1:A:543:ASP:OD2	1:B:254:SER:OG	2.35	0.44
1:K:208:LEU:HD12	1:K:208:LEU:HA	1.84	0.44
1:E:198:LEU:HD22	1:E:202:ASP:HB3	1.98	0.44
1:H:230:VAL:HG12	1:H:234:LEU:HD23	1.99	0.44
1:J:214:LEU:HD21	1:J:222:LEU:HD22	2.00	0.44
1:J:488:THR:HG21	1:J:555:SER:HA	1.99	0.44
1:A:392:MET:HE2	1:A:392:MET:HB3	1.77	0.44
1:I:174:HIS:HB3	1:K:175:PHE:CD2	2.52	0.44
1:B:360:LYS:HE3	1:B:365:VAL:HG21	1.98	0.44
1:F:321:LEU:HD11	1:F:411:TYR:HA	1.99	0.44
1:F:392:MET:HE2	1:F:392:MET:HB3	1.94	0.44
1:H:499:TYR:OH	6:H:1010:DMS:H22	2.18	0.44
1:A:126:GLY:HA2	5:A:1005:SO4:O1	2.18	0.44
1:B:328:LEU:N	1:B:328:LEU:HD12	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:320:LYS:HE3	7:D:1007:1PE:H131	1.99	0.44
1:D:320:LYS:HZ2	7:D:1007:1PE:H221	1.82	0.44
1:E:306:ASN:C	1:E:377:THR:HG21	2.42	0.44
1:H:173:LYS:HA	1:H:173:LYS:HD3	1.81	0.44
1:J:411:TYR:HE1	7:J:1009:1PE:H242	1.83	0.44
1:C:103:TYR:O	7:C:1007:1PE:H242	2.17	0.44
1:G:525:TRP:CZ3	1:L:528:PRO:HB3	2.52	0.44
1:K:590:GLY:N	10:K:1115:HOH:O	2.42	0.44
1:D:320:LYS:HZ1	7:D:1007:1PE:C13	2.30	0.44
1:E:235:PHE:HE1	1:E:269:VAL:HG11	1.81	0.44
1:F:338:MET:HE2	10:F:1130:HOH:O	2.17	0.44
1:B:230:VAL:O	1:B:277:TYR:OH	2.31	0.43
1:C:395:LEU:HD11	1:C:581:TRP:CG	2.53	0.43
1:D:522:GLU:OE1	1:D:595:LEU:N	2.40	0.43
1:J:567:GLN:NE2	7:J:1011:1PE:H152	2.33	0.43
1:L:543:ASP:HB3	7:L:1007:1PE:H232	2.00	0.43
1:C:256:ASP:O	10:C:1101:HOH:O	2.21	0.43
1:D:364:ASP:O	1:D:420:ASN:HA	2.18	0.43
1:J:364:ASP:O	1:J:420:ASN:HA	2.18	0.43
1:K:236:ARG:NH2	10:K:1104:HOH:O	2.30	0.43
1:C:174:HIS:CE1	1:C:213:MET:HG2	2.53	0.43
1:I:174:HIS:CE1	1:I:213:MET:HE2	2.54	0.43
1:J:393:ILE:HG12	1:L:441:PRO:HG2	1.99	0.43
1:L:543:ASP:HB3	7:L:1007:1PE:H131	1.99	0.43
1:D:376:ILE:HB	1:D:399:ASP:HB3	2.00	0.43
5:K:1004:SO4:O4	1:L:436:LYS:HG2	2.18	0.43
1:D:96:PRO:HG2	1:D:303:ASN:O	2.17	0.43
1:E:364:ASP:O	1:E:420:ASN:HA	2.19	0.43
1:E:440:ARG:NH2	1:F:350:TYR:HE1	2.17	0.43
1:L:131:LEU:O	1:L:227:GLU:HB2	2.19	0.43
1:L:498:SER:O	1:L:523:PRO:HG2	2.18	0.43
1:A:274:ALA:O	1:A:278:LYS:HG3	2.18	0.43
1:J:283:LYS:HE2	1:J:287:TYR:CZ	2.54	0.43
1:A:328:LEU:HD23	1:A:332:GLU:HG2	2.01	0.43
1:D:320:LYS:NZ	7:D:1007:1PE:H221	2.33	0.43
1:H:165:PHE:HB3	1:H:189:TYR:OH	2.19	0.43
1:B:168:LYS:O	1:B:171:THR:HG22	2.19	0.43
1:C:95:ASP:HA	1:C:96:PRO:HD3	1.88	0.42
1:D:190:VAL:HG11	1:D:206:VAL:HG13	2.00	0.42
1:E:90:GLN:NE2	1:E:95:ASP:O	2.48	0.42
1:G:168:LYS:HD2	1:J:260:ASN:HD21	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:207:VAL:HG11	1:I:241:THR:HG22	2.01	0.42
1:I:341:TYR:CE1	1:I:428:ALA:HB1	2.53	0.42
1:L:350:TYR:HA	1:L:351:PRO:HD3	1.93	0.42
1:I:134:ASN:ND2	1:I:141:PRO:HD2	2.34	0.42
1:J:381:GLY:HA2	1:J:459:ASP:OD1	2.19	0.42
1:E:441:PRO:HB2	1:F:394:ASP:HA	2.01	0.42
1:I:522:GLU:HA	1:I:523:PRO:HD3	1.80	0.42
1:J:441:PRO:HB2	1:K:394:ASP:HA	2.00	0.42
1:L:95:ASP:HA	1:L:96:PRO:HD3	1.92	0.42
1:D:242:LEU:O	1:D:246:TYR:HB2	2.18	0.42
1:E:204:LYS:HB2	1:E:204:LYS:HE3	1.64	0.42
1:F:127:LEU:HD11	1:F:129:ILE:HD11	2.02	0.42
1:F:400:MET:CE	1:F:404:ALA:HB2	2.49	0.42
1:K:562:LEU:CD1	1:K:573:HIS:CD2	3.01	0.42
1:B:117:ILE:HD11	1:B:146:SER:HB2	2.01	0.42
1:D:336:LEU:HD13	1:D:338:MET:HE3	2.02	0.42
1:G:216:ASP:HB3	10:G:1125:HOH:O	2.20	0.42
1:H:287:TYR:O	1:H:291:THR:HG23	2.19	0.42
1:J:332:GLU:HG3	10:J:1263:HOH:O	2.19	0.42
1:D:85:ALA:HB1	10:D:1260:HOH:O	2.19	0.42
1:D:300:ALA:HA	1:D:301:PRO:HD3	1.78	0.42
1:D:320:LYS:CE	7:D:1007:1PE:H131	2.50	0.42
1:F:328:LEU:HB2	1:F:354:PHE:HB3	2.00	0.42
1:K:487:LEU:HD12	1:K:487:LEU:HA	1.78	0.42
1:L:225:VAL:HA	1:L:270:TYR:HB2	2.02	0.42
1:L:376:ILE:HD11	1:L:465:THR:HG21	2.01	0.42
1:D:230:VAL:HG12	1:D:234:LEU:HD23	2.02	0.42
1:H:311:SER:O	1:H:315:VAL:HG23	2.19	0.42
1:E:396:MET:SD	1:E:398:PHE:HE2	2.43	0.42
1:F:333:LEU:HD21	1:F:354:PHE:HB2	2.02	0.42
1:H:321:LEU:HD11	1:H:411:TYR:HA	2.02	0.42
1:H:510:ILE:HD13	1:H:526:TRP:NE1	2.34	0.42
1:I:283:LYS:HE2	1:I:287:TYR:CZ	2.55	0.42
1:J:376:ILE:HB	1:J:399:ASP:HB3	2.02	0.42
1:J:451:LYS:HG2	7:J:1011:1PE:H241	2.02	0.42
1:C:326:LYS:HG2	1:C:328:LEU:HD12	2.00	0.42
1:G:537:LEU:HA	1:G:545:ASN:HB2	2.01	0.42
1:A:174:HIS:HB3	1:D:175:PHE:CD2	2.55	0.41
1:A:483:ASP:OD2	1:A:573:HIS:ND1	2.35	0.41
1:I:346:LYS:HB3	1:I:437:ASN:O	2.20	0.41
1:A:121:CYS:HA	1:A:270:TYR:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:207:VAL:HG11	1:H:241:THR:HG22	2.01	0.41
1:A:148:VAL:O	1:A:150:ASP:N	2.48	0.41
1:A:321:LEU:HD11	1:A:411:TYR:HA	2.01	0.41
1:C:90:GLN:HB3	1:C:95:ASP:HB2	2.02	0.41
1:F:440:ARG:NH1	1:F:443:ASP:OD2	2.52	0.41
1:A:392:MET:H	6:A:1008:DMS:H11	1.84	0.41
1:B:236:ARG:NE	1:B:240:GLU:OE2	2.43	0.41
1:I:150:ASP:OD1	1:I:179:ASN:HB2	2.20	0.41
1:J:398:PHE:C	1:J:400:MET:H	2.28	0.41
1:A:169:LEU:HG	1:A:205:ARG:HD2	2.03	0.41
1:C:525:TRP:CE2	1:D:528:PRO:HD3	2.56	0.41
1:G:361:SER:HB3	10:G:1104:HOH:O	2.21	0.41
1:H:135:PRO:HA	1:H:194:SER:O	2.20	0.41
1:I:411:TYR:HE1	7:I:1009:1PE:H242	1.84	0.41
1:E:341:TYR:CE1	1:E:428:ALA:HB1	2.56	0.41
1:F:214:LEU:HD11	1:F:222:LEU:HD22	2.03	0.41
1:G:323:LEU:HD22	1:G:359:TYR:HB2	2.03	0.41
1:A:321:LEU:O	1:A:322:ASN:HB2	2.21	0.41
1:D:273:ASN:O	1:D:277:TYR:HD2	2.04	0.41
1:H:103:TYR:CD1	9:H:1007:2PE:H182	2.56	0.41
1:H:129:ILE:HG21	1:H:190:VAL:HG23	2.02	0.41
1:I:350:TYR:HA	1:I:351:PRO:HD3	1.93	0.41
1:J:233:ASN:ND2	10:J:1120:HOH:O	2.49	0.41
1:D:132:VAL:HG11	1:D:144:ILE:HD13	2.02	0.41
1:F:316:GLU:HG3	7:F:1009:1PE:H241	2.01	0.41
1:G:138:GLU:HA	1:G:194:SER:HB3	2.02	0.41
1:G:395:LEU:O	1:G:395:LEU:HG	2.20	0.41
1:J:407:LEU:HD23	1:J:407:LEU:HA	1.89	0.41
1:B:321:LEU:HD11	1:B:411:TYR:HA	2.02	0.41
1:C:135:PRO:HA	1:C:194:SER:O	2.21	0.41
1:C:551:VAL:HG12	1:C:553:ALA:H	1.86	0.41
1:D:282:GLU:O	1:D:286:VAL:HG23	2.21	0.41
1:H:528:PRO:HD3	1:K:525:TRP:CE2	2.56	0.41
1:J:164:LYS:HB2	1:J:164:LYS:HE3	1.73	0.41
1:E:104:ASN:HB3	10:E:1278:HOH:O	2.21	0.41
1:H:169:LEU:HD23	1:H:205:ARG:HH21	1.86	0.41
1:J:132:VAL:HG11	1:J:144:ILE:HD13	2.03	0.41
7:A:1010:1PE:H131	7:A:1010:1PE:H142	1.63	0.40
1:G:187:VAL:HG12	1:G:188:GLY:N	2.36	0.40
1:G:509:LEU:O	1:G:513:ILE:HG12	2.20	0.40
1:K:338:MET:HE2	10:K:1117:HOH:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:LEU:O	1:A:395:LEU:HG	2.21	0.40
1:F:236:ARG:NE	1:F:240:GLU:OE2	2.43	0.40
1:F:498:SER:O	1:F:523:PRO:HG2	2.21	0.40
1:J:85:ALA:HA	1:J:312:ASN:OD1	2.21	0.40
1:J:411:TYR:CE1	7:J:1009:1PE:H242	2.56	0.40
1:B:341:TYR:CE1	1:B:428:ALA:HB1	2.57	0.40
1:E:466:LEU:HD23	1:E:466:LEU:HA	1.94	0.40
1:H:369:ILE:HB	1:H:423:ILE:HD12	2.03	0.40
1:B:439:TYR:OH	1:B:458:THR:O	2.32	0.40
1:C:162:MET:HA	1:C:162:MET:HE2	2.04	0.40
1:D:301:PRO:HB3	1:F:442:GLY:O	2.21	0.40
1:L:440:ARG:NH2	10:L:1122:HOH:O	2.55	0.40
1:D:156:PHE:CG	1:D:177:MET:HE1	2.57	0.40
1:F:342:LEU:HD23	1:F:342:LEU:HA	1.98	0.40
1:F:398:PHE:C	1:F:400:MET:H	2.30	0.40
1:I:209:SER:O	1:I:212:THR:OG1	2.30	0.40
1:I:440:ARG:NH2	10:I:1135:HOH:O	2.54	0.40
1:J:230:VAL:HG12	1:J:234:LEU:HD23	2.01	0.40
1:L:407:LEU:HD23	1:L:407:LEU:HA	1.90	0.40

There are no symmetry-related clashes.

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	A	510/519 (98%)	495 (97%)	15 (3%)	0	100	100
1	B	505/519 (97%)	491 (97%)	14 (3%)	0	100	100
1	C	517/519 (100%)	503 (97%)	14 (3%)	0	100	100
1	D	513/519 (99%)	499 (97%)	14 (3%)	0	100	100
1	E	506/519 (98%)	491 (97%)	15 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	503/519 (97%)	487 (97%)	16 (3%)	0	100	100
1	G	513/519 (99%)	496 (97%)	17 (3%)	0	100	100
1	H	508/519 (98%)	496 (98%)	12 (2%)	0	100	100
1	I	517/519 (100%)	510 (99%)	6 (1%)	1 (0%)	43	55
1	J	513/519 (99%)	505 (98%)	8 (2%)	0	100	100
1	K	506/519 (98%)	496 (98%)	9 (2%)	1 (0%)	43	55
1	L	504/519 (97%)	493 (98%)	11 (2%)	0	100	100
All	All	6115/6228 (98%)	5962 (98%)	151 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	386	LYS
1	I	196	ALA

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	A	423/447 (95%)	420 (99%)	3 (1%)	76	87
1	B	402/447 (90%)	398 (99%)	4 (1%)	68	82
1	C	417/447 (93%)	415 (100%)	2 (0%)	81	90
1	D	415/447 (93%)	411 (99%)	4 (1%)	68	82
1	E	410/447 (92%)	405 (99%)	5 (1%)	63	79
1	F	404/447 (90%)	397 (98%)	7 (2%)	53	72
1	G	424/447 (95%)	419 (99%)	5 (1%)	63	79
1	H	402/447 (90%)	400 (100%)	2 (0%)	81	90
1	I	415/447 (93%)	410 (99%)	5 (1%)	63	79
1	J	422/447 (94%)	414 (98%)	8 (2%)	50	69
1	K	414/447 (93%)	411 (99%)	3 (1%)	76	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	L	398/447 (89%)	391 (98%)	7 (2%)	51 70
All	All	4946/5364 (92%)	4891 (99%)	55 (1%)	65 81

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	194	SER
1	A	398	PHE
1	A	439	TYR
1	B	398	PHE
1	B	406	VAL
1	B	439	TYR
1	B	544	ILE
1	C	171	THR
1	C	398	PHE
1	D	395	LEU
1	D	398	PHE
1	D	579	VAL
1	D	600	VAL
1	E	117	ILE
1	E	145	SER
1	E	230	VAL
1	E	324	GLU
1	E	400	MET
1	F	203	MET
1	F	322	ASN
1	F	398	PHE
1	F	445	ILE
1	F	518	LYS
1	F	579	VAL
1	F	601	LEU
1	G	117	ILE
1	G	200	GLU
1	G	398	PHE
1	G	438	SER
1	G	554	SER
1	H	181	ASN
1	H	439	TYR
1	I	168	LYS
1	I	171	THR
1	I	200	GLU
1	I	239	LEU

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Mol	Chain	Res	Type
1	I	554	SER
1	J	90	GLN
1	J	164	LYS
1	J	208	LEU
1	J	228	ILE
1	J	262	GLU
1	J	398	PHE
1	J	544	ILE
1	J	579	VAL
1	K	204	LYS
1	K	332	GLU
1	K	398	PHE
1	L	88	VAL
1	L	101	ILE
1	L	200	GLU
1	L	205	ARG
1	L	392	MET
1	L	398	PHE
1	L	579	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	139	ASN
1	A	420	ASN
1	A	531	ASN
1	B	174	HIS
1	C	183	ASN
1	C	437	ASN
1	D	139	ASN
1	D	183	ASN
1	E	174	HIS
1	F	420	ASN
1	F	515	GLN
1	G	181	ASN
1	G	272	ASN
1	H	420	ASN
1	I	134	ASN
1	I	174	HIS
1	I	215	HIS
1	I	521	ASN
1	J	139	ASN

