Full wwPDB X-ray Structure Validation Report ⓘ

Nov 6, 2023 – 01:15 AM EST

PDB ID	:	8F2L
Title	:	Crystal structure of Mycobacterium tuberculosis Homoserine transacetylase in complex with L-Homoserine
Authors	:	Jayasinghe, Y.P.; Ronning, D.R.
Deposited on	:	2022-11-08
Resolution	:	2.89 Å(reported)

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

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

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

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

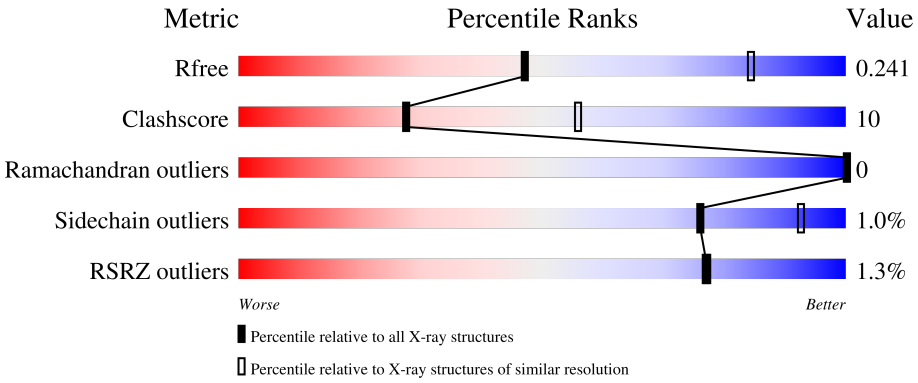
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.89 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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	368	81% 18%
1	B	368	83% 17%
1	C	368	82% 18%
1	D	368	82% 18%
1	E	368	2% 83% 15%

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Mol	Chain	Length	Quality of chain
1	F	368	4% 78% 22%
1	G	368	2% 79% 21%
1	H	368	3% 76% 23%
1	I	368	% 80% 18%
1	J	368	2% 75% 25%
1	K	368	% 76% 23%
1	L	368	2% 79% 21%

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
2	HSE	H	401	-	-	X	-

2 Entry composition (i)

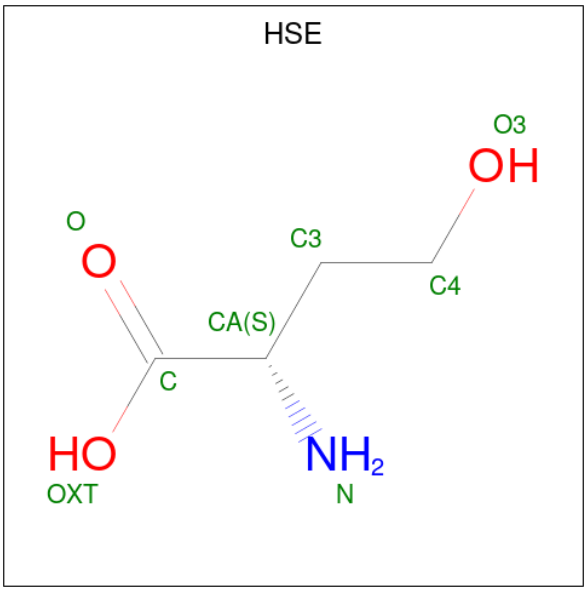
There are 2 unique types of molecules in this entry. The entry contains 33542 atoms, of which 1081 are hydrogens and 0 are deuteriums.

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 Homoserine O-acetyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	B	367	Total	C	H	N	O	S	0	1	0
			2721	1689	9	495	522	6			
1	A	367	Total	C	H	N	O	S	0	0	0
			2878	1685	172	495	520	6			
1	C	366	Total	C	H	N	O	S	0	0	0
			2870	1683	167	497	517	6			
1	D	366	Total	C	H	N	O	S	0	0	0
			2706	1680	9	494	517	6			
1	E	365	Total	C	H	N	O	S	0	0	0
			2860	1674	172	492	516	6			
1	F	367	Total	C	H	N	O	S	0	0	0
			2710	1682	9	493	520	6			
1	G	365	Total	C	H	N	O	S	0	0	0
			2856	1673	172	490	515	6			
1	H	366	Total	C	H	N	O	S	0	0	0
			2702	1677	9	493	517	6			
1	I	365	Total	C	H	N	O	S	0	0	0
			2864	1677	172	493	516	6			
1	J	367	Total	C	H	N	O	S	0	0	0
			2721	1688	9	498	520	6			
1	K	365	Total	C	H	N	O	S	0	0	0
			2860	1675	172	493	514	6			
1	L	367	Total	C	H	N	O	S	0	0	0
			2706	1681	9	491	519	6			

- Molecule 2 is L-HOMOSERINE (three-letter code: HSE) (formula: $C_4H_9NO_3$) (labeled as "Ligand of Interest" by depositor).



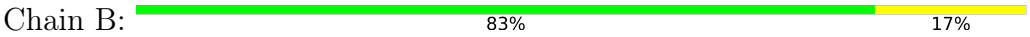
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C N O 8 4 1 3	0	0
2	A	1	Total C N O 8 4 1 3	0	0
2	C	1	Total C N O 8 4 1 3	0	0
2	D	1	Total C N O 8 4 1 3	0	0
2	F	1	Total C N O 8 4 1 3	0	0
2	G	1	Total C N O 8 4 1 3	0	0
2	H	1	Total C N O 8 4 1 3	0	0
2	I	1	Total C N O 8 4 1 3	0	0
2	J	1	Total C N O 8 4 1 3	0	0
2	K	1	Total C N O 8 4 1 3	0	0
2	L	1	Total C N O 8 4 1 3	0	0

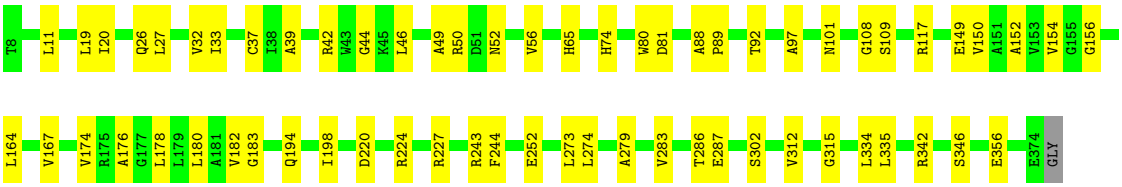
3 Residue-property plots (i)

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: Homoserine O-acetyltransferase

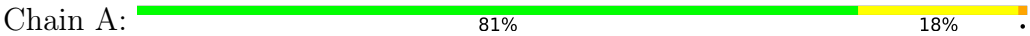
Chain B:

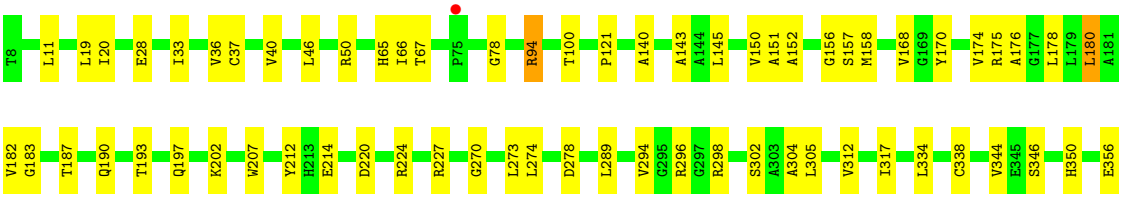




• Molecule 1: Homoserine O-acetyltransferase

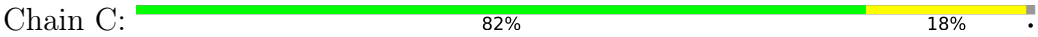
Chain A:

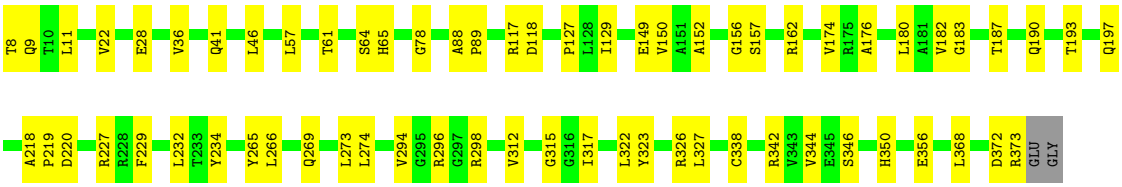




• Molecule 1: Homoserine O-acetyltransferase

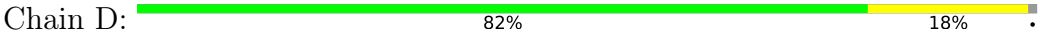
Chain C:

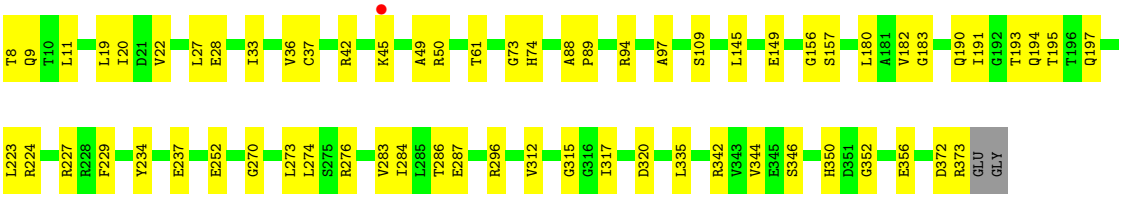




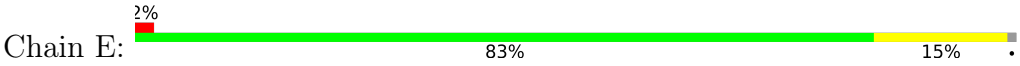
• Molecule 1: Homoserine O-acetyltransferase

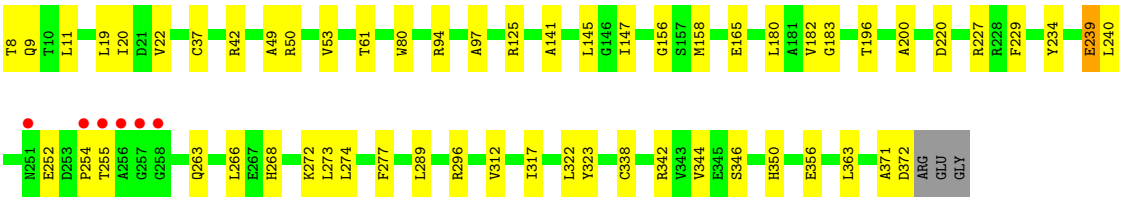
Chain D:



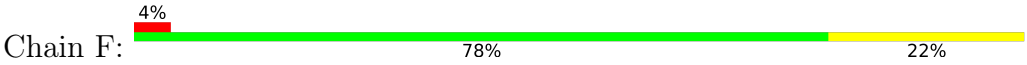


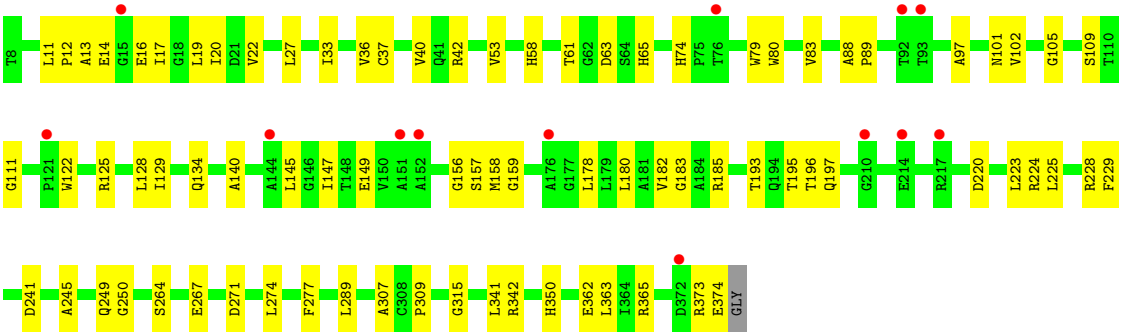
• Molecule 1: Homoserine O-acetyltransferase



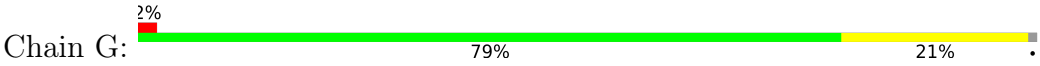


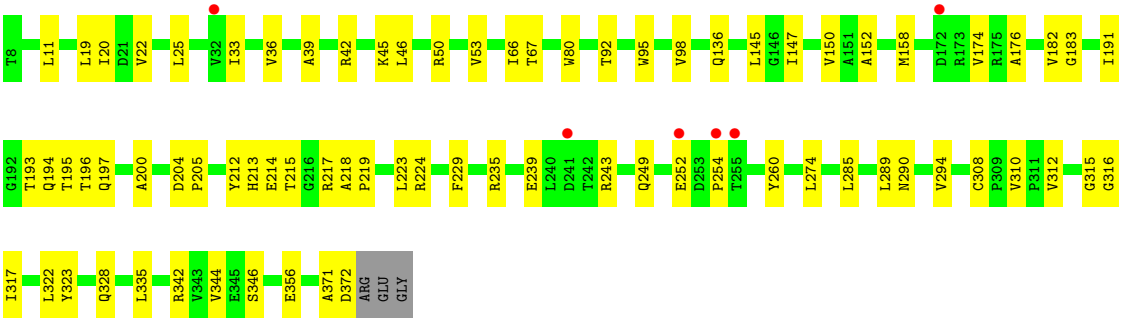
• Molecule 1: Homoserine O-acetyltransferase



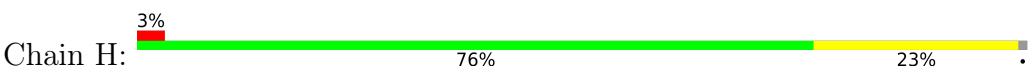


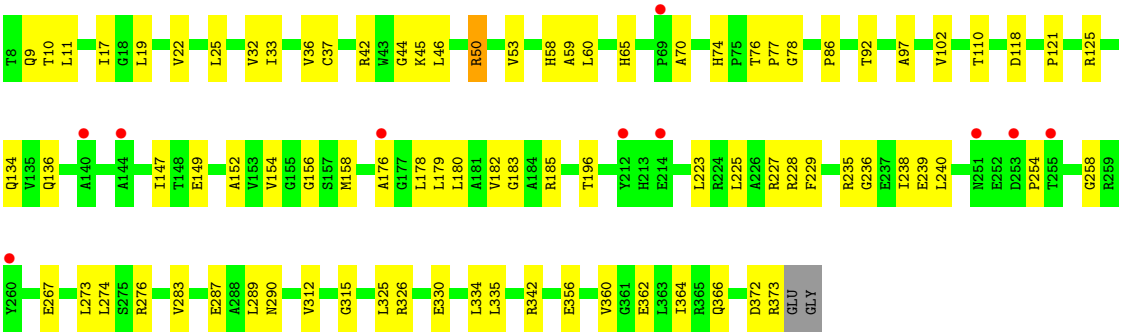
• Molecule 1: Homoserine O-acetyltransferase



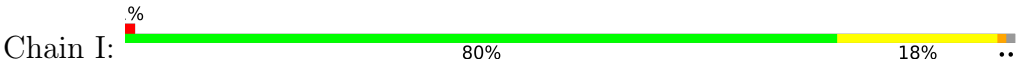


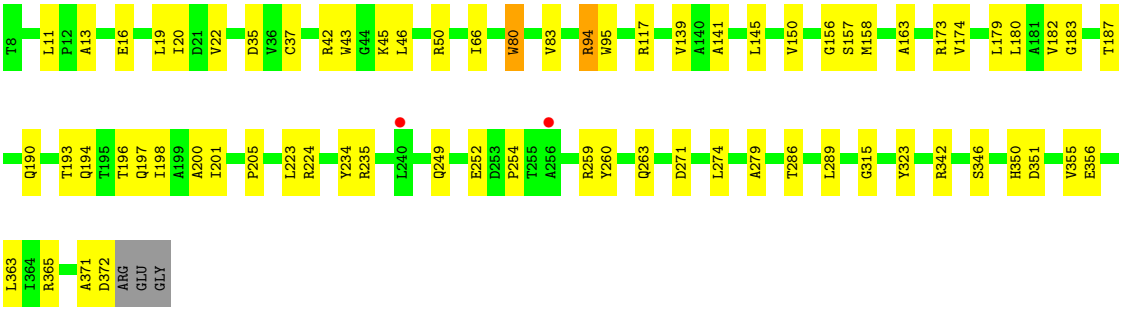
• Molecule 1: Homoserine O-acetyltransferase



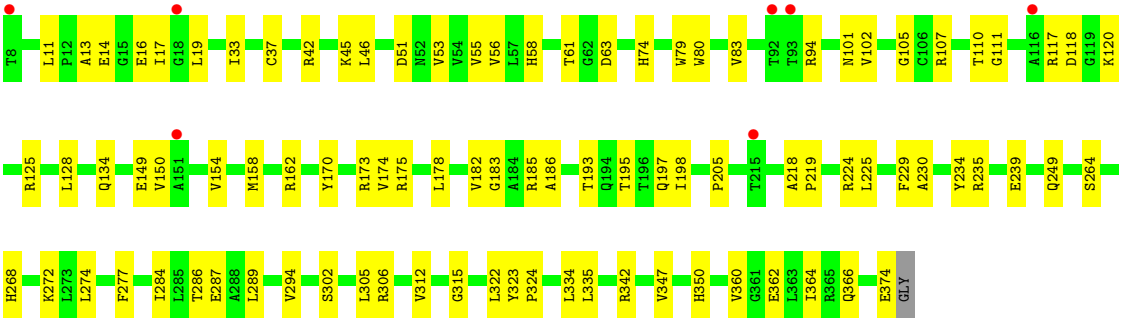


• Molecule 1: Homoserine O-acetyltransferase

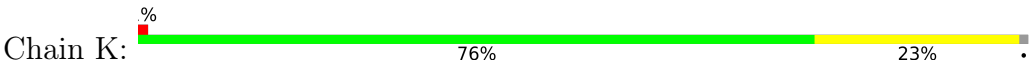


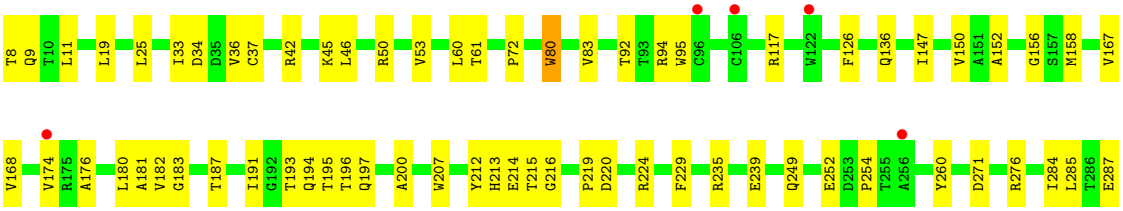


• Molecule 1: Homoserine O-acetyltransferase



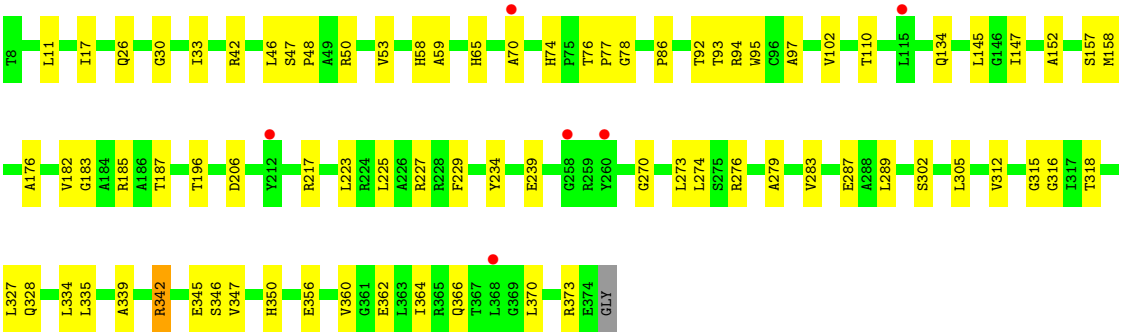
• Molecule 1: Homoserine O-acetyltransferase





• Molecule 1: Homoserine O-acetyltransferase

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	161.74Å 161.74Å 249.24Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.96 – 2.89 46.96 – 2.89	Depositor EDS
% Data completeness (in resolution range)	98.9 (46.96-2.89) 98.9 (46.96-2.89)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.91 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.18.2-3874	Depositor
R, R_{free}	0.190 , 0.243 0.191 , 0.241	Depositor DCC
R_{free} test set	2010 reflections (1.25%)	wwPDB-VP
Wilson B-factor (Å^2)	40.0	Xtriage
Anisotropy	0.477	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 7.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.002 for -h,-k,l 0.469 for h,-h-k,-l 0.003 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	33542	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.93% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.49	0/2760	0.67	0/3765
1	B	0.47	0/2769	0.71	0/3777
1	C	0.49	0/2757	0.67	0/3760
1	D	0.48	0/2751	0.73	0/3753
1	E	0.47	0/2742	0.67	0/3742
1	F	0.46	0/2754	0.65	0/3757
1	G	0.45	0/2738	0.66	0/3736
1	H	0.46	0/2747	0.63	0/3749
1	I	0.48	0/2746	0.68	0/3746
1	J	0.46	0/2766	0.67	0/3772
1	K	0.47	0/2742	0.67	0/3741
1	L	0.45	0/2751	0.65	0/3754
All	All	0.47	0/33023	0.67	0/45052

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	A	2706	172	2657	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2712	9	2663	43	0
1	C	2703	167	2662	45	0
1	D	2697	9	2651	43	0
1	E	2688	172	2638	48	0
1	F	2701	9	2652	74	0
1	G	2684	172	2633	57	0
1	H	2693	9	2640	68	0
1	I	2692	172	2649	58	0
1	J	2712	9	2668	74	0
1	K	2688	172	2645	67	0
1	L	2697	9	2642	53	0
2	A	8	0	3	0	0
2	B	8	0	3	0	0
2	C	8	0	3	3	0
2	D	8	0	3	1	0
2	F	8	0	3	0	0
2	G	8	0	3	0	0
2	H	8	0	3	5	0
2	I	8	0	3	3	0
2	J	8	0	3	1	0
2	K	8	0	3	1	0
2	L	8	0	3	1	0
All	All	32461	1081	31833	643	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 10.

