



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:51 PM UTC

PDB ID : 5B1I / pdb_00005b1i
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

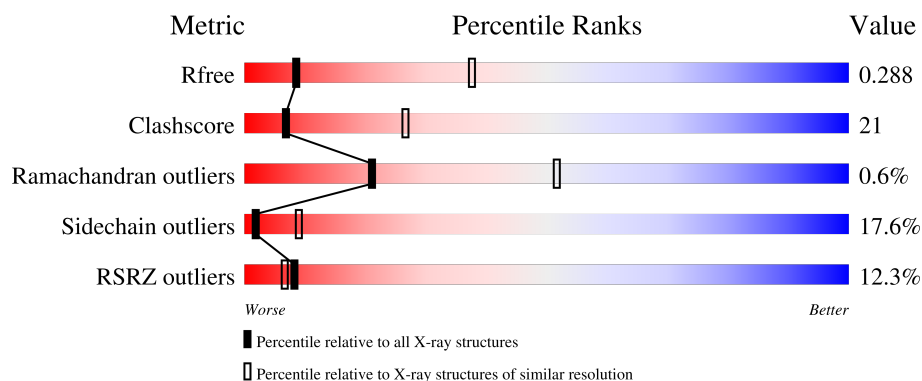
1 Overall quality at a glance

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}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	311	3% 51% 37% 9%
1	B	311	2% 56% 32% 8%
1	C	311	0% 56% 35% 5%
1	D	311	2% 51% 40% 6%
1	E	311	3% 50% 38% 8%

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Mol	Chain	Length	Quality of chain
1	F	311	% 53% 36% 8%
1	G	311	7% 50% 39% 9%
1	H	311	77% 46% 44% 7%

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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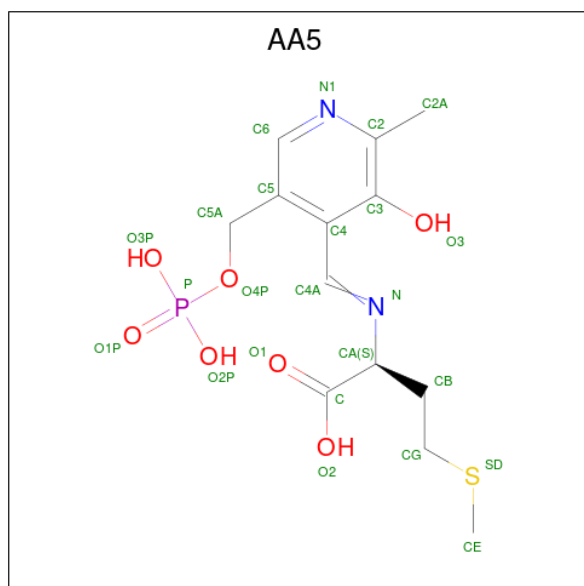
Chain	Residue	Modelled	Actual	Comment	Reference
B	307	HIS	-	expression tag	UNP F9UT54
B	308	HIS	-	expression tag	UNP F9UT54
B	309	HIS	-	expression tag	UNP F9UT54
B	310	HIS	-	expression tag	UNP F9UT54
B	311	HIS	-	expression tag	UNP F9UT54
C	42	ALA	LYS	engineered mutation	UNP F9UT54
C	304	LEU	-	expression 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 (CCD ID: AA5) (formula: C₁₃H₁₉N₂O₇PS).



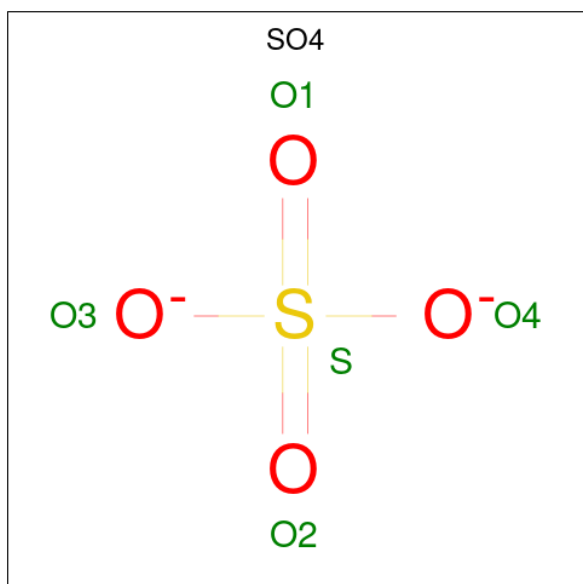
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			24	13	2	7	1	1		
2	B	1	Total	C	N	O	P	S	0	0
			24	13	2	7	1	1		

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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 (CCD ID: 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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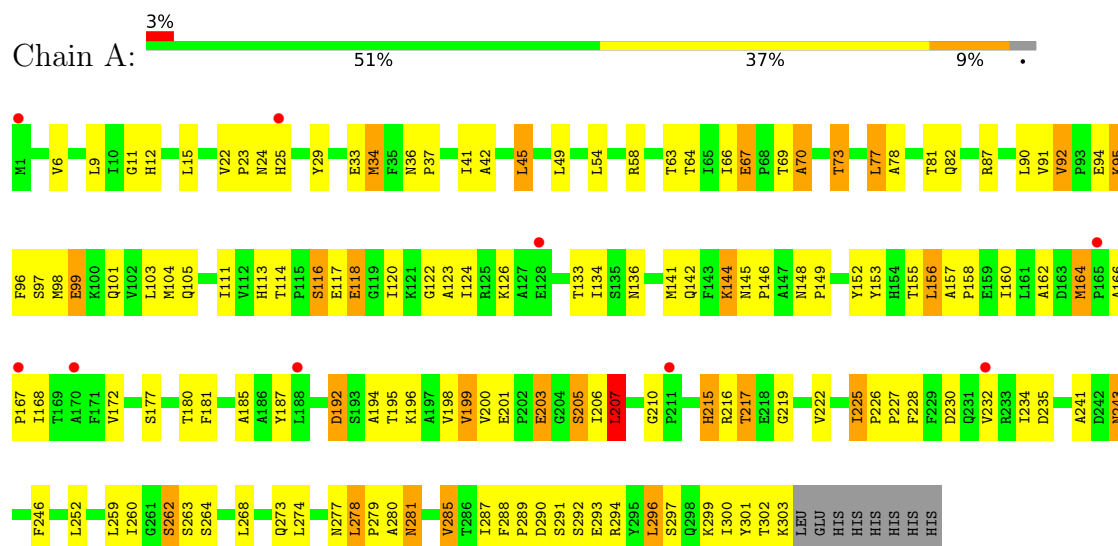
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			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		

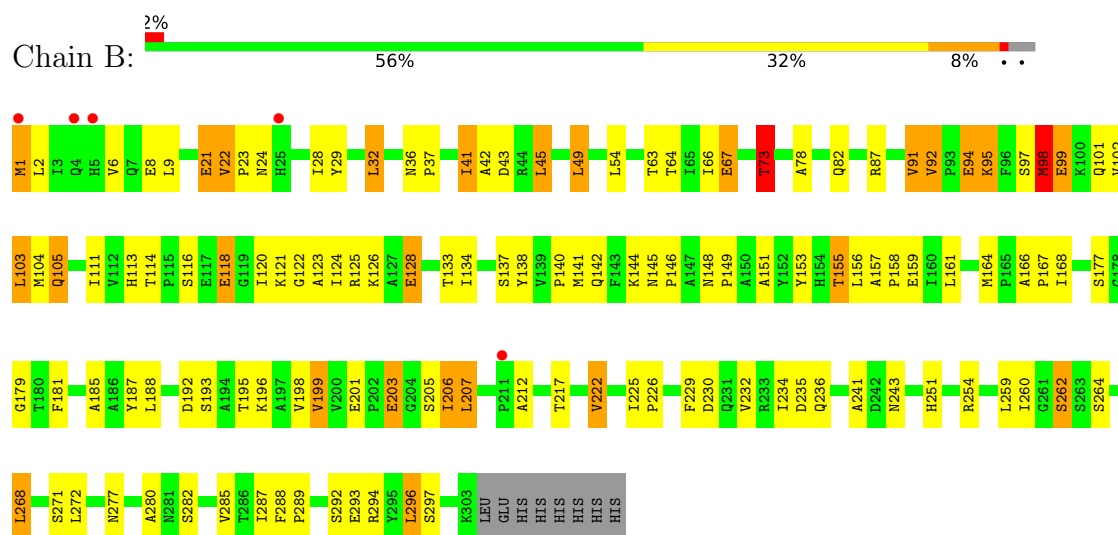
3 Residue-property plots [i](#)

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: Cystathionine beta-synthase

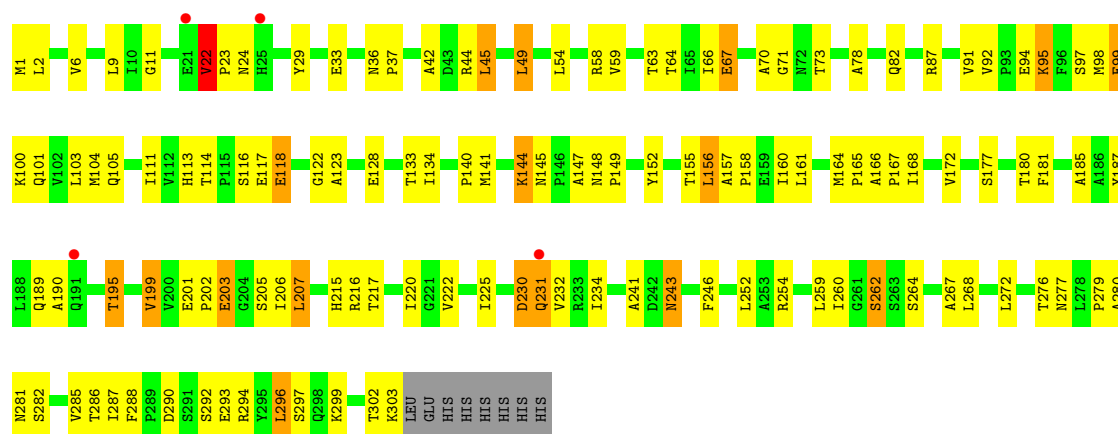


• Molecule 1: Cystathionine beta-synthase

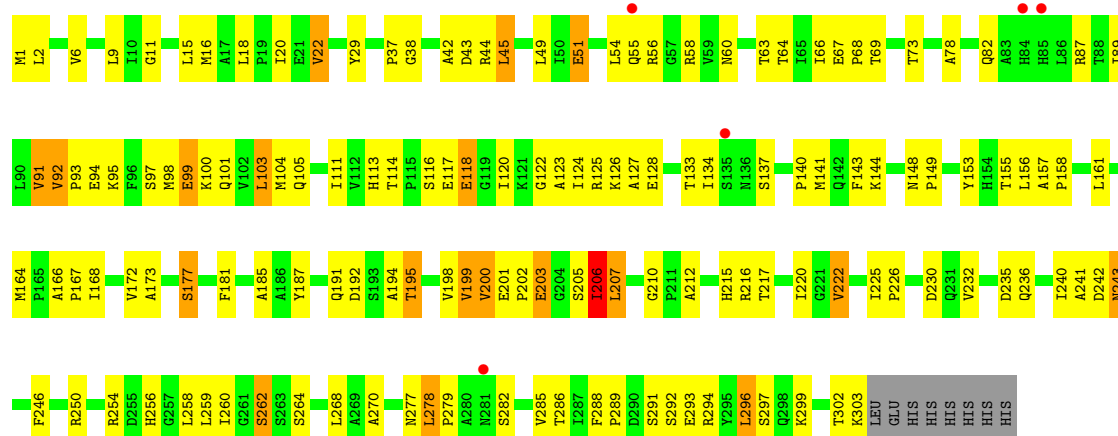


• Molecule 1: Cystathionine beta-synthase

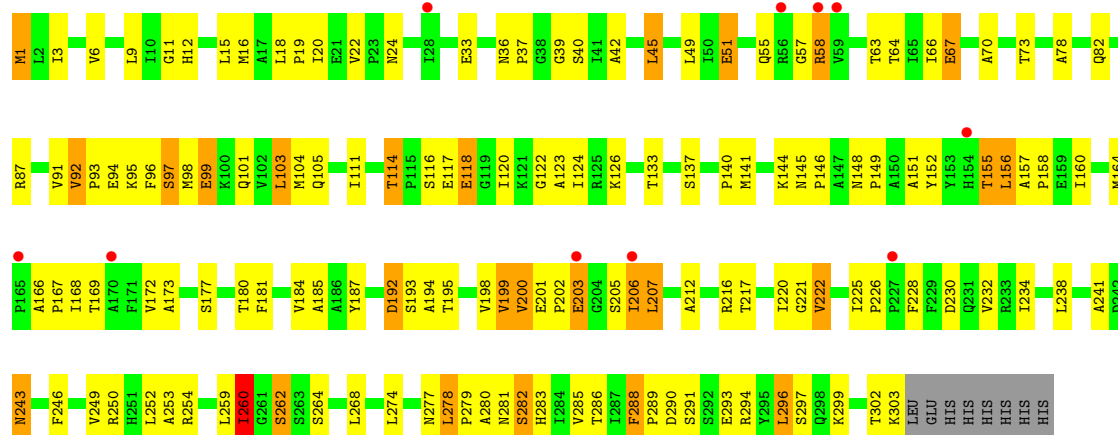




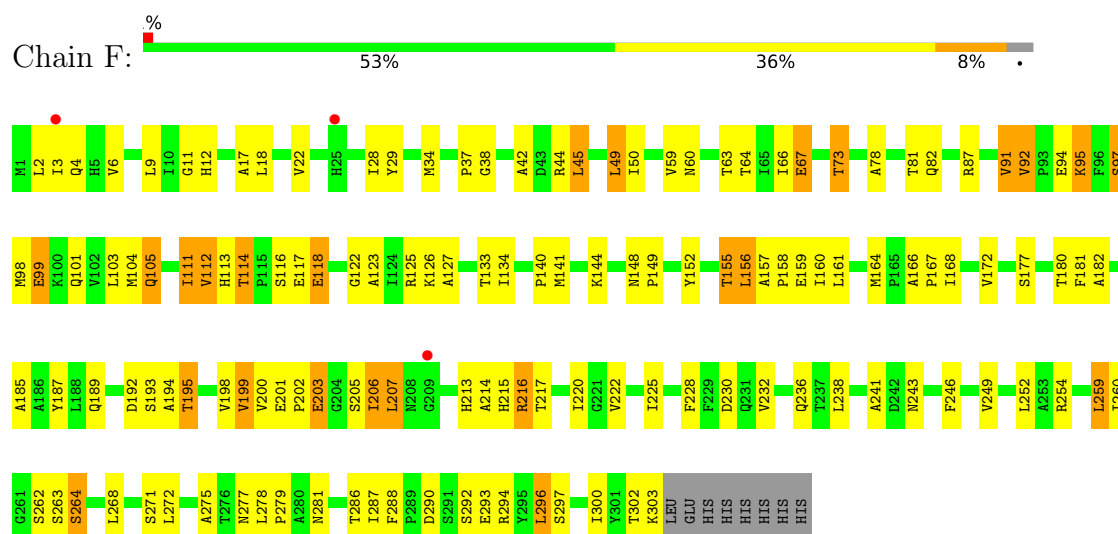
• Molecule 1: Cystathionine beta-synthase



