



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 12:37 am BST

PDB ID : 5B1I
Title : Crystal structure of K42A mutant of cystathionine beta-synthase from Lactobacillus plantarum in a complex with L-methionine
Authors : Matoba, Y.; Sugiyama, M.
Deposited on : 2015-12-04
Resolution : 3.30 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 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 : 2.11
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) : 2.11

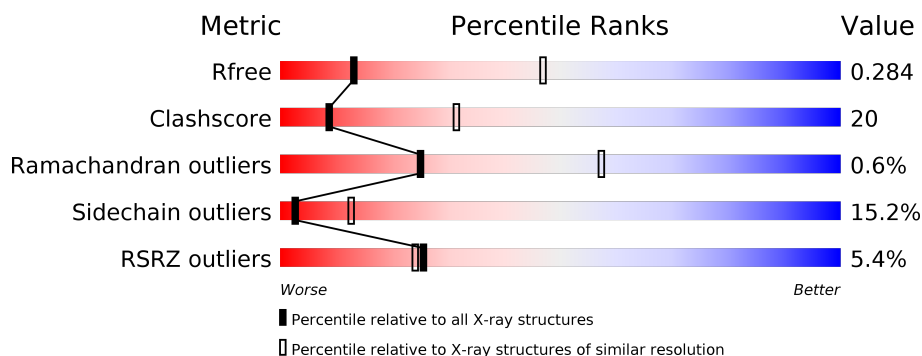
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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 on 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	311	<div> <div>2%</div> <div>55% 37% 5%</div> </div>
1	B	311	<div> <div>60% 31% 7%</div> </div>
1	C	311	<div> <div>59% 33% 5%</div> </div>
1	D	311	<div> <div>2%</div> <div>53% 38% 6%</div> </div>
1	E	311	<div> <div>%</div> <div>53% 37% 7%</div> </div>
1	F	311	<div> <div>%</div> <div>57% 35% 5%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	311	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>2%53%39%5%</div><div></div></div>
1	H	311	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>34%49%42%6%</div><div></div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 18392 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 Cystathionine beta-synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	303	Total	C	N	O	S	0	0	0
			2265	1438	394	426	7			
1	B	303	Total	C	N	O	S	0	0	0
			2265	1438	394	426	7			
1	C	303	Total	C	N	O	S	0	0	0
			2265	1438	394	426	7			
1	D	303	Total	C	N	O	S	0	0	0
			2265	1438	394	426	7			
1	E	303	Total	C	N	O	S	0	0	0
			2265	1438	394	426	7			
1	F	303	Total	C	N	O	S	0	0	0
			2265	1438	394	426	7			
1	G	303	Total	C	N	O	S	0	0	0
			2265	1438	394	426	7			
1	H	303	Total	C	N	O	S	0	0	0
			2265	1438	394	426	7			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	42	ALA	LYS	engineered mutation	UNP F9UT54
A	304	LEU	-	expression tag	UNP F9UT54
A	305	GLU	-	expression tag	UNP F9UT54
A	306	HIS	-	expression tag	UNP F9UT54
A	307	HIS	-	expression tag	UNP F9UT54
A	308	HIS	-	expression tag	UNP F9UT54
A	309	HIS	-	expression tag	UNP F9UT54
A	310	HIS	-	expression tag	UNP F9UT54
A	311	HIS	-	expression tag	UNP F9UT54
B	42	ALA	LYS	engineered mutation	UNP F9UT54
B	304	LEU	-	expression tag	UNP F9UT54
B	305	GLU	-	expression tag	UNP F9UT54
B	306	HIS	-	expression tag	UNP F9UT54

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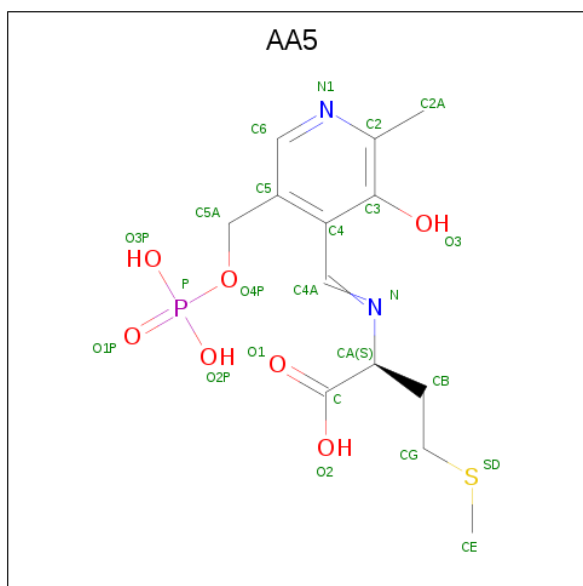
Chain	Residue	Modelled	Actual	Comment	Reference
B	307	HIS	-	expression tag	UNP F9UT54
B	308	HIS	-	expression tag	UNP F9UT54
B	309	HIS	-	expression tag	UNP F9UT54
B	310	HIS	-	expression tag	UNP F9UT54
B	311	HIS	-	expression tag	UNP F9UT54
C	42	ALA	LYS	engineered mutation	UNP F9UT54
C	304	LEU	-	expression tag	UNP F9UT54
C	305	GLU	-	expression tag	UNP F9UT54
C	306	HIS	-	expression tag	UNP F9UT54
C	307	HIS	-	expression tag	UNP F9UT54
C	308	HIS	-	expression tag	UNP F9UT54
C	309	HIS	-	expression tag	UNP F9UT54
C	310	HIS	-	expression tag	UNP F9UT54
C	311	HIS	-	expression tag	UNP F9UT54
D	42	ALA	LYS	engineered mutation	UNP F9UT54
D	304	LEU	-	expression tag	UNP F9UT54
D	305	GLU	-	expression tag	UNP F9UT54
D	306	HIS	-	expression tag	UNP F9UT54
D	307	HIS	-	expression tag	UNP F9UT54
D	308	HIS	-	expression tag	UNP F9UT54
D	309	HIS	-	expression tag	UNP F9UT54
D	310	HIS	-	expression tag	UNP F9UT54
D	311	HIS	-	expression tag	UNP F9UT54
E	42	ALA	LYS	engineered mutation	UNP F9UT54
E	304	LEU	-	expression tag	UNP F9UT54
E	305	GLU	-	expression tag	UNP F9UT54
E	306	HIS	-	expression tag	UNP F9UT54
E	307	HIS	-	expression tag	UNP F9UT54
E	308	HIS	-	expression tag	UNP F9UT54
E	309	HIS	-	expression tag	UNP F9UT54
E	310	HIS	-	expression tag	UNP F9UT54
E	311	HIS	-	expression tag	UNP F9UT54
F	42	ALA	LYS	engineered mutation	UNP F9UT54
F	304	LEU	-	expression tag	UNP F9UT54
F	305	GLU	-	expression tag	UNP F9UT54
F	306	HIS	-	expression tag	UNP F9UT54
F	307	HIS	-	expression tag	UNP F9UT54
F	308	HIS	-	expression tag	UNP F9UT54
F	309	HIS	-	expression tag	UNP F9UT54
F	310	HIS	-	expression tag	UNP F9UT54
F	311	HIS	-	expression tag	UNP F9UT54
G	42	ALA	LYS	engineered mutation	UNP F9UT54

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Chain	Residue	Modelled	Actual	Comment	Reference
G	304	LEU	-	expression tag	UNP F9UT54
G	305	GLU	-	expression tag	UNP F9UT54
G	306	HIS	-	expression tag	UNP F9UT54
G	307	HIS	-	expression tag	UNP F9UT54
G	308	HIS	-	expression tag	UNP F9UT54
G	309	HIS	-	expression tag	UNP F9UT54
G	310	HIS	-	expression tag	UNP F9UT54
G	311	HIS	-	expression tag	UNP F9UT54
H	42	ALA	LYS	engineered mutation	UNP F9UT54
H	304	LEU	-	expression tag	UNP F9UT54
H	305	GLU	-	expression tag	UNP F9UT54
H	306	HIS	-	expression tag	UNP F9UT54
H	307	HIS	-	expression tag	UNP F9UT54
H	308	HIS	-	expression tag	UNP F9UT54
H	309	HIS	-	expression tag	UNP F9UT54
H	310	HIS	-	expression tag	UNP F9UT54
H	311	HIS	-	expression tag	UNP F9UT54

- Molecule 2 is N-[(3-HYDROXY-2-METHYL-5-[(TRIHYDROXYPHOSPHORANYL)OXY]METHYL}PYRIDIN-4-YL)METHYLENE]METHIONINE (three-letter code: AA5) (formula: C₁₃H₁₉N₂O₇PS).



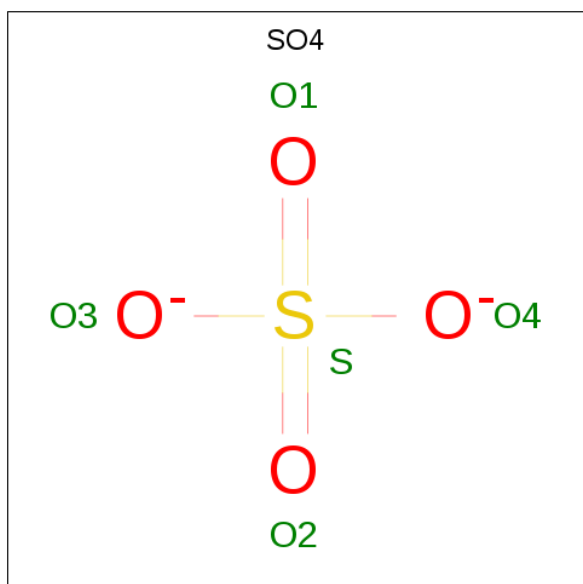
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			24	13	2	7	1	1		
2	B	1	Total	C	N	O	P	S	0	0
			24	13	2	7	1	1		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	S	0	0
			24	13	2	7	1	1		
2	D	1	Total	C	N	O	P	S	0	0
			24	13	2	7	1	1		
2	E	1	Total	C	N	O	P	S	0	0
			24	13	2	7	1	1		
2	F	1	Total	C	N	O	P	S	0	0
			24	13	2	7	1	1		
2	G	1	Total	C	N	O	P	S	0	0
			24	13	2	7	1	1		
2	H	1	Total	C	N	O	P	S	0	0
			24	13	2	7	1	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		

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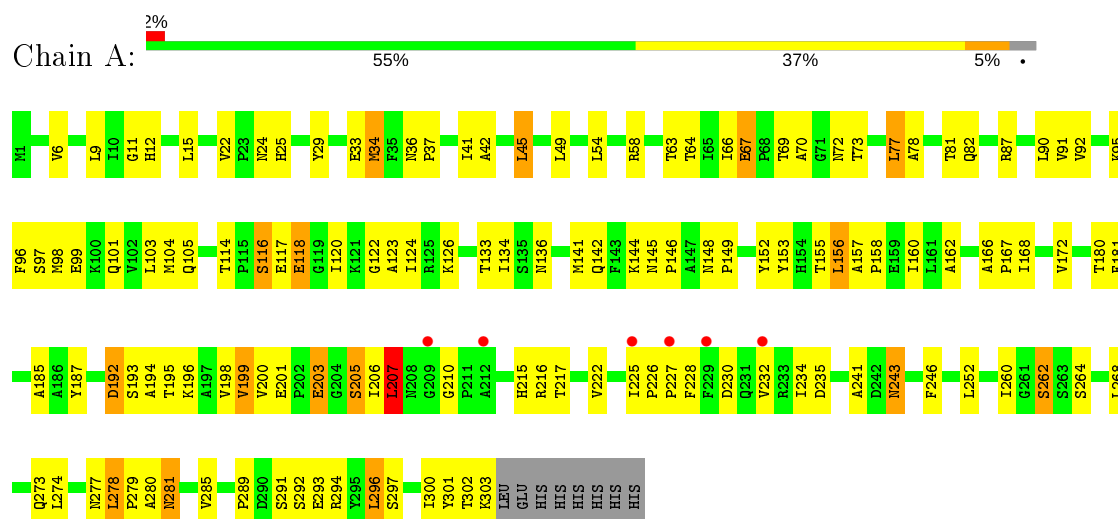
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0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

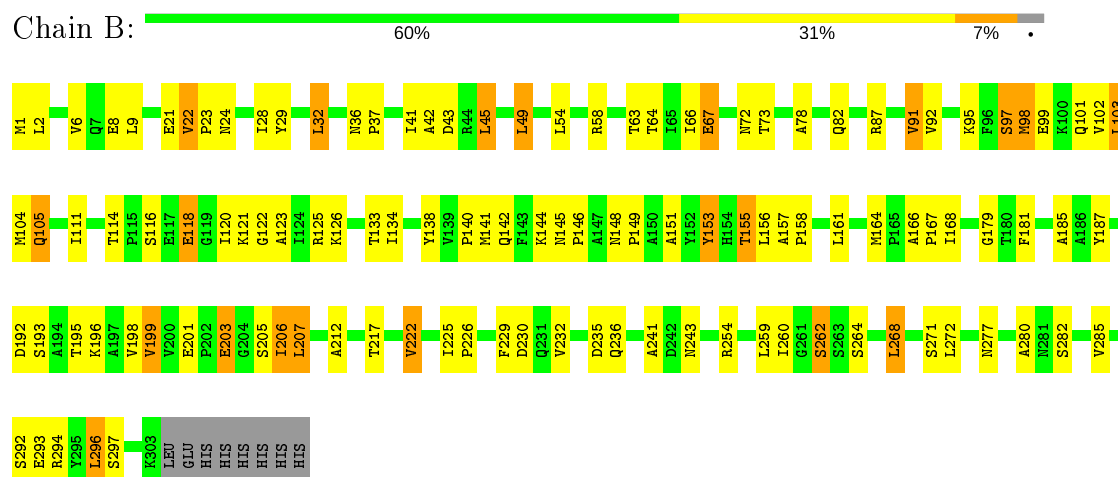
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: Cystathionine beta-synthase

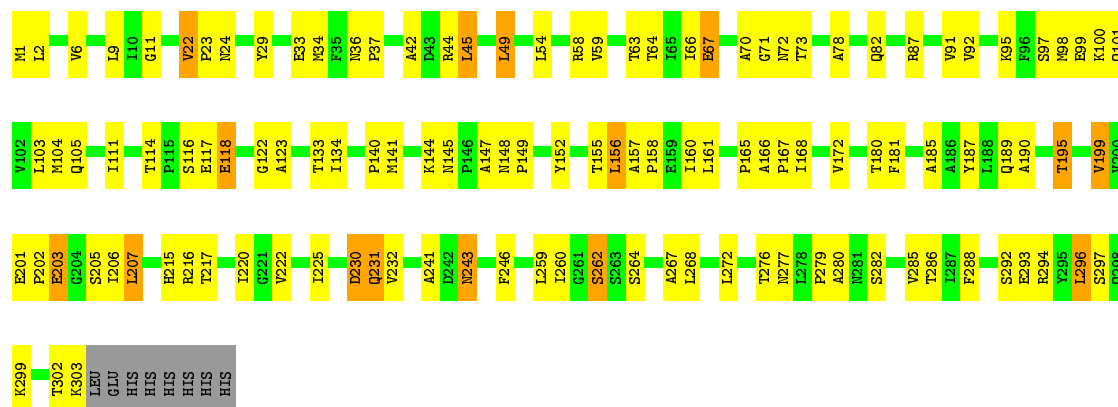


• Molecule 1: Cystathionine beta-synthase

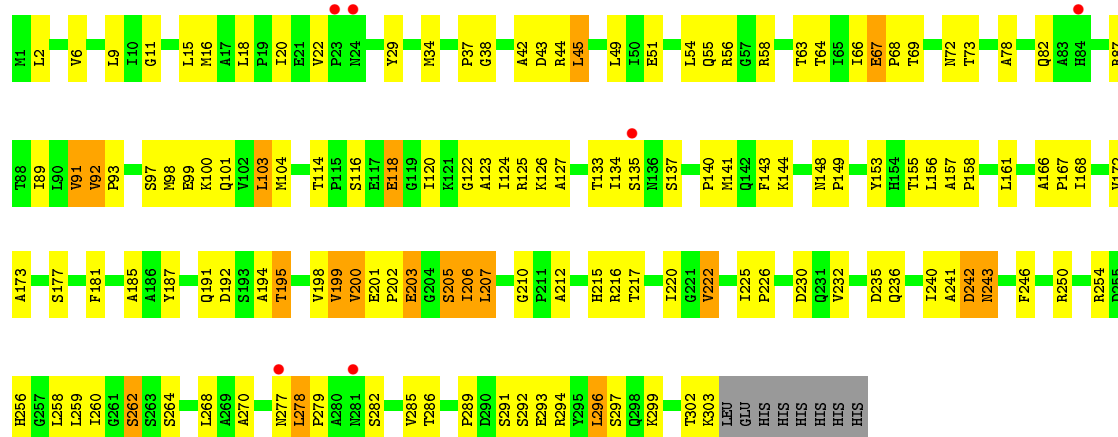


• Molecule 1: Cystathionine beta-synthase

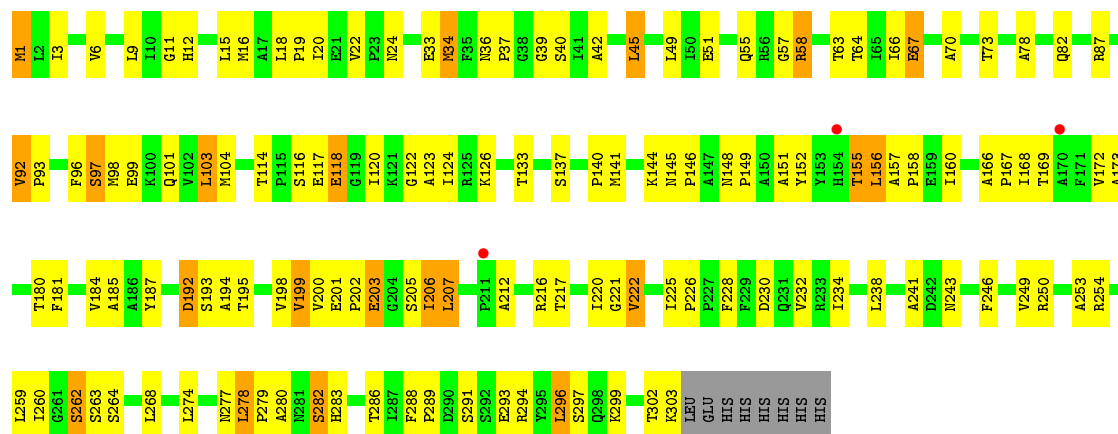




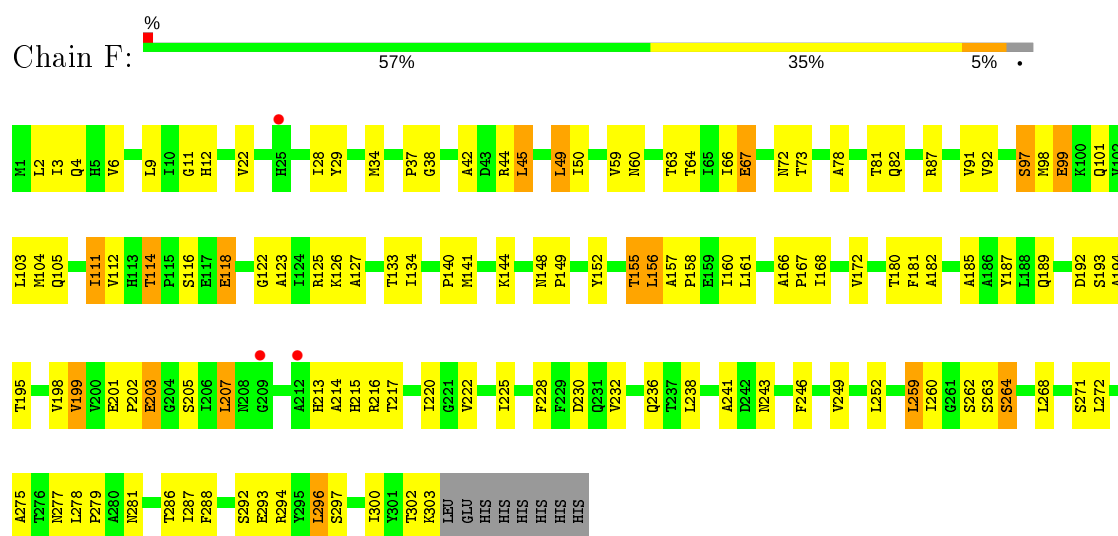
• Molecule 1: Cystathionine beta-synthase



