



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:38 PM UTC

PDB ID : 1MLV / pdb_00001mlv
Title : Structure and Catalytic Mechanism of a SET Domain Protein Methyltransferase
Authors : Trievel, R.C.; Beach, B.M.; Dirk, L.M.A.; Houtz, R.L.; Hurley, J.H.
Deposited on : 2002-08-30
Resolution : 2.60 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

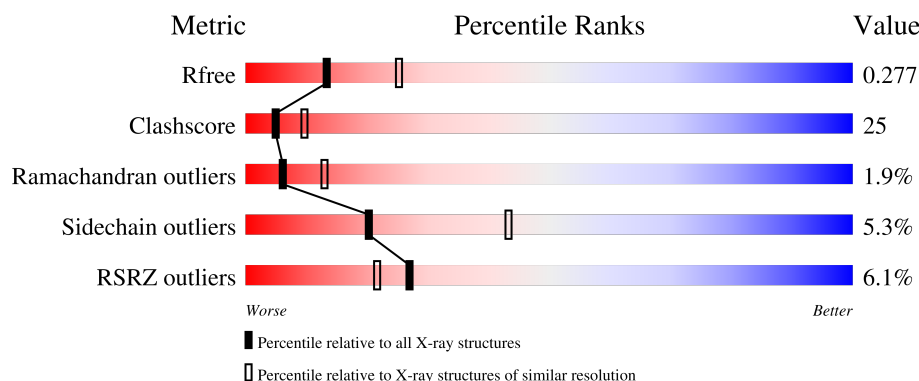
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	444	
1	B	444	
1	C	444	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11270 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.

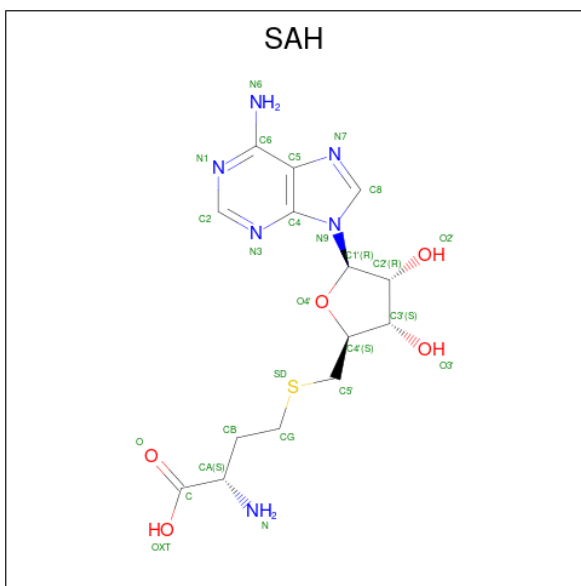
- Molecule 1 is a protein called Ribulose-1,5 biphosphate carboxylase/oxygenase large subunit N-methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	424	Total	C	N	O	S	0	0	0
			3413	2189	562	655	7			
1	B	440	Total	C	N	O	S	0	0	0
			3542	2270	585	680	7			
1	C	438	Total	C	N	O	S	0	0	0
			3526	2262	582	675	7			

There are 21 discrepancies between the modelled and reference sequences:

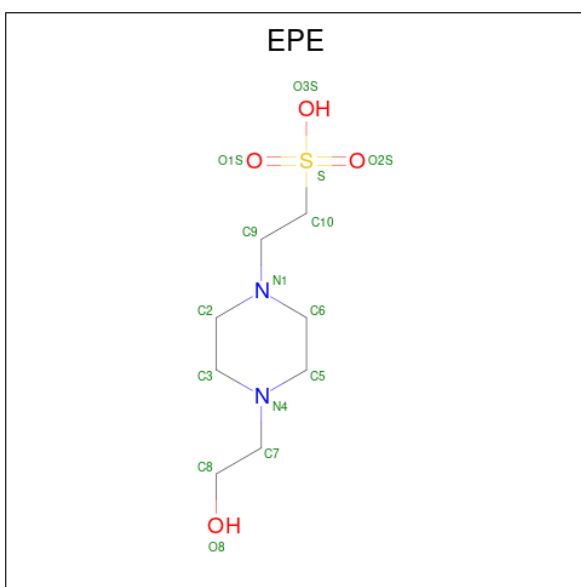
Chain	Residue	Modelled	Actual	Comment	Reference
A	45	MET	-	initiating methionine	UNP Q43088
A	483	GLU	-	engineered mutation	UNP Q43088
A	484	ASN	-	engineered mutation	UNP Q43088
A	485	LEU	-	engineered mutation	UNP Q43088
A	486	TYR	-	engineered mutation	UNP Q43088
A	487	PHE	-	engineered mutation	UNP Q43088
A	488	GLN	-	engineered mutation	UNP Q43088
B	45	MET	-	initiating methionine	UNP Q43088
B	483	GLU	-	engineered mutation	UNP Q43088
B	484	ASN	-	engineered mutation	UNP Q43088
B	485	LEU	-	engineered mutation	UNP Q43088
B	486	TYR	-	engineered mutation	UNP Q43088
B	487	PHE	-	engineered mutation	UNP Q43088
B	488	GLN	-	engineered mutation	UNP Q43088
C	45	MET	-	initiating methionine	UNP Q43088
C	483	GLU	-	engineered mutation	UNP Q43088
C	484	ASN	-	engineered mutation	UNP Q43088
C	485	LEU	-	engineered mutation	UNP Q43088
C	486	TYR	-	engineered mutation	UNP Q43088
C	487	PHE	-	engineered mutation	UNP Q43088
C	488	GLN	-	engineered mutation	UNP Q43088