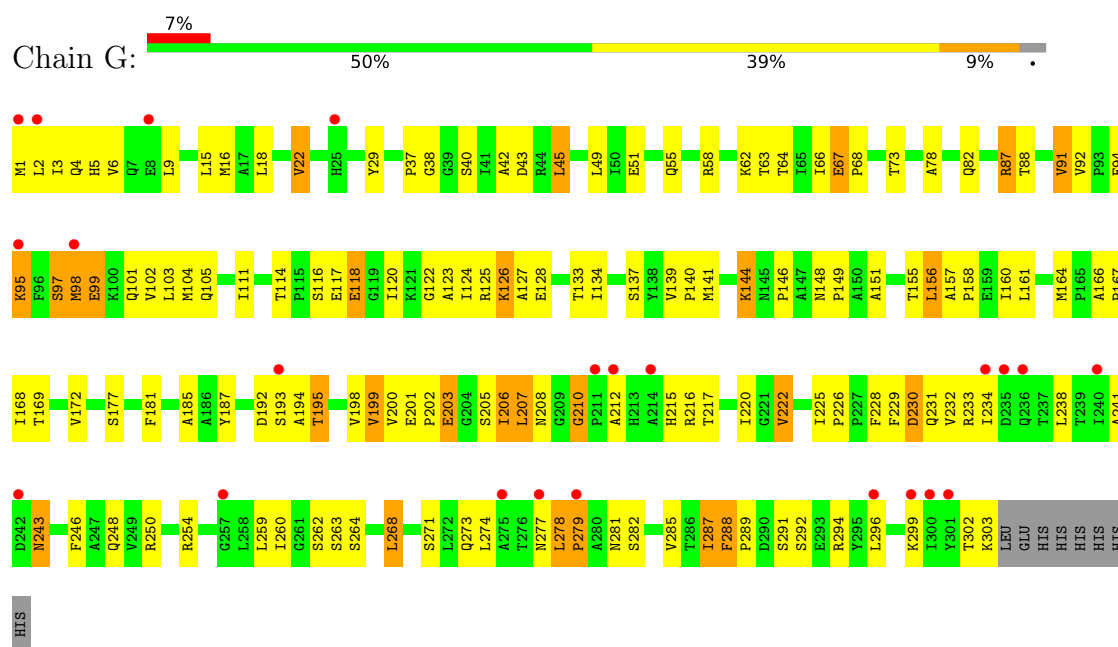
• Molecule 1: Cystathionine beta-synthase



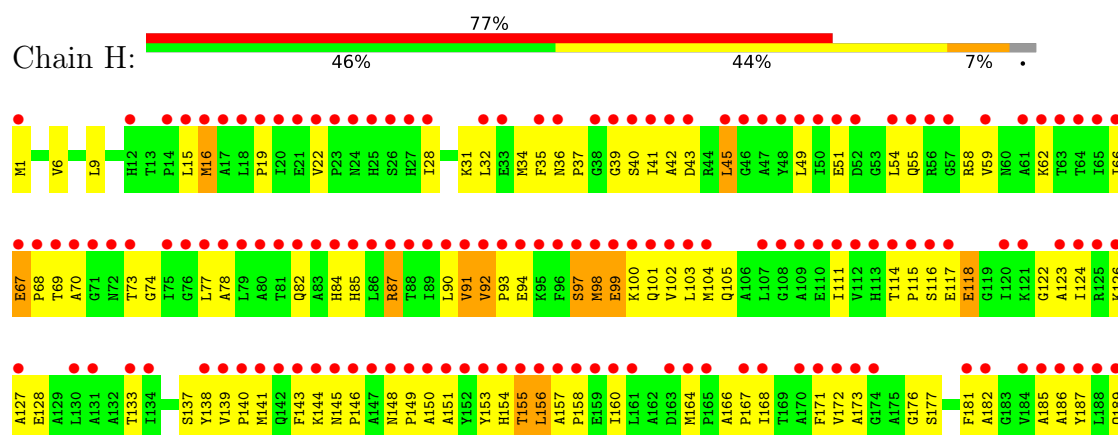
• Molecule 1: Cystathionine beta-synthase

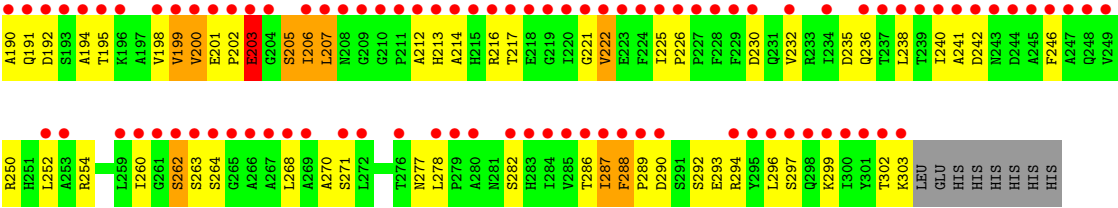


• Molecule 1: Cystathionine beta-synthase



• 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 29.98 – 3.30	Depositor EDS
% Data completeness (in resolution range)	97.7 (29.98-3.30) 99.7 (29.98-3.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtrriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.238 , 0.283 0.246 , 0.288	Depositor DCC
R_{free} test set	2797 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	(Not available)	Xtrriage
Anisotropy	(Not available)	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.3	EDS
L-test for twinning ¹	$\langle L \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available)	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	18392	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *(Not available)*

¹Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.51	0/2314	1.02	13/3152 (0.4%)
1	B	0.58	1/2314 (0.0%)	1.06	11/3152 (0.3%)
1	C	0.57	0/2314	1.01	8/3152 (0.3%)
1	D	0.55	0/2314	1.01	11/3152 (0.3%)
1	E	0.53	0/2314	1.00	8/3152 (0.3%)
1	F	0.57	0/2314	1.02	8/3152 (0.3%)
1	G	0.47	0/2314	0.98	9/3152 (0.3%)
1	H	0.55	0/2314	1.00	8/3152 (0.3%)
All	All	0.54	1/18512 (0.0%)	1.01	76/25216 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	98	MET	SD-CE	5.24	1.92	1.79

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	177	SER	N-CA-C	-9.56	101.74	113.97
1	C	177	SER	N-CA-C	-9.31	102.42	113.88
1	G	94	GLU	N-CA-C	9.06	121.99	111.11
1	F	177	SER	N-CA-C	-9.01	102.42	113.50
1	G	177	SER	N-CA-C	-8.69	102.84	113.97
1	E	95	LYS	N-CA-C	8.41	123.16	113.15
1	H	177	SER	N-CA-C	-8.13	103.57	113.97
1	B	95	LYS	N-CA-C	8.08	121.98	112.93
1	E	177	SER	N-CA-C	-8.03	102.39	112.90
1	D	177	SER	N-CA-C	-7.99	103.74	113.97
1	F	92	VAL	N-CA-C	7.47	116.50	107.61
1	C	113	HIS	N-CA-C	7.24	120.46	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	95	LYS	N-CA-C	7.14	121.64	113.15
1	H	94	GLU	N-CA-C	6.98	122.89	111.37
1	A	95	LYS	N-CA-C	6.93	121.34	113.02
1	G	288	PHE	CA-C-N	6.89	126.70	119.05
1	G	288	PHE	C-N-CA	6.89	126.70	119.05
1	A	288	PHE	CA-C-N	6.79	126.59	119.05
1	A	288	PHE	C-N-CA	6.79	126.59	119.05
1	A	92	VAL	N-CA-C	6.74	115.63	107.61
1	B	94	GLU	N-CA-C	6.61	122.28	111.37
1	D	95	LYS	N-CA-C	6.50	120.82	113.02
1	B	92	VAL	N-CA-C	6.45	115.28	107.61
1	E	94	GLU	N-CA-C	6.45	121.94	111.37
1	A	290	ASP	N-CA-C	6.40	117.95	108.60
1	B	287	ILE	N-CA-C	6.40	117.34	108.12
1	B	288	PHE	CA-C-N	6.37	126.06	119.56
1	B	288	PHE	C-N-CA	6.37	126.06	119.56
1	D	51	GLU	N-CA-C	-6.33	104.07	110.97
1	C	95	LYS	N-CA-C	6.27	120.64	112.92
1	F	95	LYS	N-CA-C	6.26	119.94	112.93
1	B	251	HIS	N-CA-C	6.26	117.77	111.07
1	C	94	GLU	N-CA-C	6.19	123.99	110.80
1	B	177	SER	N-CA-C	-6.18	105.88	113.41
1	D	288	PHE	CA-C-N	6.16	125.89	119.05
1	D	288	PHE	C-N-CA	6.16	125.89	119.05
1	H	290	ASP	N-CA-C	6.10	117.51	108.60
1	F	206	ILE	N-CA-C	6.03	118.63	111.09
1	F	94	GLU	N-CA-C	6.03	123.64	110.80
1	A	94	GLU	N-CA-C	6.01	123.60	110.80
1	H	287	ILE	N-CA-C	5.89	116.48	107.77
1	G	229	PHE	N-CA-C	5.88	119.71	112.54
1	A	287	ILE	N-CA-C	5.82	116.50	108.12
1	D	94	GLU	N-CA-C	5.78	123.10	110.80
1	F	113	HIS	N-CA-C	5.76	118.05	108.20
1	H	203	GLU	N-CA-C	-5.76	101.33	109.96
1	B	73	THR	N-CA-C	-5.66	104.48	111.33
1	A	225	ILE	CA-C-N	5.63	126.18	120.38
1	A	225	ILE	C-N-CA	5.63	126.18	120.38
1	E	260	ILE	N-CA-C	5.59	116.53	108.48
1	A	113	HIS	N-CA-C	5.55	117.69	108.20
1	B	113	HIS	N-CA-C	5.47	117.65	108.96
1	C	22	VAL	CA-C-N	5.43	125.35	119.76
1	C	22	VAL	C-N-CA	5.43	125.35	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	113	HIS	N-CA-C	5.43	117.59	108.73
1	D	206	ILE	N-CA-C	5.43	119.64	112.04
1	B	289	PRO	N-CA-C	5.42	120.88	113.84
1	C	287	ILE	N-CA-C	5.40	115.67	108.11
1	E	288	PHE	CA-C-N	5.35	124.98	119.05
1	E	288	PHE	C-N-CA	5.35	124.98	119.05
1	H	288	PHE	CA-C-N	5.29	125.35	119.32
1	H	288	PHE	C-N-CA	5.29	125.35	119.32
1	G	88	THR	N-CA-C	5.28	117.51	108.90
1	G	287	ILE	N-CA-C	5.25	115.54	107.77
1	H	16	MET	N-CA-C	5.17	116.95	108.52
1	G	22	VAL	N-CA-C	5.10	113.45	107.89
1	D	22	VAL	CA-C-N	5.08	125.07	119.89
1	D	22	VAL	C-N-CA	5.08	125.07	119.89
1	F	290	ASP	N-CA-C	5.07	116.23	108.42
1	E	290	ASP	N-CA-C	5.06	115.99	108.60
1	A	217	THR	N-CA-C	-5.06	102.37	109.96
1	E	51	GLU	N-CA-C	-5.06	105.68	111.14
1	A	70	ALA	N-CA-C	-5.05	106.89	113.16
1	D	111	ILE	N-CA-C	5.05	116.24	108.71
1	C	290	ASP	N-CA-C	5.04	115.70	108.74
1	F	34	MET	N-CA-C	-5.00	107.14	113.20

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	2265	0	2275	102	0
1	B	2265	0	2275	92	0
1	C	2265	0	2275	91	0
1	D	2265	0	2275	127	1
1	E	2265	0	2275	106	1
1	F	2265	0	2275	96	0
1	G	2265	0	2275	105	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	2265	0	2275	136	0
2	A	24	0	15	7	0
2	B	24	0	16	3	0
2	C	24	0	16	2	0
2	D	24	0	16	1	0
2	E	24	0	16	2	0
2	F	24	0	16	0	0
2	G	24	0	16	1	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	781	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 21.