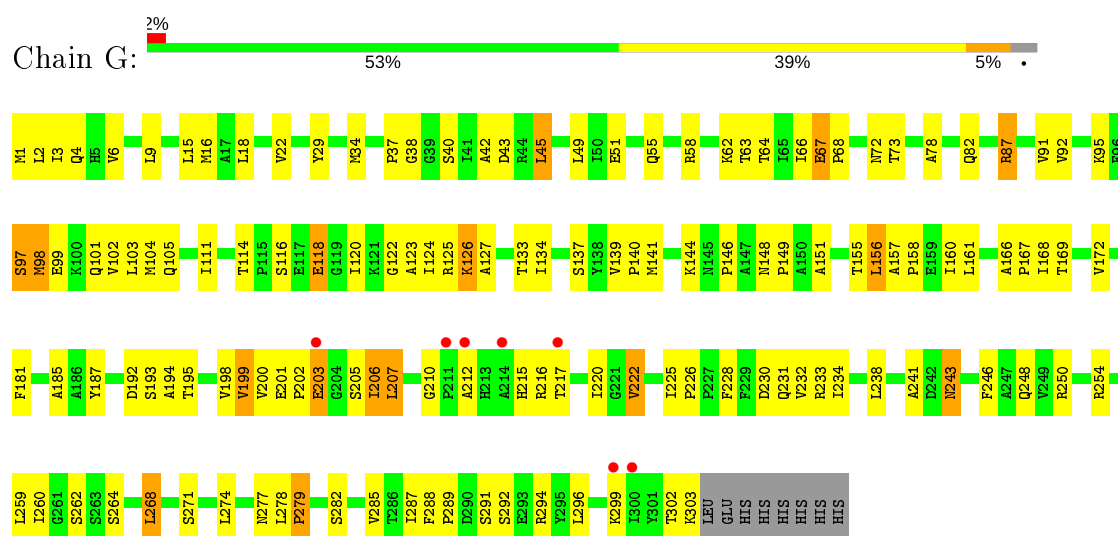
• Molecule 1: Cystathionine beta-synthase



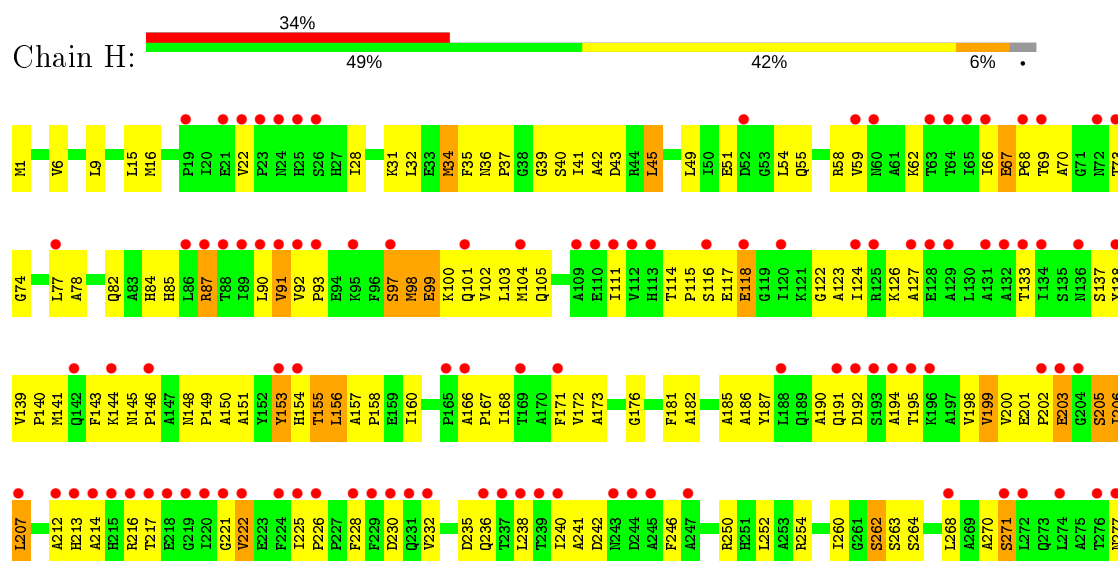
• Molecule 1: Cystathionine beta-synthase



• Molecule 1: Cystathionine beta-synthase



• Molecule 1: Cystathionine beta-synthase





4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	165.94Å 165.94Å 259.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.98 – 3.30 48.84 – 3.30	Depositor EDS
% Data completeness (in resolution range)	97.7 (29.98-3.30) 99.8 (48.84-3.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.71 (at 3.33Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.238 , 0.283 0.235 , 0.284	Depositor DCC
R_{free} test set	2797 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	43.9	Xtriage
Anisotropy	0.369	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	18392	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.92% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: AA5, SO4

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	0.39	0/2314	0.62	0/3152
1	B	0.44	0/2314	0.66	0/3152
1	C	0.44	0/2314	0.64	0/3152
1	D	0.43	0/2314	0.63	0/3152
1	E	0.41	0/2314	0.62	0/3152
1	F	0.44	0/2314	0.64	0/3152
1	G	0.38	0/2314	0.59	0/3152
1	H	0.41	0/2314	0.60	0/3152
All	All	0.42	0/18512	0.63	0/25216

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2265	0	2275	92	0
1	B	2265	0	2275	89	0
1	C	2265	0	2275	88	0
1	D	2265	0	2275	121	1
1	E	2265	0	2275	108	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2265	0	2275	92	0
1	G	2265	0	2275	98	0
1	H	2265	0	2275	130	0
2	A	24	0	15	5	0
2	B	24	0	16	5	0
2	C	24	0	16	3	0
2	D	24	0	16	2	0
2	E	24	0	16	3	0
2	F	24	0	16	2	0
2	G	24	0	16	2	0
2	H	24	0	16	4	0
3	A	10	0	0	0	0
3	B	10	0	0	1	0
3	C	10	0	0	0	0
3	D	10	0	0	0	0
3	E	10	0	0	0	0
3	F	10	0	0	0	0
3	G	10	0	0	0	0
3	H	10	0	0	0	0
All	All	18392	0	18327	751	1

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 20.