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Mol	Chain	Res	Type
1	J	174	HIS
1	J	420	ASN
1	K	181	ASN
1	K	567	GLN
1	K	573	HIS
1	L	134	ASN
1	L	521	ASN
1	L	568	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 111 ligands modelled in this entry, 12 are monoatomic - leaving 99 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	$\# Z > 2$
8	EDO	L	1006	-	3,3,3	0.39	0	2,2,2	0.50	0
8	EDO	I	1007	-	3,3,3	0.40	0	2,2,2	0.75	0
6	DMS	B	1006	-	3,3,3	0.77	0	3,3,3	0.67	0
8	EDO	J	1006	-	3,3,3	0.47	0	2,2,2	0.25	0
5	SO4	J	1004	-	4,4,4	0.19	0	6,6,6	0.14	0
5	SO4	K	1005	-	4,4,4	0.25	0	6,6,6	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SO4	I	1006	-	4,4,4	0.22	0	6,6,6	0.17	0
7	1PE	D	1008	-	6,6,15	0.45	0	5,5,14	0.36	0
7	1PE	L	1009	-	6,6,15	0.49	0	5,5,14	0.43	0
7	1PE	C	1008	-	11,11,15	0.58	0	10,10,14	0.45	0
5	SO4	D	1004	-	4,4,4	0.25	0	6,6,6	0.16	0
3	CO3	I	1002	-	3,3,3	0.49	0	2,3,3	0.23	0
5	SO4	A	1006	-	4,4,4	0.35	0	6,6,6	0.18	0
2	J4V	K	1001	4	36,37,37	2.12	5 (13%)	50,55,55	2.26	7 (14%)
5	SO4	D	1005	-	4,4,4	0.25	0	6,6,6	0.16	0
5	SO4	E	1004	-	4,4,4	0.27	0	6,6,6	0.08	0
3	CO3	C	1002	-	3,3,3	0.31	0	2,3,3	0.45	0
7	1PE	L	1010	-	4,4,15	0.46	0	3,3,14	0.36	0
8	EDO	G	1007	-	3,3,3	0.54	0	2,2,2	0.11	0
6	DMS	A	1008	-	3,3,3	0.66	0	3,3,3	0.36	0
3	CO3	K	1002	-	3,3,3	0.56	0	2,3,3	0.74	0
3	CO3	J	1002	-	3,3,3	0.98	0	2,3,3	0.52	0
5	SO4	A	1004	-	4,4,4	0.20	0	6,6,6	0.09	0
5	SO4	C	1004	-	4,4,4	0.17	0	6,6,6	0.24	0
5	SO4	J	1005	-	4,4,4	0.25	0	6,6,6	0.21	0
7	1PE	I	1009	-	8,8,15	0.46	0	7,7,14	0.44	0
5	SO4	C	1005	-	4,4,4	0.22	0	6,6,6	0.18	0
8	EDO	K	1009	-	3,3,3	0.55	0	2,2,2	0.31	0
6	DMS	B	1005	-	3,3,3	0.62	0	3,3,3	0.94	0
9	2PE	H	1007	-	24,24,27	0.56	0	23,23,26	0.30	0
8	EDO	E	1006	-	3,3,3	0.52	0	2,2,2	0.17	0
2	J4V	L	1001	4	36,37,37	2.08	8 (22%)	50,55,55	2.43	6 (12%)
5	SO4	H	1006	-	4,4,4	0.20	0	6,6,6	0.15	0
2	J4V	C	1001	4	36,37,37	1.95	8 (22%)	50,55,55	2.56	8 (16%)
5	SO4	A	1005	-	4,4,4	0.28	0	6,6,6	0.33	0
5	SO4	K	1006	-	4,4,4	0.20	0	6,6,6	0.17	0
7	1PE	F	1009	-	8,8,15	0.59	0	7,7,14	0.41	0
2	J4V	F	1001	4	36,37,37	2.39	10 (27%)	50,55,55	2.44	7 (14%)
3	CO3	E	1002	-	3,3,3	0.65	0	2,3,3	0.27	0
5	SO4	D	1006	-	4,4,4	0.18	0	6,6,6	0.14	0
7	1PE	J	1011	-	12,12,15	0.56	0	11,11,14	0.43	0
5	SO4	H	1004	-	4,4,4	0.26	0	6,6,6	0.31	0
8	EDO	F	1007	-	3,3,3	0.45	0	2,2,2	0.35	0
5	SO4	C	1006	-	4,4,4	0.34	0	6,6,6	0.18	0
7	1PE	K	1012	-	12,12,15	0.55	0	11,11,14	0.33	0
7	1PE	I	1008	-	11,11,15	0.55	0	10,10,14	0.41	0
5	SO4	E	1005	-	4,4,4	0.21	0	6,6,6	0.21	0
3	CO3	D	1002	-	3,3,3	0.91	0	2,3,3	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	EDO	J	1007	-	3,3,3	0.49	0	2,2,2	0.16	0
7	1PE	L	1007	-	12,12,15	0.57	0	11,11,14	0.54	0
5	SO4	I	1004	-	4,4,4	0.23	0	6,6,6	0.23	0
7	1PE	A	1009	-	14,14,15	0.56	0	13,13,14	0.44	0
2	J4V	E	1001	4	36,37,37	2.19	8 (22%)	50,55,55	2.41	6 (12%)
3	CO3	L	1002	-	3,3,3	0.63	0	2,3,3	0.35	0
7	1PE	J	1009	-	8,8,15	0.58	0	7,7,14	0.43	0
3	CO3	H	1002	-	3,3,3	0.88	0	2,3,3	0.09	0
3	CO3	F	1002	-	3,3,3	0.40	0	2,3,3	0.67	0
2	J4V	H	1001	4	36,37,37	2.40	8 (22%)	50,55,55	2.28	8 (16%)
3	CO3	G	1002	-	3,3,3	0.83	0	2,3,3	1.15	0
8	EDO	J	1008	-	3,3,3	0.47	0	2,2,2	0.35	0
7	1PE	G	1008	-	8,8,15	0.58	0	7,7,14	0.39	0
7	1PE	L	1008	-	11,11,15	0.57	0	10,10,14	0.43	0
7	1PE	J	1010	-	8,8,15	0.54	0	7,7,14	0.37	0
2	J4V	B	1001	4	36,37,37	1.94	6 (16%)	50,55,55	2.49	6 (12%)
8	EDO	K	1010	-	3,3,3	0.48	0	2,2,2	0.47	0
5	SO4	L	1004	-	4,4,4	0.27	0	6,6,6	0.10	0
2	J4V	J	1001	4	36,37,37	2.36	8 (22%)	50,55,55	2.31	7 (14%)
7	1PE	F	1008	-	8,8,15	0.56	0	7,7,14	0.48	0
6	DMS	H	1010	-	3,3,3	0.76	0	3,3,3	0.41	0
3	CO3	B	1002	-	3,3,3	1.03	0	2,3,3	0.54	0
5	SO4	L	1005	-	4,4,4	0.26	0	6,6,6	0.18	0
5	SO4	A	1007	-	4,4,4	0.32	0	6,6,6	0.21	0
5	SO4	F	1004	-	4,4,4	0.34	0	6,6,6	0.11	0
8	EDO	F	1006	-	3,3,3	0.45	0	2,2,2	0.51	0
8	EDO	H	1009	-	3,3,3	0.47	0	2,2,2	0.59	0
6	DMS	B	1007	-	3,3,3	0.73	0	3,3,3	0.74	0
5	SO4	F	1005	-	4,4,4	0.27	0	6,6,6	0.22	0
7	1PE	B	1008	-	8,8,15	0.52	0	7,7,14	0.47	0
2	J4V	D	1001	4	36,37,37	2.20	8 (22%)	50,55,55	2.37	6 (12%)
5	SO4	I	1005	-	4,4,4	0.27	0	6,6,6	0.19	0
3	CO3	A	1002	-	3,3,3	0.90	0	2,3,3	0.17	0
5	SO4	K	1004	-	4,4,4	0.19	0	6,6,6	0.17	0
5	SO4	B	1004	-	4,4,4	0.21	0	6,6,6	0.17	0
5	SO4	H	1005	-	4,4,4	0.25	0	6,6,6	0.19	0
7	1PE	G	1009	-	8,8,15	0.57	0	7,7,14	0.40	0
8	EDO	K	1008	-	3,3,3	0.46	0	2,2,2	0.37	0
7	1PE	D	1007	-	11,11,15	0.55	0	10,10,14	0.41	0
7	1PE	H	1008	-	8,8,15	0.49	0	7,7,14	0.54	0
7	1PE	C	1007	-	14,14,15	0.53	0	13,13,14	0.46	0
5	SO4	G	1004	-	4,4,4	0.24	0	6,6,6	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	J4V	A	1001	4	36,37,37	2.14	8 (22%)	50,55,55	2.38	7 (14%)
7	1PE	K	1013	-	14,14,15	0.57	0	13,13,14	0.44	0
5	SO4	G	1005	-	4,4,4	0.28	0	6,6,6	0.21	0
8	EDO	K	1011	-	3,3,3	0.47	0	2,2,2	0.29	0
2	J4V	I	1001	4	36,37,37	1.92	5 (13%)	50,55,55	2.38	6 (12%)
6	DMS	G	1006	-	3,3,3	0.72	0	3,3,3	0.47	0
5	SO4	K	1007	-	4,4,4	0.23	0	6,6,6	0.05	0
2	J4V	G	1001	4	36,37,37	1.94	5 (13%)	50,55,55	2.41	7 (14%)
7	1PE	A	1010	-	11,11,15	0.52	0	10,10,14	0.43	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
8	EDO	L	1006	-	-	0/1/1/1	-
7	1PE	A	1009	-	-	8/12/12/13	-
2	J4V	E	1001	4	-	2/22/50/50	0/6/5/5
7	1PE	J	1009	-	-	3/6/6/13	-
2	J4V	C	1001	4	-	2/22/50/50	0/6/5/5
2	J4V	D	1001	4	-	2/22/50/50	0/6/5/5
8	EDO	I	1007	-	-	0/1/1/1	-
2	J4V	H	1001	4	-	0/22/50/50	0/6/5/5
8	EDO	J	1006	-	-	0/1/1/1	-
7	1PE	F	1009	-	-	3/6/6/13	-
8	EDO	J	1008	-	-	1/1/1/1	-
7	1PE	D	1008	-	-	3/4/4/13	-
7	1PE	G	1009	-	-	5/6/6/13	-
7	1PE	L	1009	-	-	2/4/4/13	-
7	1PE	G	1008	-	-	2/6/6/13	-
7	1PE	D	1007	-	-	5/9/9/13	-
7	1PE	L	1008	-	-	3/9/9/13	-
2	J4V	F	1001	4	-	2/22/50/50	0/6/5/5
7	1PE	J	1010	-	-	3/6/6/13	-
8	EDO	K	1008	-	-	0/1/1/1	-
2	J4V	B	1001	4	-	2/22/50/50	0/6/5/5
7	1PE	H	1008	-	-	4/6/6/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	EDO	K	1010	-	-	1/1/1/1	-
7	1PE	C	1008	-	-	6/9/9/13	-
7	1PE	C	1007	-	-	3/12/12/13	-
8	EDO	H	1009	-	-	1/1/1/1	-
7	1PE	J	1011	-	-	5/10/10/13	-
8	EDO	F	1007	-	-	0/1/1/1	-
2	J4V	J	1001	4	-	0/22/50/50	0/6/5/5
2	J4V	K	1001	4	-	0/22/50/50	0/6/5/5
7	1PE	F	1008	-	-	5/6/6/13	-
7	1PE	K	1012	-	-	7/10/10/13	-
2	J4V	A	1001	4	-	4/22/50/50	0/6/5/5
7	1PE	L	1010	-	-	1/2/2/13	-
7	1PE	I	1008	-	-	8/9/9/13	-
7	1PE	K	1013	-	-	5/12/12/13	-
8	EDO	G	1007	-	-	0/1/1/1	-
7	1PE	I	1009	-	-	3/6/6/13	-
8	EDO	K	1011	-	-	0/1/1/1	-
2	J4V	I	1001	4	-	2/22/50/50	0/6/5/5
8	EDO	J	1007	-	-	0/1/1/1	-
8	EDO	K	1009	-	-	0/1/1/1	-
9	2PE	H	1007	-	-	7/22/22/25	-
8	EDO	F	1006	-	-	1/1/1/1	-
7	1PE	L	1007	-	-	4/10/10/13	-
2	J4V	G	1001	4	-	2/22/50/50	0/6/5/5
8	EDO	E	1006	-	-	1/1/1/1	-
2	J4V	L	1001	4	-	2/22/50/50	0/6/5/5
7	1PE	A	1010	-	-	5/9/9/13	-
7	1PE	B	1008	-	-	4/6/6/13	-

All (87) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	1001	J4V	CAC-CA	-8.33	1.39	1.52
2	E	1001	J4V	CAC-CA	-8.32	1.39	1.52
2	L	1001	J4V	CAC-CA	-7.89	1.40	1.52
2	I	1001	J4V	CAC-CA	-7.81	1.40	1.52
2	B	1001	J4V	CAC-CA	-7.80	1.40	1.52
2	F	1001	J4V	CAC-CA	-7.72	1.40	1.52
2	A	1001	J4V	CAC-CA	-7.63	1.40	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1001	J4V	CAC-CA	-7.62	1.41	1.52
2	J	1001	J4V	OAT-NAS	7.50	1.58	1.40
2	H	1001	J4V	FAN-CAJ	7.02	1.45	1.34
2	G	1001	J4V	CAC-CA	-6.90	1.42	1.52
2	D	1001	J4V	CAC-CA	-6.79	1.42	1.52
2	C	1001	J4V	CAC-CA	-6.77	1.42	1.52
2	J	1001	J4V	CAC-CA	-6.51	1.42	1.52
2	F	1001	J4V	OAT-NAS	6.26	1.55	1.40
2	D	1001	J4V	OAT-NAS	5.83	1.54	1.40
2	D	1001	J4V	CBD-CBE	-5.36	1.38	1.52
2	K	1001	J4V	CBA-CBE	-4.77	1.39	1.52
2	A	1001	J4V	CBD-CBE	-4.59	1.40	1.52
2	J	1001	J4V	CBD-CBE	-4.55	1.40	1.52
2	F	1001	J4V	FAN-CAJ	-4.54	1.28	1.34
2	H	1001	J4V	CBD-CBE	-4.52	1.40	1.52
2	F	1001	J4V	CBD-CBE	-4.41	1.40	1.52
2	E	1001	J4V	FAN-CAJ	4.40	1.41	1.34
2	H	1001	J4V	CBG-CBE	-4.30	1.41	1.52
2	K	1001	J4V	CBD-CBE	-4.23	1.41	1.52
2	C	1001	J4V	CBA-CBE	-4.22	1.41	1.52
2	H	1001	J4V	CAG-CAF	-4.19	1.39	1.49
2	E	1001	J4V	CBD-CBE	-4.15	1.41	1.52
2	L	1001	J4V	OAT-NAS	4.14	1.50	1.40
2	E	1001	J4V	CAG-CAF	-4.12	1.39	1.49
2	H	1001	J4V	CBA-CBE	-4.11	1.41	1.52
2	L	1001	J4V	CAG-CAF	-4.05	1.39	1.49
2	G	1001	J4V	CAG-CAF	-4.05	1.39	1.49
2	J	1001	J4V	CBG-CBE	-4.03	1.41	1.52
2	J	1001	J4V	FAN-CAJ	-4.02	1.29	1.34
2	I	1001	J4V	CBG-CBE	-3.98	1.41	1.52
2	B	1001	J4V	CAG-CAF	-3.94	1.39	1.49
2	B	1001	J4V	CBD-CBE	-3.93	1.42	1.52
2	A	1001	J4V	CBA-CBE	-3.92	1.42	1.52
2	G	1001	J4V	CBG-CBE	-3.90	1.42	1.52
2	G	1001	J4V	CBA-CBE	-3.79	1.42	1.52
2	J	1001	J4V	CBA-CBE	-3.78	1.42	1.52
2	A	1001	J4V	CAG-CAF	-3.77	1.40	1.49
2	K	1001	J4V	CAG-CAF	-3.75	1.40	1.49
2	K	1001	J4V	CBG-CBE	-3.69	1.42	1.52
2	E	1001	J4V	CBG-CBE	-3.67	1.42	1.52
2	I	1001	J4V	CAG-CAF	-3.67	1.40	1.49
2	J	1001	J4V	CAG-CAF	-3.57	1.40	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	1001	J4V	CBD-CBE	-3.55	1.43	1.52
2	I	1001	J4V	CBA-CBE	-3.54	1.43	1.52
2	F	1001	J4V	CAG-CAF	-3.50	1.40	1.49
2	B	1001	J4V	CBA-CBE	-3.50	1.43	1.52
2	L	1001	J4V	CBA-CBE	-3.49	1.43	1.52
2	G	1001	J4V	CBD-CBE	-3.48	1.43	1.52
2	D	1001	J4V	CBA-CBE	-3.48	1.43	1.52
2	I	1001	J4V	CBD-CBE	-3.44	1.43	1.52
2	C	1001	J4V	CAG-CAF	-3.38	1.41	1.49
2	F	1001	J4V	FAO-CAI	3.36	1.44	1.35
2	C	1001	J4V	CBD-CBE	-3.30	1.43	1.52
2	L	1001	J4V	CBG-CBE	-3.22	1.44	1.52
2	D	1001	J4V	CAG-CAF	-3.19	1.41	1.49
2	A	1001	J4V	CBG-CBE	-3.00	1.44	1.52
2	D	1001	J4V	FAM-CAK	2.96	1.43	1.35
2	D	1001	J4V	CBG-CBE	-2.88	1.44	1.52
2	C	1001	J4V	OAT-NAS	2.87	1.46	1.40
2	B	1001	J4V	CBG-CBE	-2.81	1.45	1.52
2	D	1001	J4V	FAO-CAI	2.80	1.43	1.35
2	F	1001	J4V	CBA-CBE	-2.80	1.45	1.52
2	H	1001	J4V	FAM-CAK	2.79	1.43	1.35
2	E	1001	J4V	CBA-CBE	-2.67	1.45	1.52
2	A	1001	J4V	CAW-CAY	-2.64	1.50	1.54
2	A	1001	J4V	CAW-CAV	2.64	1.56	1.51
2	F	1001	J4V	FAM-CAK	2.54	1.42	1.35
2	H	1001	J4V	OAT-NAS	2.53	1.46	1.40
2	F	1001	J4V	CBG-CBE	-2.50	1.46	1.52
2	C	1001	J4V	CAW-CAV	2.46	1.56	1.51
2	E	1001	J4V	OAT-NAS	2.37	1.45	1.40
2	J	1001	J4V	FAM-CAK	2.34	1.41	1.35
2	A	1001	J4V	CBB-CAY	2.33	1.58	1.53
2	C	1001	J4V	CBG-CBE	-2.31	1.46	1.52
2	C	1001	J4V	FAN-CAJ	2.26	1.38	1.34
2	F	1001	J4V	CAW-CAV	2.20	1.55	1.51
2	L	1001	J4V	CAW-CAV	2.19	1.55	1.51
2	B	1001	J4V	CAW-CAZ	2.12	1.57	1.54
2	L	1001	J4V	CBB-CBC	2.04	1.58	1.52
2	E	1001	J4V	CBF-CAZ	2.02	1.58	1.53