All (781) 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:101:GLN:HA	1:G:104:MET:HE3	1.49	0.92
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:C:157:ALA:HB3	1:C:158:PRO:HD3	1.52	0.88
1:D:101:GLN:HA	1:D:104:MET:HE3	1.52	0.88
1:E:124:ILE:HG23	1:E:141:MET:HE1	1.56	0.87
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:H:67:GLU:CD	1:H:68:PRO:HD2	2.02	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:114:THR:HG21	1:H:123:ALA:HA	1.64	0.79
1:C:101:GLN:HA	1:C:104:MET:HE3	1.63	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:H	1:A:243:ASN:ND2	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:F:101:GLN:HA	1:F:104:MET:HE3	1.67	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:F:9:LEU:HB2	1:F:37:PRO:HG3	1.68	0.75
1:A:101:GLN:HA	1:A:104:MET:HE3	1.68	0.74
1:A:296:LEU:HD23	1:B:99:GLU:HB3	1.69	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:E:101:GLN:HA	1:E:104:MET:HE3	1.68	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:GLU:OE1	1:C:205:SER:HB3	1.88	0.73
1:D:243:ASN:HD22	1:D:243:ASN:H	1.38	0.72
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:A:162:ALA:HB1	1:G:231:GLN:CD	2.16	0.70
1:C:201:GLU:CD	1:C:205:SER:HB3	2.17	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:D:54:LEU:HD13	1:H:191:GLN:CD	2.17	0.68
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:B:101:GLN:HA	1:B:104:MET:HE3	1.77	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:ND2	1:E:243:ASN:H	1.93	0.66
1:A:78:ALA:O	1:A:82:GLN:HB2	1.96	0.66
1:B:201:GLU:CD	1:B:205:SER:HB3	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:55:GLN:HB3	1:H:153:TYR:CZ	2.31	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:O	1:H:254:ARG:HG2	1.94	0.65
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:217:THR:HG23	1:H:262:SER:HB2	1.78	0.65
1:H:260:ILE:HB	1:H:264:SER:HB2	1.79	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:9:LEU:HB2	1:H:37:PRO:HG3	1.79	0.64
1:H:166:ALA:HB1	1:H:167:PRO:HD2	1.79	0.64
1:B:1:MET:SD	1:G:233:ARG:HB2	2.38	0.64
1:B:120:ILE:HG13	2:B:401:AA5:HE3	1.78	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: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:G:201:GLU:CD	1:G:205:SER:HB3	2.24	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:A:124:ILE:HG23	1:A:141:MET:HE1	1.81	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:201:GLU:CD	1:D:205:SER:HB3	2.25	0.61
1:E:201:GLU:CD	1:E:205:SER:HB3	2.25	0.61
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: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:H	1:E:243:ASN:HD22	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:D:55:GLN:CD	1:H:153:TYR:CE2	2.80	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:6:VAL:HG22	1:D:37:PRO:HB3	1.84	0.60
1:D:243:ASN:H	1:D:243:ASN:ND2	1.99	0.60
1:A:6:VAL:HG22	1:A:37:PRO:HB3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H	1:C:243:ASN:ND2	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
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: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: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:H:101:GLN:HA	1:H:104:MET:HE3	1.84	0.58
1:D:148:ASN:HB3	1:D:149:PRO:CD	2.30	0.58
1:B:243:ASN:H	1:B:243:ASN:ND2	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:D:215:HIS:HD2	1:D:217:THR:O	1.86	0.58
1:D:302:THR:HG22	1:D:303:LYS:N	2.17	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:F:201:GLU:CD	1:F:207:LEU:HB2	2.29	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:A:157:ALA:HB1	1:A:187:TYR:CD2	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:25:HIS:CD2	1:C:231:GLN:HA	2.41	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: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:B:201:GLU:CD	1:B:207:LEU:HB2	2.31	0.56
1:D:192:ASP:OD2	1:D:194:ALA:HB3	2.06	0.56
1:D:201:GLU:CD	1:D:207:LEU:HB2	2.31	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: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:C:216:ARG:HG2	1:C:246:PHE:CZ	2.42	0.55
1:E:124:ILE:HG23	1:E:141:MET:CE	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:F:201:GLU:CD	1:F:205:SER:HB3	2.32	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:C:201:GLU:CD	1:C:207:LEU:HB2	2.32	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:D:67:GLU:CD	1:D:68:PRO:HD2	2.33	0.54
1:G:5:HIS:HA	1:H:16:MET:HE3	1.88	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:A:201:GLU:CD	1:A:205:SER:HB3	2.33	0.53
1:G:99:GLU:HG3	1:G:294:ARG:O	2.08	0.53
1:B:6:VAL:HG22	1:B:37:PRO:HB3	1.90	0.53
1:B:118:GLU:HG2	1:B:125:ARG:NH2	2.22	0.53
1:H:99:GLU:HG3	1:H:294:ARG:O	2.08	0.53
1:B:124:ILE:HG23	1:B:141:MET:HE1	1.89	0.53
1:D:153:TYR:CE2	1:H:55:GLN:CD	2.87	0.53
1:E:1:MET:HE3	1:E:1:MET:HA	1.89	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:124:ILE:HG23	1:D:141:MET:HE1	1.89	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: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
1:G:91:VAL:HG11	1:G:126:LYS:HB3	1.91	0.52
1:A:117:GLU:CD	1:A:117:GLU:H	2.16	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: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:A:141:MET:HG3	1:A:144:LYS:HB2	1.91	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:293:GLU:OE2	1:B:294:ARG:HD3	2.11	0.51
1:A:300:ILE:HG23	1:A:301:TYR:N	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:MET:HG3	1:C:141:MET:O	2.10	0.51
1:D:51:GLU:HG3	1:D:55:GLN:HE21	1.75	0.51
1:D:203:GLU:OE1	1:D:242:ASP:HB2	2.10	0.51
1:E:40:SER:HA	1:E:289:PRO:O	2.10	0.51
1:F:164:MET:HE2	1:F:168:ILE:HG12	1.91	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: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:99:GLU:OE1	1:C:297:SER:HB3	2.11	0.51
1:C:185:ALA:O	1:C:189:GLN:HB2	2.11	0.51
1:E:117:GLU:CD	1:E:117:GLU:H	2.19	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:29:TYR:HB2	1:G:285:VAL:HG22	1.93	0.51
1:G:118:GLU:HB3	1:G:122:GLY:HA3	1.92	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:254:ARG:C	1:F:82:GLN:NE2	2.70	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:42:ALA:HB1	1:F:73:THR:HA	1.93	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: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:D:191:GLN:OE1	1:H:84:HIS:NE2	2.45	0.50
1:E:67:GLU:OE2	1:E:141:MET:N	2.44	0.50
1:H:66:ILE:HD12	1:H:137:SER:HB2	1.94	0.50
1:C:42:ALA:HB1	1:C:73:THR:HA	1.93	0.50
1:F:187:TYR:C	1:F:187:TYR:CD2	2.89	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:C:117:GLU:CD	1:C:117:GLU:H	2.18	0.49
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:22:VAL:HG12	1:B:23:PRO:HD2	1.94	0.49
1:B:157:ALA:CB	1:B:158:PRO:HD3	2.33	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: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:99:GLU:OE1	1:D:297:SER:HB3	2.13	0.49
1:D:206:ILE:HD11	1:D:212:ALA:HB2	1.94	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:A:33:GLU:O	1:A:36:ASN:ND2	2.45	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: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:D:55:GLN:CG	1:H:153:TYR:CE2	2.96	0.48
1:F:63:THR:HG22	1:F:64:THR:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:164:MET:HE2	1:D:285:VAL:HG23	1.96	0.48
1:E:67:GLU:HG3	1:E:140:PRO:HD2	1.94	0.48
1:E:18:LEU:O	1:E:20:ILE:N	2.43	0.48
1:E:66:ILE:HD12	1:E:137:SER:HB2	1.95	0.48
1:E:216:ARG:HG2	1:E:246:PHE:CZ	2.49	0.48
1:G:1:MET:HE3	1:G:2:LEU:H	1.78	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:A:25:HIS:CD2	1:C:230:ASP:C	2.92	0.47
1:C:296:LEU:HD12	1:C:296:LEU:HA	1.71	0.47
1:D:1:MET:HE3	1:D:1:MET:HA	1.96	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: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:D:55:GLN:CD	1:H:153:TYR:CD2	2.93	0.47
1:H:302:THR:CG2	1:H:303:LYS:N	2.78	0.47
1:D:55:GLN:CA	1:H:153:TYR:OH	2.62	0.47
1:E:172:VAL:O	1:E:286:THR:HA	2.15	0.47
1:A:77:LEU:O	1:A:81:THR:HG23	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:68:PRO:HA	1:D:91:VAL:O	2.15	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:164:MET:HE2	1:G:285:VAL:HG23	1.96	0.47
1:G:3:ILE:HG13	1:H:16:MET:HB2	1.96	0.47
1:A:67:GLU:OE2	1:A:142:GLN:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:ASN:O	1:A:228:PHE:CE2	2.68	0.47
1:C:185:ALA:HB3	1:C:232:VAL:HG21	1.96	0.47
1:D:51:GLU:OE2	1:H:187:TYR:OH	2.31	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
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:D:16:MET:HE2	1:D:258:LEU:HD11	1.96	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:A:162:ALA:CB	1:G:231:GLN:OE1	2.59	0.46
1:F:11:GLY:O	1:F:12:HIS:HB2	2.15	0.46
1:G:198:VAL:HG11	1:G:238:LEU:HD12	1.98	0.46
1:F:182:ALA:HA	1:F:232:VAL:HG21	1.97	0.46
1:F:243:ASN:H	1:F:243:ASN:ND2	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:70:ALA:CB	2:C:401:AA5:HG1	2.44	0.46
1:C:216:ARG:HG2	1:C:246:PHE:CE1	2.50	0.46
1:E:70:ALA:CB	2:E:401:AA5:HG1	2.45	0.46
1:E:157:ALA:HB1	1:E:187:TYR:CD2	2.49	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:D:51:GLU:C	1:D:55:GLN:HG3	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:1:MET:HE2	1:G:2:LEU:O	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:206:ILE:CD1	1:D:212:ALA:HB2	2.45	0.46
1:C:164:MET:HE2	1:C:285:VAL:HG23	1.98	0.46
1:D:161:LEU:HD23	1:D:161:LEU:HA	1.77	0.46
1:H:28:ILE:HD13	1:H:271:SER:HB3	1.98	0.46
1:H:90:LEU:HD13	1:H:104:MET:SD	2.56	0.46
1:A:164:MET:HE2	1:A:285:VAL:HG23	1.98	0.45
1:B:1:MET:HE3	1:B:1:MET:HA	1.99	0.45
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
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:63:THR:CG2	1:B:64:THR:N	2.80	0.45
1:B:101:GLN:O	1:B:105:GLN:HG2	2.16	0.45
1:C:302:THR:CG2	1:C:303:LYS:N	2.79	0.45
1:D:153:TYR:OH	1:H:55:GLN:HG2	2.17	0.45
1:E:99:GLU:O	1:E:103:LEU:HD22	2.17	0.45
1:E:249:VAL:HG13	1:E:260:ILE:O	2.16	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:C:254:ARG:C	1:D:82:GLN:NE2	2.75	0.45
1:A:219:GLY:O	2:A:401:AA5:HE3	2.16	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:E:164:MET:HE2	1:E:285:VAL:HG23	1.99	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:G:117:GLU:H	1:G:117:GLU:CD	2.25	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:D:153:TYR:CD2	1:H:55:GLN:NE2	2.84	0.45
1:G:66:ILE:O	1:G:139:VAL:HA	2.17	0.45
1:C:264:SER:O	1:C:267:ALA:HB3	2.17	0.45
1:E:70:ALA:HB2	2:E:401:AA5:HG1	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:149:PRO:HG2	1:E:228:PHE:CD2	2.51	0.45
1:A:156:LEU:HD22	1:A:160:ILE:HD11	1.99	0.44
1:D:92:VAL:HA	1:D:93:PRO:HD3	1.79	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: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:B:164:MET:HE2	1:B:168:ILE:HG12	1.99	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
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:D:60:ASN:C	1:D:60:ASN:OD1	2.60	0.44
1:E:141:MET:HG3	1:E:144:LYS:HB2	1.99	0.44
1:A:11:GLY:O	1:A:12:HIS:HB2	2.16	0.44
1:D:20:ILE:HG22	1:D:256:HIS:NE2	2.33	0.44
1:D:185:ALA:HB3	1:D:232:VAL:CG2	2.42	0.44
1:F:101:GLN:O	1:F:105:GLN:HG3	2.18	0.44
1:B:42:ALA:HB1	1:B:73:THR:HA	2.00	0.44
1:B:217:THR:HG23	1:B:262:SER:HB2	2.00	0.44
1:D:54:LEU:O	1:H:190:ALA:HB1	2.17	0.44
1:D:203:GLU:O	1:D:215:HIS:HB3	2.18	0.44
1:H:117:GLU:CD	1:H:117:GLU:H	2.25	0.44
1:H:181:PHE:CE2	1:H:199:VAL:HG22	2.52	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:73:THR:O	1:H:77:LEU:HB2	2.18	0.44
1:H:153:TYR:CE2	1:H:187:TYR:HD1	2.36	0.44
1:B:134:ILE:O	1:B:137:SER:OG	2.36	0.43
1:E:92:VAL:HA	1:E:93:PRO:HD3	1.83	0.43
1:F:278:LEU:HD23	1:F:278:LEU:HA	1.79	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:16:MET:HG2	1:G:18:LEU:HD23	2.00	0.43
1:G:148:ASN:O	1:G:151:ALA:HB3	2.18	0.43
1:G:264:SER:HB3	1:G:288:PHE:CD1	2.53	0.43
1:A:34:MET:HE3	1:A:34:MET:HB3	1.85	0.43
1:A:70:ALA:HB3	2:A:401:AA5:HG1	2.00	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: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
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:F:101:GLN:HA	1:F:104:MET:CE	2.44	0.43
1:G:274:LEU:O	1:G:274:LEU:HG	2.18	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:HD12	1:F:296:LEU:HA	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:HD23	1:B:161:LEU:HA	1.79	0.43
1:D:207:LEU:HD23	1:D:222:VAL:HG11	2.00	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:H:155:THR:C	1:H:158:PRO:HD2	2.43	0.43
1:A:23:PRO:C	1:A:25:HIS:N	2.76	0.43
1:A:201:GLU:CD	1:A:207:LEU:HB2	2.44	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:HD12	1:B:103:LEU:HA	1.86	0.43
1:C:71:GLY:HA2	1:C:104:MET:CE	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:97:SER:OG	1:D:99:GLU:HG2	2.19	0.43
1:E:36:ASN:O	1:E:39:GLY:N	2.44	0.43
1:E:206:ILE:CD1	1:E:212:ALA:HB2	2.48	0.43
1:G:38:GLY:N	1:G:43:ASP:OD2	2.37	0.43
1:A:25:HIS:HD2	1:C:230:ASP:C	2.26	0.43
1:A:41:ILE:HD11	1:A:156:LEU:HD11	2.01	0.43
1:B:1:MET:N	1:G:230:ASP:O	2.40	0.43
1:B:98:MET:O	1:B:102:VAL:HG23	2.19	0.43
1:B:268:LEU:HD22	1:B:272:LEU:CD1	2.49	0.43
1:E:16:MET:HB2	1:F:3:ILE:CG1	2.48	0.43
1:F:29:TYR:CD1	1:F:29:TYR:N	2.87	0.43
1:B:226:PRO:HG2	1:B:229:PHE:CE2	2.53	0.42
1:C:29:TYR:HB2	1:C:285:VAL:HG22	2.00	0.42
1:F:50:ILE:CD1	1:F:81:THR:HG22	2.48	0.42
1:F:213:HIS:CD2	1:F:214:ALA:O	2.71	0.42
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: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:24:ASN:HB3	1:E:280:ALA:HA	2.02	0.42
1:E:149:PRO:CG	1:E:228:PHE:CD2	3.02	0.42
1:F:50:ILE:HD11	1:F:81:THR:HG22	2.02	0.42
1:G:9:LEU:HB2	1:G:37:PRO:HG3	2.02	0.42
1:G:216:ARG:HG2	1:G:246:PHE:CE1	2.54	0.42
1:H:92:VAL:HA	1:H:93:PRO:HD3	1.88	0.42
1:H:150:ALA:HA	1:H:153:TYR:HB2	2.01	0.42
1:A:63:THR:HG22	1:A:64:THR:N	2.34	0.42
1:A:263:SER:OG	2:A:401:AA5:H2A3	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:215:HIS:HD2	1:F:217:THR:O	2.02	0.42
1:H:54:LEU:HD23	1:H:59:VAL:HB	2.01	0.42
1:H:99:GLU:OE1	1:H:297:SER:HB3	2.20	0.42
1:H:157:ALA:HA	1:H:160:ILE:HD12	2.02	0.42
1:D:235:ASP:O	1:D:236:GLN:HB2	2.19	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:4:GLN:O	1:H:16:MET:HE3	2.20	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:D:117:GLU:CD	1:D:117:GLU:H	2.28	0.42
1:E:19:PRO:HD3	1:F:4:GLN:O	2.20	0.42
1:E:51:GLU:HG3	1:E:55:GLN:NE2	2.33	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:C:187:TYR:CD2	1:C:187:TYR:C	2.97	0.41
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:95:LYS:HD3	1:A:116:SER:HB3	2.02	0.41
1:A:162:ALA:C	1:G:231:GLN:OE1	2.63	0.41
1:E:172:VAL:HG12	1:E:200:VAL:CG2	2.50	0.41
1:A:63:THR:HA	1:A:136:ASN:CG	2.46	0.41
1:C:99:GLU:OE1	1:C:297:SER:CB	2.69	0.41
1:C:215:HIS:HD2	1:C:217:THR:O	2.02	0.41
1:F:117:GLU:CD	1:F:117:GLU:H	2.28	0.41
1:G:42:ALA:HB1	1:G:73:THR:HA	2.03	0.41
1:G:172:VAL:HG12	1:G:200:VAL:CG2	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:161:LEU:HD23	1:G:161:LEU:HA	1.89	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:E:99:GLU:CB	1:F:296:LEU:HD23	2.50	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: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:HD23	1:A:54:LEU:HA	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:F:111:ILE:HG22	1:F:112:VAL:N	2.34	0.41
1:H:185:ALA:HB3	1:H:232:VAL:HG21	2.03	0.41
1:A:63:THR:HA	1:A:136:ASN:OD1	2.21	0.41
1:D:153:TYR:CE2	1:H:55:GLN:HG2	2.56	0.41
1:F:17:ALA:O	1:F:18:LEU:C	2.64	0.41
1:F:60:ASN:H	1:F:63:THR:HG1	1.67	0.41
1:F:148:ASN:OD1	1:F:148:ASN:C	2.64	0.41
1:F:198:VAL:HG11	1:F:238:LEU:HD12	2.02	0.41
1:F:264:SER:HB3	1:F:288:PHE:CD1	2.55	0.41
1:G:250:ARG:NH1	1:G:303:LYS:HE3	2.36	0.41
1:H:54:LEU:HD21	1:H:59:VAL:HG12	2.03	0.41
1:H:164:MET:HE3	1:H:166:ALA:O	2.21	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:22:VAL:HG11	1:B:28:ILE:HG13	2.03	0.40
1:B:101:GLN:O	1:B:105:GLN:CG	2.68	0.40
1:B:128:GLU:OE1	1:B:141:MET:HE3	2.21	0.40
1:E:33:GLU:O	1:E:36:ASN:ND2	2.50	0.40
1:E:49:LEU:HD23	1:E:49:LEU:HA	1.72	0.40
1:E:82:GLN:NE2	1:F:254:ARG:C	2.79	0.40
1:G:294:ARG:HD3	1:H:293:GLU:OE2	2.21	0.40
1:H:16:MET:HE2	1:H:19:PRO:HD3	2.02	0.40
1:C:217:THR:HG23	1:C:262:SER:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:62:LYS:HD3	1:H:87:ARG:NH2	2.37	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:A:153:TYR:O	1:A:158:PRO:HD3	2.21	0.40
1:A:219:GLY:C	2:A:401:AA5:HE3	2.46	0.40
1:D:254:ARG:O	1:D:254:ARG:HG2	2.21	0.40
1:G:42:ALA:O	1:G:43:ASP:C	2.63	0.40
1:G:67:GLU:CG	1:G:140:PRO:HD2	2.49	0.40
1:G:208:ASN:C	1:G:210:GLY:H	2.30	0.40
1:G:278:LEU:HD23	1:G:278:LEU:HA	1.86	0.40
1:H:203:GLU:H	1:H:203:GLU:HG3	1.59	0.40
1:A:215:HIS:ND1	1:A:215:HIS:N	2.69	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:D:181:PHE:CD2	1:D:199:VAL:HG13	2.56	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:B:120:ILE:CG1	2:B:401:AA5:HE3	2.51	0.40
1:C:99:GLU:CB	1:D:296:LEU:HD23	2.52	0.40
1:E:166:ALA:HB3	1:E:283:HIS:CD2	2.57	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:F:141:MET:HG3	1:F:141:MET:O	2.22	0.40
1:G:6:VAL:CG2	1:G:37:PRO:HB3	2.50	0.40
1:G:206:ILE:CD1	1:G:212:ALA:HB2	2.46	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 symmetry 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