All (751) 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:A:148:ASN:HB3	1:A:149:PRO:HD3	1.46	0.97
1:H:148:ASN:HB3	1:H:149:PRO:HD3	1.45	0.94
1:B:45:LEU:HD22	1:B:49:LEU:HG	1.51	0.93
1:A:25:HIS:NE2	1:C:230:ASP:HB2	1.83	0.93
1:G:45:LEU:HD22	1:G:49:LEU:HG	1.48	0.92
1:B:157:ALA:HB3	1:B:158:PRO:HD3	1.48	0.92
1:C:148:ASN:HB3	1:C:149:PRO:HD3	1.49	0.91
1:D:148:ASN:HB3	1:D:149:PRO:HD3	1.51	0.91
1:G:101:GLN:HA	1:G:104:MET:HE3	1.54	0.90
1:C:157:ALA:HB3	1:C:158:PRO:HD3	1.52	0.88
1:G:148:ASN:HB3	1:G:149:PRO:HD3	1.57	0.86
1:H:201:GLU:OE1	1:H:205:SER:HB3	1.75	0.86
1:F:201:GLU:OE1	1:F:207:LEU:HB2	1.77	0.85
1:A:203:GLU:HG2	1:A:241:ALA:HA	1.58	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:148:ASN:HB3	1:E:149:PRO:HD3	1.55	0.84
1:D:54:LEU:HD13	1:H:191:GLN:NE2	1.93	0.83
1:G:201:GLU:OE1	1:G:207:LEU:HB2	1.78	0.83
1:F:203:GLU:HG2	1:F:241:ALA:HA	1.59	0.83
1:B:9:LEU:HB2	1:B:37:PRO:HG3	1.61	0.82
1:D:201:GLU:OE1	1:D:207:LEU:HB2	1.79	0.82
1:B:148:ASN:HB3	1:B:149:PRO:HD3	1.62	0.82
1:G:203:GLU:HG2	1:G:241:ALA:HA	1.61	0.81
1:H:201:GLU:OE1	1:H:207:LEU:HB2	1.79	0.81
1:C:9:LEU:HB2	1:C:37:PRO:HG3	1.63	0.80
1:A:157:ALA:HB3	1:A:158:PRO:HD3	1.62	0.80
1:D:51:GLU:O	1:D:55:GLN:HG3	1.82	0.79
1:G:2:LEU:HD12	1:H:15:LEU:O	1.83	0.79
1:H:67:GLU:CD	1:H:68:PRO:HD2	2.02	0.79
1:H:114:THR:HG21	1:H:123:ALA:HA	1.64	0.79
1:A:243:ASN:HD22	1:A:243:ASN:H	1.31	0.79
1:C:201:GLU:OE1	1:C:207:LEU:HB2	1.81	0.79
1:A:243:ASN:ND2	1:A:243:ASN:H	1.80	0.78
1:A:201:GLU:OE1	1:A:205:SER:HB3	1.84	0.78
1:A:201:GLU:OE1	1:A:207:LEU:HB2	1.83	0.78
1:H:157:ALA:HB3	1:H:158:PRO:HD3	1.64	0.77
1:H:155:THR:O	1:H:158:PRO:HD2	1.85	0.77
1:D:157:ALA:HB3	1:D:158:PRO:HD3	1.67	0.77
1:G:157:ALA:HB3	1:G:158:PRO:HD3	1.68	0.76
1:C:203:GLU:HG2	1:C:241:ALA:HA	1.65	0.76
1:H:203:GLU:HG2	1:H:241:ALA:HA	1.68	0.76
1:A:166:ALA:HB1	1:A:167:PRO:HD2	1.67	0.76
1:G:192:ASP:OD2	1:G:194:ALA:HB3	1.87	0.75
1:D:101:GLN:HA	1:D:104:MET:HE3	1.67	0.75
1:F:9:LEU:HB2	1:F:37:PRO:HG3	1.68	0.75
1:A:296:LEU:HD23	1:B:99:GLU:HB3	1.69	0.74
1:C:101:GLN:HA	1:C:104:MET:HE3	1.67	0.74
1:B:201:GLU:OE1	1:B:205:SER:HB3	1.88	0.74
1:A:162:ALA:HB1	1:G:231:GLN:OE1	1.88	0.73
1:D:203:GLU:HG2	1:D:241:ALA:HA	1.70	0.73
1:D:97:SER:HB3	1:D:100:LYS:HD2	1.69	0.73
1:G:206:ILE:HD11	1:G:212:ALA:HB2	1.68	0.73
1:G:168:ILE:O	1:G:195:THR:HG23	1.89	0.73
1:H:118:GLU:HB3	1:H:122:GLY:HA3	1.70	0.73
1:C:201:GLU:OE1	1:C:205:SER:HB3	1.88	0.73
1:D:243:ASN:H	1:D:243:ASN:HD22	1.38	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3:ILE:HD13	1:E:9:LEU:HD21	1.71	0.72
1:H:91:VAL:HG21	1:H:127:ALA:HB2	1.71	0.72
1:B:222:VAL:HG21	1:B:226:PRO:HD3	1.73	0.71
1:B:203:GLU:HG2	1:B:241:ALA:HA	1.72	0.71
1:A:185:ALA:HB3	1:A:232:VAL:HG21	1.72	0.71
1:F:155:THR:O	1:F:158:PRO:HD2	1.90	0.71
1:D:185:ALA:HB3	1:D:232:VAL:HG21	1.73	0.70
1:D:118:GLU:HB3	1:D:122:GLY:HA3	1.73	0.70
1:B:72:ASN:ND2	2:B:401:AA5:H2A3	2.07	0.69
1:F:166:ALA:HB1	1:F:167:PRO:HD2	1.74	0.69
1:E:201:GLU:OE1	1:E:207:LEU:HB2	1.92	0.69
1:B:24:ASN:HB3	1:B:280:ALA:HA	1.75	0.68
1:B:120:ILE:HG13	2:B:401:AA5:CE	2.23	0.68
1:D:153:TYR:CE2	1:H:55:GLN:NE2	2.61	0.68
1:E:203:GLU:HG2	1:E:241:ALA:HA	1.74	0.68
1:A:181:PHE:CD2	1:A:199:VAL:HG13	2.29	0.68
1:E:45:LEU:HD22	1:E:49:LEU:HG	1.76	0.68
1:D:67:GLU:OE1	1:D:68:PRO:HD2	1.92	0.68
1:F:216:ARG:HG2	1:F:246:PHE:CZ	2.28	0.68
1:B:168:ILE:O	1:B:195:THR:HG23	1.94	0.68
1:D:120:ILE:O	1:D:124:ILE:HG13	1.92	0.68
1:H:222:VAL:HG21	1:H:226:PRO:HD3	1.76	0.68
1:G:78:ALA:O	1:G:82:GLN:HB2	1.94	0.67
1:D:166:ALA:HB1	1:D:167:PRO:HD2	1.77	0.67
1:B:49:LEU:HD13	1:B:140:PRO:HB3	1.74	0.67
1:H:302:THR:HG22	1:H:303:LYS:N	2.10	0.67
1:E:9:LEU:HB2	1:E:37:PRO:HG3	1.78	0.66
1:F:152:TYR:CD1	1:F:180:THR:HA	2.30	0.66
1:G:62:LYS:HD3	1:G:87:ARG:NH2	2.09	0.66
1:D:99:GLU:HG3	1:D:294:ARG:O	1.95	0.66
1:G:156:LEU:HD22	1:G:160:ILE:HD11	1.77	0.66
1:E:243:ASN:H	1:E:243:ASN:ND2	1.93	0.66
1:A:78:ALA:O	1:A:82:GLN:HB2	1.96	0.66
1:F:101:GLN:HA	1:F:104:MET:HE3	1.78	0.66
1:H:45:LEU:HD22	1:H:49:LEU:HG	1.77	0.66
1:A:45:LEU:HD22	1:A:49:LEU:HG	1.78	0.66
1:D:55:GLN:HB3	1:H:153:TYR:CZ	2.31	0.66
1:A:162:ALA:HB1	1:G:231:GLN:CD	2.16	0.66
1:E:67:GLU:CG	1:E:140:PRO:HD2	2.26	0.66
1:C:293:GLU:OE2	1:D:294:ARG:HD3	1.96	0.65
1:H:254:ARG:HG2	1:H:254:ARG:O	1.94	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:216:ARG:HG2	1:F:246:PHE:CE1	2.31	0.65
1:E:67:GLU:HG2	1:E:140:PRO:HD2	1.78	0.65
1:B:29:TYR:HB2	1:B:285:VAL:HG22	1.78	0.65
1:D:54:LEU:CD1	1:H:191:GLN:NE2	2.59	0.65
1:H:260:ILE:HB	1:H:264:SER:HB2	1.79	0.65
1:H:217:THR:HG23	1:H:262:SER:HB2	1.78	0.65
1:C:201:GLU:CD	1:C:205:SER:HB3	2.17	0.65
1:E:294:ARG:HD3	1:F:293:GLU:OE2	1.97	0.65
1:E:201:GLU:OE1	1:E:205:SER:HB3	1.96	0.65
1:D:55:GLN:HA	1:H:153:TYR:OH	1.96	0.65
1:G:3:ILE:O	1:H:16:MET:HA	1.97	0.65
1:H:302:THR:HG22	1:H:303:LYS:H	1.61	0.65
1:A:66:ILE:HD11	1:A:134:ILE:HD12	1.79	0.64
1:D:278:LEU:HD22	1:D:279:PRO:HD2	1.78	0.64
1:D:201:GLU:OE1	1:D:205:SER:HB3	1.97	0.64
1:H:166:ALA:HB1	1:H:167:PRO:HD2	1.79	0.64
1:H:9:LEU:HB2	1:H:37:PRO:HG3	1.79	0.64
1:B:1:MET:SD	1:G:233:ARG:HB2	2.38	0.64
1:G:2:LEU:HA	1:H:15:LEU:O	1.97	0.64
1:H:206:ILE:HD11	1:H:212:ALA:HB2	1.80	0.64
1:C:49:LEU:HD13	1:C:140:PRO:HB3	1.80	0.64
1:D:54:LEU:HD13	1:H:191:GLN:CD	2.17	0.64
1:F:114:THR:HG21	1:F:123:ALA:HA	1.80	0.64
1:F:118:GLU:HG2	1:F:125:ARG:HH22	1.63	0.63
1:C:181:PHE:CD2	1:C:199:VAL:HG13	2.33	0.63
1:D:9:LEU:HB2	1:D:37:PRO:HG3	1.79	0.63
1:E:166:ALA:HB1	1:E:167:PRO:HD2	1.80	0.63
1:A:99:GLU:HB3	1:B:296:LEU:HD23	1.79	0.63
1:H:141:MET:HG3	1:H:144:LYS:HB2	1.79	0.63
1:B:260:ILE:O	1:B:292:SER:HB3	1.99	0.63
1:H:260:ILE:O	1:H:292:SER:HB3	1.99	0.63
1:D:51:GLU:OE2	1:H:187:TYR:CE1	2.52	0.63
1:A:99:GLU:OE1	1:A:297:SER:HB3	1.99	0.62
1:B:185:ALA:HB3	1:B:232:VAL:HG21	1.81	0.62
1:E:78:ALA:O	1:E:82:GLN:HB2	2.00	0.62
1:E:173:ALA:O	1:E:200:VAL:HG23	2.00	0.62
1:C:97:SER:OG	1:C:99:GLU:HG2	1.99	0.62
1:D:217:THR:HG23	1:D:262:SER:HB2	1.81	0.62
1:H:153:TYR:CE2	1:H:187:TYR:HB2	2.35	0.62
1:H:148:ASN:HB3	1:H:149:PRO:CD	2.27	0.61
1:D:153:TYR:CE2	1:D:187:TYR:HD1	2.18	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:51:GLU:O	1:H:55:GLN:HG3	2.00	0.61
1:B:118:GLU:HG2	1:B:125:ARG:HH22	1.65	0.61
1:B:146:PRO:O	1:B:149:PRO:HD2	2.00	0.61
1:B:201:GLU:CD	1:B:205:SER:HB3	2.21	0.61
1:G:9:LEU:HD13	1:H:35:PHE:CE2	2.35	0.61
1:C:166:ALA:HB1	1:C:167:PRO:HD2	1.82	0.61
1:C:296:LEU:HD23	1:D:99:GLU:HB3	1.83	0.61
1:E:181:PHE:CD2	1:E:199:VAL:HG13	2.35	0.61
1:G:6:VAL:HG22	1:G:37:PRO:HB3	1.82	0.61
1:B:157:ALA:HB3	1:B:158:PRO:CD	2.25	0.61
1:G:141:MET:HG3	1:G:144:LYS:HB2	1.81	0.61
1:A:217:THR:HG23	1:A:262:SER:HB2	1.83	0.61
1:C:296:LEU:HD21	1:D:103:LEU:HD13	1.80	0.61
1:G:185:ALA:HB3	1:G:232:VAL:HG21	1.83	0.61
1:H:98:MET:O	1:H:102:VAL:HG23	2.01	0.61
1:A:216:ARG:HG2	1:A:246:PHE:CZ	2.34	0.61
1:E:181:PHE:CZ	1:E:199:VAL:HG22	2.35	0.61
1:G:114:THR:HG21	1:G:123:ALA:HA	1.83	0.61
1:D:114:THR:HG21	1:D:123:ALA:HA	1.82	0.61
1:E:152:TYR:CD1	1:E:180:THR:HA	2.36	0.61
1:E:243:ASN:HD22	1:E:243:ASN:H	1.46	0.61
1:G:166:ALA:HB1	1:G:167:PRO:HD2	1.83	0.61
1:G:243:ASN:HD22	1:G:243:ASN:H	1.49	0.61
1:F:97:SER:OG	1:F:99:GLU:HG2	2.01	0.60
1:G:157:ALA:HB1	1:G:187:TYR:CD2	2.36	0.60
1:G:243:ASN:H	1:G:243:ASN:ND2	1.99	0.60
1:F:99:GLU:HG3	1:F:294:ARG:O	2.01	0.60
1:H:6:VAL:HG22	1:H:37:PRO:HB3	1.83	0.60
1:C:243:ASN:H	1:C:243:ASN:HD22	1.49	0.60
1:D:260:ILE:O	1:D:292:SER:HB3	2.01	0.60
1:G:67:GLU:HG2	1:G:140:PRO:HD2	1.83	0.60
1:D:243:ASN:H	1:D:243:ASN:ND2	1.99	0.60
1:D:6:VAL:HG22	1:D:37:PRO:HB3	1.84	0.60
1:A:6:VAL:HG22	1:A:37:PRO:HB3	1.84	0.60
1:B:201:GLU:OE1	1:B:207:LEU:HB2	2.01	0.60
1:D:45:LEU:HD22	1:D:49:LEU:HG	1.82	0.60
1:A:29:TYR:HB2	1:A:285:VAL:HG22	1.84	0.59
1:E:264:SER:HB3	1:E:288:PHE:CD1	2.37	0.59
1:C:243:ASN:ND2	1:C:243:ASN:H	2.00	0.59
1:H:66:ILE:O	1:H:139:VAL:HA	2.02	0.59
1:G:278:LEU:HD22	1:G:279:PRO:HD2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:216:ARG:HG2	1:H:246:PHE:CZ	2.37	0.59
1:A:232:VAL:O	1:A:234:ILE:HD12	2.02	0.59
1:E:114:THR:HG21	1:E:123:ALA:HA	1.85	0.59
1:B:28:ILE:HD13	1:B:271:SER:HB3	1.84	0.59
1:D:67:GLU:HG2	1:D:140:PRO:HD2	1.83	0.59
1:E:101:GLN:HA	1:E:104:MET:HE3	1.84	0.59
1:H:124:ILE:HD11	1:H:143:PHE:CD2	2.37	0.59
1:G:146:PRO:O	1:G:149:PRO:HD2	2.01	0.59
1:B:166:ALA:HB1	1:B:167:PRO:HD2	1.84	0.59
1:E:192:ASP:OD2	1:E:194:ALA:HB3	2.03	0.59
1:F:148:ASN:HB3	1:F:149:PRO:CD	2.33	0.59
1:H:36:ASN:HB3	1:H:43:ASP:OD2	2.03	0.59
1:D:302:THR:HG22	1:D:303:LYS:N	2.17	0.59
1:D:78:ALA:O	1:D:82:GLN:HB2	2.03	0.59
1:E:222:VAL:HG21	1:E:226:PRO:HD3	1.85	0.59
1:B:36:ASN:HB3	1:B:43:ASP:OD2	2.03	0.58
1:C:99:GLU:HB3	1:D:296:LEU:HD23	1.85	0.58
1:D:148:ASN:HB3	1:D:149:PRO:CD	2.30	0.58
1:E:124:ILE:HG23	1:E:141:MET:CE	2.33	0.58
1:B:243:ASN:ND2	1:B:243:ASN:H	2.01	0.58
1:D:51:GLU:OE2	1:H:187:TYR:HE1	1.86	0.58
1:A:162:ALA:HB1	1:G:231:GLN:NE2	2.17	0.58
1:A:148:ASN:HB3	1:A:149:PRO:CD	2.28	0.58
1:F:72:ASN:ND2	2:F:401:AA5:H2A3	2.18	0.58
1:D:215:HIS:HD2	1:D:217:THR:O	1.86	0.58
1:G:201:GLU:CD	1:G:205:SER:HB3	2.24	0.58
1:B:97:SER:OG	1:B:99:GLU:HG2	2.03	0.58
1:C:99:GLU:HG3	1:C:294:ARG:O	2.04	0.58
1:C:45:LEU:HD22	1:C:49:LEU:HG	1.84	0.58
1:E:250:ARG:NH1	1:E:303:LYS:HE3	2.18	0.58
1:C:70:ALA:HB2	2:C:401:AA5:HG1	1.86	0.58
1:B:181:PHE:CD2	1:B:199:VAL:HG13	2.38	0.57
1:B:157:ALA:HB1	1:B:187:TYR:CD2	2.39	0.57
1:F:118:GLU:HB3	1:F:122:GLY:HA3	1.86	0.57
1:F:156:LEU:HD22	1:F:160:ILE:HD11	1.86	0.57
1:H:101:GLN:HA	1:H:104:MET:HE3	1.86	0.57
1:A:157:ALA:HB1	1:A:187:TYR:CD2	2.40	0.57
1:H:172:VAL:O	1:H:286:THR:HA	2.04	0.57
1:C:302:THR:HG22	1:C:303:LYS:N	2.20	0.57
1:D:201:GLU:CD	1:D:205:SER:HB3	2.25	0.57
1:E:201:GLU:CD	1:E:205:SER:HB3	2.25	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:228:PHE:O	1:G:231:GLN:HG2	2.05	0.57
1:H:6:VAL:CG2	1:H:37:PRO:HB3	2.35	0.57
1:C:294:ARG:HD3	1:D:293:GLU:OE2	2.05	0.57
1:D:99:GLU:CG	1:D:294:ARG:O	2.53	0.57
1:E:99:GLU:HB3	1:F:296:LEU:HD23	1.87	0.57
1:G:181:PHE:CD2	1:G:199:VAL:HG13	2.39	0.57
1:B:294:ARG:O	1:B:294:ARG:HG3	2.05	0.56
1:E:206:ILE:HD11	1:E:212:ALA:HB2	1.87	0.56
1:H:40:SER:OG	1:H:42:ALA:HB3	2.03	0.56
1:B:114:THR:HG21	1:B:123:ALA:HA	1.87	0.56
1:B:151:ALA:O	1:B:155:THR:OG1	2.23	0.56
1:F:148:ASN:HB3	1:F:149:PRO:HD3	1.87	0.56
1:H:101:GLN:O	1:H:105:GLN:HG3	2.06	0.56
1:A:25:HIS:CD2	1:C:231:GLN:HA	2.41	0.56
1:G:4:GLN:O	1:H:16:MET:HE3	2.05	0.56
1:A:168:ILE:O	1:A:195:THR:HG23	2.05	0.56
1:G:260:ILE:HB	1:G:264:SER:HB2	1.87	0.56
1:H:138:TYR:O	1:H:140:PRO:HD3	2.05	0.56
1:C:97:SER:HB3	1:C:100:LYS:HD2	1.87	0.56
1:G:120:ILE:O	1:G:124:ILE:HG13	2.06	0.56
1:C:161:LEU:HD12	1:C:187:TYR:HE2	1.69	0.56
1:F:99:GLU:OE1	1:F:297:SER:HB3	2.05	0.56
1:A:302:THR:HG22	1:A:303:LYS:N	2.20	0.56
1:G:15:LEU:HD11	1:G:29:TYR:HB3	1.86	0.56
1:D:192:ASP:OD2	1:D:194:ALA:HB3	2.06	0.56
1:A:73:THR:HB	2:A:401:AA5:O1	2.06	0.56
1:C:67:GLU:CG	1:C:140:PRO:HD2	2.36	0.56
1:D:55:GLN:CD	1:H:153:TYR:CE2	2.80	0.56
1:F:201:GLU:OE1	1:F:205:SER:HB3	2.06	0.55
1:G:97:SER:OG	1:G:99:GLU:HG2	2.06	0.55
1:E:124:ILE:HG23	1:E:141:MET:HE3	1.89	0.55
1:C:216:ARG:HG2	1:C:246:PHE:CZ	2.42	0.55
1:E:302:THR:HG22	1:E:303:LYS:N	2.21	0.55
1:A:172:VAL:HG12	1:A:200:VAL:CG2	2.37	0.55
1:E:118:GLU:HB3	1:E:122:GLY:HA3	1.87	0.55
1:E:155:THR:O	1:E:158:PRO:HD2	2.07	0.55
1:E:70:ALA:HB1	1:E:96:PHE:CE2	2.42	0.55
1:H:156:LEU:HD22	1:H:160:ILE:HD11	1.89	0.55
1:D:141:MET:HG3	1:D:144:LYS:HB2	1.88	0.55
1:G:216:ARG:HG2	1:G:246:PHE:CZ	2.41	0.55
1:H:91:VAL:HG21	1:H:127:ALA:CB	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:MET:HG3	1:C:144:LYS:HB2	1.89	0.55
1:E:278:LEU:HD22	1:E:279:PRO:HD2	1.89	0.55
1:F:6:VAL:HG22	1:F:37:PRO:HB3	1.89	0.55
1:H:157:ALA:HB1	1:H:187:TYR:CD2	2.42	0.55
1:H:78:ALA:O	1:H:82:GLN:HB2	2.06	0.55
1:A:146:PRO:O	1:A:149:PRO:HD2	2.06	0.54
1:B:45:LEU:CD2	1:B:49:LEU:HG	2.32	0.54
1:D:202:PRO:HD3	1:D:220:ILE:HD12	1.89	0.54
1:F:149:PRO:HG3	1:F:228:PHE:CD2	2.42	0.54
1:B:260:ILE:HB	1:B:264:SER:HB2	1.87	0.54
1:A:33:GLU:OE1	1:A:41:ILE:HG13	2.07	0.54
1:F:185:ALA:O	1:F:189:GLN:HB2	2.07	0.54
1:B:101:GLN:HA	1:B:104:MET:HE3	1.90	0.54
1:C:148:ASN:HB3	1:C:149:PRO:CD	2.31	0.54
1:D:172:VAL:O	1:D:286:THR:HA	2.07	0.54
1:F:213:HIS:HD2	1:F:214:ALA:O	1.91	0.54
1:G:201:GLU:OE1	1:G:205:SER:HB3	2.07	0.54
1:C:6:VAL:CG2	1:C:37:PRO:HB3	2.37	0.54
1:D:173:ALA:O	1:D:200:VAL:HG23	2.07	0.54
1:G:67:GLU:OE2	1:G:141:MET:N	2.41	0.54
1:B:120:ILE:HG13	2:B:401:AA5:HE2	1.89	0.54
1:H:213:HIS:HD2	1:H:214:ALA:O	1.91	0.54
1:H:250:ARG:NH1	1:H:303:LYS:HE3	2.23	0.54
1:E:146:PRO:O	1:E:149:PRO:HD2	2.08	0.53
1:E:185:ALA:HB3	1:E:232:VAL:HG21	1.89	0.53
1:G:99:GLU:HG3	1:G:294:ARG:O	2.08	0.53
1:B:118:GLU:HG2	1:B:125:ARG:NH2	2.22	0.53
1:B:6:VAL:HG22	1:B:37:PRO:HB3	1.90	0.53
1:H:99:GLU:HG3	1:H:294:ARG:O	2.08	0.53
1:E:120:ILE:O	1:E:124:ILE:HG13	2.08	0.53
1:D:67:GLU:OE2	1:D:141:MET:N	2.42	0.53
1:C:33:GLU:O	1:C:36:ASN:ND2	2.42	0.53
1:D:54:LEU:CD1	1:H:191:GLN:HE22	2.21	0.53
1:H:15:LEU:HD13	1:H:31:LYS:HG2	1.91	0.53
1:F:157:ALA:HB3	1:F:158:PRO:HD3	1.90	0.53
1:A:9:LEU:HB2	1:A:37:PRO:HG3	1.90	0.53
1:F:201:GLU:CD	1:F:207:LEU:HB2	2.29	0.53
1:E:16:MET:HB2	1:F:3:ILE:HG13	1.90	0.53
1:H:148:ASN:O	1:H:151:ALA:HB3	2.09	0.53
1:A:97:SER:OG	1:A:99:GLU:HG2	2.09	0.53
1:F:118:GLU:HG2	1:F:125:ARG:NH2	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:91:VAL:HG11	1:G:126:LYS:HB3	1.91	0.52
1:C:201:GLU:OE1	1:C:205:SER:CB	2.58	0.52
1:A:120:ILE:O	1:A:124:ILE:HG13	2.09	0.52
1:A:281:ASN:OD1	1:C:190:ALA:HB2	2.09	0.52
1:C:296:LEU:HD23	1:D:99:GLU:CB	2.40	0.52
1:A:294:ARG:NH1	1:B:293:GLU:OE2	2.42	0.52
1:C:157:ALA:HB1	1:C:187:TYR:CD2	2.43	0.52
1:H:173:ALA:O	1:H:200:VAL:HG23	2.10	0.52
1:D:191:GLN:OE1	1:H:84:HIS:CD2	2.63	0.52
1:H:171:PHE:CZ	1:H:173:ALA:HB2	2.45	0.52
1:A:141:MET:HG3	1:A:144:LYS:HB2	1.91	0.52
1:A:24:ASN:HB3	1:A:280:ALA:HA	1.92	0.52
1:A:42:ALA:HB1	1:A:73:THR:HA	1.92	0.52
1:D:51:GLU:HG3	1:D:55:GLN:NE2	2.25	0.52
1:F:78:ALA:O	1:F:82:GLN:HB2	2.09	0.52
1:A:99:GLU:HG3	1:A:294:ARG:O	2.10	0.52
1:C:202:PRO:HD3	1:C:220:ILE:HG13	1.91	0.52
1:D:222:VAL:HG21	1:D:226:PRO:HD3	1.90	0.52
1:E:15:LEU:O	1:F:2:LEU:HD12	2.09	0.52
1:H:240:ILE:HD11	1:H:270:ALA:HA	1.91	0.52
1:A:260:ILE:O	1:A:292:SER:HB3	2.10	0.52
1:D:157:ALA:HB1	1:D:187:TYR:CD2	2.46	0.52
1:E:42:ALA:HB1	1:E:73:THR:HA	1.92	0.52
1:B:254:ARG:O	1:B:254:ARG:HG2	2.09	0.51
1:C:168:ILE:O	1:C:195:THR:HG23	2.11	0.51
1:F:141:MET:HG3	1:F:144:LYS:HB2	1.92	0.51
1:A:300:ILE:HG23	1:A:301:TYR:N	2.25	0.51
1:A:293:GLU:OE2	1:B:294:ARG:HD3	2.11	0.51
1:C:157:ALA:CB	1:C:158:PRO:HD3	2.35	0.51
1:D:168:ILE:O	1:D:195:THR:HG23	2.10	0.51
1:E:99:GLU:HG3	1:E:294:ARG:O	2.10	0.51
1:H:97:SER:HB3	1:H:100:LYS:HD2	1.93	0.51
1:C:141:MET:HG3	1:C:141:MET:O	2.10	0.51
1:D:203:GLU:OE1	1:D:242:ASP:HB2	2.10	0.51
1:D:51:GLU:HG3	1:D:55:GLN:HE21	1.75	0.51
1:E:40:SER:HA	1:E:289:PRO:O	2.10	0.51
1:B:201:GLU:CD	1:B:207:LEU:HB2	2.31	0.51
1:C:260:ILE:O	1:C:292:SER:HB3	2.09	0.51
1:G:169:THR:HG21	1:G:278:LEU:HD13	1.93	0.51
1:D:187:TYR:HE1	1:H:51:GLU:OE2	1.92	0.51
1:D:201:GLU:CD	1:D:207:LEU:HB2	2.31	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:114:THR:HG21	1:C:123:ALA:HA	1.92	0.51
1:G:91:VAL:HG21	1:G:127:ALA:HA	1.92	0.51
1:H:70:ALA:HB3	2:H:401:AA5:O1	2.11	0.51
1:C:185:ALA:O	1:C:189:GLN:HB2	2.11	0.51
1:C:99:GLU:OE1	1:C:297:SER:HB3	2.11	0.51
1:F:259:LEU:CD1	1:F:259:LEU:N	2.73	0.51
1:A:118:GLU:HB3	1:A:122:GLY:HA3	1.91	0.51
1:C:118:GLU:HB3	1:C:122:GLY:HA3	1.92	0.51
1:E:169:THR:HG21	1:E:278:LEU:HD13	1.92	0.51
1:B:138:TYR:O	1:B:140:PRO:HD3	2.11	0.51
1:C:6:VAL:HG22	1:C:37:PRO:HB3	1.93	0.51
1:G:118:GLU:HB3	1:G:122:GLY:HA3	1.92	0.51
1:G:29:TYR:HB2	1:G:285:VAL:HG22	1.93	0.51
1:H:202:PRO:HD2	1:H:221:GLY:HA2	1.94	0.50
1:H:205:SER:OG	1:H:221:GLY:HA2	2.11	0.50
1:E:1:MET:HE3	1:E:1:MET:HA	1.93	0.50
1:G:156:LEU:HD22	1:G:160:ILE:CD1	2.40	0.50
1:D:187:TYR:CE1	1:H:51:GLU:OE2	2.64	0.50
1:E:63:THR:HG22	1:E:64:THR:N	2.27	0.50
1:F:49:LEU:HD13	1:F:140:PRO:HB3	1.92	0.50
1:F:202:PRO:HD3	1:F:220:ILE:HD12	1.93	0.50
1:F:42:ALA:HB1	1:F:73:THR:HA	1.93	0.50
1:G:260:ILE:O	1:G:292:SER:HB3	2.12	0.50
1:D:16:MET:HG2	1:D:18:LEU:HD23	1.92	0.50
1:E:67:GLU:OE2	1:E:141:MET:N	2.44	0.50
1:F:201:GLU:CD	1:F:205:SER:HB3	2.32	0.50
1:H:66:ILE:HD12	1:H:137:SER:HB2	1.94	0.50
1:D:191:GLN:OE1	1:H:84:HIS:NE2	2.45	0.50
1:C:42:ALA:HB1	1:C:73:THR:HA	1.93	0.50
2:H:401:AA5:H4A	2:H:401:AA5:O1P	2.11	0.50
1:C:67:GLU:OE2	1:C:141:MET:N	2.45	0.50
1:B:21:GLU:HB2	3:B:403:SO4:O3	2.12	0.50