All (643) 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:H:60:LEU:H	2:H:401:HSE:H42	1.08	1.15
1:H:223:LEU:HD23	1:H:274:LEU:HD23	1.39	1.05
1:G:20:ILE:HD12	1:G:145:LEU:HD21	1.37	1.01
1:H:70:ALA:HB2	1:H:77:PRO:HD3	1.48	0.96
1:E:11:LEU:HD13	1:E:42:ARG:HD3	1.47	0.95
1:H:46:LEU:HD21	1:H:50:ARG:HG3	1.49	0.95
1:A:20:ILE:HD12	1:A:145:LEU:HD21	1.51	0.93
1:J:193:THR:O	1:J:197:GLN:HG3	1.69	0.93
1:J:55:VAL:HG23	1:J:150:VAL:HG11	1.52	0.91
1:C:220:ASP:HB3	1:C:274:LEU:HD21	1.54	0.91
1:B:150:VAL:HG23	1:B:174:VAL:HG23	1.54	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:53:VAL:HG21	1:H:147:ILE:HD13	1.56	0.86
1:E:255:THR:O	1:F:128:LEU:HD12	1.78	0.83
1:D:190:GLN:O	1:D:194:GLN:HG3	1.81	0.81
1:I:13:ALA:HB3	1:I:16:GLU:HG3	1.61	0.81
1:K:11:LEU:HB3	1:K:42:ARG:HD3	1.62	0.80
1:J:11:LEU:HD13	1:J:42:ARG:CD	2.11	0.80
1:K:249:GLN:O	1:K:252:GLU:HG2	1.82	0.79
1:F:19:LEU:HD12	1:F:37:CYS:SG	2.22	0.79
1:A:220:ASP:HB3	1:A:274:LEU:HD21	1.64	0.78
1:L:65:HIS:O	1:L:78:GLY:HA2	1.83	0.78
1:L:223:LEU:HD23	1:L:274:LEU:HD13	1.66	0.77
1:J:33:ILE:HD11	1:J:110:THR:HG21	1.67	0.77
1:K:294:VAL:O	1:K:298:ARG:HD2	1.85	0.77
1:G:150:VAL:HG23	1:G:174:VAL:HG23	1.66	0.76
1:A:20:ILE:CD1	1:A:145:LEU:HD21	2.14	0.76
1:G:252:GLU:HB3	1:I:252:GLU:HG2	1.68	0.76
1:D:372:ASP:O	1:D:373:ARG:HB2	1.86	0.76
1:L:356:GLU:O	1:L:360:VAL:HG23	1.85	0.76
1:F:11:LEU:HD23	1:F:42:ARG:HE	1.49	0.75
1:H:223:LEU:HD23	1:H:274:LEU:CD2	2.14	0.75
1:I:42:ARG:HH12	1:I:45:LYS:HD2	1.52	0.75
1:F:13:ALA:HB3	1:F:16:GLU:OE1	1.87	0.74
1:E:268:HIS:O	1:E:272:LYS:HG3	1.87	0.74
1:J:158:MET:HG3	1:J:289:LEU:HD21	1.70	0.74
1:H:59:ALA:HB1	2:H:401:HSE:C4	2.18	0.74
1:A:11:LEU:HD11	1:A:46:LEU:HD22	1.68	0.73
1:A:150:VAL:HG23	1:A:174:VAL:HG23	1.71	0.73
1:I:157:SER:HB2	1:I:350:HIS:NE2	2.04	0.73
1:F:11:LEU:HD23	1:F:42:ARG:NE	2.03	0.73
1:H:239:GLU:HG3	1:H:240:LEU:N	2.02	0.73
1:H:60:LEU:N	2:H:401:HSE:H42	1.94	0.72
1:I:223:LEU:HD23	1:I:274:LEU:HD23	1.72	0.72
1:B:154:VAL:HG12	1:B:178:LEU:HB3	1.72	0.72
1:G:193:THR:O	1:G:197:GLN:HG3	1.89	0.71
1:G:42:ARG:HH12	1:G:45:LYS:HD2	1.55	0.71
1:J:11:LEU:HD13	1:J:42:ARG:HD3	1.71	0.71
1:B:26:GLN:HG3	1:B:32:VAL:HG22	1.71	0.71
1:B:220:ASP:HB3	1:B:274:LEU:HD21	1.73	0.71
1:H:19:LEU:HD12	1:H:37:CYS:SG	2.31	0.71
1:A:346:SER:HB2	1:A:356:GLU:HG3	1.73	0.70
1:H:65:HIS:O	1:H:78:GLY:HA2	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:46:LEU:HD23	1:L:47:SER:O	1.91	0.70
1:I:187:THR:OG1	1:I:190:GLN:HG3	1.91	0.70
1:I:196:THR:HG22	1:J:229:PHE:CZ	2.27	0.70
1:A:294:VAL:O	1:A:298:ARG:HD2	1.93	0.69
1:G:11:LEU:HB3	1:G:42:ARG:HD3	1.73	0.69
1:L:227:ARG:HD3	1:L:273:LEU:HD22	1.75	0.69
1:E:8:THR:HG22	1:E:9:GLN:HG3	1.73	0.69
1:C:372:ASP:O	1:C:373:ARG:HB2	1.93	0.69
1:E:239:GLU:HG3	1:E:240:LEU:N	2.06	0.69
1:F:373:ARG:O	1:F:374:GLU:HG2	1.92	0.68
1:G:194:GLN:NE2	1:G:290:ASN:OD1	2.27	0.68
1:J:185:ARG:HH11	1:J:185:ARG:HG3	1.59	0.68
1:C:11:LEU:HD11	1:C:46:LEU:HD22	1.76	0.67
1:L:206:ASP:OD1	1:L:217:ARG:NH1	2.27	0.67
1:H:59:ALA:HB1	2:H:401:HSE:H41	1.76	0.67
1:D:227:ARG:HD3	1:D:273:LEU:HD22	1.76	0.67
1:I:263:GLN:HG3	1:J:195:THR:HG21	1.76	0.67
1:J:45:LYS:HG2	1:J:46:LEU:N	2.10	0.67
1:E:227:ARG:HD3	1:E:273:LEU:HD22	1.75	0.66
1:G:317:ILE:HD13	1:G:344:VAL:HB	1.77	0.66
1:G:371:ALA:O	1:G:372:ASP:HB2	1.94	0.66
1:F:27:LEU:HD13	1:F:129:ILE:HG22	1.76	0.66
1:K:191:ILE:O	1:K:195:THR:HG23	1.95	0.66
1:K:193:THR:O	1:K:197:GLN:HG3	1.95	0.66
1:G:33:ILE:HG23	1:G:36:VAL:CG2	2.26	0.66
1:F:11:LEU:CD1	1:F:145:LEU:HD23	2.25	0.66
1:D:191:ILE:O	1:D:195:THR:HG23	1.97	0.65
1:J:13:ALA:HB3	1:J:16:GLU:OE2	1.96	0.65
1:E:196:THR:HG22	1:F:229:PHE:CE2	2.32	0.65
1:B:46:LEU:HD11	1:B:50:ARG:HA	1.79	0.65
1:D:42:ARG:HA	1:D:97:ALA:O	1.96	0.65
1:D:317:ILE:HG23	1:D:346:SER:HB3	1.80	0.64
1:K:61:THR:HB	1:K:276:ARG:HH21	1.62	0.64
1:L:33:ILE:HD11	1:L:110:THR:HG21	1.79	0.64
1:K:224:ARG:NH1	1:K:271:ASP:OD1	2.30	0.64
1:E:317:ILE:CD1	1:E:344:VAL:HB	2.27	0.63
1:I:196:THR:HG22	1:J:229:PHE:CE2	2.33	0.63
1:L:70:ALA:HB2	1:L:77:PRO:HD3	1.80	0.63
1:E:196:THR:HG22	1:F:229:PHE:CZ	2.33	0.63
1:F:14:GLU:HG3	1:F:42:ARG:NH2	2.14	0.63
1:B:312:VAL:HG21	1:B:335:LEU:HD13	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:42:ARG:HH12	1:K:45:LYS:HD2	1.64	0.63
1:C:41:GLN:HG3	1:C:64:SER:HB2	1.79	0.62
1:K:220:ASP:O	1:K:224:ARG:HG3	1.99	0.62
1:G:20:ILE:CD1	1:G:145:LEU:HD21	2.22	0.62
1:F:17:ILE:HD12	1:F:17:ILE:H	1.64	0.62
1:C:220:ASP:HB3	1:C:274:LEU:CD2	2.28	0.62
1:J:14:GLU:HG3	1:J:42:ARG:NH1	2.14	0.62
1:C:193:THR:O	1:C:197:GLN:HG3	2.00	0.62
1:F:224:ARG:NH1	1:F:271:ASP:OD1	2.33	0.61
1:B:227:ARG:HD3	1:B:273:LEU:HD22	1.82	0.61
1:G:200:ALA:HA	1:H:225:LEU:HD11	1.81	0.61
1:A:227:ARG:HD3	1:A:273:LEU:HD22	1.82	0.61
1:H:59:ALA:HB1	2:H:401:HSE:H42	1.81	0.61
1:F:185:ARG:HG3	1:F:185:ARG:HH11	1.65	0.61
1:B:346:SER:HB2	1:B:356:GLU:HG3	1.82	0.60
1:K:33:ILE:HG23	1:K:36:VAL:CG2	2.30	0.60
1:L:42:ARG:HA	1:L:97:ALA:O	2.02	0.60
1:H:86:PRO:HD3	1:H:92:THR:OG1	2.00	0.60
1:F:58:HIS:HA	1:F:79:TRP:CH2	2.36	0.60
1:L:33:ILE:HD11	1:L:110:THR:CG2	2.32	0.60
2:I:401:HSE:OXT	2:I:401:HSE:H41	1.90	0.60
1:L:46:LEU:HD21	1:L:50:ARG:HG2	1.83	0.60
1:F:22:VAL:CG1	1:F:140:ALA:HB1	2.31	0.60
1:B:44:GLY:CA	1:B:92:THR:HB	2.31	0.59
1:K:254:PRO:HG2	1:K:260:TYR:CE1	2.37	0.59
1:L:102:VAL:HG23	1:L:134:GLN:HB3	1.84	0.59
1:D:223:LEU:HD12	1:D:223:LEU:O	2.02	0.59
1:J:11:LEU:HD13	1:J:42:ARG:HD2	1.85	0.59
1:D:312:VAL:HG21	1:D:335:LEU:HD13	1.83	0.59
1:H:185:ARG:HG3	1:H:185:ARG:HH11	1.67	0.59
1:F:11:LEU:HD12	1:F:145:LEU:HD23	1.83	0.59
1:H:33:ILE:HD11	1:H:110:THR:HG21	1.84	0.59
1:L:223:LEU:HD13	1:L:279:ALA:HA	1.84	0.59
1:E:371:ALA:O	1:E:372:ASP:HB2	2.03	0.59
1:G:312:VAL:HG21	1:G:335:LEU:HD13	1.85	0.58
1:I:35:ASP:OD2	1:I:117:ARG:HD2	2.04	0.58
1:F:17:ILE:HD11	1:F:74:HIS:NE2	2.17	0.58
1:J:239:GLU:HG2	1:J:347:VAL:O	2.03	0.58
1:K:8:THR:HG22	1:K:9:GLN:H	1.67	0.58
1:J:33:ILE:HD11	1:J:110:THR:CG2	2.33	0.58
1:J:51:ASP:O	1:J:175:ARG:NH2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:158:MET:HB2	1:I:289:LEU:HD21	1.86	0.58
1:I:193:THR:O	1:I:197:GLN:HG3	2.04	0.58
1:B:224:ARG:HG3	1:B:274:LEU:HD11	1.85	0.58
1:F:33:ILE:HG23	1:F:36:VAL:CG2	2.34	0.58
1:F:223:LEU:HD23	1:F:274:LEU:HD12	1.86	0.57
1:L:227:ARG:CD	1:L:273:LEU:HD22	2.33	0.57
1:H:121:PRO:O	1:H:125:ARG:NH2	2.37	0.57
1:I:182:VAL:HG22	1:I:183:GLY:N	2.18	0.57
1:F:373:ARG:HH11	1:F:373:ARG:HG2	1.69	0.57
1:J:120:LYS:HB2	1:J:125:ARG:HH22	1.69	0.57
1:A:121:PRO:HG3	1:A:214:GLU:OE1	2.04	0.57
1:E:317:ILE:HD13	1:E:344:VAL:HB	1.86	0.57
1:C:326:ARG:HH21	1:D:237:GLU:CD	2.08	0.57
1:G:317:ILE:CD1	1:G:344:VAL:HB	2.35	0.57
1:F:122:TRP:O	1:F:125:ARG:HB2	2.04	0.56
1:B:252:GLU:HA	1:K:216:GLY:O	2.05	0.56
2:D:401:HSE:H41	2:D:401:HSE:OXT	2.04	0.56
1:E:239:GLU:HG3	1:E:240:LEU:H	1.70	0.56
1:H:228:ARG:NH1	1:H:267:GLU:HG2	2.20	0.56
1:K:158:MET:HB2	1:K:289:LEU:HD21	1.86	0.56
1:H:326:ARG:NH1	1:H:326:ARG:HG3	2.20	0.56
1:K:42:ARG:HH12	1:K:45:LYS:HA	1.69	0.56
1:K:168:VAL:HG12	1:K:298:ARG:NH1	2.20	0.56
1:G:229:PHE:CE2	1:H:196:THR:HG22	2.40	0.56
1:G:249:GLN:O	1:G:252:GLU:HG2	2.06	0.56
1:H:356:GLU:O	1:H:360:VAL:HG23	2.06	0.56
1:K:213:HIS:O	1:K:214:GLU:HB2	2.06	0.56
1:G:152:ALA:HA	1:G:176:ALA:O	2.06	0.56
1:K:19:LEU:HD22	1:K:37:CYS:SG	2.46	0.56
1:I:234:TYR:OH	2:I:401:HSE:H42	2.06	0.56
1:J:58:HIS:CE1	1:J:102:VAL:HG12	2.41	0.56
1:B:44:GLY:HA3	1:B:92:THR:HB	1.87	0.56
1:A:224:ARG:HG2	1:A:270:GLY:HA3	1.88	0.56
1:F:193:THR:O	1:F:197:GLN:HG3	2.07	0.55
1:H:227:ARG:NE	1:H:273:LEU:HD22	2.21	0.55
1:C:346:SER:HB2	1:C:356:GLU:HG3	1.86	0.55
1:I:371:ALA:O	1:I:372:ASP:HB2	2.05	0.55
1:G:322:LEU:HD23	1:G:323:TYR:CE1	2.42	0.55
1:H:45:LYS:HG3	1:H:46:LEU:N	2.22	0.55
1:H:182:VAL:HG22	1:H:183:GLY:N	2.22	0.55
1:H:227:ARG:HB2	1:H:273:LEU:HD23	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:58:HIS:CE1	1:F:102:VAL:HG12	2.42	0.55
1:I:150:VAL:HG23	1:I:174:VAL:HG23	1.88	0.55
1:J:234:TYR:OH	2:J:401:HSE:H42	2.07	0.55
1:K:34:ASP:HB3	1:K:117:ARG:HE	1.71	0.55
1:A:150:VAL:CG2	1:A:174:VAL:HG23	2.36	0.55
1:F:315:GLY:HA2	1:F:342:ARG:O	2.06	0.55
1:F:307:ALA:O	1:F:309:PRO:HD3	2.07	0.55
1:I:223:LEU:HD23	1:I:274:LEU:CD2	2.37	0.55
1:I:50:ARG:HG3	1:I:50:ARG:HH11	1.72	0.54
1:J:360:VAL:O	1:J:364:ILE:HG13	2.08	0.54
1:A:212:TYR:OH	1:A:278:ASP:OD1	2.22	0.54
1:J:182:VAL:HG22	1:J:183:GLY:N	2.22	0.54
1:E:342:ARG:HD3	1:E:363:LEU:HD22	1.89	0.54
1:I:200:ALA:HA	1:J:225:LEU:HD11	1.90	0.54
1:F:182:VAL:HG22	1:F:183:GLY:N	2.23	0.54
1:A:121:PRO:CG	1:A:214:GLU:OE1	2.56	0.54
1:D:182:VAL:HG22	1:D:183:GLY:N	2.23	0.54
1:K:25:LEU:HD22	1:K:136:GLN:OE1	2.08	0.54
1:A:193:THR:O	1:A:197:GLN:HG3	2.08	0.54
1:I:198:ILE:HD11	1:I:286:THR:HG22	1.90	0.54
1:D:156:GLY:HA2	1:D:180:LEU:O	2.08	0.53
1:I:20:ILE:HD11	1:I:145:LEU:HD11	1.90	0.53
1:J:14:GLU:HG3	1:J:42:ARG:HH12	1.71	0.53
1:J:17:ILE:HD12	1:J:17:ILE:H	1.73	0.53
1:J:362:GLU:OE1	1:J:362:GLU:HA	2.07	0.53
1:K:152:ALA:HA	1:K:176:ALA:O	2.09	0.53
1:E:346:SER:HB2	1:E:356:GLU:HG3	1.91	0.53
1:C:232:LEU:HD21	1:C:266:LEU:HD11	1.91	0.53
1:I:224:ARG:NH1	1:I:271:ASP:OD2	2.42	0.53
1:J:268:HIS:NE2	1:J:272:LYS:HD2	2.24	0.53
1:A:317:ILE:HG23	1:A:346:SER:HB3	1.91	0.53
1:F:157:SER:HB2	1:F:350:HIS:NE2	2.23	0.53
1:G:158:MET:HB2	1:G:289:LEU:HD21	1.90	0.53
1:L:185:ARG:HG3	1:L:185:ARG:HH11	1.74	0.53
1:F:58:HIS:HB3	1:F:79:TRP:CZ2	2.44	0.52
1:G:229:PHE:CZ	1:H:196:THR:HG22	2.44	0.52
1:J:45:LYS:HG2	1:J:46:LEU:H	1.72	0.52
1:B:198:ILE:HG23	1:B:283:VAL:HG13	1.91	0.52
1:E:156:GLY:HA2	1:E:180:LEU:O	2.09	0.52
1:F:11:LEU:HG	1:F:42:ARG:HD2	1.90	0.52
1:F:12:PRO:O	1:F:42:ARG:HD3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:102:VAL:HG23	1:H:134:GLN:HB3	1.91	0.52
1:L:76:THR:HG23	1:L:276:ARG:HD3	1.92	0.52
1:D:194:GLN:HB3	1:D:286:THR:HG23	1.92	0.52
1:C:187:THR:HG21	1:C:327:LEU:HD11	1.92	0.52
1:H:154:VAL:HG12	1:H:178:LEU:HB3	1.91	0.52
1:J:185:ARG:HG3	1:J:185:ARG:NH1	2.24	0.52
1:K:229:PHE:CZ	1:L:196:THR:HG22	2.44	0.52
1:L:58:HIS:CE1	1:L:102:VAL:HG12	2.44	0.52
1:A:168:VAL:HG12	1:A:298:ARG:NH1	2.24	0.52
1:H:76:THR:HG23	1:H:276:ARG:HD3	1.92	0.52
1:L:11:LEU:HG	1:L:145:LEU:HD13	1.90	0.52
1:G:46:LEU:HG	1:G:50:ARG:HG2	1.92	0.52
1:K:182:VAL:HG22	1:K:183:GLY:N	2.24	0.52
1:A:152:ALA:HA	1:A:176:ALA:O	2.10	0.51
1:J:63:ASP:HA	1:J:101:ASN:ND2	2.25	0.51
1:B:150:VAL:CG2	1:B:174:VAL:HG23	2.33	0.51
1:D:182:VAL:HG22	1:D:183:GLY:H	1.75	0.51
1:J:305:LEU:HD22	1:J:335:LEU:HD21	1.92	0.51
1:J:302:SER:HA	1:J:334:LEU:HD13	1.92	0.51
1:A:28:GLU:CD	1:A:296:ARG:HH21	2.12	0.51
1:G:322:LEU:HD23	1:G:323:TYR:HE1	1.74	0.51
1:H:17:ILE:HD11	1:H:74:HIS:NE2	2.25	0.51
1:F:58:HIS:HE1	1:F:102:VAL:HG12	1.74	0.51
1:I:182:VAL:HG22	1:I:183:GLY:H	1.74	0.51
1:A:157:SER:HB2	1:A:350:HIS:NE2	2.24	0.51
1:C:373:ARG:NE	1:C:373:ARG:HA	2.25	0.51
1:D:270:GLY:O	1:D:274:LEU:HD23	2.10	0.51
1:G:235:ARG:NH2	1:G:239:GLU:OE2	2.43	0.51
1:H:33:ILE:HD11	1:H:110:THR:CG2	2.41	0.51
1:J:53:VAL:HB	1:J:150:VAL:HG13	1.92	0.51
1:K:46:LEU:HD21	1:K:50:ARG:HG3	1.91	0.51
1:L:182:VAL:HG22	1:L:183:GLY:N	2.26	0.51
1:C:65:HIS:O	1:C:78:GLY:HA2	2.11	0.51
1:C:157:SER:HB2	1:C:350:HIS:NE2	2.25	0.51
1:D:37:CYS:O	1:D:109:SER:HA	2.10	0.51
1:L:157:SER:HB2	1:L:350:HIS:NE2	2.25	0.51
1:J:323:TYR:CD1	1:J:350:HIS:CE1	2.99	0.51
1:I:156:GLY:HA2	1:I:180:LEU:O	2.10	0.51
1:F:22:VAL:HG11	1:F:140:ALA:CB	2.40	0.51
1:L:102:VAL:CG2	1:L:134:GLN:HB3	2.41	0.51
1:H:46:LEU:HD11	1:H:50:ARG:HA	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:139:VAL:CG1	1:I:173:ARG:HH12	2.24	0.50
1:L:187:THR:HG21	1:L:327:LEU:HD11	1.94	0.50
1:K:187:THR:HG21	1:K:327:LEU:HD11	1.91	0.50
1:L:86:PRO:HA	1:L:93:THR:HG23	1.93	0.50
1:B:46:LEU:HD12	1:B:52:ASN:OD1	2.11	0.50
1:D:61:THR:HB	1:D:276:ARG:HH22	1.76	0.50
1:J:198:ILE:HD11	1:J:286:THR:HG22	1.93	0.50
1:A:298:ARG:HG3	1:A:304:ALA:HB2	1.93	0.50
1:F:17:ILE:HD12	1:F:17:ILE:N	2.26	0.50
1:B:101:ASN:HB3	1:B:109:SER:OG	2.12	0.50
1:C:182:VAL:HG22	1:C:183:GLY:N	2.26	0.50
1:I:190:GLN:O	1:I:194:GLN:HG3	2.11	0.50
1:A:187:THR:OG1	1:A:190:GLN:HG3	2.12	0.50
1:G:42:ARG:HH12	1:G:45:LYS:HA	1.77	0.50
1:K:346:SER:HB2	1:K:356:GLU:HG3	1.94	0.50
1:C:312:VAL:HG23	1:C:338:CYS:HB2	1.92	0.50
1:F:20:ILE:HD11	1:F:40:VAL:HG11	1.94	0.50
1:G:223:LEU:HD23	1:G:274:LEU:HD23	1.94	0.50
1:J:11:LEU:HD22	1:J:42:ARG:HD3	1.94	0.50
1:E:182:VAL:HG22	1:E:183:GLY:N	2.26	0.49
1:I:346:SER:HB2	1:I:356:GLU:HG3	1.93	0.49
1:L:312:VAL:HG21	1:L:335:LEU:HD13	1.93	0.49
1:L:362:GLU:O	1:L:366:GLN:HG3	2.12	0.49
1:A:40:VAL:HG22	1:A:100:THR:HG22	1.94	0.49
1:F:63:ASP:HA	1:F:101:ASN:ND2	2.28	0.49
1:J:63:ASP:HA	1:J:101:ASN:HD22	1.77	0.49
1:B:243:ARG:HG2	1:B:244:PHE:CE2	2.47	0.49
1:A:94:ARG:HH12	1:A:372:ASP:CG	2.14	0.49
1:E:252:GLU:HG2	1:K:252:GLU:HB3	1.95	0.49
1:H:42:ARG:HA	1:H:97:ALA:O	2.12	0.49
1:J:45:LYS:CG	1:J:46:LEU:N	2.76	0.49
1:A:33:ILE:HG23	1:A:36:VAL:HG23	1.95	0.49
1:K:212:TYR:O	1:K:215:THR:HG23	2.11	0.49
1:K:315:GLY:HA2	1:K:342:ARG:O	2.12	0.49
1:D:194:GLN:HB3	1:D:286:THR:CG2	2.42	0.49
1:H:326:ARG:HG3	1:H:326:ARG:HH11	1.78	0.49
1:I:365:ARG:HG2	1:I:365:ARG:HH11	1.77	0.49
1:G:346:SER:HB2	1:G:356:GLU:HG3	1.95	0.49
1:I:363:LEU:HD12	1:I:363:LEU:N	2.28	0.49
1:B:220:ASP:HB3	1:B:274:LEU:CD2	2.42	0.49
1:B:224:ARG:HG3	1:B:274:LEU:CD1	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:150:VAL:HG23	1:C:174:VAL:HG23	1.94	0.49
1:F:22:VAL:HG12	1:F:22:VAL:O	2.12	0.49
1:G:182:VAL:HG22	1:G:183:GLY:N	2.27	0.49
1:K:194:GLN:NE2	1:K:290:ASN:OD1	2.46	0.49
1:A:302:SER:HA	1:A:334:LEU:HD13	1.94	0.49
1:D:88:ALA:HB1	1:D:89:PRO:CD	2.43	0.49
1:G:213:HIS:O	1:G:214:GLU:HB2	2.12	0.49
1:C:61:THR:OG1	2:C:401:HSE:OXT	2.24	0.49
1:G:204:ASP:OD1	1:G:205:PRO:HD2	2.12	0.49
1:H:360:VAL:O	1:H:364:ILE:HG13	2.13	0.49
1:K:196:THR:HG22	1:L:229:PHE:CE2	2.48	0.49
1:K:302:SER:HA	1:K:334:LEU:HD23	1.95	0.49
1:B:11:LEU:HD13	1:B:42:ARG:CD	2.43	0.48
1:A:66:ILE:HG13	1:A:67:THR:HG22	1.95	0.48
1:F:341:LEU:HD12	1:F:342:ARG:N	2.27	0.48
1:I:11:LEU:HB3	1:I:42:ARG:HD3	1.94	0.48
1:J:218:ALA:HB1	1:J:219:PRO:HD2	1.95	0.48
1:B:39:ALA:HB2	1:B:108:GLY:HA3	1.94	0.48
1:K:92:THR:HA	1:K:95:TRP:O	2.14	0.48
1:C:234:TYR:CD1	2:C:401:HSE:H41	2.48	0.48
1:D:157:SER:HB2	1:D:350:HIS:NE2	2.27	0.48
1:G:22:VAL:HG23	1:G:36:VAL:HB	1.93	0.48
1:A:65:HIS:O	1:A:78:GLY:HA2	2.13	0.48
1:F:249:GLN:HE21	1:F:250:GLY:N	2.12	0.48
1:K:187:THR:CG2	1:K:327:LEU:HD11	2.43	0.48
1:B:56:VAL:HG22	1:B:154:VAL:CG2	2.44	0.48
1:C:227:ARG:HD3	1:C:273:LEU:HD22	1.95	0.48
1:G:191:ILE:O	1:G:195:THR:HG23	2.14	0.48
1:J:312:VAL:HG21	1:J:335:LEU:HD13	1.96	0.48
1:K:168:VAL:CG1	1:K:298:ARG:NH1	2.76	0.48
1:D:224:ARG:HG3	1:D:274:LEU:HD21	1.95	0.48
1:F:228:ARG:NH1	1:F:267:GLU:HG2	2.28	0.48
1:G:260:TYR:CE2	1:H:290:ASN:HB3	2.48	0.48
1:B:42:ARG:HA	1:B:97:ALA:O	2.13	0.48
1:F:53:VAL:HG21	1:F:147:ILE:HD13	1.96	0.48
1:F:178:LEU:HD11	1:F:180:LEU:HD13	1.95	0.48