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	B	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	C	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

- Molecule 3 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

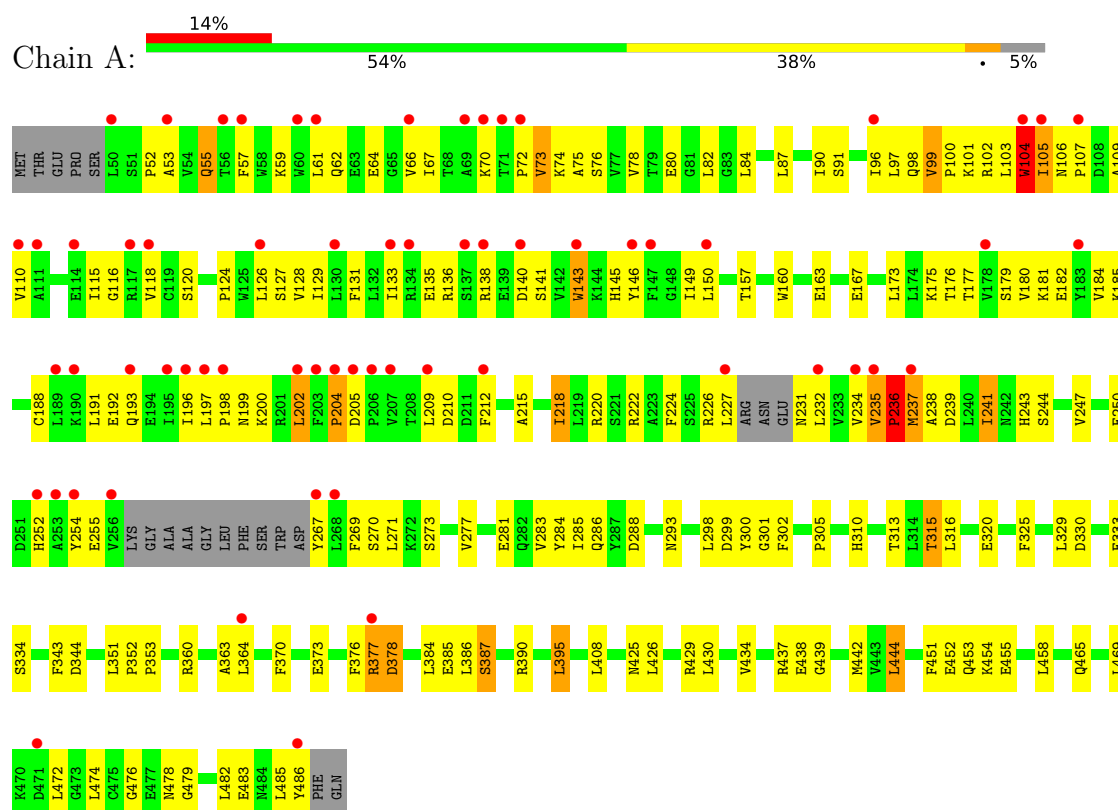
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	220	Total	O	0	0
			220	220		
4	B	228	Total	O	0	0
			228	228		
4	C	218	Total	O	0	0
			218	218		