All (81) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1001	J4V	CAY-CBG-CBE	-8.72	94.88	110.16
2	B	1001	J4V	CAZ-CBA-CBE	-8.66	94.99	110.16
2	E	1001	J4V	CAY-CBG-CBE	-8.64	95.02	110.16
2	I	1001	J4V	CAY-CBG-CBE	-8.63	95.04	110.16
2	C	1001	J4V	CAZ-CBA-CBE	-8.62	95.05	110.16
2	L	1001	J4V	CAY-CBG-CBE	-8.55	95.18	110.16
2	G	1001	J4V	CAZ-CBA-CBE	-8.53	95.22	110.16
2	B	1001	J4V	CAY-CBG-CBE	-8.38	95.48	110.16
2	D	1001	J4V	CAY-CBG-CBE	-8.37	95.49	110.16
2	C	1001	J4V	CAY-CBG-CBE	-8.33	95.57	110.16
2	A	1001	J4V	CAY-CBG-CBE	-8.01	96.12	110.16
2	J	1001	J4V	CAY-CBG-CBE	-7.92	96.29	110.16
2	L	1001	J4V	CAZ-CBA-CBE	-7.83	96.45	110.16
2	I	1001	J4V	CAZ-CBA-CBE	-7.75	96.58	110.16
2	A	1001	J4V	CAZ-CBA-CBE	-7.71	96.65	110.16
2	D	1001	J4V	CAZ-CBA-CBE	-7.69	96.69	110.16
2	F	1001	J4V	CAZ-CBA-CBE	-7.62	96.80	110.16
2	E	1001	J4V	CAZ-CBA-CBE	-7.56	96.91	110.16
2	G	1001	J4V	CAY-CBG-CBE	-7.51	97.00	110.16
2	C	1001	J4V	CBE-CBD-CBC	-7.30	94.69	109.90
2	F	1001	J4V	CBE-CBD-CBC	-7.27	94.75	109.90
2	K	1001	J4V	CAY-CBG-CBE	-7.11	97.70	110.16
2	K	1001	J4V	CAZ-CBA-CBE	-7.08	97.75	110.16
2	L	1001	J4V	CBE-CBD-CBC	-7.03	95.25	109.90
2	H	1001	J4V	CAY-CBG-CBE	-7.01	97.88	110.16
2	H	1001	J4V	CAZ-CBA-CBE	-7.00	97.89	110.16
2	B	1001	J4V	CBE-CBD-CBC	-6.91	95.50	109.90
2	D	1001	J4V	CBE-CBD-CBC	-6.91	95.51	109.90
2	J	1001	J4V	CAZ-CBA-CBE	-6.85	98.16	110.16
2	E	1001	J4V	CBE-CBD-CBC	-6.80	95.73	109.90
2	H	1001	J4V	CBE-CBD-CBC	-6.68	95.99	109.90
2	I	1001	J4V	CBE-CBD-CBC	-6.66	96.03	109.90
2	J	1001	J4V	CBE-CBD-CBC	-6.63	96.08	109.90
2	G	1001	J4V	CBE-CBD-CBC	-6.56	96.22	109.90
2	K	1001	J4V	CBE-CBD-CBC	-6.36	96.64	109.90
2	A	1001	J4V	CBE-CBD-CBC	-6.36	96.65	109.90
2	L	1001	J4V	CBG-CBE-CBD	5.96	121.03	109.69
2	A	1001	J4V	CBG-CBE-CBD	5.77	120.66	109.69
2	G	1001	J4V	CBG-CBE-CBD	5.71	120.55	109.69
2	I	1001	J4V	CBG-CBE-CBD	5.62	120.38	109.69
2	F	1001	J4V	CBG-CBE-CBD	5.60	120.34	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1001	J4V	CBG-CBE-CBD	5.59	120.32	109.69
2	J	1001	J4V	CBG-CBE-CBD	5.57	120.27	109.69
2	B	1001	J4V	CBG-CBE-CBD	5.45	120.05	109.69
2	C	1001	J4V	CBG-CBE-CBA	5.36	119.88	109.69
2	H	1001	J4V	CBD-CBE-CBA	5.27	119.70	109.69
2	B	1001	J4V	CBG-CBE-CBA	5.24	119.65	109.69
2	E	1001	J4V	CBD-CBE-CBA	5.20	119.57	109.69
2	C	1001	J4V	CBG-CBE-CBD	5.17	119.52	109.69
2	A	1001	J4V	CBD-CBE-CBA	5.16	119.50	109.69
2	E	1001	J4V	CBG-CBE-CBA	5.15	119.49	109.69
2	K	1001	J4V	CBG-CBE-CBD	5.11	119.40	109.69
2	K	1001	J4V	CBD-CBE-CBA	5.10	119.39	109.69
2	D	1001	J4V	CBG-CBE-CBA	5.09	119.37	109.69
2	I	1001	J4V	CBG-CBE-CBA	5.09	119.37	109.69
2	C	1001	J4V	CBD-CBE-CBA	5.07	119.33	109.69
2	F	1001	J4V	CBG-CBE-CBA	5.07	119.33	109.69
2	E	1001	J4V	CBG-CBE-CBD	5.05	119.30	109.69
2	G	1001	J4V	CBD-CBE-CBA	4.96	119.12	109.69
2	H	1001	J4V	CBG-CBE-CBA	4.96	119.11	109.69
2	B	1001	J4V	CBD-CBE-CBA	4.95	119.09	109.69
2	J	1001	J4V	CBD-CBE-CBA	4.94	119.09	109.69
2	D	1001	J4V	CBD-CBE-CBA	4.84	118.90	109.69
2	F	1001	J4V	CBD-CBE-CBA	4.84	118.89	109.69
2	L	1001	J4V	CBD-CBE-CBA	4.82	118.85	109.69
2	G	1001	J4V	CBG-CBE-CBA	4.79	118.79	109.69
2	K	1001	J4V	CBG-CBE-CBA	4.77	118.75	109.69
2	L	1001	J4V	CBG-CBE-CBA	4.73	118.68	109.69
2	H	1001	J4V	CBG-CBE-CBD	4.71	118.64	109.69
2	J	1001	J4V	CBG-CBE-CBA	4.68	118.58	109.69
2	I	1001	J4V	CBD-CBE-CBA	4.56	118.36	109.69
2	A	1001	J4V	CBG-CBE-CBA	4.38	118.02	109.69
2	C	1001	J4V	CAW-CAV-N	2.82	121.22	114.82
2	F	1001	J4V	CAK-CAJ-CAI	2.37	120.85	118.71
2	A	1001	J4V	CAC-CA-C	2.30	113.84	108.42
2	C	1001	J4V	CA-N-CAV	-2.27	116.54	121.18
2	G	1001	J4V	CAW-CAV-N	2.26	119.94	114.82
2	K	1001	J4V	CA-N-CAV	2.20	125.69	121.18
2	J	1001	J4V	CBA-CAZ-CAW	-2.19	106.71	109.35
2	H	1001	J4V	CAD-CAE-CAF	-2.09	118.44	121.12
2	H	1001	J4V	CA-N-CAV	2.03	125.35	121.18

There are no chirality outliers.

All (129) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1001	J4V	OAX-CAV-CAW-CAZ
2	B	1001	J4V	N-CAV-CAW-CAZ
2	C	1001	J4V	N-CAV-CAW-CAZ
2	G	1001	J4V	N-CAV-CAW-CAZ
7	D	1007	1PE	C13-C23-OH3-C22
7	A	1009	1PE	OH4-C13-C23-OH3
7	K	1012	1PE	OH5-C14-C24-OH4
7	C	1008	1PE	OH4-C13-C23-OH3
7	G	1009	1PE	OH5-C14-C24-OH4
7	K	1013	1PE	OH5-C14-C24-OH4
9	H	1007	2PE	O13-C14-C15-O16
7	B	1008	1PE	OH4-C13-C23-OH3
7	C	1007	1PE	OH4-C13-C23-OH3
7	K	1012	1PE	OH4-C13-C23-OH3
7	I	1009	1PE	OH4-C13-C23-OH3
7	B	1008	1PE	OH5-C14-C24-OH4
7	A	1010	1PE	C14-C24-OH4-C13
7	G	1009	1PE	OH6-C15-C25-OH5
7	L	1009	1PE	OH5-C14-C24-OH4
7	H	1008	1PE	OH5-C14-C24-OH4
7	L	1008	1PE	OH4-C13-C23-OH3
7	K	1013	1PE	OH4-C13-C23-OH3
7	G	1008	1PE	OH6-C15-C25-OH5
7	I	1008	1PE	OH4-C13-C23-OH3
7	L	1007	1PE	OH4-C13-C23-OH3
7	L	1007	1PE	OH7-C16-C26-OH6
7	L	1010	1PE	OH5-C14-C24-OH4
7	I	1008	1PE	OH5-C14-C24-OH4
7	A	1009	1PE	OH7-C16-C26-OH6
7	F	1009	1PE	OH6-C15-C25-OH5
7	A	1009	1PE	OH5-C14-C24-OH4
7	H	1008	1PE	OH4-C13-C23-OH3
7	F	1008	1PE	OH5-C14-C24-OH4
7	A	1009	1PE	OH6-C15-C25-OH5
7	D	1008	1PE	OH6-C15-C25-OH5
7	F	1008	1PE	OH6-C15-C25-OH5
7	J	1010	1PE	OH6-C15-C25-OH5
7	L	1009	1PE	OH4-C13-C23-OH3
9	H	1007	2PE	O4-C5-C6-O7
7	D	1007	1PE	OH6-C15-C25-OH5
8	K	1010	EDO	O1-C1-C2-O2
7	C	1007	1PE	OH6-C15-C25-OH5

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Mol	Chain	Res	Type	Atoms
9	H	1007	2PE	O16-C17-C18-O19
7	J	1009	1PE	C23-C13-OH4-C24
7	K	1012	1PE	OH6-C15-C25-OH5
7	I	1008	1PE	C16-C26-OH6-C15
7	B	1008	1PE	C13-C23-OH3-C22
8	E	1006	EDO	O1-C1-C2-O2
8	J	1008	EDO	O1-C1-C2-O2
7	C	1008	1PE	C12-C22-OH3-C23
7	K	1012	1PE	C25-C15-OH6-C26
7	L	1008	1PE	OH5-C14-C24-OH4
7	K	1013	1PE	C13-C23-OH3-C22
7	D	1008	1PE	C15-C25-OH5-C14
7	D	1007	1PE	C15-C25-OH5-C14
7	K	1012	1PE	C13-C23-OH3-C22
7	A	1009	1PE	C25-C15-OH6-C26
7	I	1008	1PE	C23-C13-OH4-C24
7	F	1009	1PE	C24-C14-OH5-C25
7	G	1009	1PE	C14-C24-OH4-C13
7	C	1007	1PE	C23-C13-OH4-C24
7	A	1010	1PE	C24-C14-OH5-C25
2	C	1001	J4V	OAX-CAV-CAW-CAZ
2	D	1001	J4V	OAX-CAV-CAW-CAZ
2	D	1001	J4V	N-CAV-CAW-CAZ
2	G	1001	J4V	OAX-CAV-CAW-CAZ
7	D	1008	1PE	C24-C14-OH5-C25
7	L	1008	1PE	C14-C24-OH4-C13
8	F	1006	EDO	O1-C1-C2-O2
7	L	1007	1PE	C25-C15-OH6-C26
7	I	1009	1PE	C23-C13-OH4-C24
7	C	1008	1PE	C15-C25-OH5-C14
7	I	1008	1PE	OH6-C15-C25-OH5
7	G	1008	1PE	C23-C13-OH4-C24
9	H	1007	2PE	C14-C15-O16-C17
7	J	1010	1PE	OH5-C14-C24-OH4
7	F	1008	1PE	C24-C14-OH5-C25
9	H	1007	2PE	C11-C12-O13-C14
7	F	1008	1PE	C14-C24-OH4-C13
7	J	1011	1PE	C23-C13-OH4-C24
7	D	1007	1PE	OH5-C14-C24-OH4
7	A	1010	1PE	OH6-C15-C25-OH5
7	H	1008	1PE	C14-C24-OH4-C13
7	C	1008	1PE	C14-C24-OH4-C13

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Mol	Chain	Res	Type	Atoms
7	A	1009	1PE	C24-C14-OH5-C25
7	G	1009	1PE	C23-C13-OH4-C24
7	I	1009	1PE	C14-C24-OH4-C13
7	I	1008	1PE	C24-C14-OH5-C25
7	J	1011	1PE	C13-C23-OH3-C22
9	H	1007	2PE	O7-C8-C9-O10
7	C	1008	1PE	OH5-C14-C24-OH4
7	K	1012	1PE	C24-C14-OH5-C25
7	B	1008	1PE	C24-C14-OH5-C25
7	K	1013	1PE	C12-C22-OH3-C23
7	A	1009	1PE	C13-C23-OH3-C22
9	H	1007	2PE	C15-C14-O13-C12
7	J	1009	1PE	OH6-C15-C25-OH5
7	G	1009	1PE	C24-C14-OH5-C25
7	F	1009	1PE	C23-C13-OH4-C24
7	J	1011	1PE	OH5-C14-C24-OH4
7	A	1009	1PE	C12-C22-OH3-C23
7	I	1008	1PE	C15-C25-OH5-C14
7	D	1007	1PE	OH4-C13-C23-OH3
2	A	1001	J4V	OAX-CAV-CAW-CAZ
2	A	1001	J4V	N-CAV-CAW-CAZ
2	E	1001	J4V	OAX-CAV-CAW-CAZ
2	E	1001	J4V	N-CAV-CAW-CAZ
2	F	1001	J4V	OAX-CAV-CAW-CAZ
2	F	1001	J4V	N-CAV-CAW-CAZ
2	I	1001	J4V	OAX-CAV-CAW-CAZ
2	I	1001	J4V	N-CAV-CAW-CAZ
2	L	1001	J4V	OAX-CAV-CAW-CAZ
2	L	1001	J4V	N-CAV-CAW-CAZ
7	H	1008	1PE	C13-C23-OH3-C22
7	A	1010	1PE	OH5-C14-C24-OH4
8	H	1009	EDO	O1-C1-C2-O2
2	A	1001	J4V	N-CA-CAC-CAB
7	J	1010	1PE	C24-C14-OH5-C25
7	K	1012	1PE	C12-C22-OH3-C23
7	I	1008	1PE	C14-C24-OH4-C13
7	C	1008	1PE	C23-C13-OH4-C24
7	L	1007	1PE	C15-C25-OH5-C14
7	K	1013	1PE	OH7-C16-C26-OH6
7	J	1009	1PE	C24-C14-OH5-C25
7	F	1008	1PE	C23-C13-OH4-C24
7	J	1011	1PE	OH4-C13-C23-OH3