5.3.1 Protein backbone

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	301/311 (97%)	271 (90%)	26 (9%)	4 (1%)	9	35
1	B	301/311 (97%)	276 (92%)	23 (8%)	2 (1%)	18	49
1	C	301/311 (97%)	278 (92%)	22 (7%)	1 (0%)	36	65
1	D	301/311 (97%)	276 (92%)	25 (8%)	0	100	100
1	E	301/311 (97%)	274 (91%)	24 (8%)	3 (1%)	12	40
1	F	301/311 (97%)	275 (91%)	25 (8%)	1 (0%)	36	65
1	G	301/311 (97%)	271 (90%)	28 (9%)	2 (1%)	18	49
1	H	301/311 (97%)	276 (92%)	24 (8%)	1 (0%)	36	65
All	All	2408/2488 (97%)	2197 (91%)	197 (8%)	14 (1%)	21	52

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
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%)	191 (81%)	44 (19%)	1	7
1	B	235/243 (97%)	192 (82%)	43 (18%)	2	7
1	C	235/243 (97%)	193 (82%)	42 (18%)	2	8
1	D	235/243 (97%)	200 (85%)	35 (15%)	3	13
1	E	235/243 (97%)	192 (82%)	43 (18%)	2	7
1	F	235/243 (97%)	192 (82%)	43 (18%)	2	7
1	G	235/243 (97%)	192 (82%)	43 (18%)	2	7
1	H	235/243 (97%)	197 (84%)	38 (16%)	2	11
All	All	1880/1944 (97%)	1549 (82%)	331 (18%)	2	9

All (331) 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	73	THR
1	A	77	LEU
1	A	87	ARG
1	A	91	VAL
1	A	92	VAL
1	A	98	MET
1	A	99	GLU
1	A	103	LEU
1	A	111	ILE
1	A	116	SER
1	A	118	GLU
1	A	126	LYS
1	A	133	THR
1	A	144	LYS
1	A	155	THR
1	A	156	LEU
1	A	164	MET
1	A	199	VAL
1	A	203	GLU
1	A	205	SER
1	A	206	ILE

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Mol	Chain	Res	Type
1	A	207	LEU
1	A	215	HIS
1	A	222	VAL
1	A	225	ILE
1	A	230	ASP
1	A	243	ASN
1	A	252	LEU
1	A	259	LEU
1	A	262	SER
1	A	268	LEU
1	A	273	GLN
1	A	277	ASN
1	A	278	LEU
1	A	285	VAL
1	A	291	SER
1	A	296	LEU
1	A	299	LYS
1	B	1	MET
1	B	21	GLU
1	B	22	VAL
1	B	32	LEU
1	B	41	ILE
1	B	45	LEU
1	B	49	LEU
1	B	67	GLU
1	B	73	THR
1	B	87	ARG
1	B	91	VAL
1	B	92	VAL
1	B	94	GLU
1	B	95	LYS
1	B	98	MET
1	B	99	GLU
1	B	103	LEU
1	B	105	GLN
1	B	111	ILE
1	B	116	SER
1	B	118	GLU
1	B	121	LYS
1	B	128	GLU
1	B	133	THR
1	B	155	THR

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Mol	Chain	Res	Type
1	B	156	LEU
1	B	159	GLU
1	B	188	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	234	ILE
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	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	99	GLU
1	C	103	LEU
1	C	105	GLN
1	C	111	ILE
1	C	116	SER
1	C	118	GLU
1	C	128	GLU
1	C	133	THR
1	C	144	LYS
1	C	155	THR
1	C	156	LEU
1	C	195	THR
1	C	199	VAL

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Mol	Chain	Res	Type
1	C	203	GLU
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	234	ILE
1	C	243	ASN
1	C	252	LEU
1	C	259	LEU
1	C	262	SER
1	C	268	LEU
1	C	277	ASN
1	C	281	ASN
1	C	282	SER
1	C	296	LEU
1	C	299	LYS
1	D	22	VAL
1	D	45	LEU
1	D	87	ARG
1	D	91	VAL
1	D	92	VAL
1	D	98	MET
1	D	99	GLU
1	D	103	LEU
1	D	105	GLN
1	D	116	SER
1	D	118	GLU
1	D	126	LYS
1	D	128	GLU
1	D	133	THR
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	206	ILE
1	D	207	LEU
1	D	222	VAL
1	D	225	ILE

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Mol	Chain	Res	Type
1	D	230	ASP
1	D	243	ASN
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	45	LEU
1	E	58	ARG
1	E	67	GLU
1	E	87	ARG
1	E	91	VAL
1	E	92	VAL
1	E	97	SER
1	E	98	MET
1	E	99	GLU
1	E	103	LEU
1	E	105	GLN
1	E	111	ILE
1	E	114	THR
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	200	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	243	ASN

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Mol	Chain	Res	Type
1	E	252	LEU
1	E	259	LEU
1	E	260	ILE
1	E	262	SER
1	E	268	LEU
1	E	277	ASN
1	E	278	LEU
1	E	281	ASN
1	E	282	SER
1	E	291	SER
1	E	296	LEU
1	E	299	LYS
1	F	22	VAL
1	F	45	LEU
1	F	49	LEU
1	F	67	GLU
1	F	73	THR
1	F	87	ARG
1	F	91	VAL
1	F	92	VAL
1	F	95	LYS
1	F	98	MET
1	F	99	GLU
1	F	103	LEU
1	F	105	GLN
1	F	111	ILE
1	F	112	VAL
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	159	GLU
1	F	193	SER
1	F	195	THR
1	F	199	VAL
1	F	200	VAL
1	F	203	GLU
1	F	206	ILE
1	F	207	LEU

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Mol	Chain	Res	Type
1	F	216	ARG
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	45	LEU
1	G	58	ARG
1	G	67	GLU
1	G	87	ARG
1	G	91	VAL
1	G	92	VAL
1	G	95	LYS
1	G	97	SER
1	G	98	MET
1	G	99	GLU
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	128	GLU
1	G	133	THR
1	G	144	LYS
1	G	155	THR
1	G	156	LEU
1	G	195	THR
1	G	199	VAL
1	G	203	GLU
1	G	206	ILE
1	G	207	LEU
1	G	222	VAL
1	G	225	ILE

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Mol	Chain	Res	Type
1	G	230	ASP
1	G	243	ASN
1	G	259	LEU
1	G	262	SER
1	G	263	SER
1	G	268	LEU
1	G	273	GLN
1	G	277	ASN
1	G	278	LEU
1	G	281	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	45	LEU
1	H	58	ARG
1	H	67	GLU
1	H	87	ARG
1	H	91	VAL
1	H	92	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
1	H	126	LYS
1	H	128	GLU
1	H	133	THR
1	H	155	THR
1	H	156	LEU
1	H	189	GLN
1	H	199	VAL
1	H	200	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

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Mol	Chain	Res	Type
1	H	230	ASP
1	H	252	LEU
1	H	262	SER
1	H	263	SER
1	H	268	LEU
1	H	277	ASN
1	H	278	LEU
1	H	282	SER
1	H	296	LEU
1	H	299	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	25	HIS
1	A	72	ASN
1	A	113	HIS
1	A	154	HIS
1	A	213	HIS
1	A	236	GLN
1	A	243	ASN
1	A	298	GLN
1	B	72	ASN
1	B	215	HIS
1	B	236	GLN
1	B	243	ASN
1	B	283	HIS
1	B	298	GLN
1	C	4	GLN
1	C	5	HIS
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	215	HIS
1	D	236	GLN
1	D	243	ASN
1	D	283	HIS

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Mol	Chain	Res	Type
1	D	298	GLN
1	E	4	GLN
1	E	55	GLN
1	E	72	ASN
1	E	213	HIS
1	E	215	HIS
1	E	236	GLN
1	E	243	ASN
1	E	283	HIS
1	E	298	GLN
1	F	4	GLN
1	F	27	HIS
1	F	213	HIS
1	F	215	HIS
1	F	236	GLN
1	F	243	ASN
1	F	283	HIS
1	F	298	GLN
1	G	55	GLN
1	G	72	ASN
1	G	213	HIS
1	G	215	HIS
1	G	236	GLN
1	G	243	ASN
1	G	256	HIS
1	G	283	HIS
1	G	298	GLN
1	H	55	GLN
1	H	113	HIS
1	H	213	HIS
1	H	215	HIS
1	H	236	GLN
1	H	243	ASN
1	H	283	HIS
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 [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	E	401	-	24,24,24	1.63	4 (16%)	30,33,33	1.23	3 (10%)
3	SO4	H	402	-	4,4,4	0.40	0	6,6,6	0.10	0
2	AA5	D	401	-	24,24,24	1.42	4 (16%)	30,33,33	1.19	3 (10%)
2	AA5	F	401	-	24,24,24	1.39	3 (12%)	30,33,33	1.25	3 (10%)
2	AA5	C	401	-	24,24,24	1.34	3 (12%)	30,33,33	1.27	4 (13%)
3	SO4	F	403	-	4,4,4	0.42	0	6,6,6	0.07	0
3	SO4	A	403	-	4,4,4	0.45	0	6,6,6	0.17	0
2	AA5	G	401	-	24,24,24	1.47	4 (16%)	30,33,33	1.23	3 (10%)
3	SO4	A	402	-	4,4,4	0.40	0	6,6,6	0.15	0
3	SO4	F	402	-	4,4,4	0.33	0	6,6,6	0.18	0
2	AA5	A	401	-	24,24,24	1.21	3 (12%)	30,33,33	1.14	3 (10%)
3	SO4	D	403	-	4,4,4	0.39	0	6,6,6	0.13	0
3	SO4	C	402	-	4,4,4	0.38	0	6,6,6	0.24	0
3	SO4	B	402	-	4,4,4	0.37	0	6,6,6	0.30	0
3	SO4	E	403	-	4,4,4	0.37	0	6,6,6	0.09	0
2	AA5	B	401	-	24,24,24	1.48	5 (20%)	30,33,33	1.37	3 (10%)
2	AA5	H	401	-	24,24,24	1.75	6 (25%)	30,33,33	1.54	4 (13%)
3	SO4	B	403	-	4,4,4	0.37	0	6,6,6	0.10	0
3	SO4	C	403	-	4,4,4	0.39	0	6,6,6	0.15	0
3	SO4	G	402	-	4,4,4	0.39	0	6,6,6	0.06	0
3	SO4	H	403	-	4,4,4	0.39	0	6,6,6	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	E	402	-	4,4,4	0.37	0	6,6,6	0.17	0
3	SO4	G	403	-	4,4,4	0.37	0	6,6,6	0.11	0
3	SO4	D	402	-	4,4,4	0.37	0	6,6,6	0.20	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	E	401	-	-	2/19/19/19	0/1/1/1
2	AA5	D	401	-	-	3/19/19/19	0/1/1/1
2	AA5	F	401	-	-	1/19/19/19	0/1/1/1
2	AA5	G	401	-	-	3/19/19/19	0/1/1/1
2	AA5	C	401	-	-	2/19/19/19	0/1/1/1
2	AA5	B	401	-	-	4/19/19/19	0/1/1/1
2	AA5	H	401	-	-	2/19/19/19	0/1/1/1
2	AA5	A	401	-	-	3/19/19/19	0/1/1/1

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	401	AA5	C4-C3	4.06	1.47	1.41
2	B	401	AA5	C4-C3	3.77	1.47	1.41
2	H	401	AA5	P-O1P	3.75	1.62	1.50
2	H	401	AA5	CB-CA	3.62	1.57	1.53
2	E	401	AA5	C4-C3	3.60	1.47	1.41
2	F	401	AA5	C4-C3	3.57	1.47	1.41
2	E	401	AA5	CB-CA	3.45	1.57	1.53
2	G	401	AA5	P-O1P	3.41	1.61	1.50
2	G	401	AA5	C4-C5	3.10	1.46	1.42
2	B	401	AA5	CB-CA	3.02	1.56	1.53
2	D	401	AA5	CB-CA	2.99	1.56	1.53
2	C	401	AA5	C4-C3	2.89	1.45	1.41
2	E	401	AA5	C4-C5	2.87	1.46	1.42
2	C	401	AA5	CB-CA	2.76	1.56	1.53
2	G	401	AA5	CB-CA	2.69	1.56	1.53
2	D	401	AA5	C4-C3	2.67	1.45	1.41
2	H	401	AA5	C4-C5	2.64	1.45	1.42
2	E	401	AA5	P-O1P	2.57	1.58	1.50
2	C	401	AA5	C4-C5	2.44	1.45	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	AA5	P-O1P	2.38	1.57	1.50
2	B	401	AA5	P-O1P	2.34	1.57	1.50
2	A	401	AA5	P-O1P	2.29	1.57	1.50
2	D	401	AA5	C4-C5	2.27	1.45	1.42
2	B	401	AA5	C4-C5	2.27	1.45	1.42
2	F	401	AA5	P-O1P	2.19	1.57	1.50
2	A	401	AA5	C4-C5	2.18	1.45	1.42
2	B	401	AA5	O1-C	2.18	1.28	1.22
2	G	401	AA5	C4-C3	2.17	1.44	1.41
2	F	401	AA5	CA-C	-2.16	1.49	1.52
2	H	401	AA5	O1-C	2.16	1.28	1.22
2	A	401	AA5	C4-C3	2.13	1.44	1.41
2	H	401	AA5	CA-C	2.12	1.54	1.52

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	401	AA5	CA-N-C4A	5.17	124.45	116.77
2	B	401	AA5	CA-N-C4A	3.81	122.43	116.77
2	B	401	AA5	C4-C3-C2	-3.67	118.08	120.14
2	C	401	AA5	CA-N-C4A	3.52	121.99	116.77
2	E	401	AA5	CA-N-C4A	3.50	121.97	116.77
2	G	401	AA5	CA-N-C4A	3.45	121.89	116.77
2	F	401	AA5	C4-C3-C2	-3.41	118.23	120.14
2	F	401	AA5	CA-N-C4A	3.30	121.66	116.77
2	H	401	AA5	C4-C3-C2	-3.28	118.30	120.14
2	D	401	AA5	C4-C3-C2	-3.20	118.34	120.14
2	C	401	AA5	C4-C3-C2	-3.13	118.38	120.14
2	E	401	AA5	C4-C3-C2	-3.03	118.44	120.14
2	D	401	AA5	CA-N-C4A	2.94	121.13	116.77
2	G	401	AA5	C4-C3-C2	-2.73	118.60	120.14
2	A	401	AA5	C4-C3-C2	-2.63	118.67	120.14
2	H	401	AA5	C6-N1-C2	2.58	123.89	119.20
2	A	401	AA5	CA-N-C4A	2.58	120.60	116.77
2	H	401	AA5	O2-C-O1	-2.43	118.57	124.08
2	B	401	AA5	C6-N1-C2	2.35	123.46	119.20
2	A	401	AA5	C6-N1-C2	2.30	123.37	119.20
2	C	401	AA5	C6-N1-C2	2.30	123.37	119.20
2	E	401	AA5	C6-N1-C2	2.28	123.33	119.20
2	C	401	AA5	O2-C-O1	-2.24	119.00	124.08
2	D	401	AA5	C6-N1-C2	2.20	123.19	119.20
2	G	401	AA5	C6-N1-C2	2.17	123.13	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	401	AA5	C6-N1-C2	2.05	122.92	119.20

There are no chirality outliers.