1:C:67:GLU:HG3	1:C:140:PRO:HD2	1.93	0.50
1:E:202:PRO:HD3	1:E:220:ILE:HG13	1.94	0.49
1:A:196:LYS:HA	1:A:235:ASP:OD2	2.12	0.49
1:B:196:LYS:HA	1:B:235:ASP:OD2	2.12	0.49
1:C:201:GLU:CD	1:C:207:LEU:HB2	2.32	0.49
1:C:24:ASN:HB3	1:C:280:ALA:HA	1.94	0.49
1:D:302:THR:CG2	1:D:303:LYS:N	2.75	0.49
1:E:148:ASN:CB	1:E:149:PRO:HD3	2.37	0.49
1:H:69:THR:HG23	1:H:92:VAL:HG12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:302:THR:HG22	1:G:303:LYS:N	2.27	0.49
1:C:54:LEU:HD23	1:C:59:VAL:HB	1.93	0.49
1:E:157:ALA:HB3	1:E:158:PRO:HD3	1.93	0.49
1:B:118:GLU:HB3	1:B:122:GLY:HA3	1.94	0.49
1:B:157:ALA:CB	1:B:158:PRO:HD3	2.33	0.49
1:B:22:VAL:HG12	1:B:23:PRO:HD2	1.94	0.49
1:D:67:GLU:CD	1:D:68:PRO:HD2	2.33	0.49
1:A:117:GLU:H	1:A:117:GLU:CD	2.16	0.49
1:B:206:ILE:HD11	1:B:212:ALA:HB2	1.95	0.49
1:D:67:GLU:CG	1:D:140:PRO:HD2	2.43	0.49
1:A:201:GLU:CD	1:A:205:SER:HB3	2.33	0.49
1:A:296:LEU:HD23	1:B:99:GLU:CB	2.41	0.49
1:B:66:ILE:HD11	1:B:134:ILE:HD12	1.94	0.49
1:B:78:ALA:O	1:B:82:GLN:HB2	2.12	0.49
1:D:206:ILE:HD11	1:D:212:ALA:HB2	1.94	0.49
1:D:99:GLU:OE1	1:D:297:SER:HB3	2.13	0.49
1:G:198:VAL:HG21	1:G:274:LEU:HD13	1.95	0.49
1:H:264:SER:HB3	1:H:288:PHE:CD1	2.48	0.49
1:A:70:ALA:CB	2:A:401:AA5:HG1	2.43	0.48
1:E:296:LEU:HD23	1:F:99:GLU:HB3	1.95	0.48
1:G:202:PRO:HD3	1:G:220:ILE:HD12	1.95	0.48
1:F:101:GLN:HA	1:F:104:MET:CE	2.44	0.48
1:A:33:GLU:O	1:A:36:ASN:ND2	2.45	0.48
1:D:153:TYR:CE2	1:H:55:GLN:CD	2.87	0.48
1:F:168:ILE:O	1:F:195:THR:HG23	2.13	0.48
1:G:66:ILE:HD12	1:G:137:SER:HB2	1.95	0.48
1:H:181:PHE:CD2	1:H:199:VAL:HG13	2.49	0.48
1:A:260:ILE:HB	1:A:264:SER:HB2	1.94	0.48
1:E:181:PHE:CE2	1:E:199:VAL:HG22	2.47	0.48
1:E:263:SER:OG	2:E:401:AA5:H2A1	2.13	0.48
1:F:45:LEU:HD22	1:F:49:LEU:HG	1.95	0.48
1:E:16:MET:HG2	1:E:18:LEU:HD23	1.95	0.48
1:E:250:ARG:HH12	1:E:303:LYS:HE3	1.76	0.48
1:A:101:GLN:O	1:A:105:GLN:HG3	2.12	0.48
1:B:32:LEU:N	1:B:32:LEU:HD23	2.29	0.48
1:C:148:ASN:CB	1:C:149:PRO:HD3	2.34	0.48
1:F:63:THR:HG22	1:F:64:THR:N	2.29	0.48
1:D:55:GLN:CG	1:H:153:TYR:CE2	2.96	0.48
1:E:67:GLU:HG3	1:E:140:PRO:HD2	1.94	0.48
1:E:66:ILE:HD12	1:E:137:SER:HB2	1.95	0.48
1:E:18:LEU:O	1:E:20:ILE:N	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:216:ARG:HG2	1:E:246:PHE:CZ	2.49	0.48
1:H:222:VAL:HG21	1:H:226:PRO:CD	2.44	0.48
1:A:145:ASN:O	1:A:228:PHE:HE2	1.96	0.48
1:B:226:PRO:HG2	1:B:229:PHE:CZ	2.49	0.48
1:C:140:PRO:O	1:C:145:ASN:HB2	2.14	0.48
1:D:63:THR:HG22	1:D:64:THR:N	2.29	0.48
1:F:260:ILE:O	1:F:292:SER:HB3	2.14	0.48
1:C:296:LEU:HA	1:C:296:LEU:HD12	1.71	0.47
1:F:198:VAL:HG13	1:F:236:GLN:O	2.13	0.47
1:F:243:ASN:HD22	1:F:243:ASN:H	1.62	0.47
1:G:222:VAL:HG21	1:G:226:PRO:HG3	1.95	0.47
1:E:260:ILE:HB	1:E:264:SER:HB2	1.96	0.47
1:F:91:VAL:HG12	1:F:114:THR:CG2	2.45	0.47
1:H:34:MET:HA	1:H:39:GLY:O	2.14	0.47
1:A:192:ASP:OD2	1:A:194:ALA:HB3	2.15	0.47
1:C:22:VAL:HG13	1:C:272:LEU:HD23	1.96	0.47
1:C:72:ASN:ND2	2:C:401:AA5:H2A3	2.29	0.47
1:E:157:ALA:HA	1:E:160:ILE:HD12	1.97	0.47
1:E:198:VAL:HG11	1:E:238:LEU:HD12	1.96	0.47
1:F:6:VAL:CG2	1:F:37:PRO:HB3	2.44	0.47
1:A:99:GLU:OE1	1:A:297:SER:CB	2.62	0.47
1:A:294:ARG:HD3	1:B:293:GLU:OE2	2.14	0.47
1:F:72:ASN:HD22	2:F:401:AA5:H2A3	1.78	0.47
1:H:302:THR:CG2	1:H:303:LYS:N	2.78	0.47
1:E:172:VAL:O	1:E:286:THR:HA	2.15	0.47
1:D:55:GLN:CA	1:H:153:TYR:OH	2.62	0.47
1:A:77:LEU:O	1:A:81:THR:HG23	2.15	0.47
1:D:68:PRO:HA	1:D:91:VAL:O	2.15	0.47
1:B:67:GLU:OE2	1:B:142:GLN:N	2.46	0.47
1:C:63:THR:HG22	1:C:64:THR:N	2.28	0.47
1:D:264:SER:OG	1:D:289:PRO:HD2	2.14	0.47
1:E:249:VAL:HA	1:E:260:ILE:HD11	1.96	0.47
1:G:3:ILE:HG13	1:H:16:MET:HB2	1.96	0.47
1:A:145:ASN:O	1:A:228:PHE:CE2	2.68	0.47
1:A:67:GLU:OE2	1:A:142:GLN:N	2.46	0.47
1:C:185:ALA:HB3	1:C:232:VAL:HG21	1.96	0.47
1:D:118:GLU:HG2	1:D:125:ARG:NH2	2.29	0.47
1:G:148:ASN:HB3	1:G:149:PRO:CD	2.37	0.47
1:H:235:ASP:O	1:H:236:GLN:HB2	2.14	0.47
1:A:198:VAL:HG21	1:A:274:LEU:HD13	1.97	0.46
1:B:198:VAL:HG13	1:B:236:GLN:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:272:LEU:O	1:F:275:ALA:HB3	2.15	0.46
1:B:201:GLU:OE1	1:B:205:SER:CB	2.60	0.46
1:E:156:LEU:HD13	1:E:184:VAL:HG21	1.97	0.46
1:G:215:HIS:HD2	1:G:217:THR:O	1.98	0.46
1:H:153:TYR:CD2	1:H:187:TYR:HB2	2.50	0.46
1:H:302:THR:CG2	1:H:303:LYS:H	2.28	0.46
1:F:11:GLY:O	1:F:12:HIS:HB2	2.15	0.46
1:A:162:ALA:CB	1:G:231:GLN:OE1	2.59	0.46
1:G:198:VAL:HG11	1:G:238:LEU:HD12	1.98	0.46
1:E:117:GLU:CD	1:E:117:GLU:H	2.19	0.46
1:F:182:ALA:HA	1:F:232:VAL:HG21	1.97	0.46
1:F:243:ASN:ND2	1:F:243:ASN:H	2.13	0.46
1:G:118:GLU:HG2	1:G:125:ARG:NH2	2.31	0.46
1:G:287:ILE:O	1:G:289:PRO:HD3	2.15	0.46
1:H:153:TYR:HE2	1:H:187:TYR:HD1	1.62	0.46
1:C:216:ARG:HG2	1:C:246:PHE:CE1	2.50	0.46
1:C:70:ALA:CB	2:C:401:AA5:HG1	2.44	0.46
1:E:157:ALA:HB1	1:E:187:TYR:CD2	2.49	0.46
1:E:70:ALA:CB	2:E:401:AA5:HG1	2.45	0.46
1:F:181:PHE:CD2	1:F:199:VAL:HG13	2.51	0.46
1:B:153:TYR:CE2	1:B:187:TYR:HD1	2.34	0.46
1:D:278:LEU:HD22	1:D:279:PRO:CD	2.43	0.46
1:G:67:GLU:HG3	1:G:140:PRO:HG2	1.97	0.46
1:B:6:VAL:CG2	1:B:37:PRO:HB3	2.45	0.46
1:D:11:GLY:HA2	1:D:44:ARG:CZ	2.46	0.46
1:F:156:LEU:HD22	1:F:160:ILE:CD1	2.46	0.46
1:G:1:MET:HE2	1:G:2:LEU:O	2.16	0.46
1:D:101:GLN:HA	1:D:104:MET:CE	2.41	0.46
1:E:302:THR:CG2	1:E:303:LYS:N	2.78	0.46
1:F:278:LEU:HD22	1:F:279:PRO:HD2	1.98	0.46
1:G:98:MET:O	1:G:102:VAL:HG23	2.15	0.46
1:H:97:SER:OG	1:H:99:GLU:HG2	2.16	0.46
1:A:90:LEU:HD13	1:A:104:MET:SD	2.55	0.46
1:D:206:ILE:CD1	1:D:212:ALA:HB2	2.45	0.46
1:D:161:LEU:HA	1:D:161:LEU:HD23	1.77	0.46
1:E:254:ARG:C	1:F:82:GLN:NE2	2.70	0.46
1:H:90:LEU:HD13	1:H:104:MET:SD	2.56	0.46
1:H:28:ILE:HD13	1:H:271:SER:HB3	1.98	0.46
1:C:2:LEU:HD12	1:D:15:LEU:O	2.17	0.45
1:E:148:ASN:HB3	1:E:149:PRO:CD	2.38	0.45
1:E:198:VAL:HG21	1:E:274:LEU:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:66:ILE:HD11	1:F:134:ILE:HD12	1.98	0.45
1:A:157:ALA:HB3	1:A:158:PRO:CD	2.39	0.45
1:B:41:ILE:HG12	1:B:41:ILE:O	2.16	0.45
1:C:145:ASN:OD1	1:C:147:ALA:HB3	2.16	0.45
1:D:56:ARG:O	1:D:58:ARG:HG2	2.16	0.45
1:D:69:THR:HG23	1:D:92:VAL:HG12	1.98	0.45
1:B:101:GLN:O	1:B:105:GLN:HG2	2.16	0.45
1:B:63:THR:CG2	1:B:64:THR:N	2.80	0.45
1:F:187:TYR:CD2	1:F:187:TYR:C	2.89	0.45
1:C:302:THR:CG2	1:C:303:LYS:N	2.79	0.45
1:E:249:VAL:HG13	1:E:260:ILE:O	2.16	0.45
1:E:99:GLU:O	1:E:103:LEU:HD22	2.17	0.45
1:F:161:LEU:HD12	1:F:187:TYR:HE2	1.82	0.45
1:G:68:PRO:HA	1:G:91:VAL:O	2.16	0.45
1:D:153:TYR:OH	1:H:55:GLN:HG2	2.17	0.45
1:G:72:ASN:ND2	2:G:401:AA5:H2A3	2.31	0.45
1:C:260:ILE:HB	1:C:264:SER:HB2	1.99	0.45
1:D:6:VAL:CG2	1:D:37:PRO:HB3	2.46	0.45
1:G:91:VAL:HG21	1:G:127:ALA:CA	2.47	0.45
1:C:157:ALA:HB3	1:C:158:PRO:CD	2.35	0.45
1:G:3:ILE:HD11	1:H:32:LEU:HD11	1.99	0.45
1:E:6:VAL:HG22	1:E:37:PRO:HB3	1.99	0.45
1:F:302:THR:HG22	1:F:303:LYS:N	2.32	0.45
1:A:114:THR:HG21	1:A:123:ALA:HA	1.99	0.45
1:D:42:ALA:HB1	1:D:73:THR:HA	1.99	0.45
1:E:34:MET:HE1	1:E:260:ILE:HG22	1.99	0.45
1:G:66:ILE:O	1:G:139:VAL:HA	2.17	0.45
1:D:153:TYR:CD2	1:H:55:GLN:NE2	2.84	0.45
1:C:264:SER:O	1:C:267:ALA:HB3	2.17	0.45
1:E:149:PRO:HG2	1:E:228:PHE:CD2	2.51	0.45
1:E:70:ALA:HB2	2:E:401:AA5:HG1	1.98	0.45
1:A:156:LEU:HD22	1:A:160:ILE:HD11	1.99	0.44
1:D:216:ARG:HG2	1:D:246:PHE:CZ	2.53	0.44
1:D:240:ILE:HD11	1:D:270:ALA:HB2	1.98	0.44
1:D:92:VAL:HA	1:D:93:PRO:HD3	1.79	0.44
1:F:38:GLY:O	1:F:294:ARG:NH2	2.34	0.44
1:B:8:GLU:HG2	1:G:193:SER:OG	2.18	0.44
1:D:134:ILE:HG22	1:D:137:SER:HB3	1.98	0.44
1:E:6:VAL:CG2	1:E:37:PRO:HB3	2.47	0.44
1:H:143:PHE:HE1	2:H:401:AA5:SD	2.41	0.44
1:A:15:LEU:O	1:B:2:LEU:HD12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:PRO:HG3	2:A:401:AA5:N1	2.32	0.44
1:B:99:GLU:OE1	1:B:297:SER:HB3	2.16	0.44
1:C:172:VAL:O	1:C:286:THR:HA	2.16	0.44
1:E:70:ALA:HB1	1:E:96:PHE:CD2	2.52	0.44
1:G:172:VAL:HG21	1:G:271:SER:HA	1.99	0.44
1:E:217:THR:HG23	1:E:262:SER:HB2	1.98	0.44
1:A:25:HIS:HD2	1:C:231:GLN:HA	1.79	0.44
1:A:278:LEU:HD22	1:A:279:PRO:HD2	1.99	0.44
1:B:67:GLU:OE2	1:B:141:MET:N	2.51	0.44
1:D:29:TYR:HB2	1:D:285:VAL:HG22	2.00	0.44
1:E:141:MET:HG3	1:E:144:LYS:HB2	1.99	0.44
1:G:274:LEU:HG	1:G:274:LEU:O	2.18	0.44
1:A:11:GLY:O	1:A:12:HIS:HB2	2.16	0.44
1:D:185:ALA:HB3	1:D:232:VAL:CG2	2.42	0.44
1:D:20:ILE:HG22	1:D:256:HIS:NE2	2.33	0.44
1:F:101:GLN:O	1:F:105:GLN:HG3	2.18	0.44
1:B:217:THR:HG23	1:B:262:SER:HB2	2.00	0.44
1:B:42:ALA:HB1	1:B:73:THR:HA	2.00	0.44
1:D:203:GLU:O	1:D:215:HIS:HB3	2.18	0.44
1:H:181:PHE:CE2	1:H:199:VAL:HG22	2.52	0.44
1:D:54:LEU:O	1:H:190:ALA:HB1	2.17	0.44
1:A:34:MET:HE1	1:A:260:ILE:HG22	1.98	0.44
1:B:45:LEU:HD22	1:B:45:LEU:O	2.17	0.44
1:C:11:GLY:HA2	1:C:44:ARG:NH1	2.32	0.44
1:H:153:TYR:CE2	1:H:187:TYR:HD1	2.36	0.44
1:H:73:THR:O	1:H:77:LEU:HB2	2.18	0.44
1:E:92:VAL:HA	1:E:93:PRO:HD3	1.83	0.43
1:F:278:LEU:HA	1:F:278:LEU:HD23	1.79	0.43
1:G:148:ASN:O	1:G:151:ALA:HB3	2.18	0.43
1:G:16:MET:HG2	1:G:18:LEU:HD23	2.00	0.43
1:G:264:SER:HB3	1:G:288:PHE:CD1	2.53	0.43
1:A:101:GLN:O	1:A:105:GLN:CG	2.67	0.43
1:A:152:TYR:CD1	1:A:180:THR:HA	2.53	0.43
1:A:70:ALA:HB3	2:A:401:AA5:HG1	2.00	0.43
1:E:99:GLU:OE1	1:E:297:SER:HB3	2.17	0.43
1:B:235:ASP:O	1:B:236:GLN:HB2	2.18	0.43
1:D:124:ILE:HD11	1:D:143:PHE:CD2	2.53	0.43
1:E:293:GLU:OE2	1:F:294:ARG:HD3	2.18	0.43
1:G:118:GLU:HG2	1:G:125:ARG:HH22	1.83	0.43
1:H:192:ASP:OD2	1:H:194:ALA:HB3	2.17	0.43
1:A:216:ARG:HG2	1:A:246:PHE:CE1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:264:SER:HB3	1:C:288:PHE:CD1	2.54	0.43
1:D:198:VAL:HG13	1:D:236:GLN:HB3	1.99	0.43
1:H:154:HIS:O	1:H:158:PRO:HG2	2.19	0.43
1:C:22:VAL:HG12	1:C:23:PRO:HD2	2.00	0.43
1:F:296:LEU:HA	1:F:296:LEU:HD12	1.75	0.43
1:G:254:ARG:O	1:G:254:ARG:HG2	2.18	0.43
1:H:198:VAL:HG11	1:H:238:LEU:HD12	2.00	0.43
1:C:66:ILE:HD11	1:C:134:ILE:HD12	2.00	0.43
1:D:38:GLY:N	1:D:43:ASP:OD2	2.33	0.43
1:F:192:ASP:OD2	1:F:194:ALA:HB3	2.19	0.43
1:H:115:PRO:HB3	1:H:117:GLU:OE1	2.18	0.43
1:H:287:ILE:O	1:H:289:PRO:HD3	2.17	0.43
1:B:91:VAL:HG11	1:B:126:LYS:HB3	2.00	0.43
1:B:161:LEU:HA	1:B:161:LEU:HD23	1.79	0.43
1:D:207:LEU:HD23	1:D:222:VAL:HG11	2.00	0.43
1:D:235:ASP:O	1:D:236:GLN:HB2	2.19	0.43
1:D:243:ASN:ND2	1:D:243:ASN:N	2.66	0.43
1:E:145:ASN:O	1:E:228:PHE:HE2	2.01	0.43
1:A:25:HIS:CD2	1:C:230:ASP:C	2.92	0.43
1:D:250:ARG:NH1	1:D:303:LYS:HE3	2.34	0.43
1:G:66:ILE:HD11	1:G:134:ILE:HD12	2.00	0.43
1:A:145:ASN:HA	1:A:146:PRO:HD3	1.81	0.43
1:B:103:LEU:HA	1:B:103:LEU:HD12	1.86	0.43
1:C:71:GLY:HA2	1:C:104:MET:CE	2.49	0.43
1:D:72:ASN:ND2	2:D:401:AA5:H2A3	2.34	0.43
1:D:97:SER:OG	1:D:99:GLU:HG2	2.19	0.43
1:E:206:ILE:CD1	1:E:212:ALA:HB2	2.48	0.43
1:E:36:ASN:O	1:E:39:GLY:N	2.44	0.43
1:G:38:GLY:N	1:G:43:ASP:OD2	2.37	0.43
1:A:41:ILE:HD11	1:A:156:LEU:HD11	2.01	0.43
1:B:268:LEU:HD22	1:B:272:LEU:CD1	2.49	0.43
1:B:98:MET:O	1:B:102:VAL:HG23	2.19	0.43
1:C:117:GLU:CD	1:C:117:GLU:H	2.18	0.43
1:E:16:MET:HB2	1:F:3:ILE:CG1	2.48	0.43
1:F:29:TYR:N	1:F:29:TYR:CD1	2.87	0.43
1:B:226:PRO:HG2	1:B:229:PHE:CE2	2.53	0.42
1:B:164:MET:HE2	1:B:285:VAL:HG23	2.00	0.42
1:C:29:TYR:HB2	1:C:285:VAL:HG22	2.00	0.42
1:F:213:HIS:CD2	1:F:214:ALA:O	2.71	0.42
1:F:50:ILE:CD1	1:F:81:THR:HG22	2.48	0.42
1:D:55:GLN:CD	1:H:153:TYR:CD2	2.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:LEU:HD23	1:B:294:ARG:NH1	2.35	0.42
1:B:243:ASN:H	1:B:243:ASN:HD22	1.66	0.42
1:D:15:LEU:HD11	1:D:29:TYR:HB3	2.00	0.42
1:D:91:VAL:HG21	1:D:127:ALA:HB2	2.00	0.42
1:E:101:GLN:HA	1:E:104:MET:CE	2.48	0.42
1:B:141:MET:HG3	1:B:144:LYS:HB2	2.01	0.42
1:C:67:GLU:HG2	1:C:140:PRO:HD2	2.00	0.42
1:C:156:LEU:HD22	1:C:160:ILE:HD11	2.00	0.42
1:D:177:SER:N	2:D:401:AA5:O2P	2.52	0.42
1:E:168:ILE:O	1:E:195:THR:HG23	2.19	0.42
1:F:44:ARG:HH11	1:F:155:THR:HB	1.85	0.42
1:F:67:GLU:CG	1:F:140:PRO:HD2	2.50	0.42
1:G:73:THR:HB	2:G:401:AA5:O1	2.18	0.42
1:C:23:PRO:HB3	1:C:276:THR:HG22	2.01	0.42
1:D:258:LEU:HD23	1:D:258:LEU:HA	1.92	0.42
1:E:149:PRO:CG	1:E:228:PHE:CD2	3.02	0.42
1:E:24:ASN:HB3	1:E:280:ALA:HA	2.02	0.42
1:F:111:ILE:HG22	1:F:112:VAL:N	2.34	0.42
1:F:50:ILE:HD11	1:F:81:THR:HG22	2.02	0.42
1:G:216:ARG:HG2	1:G:246:PHE:CE1	2.54	0.42
1:G:9:LEU:HB2	1:G:37:PRO:HG3	2.02	0.42
1:H:150:ALA:HA	1:H:153:TYR:HB2	2.01	0.42
1:H:92:VAL:HA	1:H:93:PRO:HD3	1.88	0.42
1:A:63:THR:HG22	1:A:64:THR:N	2.34	0.42
1:F:67:GLU:HG3	1:F:140:PRO:HD2	2.00	0.42
1:E:264:SER:OG	1:E:289:PRO:HD2	2.20	0.42
1:F:45:LEU:HB2	1:F:152:TYR:OH	2.19	0.42
1:F:215:HIS:HD2	1:F:217:THR:O	2.02	0.42
1:H:157:ALA:HA	1:H:160:ILE:HD12	2.02	0.42
1:H:99:GLU:OE1	1:H:297:SER:HB3	2.20	0.42
1:H:54:LEU:HD23	1:H:59:VAL:HB	2.01	0.42
1:F:28:ILE:HD13	1:F:271:SER:HB3	2.01	0.42
1:F:91:VAL:HG21	1:F:127:ALA:HA	2.01	0.42
1:G:198:VAL:CG1	1:G:238:LEU:HD12	2.50	0.42
1:H:168:ILE:HG22	1:H:195:THR:HG23	2.01	0.42
1:H:182:ALA:O	1:H:186:ALA:HB2	2.19	0.42
1:A:67:GLU:OE2	1:A:141:MET:N	2.53	0.42
1:A:70:ALA:HB1	1:A:96:PHE:CE2	2.55	0.42
1:B:145:ASN:HA	1:B:146:PRO:HD3	1.90	0.42
1:E:278:LEU:HD22	1:E:279:PRO:CD	2.49	0.42
1:E:51:GLU:HG3	1:E:55:GLN:NE2	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:19:PRO:HD3	1:F:4:GLN:O	2.20	0.42
1:G:51:GLU:HG3	1:G:55:GLN:NE2	2.35	0.42
1:H:99:GLU:CG	1:H:294:ARG:O	2.68	0.42
1:E:11:GLY:O	1:E:12:HIS:HB2	2.19	0.41
1:F:59:VAL:HG12	1:F:60:ASN:N	2.34	0.41
1:G:63:THR:HG22	1:G:64:THR:N	2.34	0.41
1:H:145:ASN:HA	1:H:146:PRO:HD3	1.88	0.41
1:A:72:ASN:ND2	2:A:401:AA5:H2A3	2.35	0.41
1:A:95:LYS:HD3	1:A:116:SER:HB3	2.02	0.41
1:E:172:VAL:HG12	1:E:200:VAL:CG2	2.50	0.41
1:C:215:HIS:HD2	1:C:217:THR:O	2.02	0.41
1:C:99:GLU:OE1	1:C:297:SER:CB	2.69	0.41
1:G:172:VAL:HG12	1:G:200:VAL:CG2	2.50	0.41
1:G:42:ALA:HB1	1:G:73:THR:HA	2.03	0.41
1:H:69:THR:HG21	1:H:74:GLY:CA	2.50	0.41
1:G:40:SER:HA	1:G:289:PRO:O	2.21	0.41
1:H:69:THR:HG21	1:H:74:GLY:HA3	2.02	0.41
1:A:226:PRO:HA	1:A:227:PRO:HD2	1.95	0.41
1:A:243:ASN:ND2	1:A:243:ASN:N	2.56	0.41
1:D:99:GLU:OE1	1:D:297:SER:CB	2.68	0.41
1:F:249:VAL:HG11	1:F:300:ILE:HG12	2.02	0.41
1:G:161:LEU:HA	1:G:161:LEU:HD23	1.89	0.41
1:D:51:GLU:C	1:D:55:GLN:HG3	2.41	0.41
1:E:148:ASN:O	1:E:151:ALA:HB3	2.21	0.41
1:F:286:THR:OG1	1:F:287:ILE:N	2.54	0.41
1:G:248:GLN:OE1	1:G:268:LEU:HD13	2.20	0.41
1:B:63:THR:HG22	1:B:64:THR:N	2.35	0.41
1:C:78:ALA:O	1:C:82:GLN:HB2	2.20	0.41
1:F:172:VAL:O	1:F:286:THR:HA	2.20	0.41
1:F:260:ILE:HB	1:F:264:SER:HB2	2.03	0.41
1:E:99:GLU:CB	1:F:296:LEU:HD23	2.50	0.41
1:H:176:GLY:O	2:H:401:AA5:SD	2.79	0.41
1:H:203:GLU:OE1	1:H:242:ASP:HB2	2.21	0.41
1:H:250:ARG:HH12	1:H:303:LYS:HE3	1.85	0.41
1:A:54:LEU:HA	1:A:54:LEU:HD23	1.90	0.41
1:C:152:TYR:CD1	1:C:180:THR:HA	2.56	0.41
1:E:253:ALA:O	1:F:82:GLN:NE2	2.53	0.41
1:H:185:ALA:HB3	1:H:232:VAL:HG21	2.03	0.41
1:G:250:ARG:NH1	1:G:303:LYS:HE3	2.36	0.41
1:A:63:THR:HA	1:A:136:ASN:OD1	2.21	0.41
1:F:198:VAL:HG11	1:F:238:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:264:SER:HB3	1:F:288:PHE:CD1	2.55	0.41
1:H:54:LEU:HD21	1:H:59:VAL:HG12	2.03	0.41
1:D:153:TYR:CE2	1:H:55:GLN:HG2	2.56	0.41
1:B:120:ILE:HG13	2:B:401:AA5:HE1	2.02	0.41
1:B:54:LEU:HD23	1:B:54:LEU:HA	1.93	0.41
1:D:54:LEU:HD23	1:D:54:LEU:HA	1.91	0.41
1:F:99:GLU:CG	1:F:294:ARG:O	2.68	0.41
1:G:234:ILE:H	1:G:234:ILE:HD12	1.86	0.41
1:H:45:LEU:HD21	1:H:148:ASN:HA	2.02	0.41
1:B:101:GLN:O	1:B:105:GLN:CG	2.68	0.40
1:B:22:VAL:HG11	1:B:28:ILE:HG13	2.03	0.40
1:E:33:GLU:O	1:E:36:ASN:ND2	2.50	0.40
1:E:49:LEU:HA	1:E:49:LEU:HD23	1.72	0.40
1:G:294:ARG:HD3	1:H:293:GLU:OE2	2.21	0.40
1:B:72:ASN:HD22	2:B:401:AA5:H2A3	1.81	0.40
1:C:217:THR:HG23	1:C:262:SER:HB2	2.02	0.40
1:E:124:ILE:HG23	1:E:141:MET:HE1	2.02	0.40
1:H:140:PRO:O	1:H:145:ASN:HB2	2.21	0.40
1:H:240:ILE:HD11	1:H:270:ALA:CA	2.51	0.40
1:H:62:LYS:HD3	1:H:87:ARG:NH2	2.37	0.40
1:A:153:TYR:O	1:A:158:PRO:HD3	2.21	0.40
1:D:254:ARG:HG2	1:D:254:ARG:O	2.21	0.40
1:G:67:GLU:CG	1:G:140:PRO:HD2	2.49	0.40
1:G:278:LEU:HA	1:G:278:LEU:HD23	1.86	0.40
1:H:203:GLU:HG3	1:H:203:GLU:H	1.59	0.40
1:A:215:HIS:ND1	1:A:215:HIS:N	2.69	0.40
1:D:181:PHE:CD2	1:D:199:VAL:HG13	2.56	0.40
1:C:165:PRO:HG3	1:D:2:LEU:HD21	2.03	0.40
1:D:66:ILE:HA	1:D:89:ILE:O	2.22	0.40
1:E:169:THR:HG21	1:E:282:SER:OG	2.22	0.40
1:H:68:PRO:HG3	1:H:124:ILE:HG12	2.03	0.40
1:H:84:HIS:O	1:H:85:HIS:HB2	2.21	0.40
1:C:99:GLU:CB	1:D:296:LEU:HD23	2.52	0.40
1:E:202:PRO:HD2	1:E:221:GLY:HA2	2.04	0.40
1:E:232:VAL:O	1:E:234:ILE:HD12	2.22	0.40
1:E:166:ALA:HB3	1:E:283:HIS:CD2	2.57	0.40
1:F:141:MET:HG3	1:F:141:MET:O	2.22	0.40
1:G:206:ILE:CD1	1:G:212:ALA:HB2	2.46	0.40
1:G:6:VAL:CG2	1:G:37:PRO:HB3	2.50	0.40
1:H:41:ILE:HD11	1:H:156:LEU:CD1	2.52	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:210:GLY:N	1:E:58:ARG:NH2[1_455]	2.11	0.09