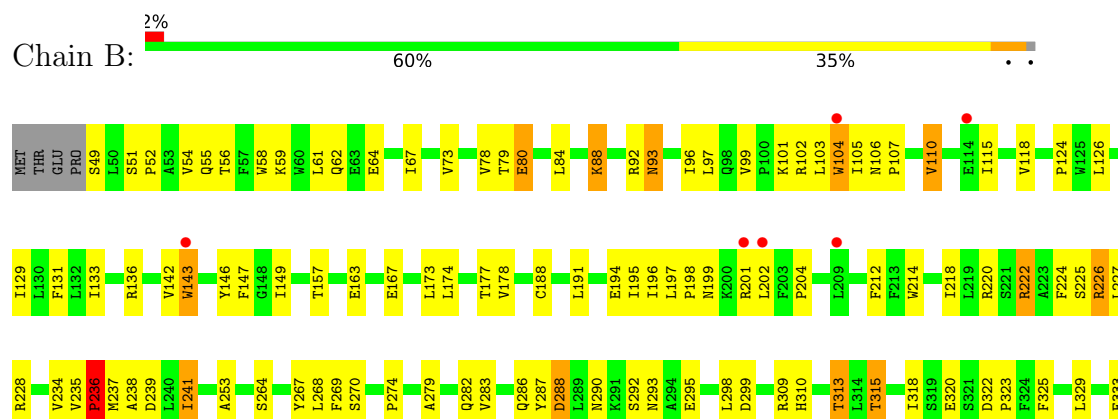
3 Residue-property plots

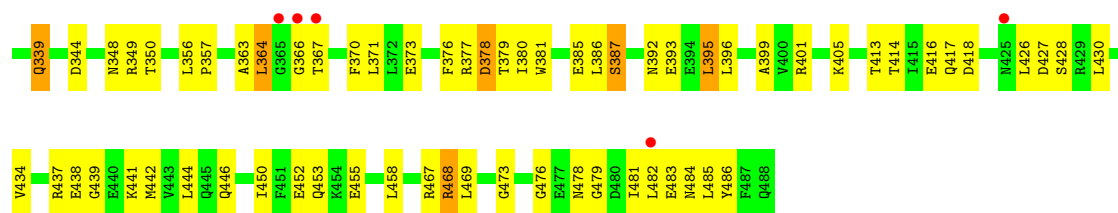
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Ribulose-1,5 biphosphate carboxylase/oxygenase large subunit N-methyltransferase

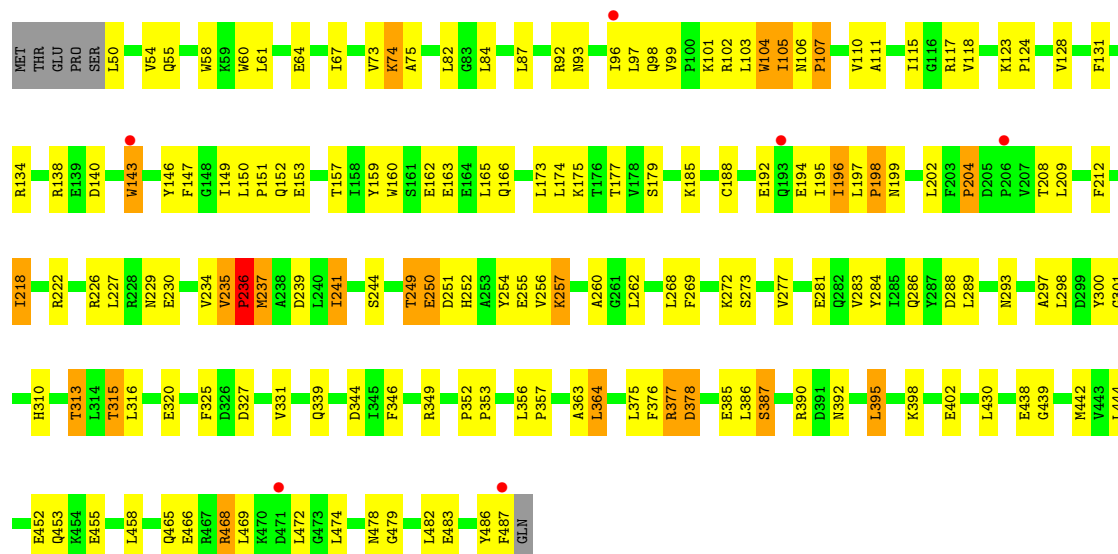


- Molecule 1: Ribulose-1,5 biphosphate carboxylase/oxygenase large subunit N-methyltransferase





- Molecule 1: Ribulose-1,5 biphosphate carboxylase/oxygenase large subunit N-methyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	132.16Å 156.68Å 268.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.78 – 2.60 30.78 – 2.60	Depositor EDS
% Data completeness (in resolution range)	87.4 (30.78-2.60) 87.4 (30.78-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.73 (at 2.61Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.232 , 0.277 0.232 , 0.277	Depositor DCC
R_{free} test set	4270 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	55.0	Xtriage
Anisotropy	0.626	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 50.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11270	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% 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: EPE, SAH

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	0.48	0/3482	0.89	7/4723 (0.1%)
1	B	0.49	0/3617	0.92	9/4906 (0.2%)
1	C	0.47	0/3601	0.90	7/4886 (0.1%)
All	All	0.48	0/10700	0.91	23/14515 (0.2%)

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	235	VAL	CA-C-N	8.44	130.39	119.84
1	C	235	VAL	C-N-CA	8.44	130.39	119.84
1	A	99	VAL	CA-C-N	7.02	127.27	119.90
1	A	99	VAL	C-N-CA	7.02	127.27	119.90
1	A	235	VAL	CA-C-N	6.27	127.67	119.84
1	A	235	VAL	C-N-CA	6.27	127.67	119.84
1	B	235	VAL	CA-C-N	6.21	127.60	119.84
1	B	235	VAL	C-N-CA	6.21	127.60	119.84
1	B	452	GLU	N-CA-C	-6.00	104.31	111.69
1	B	290	ASN	N-CA-C	5.82	120.53	113.38
1	A	300	TYR	N-CA-C	-5.75	101.41	109.69
1	C	236	PRO	N-CA-C	5.71	124.23	112.47
1	B	222	ARG	N-CA-C	5.66	120.45	112.93
1	A	64	GLU	N-CA-C	-5.49	106.59	113.72
1	C	452	GLU	N-CA-C	-5.49	105.38	111.36
1	B	268	LEU	N-CA-C	5.47	118.40	109.59
1	C	196	ILE	N-CA-C	5.47	115.67	110.53
1	C	430	LEU	N-CA-C	-5.41	105.46	111.36
1	B	236	PRO	N-CA-C	5.32	123.42	112.47
1	C	339	GLN	N-CA-C	-5.30	105.92	112.38
1	A	452	GLU	N-CA-C	-5.29	105.59	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	339	GLN	N-CA-C	-5.10	106.16	112.38
1	B	196	ILE	N-CA-C	5.09	115.31	110.42

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	3413	0	3384	194	0
1	B	3542	0	3501	167	0
1	C	3526	0	3488	191	0
2	A	26	0	19	1	0
2	B	26	0	19	1	0
2	C	26	0	19	2	0
3	A	15	0	18	3	0
3	B	15	0	17	5	0
3	C	15	0	18	3	0
4	A	220	0	0	22	0
4	B	228	0	0	21	0
4	C	218	0	0	23	0
All	All	11270	0	10483	529	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 25.