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Mol	Chain	Res	Type	Atoms
2	A	1001	J4V	N-CA-CAC-CAD
7	A	1010	1PE	OH4-C13-C23-OH3
7	J	1011	1PE	C15-C25-OH5-C14

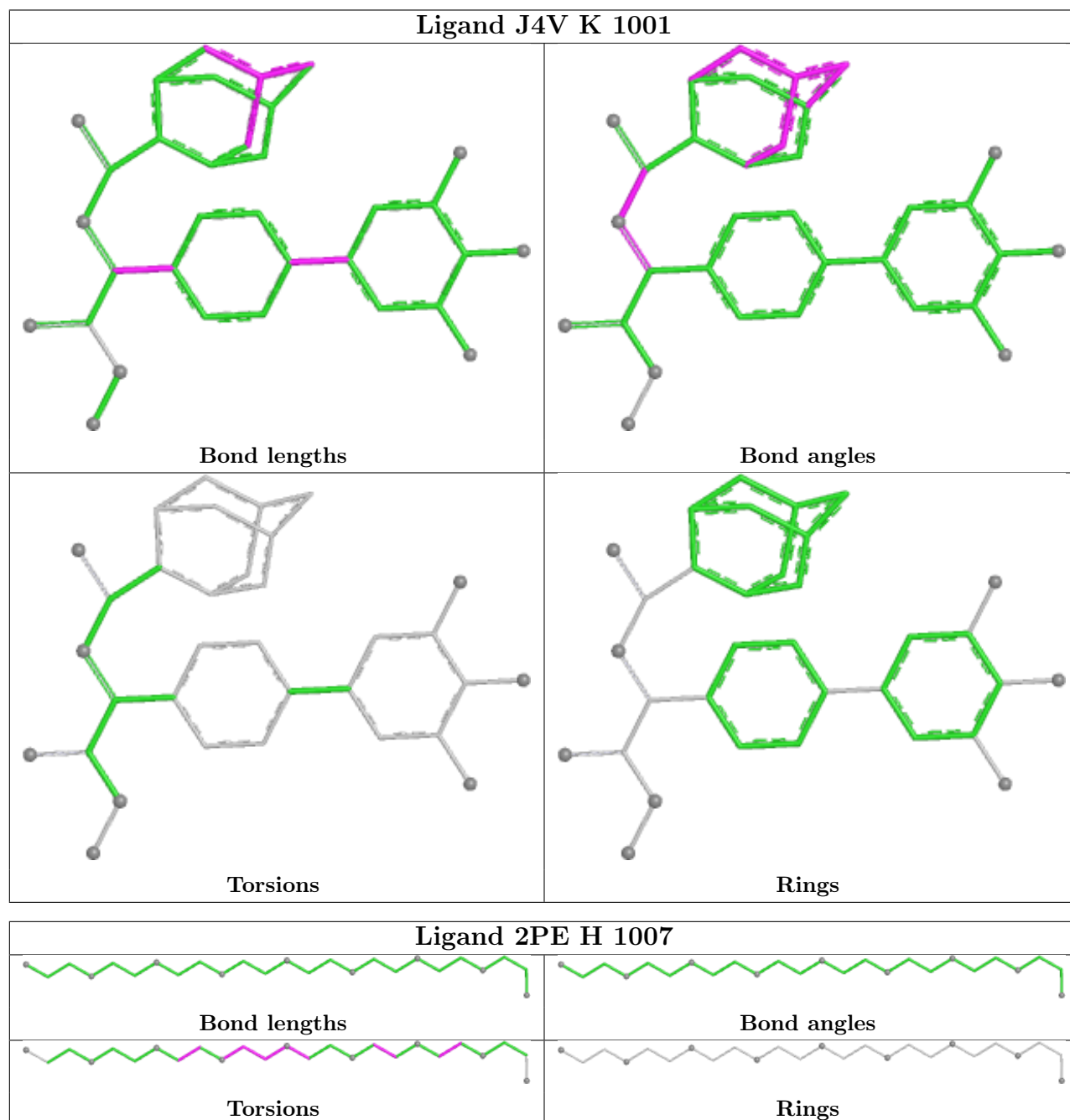
There are no ring outliers.

29 monomers are involved in 53 short contacts:

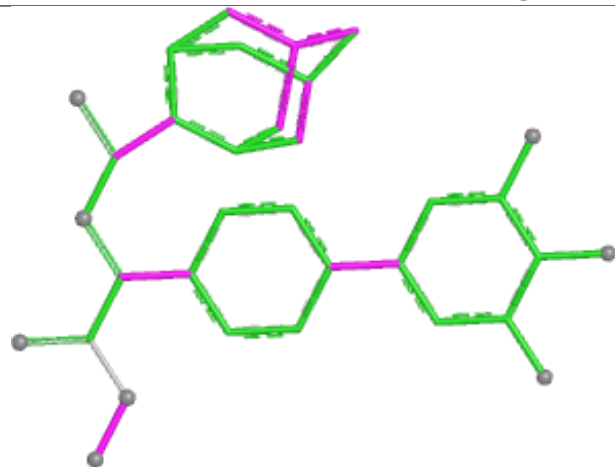
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	I	1007	EDO	2	0
6	B	1006	DMS	1	0
6	A	1008	DMS	1	0
5	C	1004	SO4	1	0
7	I	1009	1PE	1	0
6	B	1005	DMS	1	0
9	H	1007	2PE	3	0
5	H	1006	SO4	1	0
5	A	1005	SO4	1	0
7	F	1009	1PE	1	0
7	J	1011	1PE	5	0
7	K	1012	1PE	1	0
8	J	1007	EDO	1	0
7	L	1007	1PE	2	0
7	J	1009	1PE	3	0
7	L	1008	1PE	1	0
2	J	1001	J4V	1	0
7	F	1008	1PE	2	0
6	H	1010	DMS	1	0
8	F	1006	EDO	2	0
6	B	1007	DMS	1	0
5	K	1004	SO4	1	0
7	G	1009	1PE	1	0
7	D	1007	1PE	11	0
7	C	1007	1PE	2	0
2	A	1001	J4V	1	0
6	G	1006	DMS	2	0
2	G	1001	J4V	1	0
7	A	1010	1PE	1	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

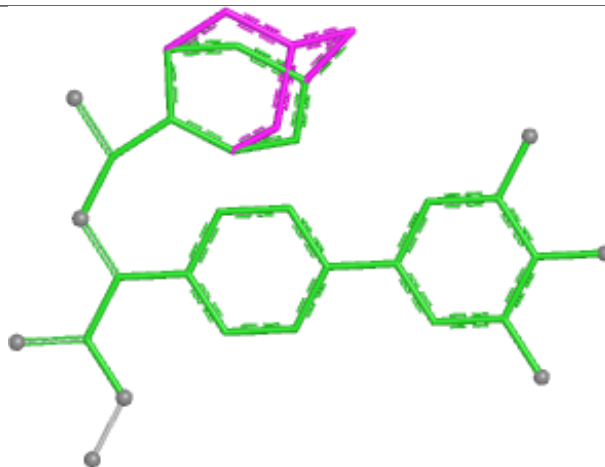
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.