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	301/311 (97%)	271 (90%)	26 (9%)	4 (1%)	12	40
1	B	301/311 (97%)	276 (92%)	23 (8%)	2 (1%)	22	54
1	C	301/311 (97%)	278 (92%)	22 (7%)	1 (0%)	41	71
1	D	301/311 (97%)	276 (92%)	25 (8%)	0	100	100
1	E	301/311 (97%)	274 (91%)	24 (8%)	3 (1%)	15	46
1	F	301/311 (97%)	275 (91%)	25 (8%)	1 (0%)	41	71
1	G	301/311 (97%)	271 (90%)	28 (9%)	2 (1%)	22	54
1	H	301/311 (97%)	276 (92%)	24 (8%)	1 (0%)	41	71
All	All	2408/2488 (97%)	2197 (91%)	197 (8%)	14 (1%)	25	57

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	57	GLY
1	B	192	ASP
1	E	97	SER
1	E	192	ASP
1	F	97	SER
1	H	97	SER
1	A	192	ASP
1	A	207	LEU
1	A	281	ASN
1	B	179	GLY

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Mol	Chain	Res	Type
1	C	279	PRO
1	A	210	GLY
1	G	210	GLY
1	G	279	PRO

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	235/243 (97%)	199 (85%)	36 (15%)	2	12
1	B	235/243 (97%)	199 (85%)	36 (15%)	2	12
1	C	235/243 (97%)	198 (84%)	37 (16%)	2	12
1	D	235/243 (97%)	198 (84%)	37 (16%)	2	12
1	E	235/243 (97%)	201 (86%)	34 (14%)	3	14
1	F	235/243 (97%)	201 (86%)	34 (14%)	3	14
1	G	235/243 (97%)	200 (85%)	35 (15%)	3	13
1	H	235/243 (97%)	199 (85%)	36 (15%)	2	12
All	All	1880/1944 (97%)	1595 (85%)	285 (15%)	3	13

All (285) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	VAL
1	A	34	MET
1	A	45	LEU
1	A	58	ARG
1	A	67	GLU
1	A	69	THR
1	A	77	LEU
1	A	87	ARG
1	A	91	VAL
1	A	92	VAL
1	A	98	MET

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Mol	Chain	Res	Type
1	A	103	LEU
1	A	116	SER
1	A	118	GLU
1	A	126	LYS
1	A	133	THR
1	A	155	THR
1	A	156	LEU
1	A	193	SER
1	A	199	VAL
1	A	203	GLU
1	A	205	SER
1	A	206	ILE
1	A	207	LEU
1	A	222	VAL
1	A	225	ILE
1	A	230	ASP
1	A	243	ASN
1	A	252	LEU
1	A	262	SER
1	A	268	LEU
1	A	273	GLN
1	A	277	ASN
1	A	278	LEU
1	A	291	SER
1	A	296	LEU
1	B	22	VAL
1	B	32	LEU
1	B	45	LEU
1	B	49	LEU
1	B	58	ARG
1	B	67	GLU
1	B	87	ARG
1	B	91	VAL
1	B	92	VAL
1	B	95	LYS
1	B	97	SER
1	B	98	MET
1	B	103	LEU
1	B	105	GLN
1	B	111	ILE
1	B	116	SER
1	B	118	GLU

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Mol	Chain	Res	Type
1	B	121	LYS
1	B	133	THR
1	B	153	TYR
1	B	155	THR
1	B	156	LEU
1	B	193	SER
1	B	199	VAL
1	B	203	GLU
1	B	206	ILE
1	B	207	LEU
1	B	222	VAL
1	B	225	ILE
1	B	230	ASP
1	B	259	LEU
1	B	262	SER
1	B	268	LEU
1	B	277	ASN
1	B	282	SER
1	B	296	LEU
1	C	1	MET
1	C	22	VAL
1	C	34	MET
1	C	45	LEU
1	C	49	LEU
1	C	58	ARG
1	C	67	GLU
1	C	87	ARG
1	C	91	VAL
1	C	92	VAL
1	C	95	LYS
1	C	98	MET
1	C	103	LEU
1	C	105	GLN
1	C	111	ILE
1	C	116	SER
1	C	118	GLU
1	C	133	THR
1	C	155	THR
1	C	156	LEU
1	C	195	THR
1	C	199	VAL
1	C	203	GLU

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Mol	Chain	Res	Type
1	C	206	ILE
1	C	207	LEU
1	C	222	VAL
1	C	225	ILE
1	C	230	ASP
1	C	231	GLN
1	C	243	ASN
1	C	259	LEU
1	C	262	SER
1	C	268	LEU
1	C	277	ASN
1	C	282	SER
1	C	296	LEU
1	C	299	LYS
1	D	22	VAL
1	D	34	MET
1	D	45	LEU
1	D	67	GLU
1	D	87	ARG
1	D	91	VAL
1	D	92	VAL
1	D	98	MET
1	D	103	LEU
1	D	116	SER
1	D	118	GLU
1	D	126	LYS
1	D	133	THR
1	D	135	SER
1	D	155	THR
1	D	156	LEU
1	D	195	THR
1	D	199	VAL
1	D	200	VAL
1	D	203	GLU
1	D	205	SER
1	D	206	ILE
1	D	207	LEU
1	D	222	VAL
1	D	225	ILE
1	D	230	ASP
1	D	242	ASP
1	D	243	ASN

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Mol	Chain	Res	Type
1	D	259	LEU
1	D	262	SER
1	D	268	LEU
1	D	277	ASN
1	D	278	LEU
1	D	282	SER
1	D	291	SER
1	D	296	LEU
1	D	299	LYS
1	E	1	MET
1	E	22	VAL
1	E	34	MET
1	E	45	LEU
1	E	58	ARG
1	E	67	GLU
1	E	87	ARG
1	E	92	VAL
1	E	97	SER
1	E	98	MET
1	E	103	LEU
1	E	116	SER
1	E	118	GLU
1	E	126	LYS
1	E	133	THR
1	E	155	THR
1	E	156	LEU
1	E	193	SER
1	E	199	VAL
1	E	203	GLU
1	E	206	ILE
1	E	207	LEU
1	E	222	VAL
1	E	225	ILE
1	E	230	ASP
1	E	259	LEU
1	E	262	SER
1	E	268	LEU
1	E	277	ASN
1	E	278	LEU
1	E	282	SER
1	E	291	SER
1	E	296	LEU

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Mol	Chain	Res	Type
1	E	299	LYS
1	F	22	VAL
1	F	34	MET
1	F	45	LEU
1	F	49	LEU
1	F	67	GLU
1	F	87	ARG
1	F	92	VAL
1	F	98	MET
1	F	99	GLU
1	F	103	LEU
1	F	111	ILE
1	F	114	THR
1	F	116	SER
1	F	118	GLU
1	F	126	LYS
1	F	133	THR
1	F	155	THR
1	F	156	LEU
1	F	193	SER
1	F	199	VAL
1	F	203	GLU
1	F	207	LEU
1	F	222	VAL
1	F	225	ILE
1	F	230	ASP
1	F	252	LEU
1	F	259	LEU
1	F	262	SER
1	F	263	SER
1	F	264	SER
1	F	268	LEU
1	F	277	ASN
1	F	281	ASN
1	F	296	LEU
1	G	22	VAL
1	G	34	MET
1	G	45	LEU
1	G	58	ARG
1	G	67	GLU
1	G	87	ARG
1	G	92	VAL

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Mol	Chain	Res	Type
1	G	95	LYS
1	G	97	SER
1	G	98	MET
1	G	103	LEU
1	G	105	GLN
1	G	111	ILE
1	G	116	SER
1	G	118	GLU
1	G	126	LYS
1	G	133	THR
1	G	155	THR
1	G	156	LEU
1	G	199	VAL
1	G	203	GLU
1	G	206	ILE
1	G	207	LEU
1	G	222	VAL
1	G	225	ILE
1	G	230	ASP
1	G	243	ASN
1	G	259	LEU
1	G	262	SER
1	G	268	LEU
1	G	277	ASN
1	G	282	SER
1	G	291	SER
1	G	296	LEU
1	G	299	LYS
1	H	1	MET
1	H	22	VAL
1	H	34	MET
1	H	45	LEU
1	H	58	ARG
1	H	67	GLU
1	H	87	ARG
1	H	91	VAL
1	H	98	MET
1	H	99	GLU
1	H	103	LEU
1	H	111	ILE
1	H	116	SER
1	H	118	GLU

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Mol	Chain	Res	Type
1	H	126	LYS
1	H	133	THR
1	H	153	TYR
1	H	155	THR
1	H	156	LEU
1	H	199	VAL
1	H	203	GLU
1	H	205	SER
1	H	206	ILE
1	H	207	LEU
1	H	222	VAL
1	H	225	ILE
1	H	228	PHE
1	H	230	ASP
1	H	252	LEU
1	H	262	SER
1	H	263	SER
1	H	268	LEU
1	H	271	SER
1	H	277	ASN
1	H	282	SER
1	H	296	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	213	HIS
1	A	236	GLN
1	A	243	ASN
1	A	298	GLN
1	B	236	GLN
1	B	243	ASN
1	B	298	GLN
1	C	27	HIS
1	C	213	HIS
1	C	215	HIS
1	C	236	GLN
1	C	243	ASN
1	C	283	HIS
1	C	298	GLN
1	D	55	GLN
1	D	213	HIS

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Mol	Chain	Res	Type
1	D	215	HIS
1	D	236	GLN
1	D	243	ASN
1	D	298	GLN
1	E	55	GLN
1	E	213	HIS
1	E	215	HIS
1	E	236	GLN
1	E	243	ASN
1	E	298	GLN
1	F	27	HIS
1	F	213	HIS
1	F	215	HIS
1	F	236	GLN
1	F	243	ASN
1	F	298	GLN
1	G	213	HIS
1	G	215	HIS
1	G	236	GLN
1	G	243	ASN
1	G	298	GLN
1	H	55	GLN
1	H	191	GLN
1	H	213	HIS
1	H	215	HIS
1	H	236	GLN
1	H	243	ASN
1	H	298	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

24 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	AA5	F	401	-	21,24,24	1.39	3 (14%)	25,33,33	1.23	3 (12%)
3	SO4	B	402	-	4,4,4	0.26	0	6,6,6	0.28	0
3	SO4	F	402	-	4,4,4	0.22	0	6,6,6	0.18	0
3	SO4	D	403	-	4,4,4	0.28	0	6,6,6	0.12	0
3	SO4	B	403	-	4,4,4	0.26	0	6,6,6	0.12	0
3	SO4	E	403	-	4,4,4	0.26	0	6,6,6	0.09	0
3	SO4	A	402	-	4,4,4	0.29	0	6,6,6	0.11	0
3	SO4	D	402	-	4,4,4	0.26	0	6,6,6	0.18	0
3	SO4	H	402	-	4,4,4	0.30	0	6,6,6	0.09	0
2	AA5	E	401	-	21,24,24	1.72	5 (23%)	25,33,33	1.22	3 (12%)
2	AA5	G	401	-	21,24,24	1.53	4 (19%)	25,33,33	1.24	3 (12%)
2	AA5	C	401	-	21,24,24	1.39	3 (14%)	25,33,33	1.25	3 (12%)
3	SO4	G	403	-	4,4,4	0.27	0	6,6,6	0.10	0
2	AA5	D	401	-	21,24,24	1.48	4 (19%)	25,33,33	1.18	3 (12%)
3	SO4	C	402	-	4,4,4	0.28	0	6,6,6	0.22	0
3	SO4	G	402	-	4,4,4	0.28	0	6,6,6	0.05	0
2	AA5	B	401	-	21,24,24	1.57	4 (19%)	25,33,33	1.36	3 (12%)
3	SO4	H	403	-	4,4,4	0.28	0	6,6,6	0.07	0
2	AA5	H	401	-	21,24,24	1.79	4 (19%)	25,33,33	1.54	3 (12%)
2	AA5	A	401	-	21,24,24	1.24	3 (14%)	25,33,33	1.11	3 (12%)
3	SO4	C	403	-	4,4,4	0.28	0	6,6,6	0.13	0
3	SO4	A	403	-	4,4,4	0.35	0	6,6,6	0.14	0
3	SO4	F	403	-	4,4,4	0.32	0	6,6,6	0.06	0
3	SO4	E	402	-	4,4,4	0.26	0	6,6,6	0.15	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	AA5	D	401	-	-	2/15/19/19	0/1/1/1
2	AA5	F	401	-	-	1/15/19/19	0/1/1/1
2	AA5	B	401	-	-	4/15/19/19	0/1/1/1
2	AA5	H	401	-	-	2/15/19/19	0/1/1/1
2	AA5	E	401	-	-	2/15/19/19	0/1/1/1
2	AA5	G	401	-	-	3/15/19/19	0/1/1/1
2	AA5	A	401	-	-	3/15/19/19	0/1/1/1
2	AA5	C	401	-	-	2/15/19/19	0/1/1/1

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	401	AA5	C4-C3	4.64	1.47	1.40
2	B	401	AA5	C4-C3	4.32	1.47	1.40
2	E	401	AA5	C4-C3	4.14	1.47	1.40
2	F	401	AA5	C4-C3	4.10	1.47	1.40
2	H	401	AA5	P-O1P	3.59	1.62	1.50
2	G	401	AA5	C4-C5	3.42	1.46	1.42
2	H	401	AA5	CB-CA	3.39	1.57	1.53
2	C	401	AA5	C4-C3	3.35	1.45	1.40
2	G	401	AA5	P-O1P	3.26	1.61	1.50
2	E	401	AA5	CB-CA	3.23	1.57	1.53
2	E	401	AA5	C4-C5	3.18	1.46	1.42
2	D	401	AA5	C4-C3	3.11	1.45	1.40
2	H	401	AA5	C4-C5	2.92	1.45	1.42
2	B	401	AA5	CB-CA	2.82	1.56	1.53
2	D	401	AA5	CB-CA	2.80	1.56	1.53
2	C	401	AA5	C4-C5	2.70	1.45	1.42
2	C	401	AA5	CB-CA	2.57	1.56	1.53
2	G	401	AA5	C4-C3	2.57	1.44	1.40
2	A	401	AA5	C4-C3	2.52	1.44	1.40
2	G	401	AA5	CB-CA	2.51	1.56	1.53
2	D	401	AA5	C4-C5	2.51	1.45	1.42
2	B	401	AA5	C4-C5	2.50	1.45	1.42
2	E	401	AA5	P-O1P	2.46	1.58	1.50
2	A	401	AA5	C4-C5	2.41	1.45	1.42
2	D	401	AA5	P-O1P	2.27	1.57	1.50
2	B	401	AA5	P-O1P	2.23	1.57	1.50
2	A	401	AA5	P-O1P	2.19	1.57	1.50
2	E	401	AA5	C4-C4A	2.17	1.50	1.46
2	F	401	AA5	C3-C2	2.11	1.43	1.40
2	F	401	AA5	P-O1P	2.09	1.57	1.50