1:G:254:PRO:HG2	1:G:260:TYR:CE1	2.49	0.48
1:J:249:GLN:OE1	1:J:264:SER:HB3	2.14	0.48
1:L:53:VAL:HG21	1:L:147:ILE:HG21	1.96	0.47
1:B:182:VAL:HG22	1:B:183:GLY:N	2.28	0.47
1:C:372:ASP:O	1:C:373:ARG:CB	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:20:ILE:HD11	1:E:145:LEU:HD11	1.96	0.47
1:A:294:VAL:HG11	1:A:305:LEU:HD21	1.95	0.47
1:H:25:LEU:HD22	1:H:136:GLN:OE1	2.13	0.47
1:J:224:ARG:NH2	1:J:274:LEU:HD12	2.29	0.47
1:K:285:LEU:HA	1:K:285:LEU:HD23	1.62	0.47
1:D:193:THR:O	1:D:197:GLN:HG3	2.14	0.47
1:G:158:MET:HG3	1:G:289:LEU:HD21	1.97	0.47
1:H:254:PRO:HA	1:H:258:GLY:O	2.14	0.47
1:A:19:LEU:HB3	1:A:37:CYS:SG	2.54	0.47
1:F:158:MET:HG3	1:F:289:LEU:HD21	1.97	0.47
1:K:34:ASP:CB	1:K:117:ARG:HE	2.27	0.47
1:K:60:LEU:H	2:K:401:HSE:H41	1.80	0.47
1:H:185:ARG:HG3	1:H:185:ARG:NH1	2.30	0.47
1:K:181:ALA:HB1	1:K:350:HIS:CE1	2.49	0.47
1:L:360:VAL:O	1:L:364:ILE:HG13	2.14	0.47
1:A:178:LEU:HB2	1:A:367:THR:OG1	2.15	0.47
1:E:229:PHE:CE2	1:F:196:THR:HG22	2.50	0.47
1:E:312:VAL:CG2	1:E:338:CYS:HB2	2.45	0.47
1:F:65:HIS:HB2	1:F:74:HIS:CE1	2.49	0.47
1:I:286:THR:HA	1:I:289:LEU:HD12	1.97	0.47
1:A:46:LEU:HD11	1:A:50:ARG:HA	1.95	0.47
1:I:19:LEU:HD22	1:I:37:CYS:HB3	1.97	0.47
1:L:270:GLY:O	1:L:274:LEU:HD23	2.14	0.47
1:C:28:GLU:CD	1:C:296:ARG:HH21	2.18	0.47
1:C:232:LEU:CD2	1:C:266:LEU:HD21	2.45	0.47
1:K:235:ARG:NH2	1:K:239:GLU:OE2	2.47	0.47
1:L:17:ILE:HD11	1:L:74:HIS:NE2	2.30	0.47
1:D:88:ALA:HB1	1:D:89:PRO:HD2	1.96	0.46
1:D:227:ARG:CD	1:D:273:LEU:HD22	2.43	0.46
1:G:158:MET:CG	1:G:289:LEU:HD21	2.45	0.46
1:L:283:VAL:O	1:L:287:GLU:HG2	2.15	0.46
1:C:187:THR:OG1	1:C:190:GLN:HG3	2.15	0.46
1:E:8:THR:HG22	1:E:9:GLN:CG	2.42	0.46
1:I:139:VAL:HG13	1:I:173:ARG:HH12	1.80	0.46
1:I:11:LEU:HD13	1:I:42:ARG:HD2	1.97	0.46
1:J:61:THR:HA	1:J:277:PHE:CE1	2.50	0.46
1:A:202:LYS:HG2	1:A:207:TRP:NE1	2.31	0.46
1:F:11:LEU:HD13	1:F:145:LEU:HD23	1.96	0.46
1:I:43:TRP:CZ3	1:I:66:ILE:HG12	2.51	0.46
1:I:254:PRO:HB3	1:I:260:TYR:CE2	2.49	0.46
1:J:158:MET:HG3	1:J:289:LEU:CD2	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:318:THR:HG23	1:L:345:GLU:HA	1.97	0.46
1:C:152:ALA:HA	1:C:176:ALA:O	2.16	0.46
1:E:252:GLU:O	1:E:254:PRO:HD3	2.15	0.46
1:I:22:VAL:HG12	1:I:141:ALA:HA	1.97	0.46
1:J:17:ILE:HD11	1:J:74:HIS:NE2	2.31	0.46
1:A:11:LEU:CD1	1:A:46:LEU:HD22	2.40	0.46
1:C:22:VAL:HG23	1:C:36:VAL:HB	1.98	0.46
1:E:53:VAL:HG21	1:E:147:ILE:HD13	1.98	0.46
1:F:58:HIS:HE1	1:F:102:VAL:CG1	2.29	0.46
1:I:223:LEU:HD13	1:I:279:ALA:HA	1.97	0.46
1:E:49:ALA:O	1:E:50:ARG:HB2	2.16	0.46
1:E:182:VAL:HA	1:E:323:TYR:CD2	2.51	0.46
1:F:22:VAL:HG11	1:F:140:ALA:HB3	1.98	0.46
1:G:22:VAL:HG22	1:G:36:VAL:O	2.15	0.46
1:H:178:LEU:C	1:H:179:LEU:HD23	2.37	0.46
1:J:105:GLY:O	1:J:111:GLY:HA3	2.15	0.46
1:F:11:LEU:CD2	1:F:42:ARG:HE	2.24	0.46
1:H:76:THR:CG2	1:H:276:ARG:HD3	2.45	0.46
1:K:326:ARG:HG3	1:K:327:LEU:HD23	1.97	0.46
1:L:315:GLY:HA2	1:L:342:ARG:O	2.16	0.46
1:B:224:ARG:NH1	1:B:274:LEU:HD22	2.31	0.45
1:D:317:ILE:HD13	1:D:344:VAL:HB	1.98	0.45
1:D:346:SER:HB2	1:D:356:GLU:HG3	1.98	0.45
1:C:156:GLY:HA2	1:C:180:LEU:O	2.16	0.45
1:E:229:PHE:CZ	1:F:196:THR:HG22	2.51	0.45
1:K:42:ARG:NH1	1:K:45:LYS:HD2	2.30	0.45
1:L:305:LEU:HD22	1:L:335:LEU:HD21	1.97	0.45
1:K:229:PHE:CE2	1:L:196:THR:HG22	2.51	0.45
1:B:37:CYS:O	1:B:109:SER:HA	2.17	0.45
1:C:88:ALA:HB1	1:C:89:PRO:HD2	1.99	0.45
1:D:317:ILE:HB	1:D:320:ASP:HB2	1.98	0.45
1:E:342:ARG:HD3	1:E:363:LEU:CD2	2.46	0.45
1:F:11:LEU:HD12	1:F:145:LEU:CD2	2.46	0.45
1:F:101:ASN:HB3	1:F:109:SER:OG	2.16	0.45
1:G:315:GLY:HA2	1:G:342:ARG:O	2.17	0.45
1:H:45:LYS:CG	1:H:46:LEU:N	2.79	0.45
1:A:182:VAL:HG22	1:A:183:GLY:N	2.31	0.45
1:C:317:ILE:HD13	1:C:344:VAL:HB	1.98	0.45
1:H:22:VAL:CG2	1:H:36:VAL:HB	2.46	0.45
1:H:312:VAL:HG21	1:H:335:LEU:HD13	1.97	0.45
1:B:152:ALA:HA	1:B:176:ALA:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:ILE:HG23	1:A:36:VAL:CG2	2.47	0.45
1:F:63:ASP:HA	1:F:101:ASN:HD22	1.81	0.45
1:F:89:PRO:HA	1:F:365:ARG:HE	1.82	0.45
1:F:274:LEU:HD12	1:F:274:LEU:HA	1.80	0.45
1:J:374:GLU:O	1:J:374:GLU:HG3	2.16	0.45
1:C:57:LEU:HD13	1:C:162:ARG:HB2	1.99	0.45
1:L:158:MET:HB2	1:L:289:LEU:HD21	1.99	0.45
1:L:234:TYR:HA	1:L:350:HIS:HB3	1.99	0.45
1:G:92:THR:HA	1:G:95:TRP:O	2.17	0.45
1:G:196:THR:HG22	1:H:229:PHE:CE2	2.52	0.45
1:K:200:ALA:HA	1:L:225:LEU:HD11	1.98	0.45
1:L:76:THR:CG2	1:L:276:ARG:HD3	2.47	0.45
1:H:156:GLY:HA2	1:H:180:LEU:O	2.17	0.44
1:B:80:TRP:O	1:B:81:ASP:C	2.55	0.44
1:B:315:GLY:HA2	1:B:342:ARG:O	2.16	0.44
1:B:334:LEU:HD23	1:B:334:LEU:HA	1.67	0.44
1:A:156:GLY:HA2	1:A:180:LEU:O	2.17	0.44
1:I:234:TYR:CZ	2:I:401:HSE:H42	2.52	0.44
1:F:180:LEU:HD11	1:F:363:LEU:HD12	2.00	0.44
1:K:33:ILE:HD11	1:K:126:PHE:CE1	2.53	0.44
1:K:235:ARG:HD2	1:K:235:ARG:HA	1.79	0.44
1:L:26:GLN:NE2	1:L:30:GLY:O	2.49	0.44
1:A:66:ILE:HG13	1:A:67:THR:N	2.33	0.44
1:D:252:GLU:HG2	1:G:217:ARG:HD3	1.99	0.44
1:G:158:MET:CB	1:G:289:LEU:HD21	2.47	0.44
1:L:302:SER:HA	1:L:334:LEU:HD13	2.00	0.44
1:A:312:VAL:HG23	1:A:338:CYS:HB2	1.99	0.44
1:C:8:THR:HG23	1:C:9:GLN:HG3	1.99	0.44
1:C:326:ARG:NH2	1:D:237:GLU:OE2	2.51	0.44
1:D:283:VAL:O	1:D:287:GLU:HG2	2.18	0.44
1:F:88:ALA:HB1	1:F:89:PRO:HD2	1.98	0.44
1:L:59:ALA:HB1	2:L:401:HSE:H42	1.99	0.44
1:B:49:ALA:O	1:B:50:ARG:HB2	2.17	0.44
1:E:158:MET:HB2	1:E:289:LEU:HD21	1.99	0.44
1:G:46:LEU:CD2	1:G:50:ARG:HG2	2.47	0.44
1:H:236:GLY:O	1:H:239:GLU:HG2	2.18	0.44
1:H:372:ASP:O	1:H:373:ARG:C	2.56	0.44
1:E:61:THR:HA	1:E:277:PHE:CE1	2.53	0.44
1:J:17:ILE:HD12	1:J:17:ILE:N	2.32	0.44
1:A:363:LEU:N	1:A:363:LEU:HD23	2.33	0.44
1:H:45:LYS:HD2	1:H:46:LEU:H	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:158:MET:HG3	1:H:289:LEU:HD21	1.98	0.44
1:I:235:ARG:HA	1:I:235:ARG:HD2	1.85	0.44
1:I:252:GLU:OE1	1:I:259:ARG:N	2.48	0.44
1:L:239:GLU:HG2	1:L:347:VAL:O	2.17	0.44
1:A:170:TYR:CZ	1:K:72:PRO:HG2	2.53	0.44
1:C:61:THR:HG21	1:C:273:LEU:HD11	2.00	0.44
1:C:234:TYR:CE1	2:C:401:HSE:H41	2.52	0.44
1:D:28:GLU:CD	1:D:296:ARG:HH21	2.20	0.44
1:F:228:ARG:HH12	1:F:267:GLU:HG2	1.82	0.44
1:G:212:TYR:O	1:G:215:THR:HG23	2.18	0.44
1:A:158:MET:HB2	1:A:289:LEU:HD21	2.00	0.43
1:G:308:CYS:SG	1:G:310:VAL:HG23	2.58	0.43
1:I:249:GLN:O	1:I:252:GLU:HG3	2.18	0.43
1:K:284:ILE:HA	1:K:284:ILE:HD13	1.85	0.43
1:C:234:TYR:HA	1:C:350:HIS:HB3	2.00	0.43
1:E:263:GLN:HG3	1:F:195:THR:HG21	2.00	0.43
1:J:322:LEU:C	1:J:324:PRO:HD3	2.39	0.43
1:K:150:VAL:HG23	1:K:174:VAL:HG23	1.99	0.43
1:K:302:SER:O	1:K:306:ARG:HG3	2.18	0.43
1:G:33:ILE:HG23	1:G:36:VAL:HG22	1.97	0.43
1:G:53:VAL:HG21	1:G:147:ILE:HD13	2.01	0.43
1:J:45:LYS:CG	1:J:46:LEU:H	2.31	0.43
1:J:170:TYR:O	1:J:174:VAL:HG12	2.18	0.43
1:B:19:LEU:C	1:B:20:ILE:HD13	2.38	0.43
1:F:42:ARG:HA	1:F:97:ALA:O	2.18	0.43
1:G:294:VAL:HG22	1:G:294:VAL:O	2.19	0.43
1:J:58:HIS:HA	1:J:79:TRP:CH2	2.53	0.43
1:A:317:ILE:HD13	1:A:344:VAL:HB	2.00	0.43
1:D:284:ILE:HD13	1:D:284:ILE:HA	1.87	0.43
1:D:372:ASP:O	1:D:373:ARG:CB	2.63	0.43
1:G:19:LEU:HD23	1:G:39:ALA:HA	2.01	0.43
1:I:11:LEU:HD13	1:I:42:ARG:CD	2.48	0.43
1:B:279:ALA:O	1:B:283:VAL:HG23	2.19	0.43
1:K:8:THR:HG22	1:K:9:GLN:N	2.31	0.43
1:L:339:ALA:HB3	1:L:342:ARG:HH12	1.84	0.43
1:C:294:VAL:O	1:C:298:ARG:HD2	2.19	0.43
1:D:22:VAL:CG2	1:D:36:VAL:HG12	2.49	0.43
1:K:19:LEU:HD13	1:K:37:CYS:SG	2.58	0.43
1:C:265:TYR:O	1:C:269:GLN:HG2	2.19	0.43
1:F:185:ARG:HG3	1:F:185:ARG:NH1	2.30	0.43
1:J:80:TRP:HB3	1:J:83:VAL:HB	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:47:SER:HB2	1:L:48:PRO:CD	2.48	0.43
1:F:362:GLU:HA	1:F:362:GLU:OE1	2.19	0.43
1:H:228:ARG:HH12	1:H:267:GLU:HG2	1.84	0.43
1:F:102:VAL:HG21	1:F:134:GLN:OE1	2.18	0.43
1:H:11:LEU:HD12	1:H:11:LEU:H	1.84	0.43
1:D:350:HIS:C	1:D:352:GLY:H	2.22	0.42
1:H:9:GLN:HG2	1:H:10:THR:N	2.34	0.42
1:H:330:GLU:O	1:H:334:LEU:HG	2.18	0.42
1:H:362:GLU:O	1:H:366:GLN:HG3	2.18	0.42
1:J:185:ARG:NH1	1:J:186:ALA:O	2.52	0.42
1:A:140:ALA:O	1:A:143:ALA:HB3	2.19	0.42
1:E:8:THR:HG22	1:E:9:GLN:N	2.33	0.42
1:F:61:THR:HA	1:F:277:PHE:CE1	2.53	0.42
1:I:254:PRO:CB	1:I:260:TYR:CZ	3.02	0.42
1:L:152:ALA:HA	1:L:176:ALA:O	2.19	0.42
1:B:283:VAL:O	1:B:287:GLU:HG2	2.19	0.42
1:A:168:VAL:CG1	1:A:298:ARG:NH1	2.82	0.42
1:I:94:ARG:HD3	1:I:95:TRP:CE2	2.54	0.42
1:E:42:ARG:HA	1:E:97:ALA:O	2.19	0.42
1:I:201:ILE:HD11	1:I:223:LEU:HD12	2.02	0.42
1:J:342:ARG:NH1	1:J:366:GLN:OE1	2.52	0.42
1:F:158:MET:HG3	1:F:289:LEU:CD2	2.50	0.42
1:H:152:ALA:HA	1:H:176:ALA:O	2.19	0.42
1:K:156:GLY:HA2	1:K:180:LEU:O	2.19	0.42
1:K:182:VAL:HA	1:K:323:TYR:CD2	2.55	0.42
1:B:88:ALA:HB1	1:B:89:PRO:HD2	2.01	0.42
1:A:220:ASP:HB3	1:A:274:LEU:CD2	2.43	0.42
1:D:19:LEU:C	1:D:20:ILE:HD13	2.40	0.42
1:D:234:TYR:HA	1:D:350:HIS:HB3	2.02	0.42
1:E:182:VAL:HG22	1:E:183:GLY:H	1.83	0.42
1:E:220:ASP:HB3	1:E:274:LEU:HD21	2.02	0.42
1:E:252:GLU:HA	1:K:252:GLU:HB3	2.02	0.42
1:E:317:ILE:HG23	1:E:346:SER:HB3	2.02	0.42
1:F:105:GLY:O	1:F:111:GLY:HA3	2.20	0.42
1:I:163:ALA:HB3	1:I:179:LEU:CD2	2.50	0.42
1:L:346:SER:OG	1:L:356:GLU:OE2	2.30	0.42
1:B:27:LEU:HD11	1:B:33:ILE:HD11	2.02	0.42
1:C:22:VAL:CG2	1:C:36:VAL:HB	2.49	0.42
1:E:165:GLU:OE1	1:E:165:GLU:HA	2.19	0.42
1:F:220:ASP:HB3	1:F:274:LEU:HD21	2.01	0.42
1:G:33:ILE:CG2	1:G:36:VAL:CG2	2.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:11:LEU:CD2	1:I:145:LEU:HD13	2.49	0.42
1:K:372:ASP:N	1:K:372:ASP:OD1	2.53	0.42
1:F:80:TRP:HB3	1:F:83:VAL:CG1	2.49	0.42
1:H:25:LEU:HD23	1:H:25:LEU:HA	1.82	0.42
1:I:205:PRO:HG3	1:J:205:PRO:HG3	2.01	0.42
1:I:263:GLN:HG3	1:J:195:THR:CG2	2.48	0.42
1:K:8:THR:CG2	1:K:9:GLN:H	2.30	0.42
1:K:80:TRP:CD1	1:K:83:VAL:HB	2.55	0.42
1:B:56:VAL:HG22	1:B:154:VAL:HG23	2.01	0.42
1:C:118:ASP:OD1	1:C:118:ASP:N	2.42	0.42
1:E:200:ALA:HA	1:F:225:LEU:HD11	2.01	0.42
1:G:316:GLY:HA3	1:G:328:GLN:OE1	2.20	0.42
1:H:102:VAL:CG2	1:H:134:GLN:HB3	2.50	0.42
1:J:284:ILE:HD13	1:J:284:ILE:HA	1.77	0.42
1:K:19:LEU:HD23	1:K:19:LEU:HA	1.85	0.42
1:L:58:HIS:HE1	1:L:102:VAL:HG12	1.84	0.42
1:B:156:GLY:HA2	1:B:180:LEU:O	2.19	0.42
1:D:315:GLY:HA2	1:D:342:ARG:O	2.19	0.42
1:E:322:LEU:HD23	1:E:323:TYR:HE1	1.85	0.42
1:K:167:VAL:HB	1:K:310:VAL:HG21	2.01	0.42
1:K:249:GLN:HB3	1:K:252:GLU:OE2	2.19	0.42
1:B:88:ALA:HB1	1:B:89:PRO:CD	2.50	0.41
1:D:8:THR:HG22	1:D:9:GLN:O	2.20	0.41
1:E:22:VAL:HG12	1:E:141:ALA:HA	2.02	0.41
1:G:66:ILE:HG13	1:G:67:THR:N	2.34	0.41
1:J:154:VAL:HG12	1:J:178:LEU:HB3	2.00	0.41
1:J:197:GLN:OE1	1:J:230:ALA:HB2	2.19	0.41
1:J:315:GLY:HA2	1:J:342:ARG:O	2.20	0.41
1:C:317:ILE:HG23	1:C:346:SER:HB3	2.02	0.41
1:H:315:GLY:HA2	1:H:342:ARG:O	2.20	0.41
1:I:182:VAL:CG2	1:I:183:GLY:N	2.83	0.41
1:J:128:LEU:HD23	1:J:128:LEU:HA	1.86	0.41
1:K:53:VAL:HG21	1:K:147:ILE:HD13	2.02	0.41
1:B:164:LEU:HA	1:B:167:VAL:HG22	2.02	0.41
1:A:151:ALA:O	1:A:175:ARG:HB2	2.19	0.41
1:H:58:HIS:CE1	1:H:102:VAL:HG12	2.55	0.41
1:E:263:GLN:HG3	1:F:195:THR:CB	2.51	0.41
1:F:249:GLN:OE1	1:F:264:SER:HB3	2.20	0.41
1:J:294:VAL:HG22	1:J:294:VAL:O	2.20	0.41
1:G:25:LEU:HD22	1:G:136:GLN:OE1	2.20	0.41
1:I:80:TRP:CD1	1:I:83:VAL:HB	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:107:ARG:HA	1:J:107:ARG:HD2	1.82	0.41
1:C:322:LEU:HG	1:C:323:TYR:CE1	2.56	0.41
1:F:241:ASP:OD1	1:F:245:ALA:HA	2.20	0.41
1:G:285:LEU:HD23	1:G:285:LEU:HA	1.73	0.41
1:J:128:LEU:HD21	1:J:287:GLU:HG3	2.03	0.41
1:D:49:ALA:O	1:D:50:ARG:HB2	2.21	0.41
1:E:229:PHE:CE2	1:F:229:PHE:CD2	3.09	0.41
1:I:315:GLY:HA2	1:I:342:ARG:O	2.20	0.41
1:J:268:HIS:CE1	1:J:272:LYS:HD2	2.55	0.41
1:L:270:GLY:O	1:L:274:LEU:CD2	2.69	0.41
1:L:370:LEU:HD22	1:L:373:ARG:HH21	1.84	0.41
1:G:53:VAL:HG13	1:G:98:VAL:CG2	2.51	0.41
1:J:19:LEU:HD22	1:J:37:CYS:SG	2.60	0.41
1:C:218:ALA:HB1	1:C:219:PRO:CD	2.51	0.41
1:D:11:LEU:HD12	1:D:145:LEU:HD13	2.02	0.41
1:D:73:GLY:C	1:D:74:HIS:HD1	2.23	0.41
1:E:322:LEU:HD23	1:E:323:TYR:CE1	2.56	0.41
1:F:156:GLY:O	1:F:159:GLY:N	2.54	0.41
1:H:325:LEU:HD12	1:H:325:LEU:HA	1.85	0.41
1:I:45:LYS:HG3	1:I:46:LEU:N	2.36	0.41
1:J:149:GLU:HB3	1:J:173:ARG:HB2	2.03	0.41
1:L:92:THR:HA	1:L:95:TRP:O	2.21	0.41
1:C:127:PRO:O	1:C:129:ILE:HG23	2.21	0.41
1:E:234:TYR:HA	1:E:350:HIS:HB3	2.03	0.41
1:H:25:LEU:O	1:H:32:VAL:HG13	2.21	0.41
1:J:58:HIS:CD2	1:J:162:ARG:HH12	2.39	0.41
1:K:207:TRP:HE3	1:K:219:PRO:HG3	1.85	0.41
1:K:287:GLU:OE1	1:K:287:GLU:HA	2.21	0.41
1:C:229:PHE:CE2	1:D:229:PHE:CD2	3.09	0.40
1:C:315:GLY:HA2	1:C:342:ARG:O	2.21	0.40
1:C:368:LEU:HA	1:C:368:LEU:HD23	1.85	0.40
1:E:19:LEU:HD22	1:E:37:CYS:HB3	2.03	0.40
1:G:196:THR:HG22	1:H:229:PHE:CZ	2.56	0.40
1:G:218:ALA:HB1	1:G:219:PRO:HD2	2.02	0.40
1:I:182:VAL:HA	1:I:323:TYR:CD2	2.57	0.40
1:J:102:VAL:HG21	1:J:134:GLN:OE1	2.21	0.40
1:J:182:VAL:CG2	1:J:183:GLY:N	2.84	0.40
1:B:194:GLN:HB3	1:B:286:THR:HG23	2.04	0.40
1:E:252:GLU:HG2	1:K:252:GLU:CB	2.51	0.40
1:H:44:GLY:HA3	1:H:92:THR:HB	2.03	0.40
1:I:42:ARG:HH12	1:I:45:LYS:HA	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:HIS:CG	1:B:74:HIS:ND1	2.89	0.40
1:B:302:SER:HA	1:B:334:LEU:HD13	2.03	0.40
1:D:27:LEU:HD11	1:D:33:ILE:HD11	2.03	0.40
1:E:266:LEU:HA	1:E:266:LEU:HD23	1.74	0.40
1:E:296:ARG:HH11	1:E:296:ARG:HD3	1.76	0.40
1:I:351:ASP:O	1:I:355:VAL:HG23	2.21	0.40
1:H:227:ARG:CD	1:H:273:LEU:HD22	2.51	0.40
1:H:283:VAL:O	1:H:287:GLU:HG2	2.21	0.40
1:J:14:GLU:CG	1:J:42:ARG:HH12	2.34	0.40
1:K:182:VAL:CG2	1:K:183:GLY:N	2.84	0.40
1:L:316:GLY:HA3	1:L:328:GLN:OE1	2.21	0.40
1:G:224:ARG:HG3	1:G:274:LEU:HD11	2.03	0.40
1:H:238:ILE:O	1:H:239:GLU:C	2.59	0.40
1:I:11:LEU:HD23	1:I:145:LEU:HD13	2.03	0.40
1:J:11:LEU:HD23	1:J:11:LEU:HA	1.95	0.40
1:J:56:VAL:HG13	1:J:80:TRP:HZ3	1.87	0.40
1:K:342:ARG:NH1	1:K:366:GLN:OE1	2.40	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	365/368 (99%)	353 (97%)	12 (3%)	0	100	100
1	B	366/368 (100%)	351 (96%)	15 (4%)	0	100	100
1	C	364/368 (99%)	353 (97%)	11 (3%)	0	100	100
1	D	364/368 (99%)	352 (97%)	12 (3%)	0	100	100
1	E	363/368 (99%)	350 (96%)	13 (4%)	0	100	100
1	F	365/368 (99%)	349 (96%)	16 (4%)	0	100	100
1	G	363/368 (99%)	349 (96%)	14 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	364/368 (99%)	349 (96%)	15 (4%)	0	100	100
1	I	363/368 (99%)	350 (96%)	13 (4%)	0	100	100
1	J	365/368 (99%)	349 (96%)	16 (4%)	0	100	100
1	K	363/368 (99%)	350 (96%)	13 (4%)	0	100	100
1	L	365/368 (99%)	349 (96%)	16 (4%)	0	100	100
All	All	4370/4416 (99%)	4204 (96%)	166 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	273/274 (100%)	270 (99%)	3 (1%)	73	92
1	B	274/274 (100%)	272 (99%)	2 (1%)	84	95
1	C	273/274 (100%)	271 (99%)	2 (1%)	84	95
1	D	272/274 (99%)	269 (99%)	3 (1%)	73	92
1	E	271/274 (99%)	267 (98%)	4 (2%)	65	87
1	F	272/274 (99%)	271 (100%)	1 (0%)	91	97
1	G	270/274 (98%)	268 (99%)	2 (1%)	84	95
1	H	271/274 (99%)	267 (98%)	4 (2%)	65	87
1	I	272/274 (99%)	270 (99%)	2 (1%)	84	95
1	J	274/274 (100%)	269 (98%)	5 (2%)	59	85
1	K	271/274 (99%)	269 (99%)	2 (1%)	84	95
1	L	271/274 (99%)	269 (99%)	2 (1%)	84	95
All	All	3264/3288 (99%)	3232 (99%)	32 (1%)	76	92