All (529) 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:C:50:LEU:HD22	1:C:54:VAL:HG11	1.42	1.02
1:B:468:ARG:HB3	1:B:468:ARG:HH11	1.22	1.00
1:A:74:LYS:HB3	1:A:87:LEU:HD21	1.44	0.98
1:B:438:GLU:HG2	1:B:442:MET:HE2	1.46	0.97
1:B:364:LEU:HB3	4:B:947:HOH:O	1.66	0.95
1:A:469:LEU:HD12	1:C:395:LEU:HD22	1.51	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:177:THR:HB	4:C:851:HOH:O	1.71	0.91
1:B:173:LEU:O	1:B:177:THR:HG23	1.72	0.89
1:A:97:LEU:HD22	1:A:237:MET:HG3	1.51	0.89
1:C:249:THR:HG22	1:C:251:ASP:HB2	1.53	0.89
1:B:439:GLY:HA2	1:B:442:MET:HE3	1.57	0.87
1:A:84:LEU:HD12	1:A:241:ILE:HG23	1.59	0.84
1:C:104:TRP:HH2	1:C:269:PHE:H	1.26	0.84
1:C:222:ARG:HA	3:C:802:EPE:H71	1.59	0.84
1:A:97:LEU:HD11	1:A:238:ALA:HB2	1.60	0.82
1:B:67:ILE:HD11	1:B:237:MET:SD	2.20	0.82
1:A:395:LEU:HD22	1:B:469:LEU:HD12	1.61	0.81
1:C:315:THR:HG22	4:C:804:HOH:O	1.81	0.81
1:B:78:VAL:HG11	1:B:282:GLN:HE22	1.46	0.81
1:B:367:THR:HA	4:B:892:HOH:O	1.78	0.80
1:C:237:MET:N	4:C:951:HOH:O	2.10	0.80
1:A:199:ASN:HB3	1:A:202:LEU:HD13	1.65	0.79
1:A:472:LEU:HD13	1:A:474:LEU:HD21	1.65	0.79
1:B:468:ARG:HH11	1:B:468:ARG:CB	1.96	0.79
1:B:222:ARG:HA	3:B:801:EPE:H71	1.66	0.78
1:B:84:LEU:HD12	1:B:241:ILE:HG23	1.65	0.78
1:B:286:GLN:HE21	1:B:288:ASP:H	1.32	0.78
1:A:101:LYS:HB2	1:A:267:TYR:HB2	1.65	0.78
1:C:226:ARG:HB3	1:C:252:HIS:NE2	1.99	0.77
1:A:101:LYS:HA	1:A:104:TRP:CD2	2.20	0.77
1:A:226:ARG:O	1:A:227:LEU:HD22	1.86	0.76
1:B:395:LEU:HD22	1:C:469:LEU:HD12	1.68	0.76
1:B:428:SER:HB2	4:B:851:HOH:O	1.85	0.75
1:B:96:ILE:HD11	1:B:283:VAL:HG11	1.67	0.74
1:A:101:LYS:HA	1:A:104:TRP:CE2	2.22	0.74
1:B:110:VAL:HG13	1:B:131:PHE:HB2	1.68	0.74
1:B:315:THR:HG22	4:C:806:HOH:O	1.89	0.73
1:C:104:TRP:CH2	1:C:269:PHE:HB2	2.24	0.73
1:B:107:PRO:O	1:B:110:VAL:HG23	1.89	0.72
1:A:59:LYS:HD3	1:A:62:GLN:OE1	1.89	0.72
1:B:313:THR:HG21	1:C:478:ASN:CG	2.15	0.72
1:C:146:TYR:CE1	1:C:236:PRO:HA	2.25	0.72
1:C:468:ARG:HH11	1:C:468:ARG:HB3	1.55	0.71
1:A:73:VAL:H	1:A:87:LEU:HD12	1.54	0.71
1:A:150:LEU:HD13	1:A:218:ILE:CD1	2.21	0.71
1:C:173:LEU:O	1:C:177:THR:HG23	1.91	0.71
1:B:199:ASN:HB3	1:B:202:LEU:HD13	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:LEU:O	1:B:333:GLU:HG3	1.90	0.70
1:C:286:GLN:HE21	1:C:288:ASP:N	1.88	0.70
1:C:107:PRO:O	1:C:110:VAL:HG22	1.90	0.70
1:C:67:ILE:HD11	1:C:237:MET:SD	2.32	0.70
1:A:286:GLN:HE21	1:A:288:ASP:C	2.00	0.70
1:B:99:VAL:O	1:B:104:TRP:HH2	1.73	0.70
1:C:286:GLN:HE21	1:C:288:ASP:H	1.41	0.69
1:C:74:LYS:HD2	1:C:75:ALA:O	1.92	0.69
1:A:177:THR:HG22	1:A:298:LEU:HD12	1.73	0.69
1:A:439:GLY:HA2	1:A:442:MET:HE3	1.75	0.69