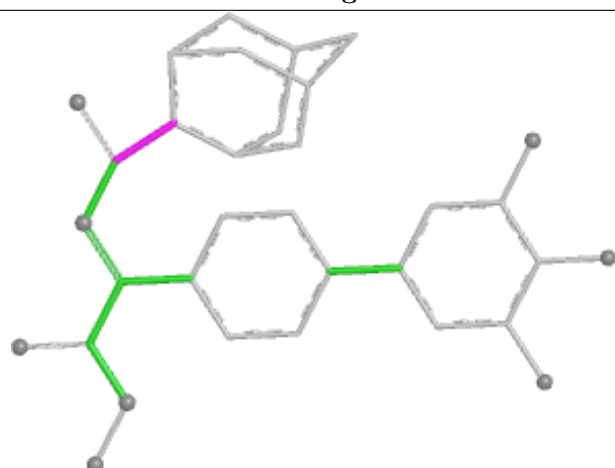
Ligand J4V L 1001



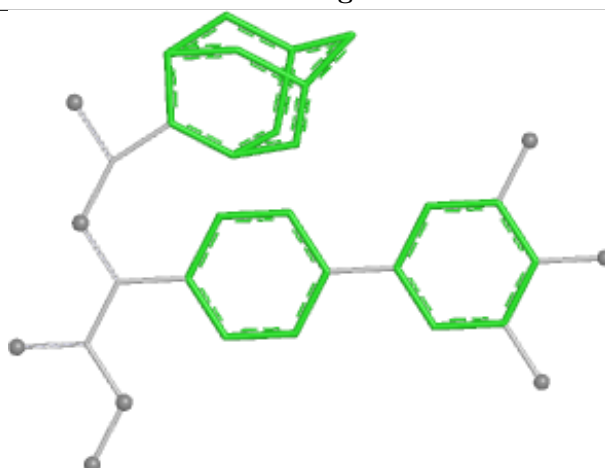
Bond lengths



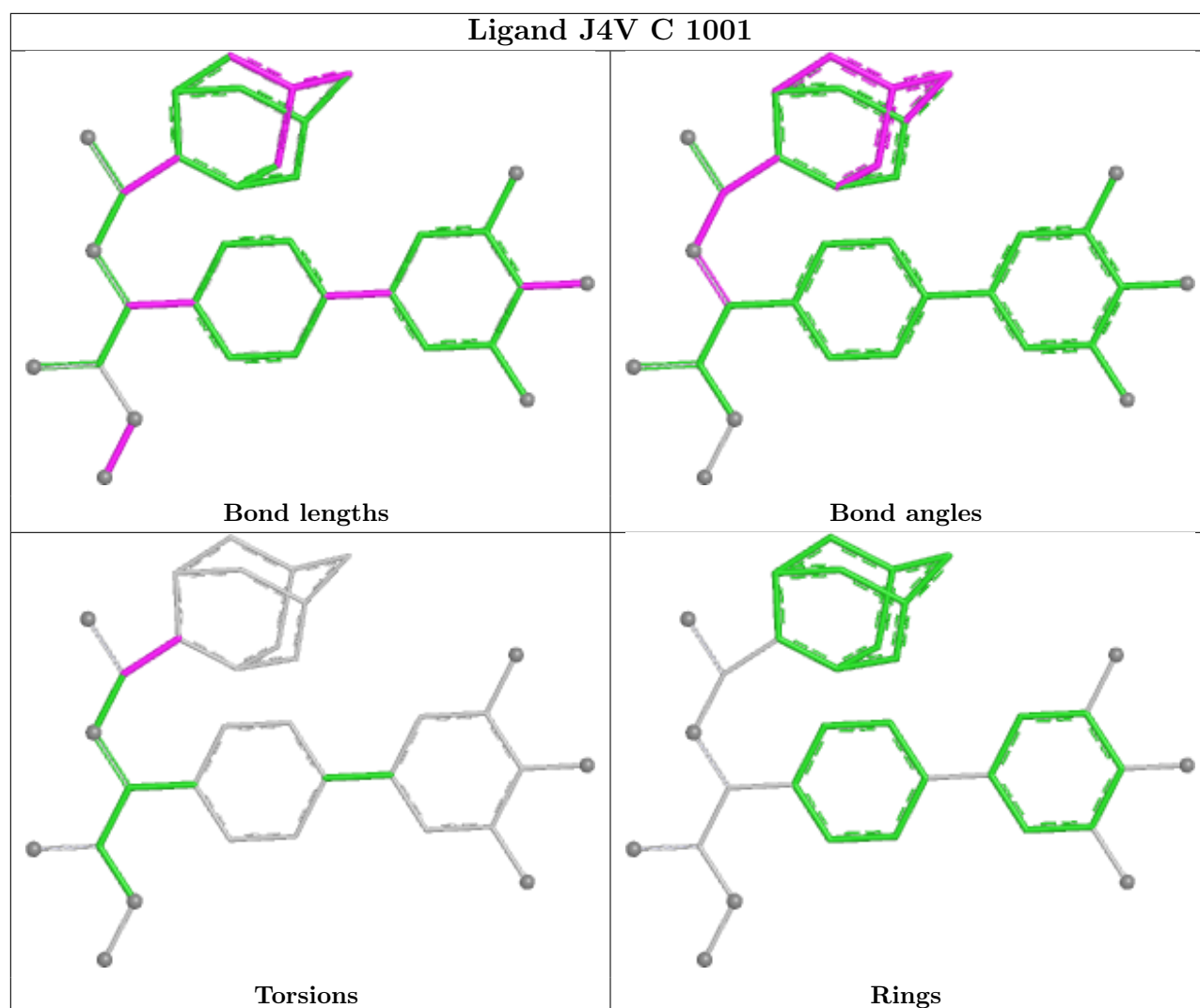
Bond angles



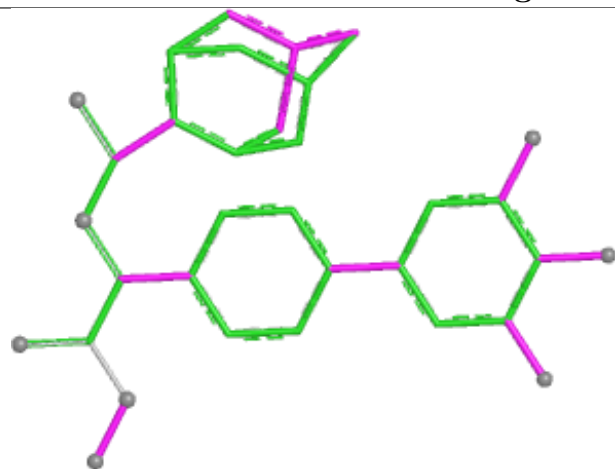
Torsions



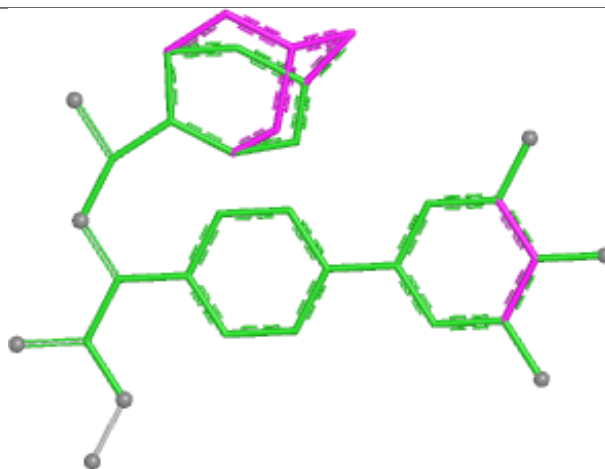
Rings



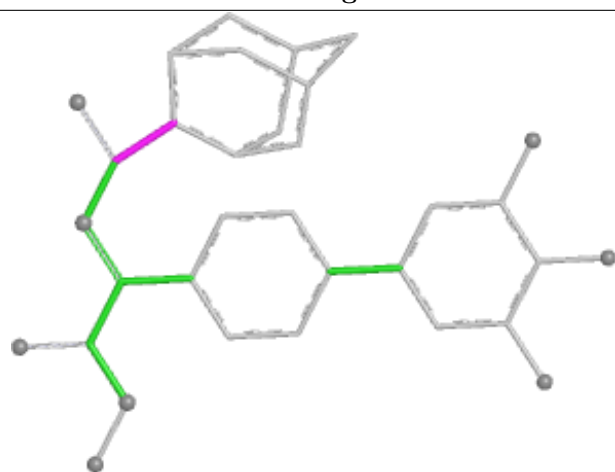
Ligand J4V F 1001



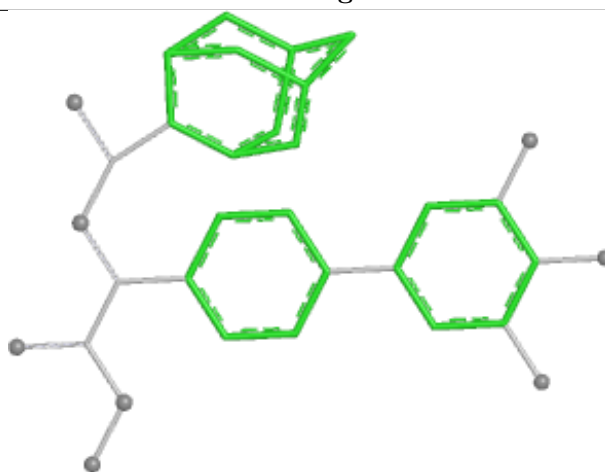
Bond lengths



Bond angles

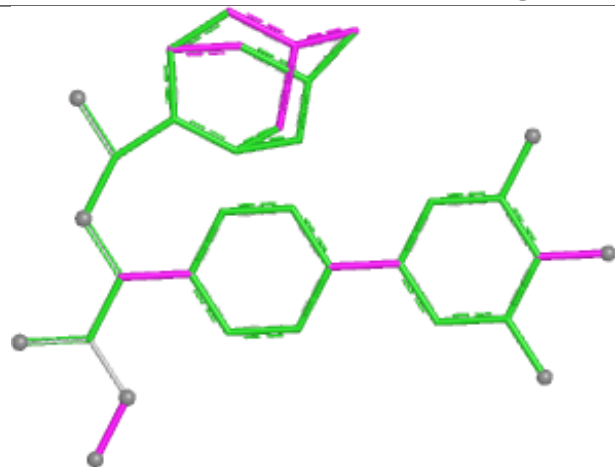


Torsions

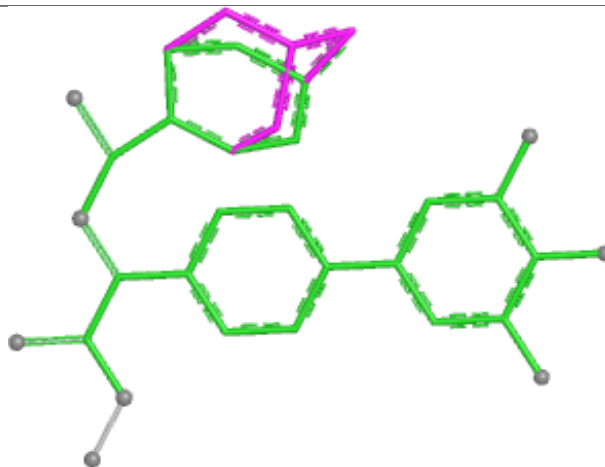


Rings

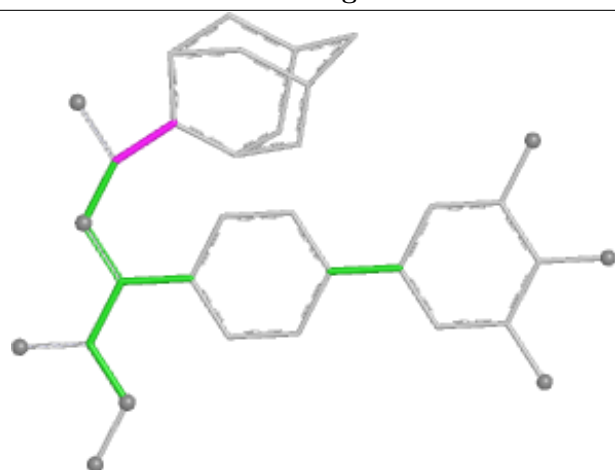
Ligand J4V E 1001



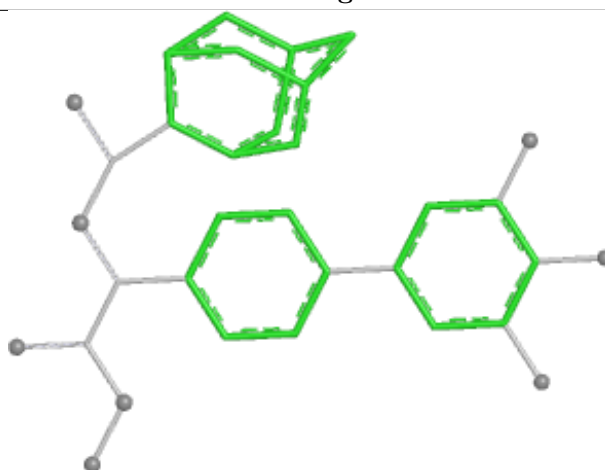
Bond lengths



Bond angles

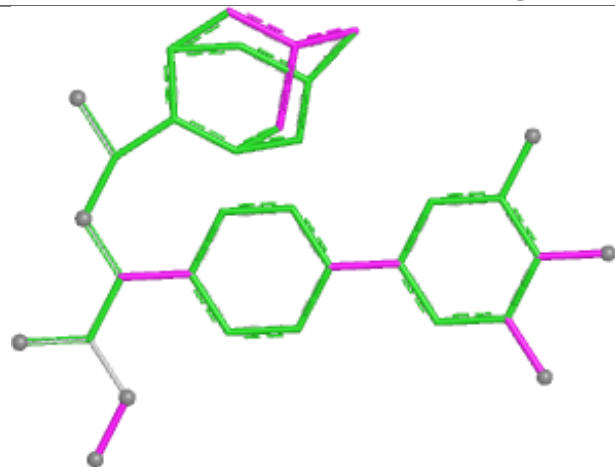


Torsions

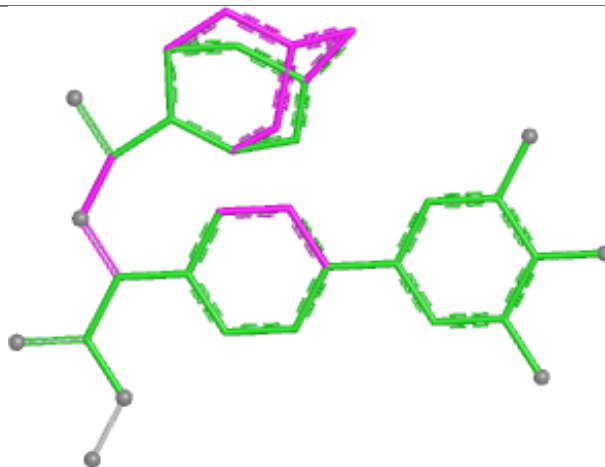


Rings

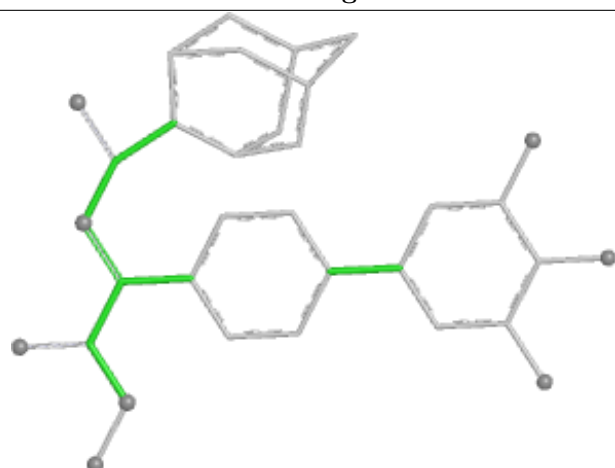
Ligand J4V H 1001



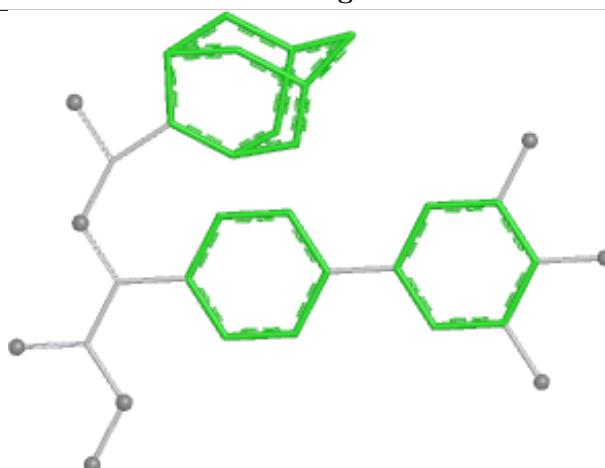
Bond lengths



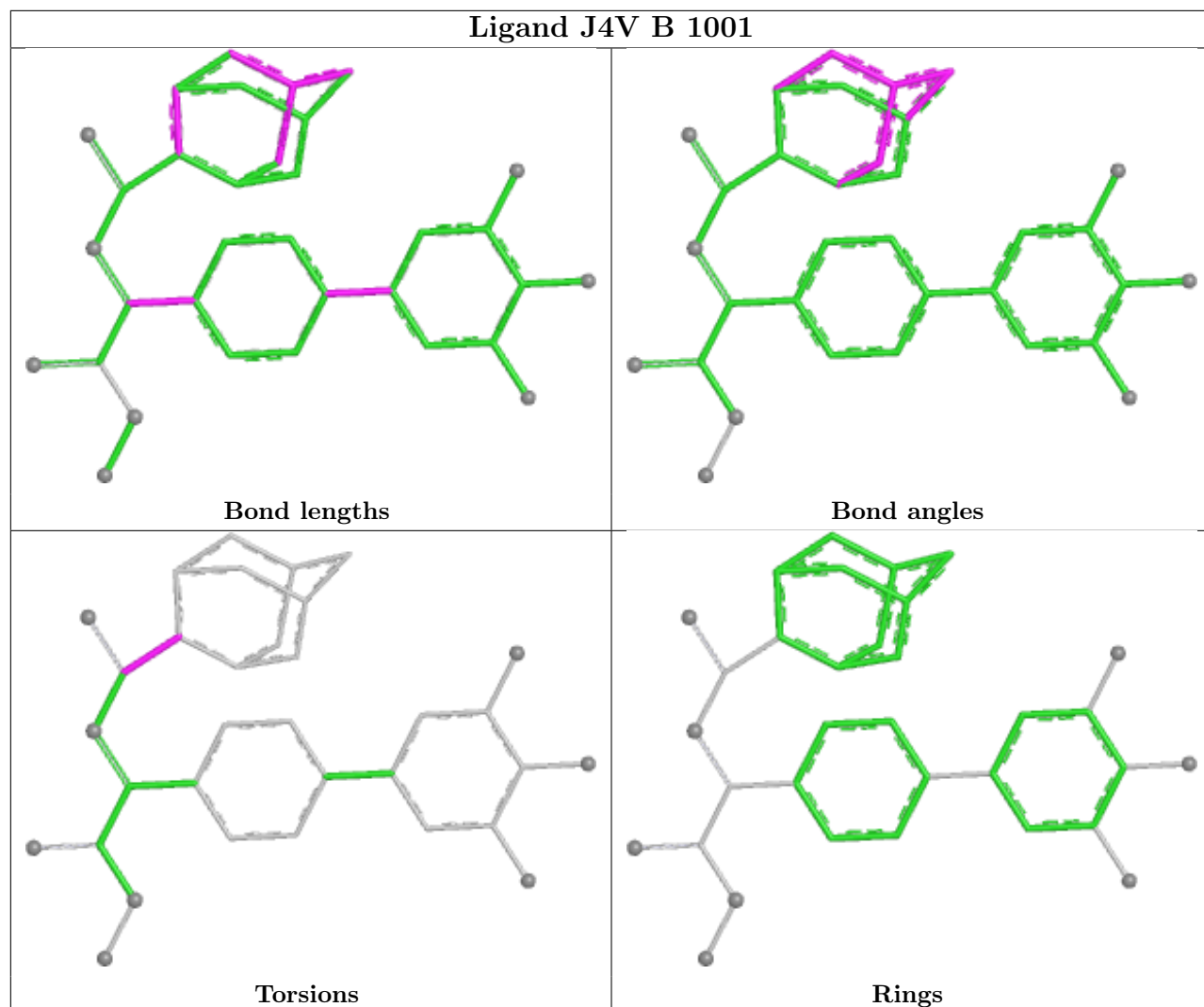
Bond angles



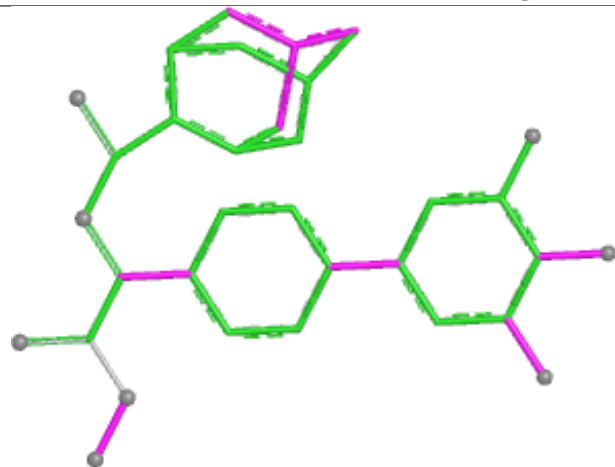
Torsions



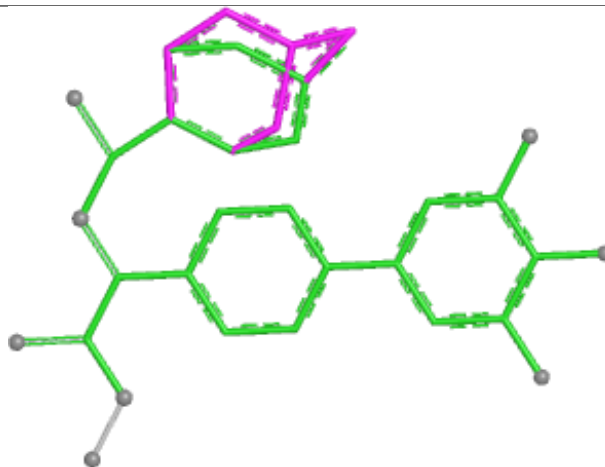
Rings



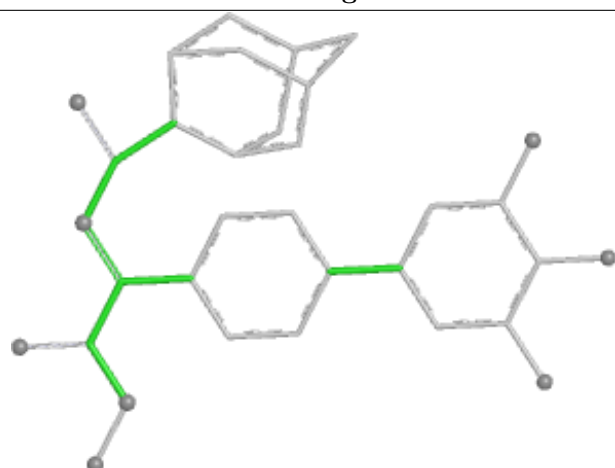
Ligand J4V J 1001



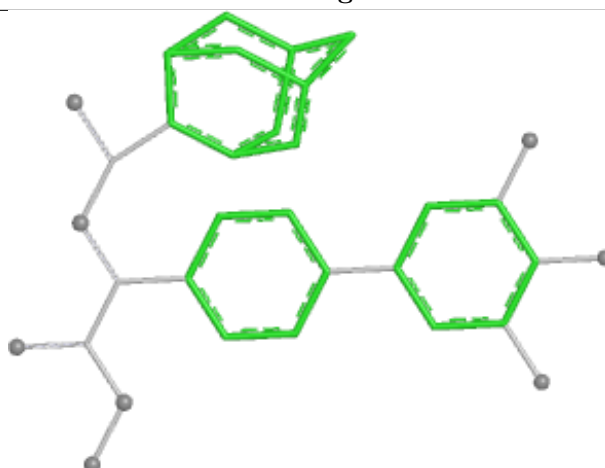