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	401	AA5	CA-N-C4A	5.20	124.45	117.40
2	B	401	AA5	CA-N-C4A	3.71	122.43	117.40
2	B	401	AA5	C4-C3-C2	-3.41	118.08	120.19
2	C	401	AA5	CA-N-C4A	3.39	121.99	117.40
2	E	401	AA5	CA-N-C4A	3.37	121.97	117.40
2	G	401	AA5	CA-N-C4A	3.31	121.89	117.40
2	F	401	AA5	C4-C3-C2	-3.17	118.23	120.19
2	F	401	AA5	CA-N-C4A	3.14	121.66	117.40
2	H	401	AA5	C4-C3-C2	-3.06	118.30	120.19
2	D	401	AA5	C4-C3-C2	-2.99	118.34	120.19
2	C	401	AA5	C4-C3-C2	-2.92	118.38	120.19
2	E	401	AA5	C4-C3-C2	-2.83	118.44	120.19
2	D	401	AA5	CA-N-C4A	2.75	121.13	117.40
2	G	401	AA5	C4-C3-C2	-2.56	118.60	120.19
2	H	401	AA5	C6-N1-C2	2.55	123.89	119.17
2	A	401	AA5	C4-C3-C2	-2.46	118.67	120.19
2	A	401	AA5	CA-N-C4A	2.36	120.60	117.40
2	B	401	AA5	C6-N1-C2	2.32	123.46	119.17
2	C	401	AA5	C6-N1-C2	2.27	123.37	119.17
2	A	401	AA5	C6-N1-C2	2.27	123.37	119.17
2	E	401	AA5	C6-N1-C2	2.24	123.33	119.17
2	D	401	AA5	C6-N1-C2	2.17	123.19	119.17
2	G	401	AA5	C6-N1-C2	2.14	123.13	119.17
2	F	401	AA5	C6-N1-C2	2.03	122.92	119.17

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	401	AA5	C-CA-N-C4A
2	E	401	AA5	CB-CA-N-C4A
2	G	401	AA5	C-CA-N-C4A
2	G	401	AA5	CB-CA-N-C4A
2	C	401	AA5	C-CA-N-C4A
2	C	401	AA5	CB-CA-N-C4A
2	D	401	AA5	C-CA-N-C4A
2	D	401	AA5	CB-CA-N-C4A
2	B	401	AA5	C-CA-N-C4A
2	B	401	AA5	CB-CA-N-C4A
2	H	401	AA5	C-CA-N-C4A
2	H	401	AA5	CB-CA-N-C4A

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Mol	Chain	Res	Type	Atoms
2	A	401	AA5	C-CA-N-C4A
2	A	401	AA5	CB-CA-N-C4A
2	B	401	AA5	CA-CB-CG-SD
2	F	401	AA5	CB-CG-SD-CE
2	B	401	AA5	CB-CG-SD-CE
2	A	401	AA5	CB-CG-SD-CE
2	G	401	AA5	CA-CB-CG-SD

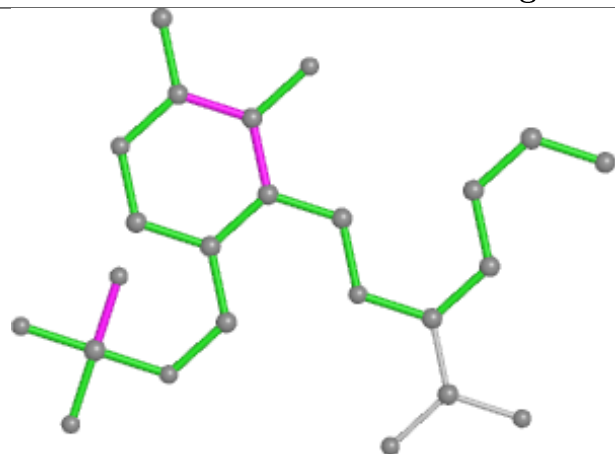
There are no ring outliers.

9 monomers are involved in 27 short contacts:

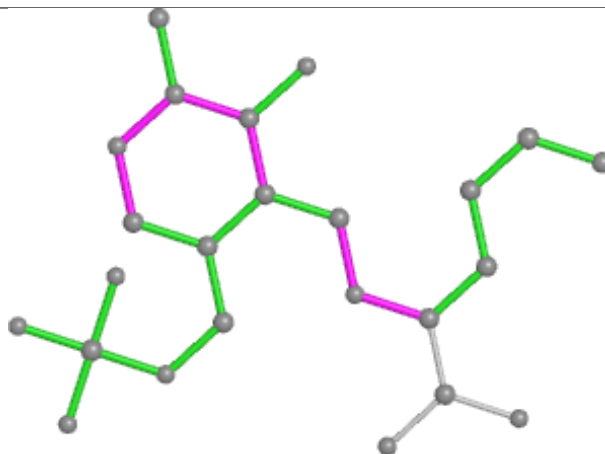
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	401	AA5	2	0
3	B	403	SO4	1	0
2	E	401	AA5	3	0
2	G	401	AA5	2	0
2	C	401	AA5	3	0
2	D	401	AA5	2	0
2	B	401	AA5	5	0
2	H	401	AA5	4	0
2	A	401	AA5	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