1:C:54:VAL:HA	1:C:149:ILE:HD11	1.74	0.69
1:C:250:GLU:C	1:C:252:HIS:H	2.00	0.69
1:C:286:GLN:NE2	1:C:288:ASP:H	1.91	0.69
1:C:479:GLY:O	1:C:483:GLU:HG2	1.92	0.69
1:C:97:LEU:HD22	1:C:237:MET:SD	2.34	0.68
1:B:478:ASN:ND2	1:B:481:ILE:HG13	2.07	0.68
1:A:239:ASP:HB3	4:A:994:HOH:O	1.93	0.68
1:A:97:LEU:HD22	1:A:237:MET:CG	2.24	0.67
1:B:99:VAL:O	1:B:104:TRP:CH2	2.46	0.67
1:A:124:PRO:HA	4:A:1001:HOH:O	1.94	0.67
1:B:286:GLN:NE2	1:B:288:ASP:H	1.92	0.67
1:A:197:LEU:HB2	1:A:198:PRO:HD3	1.77	0.67
1:C:97:LEU:HD22	1:C:237:MET:HE3	1.76	0.67
1:C:188:CYS:HB3	1:C:212:PHE:CD2	2.29	0.67
1:A:124:PRO:O	1:A:128:VAL:HG23	1.96	0.66
1:A:202:LEU:H	1:A:202:LEU:HD12	1.61	0.66
1:B:174:LEU:O	1:B:178:VAL:HG23	1.95	0.66
1:C:99:VAL:O	1:C:104:TRP:HH2	1.79	0.66
1:B:97:LEU:HD22	1:B:237:MET:SD	2.36	0.65
1:A:241:ILE:O	1:A:241:ILE:HD12	1.96	0.65
1:C:438:GLU:HG2	1:C:442:MET:HE2	1.76	0.65
1:A:99:VAL:O	1:A:104:TRP:HH2	1.80	0.65
1:A:131:PHE:CE2	1:A:135:GLU:HG3	2.32	0.65
1:A:247:VAL:HG11	4:A:920:HOH:O	1.97	0.65
1:C:97:LEU:HD22	1:C:237:MET:CE	2.26	0.64
1:A:202:LEU:O	1:A:204:PRO:HD3	1.98	0.64
1:B:226:ARG:HD3	4:B:1004:HOH:O	1.96	0.64
1:A:109:ALA:HB2	4:A:827:HOH:O	1.97	0.64
1:A:98:GLN:HA	1:A:269:PHE:O	1.98	0.64
1:B:101:LYS:HA	1:B:104:TRP:CD2	2.33	0.63
1:C:96:ILE:HD11	1:C:273:SER:HB2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:GLN:HE21	1:B:288:ASP:C	2.07	0.63
1:A:73:VAL:CG2	1:A:84:LEU:HB3	2.29	0.62
1:B:399:ALA:HB1	1:C:472:LEU:HD12	1.81	0.62
1:B:241:ILE:HD12	1:B:241:ILE:O	1.99	0.62
1:C:61:LEU:HB3	1:C:67:ILE:HG12	1.82	0.62
1:C:250:GLU:HG3	1:C:250:GLU:O	1.98	0.62
1:C:73:VAL:HG21	1:C:84:LEU:HB3	1.82	0.62
1:C:149:ILE:HG22	4:C:944:HOH:O	1.98	0.62
1:A:97:LEU:CD1	1:A:238:ALA:HB2	2.30	0.61
1:A:286:GLN:NE2	1:A:288:ASP:H	1.97	0.61
1:B:78:VAL:HG12	1:B:80:GLU:H	1.65	0.61
1:B:142:VAL:HG23	4:B:914:HOH:O	2.00	0.61
1:C:150:LEU:HD13	1:C:218:ILE:CD1	2.31	0.61
1:A:110:VAL:HG12	1:A:131:PHE:HB2	1.82	0.61
1:B:286:GLN:HE21	1:B:288:ASP:N	1.99	0.61
1:A:286:GLN:HE21	1:A:288:ASP:N	1.97	0.61
1:A:74:LYS:HB3	1:A:87:LEU:CD2	2.28	0.60
1:B:376:PHE:C	1:B:378:ASP:H	2.09	0.60
1:B:414:THR:HG23	1:B:417:GLN:OE1	2.01	0.60
1:A:192:GLU:HA	1:A:196:ILE:HB	1.83	0.60
1:C:124:PRO:O	1:C:128:VAL:HG23	2.01	0.60
1:A:96:ILE:HD11	1:A:273:SER:HB2	1.83	0.60
1:B:202:LEU:HD12	1:B:202:LEU:N	2.17	0.60
1:B:483:GLU:HA	1:B:486:TYR:CD2	2.37	0.60
1:C:466:GLU:HB2	4:C:836:HOH:O	2.02	0.60
1:B:118:VAL:HG22	4:B:992:HOH:O	2.02	0.59
1:B:228:ARG:HA	4:B:994:HOH:O	2.00	0.59
1:A:286:GLN:HE21	1:A:288:ASP:H	1.50	0.59
1:C:468:ARG:HH11	1:C:468:ARG:CB	2.14	0.59