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

Mol	Chain	Res	Type
1	B	117	ARG
1	B	149	GLU
1	A	94	ARG
1	A	180	LEU
1	A	372	ASP
1	C	117	ARG
1	C	149	GLU
1	D	45	LYS
1	D	94	ARG
1	D	149	GLU
1	E	80	TRP
1	E	94	ARG
1	E	125	ARG
1	E	239	GLU
1	F	149	GLU
1	G	80	TRP
1	G	243	ARG
1	H	50	ARG
1	H	118	ASP
1	H	149	GLU
1	H	235	ARG
1	I	80	TRP
1	I	94	ARG
1	J	94	ARG
1	J	117	ARG
1	J	118	ASP
1	J	235	ARG
1	J	306	ARG
1	K	80	TRP
1	K	94	ARG
1	L	94	ARG
1	L	342	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	101	ASN
1	J	101	ASN

5.3.3 RNA

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)

11 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	HSE	A	401	-	6,7,7	1.16	1 (16%)	6,8,8	1.00	0
2	HSE	C	401	-	6,7,7	1.11	1 (16%)	6,8,8	0.98	0
2	HSE	L	401	-	6,7,7	0.91	0	6,8,8	1.02	0
2	HSE	F	401	-	6,7,7	0.95	1 (16%)	6,8,8	0.85	0
2	HSE	G	401	-	6,7,7	1.01	0	6,8,8	2.06	3 (50%)
2	HSE	I	401	-	6,7,7	1.26	1 (16%)	6,8,8	1.60	2 (33%)
2	HSE	B	401	-	6,7,7	0.99	1 (16%)	6,8,8	0.60	0
2	HSE	D	401	-	6,7,7	0.59	0	6,8,8	0.78	0
2	HSE	K	401	-	6,7,7	0.64	0	6,8,8	0.88	0
2	HSE	H	401	-	6,7,7	0.73	0	6,8,8	0.82	0
2	HSE	J	401	-	6,7,7	0.96	1 (16%)	6,8,8	0.71	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HSE	A	401	-	-	0/7/7/7	-
2	HSE	C	401	-	-	6/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HSE	L	401	-	-	1/7/7/7	-
2	HSE	F	401	-	-	3/7/7/7	-
2	HSE	G	401	-	-	1/7/7/7	-
2	HSE	I	401	-	-	3/7/7/7	-
2	HSE	B	401	-	-	2/7/7/7	-
2	HSE	D	401	-	-	3/7/7/7	-
2	HSE	K	401	-	-	5/7/7/7	-
2	HSE	H	401	-	-	4/7/7/7	-
2	HSE	J	401	-	-	3/7/7/7	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	HSE	OXT-C	-2.46	1.22	1.30
2	I	401	HSE	OXT-C	-2.24	1.23	1.30
2	B	401	HSE	OXT-C	-2.19	1.23	1.30
2	C	401	HSE	OXT-C	-2.12	1.23	1.30
2	J	401	HSE	OXT-C	-2.09	1.23	1.30
2	F	401	HSE	OXT-C	-2.01	1.24	1.30

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	401	HSE	O-C-CA	-3.65	109.26	122.14
2	G	401	HSE	OXT-C-O	2.63	130.06	124.09
2	I	401	HSE	C3-CA-C	-2.27	104.90	110.30
2	G	401	HSE	OXT-C-CA	2.14	120.66	113.38
2	I	401	HSE	O-C-CA	-2.09	114.77	122.14

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	401	HSE	O-C-CA-N
2	C	401	HSE	C4-C3-CA-N
2	D	401	HSE	CA-C3-C4-O3
2	F	401	HSE	C4-C3-CA-N
2	F	401	HSE	C4-C3-CA-C
2	F	401	HSE	CA-C3-C4-O3
2	G	401	HSE	C4-C3-CA-C

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Mol	Chain	Res	Type	Atoms
2	H	401	HSE	C4-C3-CA-N
2	H	401	HSE	C4-C3-CA-C
2	I	401	HSE	C4-C3-CA-N
2	I	401	HSE	C4-C3-CA-C
2	I	401	HSE	CA-C3-C4-O3
2	J	401	HSE	C4-C3-CA-N
2	J	401	HSE	C4-C3-CA-C
2	J	401	HSE	CA-C3-C4-O3
2	K	401	HSE	C4-C3-CA-N
2	K	401	HSE	C4-C3-CA-C
2	K	401	HSE	CA-C3-C4-O3
2	L	401	HSE	CA-C3-C4-O3
2	C	401	HSE	OXT-C-CA-N
2	B	401	HSE	OXT-C-CA-N
2	B	401	HSE	O-C-CA-N
2	D	401	HSE	O-C-CA-N
2	K	401	HSE	O-C-CA-N
2	C	401	HSE	C4-C3-CA-C
2	H	401	HSE	OXT-C-CA-C3
2	H	401	HSE	O-C-CA-C3
2	D	401	HSE	OXT-C-CA-N
2	K	401	HSE	OXT-C-CA-N
2	C	401	HSE	OXT-C-CA-C3
2	C	401	HSE	O-C-CA-C3

There are no ring outliers.