All (20) torsion outliers are listed below:

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	C-CA-N-C4A
2	B	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	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	H	401	AA5	C-CA-N-C4A
2	H	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	D	401	AA5	O1-C-CA-N
2	A	401	AA5	CB-CG-SD-CE
2	G	401	AA5	CA-CB-CG-SD

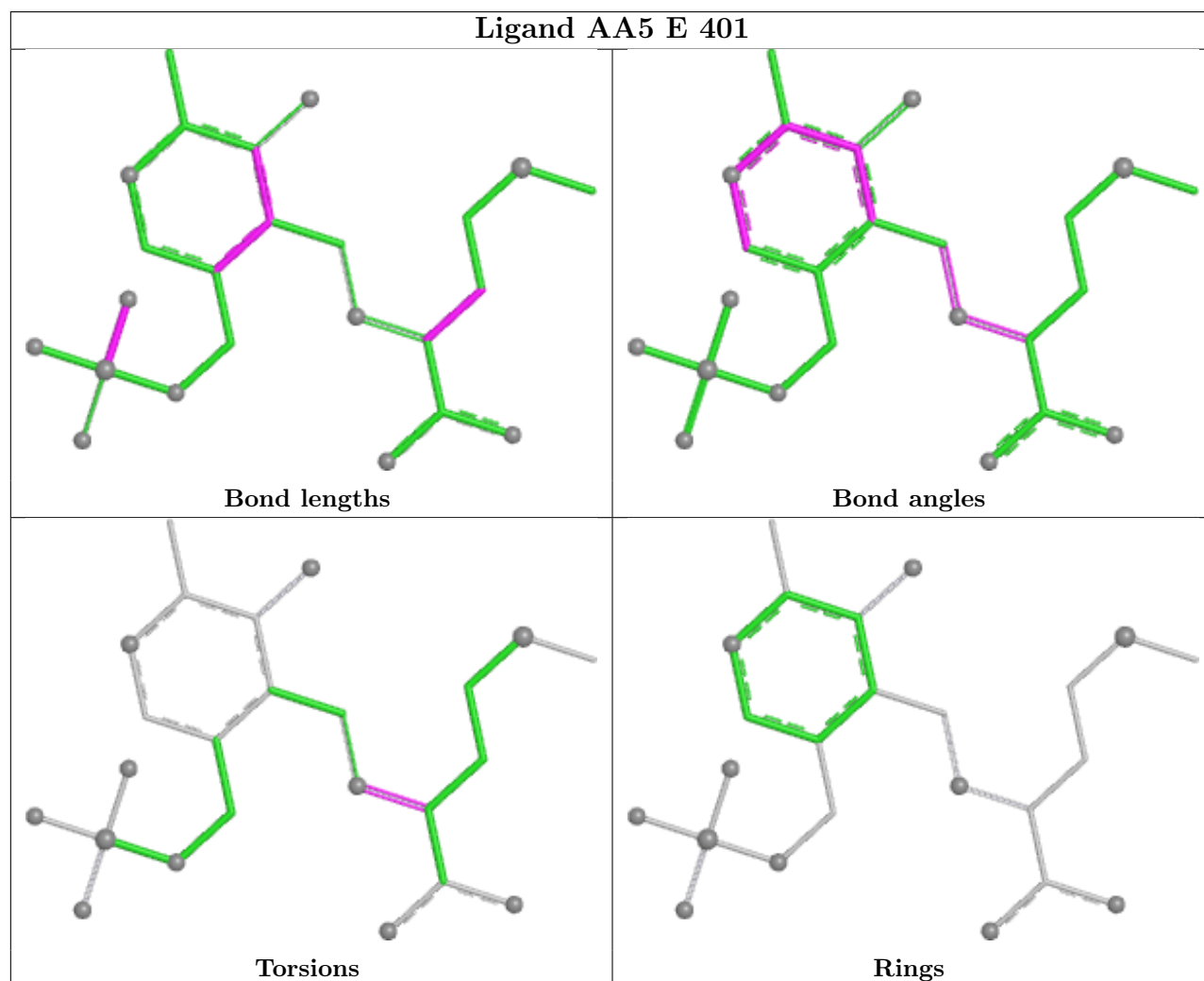
There are no ring outliers.

8 monomers are involved in 21 short contacts:

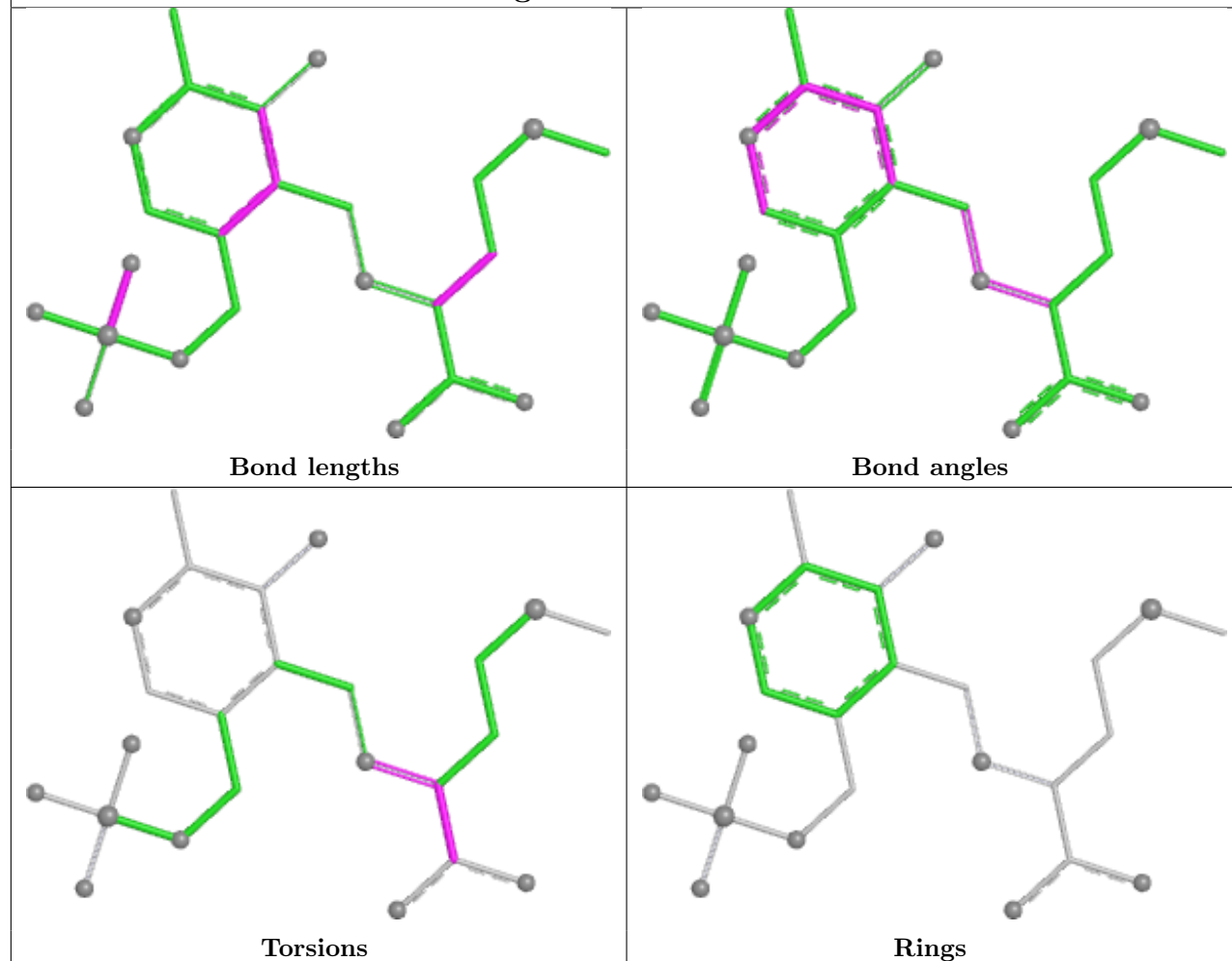
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	401	AA5	2	0
2	D	401	AA5	1	0
2	C	401	AA5	2	0
2	G	401	AA5	1	0
2	A	401	AA5	7	0
2	B	401	AA5	3	0
2	H	401	AA5	4	0
3	B	403	SO4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

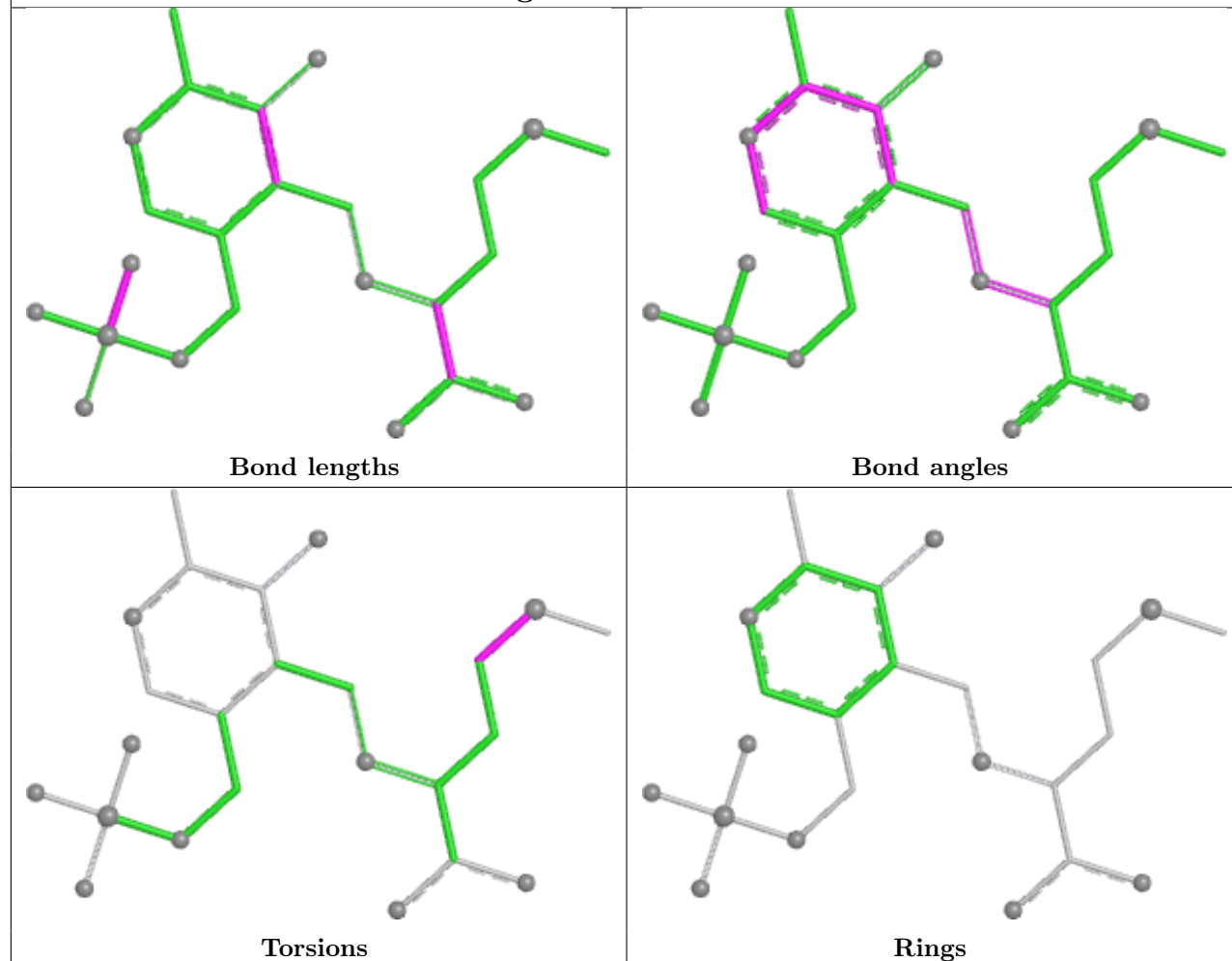
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within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