1:B:320:GLU:HA	1:B:325:PHE:CD1	2.38	0.59
1:B:484:ASN:HB2	4:B:874:HOH:O	2.01	0.59
1:C:286:GLN:HE21	1:C:288:ASP:C	2.10	0.59
1:B:78:VAL:CG1	1:B:80:GLU:OE2	2.51	0.59
1:C:202:LEU:O	1:C:204:PRO:HD3	2.03	0.59
1:C:239:ASP:O	3:C:802:EPE:O8	2.21	0.59
1:C:99:VAL:O	1:C:104:TRP:CH2	2.56	0.59
1:C:320:GLU:HA	1:C:325:PHE:CD1	2.38	0.59
1:C:208:THR:HB	4:C:967:HOH:O	2.03	0.58
1:A:210:ASP:HB3	4:A:998:HOH:O	2.02	0.58
1:B:202:LEU:O	1:B:204:PRO:HD3	2.03	0.58
1:B:104:TRP:CH2	1:B:269:PHE:HB2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:GLU:HG2	4:B:1011:HOH:O	2.03	0.58
1:C:227:LEU:HD11	1:C:256:VAL:HG23	1.84	0.58
1:A:185:LYS:HG3	1:A:209:LEU:HD21	1.86	0.58
1:A:395:LEU:CD2	1:B:469:LEU:HD12	2.33	0.58
1:A:99:VAL:O	1:A:104:TRP:CH2	2.56	0.58
1:A:110:VAL:HG12	1:A:131:PHE:CG	2.39	0.58
1:A:330:ASP:O	1:A:334:SER:HB2	2.04	0.58
1:B:197:LEU:HB2	1:B:198:PRO:HD3	1.85	0.58
1:C:103:LEU:O	1:C:143:TRP:CZ3	2.57	0.58
1:A:110:VAL:HG12	1:A:131:PHE:CB	2.34	0.57
1:B:124:PRO:HG2	4:B:949:HOH:O	2.03	0.57
1:A:150:LEU:HD13	1:A:218:ILE:HD13	1.84	0.57
1:A:222:ARG:NH1	1:A:239:ASP:OD2	2.34	0.57
1:C:386:LEU:HB3	4:C:1016:HOH:O	2.05	0.57
1:C:185:LYS:HG3	1:C:209:LEU:HD21	1.86	0.57
1:A:227:LEU:HD12	1:A:255:GLU:OE1	2.04	0.57
1:B:395:LEU:CD2	1:C:469:LEU:HD12	2.35	0.57
1:A:57:PHE:O	1:A:61:LEU:HG	2.05	0.57
1:A:438:GLU:CD	1:A:442:MET:HE2	2.30	0.57
1:A:104:TRP:CH2	1:A:269:PHE:HB2	2.40	0.56
1:C:110:VAL:HG12	1:C:131:PHE:CG	2.39	0.56
1:B:286:GLN:HE22	1:B:309:ARG:HH22	1.54	0.56
1:B:376:PHE:O	1:B:378:ASP:N	2.37	0.56
1:B:467:ARG:HD2	4:B:1021:HOH:O	2.05	0.56
1:B:363:ALA:O	1:B:364:LEU:C	2.48	0.56
1:A:454:LYS:NZ	1:A:454:LYS:HB3	2.20	0.56
1:B:61:LEU:HB3	1:B:67:ILE:HG12	1.87	0.56
1:A:173:LEU:O	1:A:177:THR:HG23	2.05	0.56
1:C:92:ARG:HB2	1:C:92:ARG:HH11	1.71	0.56
1:C:376:PHE:C	1:C:378:ASP:H	2.14	0.56
1:A:286:GLN:NE2	1:A:288:ASP:C	2.64	0.56
1:A:320:GLU:HA	1:A:325:PHE:CD1	2.41	0.56
1:A:465:GLN:HB3	1:C:395:LEU:HD11	1.87	0.56
1:B:110:VAL:CG1	1:B:131:PHE:HB2	2.34	0.56
1:A:118:VAL:HG22	4:A:812:HOH:O	2.06	0.56
1:C:157:THR:OG1	1:C:177:THR:HG21	2.06	0.56
1:C:194:GLU:C	1:C:195:ILE:HD12	2.31	0.56
1:A:115:ILE:HA	4:A:812:HOH:O	2.06	0.55
1:B:92:ARG:O	1:B:93:ASN:HB2	2.04	0.55
1:B:202:LEU:C	1:B:204:PRO:HD3	2.32	0.55
1:B:367:THR:HG23	4:B:892:HOH:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:LYS:HD2	4:A:956:HOH:O	2.05	0.55
1:C:188:CYS:HB3	1:C:212:PHE:CE2	2.41	0.55
1:C:97:LEU:C	1:C:97:LEU:HD12	2.32	0.55
1:B:222:ARG:O	3:B:801:EPE:H32	2.07	0.55
1:B:313:THR:HB	1:B:344:ASP:OD1	2.07	0.55
1:A:192:GLU:O	1:A:197:LEU:HG	2.07	0.55