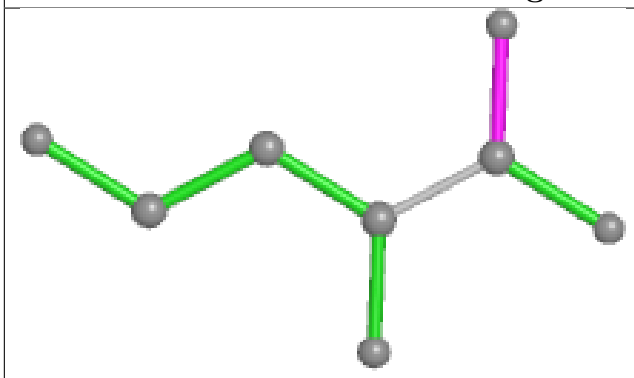
7 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	HSE	3	0
2	L	401	HSE	1	0
2	I	401	HSE	3	0
2	D	401	HSE	1	0
2	K	401	HSE	1	0
2	H	401	HSE	5	0
2	J	401	HSE	1	0

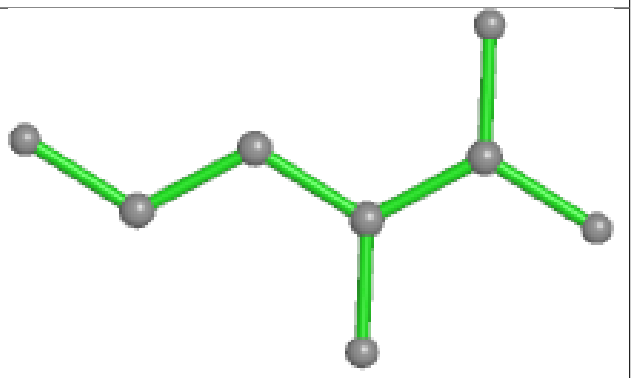
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

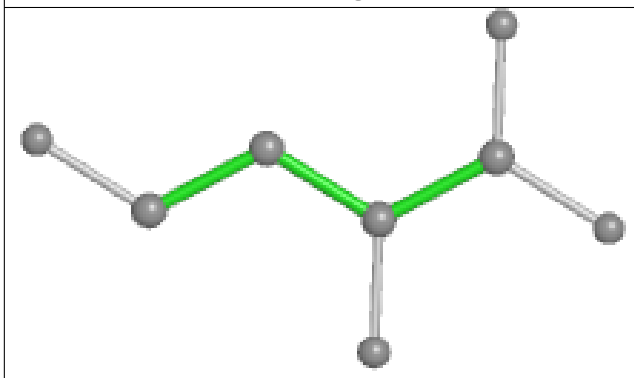
Ligand HSE A 401



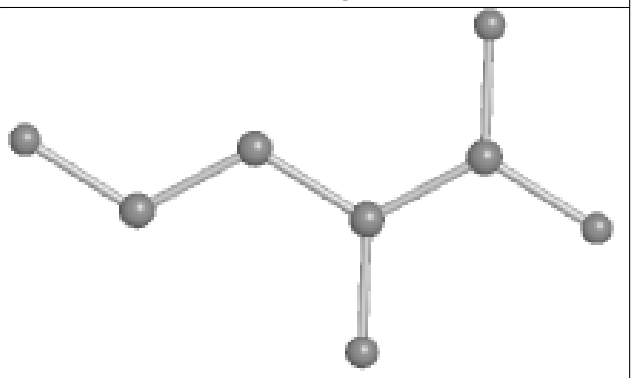
Bond lengths



Bond angles

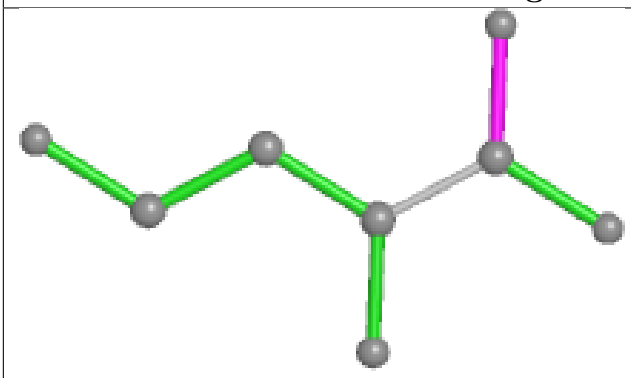


Torsions



Rings

Ligand HSE C 401



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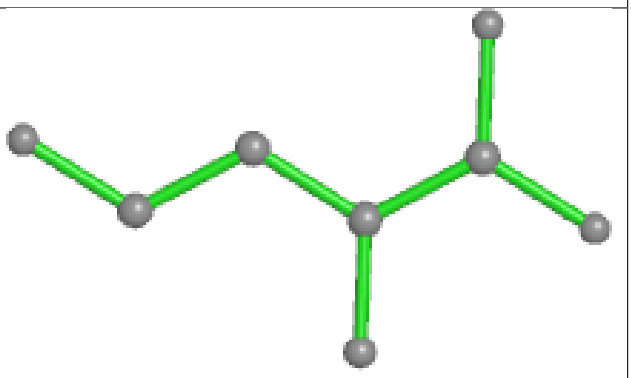
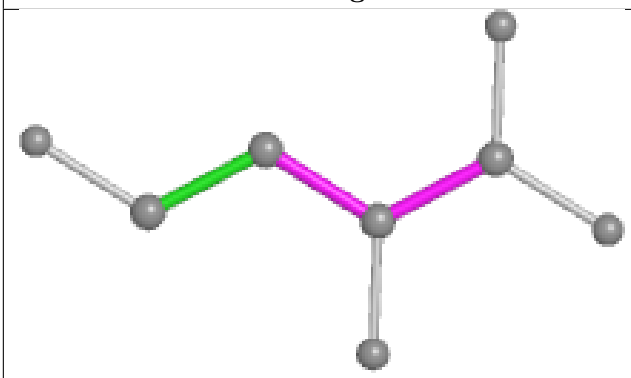
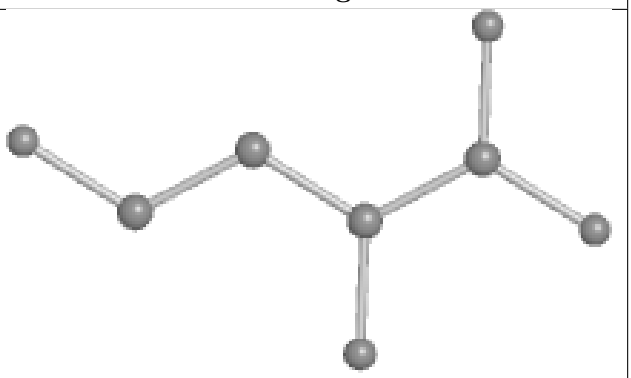


Bond angles

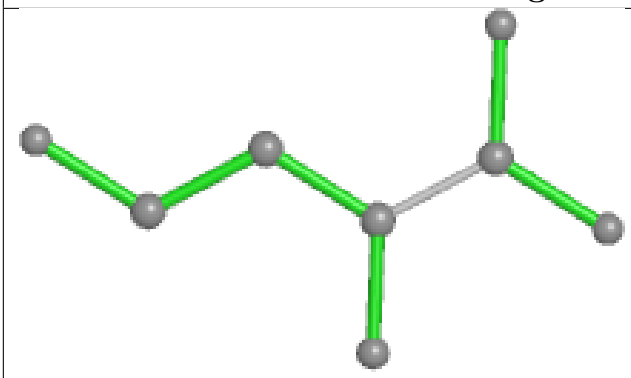


Torsions

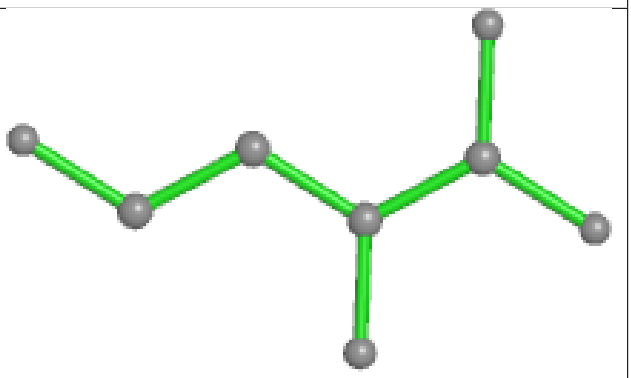


Rings

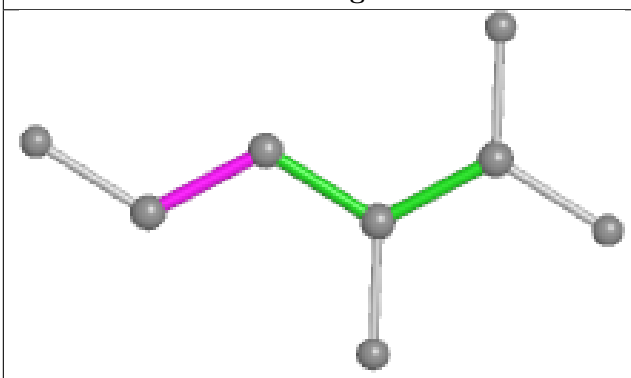
Ligand HSE L 401



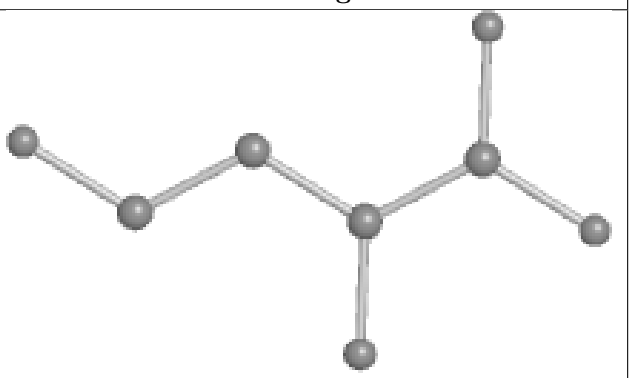
Bond lengths



Bond angles

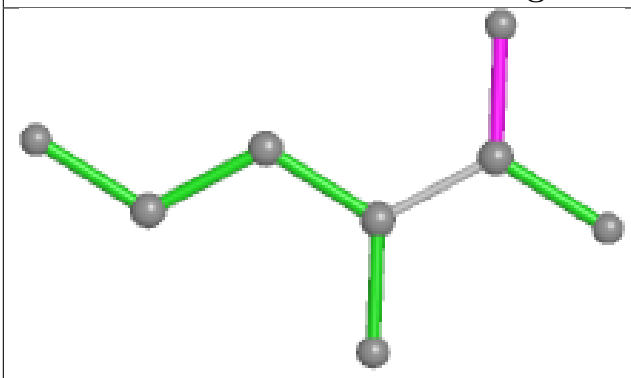


Torsions

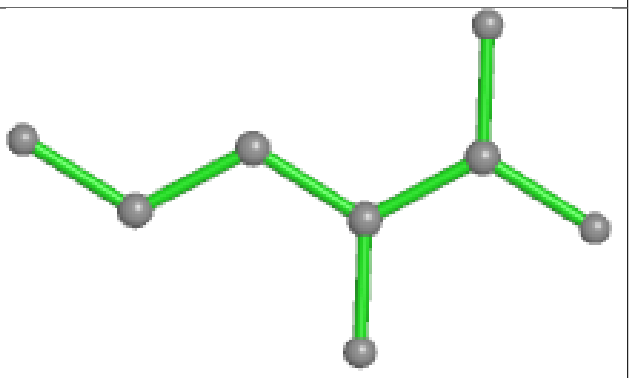


Rings

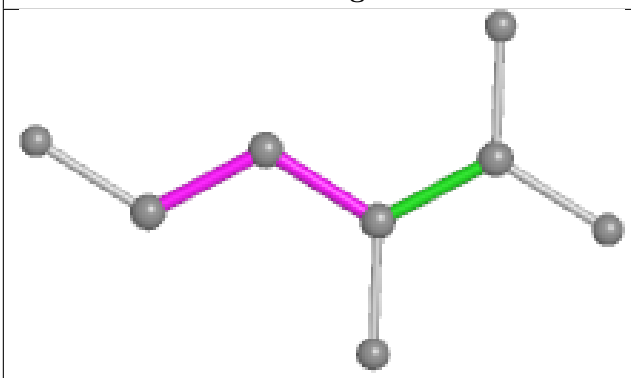
Ligand HSE F 401



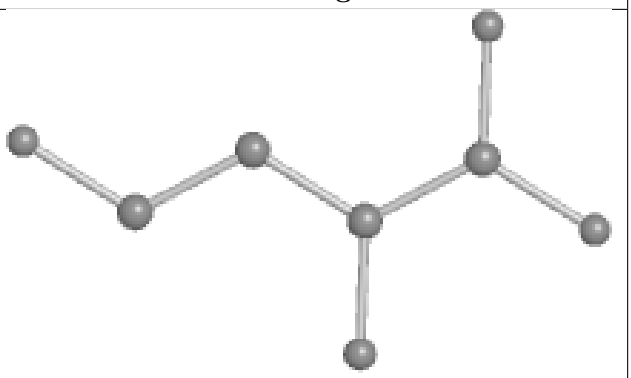
Bond lengths



Bond angles

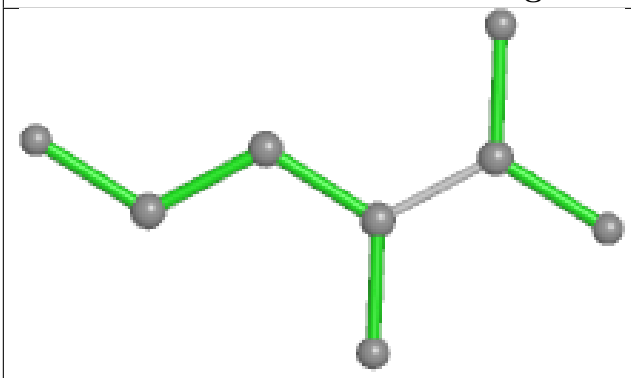


Torsions

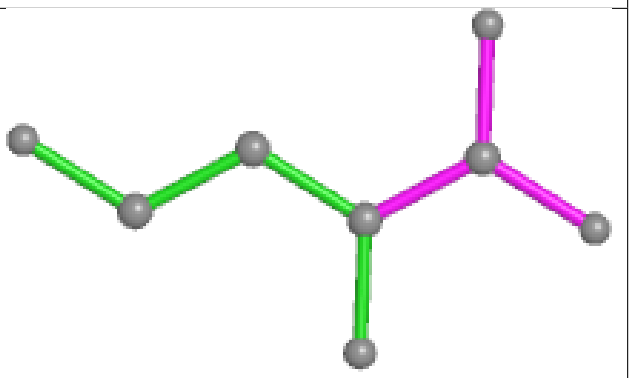


Rings

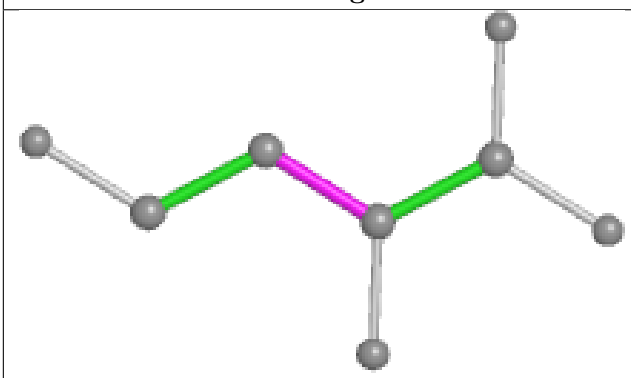
Ligand HSE G 401



Bond lengths



Bond angles



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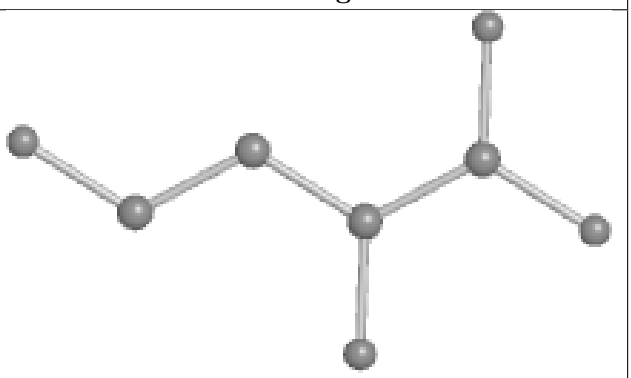
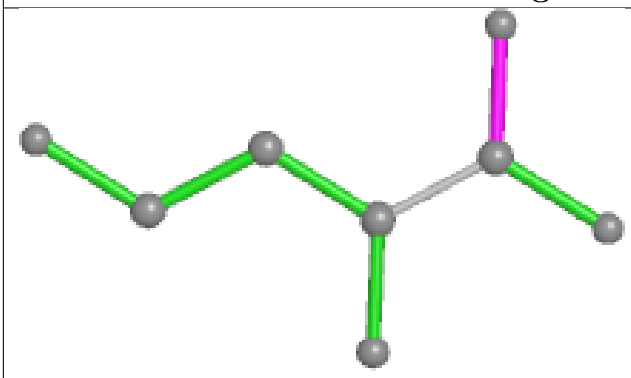
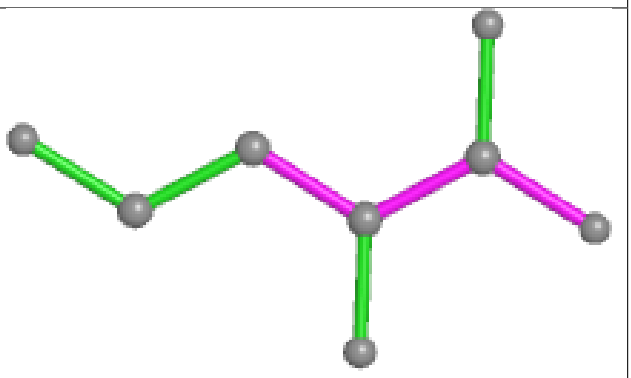