Bond lengths



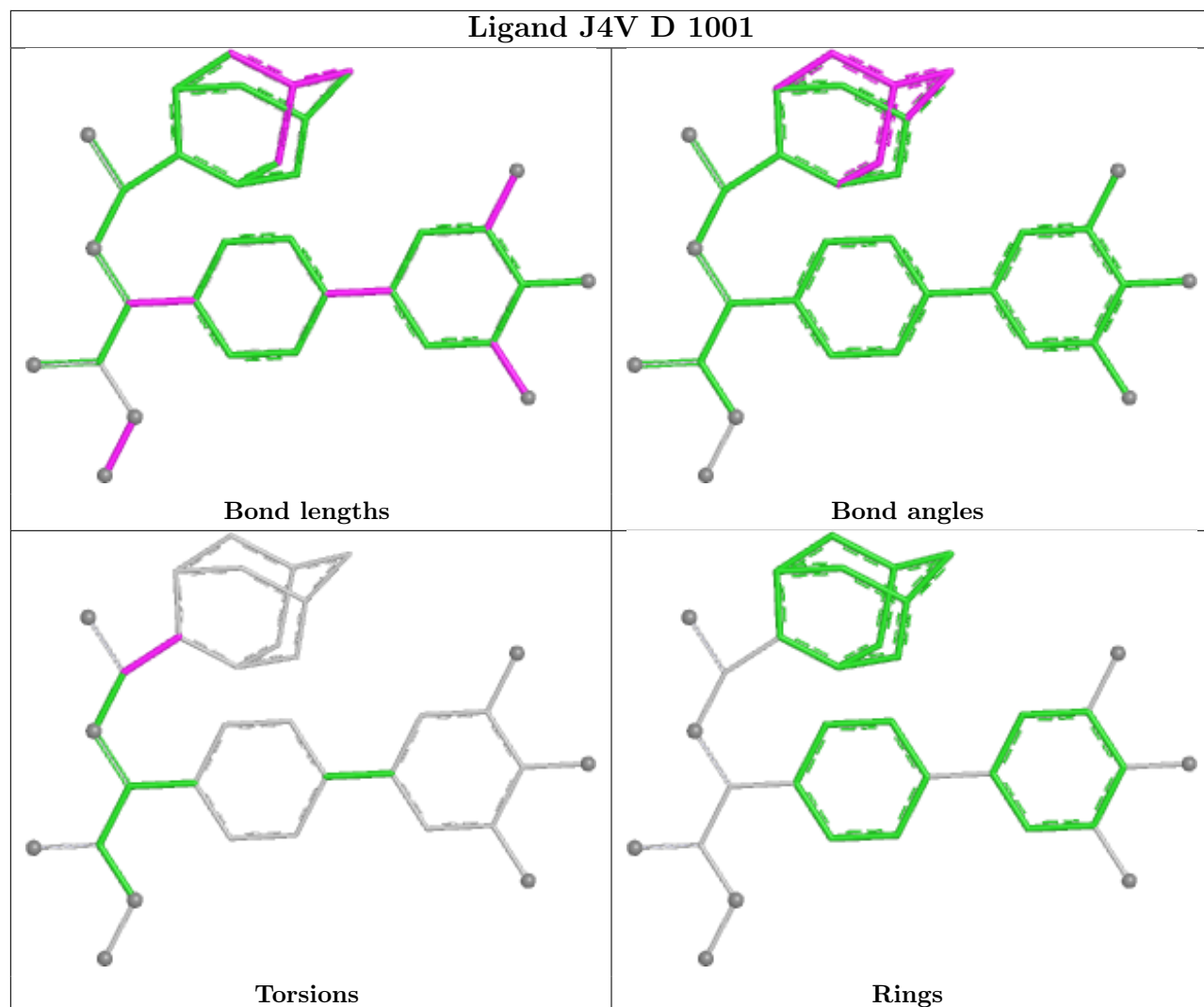
Bond angles

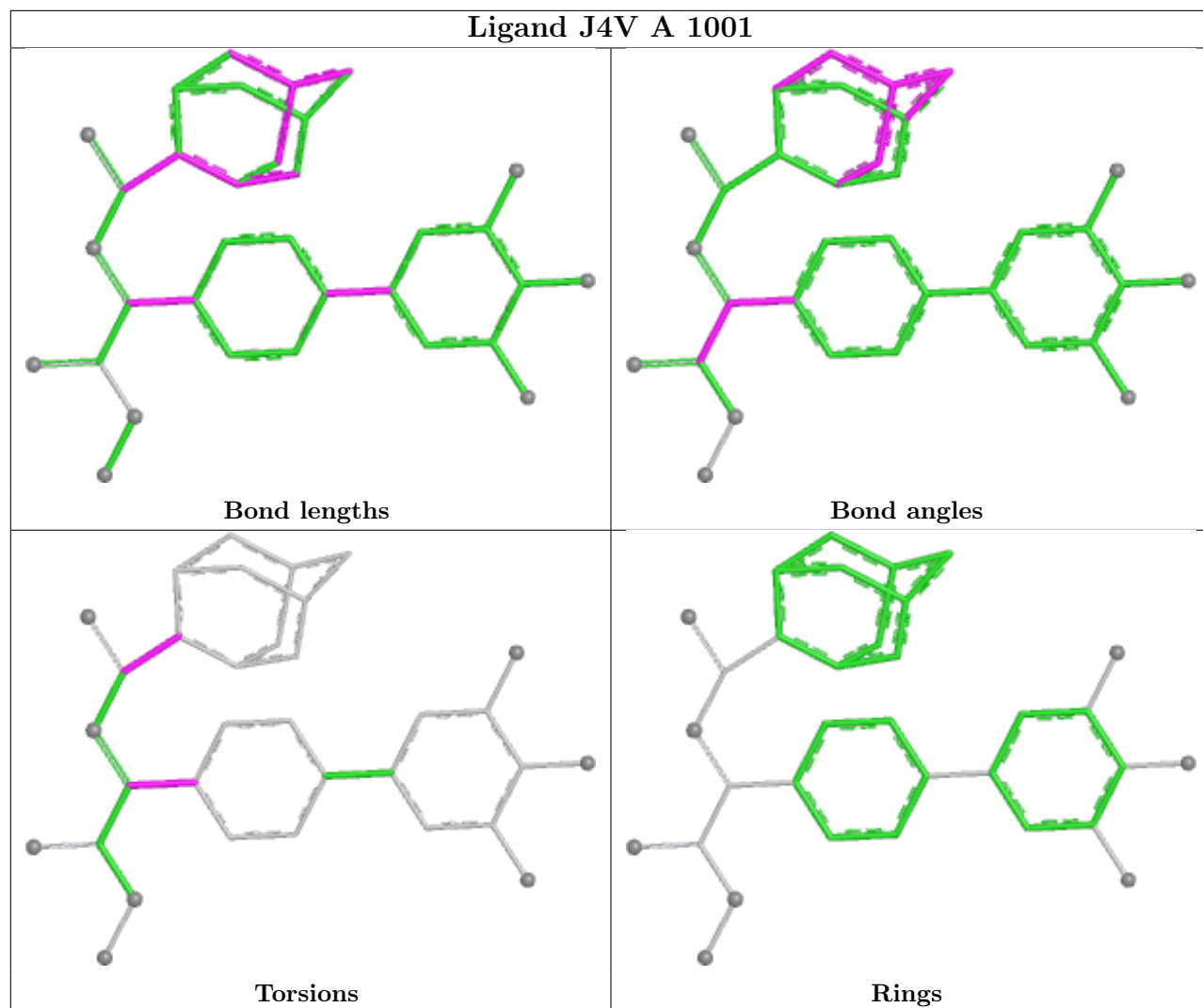


Torsions

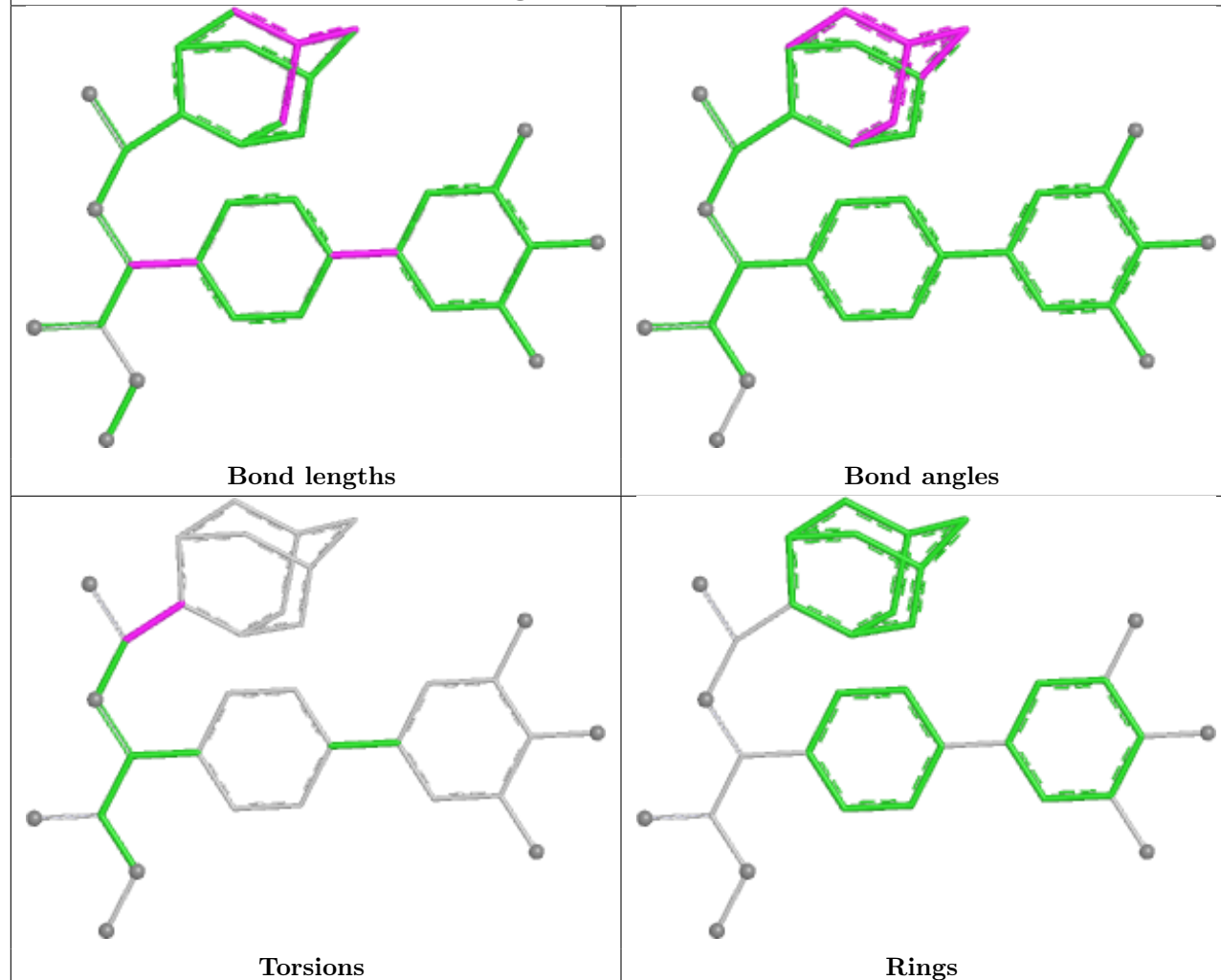


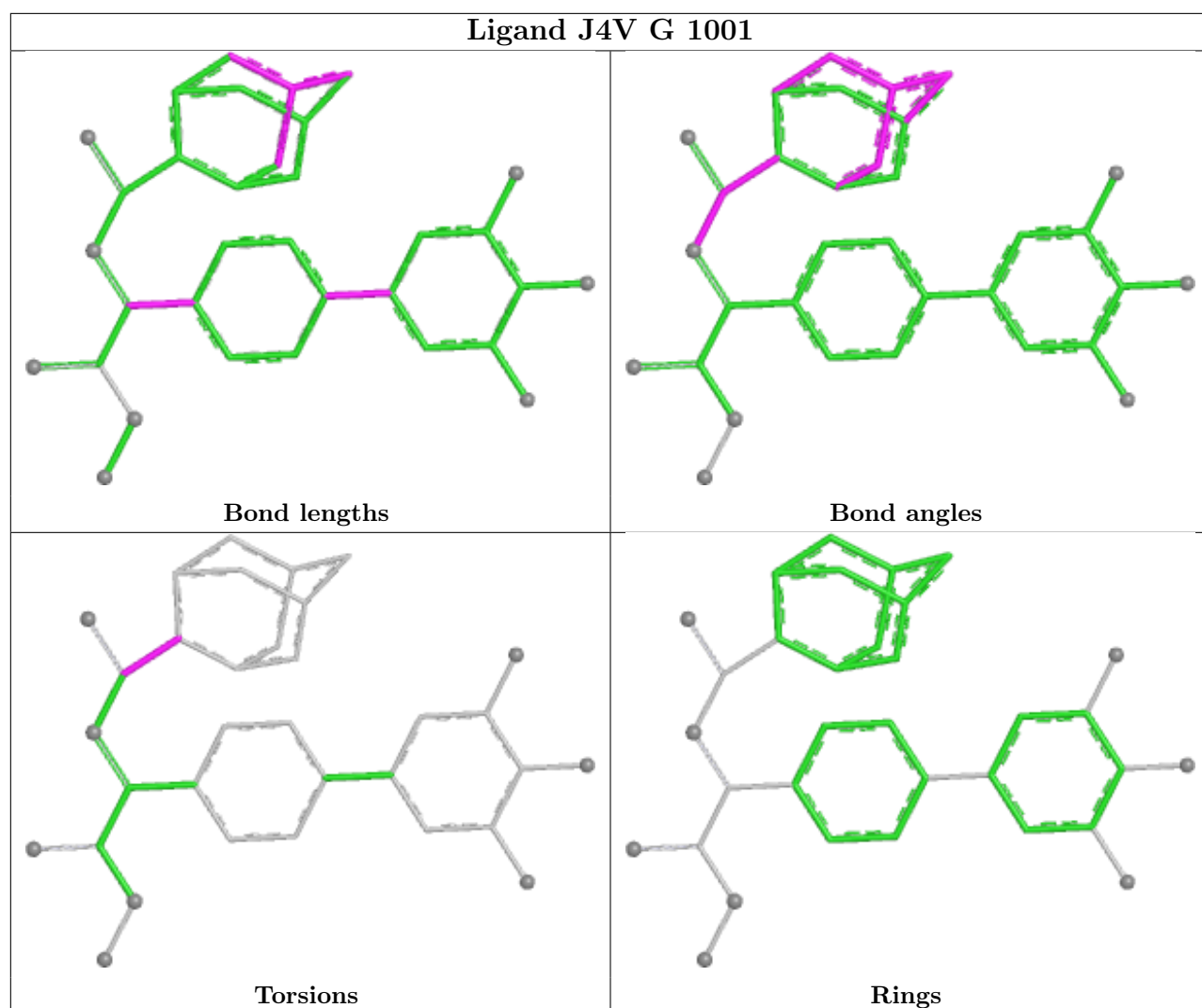
Rings





Ligand J4V I 1001





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 ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	514/519 (99%)	-0.05	3 (0%) 85 86	19, 28, 45, 63	9 (1%)
1	B	511/519 (98%)	0.21	16 (3%) 51 53	19, 29, 60, 75	4 (0%)
1	C	518/519 (99%)	-0.03	4 (0%) 82 83	19, 29, 47, 70	5 (0%)
1	D	516/519 (99%)	-0.06	4 (0%) 82 83	19, 28, 43, 67	3 (0%)
1	E	510/519 (98%)	-0.14	3 (0%) 85 86	20, 27, 38, 53	6 (1%)
1	F	509/519 (98%)	0.20	12 (2%) 59 62	22, 31, 58, 67	8 (1%)
1	G	517/519 (99%)	-0.07	4 (0%) 82 83	19, 29, 47, 65	9 (1%)
1	H	513/519 (98%)	0.19	13 (2%) 58 60	18, 29, 62, 74	18 (3%)
1	I	518/519 (99%)	-0.01	4 (0%) 82 83	19, 28, 47, 66	6 (1%)
1	J	516/519 (99%)	-0.07	5 (0%) 79 80	19, 27, 44, 69	11 (2%)
1	K	510/519 (98%)	-0.16	3 (0%) 85 86	19, 26, 37, 49	7 (1%)
1	L	510/519 (98%)	0.23	13 (2%) 58 60	21, 32, 61, 68	11 (2%)
All	All	6162/6228 (98%)	0.02	84 (1%) 73 75	18, 28, 53, 75	97 (1%)