1:B:438:GLU:CG	1:B:442:MET:HE2	2.29	0.55
1:A:53:ALA:C	1:A:149:ILE:HD11	2.32	0.54
1:A:100:PRO:HD2	1:A:103:LEU:HD12	1.87	0.54
1:B:446:GLN:O	1:B:450:ILE:HG13	2.08	0.54
1:A:167:GLU:HG3	1:A:437:ARG:NH1	2.22	0.54
1:A:202:LEU:HD12	1:A:202:LEU:N	2.21	0.54
1:A:313:THR:HB	1:A:344:ASP:OD1	2.07	0.54
1:B:386:LEU:O	1:B:387:SER:CB	2.55	0.54
1:B:386:LEU:O	1:B:387:SER:HB3	2.06	0.54
1:A:315:THR:HG22	4:B:893:HOH:O	2.06	0.54
1:B:78:VAL:HG11	1:B:282:GLN:NE2	2.17	0.54
1:A:182:GLU:HG3	4:A:1014:HOH:O	2.08	0.54
1:A:376:PHE:C	1:A:378:ASP:H	2.15	0.54
1:C:222:ARG:NH2	2:C:702:SAH:O	2.41	0.54
1:C:250:GLU:HG2	1:C:289:LEU:CD1	2.37	0.54
1:A:160:TRP:CD1	1:A:429:ARG:HD3	2.43	0.54
1:A:474:LEU:HD22	1:C:316:LEU:CD2	2.37	0.54
1:C:455:GLU:O	1:C:458:LEU:HB2	2.07	0.53
1:A:301:GLY:HA3	4:A:805:HOH:O	2.08	0.53
1:A:479:GLY:O	1:A:483:GLU:HG2	2.08	0.53
1:B:118:VAL:HG13	4:B:992:HOH:O	2.08	0.53
1:C:222:ARG:NH1	1:C:239:ASP:CG	2.67	0.53
1:A:386:LEU:O	1:A:387:SER:CB	2.56	0.53
1:B:239:ASP:HB2	3:B:801:EPE:O8	2.08	0.53
1:C:99:VAL:O	1:C:268:LEU:HB2	2.09	0.53
1:A:224:PHE:HA	3:A:800:EPE:H101	1.89	0.53
1:A:238:ALA:HB1	1:A:271:LEU:HD22	1.90	0.53
1:B:103:LEU:O	1:B:143:TRP:HZ3	1.92	0.53
1:C:313:THR:HB	1:C:344:ASP:OD1	2.08	0.53
1:C:61:LEU:CD1	1:C:237:MET:HB2	2.39	0.53
1:C:202:LEU:N	1:C:202:LEU:HD12	2.24	0.53
1:A:110:VAL:HG12	1:A:131:PHE:CD1	2.44	0.53
1:B:88:LYS:HA	1:B:279:ALA:HB2	1.91	0.53
1:C:160:TRP:HB2	1:C:165:LEU:HD21	1.91	0.53
1:C:96:ILE:HD13	1:C:283:VAL:HG11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:GLU:O	1:A:255:GLU:HG3	2.09	0.52
1:C:293:ASN:HD22	1:C:310:HIS:CD2	2.27	0.52
1:B:202:LEU:HD12	1:B:202:LEU:H	1.75	0.52
1:C:92:ARG:HB2	1:C:92:ARG:NH1	2.25	0.52
1:C:250:GLU:C	1:C:252:HIS:N	2.67	0.52
1:C:140:ASP:HA	4:C:882:HOH:O	2.09	0.52
1:A:116:GLY:HA2	4:A:943:HOH:O	2.09	0.52
1:A:145:HIS:HA	4:A:829:HOH:O	2.08	0.52
1:B:427:ASP:HB3	4:B:977:HOH:O	2.08	0.52
1:C:74:LYS:HG2	1:C:87:LEU:HD21	1.91	0.52
1:C:84:LEU:HD12	1:C:241:ILE:HG23	1.92	0.52
1:C:301:GLY:HA3	4:C:812:HOH:O	2.10	0.52
1:B:349:ARG:NH2	4:B:941:HOH:O	2.42	0.52
1:C:96:ILE:CD1	1:C:283:VAL:HG11	2.40	0.52
1:A:430:LEU:O	1:A:434:VAL:HG23	2.10	0.52
1:A:73:VAL:HG23	1:A:84:LEU:HB3	1.92	0.52
1:A:120:SER:HA	4:A:826:HOH:O	2.10	0.51
1:C:229:ASN:O	1:C:230:GLU:HG2	2.10	0.51
1:A:150:LEU:HD13	1:A:218:ILE:HD12	1.93	0.51
1:B:348:ASN:H	1:B:446:GLN:HE22	1.59	0.51
1:C:222:ARG:HH11	1:C:239:ASP:CG	2.18	0.51
1:A:106:ASN:HB2	1:A:107:PRO:HD2	1.92	0.51
1:B:194:GLU:C	1:B:195:ILE:HD12	2.35	0.51
1:B:264:SER:HA	1:B:267:TYR:CZ	2.46	0.51
1:C:104:TRP:CH2	1:C:269:PHE:N	2.78	0.51