Rings

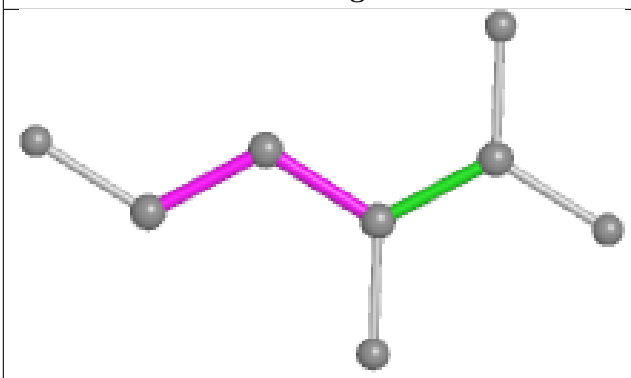
Ligand HSE I 401



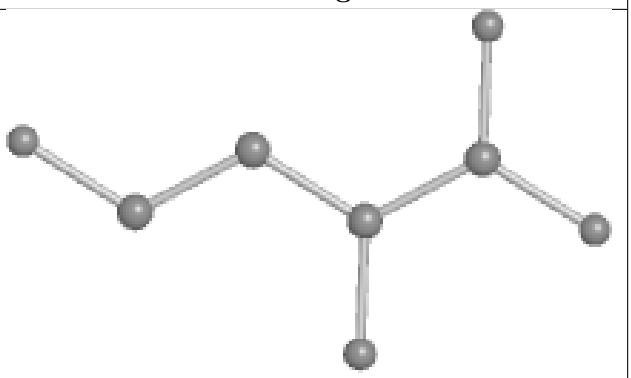
Bond lengths



Bond angles

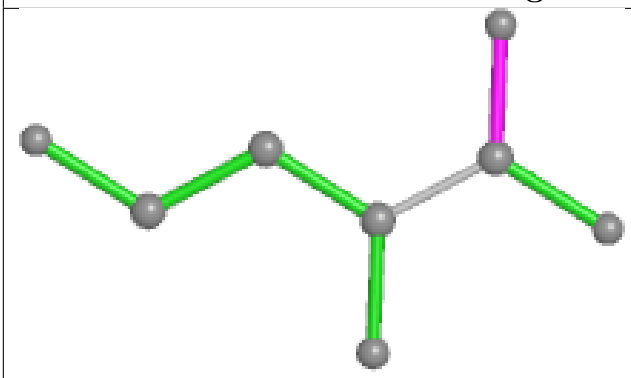


Torsions

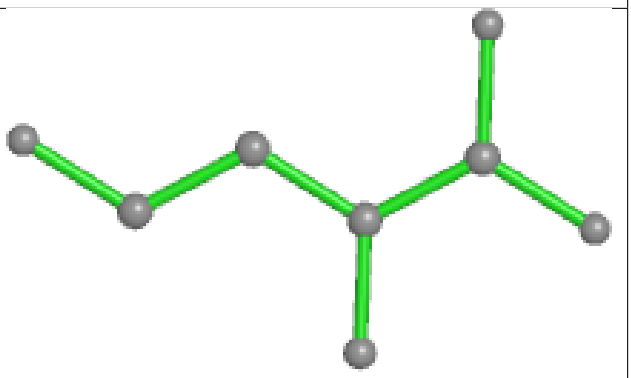


Rings

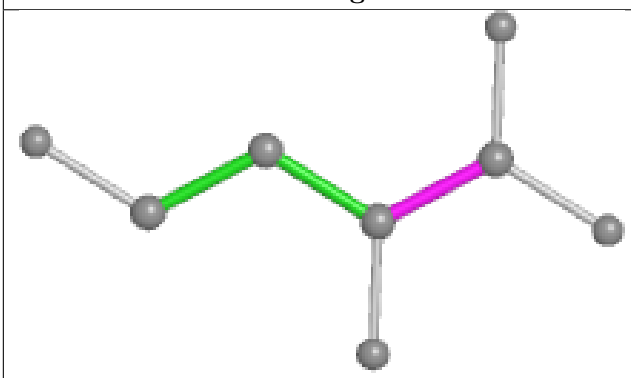
Ligand HSE B 401



Bond lengths



Bond angles



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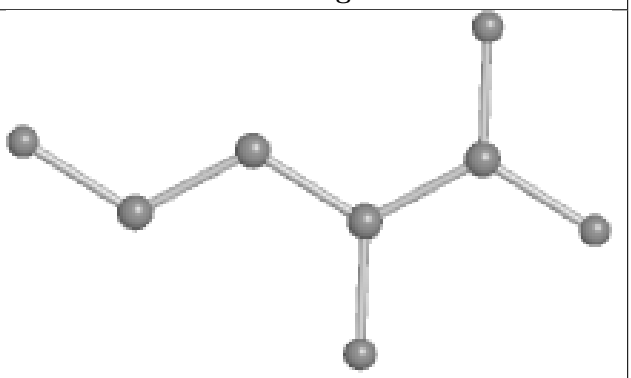
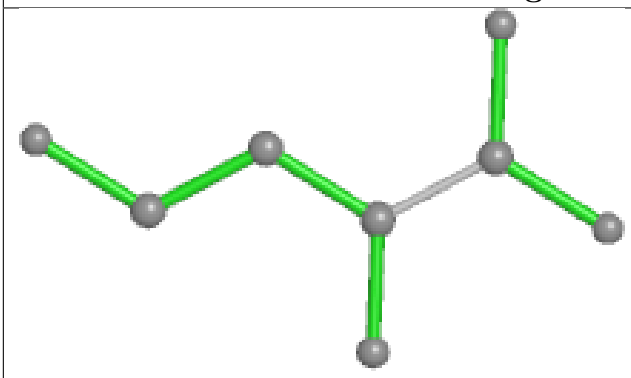


Rings

Ligand HSE D 401



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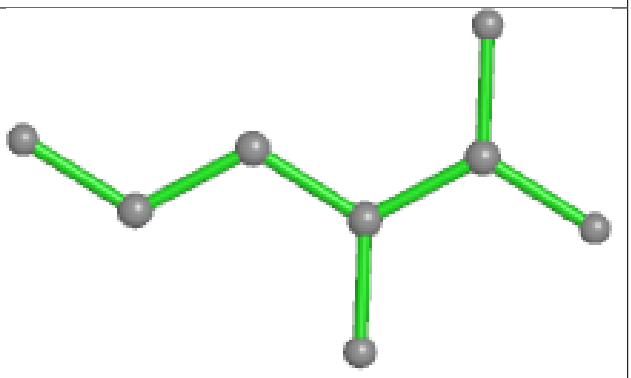
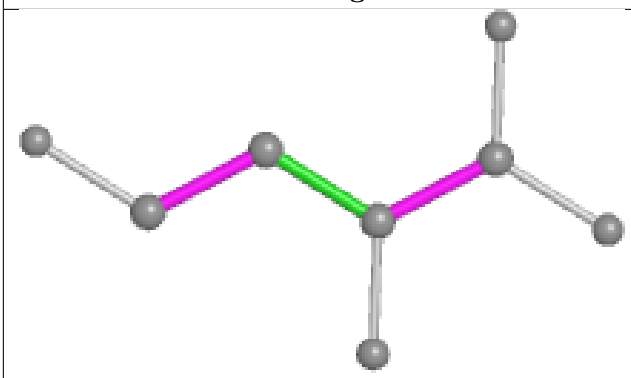
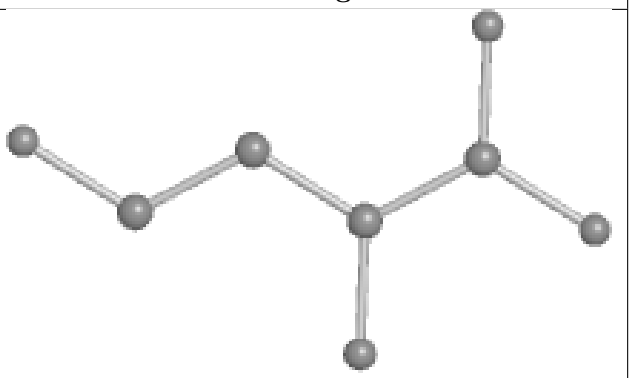


Bond angles

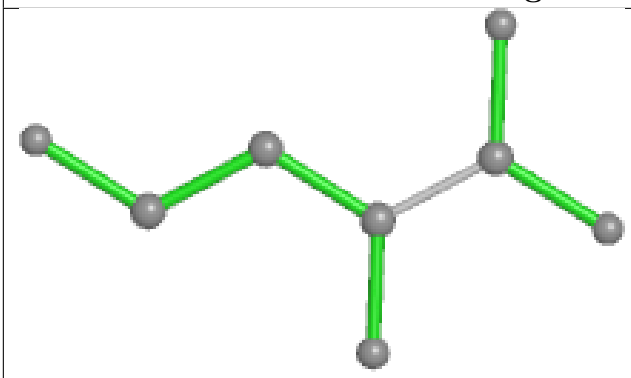


Torsions

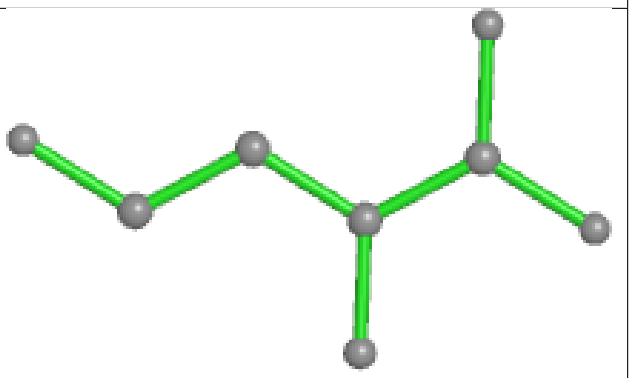


Rings

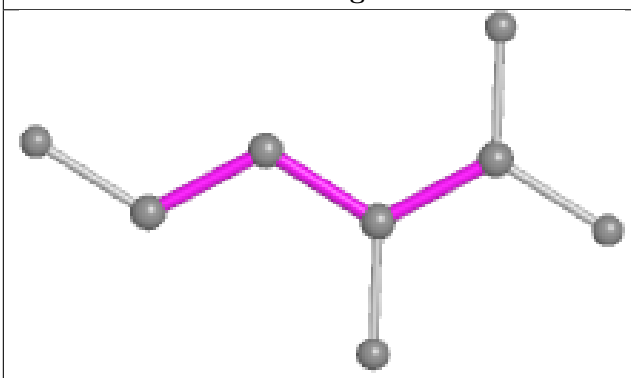
Ligand HSE K 401



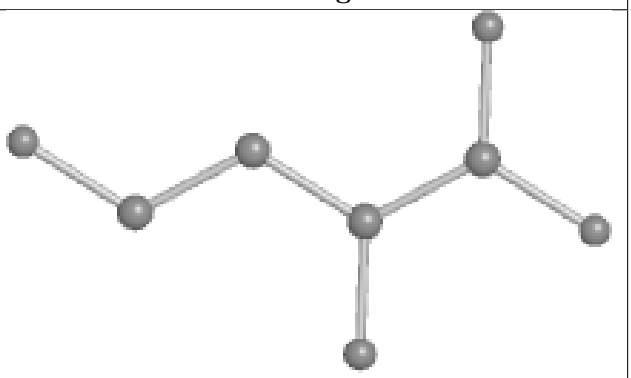
Bond lengths



Bond angles

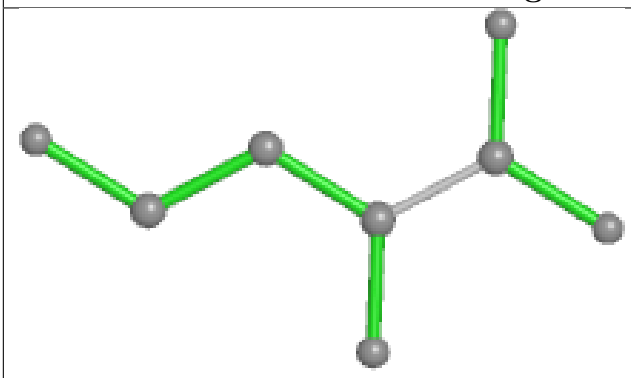


Torsions

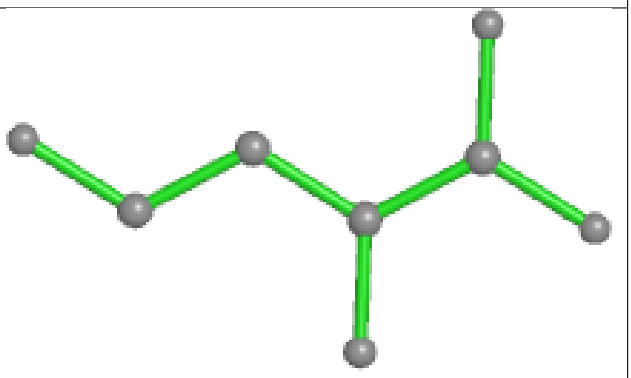


Rings

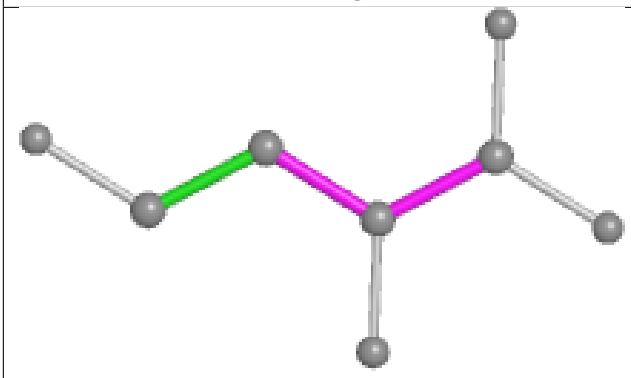
Ligand HSE H 401



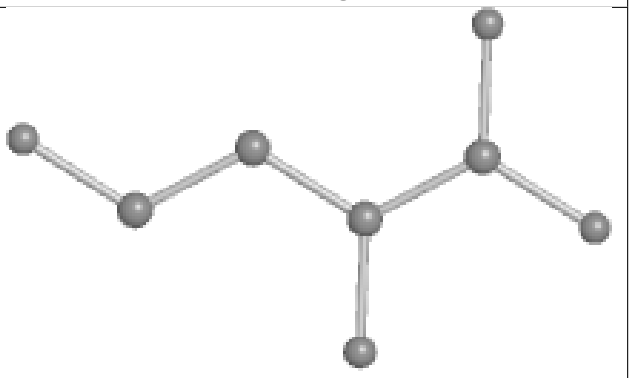
Bond lengths



Bond angles

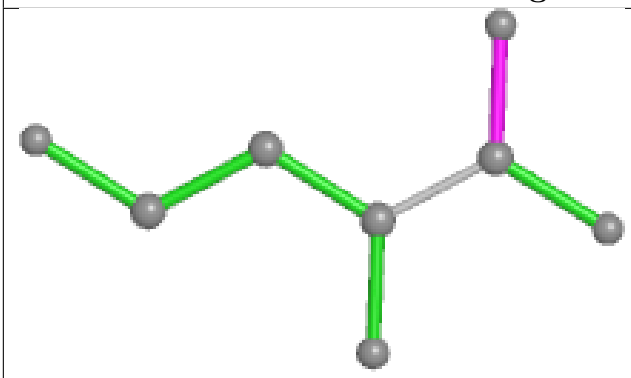


Torsions

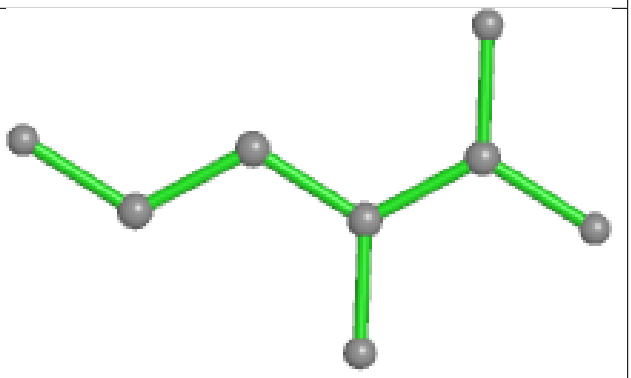


Rings

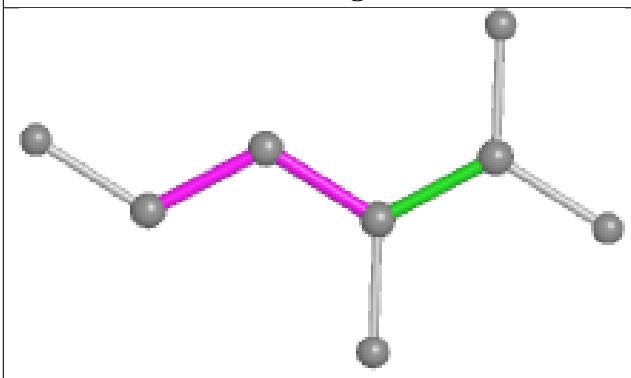
Ligand HSE J 401



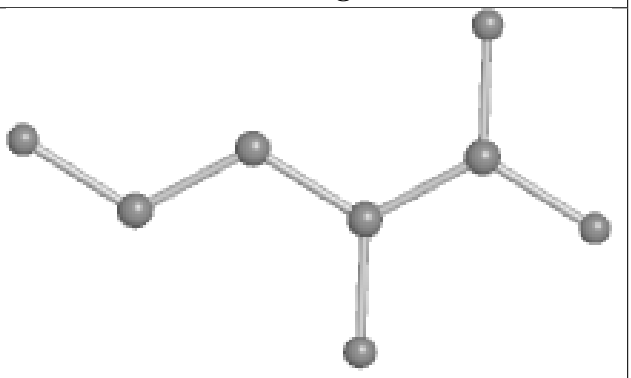
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 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, 95^{th} 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	367/368 (99%)	-0.01	1 (0%) 94 94	15, 26, 48, 77	0
1	B	367/368 (99%)	-0.06	0 100 100	16, 26, 49, 79	0
1	C	366/368 (99%)	-0.03	0 100 100	16, 26, 51, 82	0
1	D	366/368 (99%)	-0.07	1 (0%) 94 94	15, 26, 49, 72	0
1	E	365/368 (99%)	0.04	6 (1%) 72 71	18, 27, 48, 87	0
1	F	367/368 (99%)	0.15	13 (3%) 44 38	20, 39, 66, 102	0
1	G	365/368 (99%)	0.08	6 (1%) 72 71	22, 35, 61, 77	0
1	H	366/368 (99%)	0.19	10 (2%) 54 50	20, 41, 68, 86	0
1	I	365/368 (99%)	0.05	2 (0%) 91 91	17, 28, 52, 78	0
1	J	367/368 (99%)	0.20	7 (1%) 66 65	19, 38, 66, 94	0
1	K	365/368 (99%)	0.11	5 (1%) 75 75	22, 36, 60, 76	0
1	L	367/368 (99%)	0.18	6 (1%) 72 71	20, 40, 63, 84	0
All	All	4393/4416 (99%)	0.07	57 (1%) 77 77	15, 31, 60, 102	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	254	PRO	4.9
1	G	255	THR	4.2
1	E	258	GLY	4.0
1	E	256	ALA	3.4
1	J	92	THR	3.4
1	E	251	ASN	3.4
1	E	255	THR	3.3
1	K	256	ALA	3.1
1	H	144	ALA	3.1
1	H	140	ALA	3.1
1	D	45	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	92	THR	2.8
1	E	254	PRO	2.7
1	K	174	VAL	2.7
1	L	368	LEU	2.7
1	F	151	ALA	2.7
1	I	256	ALA	2.7
1	L	212	TYR	2.6
1	L	260	TYR	2.6
1	H	253	ASP	2.6
1	F	15	GLY	2.6
1	H	260	TYR	2.6
1	E	257	GLY	2.6
1	G	241	ASP	2.6
1	I	240	LEU	2.5
1	J	18	GLY	2.5
1	G	252	GLU	2.5
1	J	151	ALA	2.5
1	F	121	PRO	2.5
1	J	116	ALA	2.5
1	H	69	PRO	2.4
1	F	152	ALA	2.4
1	H	214	GLU	2.3
1	G	172	ASP	2.3
1	L	70	ALA	2.3
1	F	76	THR	2.2
1	K	96	CYS	2.2
1	K	122	TRP	2.2
1	G	32	VAL	2.2
1	H	212	TYR	2.2
1	H	176	ALA	2.2
1	F	214	GLU	2.2
1	J	93	THR	2.2
1	F	144	ALA	2.1
1	F	93	THR	2.1
1	F	372	ASP	2.1
1	K	106	CYS	2.1
1	F	176	ALA	2.1
1	L	258	GLY	2.1
1	J	8	THR	2.1
1	L	115	LEU	2.1
1	F	217	ARG	2.1
1	J	215	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	75	PRO	2.0
1	H	255	THR	2.0
1	F	210	GLY	2.0
1	H	251	ASN	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 monosaccharides in this entry.