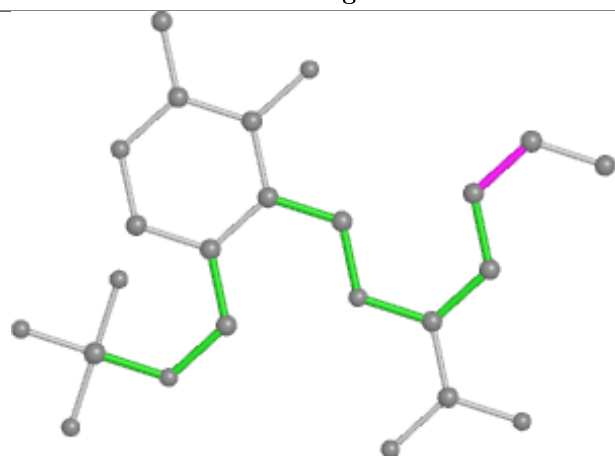
Ligand AA5 F 401



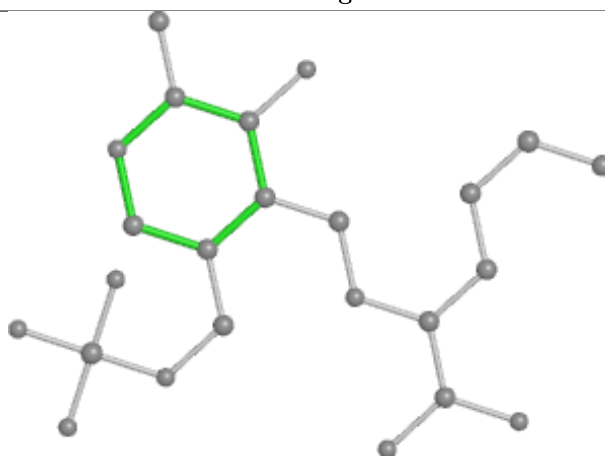
Bond lengths



Bond angles

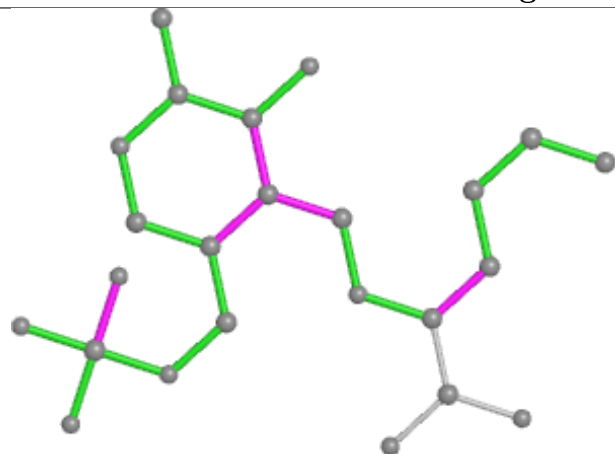


Torsions

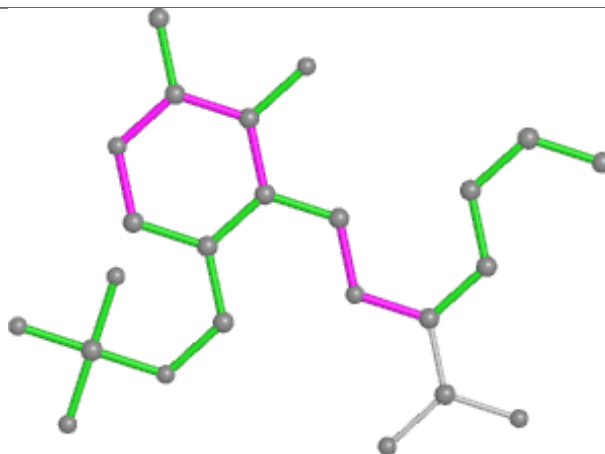


Rings

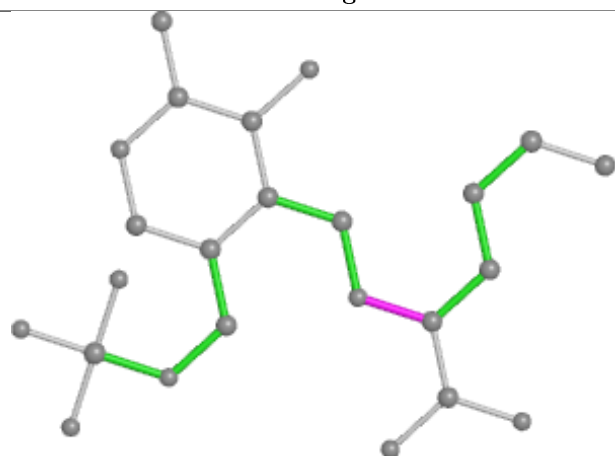
Ligand AA5 E 401



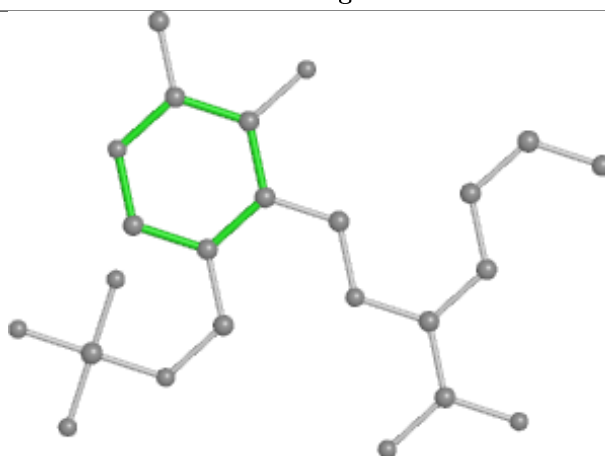
Bond lengths



Bond angles

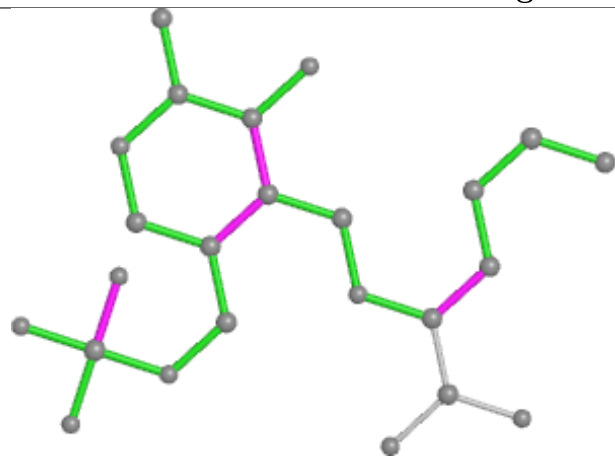


Torsions

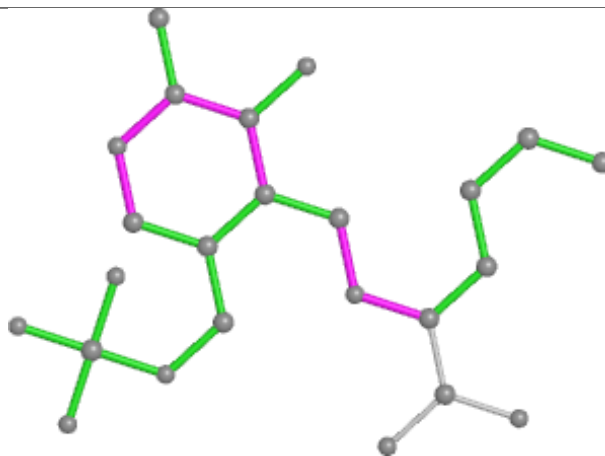


Rings

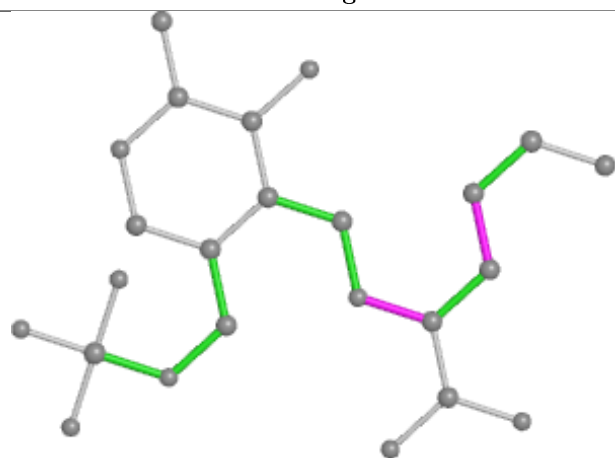
Ligand AA5 G 401



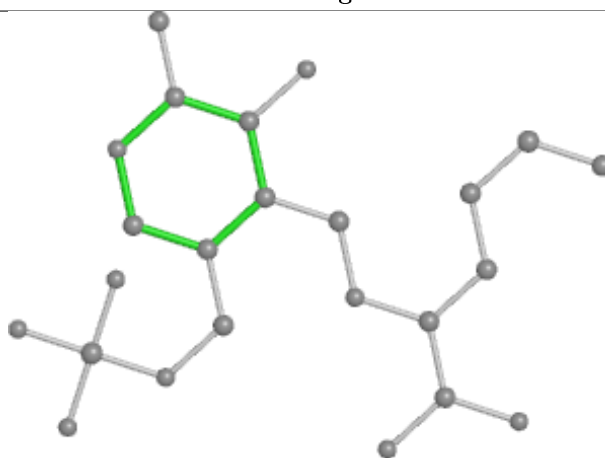
Bond lengths



Bond angles

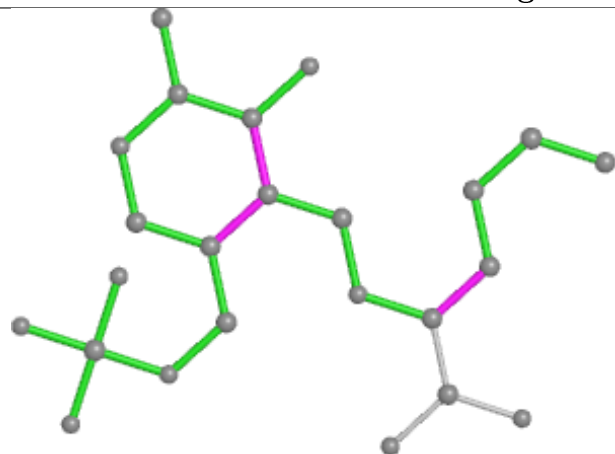


Torsions

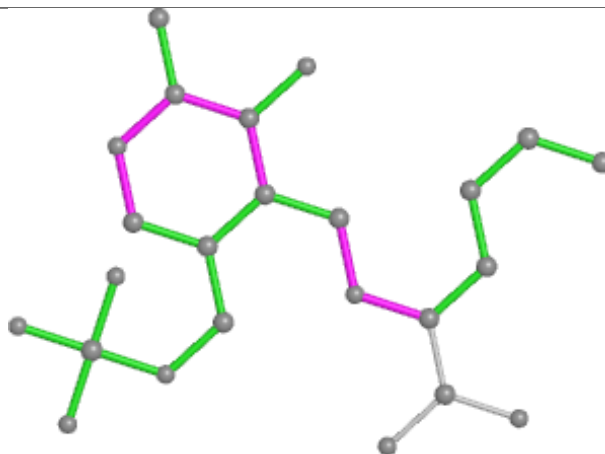


Rings

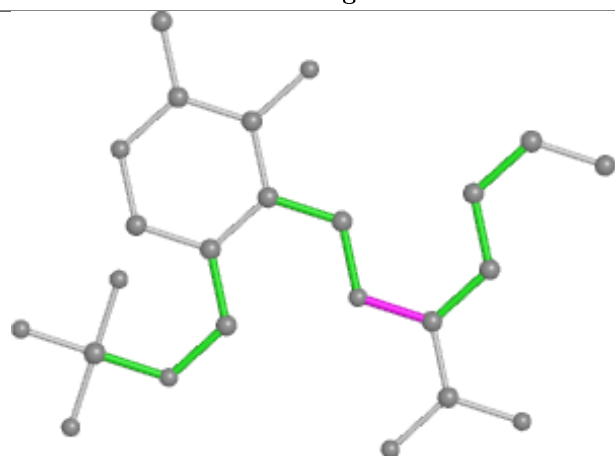
Ligand AA5 C 401



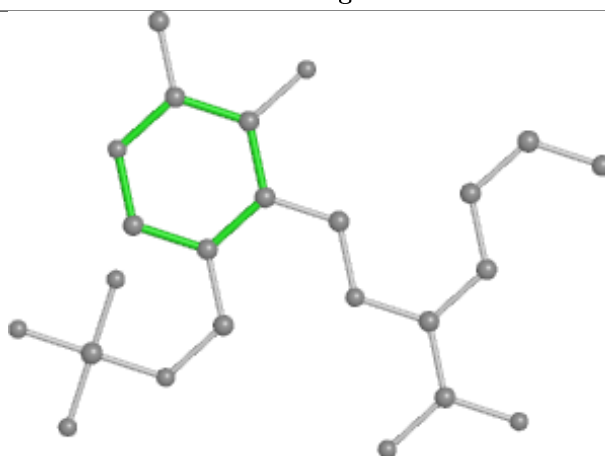
Bond lengths



Bond angles

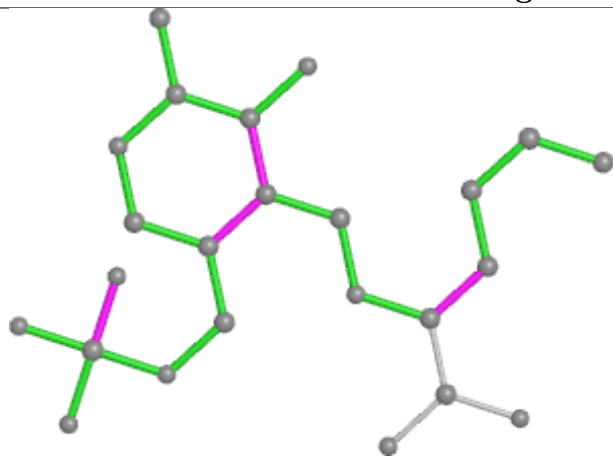


Torsions

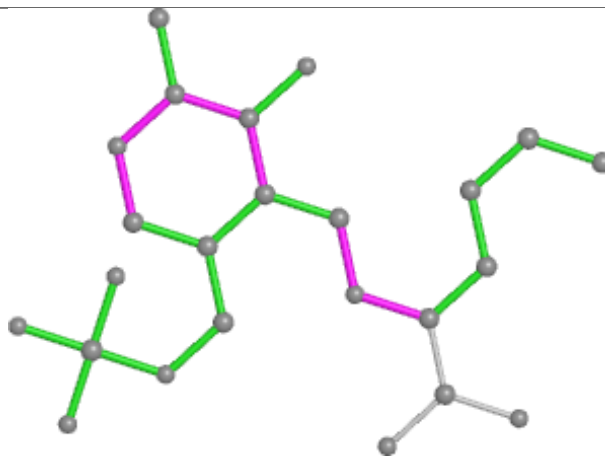


Rings

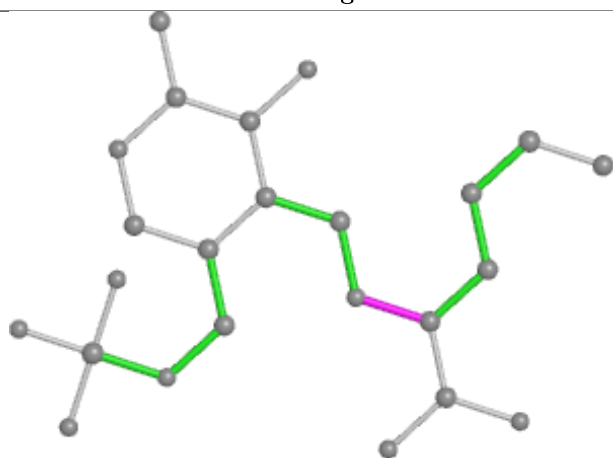
Ligand AA5 D 401



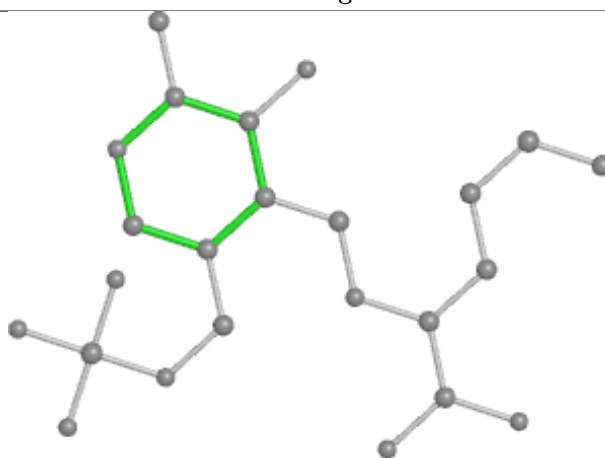
Bond lengths



Bond angles

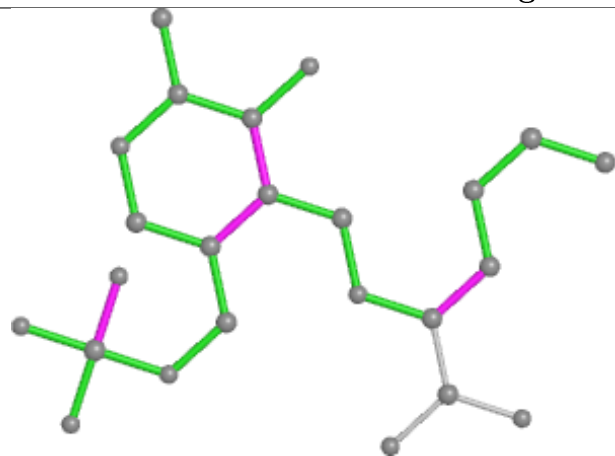


Torsions

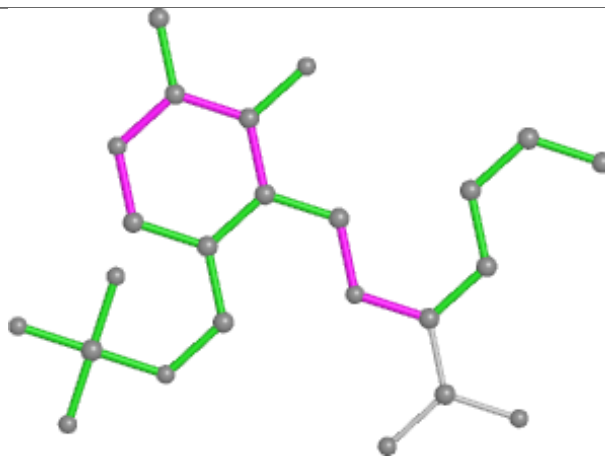


Rings

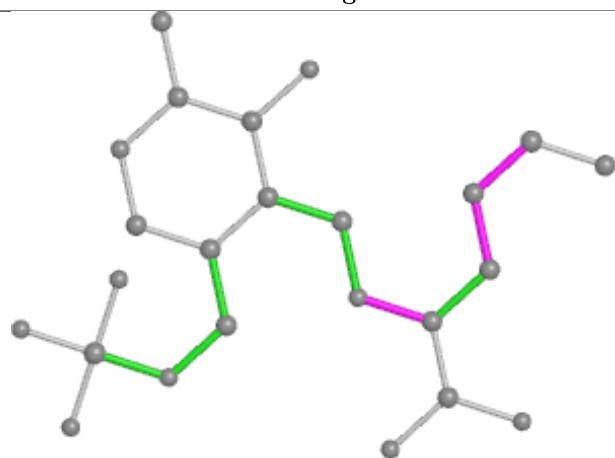
Ligand AA5 B 401



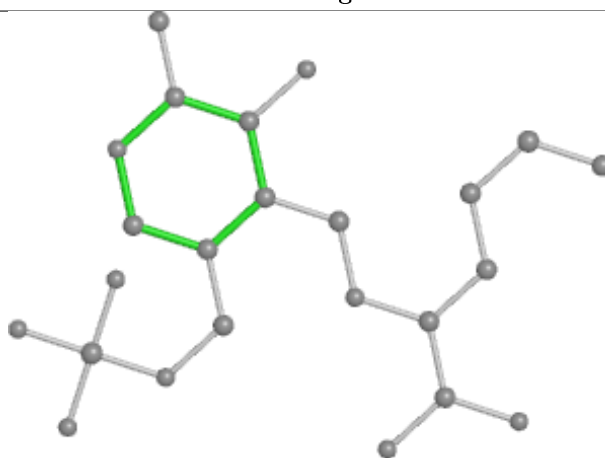
Bond lengths



Bond angles

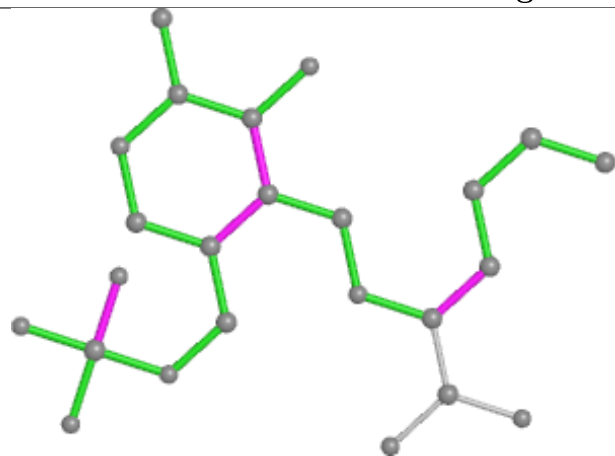


Torsions

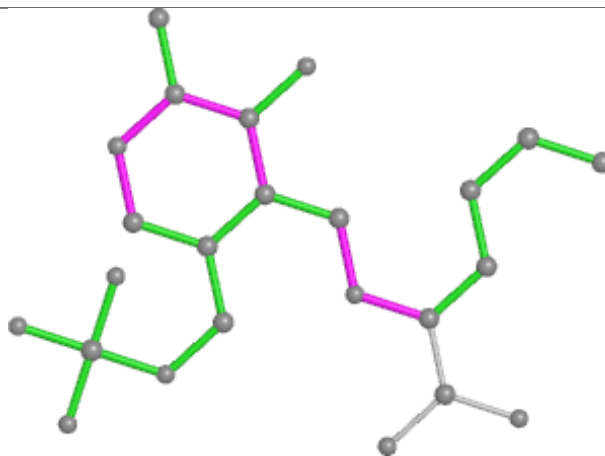


Rings

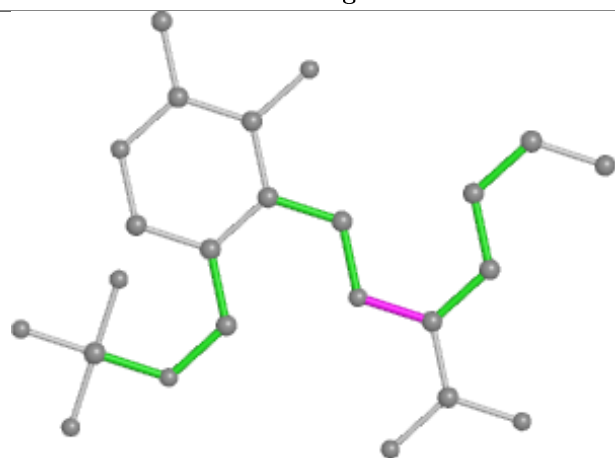
Ligand AA5 H 401



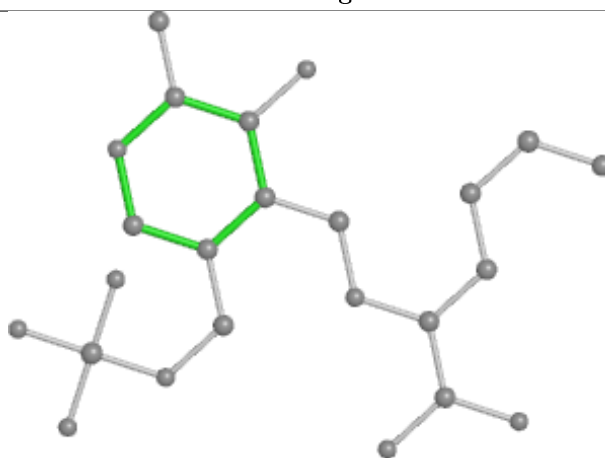
Bond lengths



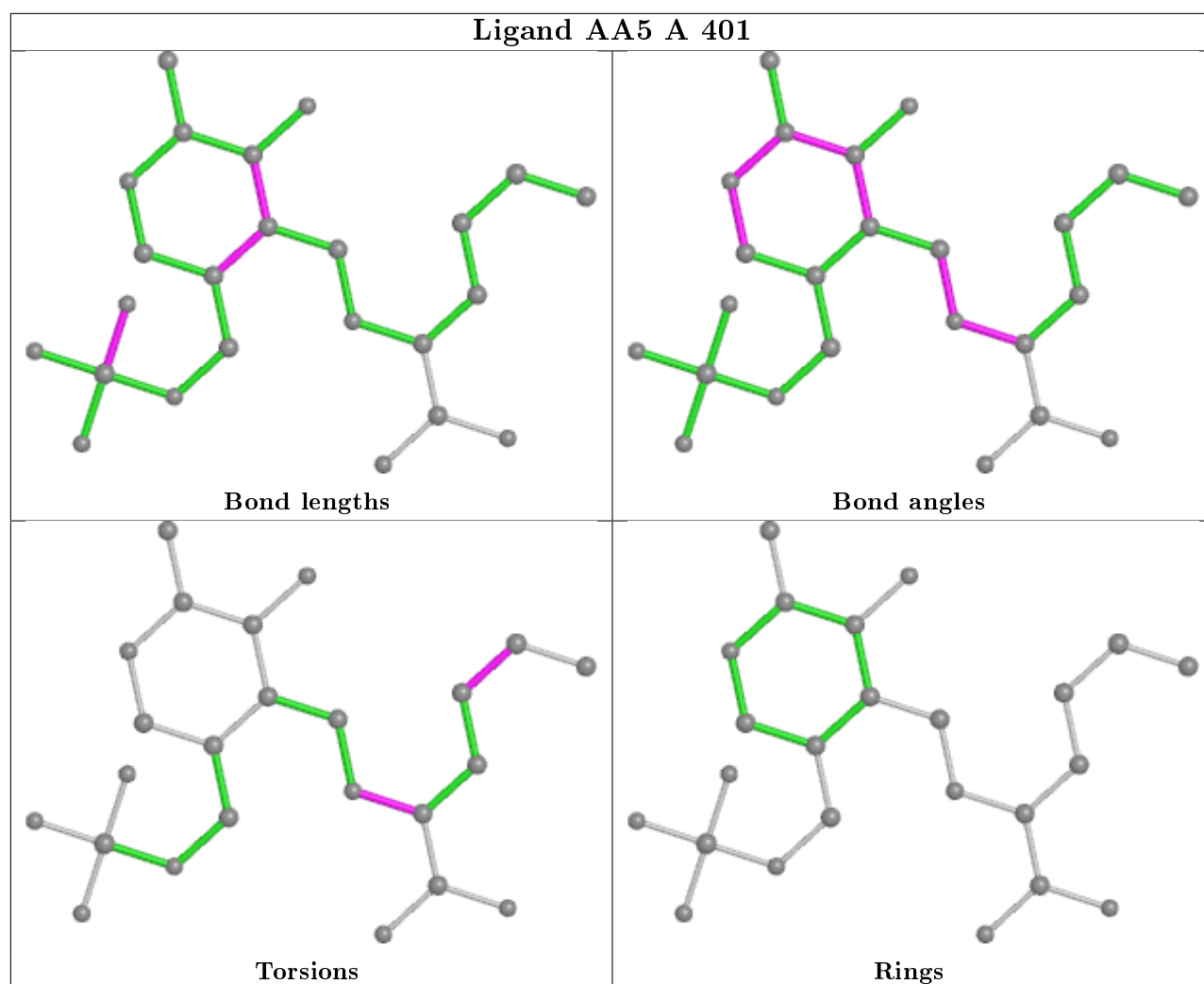
Bond angles



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, 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	303/311 (97%)	0.12	6 (1%) 65 64	14, 44, 65, 71	0
1	B	303/311 (97%)	-0.24	0 100 100	11, 26, 49, 63	0
1	C	303/311 (97%)	-0.30	0 100 100	7, 26, 47, 62	0
1	D	303/311 (97%)	-0.16	6 (1%) 65 64	16, 33, 54, 64	0
1	E	303/311 (97%)	0.11	3 (0%) 82 82	19, 45, 66, 75	0
1	F	303/311 (97%)	-0.08	3 (0%) 82 82	14, 31, 50, 63	0
1	G	303/311 (97%)	0.26	7 (2%) 60 59	24, 54, 83, 94	0
1	H	303/311 (97%)	1.65	107 (35%) 0 0	46, 93, 114, 118	0
All	All	2424/2488 (97%)	0.17	132 (5%) 25 24	7, 39, 99, 118	0

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	221	GLY	7.5
1	H	88	THR	6.0
1	H	109	ALA	5.6
1	H	193	SER	5.3
1	H	125	ARG	4.7
1	H	268	LEU	4.7
1	G	212	ALA	4.6
1	H	86	LEU	4.3
1	H	192	ASP	4.3
1	H	127	ALA	4.2
1	H	195	THR	4.2
1	H	232	VAL	4.2
1	H	111	ILE	4.1
1	H	212	ALA	4.1
1	H	24	ASN	4.0
1	H	243	ASN	3.9

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Mol	Chain	Res	Type	RSRZ
1	H	169	THR	3.9
1	H	113	HIS	3.9
1	H	120	ILE	3.9
1	G	214	ALA	3.8
1	H	68	PRO	3.8
1	H	73	THR	3.8
1	H	276	THR	3.7
1	H	89	ILE	3.7
1	H	215	HIS	3.7
1	H	222	VAL	3.6
1	H	281	ASN	3.6
1	H	191	GLN	3.6
1	H	280	ALA	3.6
1	H	65	ILE	3.5
1	H	217	THR	3.5
1	H	134	ILE	3.5
1	H	244	ASP	3.5
1	H	204	GLY	3.4
1	D	135	SER	3.4
1	H	95	LYS	3.4
1	H	124	ILE	3.3
1	H	26	SER	3.2
1	H	59	VAL	3.2
1	H	166	ALA	3.2
1	H	216	ARG	3.2
1	H	142	GLN	3.1
1	H	87	ARG	3.1
1	H	239	THR	3.1
1	H	225	ILE	3.1
1	H	132	ALA	3.1
1	H	236	GLN	3.0
1	H	165	PRO	3.0
1	H	240	ILE	3.0
1	A	225	ILE	3.0
1	H	245	ALA	2.9
1	A	212	ALA	2.9
1	H	93	PRO	2.9
1	G	211	PRO	2.9
1	H	90	LEU	2.9
1	H	19	PRO	2.8
1	H	271	SER	2.8
1	H	218	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	H	131	ALA	2.8
1	H	63	THR	2.8
1	E	211	PRO	2.8
1	H	77	LEU	2.7
1	H	144	LYS	2.7
1	H	22	VAL	2.7
1	H	213	HIS	2.7
1	H	128	GLU	2.7
1	H	129	ALA	2.6
1	H	25	HIS	2.6
1	H	92	VAL	2.6
1	H	153	TYR	2.6
1	H	188	LEU	2.6
1	H	101	GLN	2.6
1	H	171	PHE	2.6
1	H	196	LYS	2.5
1	H	116	SER	2.5
1	D	277	ASN	2.5
1	H	91	VAL	2.5
1	H	214	ALA	2.5
1	H	207	LEU	2.5
1	E	154	HIS	2.4
1	H	272	LEU	2.4
1	H	133	THR	2.4
1	H	228	PHE	2.4
1	H	231	GLN	2.4
1	H	118	GLU	2.4
1	H	23	PRO	2.4
1	H	154	HIS	2.4
1	H	69	THR	2.4
1	G	299	LYS	2.3
1	H	110	GLU	2.3
1	H	247	ALA	2.3
1	H	21	GLU	2.3
1	H	146	PRO	2.3
1	F	25	HIS	2.3
1	H	64	THR	2.3
1	H	274	LEU	2.2
1	G	300	ILE	2.2
1	A	227	PRO	2.2
1	D	23	PRO	2.2
1	H	60	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	202	PRO	2.2
1	H	72	ASN	2.2
1	H	219	GLY	2.2
1	H	66	ILE	2.2
1	H	229	PHE	2.1
1	H	104	MET	2.1
1	A	209	GLY	2.1
1	H	301	TYR	2.1
1	H	97	SER	2.1
1	H	230	ASP	2.1
1	D	24	ASN	2.1
1	E	170	ALA	2.1
1	H	220	ILE	2.1
1	F	209	GLY	2.1
1	H	52	ASP	2.1
1	A	232	VAL	2.1
1	H	136	ASN	2.1
1	H	277	ASN	2.1
1	H	138	TYR	2.1
1	H	203	GLU	2.1
1	F	212	ALA	2.1
1	H	194	ALA	2.1
1	D	84	HIS	2.1
1	H	112	VAL	2.1
1	G	203	GLU	2.0
1	H	226	PRO	2.0
1	H	224	PHE	2.0
1	A	229	PHE	2.0
1	H	238	LEU	2.0
1	D	281	ASN	2.0
1	G	217	THR	2.0
1	H	237	THR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

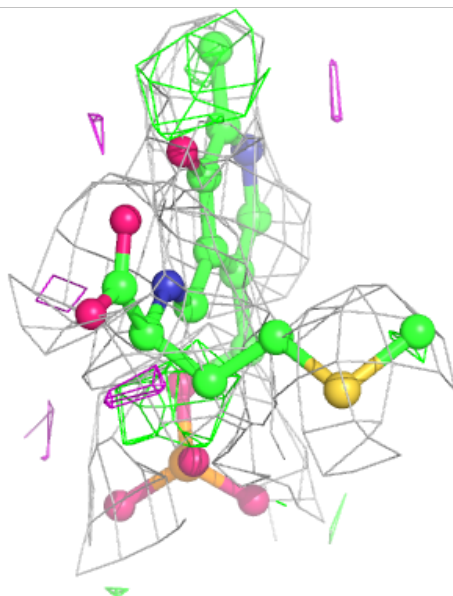
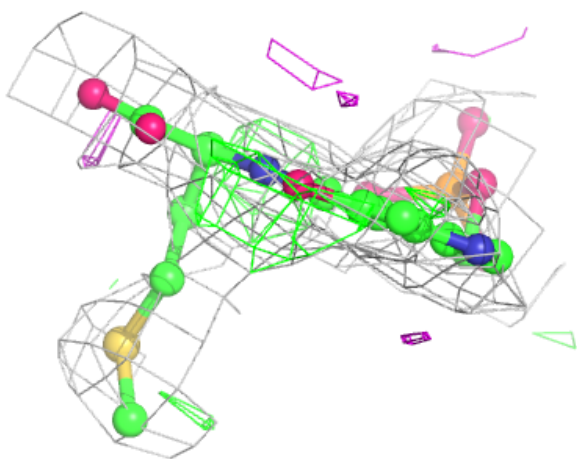
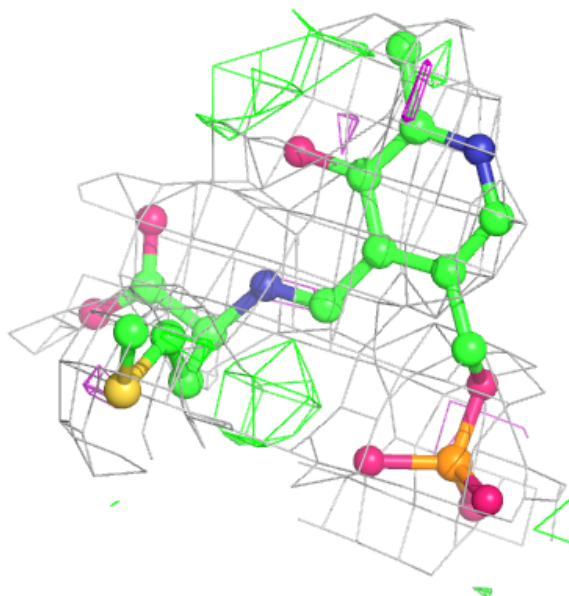
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	H	403	5/5	0.67	0.37	145,146,146,146	0
3	SO4	G	403	5/5	0.74	0.24	105,106,106,107	0
2	AA5	H	401	24/24	0.74	0.32	85,87,88,89	0
3	SO4	A	403	5/5	0.85	0.25	85,85,86,87	0
3	SO4	G	402	5/5	0.86	0.29	121,121,121,121	0
3	SO4	H	402	5/5	0.89	0.30	103,104,104,104	0
3	SO4	D	403	5/5	0.90	0.20	75,75,76,76	0
3	SO4	F	403	5/5	0.90	0.24	86,86,87,87	0
3	SO4	E	403	5/5	0.91	0.19	88,88,89,89	0
2	AA5	E	401	24/24	0.91	0.26	45,53,57,57	0
3	SO4	E	402	5/5	0.91	0.17	78,78,79,79	0
3	SO4	C	403	5/5	0.93	0.17	69,69,70,70	0
3	SO4	B	403	5/5	0.93	0.21	68,68,69,69	0
2	AA5	G	401	24/24	0.94	0.20	45,47,48,49	0
2	AA5	A	401	24/24	0.94	0.22	39,42,49,53	0
3	SO4	B	402	5/5	0.94	0.21	63,64,64,64	0
2	AA5	F	401	24/24	0.95	0.17	18,23,27,29	0
3	SO4	A	402	5/5	0.95	0.13	62,63,63,64	0
3	SO4	C	402	5/5	0.96	0.16	59,60,61,61	0
3	SO4	F	402	5/5	0.96	0.13	61,62,63,64	0
2	AA5	B	401	24/24	0.96	0.16	6,17,21,25	0
3	SO4	D	402	5/5	0.96	0.16	65,66,66,67	0
2	AA5	D	401	24/24	0.96	0.17	25,30,31,33	0
2	AA5	C	401	24/24	0.97	0.15	16,21,24,25	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.