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	256	ASP	4.9
1	B	196	ALA	4.2
1	D	603	ASP	4.2
1	J	259	VAL	4.0
1	L	121	CYS	3.9
1	I	259	VAL	3.9
1	I	195	VAL	3.7
1	F	141	PRO	3.7
1	J	258	ASN	3.7
1	J	603	ASP	3.7
1	L	276	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	L	155	GLU	3.3
1	B	255	THR	3.3
1	H	135	PRO	3.2
1	H	255	THR	3.2
1	F	135	PRO	3.1
1	H	276	THR	3.0
1	E	136	GLY	3.0
1	F	144	ILE	3.0
1	D	259	VAL	2.9
1	J	85	ALA	2.9
1	F	139	ASN	2.8
1	F	603	ASP	2.8
1	H	185	VAL	2.8
1	G	257	LYS	2.8
1	B	180	ASP	2.8
1	I	161[A]	ASN	2.8
1	L	603	ASP	2.8
1	G	258	ASN	2.7
1	H	137	LYS	2.7
1	B	142	VAL	2.7
1	E	363	GLY	2.7
1	F	231	ASP	2.6
1	A	197	ASP	2.5
1	D	258	ASN	2.5
1	F	175	PHE	2.5
1	B	140	GLY	2.5
1	F	121	CYS	2.4
1	F	171	THR	2.4
1	L	117	ILE	2.4
1	H	234	LEU	2.4
1	L	139	ASN	2.4
1	L	274	ALA	2.4
1	B	175	PHE	2.4
1	G	261	MET	2.4
1	H	121	CYS	2.4
1	F	160	GLU	2.4
1	B	156	PHE	2.3
1	L	153	VAL	2.3
1	E	161	ASN	2.3
1	H	602	ASN	2.3
1	B	136	GLY	2.3
1	C	259	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	197	ASP	2.2
1	I	261	MET	2.2
1	A	85	ALA	2.2
1	F	163	GLU	2.2
1	H	176	TYR	2.2
1	D	219	LEU	2.2
1	B	178	PHE	2.2
1	L	275	ASP	2.2
1	H	261	MET	2.2
1	K	573	HIS	2.2
1	B	276	THR	2.2
1	A	420	ASN	2.2
1	B	193	GLY	2.2
1	B	194	SER	2.2
1	L	148	VAL	2.1
1	H	178	PHE	2.1
1	B	160	GLU	2.1
1	H	197	ASP	2.1
1	K	161	ASN	2.1
1	G	146	SER	2.1
1	K	86	SER	2.1
1	J	260	ASN	2.1
1	L	113	GLN	2.1
1	C	398	PHE	2.1
1	L	178	PHE	2.1
1	B	121	CYS	2.0
1	C	121	CYS	2.0
1	B	122	ASN	2.0
1	L	119	GLY	2.0
1	C	257	LYS	2.0
1	B	138	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	1PE	F	1009	9/16	0.69	0.19	39,46,52,55	0
6	DMS	H	1010	4/4	0.74	0.21	44,48,49,55	0
8	EDO	F	1006	4/4	0.74	0.18	34,36,38,48	0
7	1PE	J	1011	13/16	0.76	0.16	35,40,50,59	0
7	1PE	L	1010	5/16	0.76	0.16	38,42,44,45	0
7	1PE	H	1008	9/16	0.76	0.18	31,40,45,48	0
8	EDO	F	1007	4/4	0.76	0.15	44,45,46,46	0
7	1PE	B	1008	9/16	0.78	0.16	37,44,48,49	0
7	1PE	L	1008	12/16	0.79	0.16	33,44,53,55	0
7	1PE	J	1010	9/16	0.79	0.15	37,37,50,55	0
8	EDO	K	1009	4/4	0.79	0.14	29,30,31,33	0
7	1PE	C	1007	15/16	0.80	0.15	35,41,58,64	0
6	DMS	A	1008	4/4	0.80	0.19	37,48,57,67	0
7	1PE	L	1007	13/16	0.81	0.14	29,42,49,50	0
8	EDO	H	1009	4/4	0.81	0.12	33,34,37,38	0
6	DMS	B	1007	4/4	0.81	0.16	35,38,53,59	0
7	1PE	D	1007	12/16	0.82	0.12	40,44,48,51	0
8	EDO	J	1007	4/4	0.82	0.14	39,39,43,44	0
8	EDO	K	1008	4/4	0.82	0.13	37,43,44,44	0
7	1PE	G	1009	9/16	0.82	0.14	37,45,47,50	0
9	2PE	H	1007	25/28	0.82	0.14	34,45,53,54	0
7	1PE	G	1008	9/16	0.83	0.14	34,40,42,43	0
8	EDO	I	1007	4/4	0.85	0.18	17,25,29,41	0
3	CO3	C	1002	4/4	0.86	0.13	19,23,31,32	0
7	1PE	J	1009	9/16	0.86	0.11	31,33,39,39	0
8	EDO	K	1011	4/4	0.86	0.11	34,40,42,44	0
7	1PE	C	1008	12/16	0.86	0.13	33,42,47,49	0
7	1PE	I	1008	12/16	0.87	0.12	31,39,44,50	0
7	1PE	A	1009	15/16	0.87	0.12	41,47,52,52	0
6	DMS	B	1005	4/4	0.87	0.15	42,48,49,54	0
6	DMS	B	1006	4/4	0.87	0.14	39,42,48,61	0
7	1PE	I	1009	9/16	0.88	0.11	29,33,38,39	0
7	1PE	K	1012	13/16	0.88	0.10	32,37,42,46	0
2	J4V	L	1001	33/33	0.89	0.10	22,30,39,41	0
2	J4V	E	1001	33/33	0.89	0.10	22,30,37,40	0
7	1PE	F	1008	9/16	0.89	0.11	31,36,41,48	0
5	SO4	A	1005	5/5	0.89	0.11	43,43,49,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	SO4	H	1005	5/5	0.89	0.13	38,39,49,49	5
7	1PE	K	1013	15/16	0.89	0.11	26,34,42,45	0
7	1PE	A	1010	12/16	0.89	0.12	33,37,49,55	0
2	J4V	F	1001	33/33	0.89	0.10	24,31,36,43	0
2	J4V	J	1001	33/33	0.89	0.10	22,29,34,36	0
2	J4V	D	1001	33/33	0.90	0.10	23,30,35,37	0
2	J4V	G	1001	33/33	0.90	0.09	23,31,41,45	0
8	EDO	J	1006	4/4	0.90	0.13	38,38,44,49	0
2	J4V	H	1001	33/33	0.90	0.10	21,30,36,43	0
6	DMS	G	1006	4/4	0.90	0.14	37,42,48,50	0
2	J4V	I	1001	33/33	0.90	0.10	23,29,35,43	0
8	EDO	K	1010	4/4	0.90	0.11	25,31,37,40	0
5	SO4	K	1007	5/5	0.90	0.12	35,37,37,38	5
2	J4V	A	1001	33/33	0.90	0.10	22,28,40,45	0
2	J4V	K	1001	33/33	0.91	0.09	21,28,35,39	0
5	SO4	F	1004	5/5	0.91	0.11	48,49,56,58	0
7	1PE	L	1009	7/16	0.91	0.10	34,38,40,41	0
2	J4V	C	1001	33/33	0.91	0.09	20,26,34,37	0
5	SO4	I	1004	5/5	0.91	0.12	42,45,51,54	0
2	J4V	B	1001	33/33	0.91	0.09	21,28,33,38	0
8	EDO	G	1007	4/4	0.91	0.09	31,33,36,40	0
5	SO4	L	1004	5/5	0.91	0.16	46,54,56,56	0
8	EDO	J	1008	4/4	0.92	0.09	32,33,42,44	0
5	SO4	G	1005	5/5	0.92	0.13	39,44,51,53	0
7	1PE	D	1008	7/16	0.92	0.09	28,32,37,37	0
3	CO3	E	1002	4/4	0.92	0.11	25,27,32,38	0
5	SO4	D	1005	5/5	0.92	0.10	31,38,43,44	5
8	EDO	L	1006	4/4	0.92	0.09	23,28,37,39	0
3	CO3	J	1002	4/4	0.92	0.13	23,24,29,30	0
5	SO4	E	1004	5/5	0.93	0.08	35,37,40,46	5
5	SO4	L	1005	5/5	0.93	0.10	46,49,58,58	0
5	SO4	H	1006	5/5	0.93	0.10	42,44,51,55	0
3	CO3	G	1002	4/4	0.93	0.10	18,23,30,31	0
5	SO4	I	1006	5/5	0.93	0.10	37,39,41,43	5
5	SO4	J	1005	5/5	0.93	0.20	41,49,52,52	0
5	SO4	K	1005	5/5	0.93	0.13	39,43,47,53	0
5	SO4	K	1006	5/5	0.93	0.09	29,32,36,46	5
3	CO3	F	1002	4/4	0.93	0.10	22,25,30,31	0
5	SO4	A	1007	5/5	0.94	0.11	39,40,49,51	0
5	SO4	B	1004	5/5	0.94	0.11	40,43,50,51	0
5	SO4	C	1004	5/5	0.94	0.12	50,50,53,54	0
5	SO4	C	1005	5/5	0.94	0.13	44,47,48,48	0

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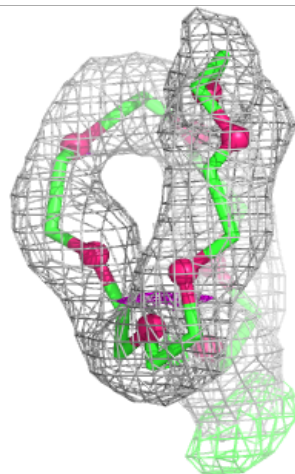
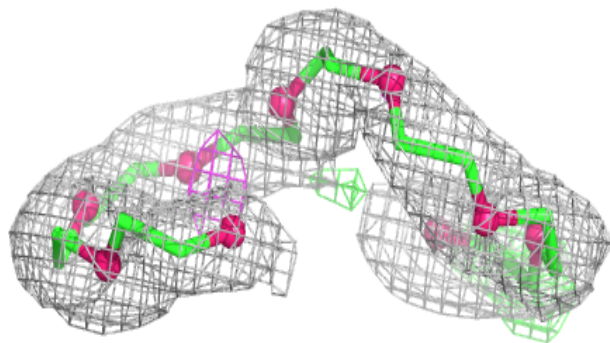
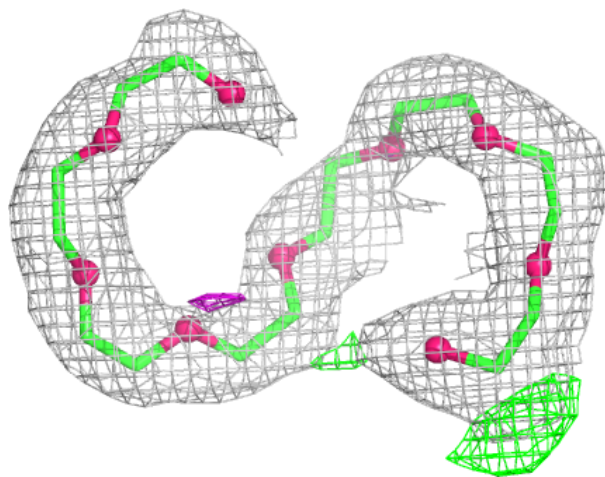
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	SO4	C	1006	5/5	0.94	0.09	31,33,36,41	0
3	CO3	H	1002	4/4	0.94	0.07	19,24,28,29	0
3	CO3	D	1002	4/4	0.94	0.10	20,24,28,30	0
5	SO4	E	1005	5/5	0.94	0.11	39,47,49,52	0
3	CO3	A	1002	4/4	0.94	0.11	22,27,32,33	0
5	SO4	F	1005	5/5	0.95	0.11	43,47,52,65	0
3	CO3	K	1002	4/4	0.95	0.08	21,22,27,27	0
3	CO3	L	1002	4/4	0.95	0.09	24,27,31,33	0
4	ZN	H	1003	1/1	0.95	0.05	40,40,40,40	1
5	SO4	D	1004	5/5	0.95	0.10	47,47,52,52	0
3	CO3	I	1002	4/4	0.96	0.07	21,27,30,33	0
5	SO4	A	1004	5/5	0.96	0.08	44,47,48,51	0
5	SO4	I	1005	5/5	0.96	0.09	40,45,46,49	0
3	CO3	B	1002	4/4	0.96	0.07	19,21,27,28	0
5	SO4	J	1004	5/5	0.96	0.09	44,46,50,54	0
4	ZN	B	1003	1/1	0.96	0.05	37,37,37,37	1
8	EDO	E	1006	4/4	0.97	0.08	24,24,25,27	0
4	ZN	I	1003	1/1	0.97	0.06	34,34,34,34	1
5	SO4	G	1004	5/5	0.97	0.07	33,36,39,44	5
4	ZN	D	1003	1/1	0.98	0.04	34,34,34,34	1
4	ZN	J	1003	1/1	0.98	0.04	35,35,35,35	1
4	ZN	K	1003	1/1	0.98	0.05	37,37,37,37	1
4	ZN	E	1003	1/1	0.98	0.05	36,36,36,36	1
4	ZN	G	1003	1/1	0.98	0.03	34,34,34,34	1
4	ZN	A	1003	1/1	0.98	0.03	35,35,35,35	1
5	SO4	H	1004	5/5	0.98	0.06	22,24,29,29	0
5	SO4	A	1006	5/5	0.99	0.05	21,24,27,30	0
4	ZN	L	1003	1/1	0.99	0.02	35,35,35,35	1
4	ZN	F	1003	1/1	0.99	0.02	33,33,33,33	1
4	ZN	C	1003	1/1	0.99	0.03	34,34,34,34	1
5	SO4	K	1004	5/5	0.99	0.05	25,27,29,29	0
5	SO4	D	1006	5/5	0.99	0.04	26,27,27,29	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

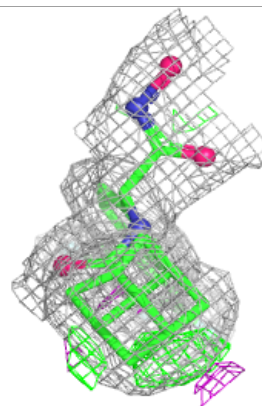
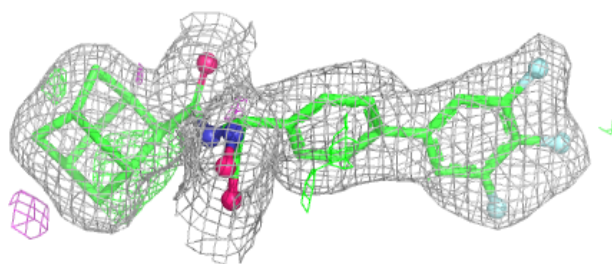
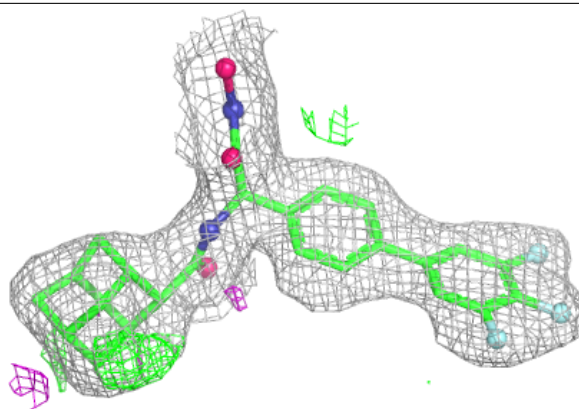
Electron density around 2PE H 1007:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

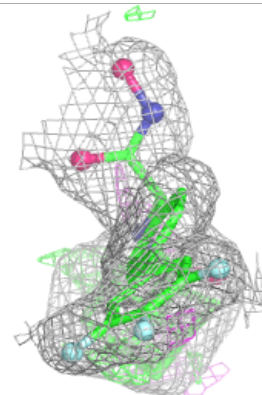
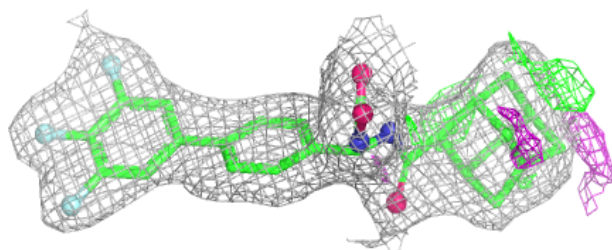
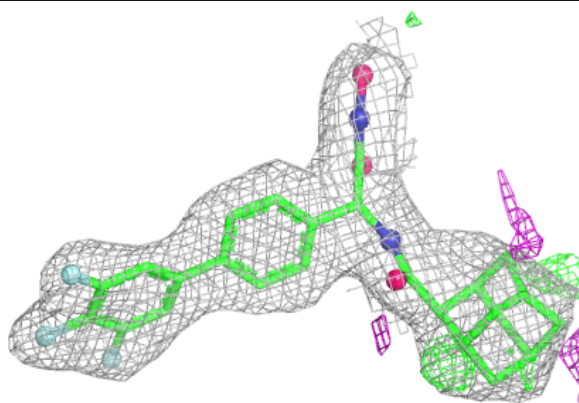


Electron density around J4V L 1001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

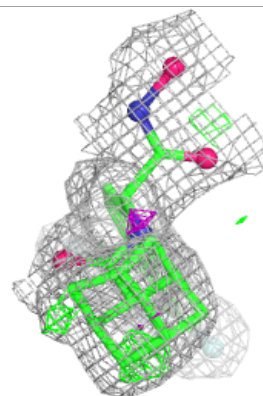
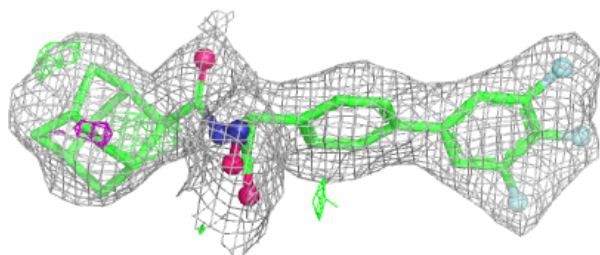
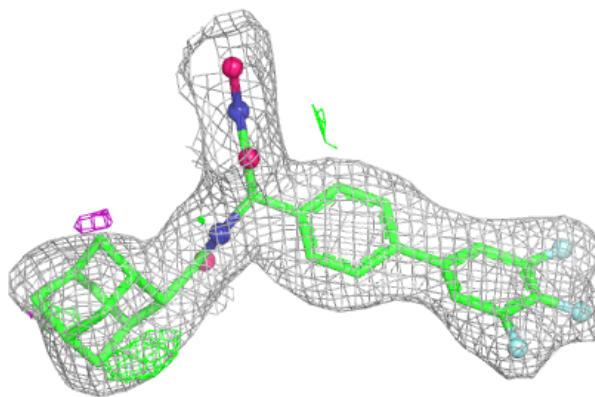
**Electron density around J4V E 1001:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