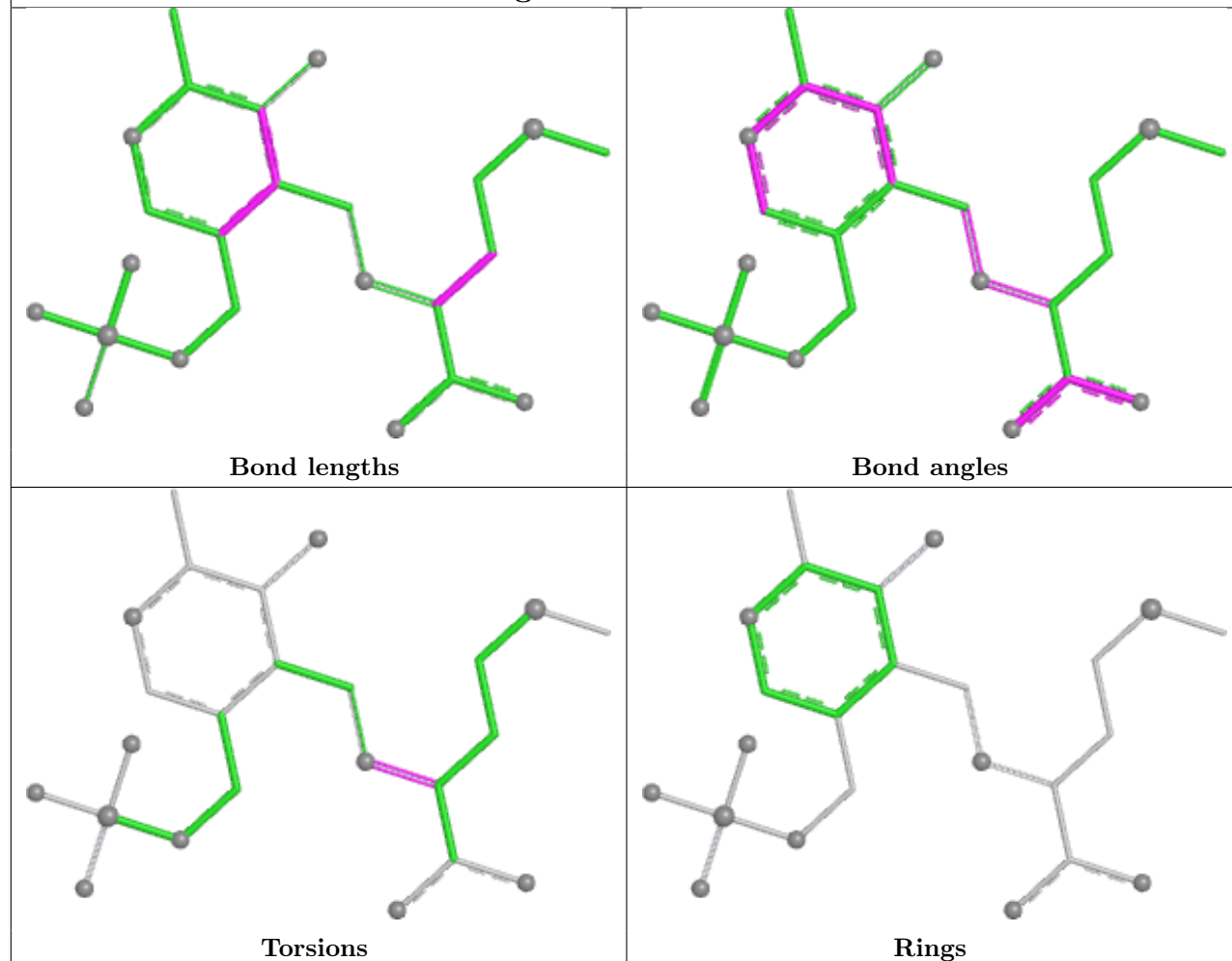
Ligand AA5 D 401



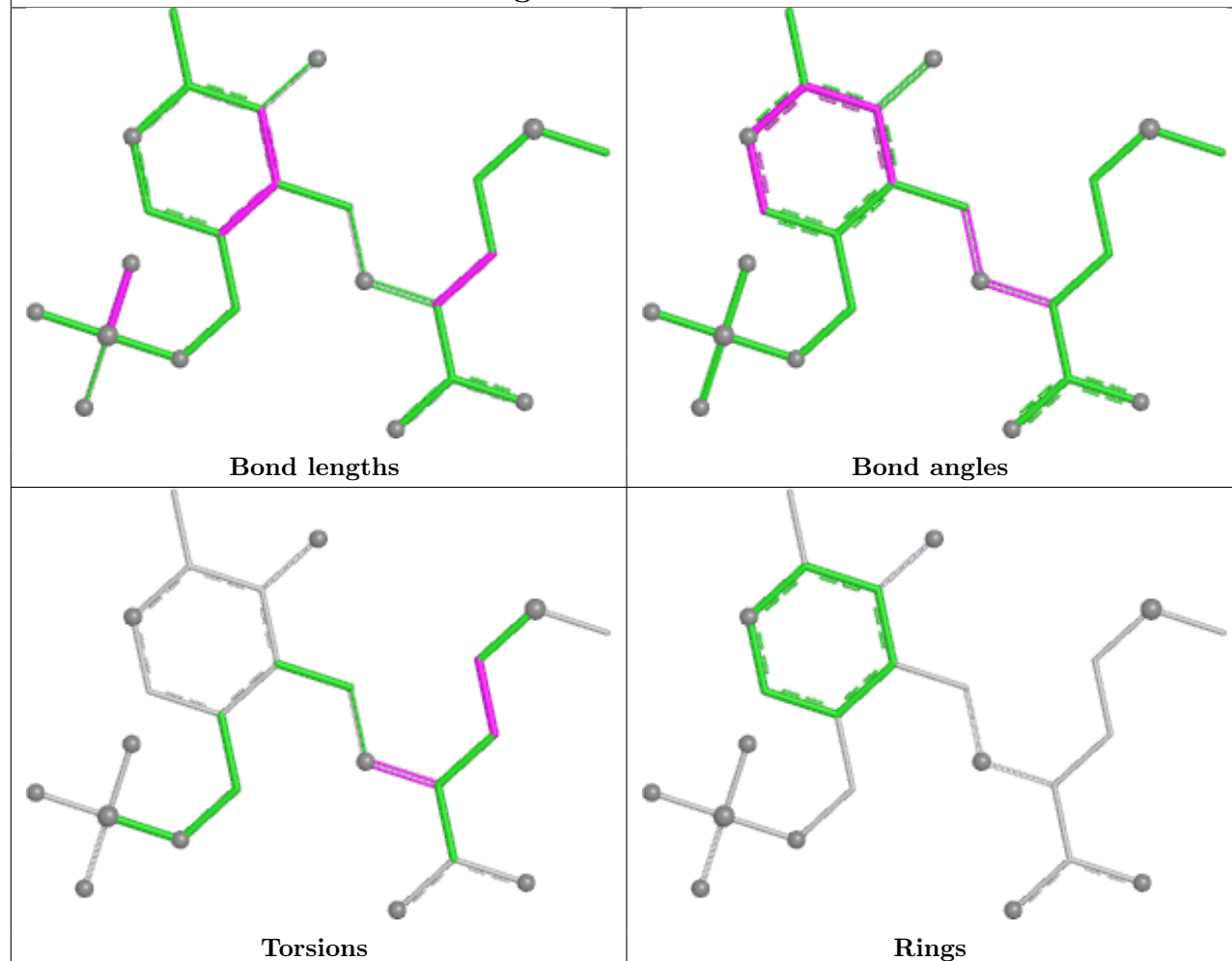
Ligand AA5 F 401



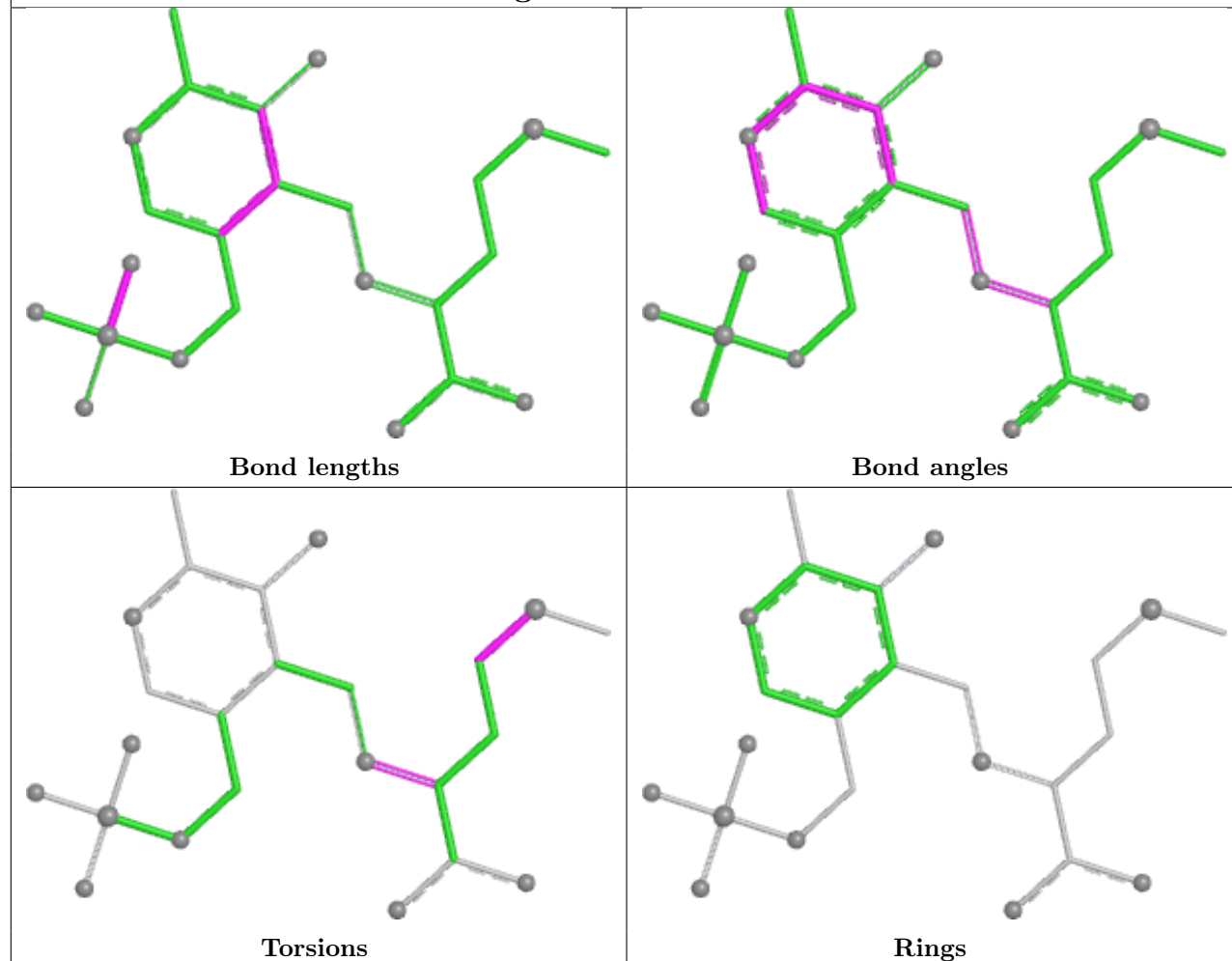
Ligand AA5 C 401



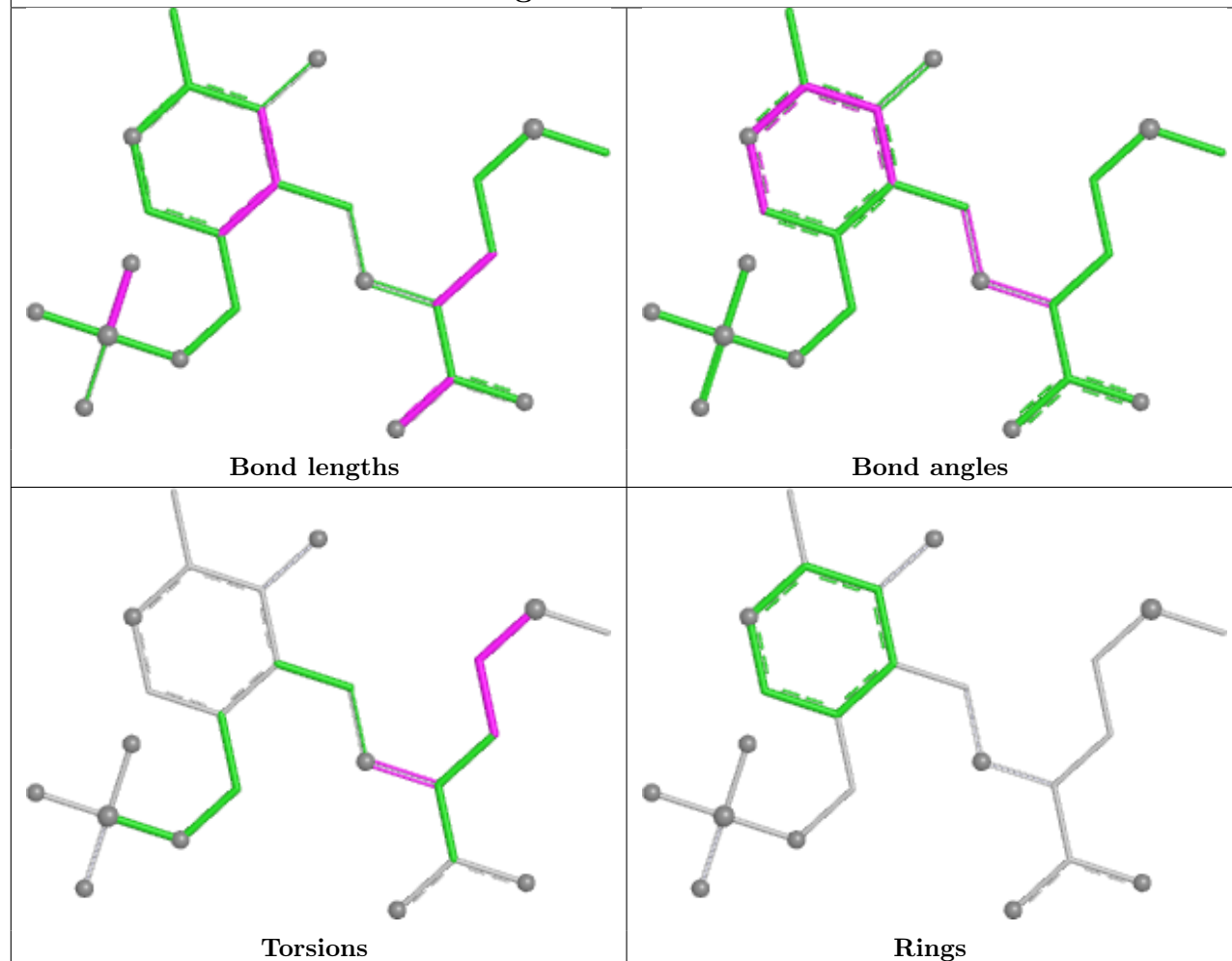
Ligand AA5 G 401

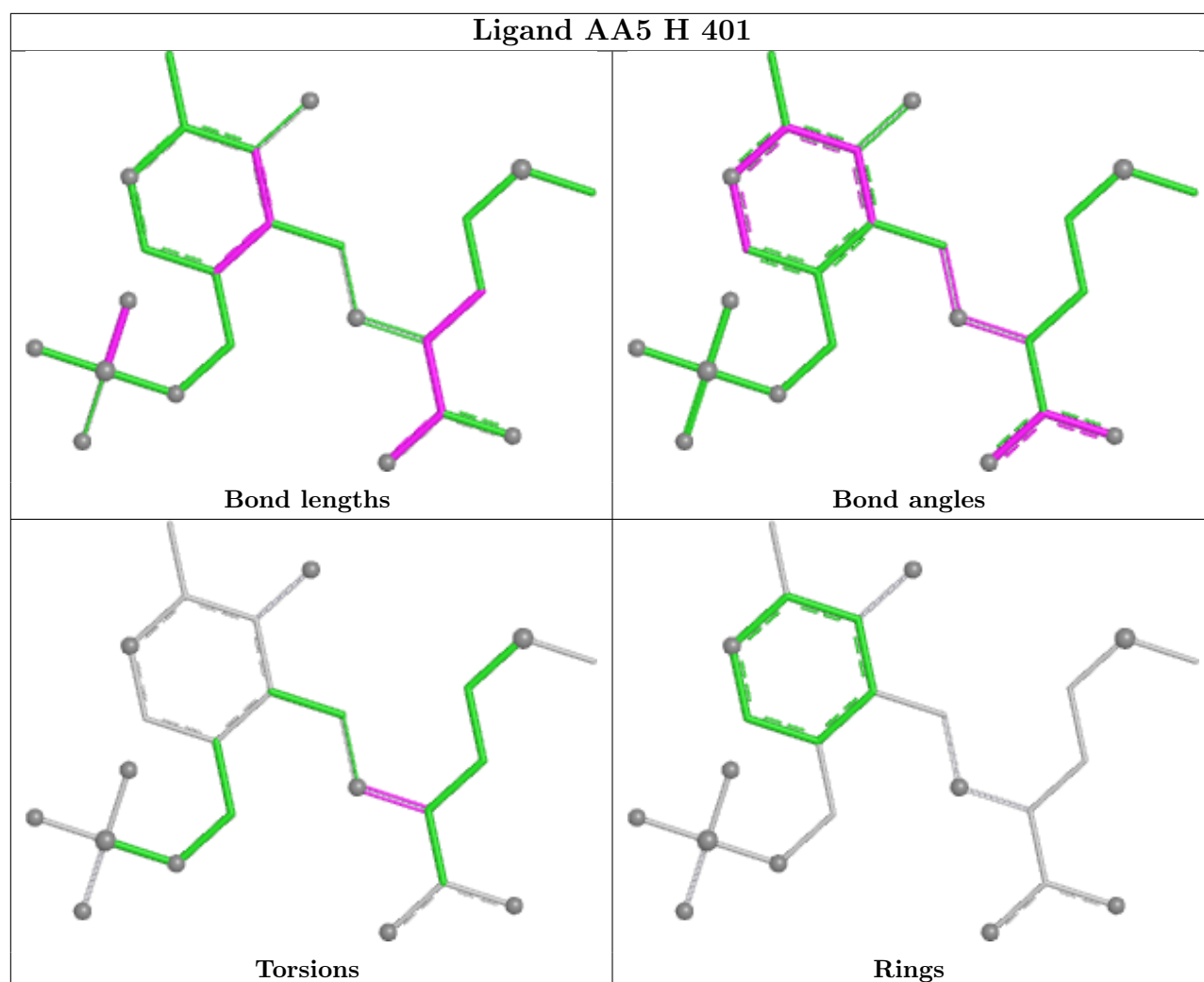


Ligand AA5 A 401



Ligand AA5 B 401





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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%)	0.41	9 (2%)	52	35	14, 44, 65, 71	0
1	B	303/311 (97%)	0.08	5 (1%)	69	50	11, 26, 49, 63	0
1	C	303/311 (97%)	-0.01	4 (1%)	75	56	7, 26, 47, 62	0
1	D	303/311 (97%)	0.13	5 (1%)	69	50	16, 33, 54, 64	0
1	E	303/311 (97%)	0.67	10 (3%)	49	33	19, 45, 66, 75	0
1	F	303/311 (97%)	0.17	3 (0%)	79	63	14, 31, 50, 63	0
1	G	303/311 (97%)	0.78	23 (7%)	20	14	24, 54, 83, 94	0
1	H	303/311 (97%)	2.96	240 (79%)	0	0	46, 93, 114, 118	0
All	All	2424/2488 (97%)	0.65	299 (12%)	8	7	7, 39, 99, 118	0

All (299) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	120	ILE	6.3
1	H	73	THR	6.1
1	H	89	ILE	5.9
1	H	218	GLU	5.9
1	H	268	LEU	5.8
1	H	212	ALA	5.7
1	H	88	THR	5.6
1	H	214	ALA	5.4
1	H	86	LEU	5.2
1	H	229	PHE	5.1
1	H	225	ILE	5.1
1	H	207	LEU	5.1
1	H	77	LEU	4.9
1	H	217	THR	4.8
1	H	232	VAL	4.8
1	H	301	TYR	4.8