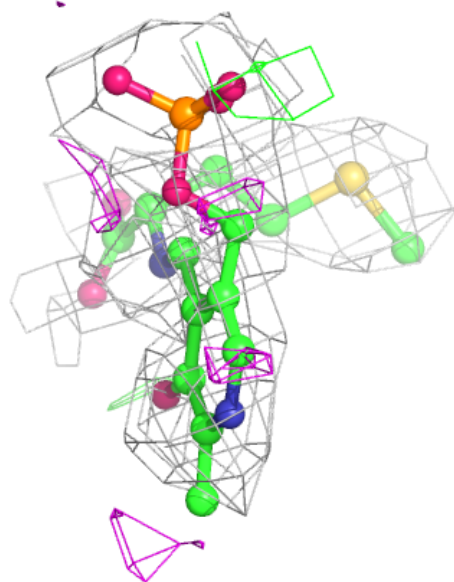
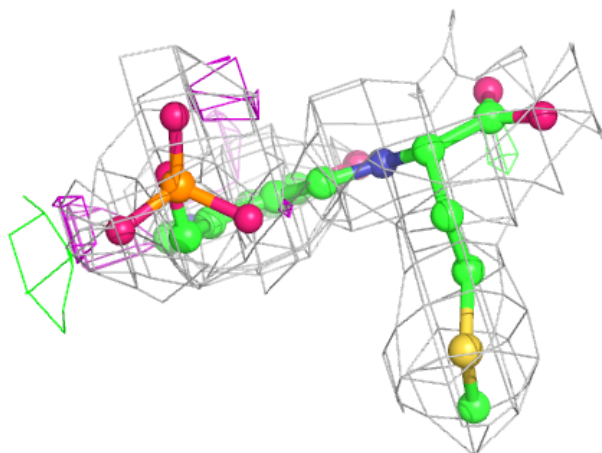
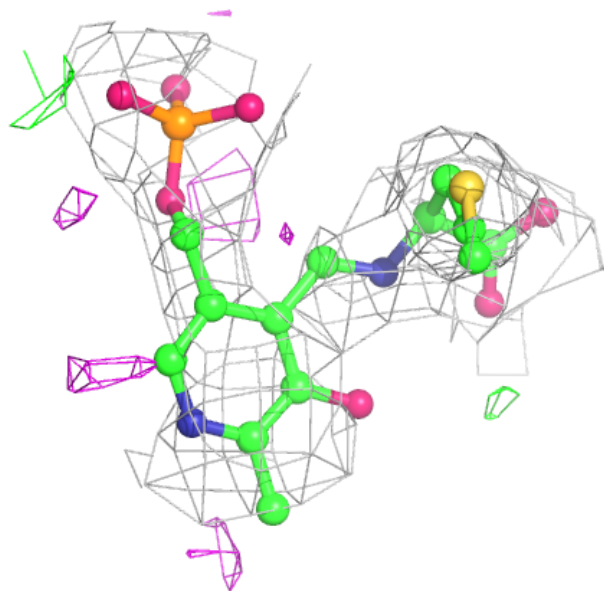
Electron density around AA5 H 401:

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



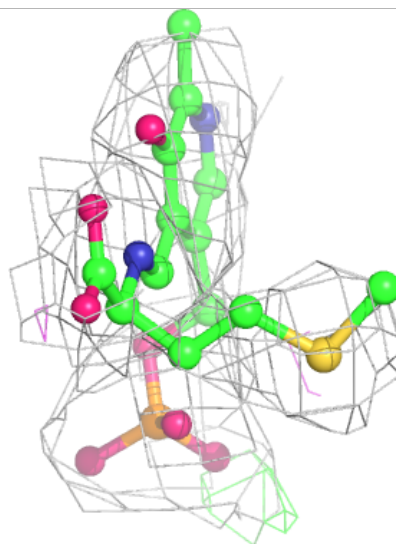
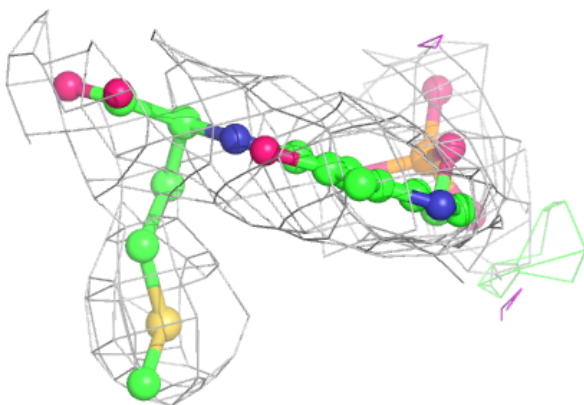
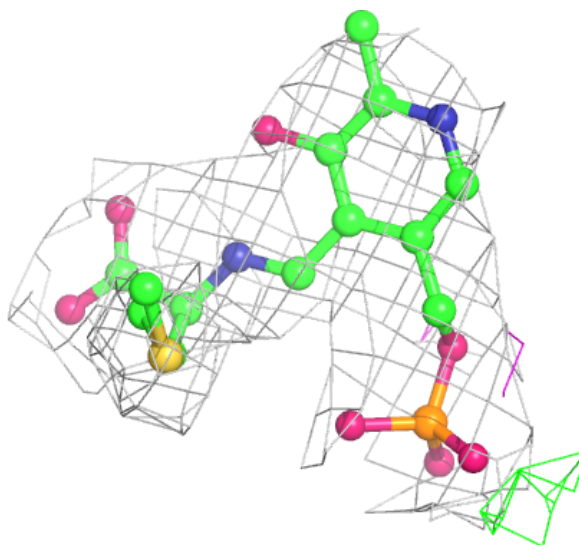
Electron density around AA5 E 401:

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



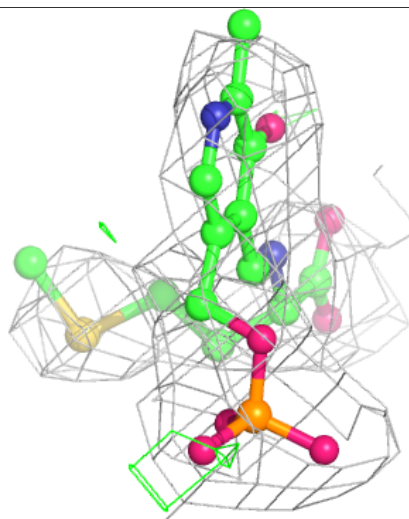
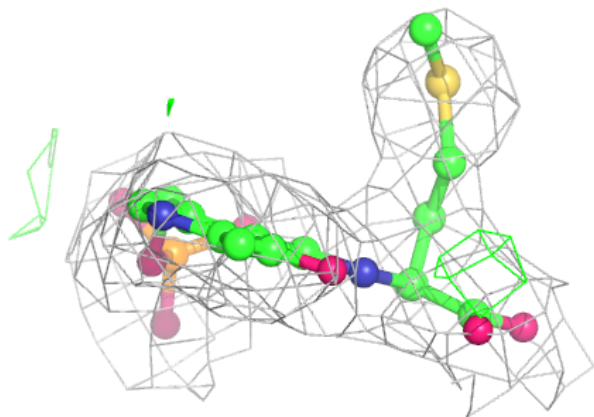
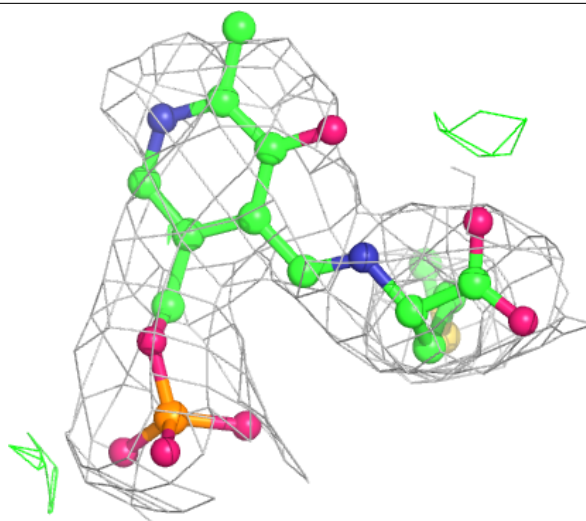
Electron density around AA5 G 401:

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



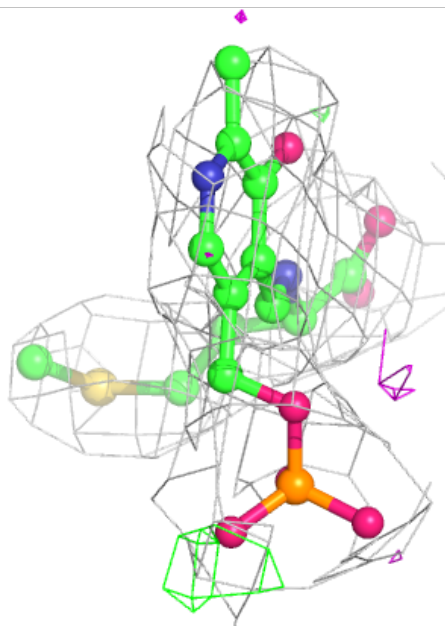
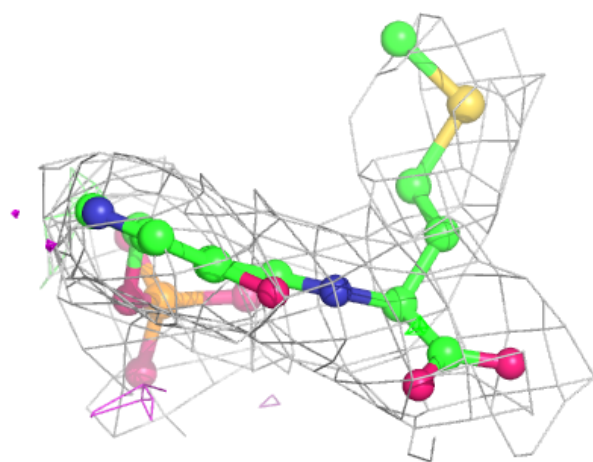
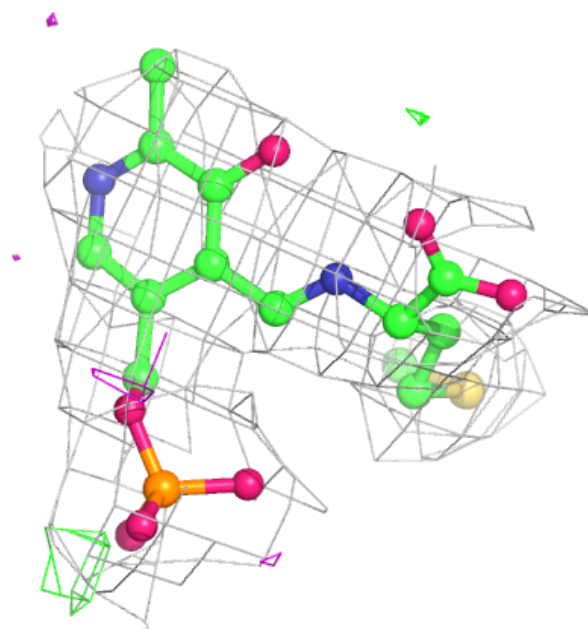
Electron density around AA5 A 401:

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



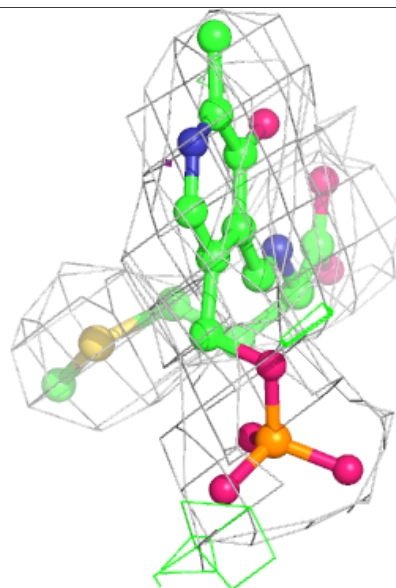
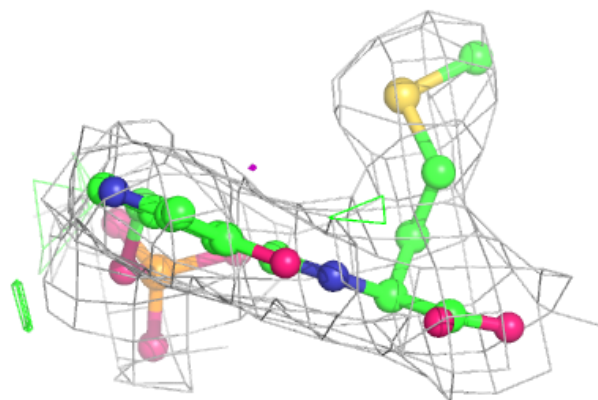
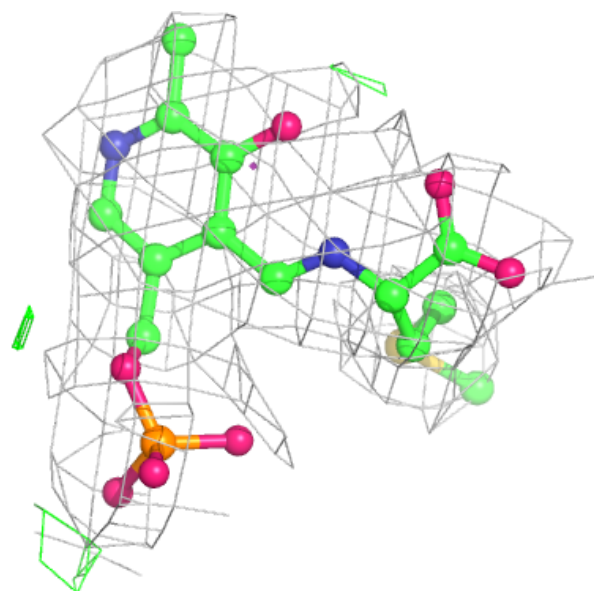
Electron density around AA5 F 401:

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



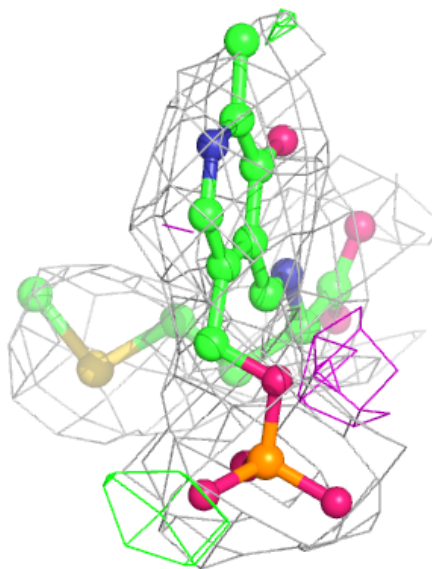
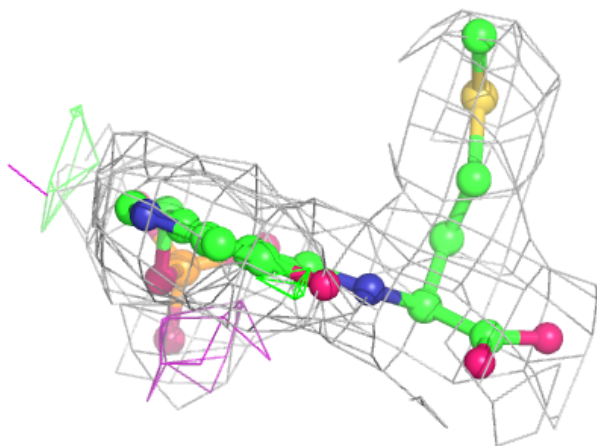
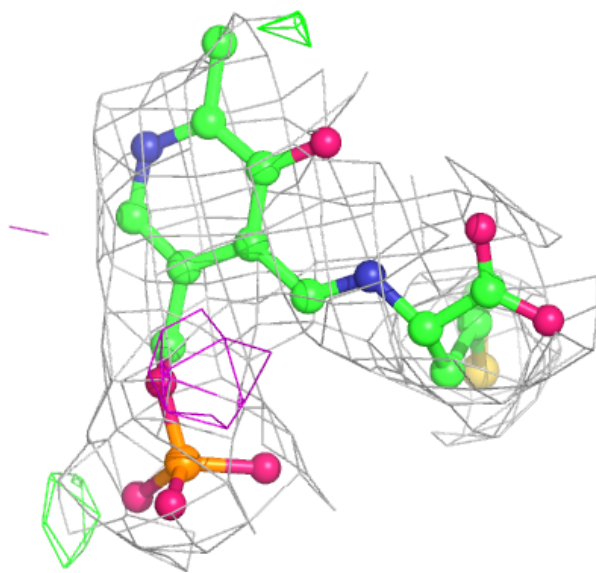
Electron density around AA5 B 401:

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



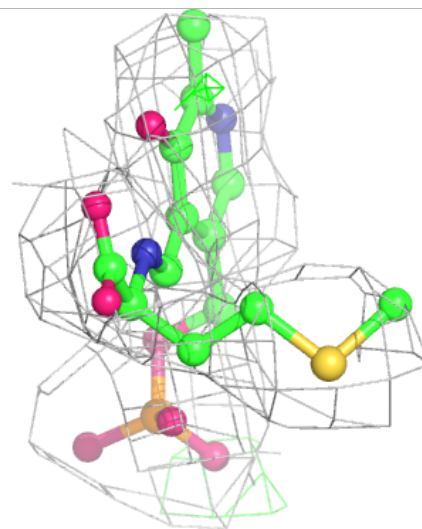
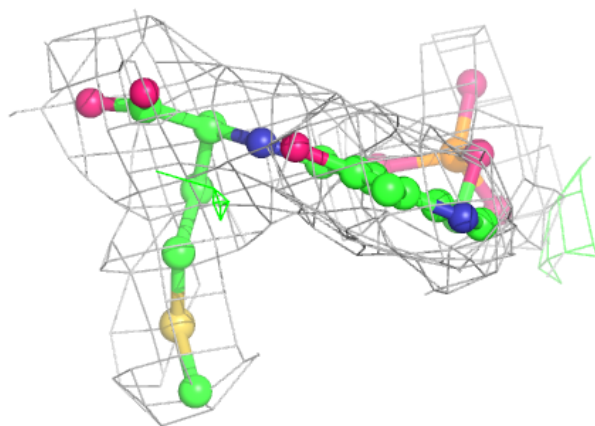
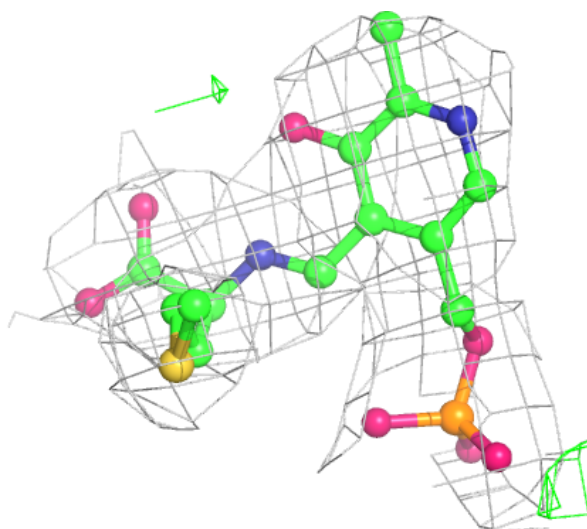
Electron density around AA5 D 401:

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



Electron density around AA5 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.