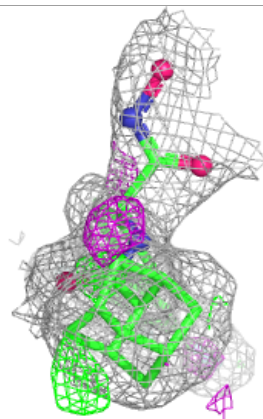
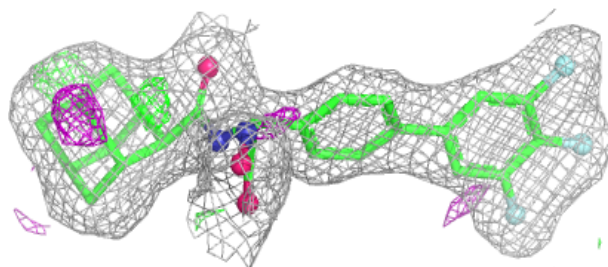
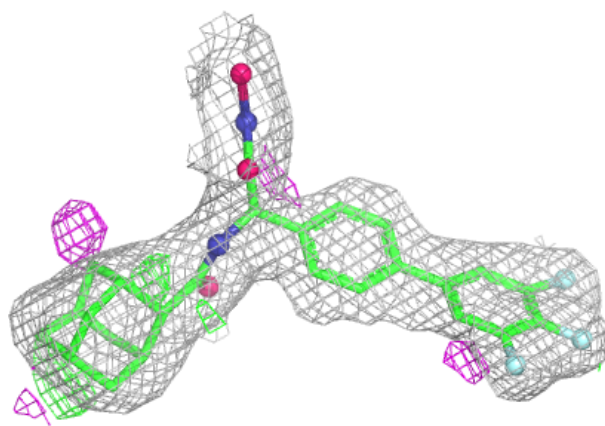


Electron density around J4V F 1001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

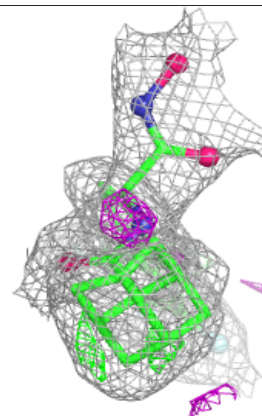
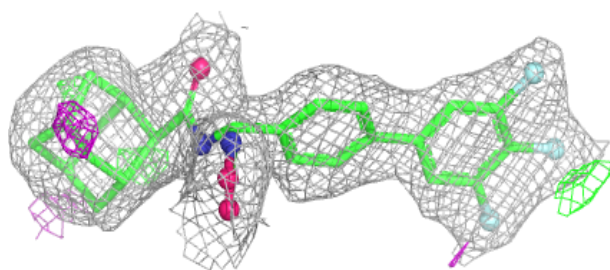
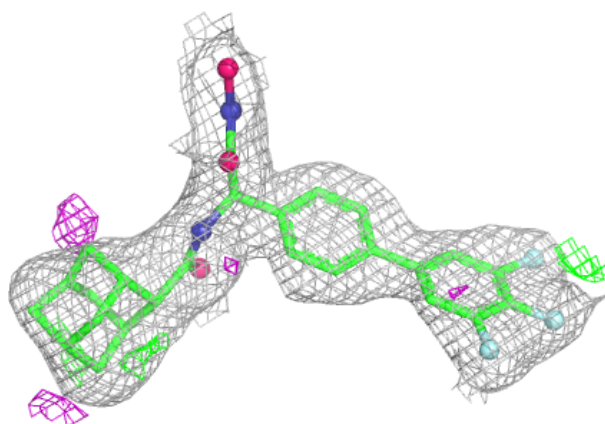
**Electron density around J4V J 1001:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



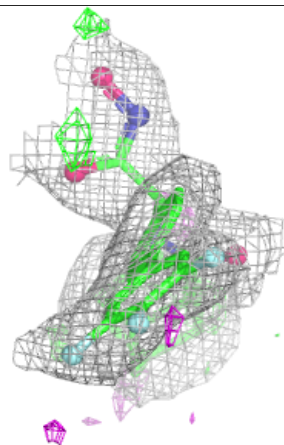
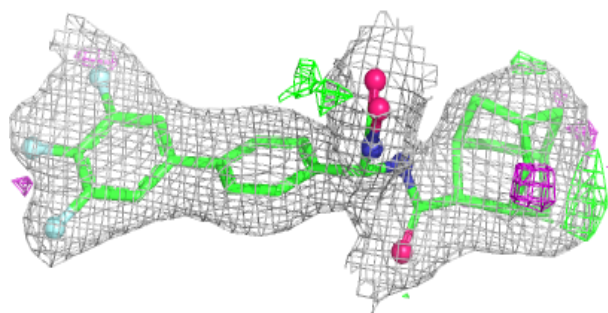
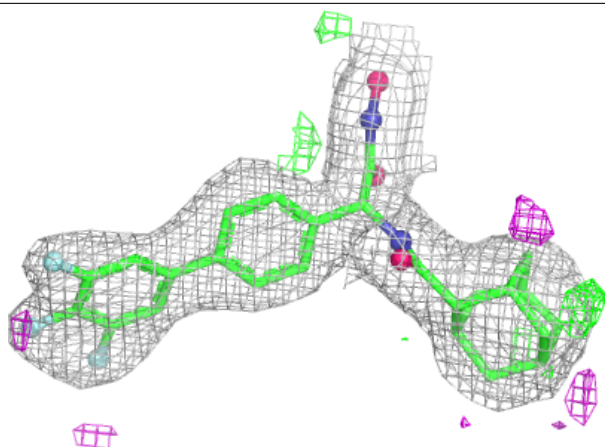
Electron density around J4V D 1001:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

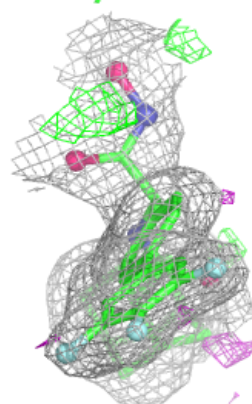
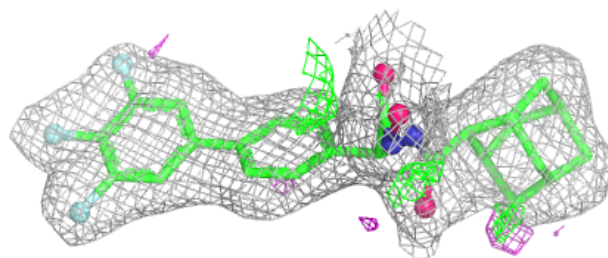
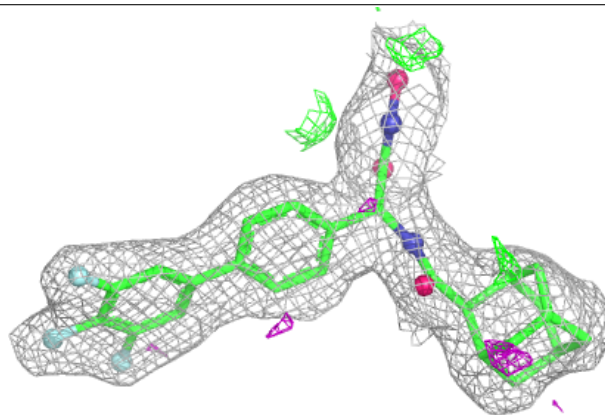


Electron density around J4V G 1001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

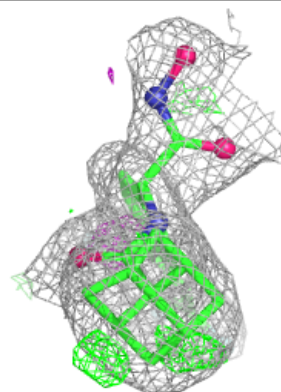
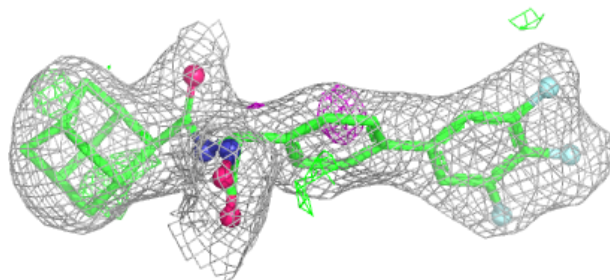
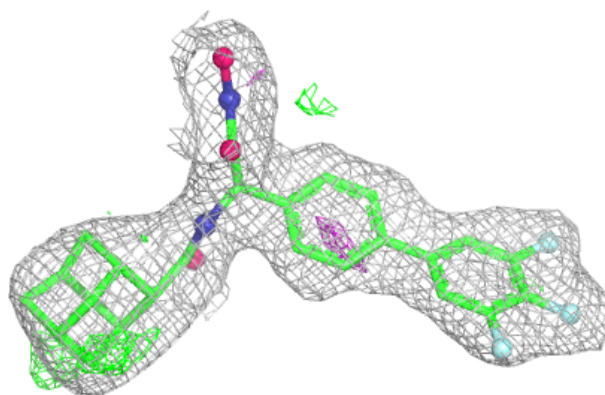
**Electron density around J4V H 1001:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

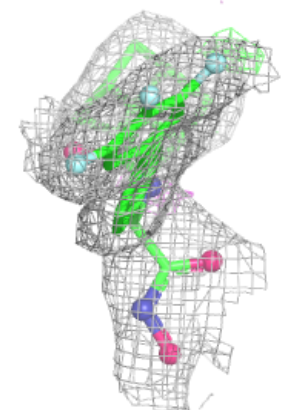
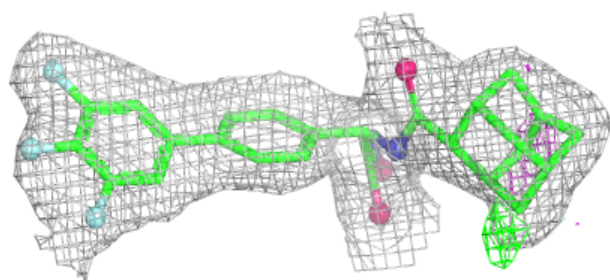
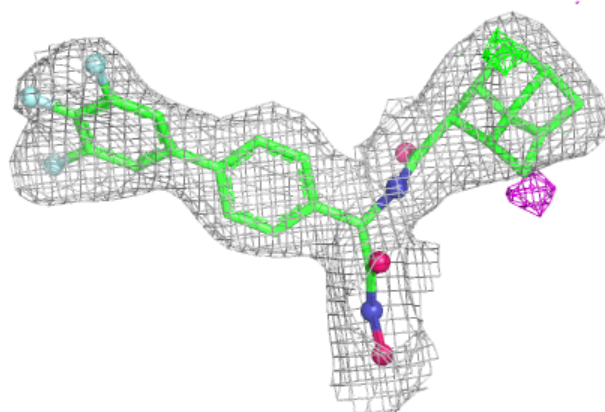


Electron density around J4V I 1001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

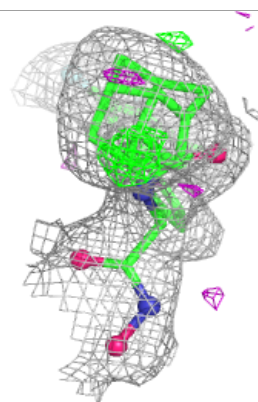
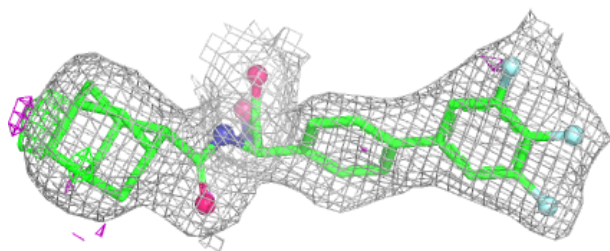
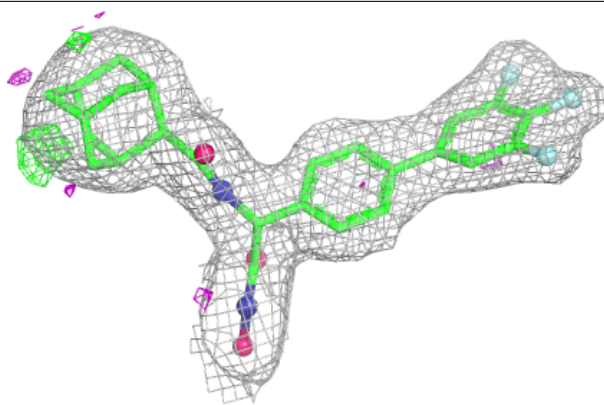
**Electron density around J4V A 1001:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

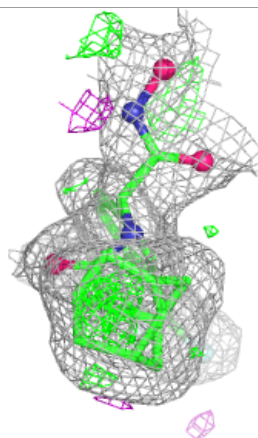
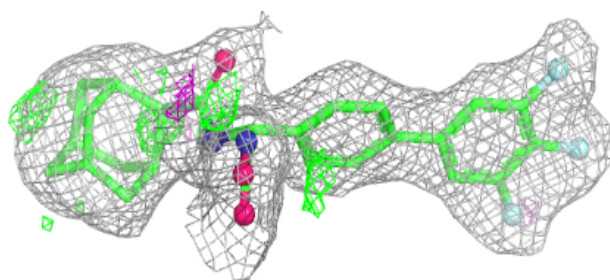
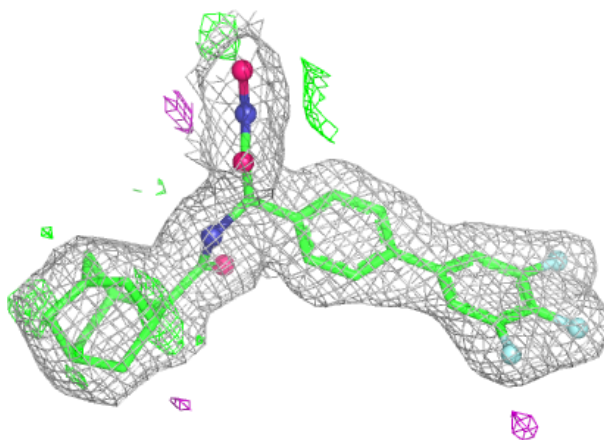


Electron density around J4V K 1001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

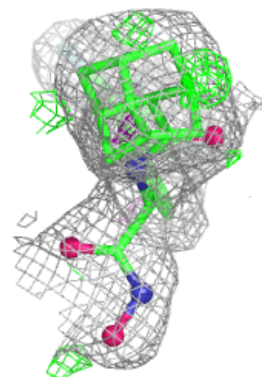
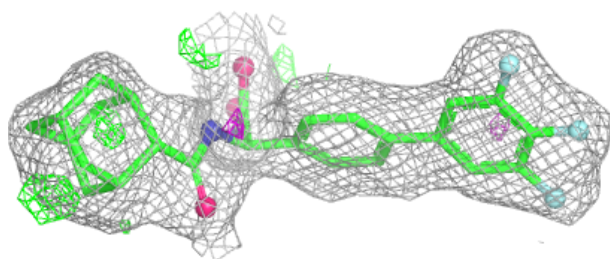
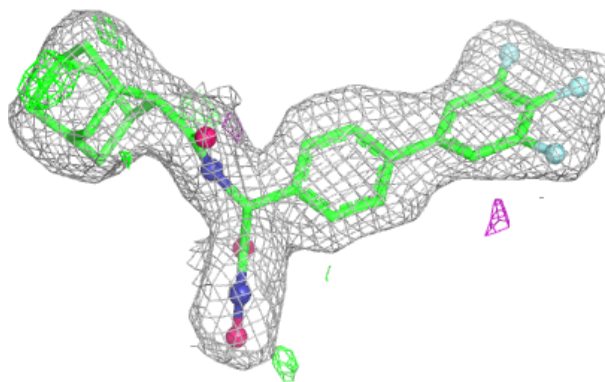
**Electron density around J4V C 1001:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around J4V B 1001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.