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Mol	Chain	Res	Type	RSRZ
1	H	84	HIS	4.8
1	H	153	TYR	4.7
1	H	240	ILE	4.7
1	H	127	ALA	4.6
1	H	222	VAL	4.6
1	H	215	HIS	4.6
1	H	302	THR	4.6
1	H	223	GLU	4.5
1	H	213	HIS	4.5
1	D	135	SER	4.5
1	H	288	PHE	4.5
1	H	49	LEU	4.4
1	H	68	PRO	4.4
1	H	85	HIS	4.4
1	H	154	HIS	4.4
1	H	146	PRO	4.4
1	H	150	ALA	4.3
1	H	124	ILE	4.3
1	H	221	GLY	4.3
1	H	216	ARG	4.3
1	H	70	ALA	4.3
1	H	193	SER	4.3
1	H	219	GLY	4.2
1	H	50	ILE	4.2
1	H	160	ILE	4.1
1	H	52	ASP	4.1
1	H	243	ASN	4.1
1	H	238	LEU	4.1
1	H	206	ILE	4.1
1	H	72	ASN	4.0
1	H	203	GLU	4.0
1	H	28	ILE	4.0
1	H	59	VAL	4.0
1	H	303	LYS	4.0
1	H	234	ILE	4.0
1	H	271	SER	4.0
1	H	194	ALA	4.0
1	H	224	PHE	4.0
1	D	84	HIS	3.9
1	H	191	GLN	3.9
1	H	111	ILE	3.9
1	H	190	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	H	93	PRO	3.9
1	H	202	PRO	3.9
1	H	228	PHE	3.9
1	H	269	ALA	3.9
1	H	188	LEU	3.8
1	H	83	ALA	3.8
1	H	300	ILE	3.8
1	H	110	GLU	3.8
1	H	171	PHE	3.8
1	H	109	ALA	3.7
1	H	211	PRO	3.7
1	H	209	GLY	3.7
1	H	99	GLU	3.7
1	H	239	THR	3.7
1	H	91	VAL	3.7
1	H	285	VAL	3.7
1	H	90	LEU	3.7
1	H	140	PRO	3.7
1	H	200	VAL	3.6
1	H	45	LEU	3.6
1	H	220	ILE	3.6
1	H	102	VAL	3.6
1	H	152	TYR	3.6
1	H	20	ILE	3.6
1	H	264	SER	3.6
1	H	18	LEU	3.6
1	H	126	LYS	3.6
1	H	66	ILE	3.6
1	H	130	LEU	3.6
1	H	266	ALA	3.6
1	H	100	LYS	3.6
1	D	55	GLN	3.5
1	H	142	GLN	3.5
1	H	23	PRO	3.5
1	H	267	ALA	3.5
1	H	65	ILE	3.5
1	H	108	GLY	3.5
1	H	92	VAL	3.5
1	H	51	GLU	3.4
1	H	165	PRO	3.4
1	H	79	LEU	3.4
1	H	156	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	H	114	THR	3.4
1	H	284	ILE	3.4
1	H	97	SER	3.4
1	H	245	ALA	3.4
1	H	121	LYS	3.4
1	H	116	SER	3.4
1	H	87	ARG	3.3
1	H	272	LEU	3.3
1	H	204	GLY	3.3
1	H	113	HIS	3.3
1	H	149	PRO	3.3
1	H	148	ASN	3.3
1	H	184	VAL	3.3
1	H	144	LYS	3.3
1	H	265	GLY	3.3
1	E	170	ALA	3.3
1	H	76	GLY	3.3
1	H	299	LYS	3.3
1	H	80	ALA	3.3
1	H	133	THR	3.2
1	H	294	ARG	3.2
1	H	297	SER	3.2
1	H	237	THR	3.2
1	H	185	ALA	3.2
1	A	25	HIS	3.2
1	H	25	HIS	3.2
1	H	262	SER	3.2
1	H	198	VAL	3.2
1	H	279	PRO	3.2
1	H	95	LYS	3.1
1	H	48	TYR	3.1
1	H	138	TYR	3.1
1	H	143	PHE	3.1
1	H	17	ALA	3.1
1	H	125	ARG	3.1
1	H	244	ASP	3.1
1	H	247	ALA	3.1
1	H	227	PRO	3.1
1	H	24	ASN	3.1
1	H	261	GLY	3.1
1	H	201	GLU	3.1
1	H	41	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	H	226	PRO	3.1
1	H	131	ALA	3.0
1	H	192	ASP	3.0
1	H	290	ASP	3.0
1	H	157	ALA	3.0
1	H	253	ALA	3.0
1	H	189	GLN	3.0
1	H	278	LEU	3.0
1	H	210	GLY	3.0
1	H	112	VAL	3.0
1	H	54	LEU	3.0
1	G	235	ASP	3.0
1	H	195	THR	3.0
1	H	287	ILE	3.0
1	H	103	LEU	2.9
1	H	134	ILE	2.9
1	H	64	THR	2.9
1	H	259	LEU	2.9
1	D	85	HIS	2.9
1	H	104	MET	2.9
1	H	164	MET	2.9
1	H	15	LEU	2.9
1	H	55	GLN	2.9
1	G	214	ALA	2.9
1	H	19	PRO	2.9
1	H	123	ALA	2.9
1	H	159	GLU	2.9
1	H	57	GLY	2.9
1	H	181	PHE	2.9
1	H	32	LEU	2.9
1	H	107	LEU	2.9
1	H	78	ALA	2.8
1	H	81	THR	2.8
1	H	246	PHE	2.8
1	E	206	ILE	2.8
1	H	158	PRO	2.8
1	H	172	VAL	2.8
1	H	199	VAL	2.8
1	H	26	SER	2.8
1	A	167	PRO	2.8
1	H	168	ILE	2.8
1	H	295	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	H	182	ALA	2.8
1	H	167	PRO	2.8
1	H	75	ILE	2.8
1	H	230	ASP	2.8
1	E	154	HIS	2.7
1	H	39	GLY	2.7
1	D	281	ASN	2.7
1	G	279	PRO	2.7
1	H	163	ASP	2.7
1	H	147	ALA	2.7
1	B	211	PRO	2.7
1	H	56	ARG	2.7
1	G	193	SER	2.7
1	H	141	MET	2.7
1	A	165	PRO	2.6
1	H	82	GLN	2.6
1	H	187	TYR	2.6
1	E	165	PRO	2.6
1	H	35	PHE	2.6
1	H	98	MET	2.6
1	H	208	ASN	2.6
1	G	2	LEU	2.6
1	G	296	LEU	2.6
1	C	191	GLN	2.6
1	H	298	GLN	2.6
1	H	96	PHE	2.6
1	B	4	GLN	2.6
1	H	101	GLN	2.6
1	H	174	GLY	2.6
1	H	22	VAL	2.6
1	H	286	THR	2.6
1	A	128	GLU	2.5
1	H	94	GLU	2.5
1	H	280	ALA	2.5
1	H	69	THR	2.5
1	A	211	PRO	2.5
1	H	38	GLY	2.5
1	G	212	ALA	2.5
1	E	58	ARG	2.5
1	G	277	ASN	2.5
1	A	1	MET	2.5
1	H	249	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	H	61	ALA	2.5
1	G	300	ILE	2.5
1	H	1	MET	2.5
1	H	14	PRO	2.5
1	H	115	PRO	2.5
1	H	252	LEU	2.5
1	H	241	ALA	2.4
1	H	71	GLY	2.4
1	H	47	ALA	2.4
1	H	36	ASN	2.4
1	H	155	THR	2.4
1	C	25	HIS	2.4
1	H	46	GLY	2.4
1	H	151	ALA	2.4
1	H	62	LYS	2.4
1	C	21	GLU	2.4
1	H	161	LEU	2.4
1	H	289	PRO	2.4
1	B	25	HIS	2.3
1	H	173	ALA	2.3
1	H	242	ASP	2.3
1	H	42	ALA	2.3
1	A	188	LEU	2.3
1	H	21	GLU	2.3
1	H	33	GLU	2.3
1	F	25	HIS	2.3
1	G	98	MET	2.3
1	H	63	THR	2.3
1	H	283	HIS	2.3
1	C	231	GLN	2.3
1	G	1	MET	2.3
1	H	170	ALA	2.3
1	H	186	ALA	2.3
1	G	299	LYS	2.3
1	A	170	ALA	2.2
1	G	211	PRO	2.2
1	H	16	MET	2.2
1	F	3	ILE	2.2
1	G	95	LYS	2.2
1	G	301	TYR	2.2
1	E	56	ARG	2.2
1	G	234	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	1	MET	2.2
1	E	59	VAL	2.1
1	H	260	ILE	2.1
1	H	236	GLN	2.1
1	H	196	LYS	2.1
1	G	275	ALA	2.1
1	H	67	GLU	2.1
1	G	236	GLN	2.1
1	A	232	VAL	2.1
1	H	43	ASP	2.1
1	H	139	VAL	2.1
1	H	12	HIS	2.1
1	H	276	THR	2.1
1	H	248	GLN	2.1
1	B	5	HIS	2.1
1	E	28	ILE	2.1
1	G	240	ILE	2.1
1	G	242	ASP	2.1
1	F	209	GLY	2.1
1	H	282	SER	2.1
1	H	27	HIS	2.1
1	G	257	GLY	2.1
1	H	40	SER	2.0
1	H	263	SER	2.0
1	H	145	ASN	2.0
1	G	25	HIS	2.0
1	E	227	PRO	2.0
1	G	8	GLU	2.0
1	H	296	LEU	2.0
1	E	203	GLU	2.0
1	H	117	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

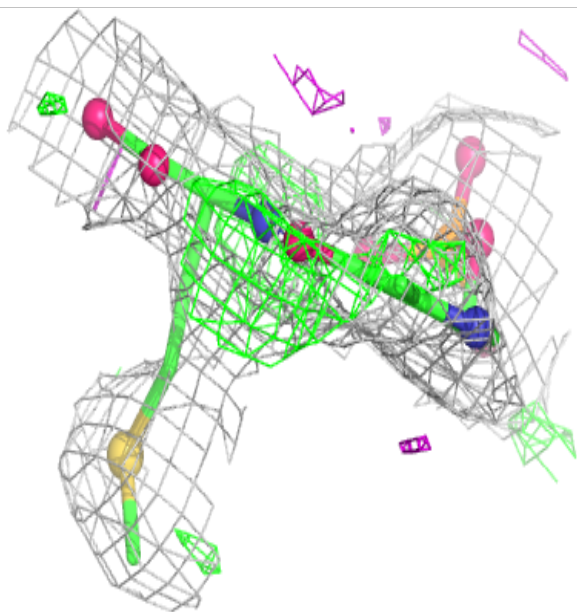
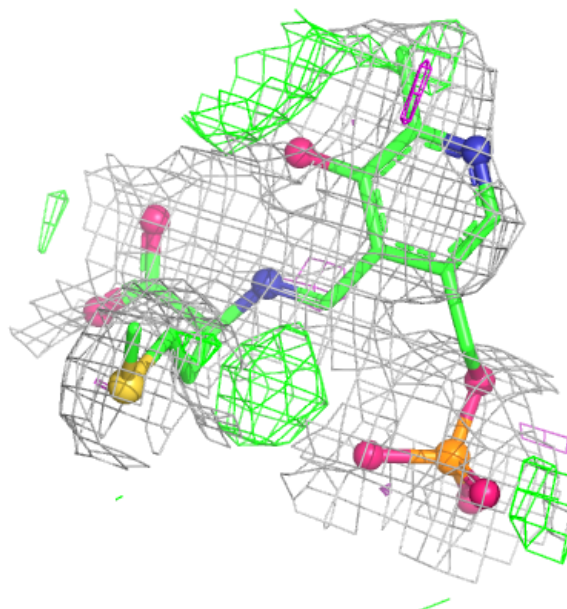
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	G	403	5/5	0.45	0.15	105,106,106,107	0
3	SO4	G	402	5/5	0.54	0.16	121,121,121,121	0
3	SO4	H	403	5/5	0.54	0.23	145,146,146,146	0
3	SO4	H	402	5/5	0.64	0.18	103,104,104,104	0
2	AA5	H	401	24/24	0.64	0.23	85,87,88,89	0
3	SO4	A	403	5/5	0.66	0.17	85,85,86,87	0
3	SO4	E	403	5/5	0.78	0.14	88,88,89,89	0
3	SO4	C	403	5/5	0.84	0.13	69,69,70,70	0
3	SO4	D	403	5/5	0.85	0.13	75,75,76,76	0
3	SO4	F	403	5/5	0.85	0.15	86,86,87,87	0
3	SO4	E	402	5/5	0.85	0.13	78,78,79,79	0
3	SO4	C	402	5/5	0.87	0.14	59,60,61,61	0
3	SO4	B	402	5/5	0.87	0.12	63,64,64,64	0
3	SO4	D	402	5/5	0.88	0.10	65,66,66,67	0
2	AA5	E	401	24/24	0.91	0.16	45,53,57,57	0
3	SO4	B	403	5/5	0.92	0.12	68,68,69,69	0
3	SO4	F	402	5/5	0.94	0.09	61,62,63,64	0
2	AA5	A	401	24/24	0.94	0.11	39,42,49,53	0
2	AA5	G	401	24/24	0.94	0.10	45,47,48,49	0
2	AA5	D	401	24/24	0.95	0.09	25,30,31,33	0
2	AA5	F	401	24/24	0.95	0.10	18,23,27,29	0
3	SO4	A	402	5/5	0.95	0.07	62,63,63,64	0
2	AA5	B	401	24/24	0.96	0.08	6,17,21,25	0
2	AA5	C	401	24/24	0.97	0.08	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.

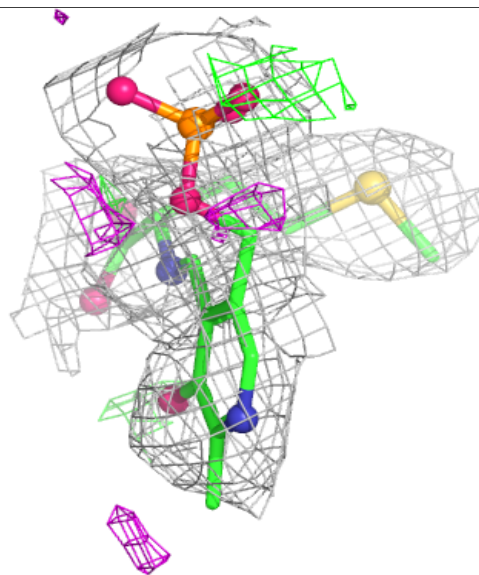
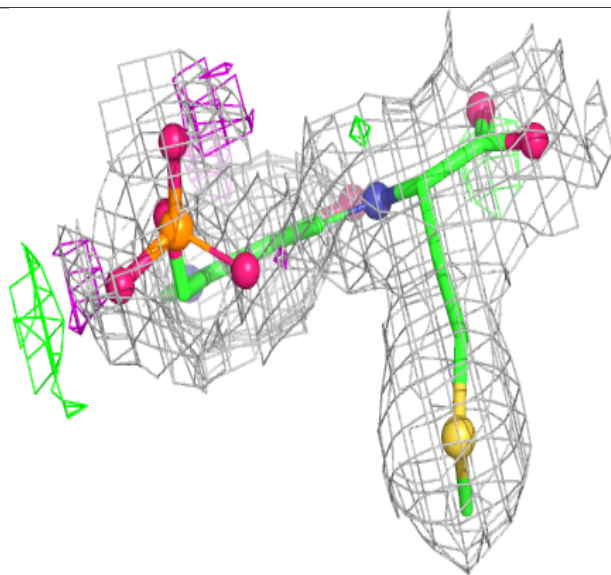
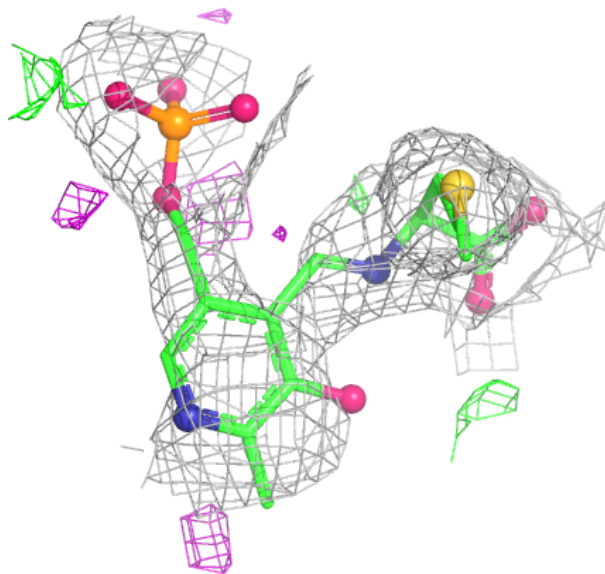
Electron density around AA5 H 401:

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



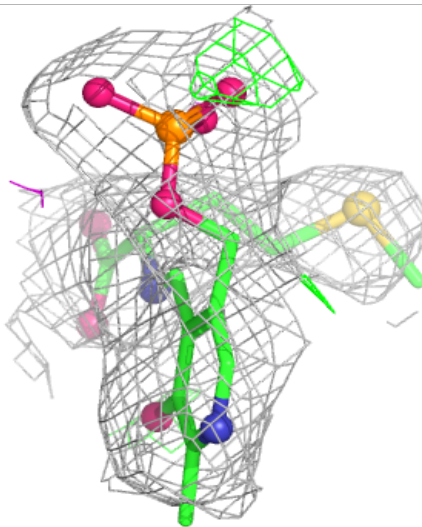
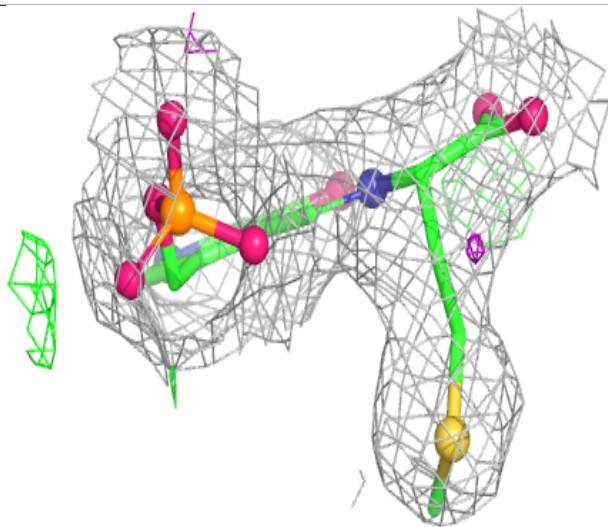
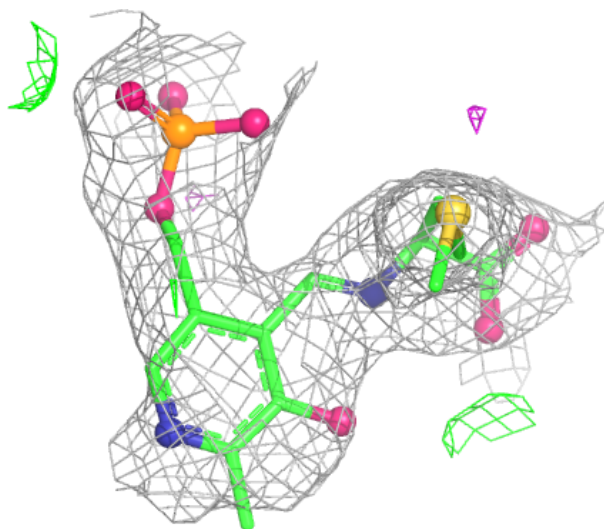
Electron density around AA5 E 401:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



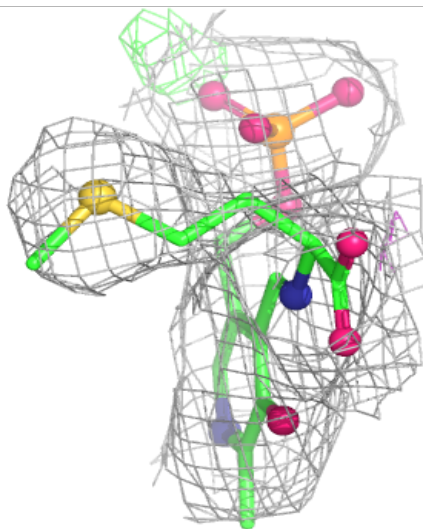
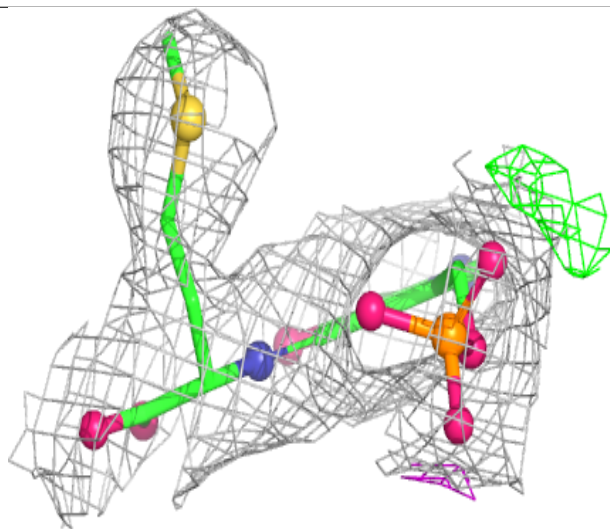
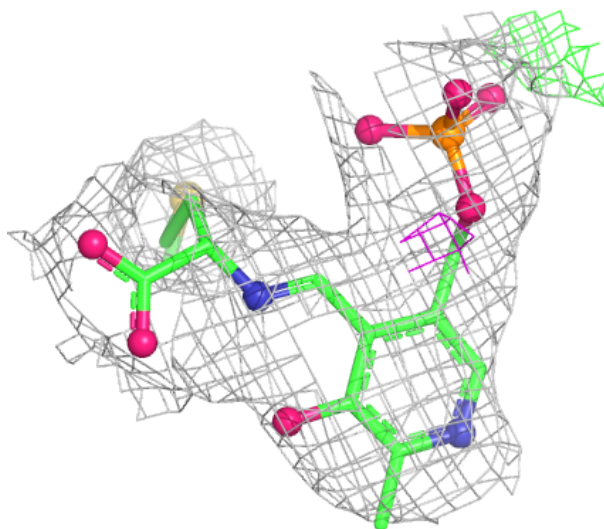
Electron density around AA5 A 401:

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and green (positive)



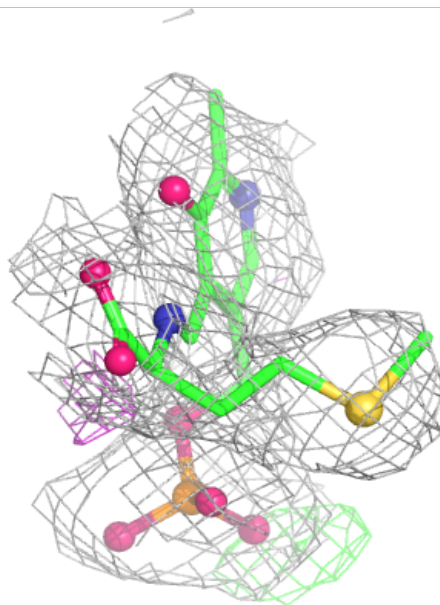
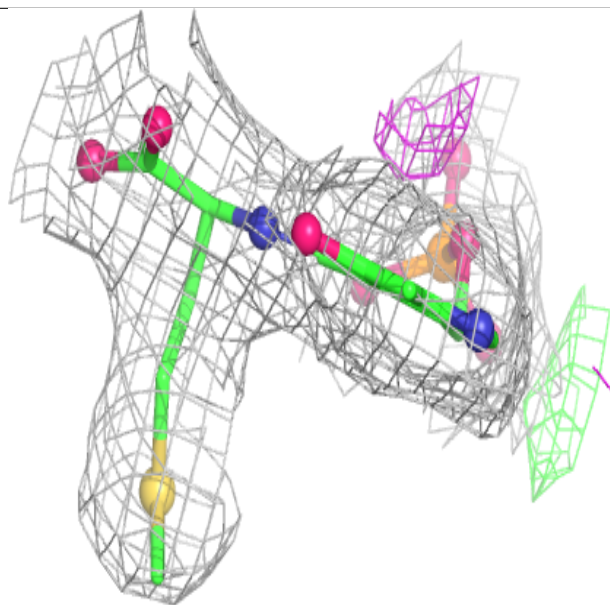
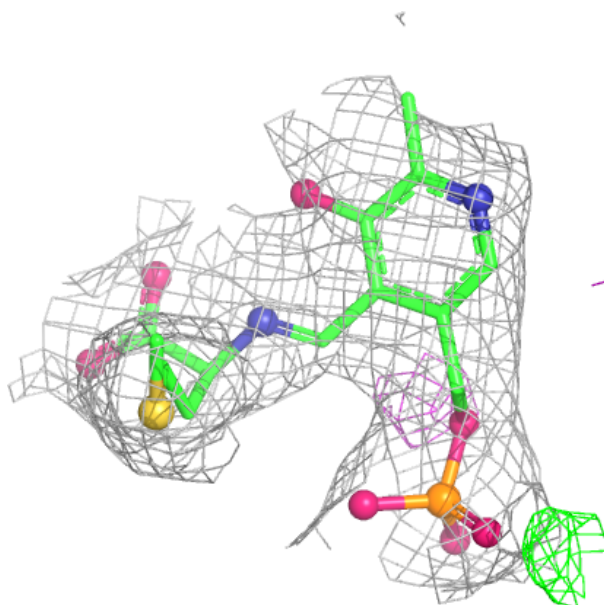
Electron density around AA5 G 401:

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and green (positive)



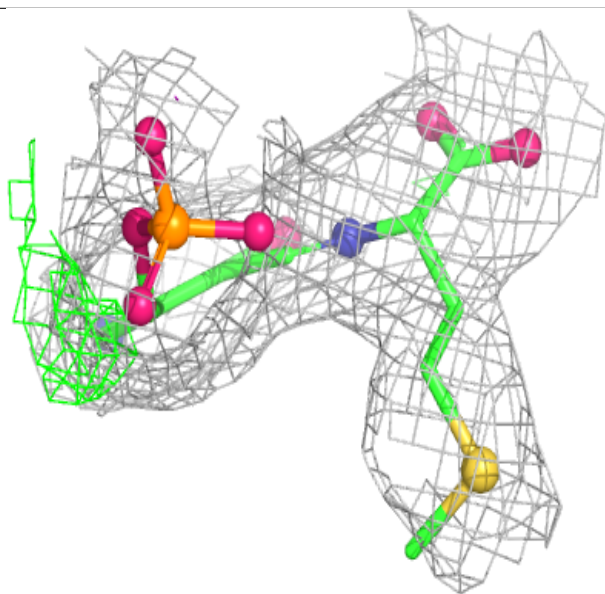
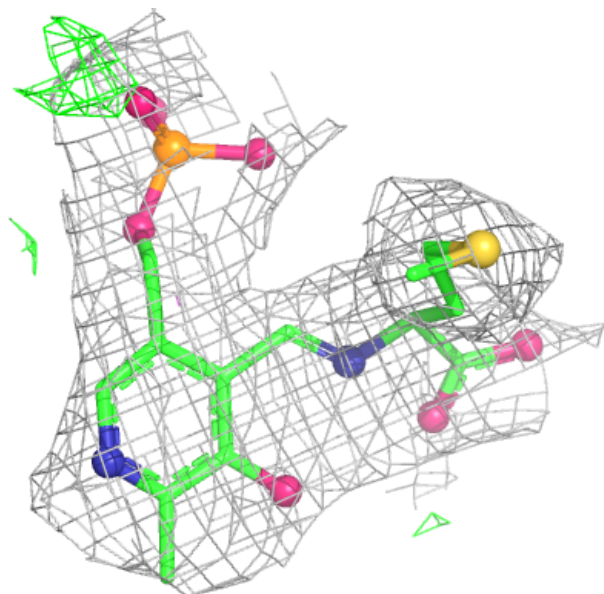
Electron density around AA5 D 401:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



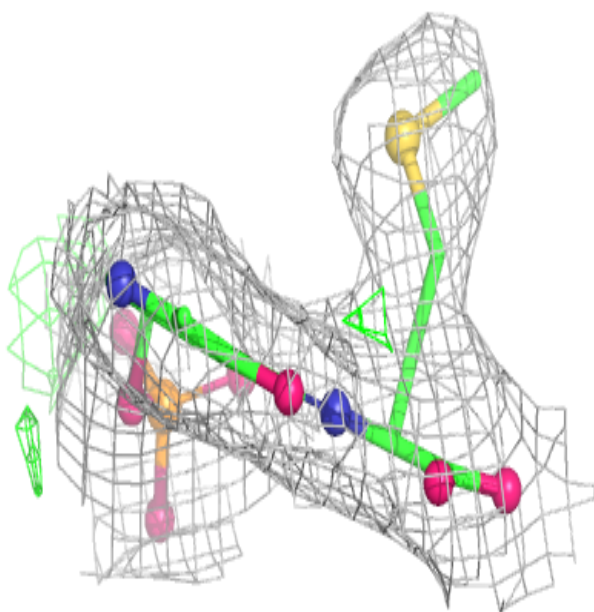
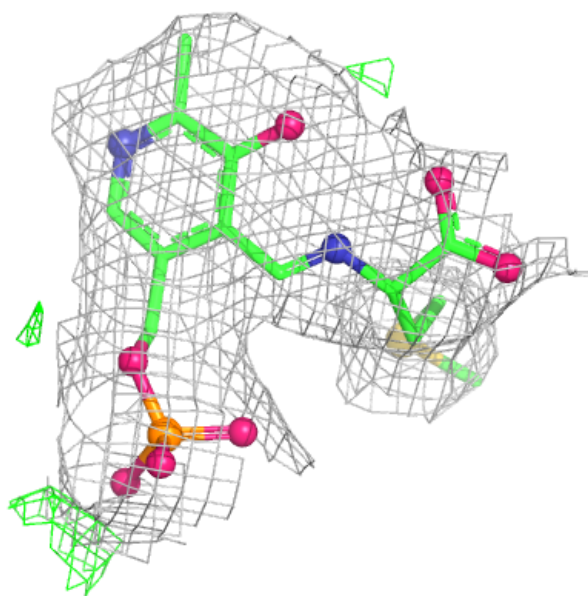
Electron density around AA5 F 401:

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and green (positive)



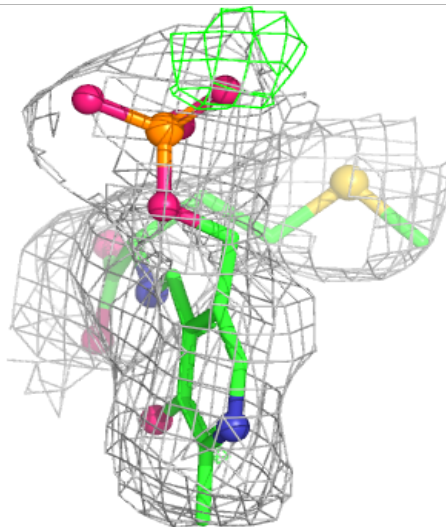
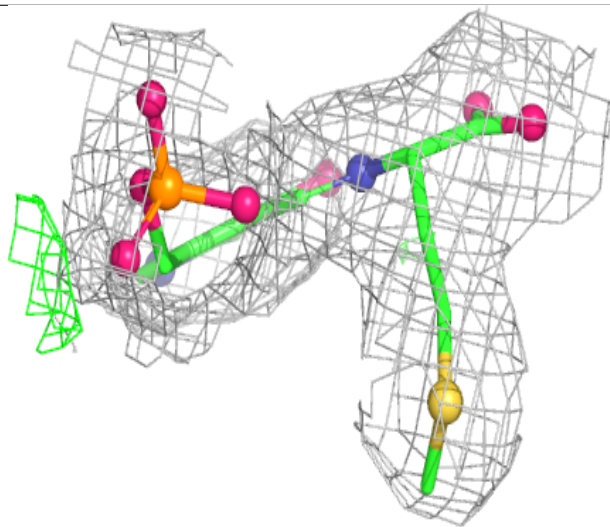
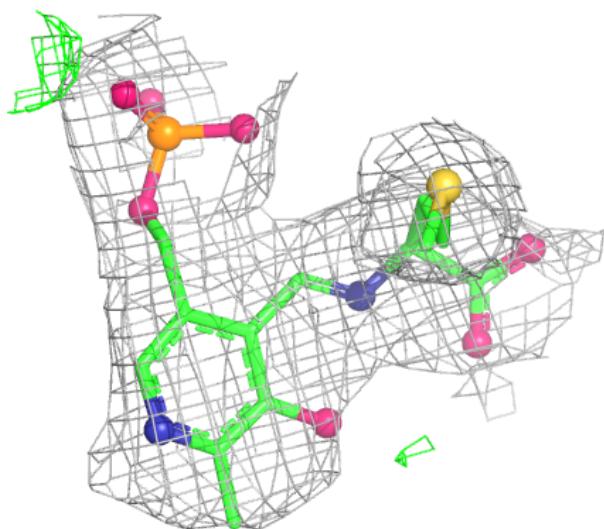
Electron density around AA5 B 401:

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 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 [i](#)

There are no such residues in this entry.