6.4 Ligands (i)

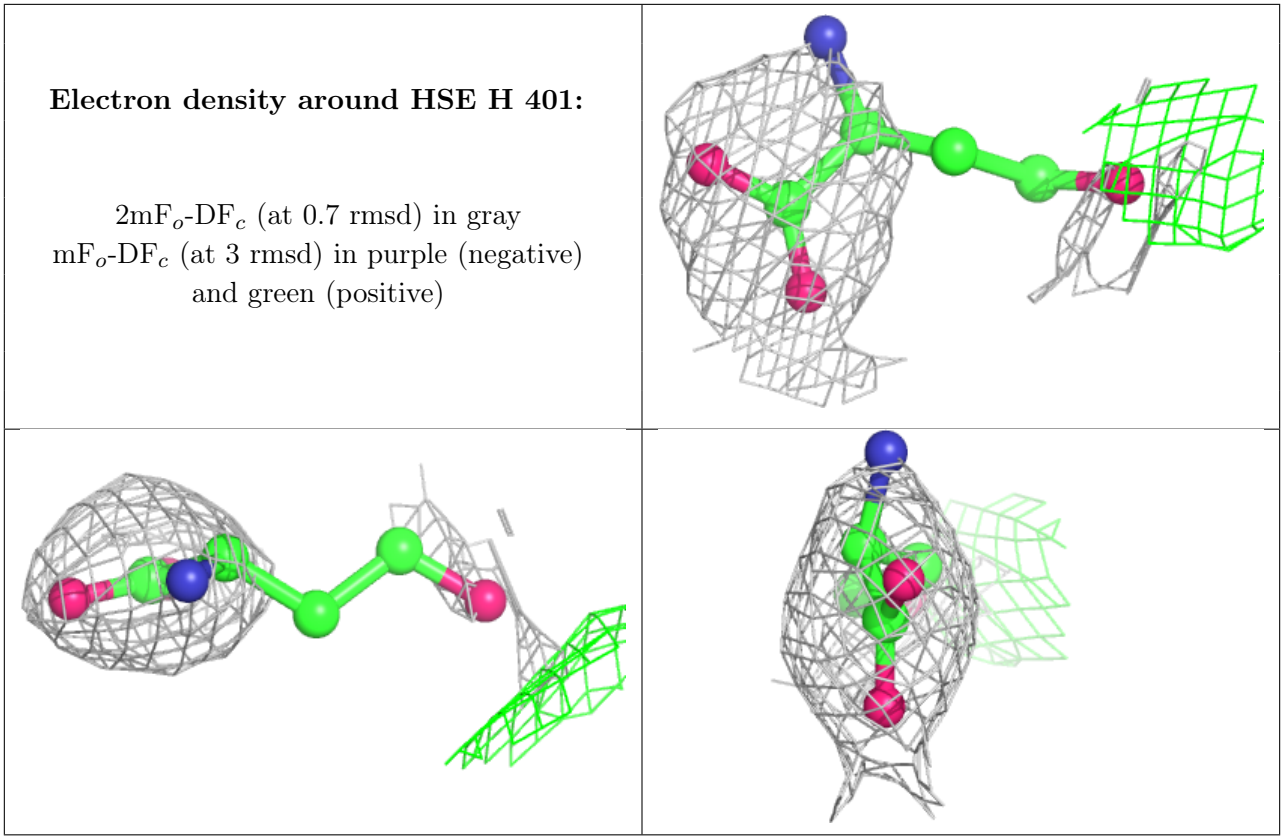
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	HSE	H	401	8/8	0.88	0.49	47,59,66,71	0
2	HSE	L	401	8/8	0.90	0.34	43,47,63,66	0
2	HSE	A	401	8/8	0.92	0.25	11,29,57,59	0
2	HSE	J	401	8/8	0.93	0.27	32,43,48,58	0
2	HSE	F	401	8/8	0.93	0.33	30,33,51,56	0
2	HSE	K	401	8/8	0.94	0.32	13,39,48,52	0
2	HSE	B	401	8/8	0.94	0.21	14,39,53,62	0
2	HSE	I	401	8/8	0.96	0.33	15,36,43,46	0
2	HSE	G	401	8/8	0.96	0.27	13,40,42,49	0
2	HSE	C	401	8/8	0.97	0.28	11,31,55,56	0
2	HSE	D	401	8/8	0.98	0.19	9,43,47,49	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.

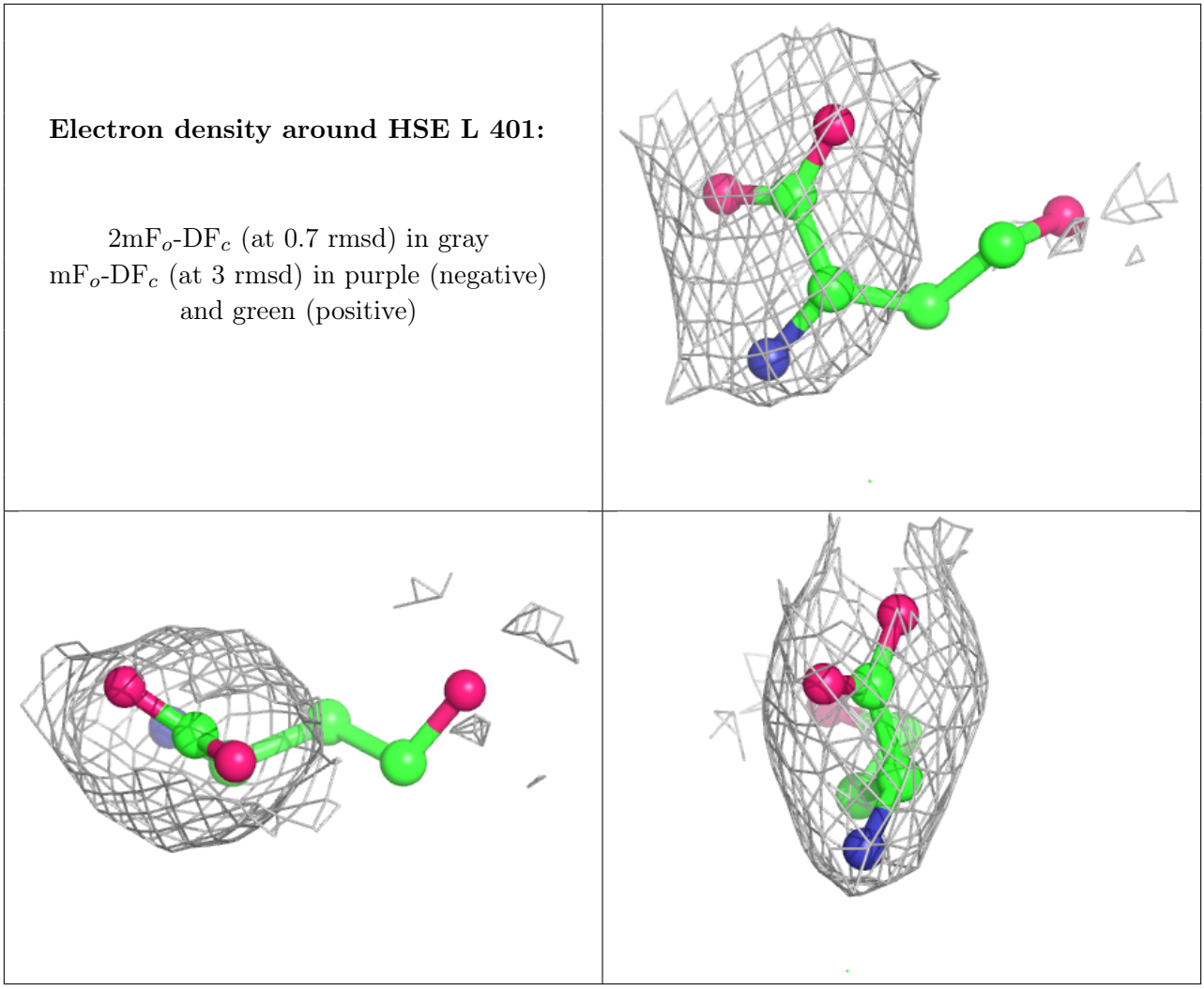
Electron density around HSE H 401:

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



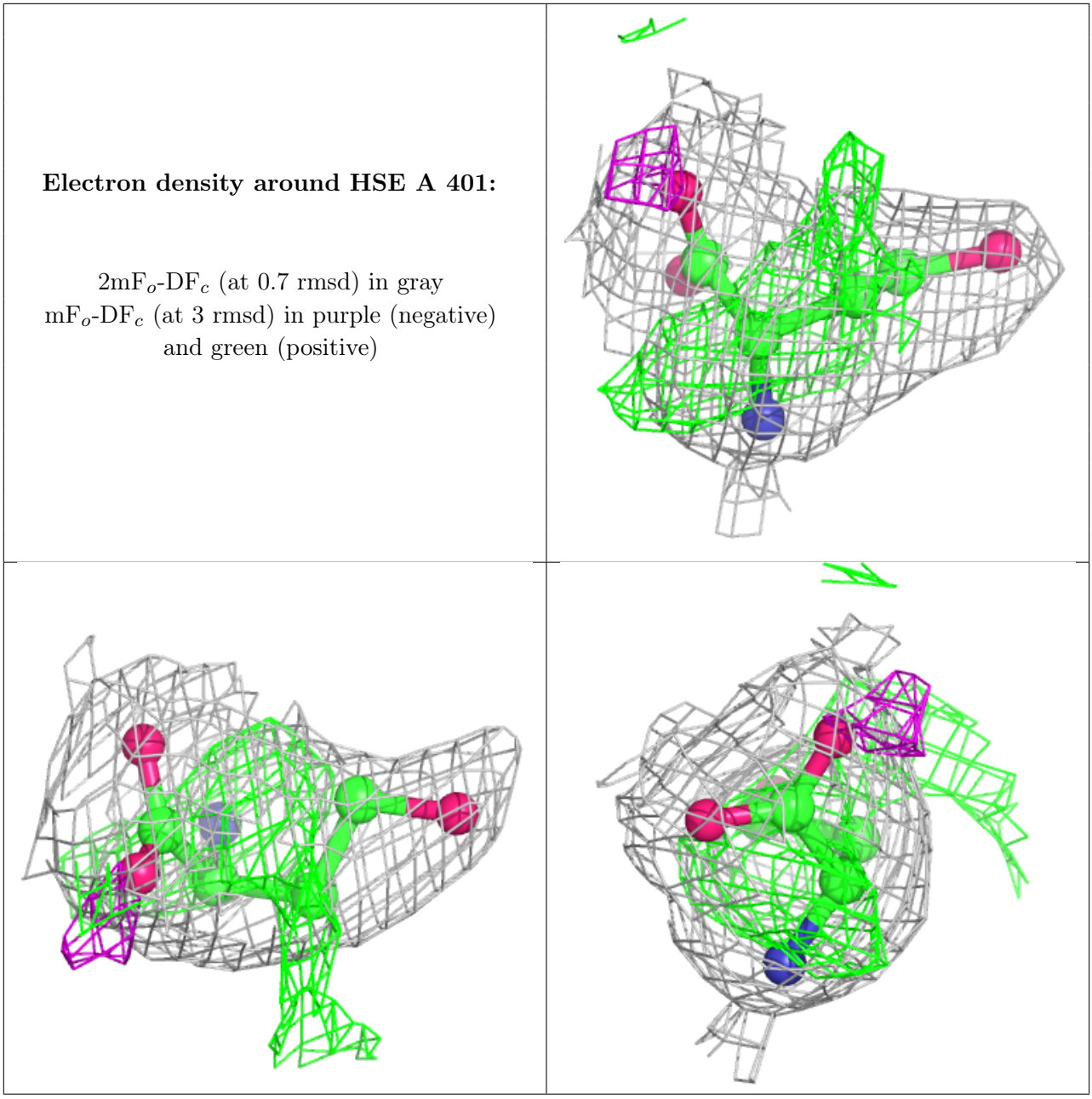
Electron density around HSE L 401:

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



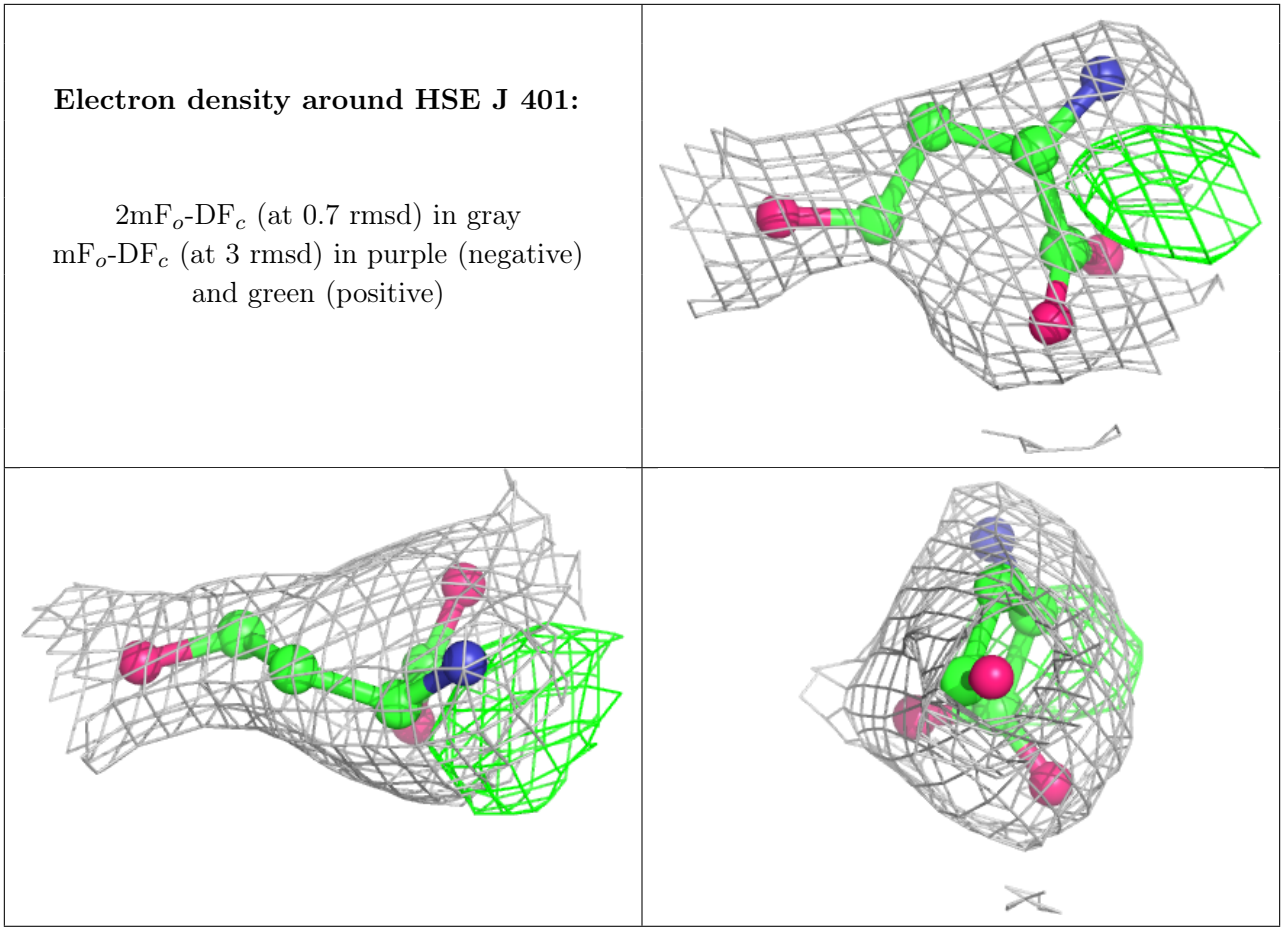
Electron density around HSE A 401:

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



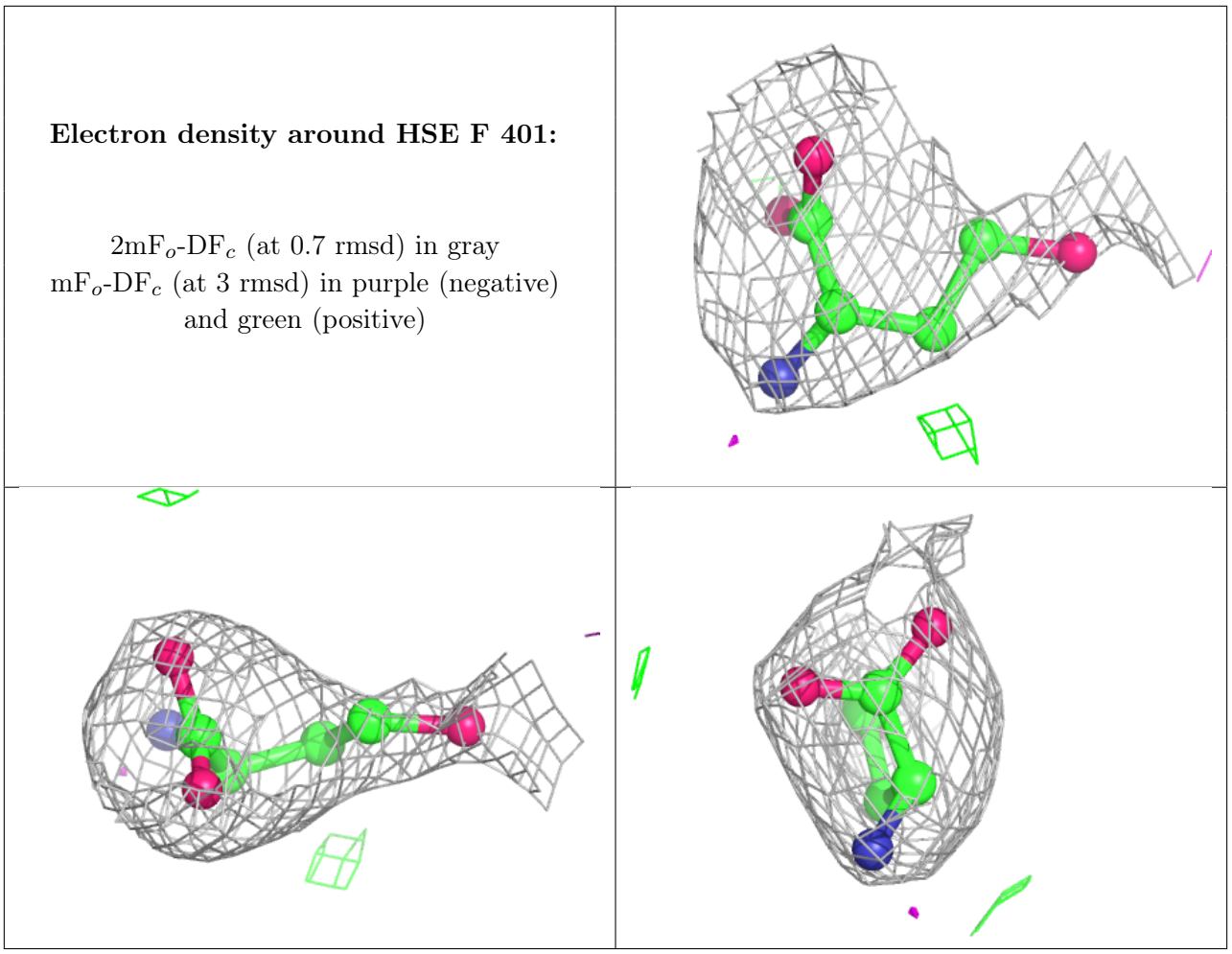
Electron density around HSE J 401:

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



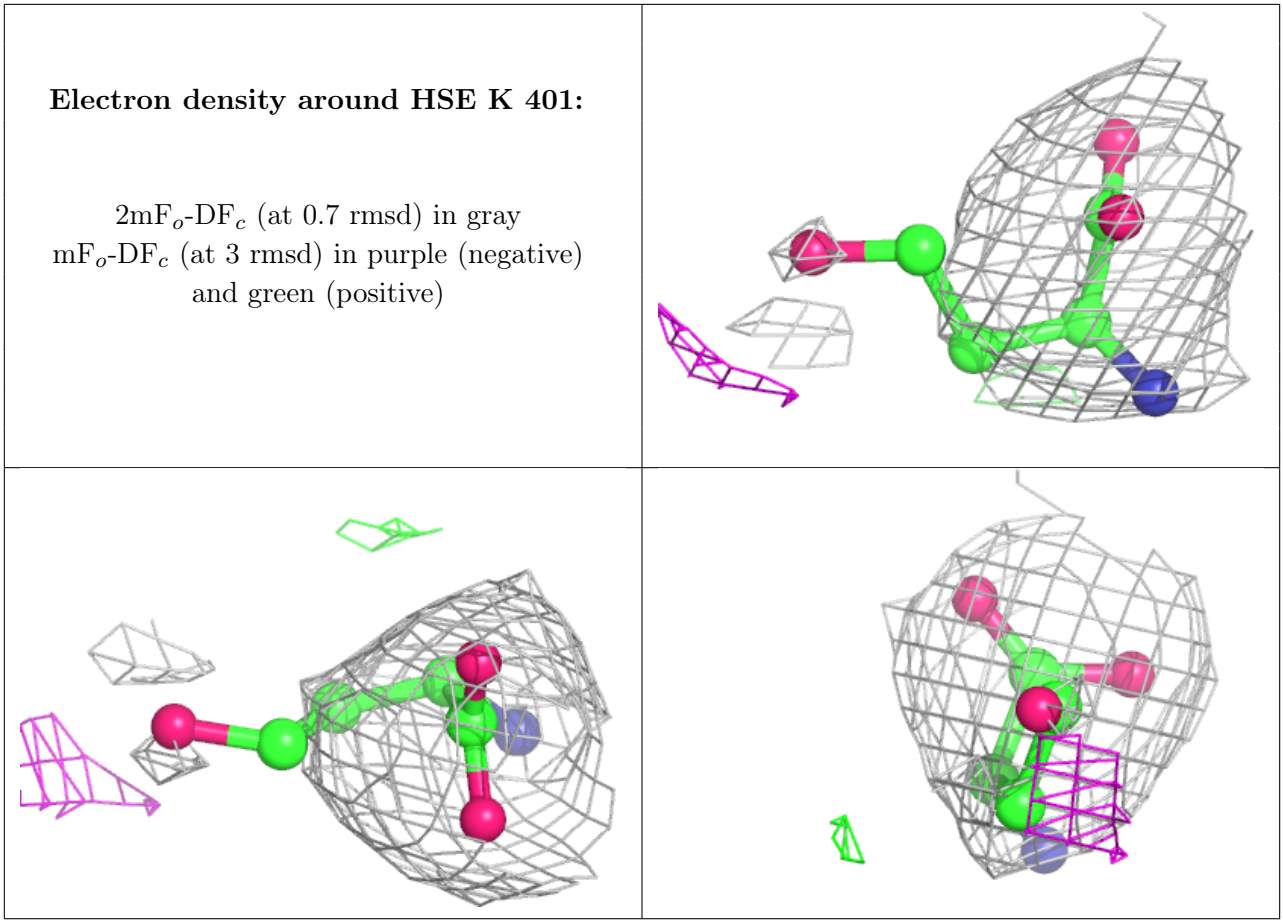
Electron density around HSE F 401:

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



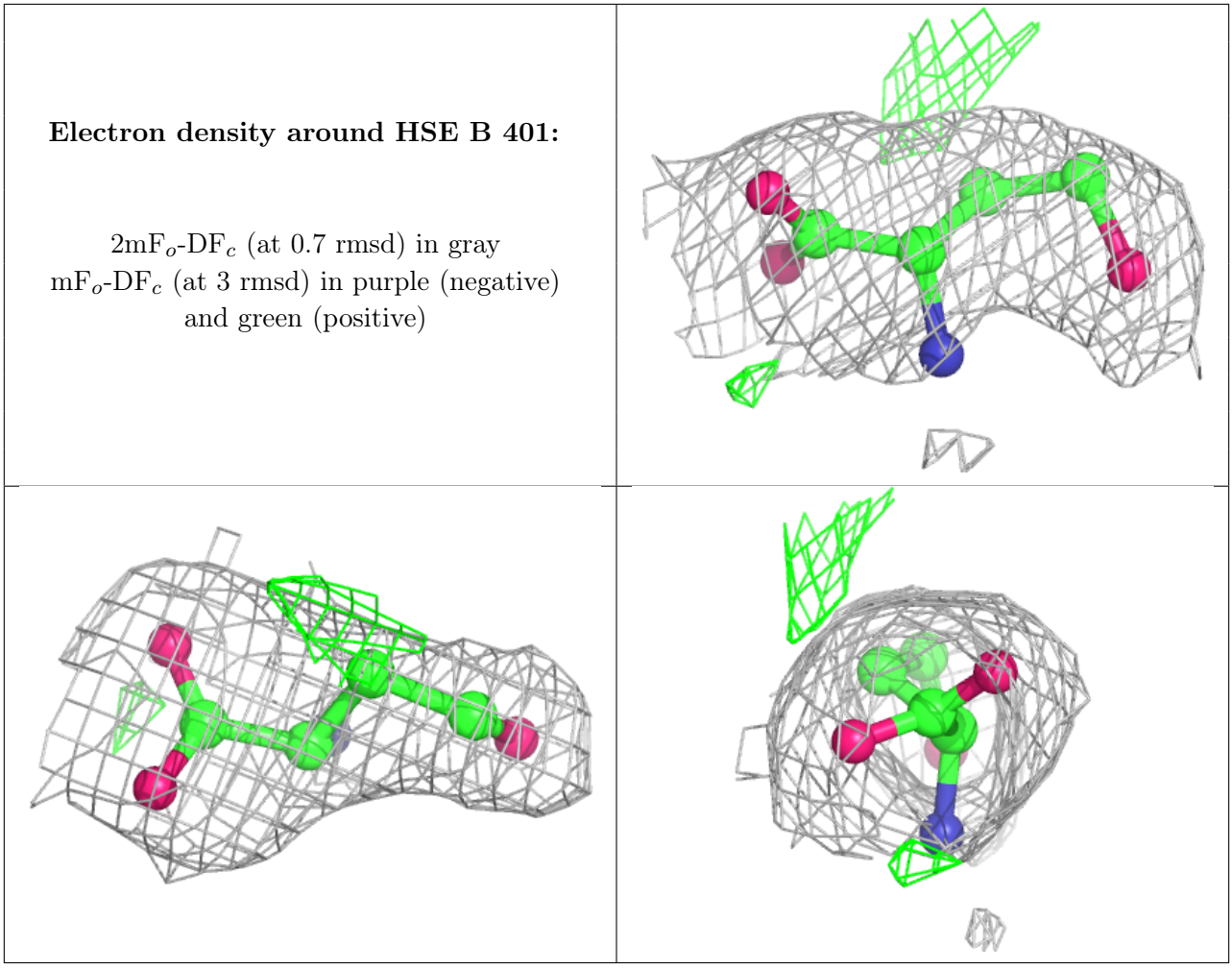
Electron density around HSE K 401:

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



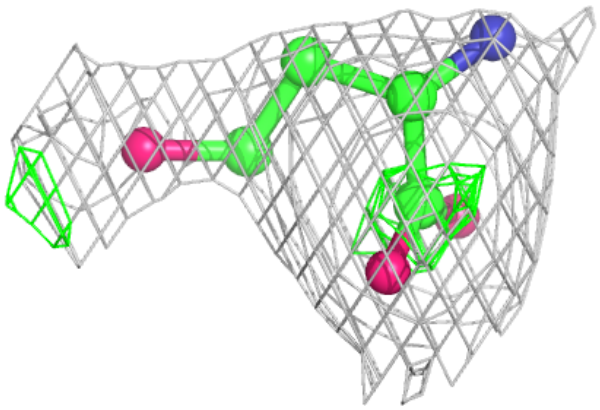
Electron density around HSE B 401:

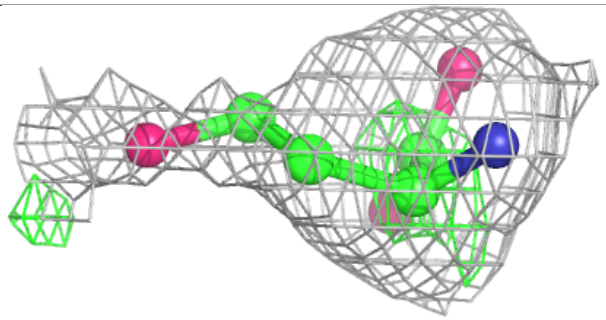
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

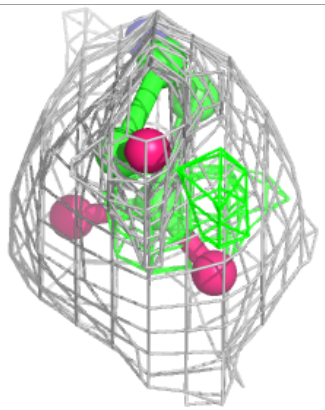


Electron density around HSE I 401:

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

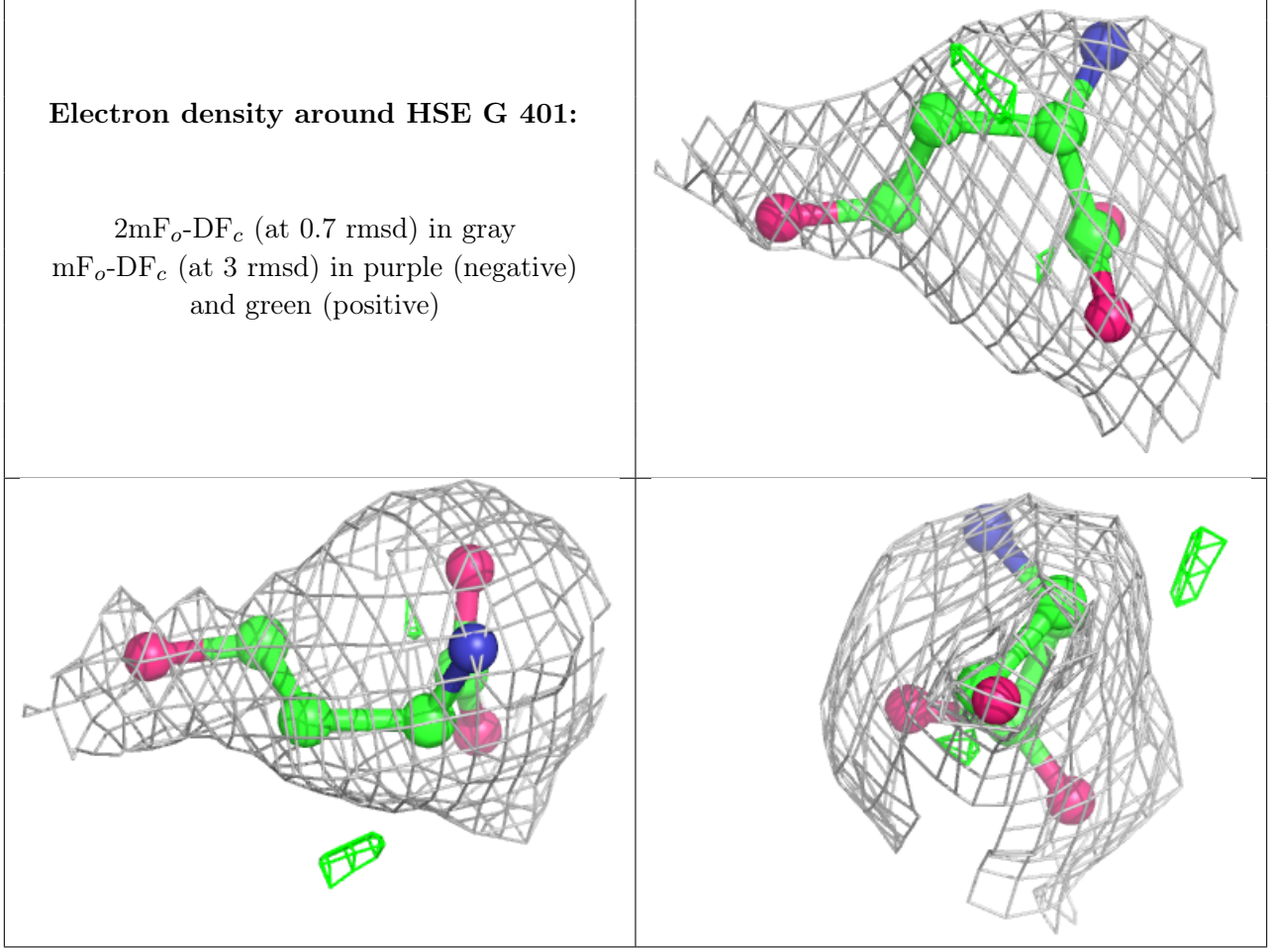






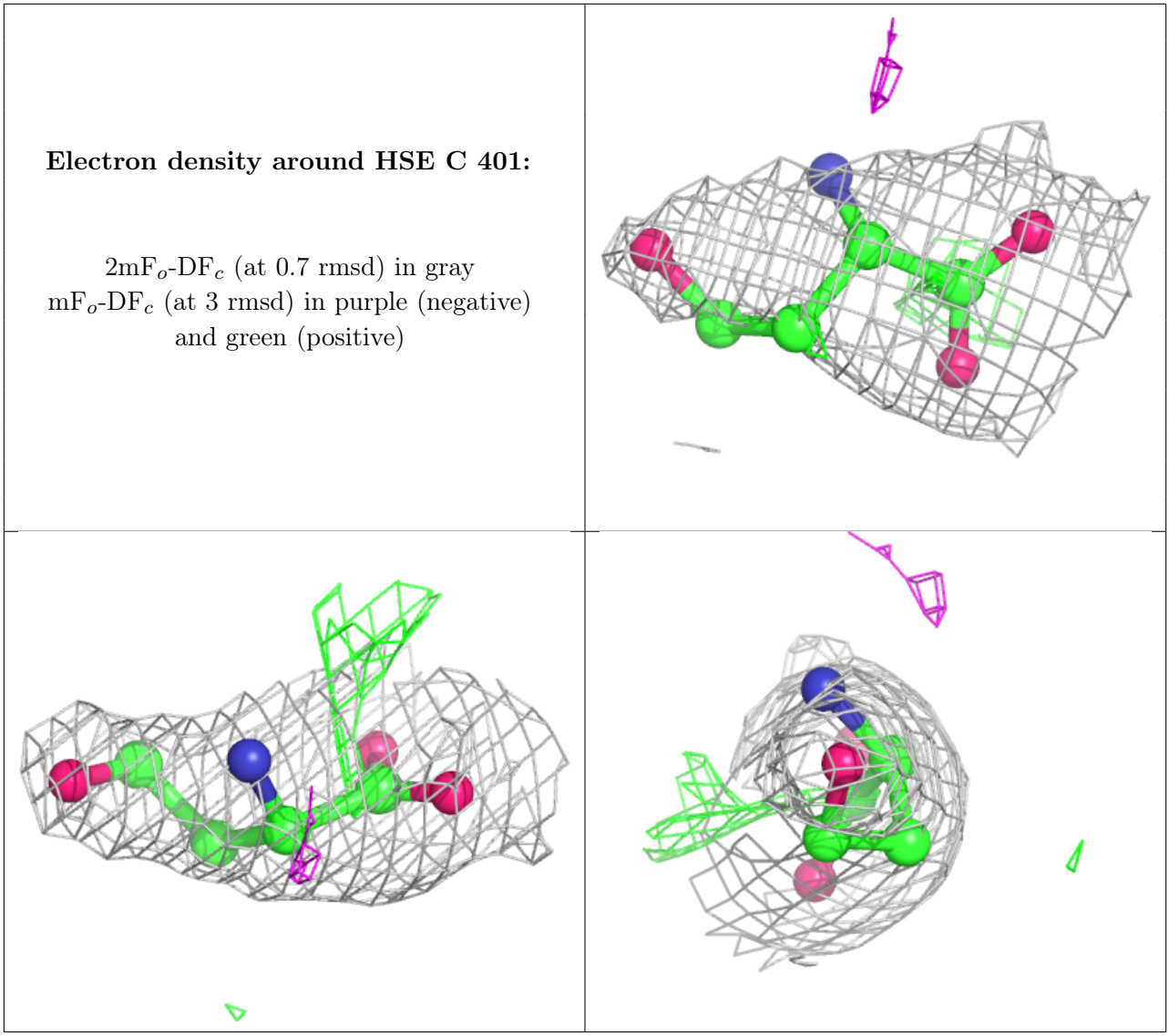
Electron density around HSE G 401:

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



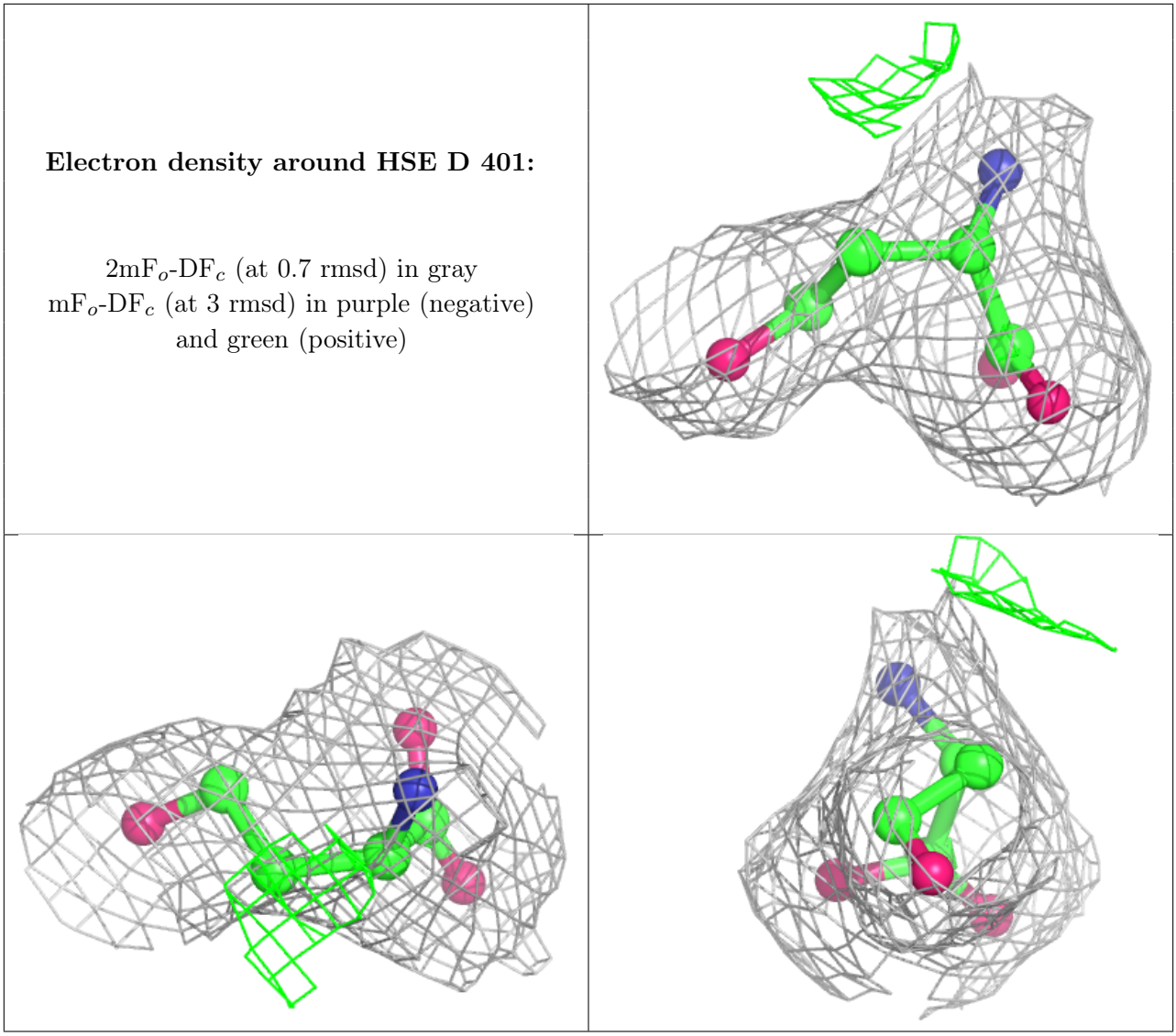
Electron density around HSE C 401:

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



Electron density around HSE D 401:

$2mF_o$-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

There are no such residues in this entry.