1:A:222:ARG:HA	3:A:800:EPE:H71	1.91	0.51
1:A:232:LEU:HD12	1:A:232:LEU:N	2.25	0.51
1:B:222:ARG:HH11	1:B:239:ASP:CG	2.18	0.51
1:B:287:TYR:O	1:B:288:ASP:HB2	2.10	0.51
1:C:386:LEU:O	1:C:387:SER:CB	2.58	0.51
1:B:49:SER:O	1:B:52:PRO:HG2	2.11	0.50
1:B:103:LEU:O	1:B:143:TRP:CZ3	2.63	0.50
1:B:224:PHE:CD2	3:B:801:EPE:H22	2.47	0.50
1:C:438:GLU:CG	1:C:442:MET:HE2	2.41	0.50
1:B:310:HIS:HE1	4:B:993:HOH:O	1.93	0.50
1:C:192:GLU:HA	1:C:196:ILE:HD12	1.93	0.50
1:A:72:PRO:HA	1:A:87:LEU:HB2	1.94	0.50
1:A:90:ILE:HG22	1:A:91:SER:N	2.26	0.50
1:C:104:TRP:NE1	4:C:895:HOH:O	2.40	0.50
1:A:110:VAL:HG21	1:A:127:SER:HB3	1.94	0.50
1:B:430:LEU:O	1:B:434:VAL:HG23	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:286:GLN:NE2	1:C:288:ASP:C	2.69	0.50
1:A:99:VAL:HG12	1:A:104:TRP:HZ3	1.77	0.50
1:A:136:ARG:NH1	4:A:803:HOH:O	2.45	0.50
1:B:323:PRO:HB3	1:C:375:LEU:HD21	1.93	0.50
1:C:153:GLU:HG2	1:C:159:TYR:CD1	2.46	0.50
1:B:51:SER:N	1:B:52:PRO:HD2	2.27	0.50
1:C:101:LYS:HA	1:C:104:TRP:CD2	2.47	0.50
1:A:486:TYR:HA	1:C:123:LYS:HD2	1.94	0.50
1:A:72:PRO:O	1:A:73:VAL:HB	2.12	0.49
1:A:220:ARG:HD3	1:A:299:ASP:OD1	2.10	0.49
1:B:293:ASN:HD22	1:B:310:HIS:CD2	2.30	0.49
1:A:78:VAL:HG23	1:A:80:GLU:HG2	1.94	0.49
1:B:227:LEU:HD21	1:B:269:PHE:HE1	1.76	0.49
1:A:188:CYS:SG	1:A:212:PHE:CD2	3.05	0.49
1:B:376:PHE:C	1:B:378:ASP:N	2.70	0.49
1:C:106:ASN:HB2	1:C:107:PRO:HD2	1.93	0.49
1:A:239:ASP:C	3:A:800:EPE:O8	2.55	0.49
1:B:92:ARG:HG3	1:B:274:PRO:O	2.11	0.49
1:B:177:THR:HG22	1:B:298:LEU:HD12	1.94	0.49
1:B:238:ALA:O	1:B:241:ILE:HG13	2.12	0.49
1:B:380:ILE:HG23	1:B:381:TRP:N	2.27	0.49
1:B:143:TRP:CD1	1:B:143:TRP:H	2.31	0.49
1:C:197:LEU:C	1:C:199:ASN:H	2.21	0.49
1:C:249:THR:CG2	1:C:251:ASP:HB2	2.35	0.49
1:B:414:THR:OG1	1:B:417:GLN:HG3	2.12	0.49
1:C:277:VAL:HG13	1:C:281:GLU:HB2	1.93	0.49
1:B:167:GLU:HG3	1:B:437:ARG:NH1	2.28	0.49
1:C:117:ARG:HG3	4:C:945:HOH:O	2.11	0.49
1:C:218:ILE:O	1:C:222:ARG:HB2	2.13	0.49
1:B:220:ARG:NH1	1:B:299:ASP:OD1	2.45	0.48
1:C:227:LEU:HB2	4:C:835:HOH:O	2.13	0.48
1:C:252:HIS:C	1:C:254:TYR:H	2.21	0.48
1:B:370:PHE:CZ	1:B:371:LEU:HG	2.48	0.48
1:B:455:GLU:O	1:B:458:LEU:HB2	2.13	0.48
1:A:167:GLU:HG3	1:A:437:ARG:HH12	1.76	0.48
1:B:106:ASN:HB2	1:B:107:PRO:HD2	1.94	0.48
1:B:195:ILE:HD12	1:B:195:ILE:N	2.28	0.48
1:A:126:LEU:HD22	1:A:191:LEU:HD11	1.94	0.48
1:A:474:LEU:HD22	1:C:316:LEU:HD23	1.96	0.48
1:B:96:ILE:CD1	1:B:283:VAL:HG11	2.39	0.48
1:C:235:VAL:HG12	4:C:951:HOH:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:ILE:HB	1:C:234:VAL:HB	1.95	0.48
1:A:105:ILE:HG22	1:A:105:ILE:O	2.12	0.48
1:A:202:LEU:C	1:A:204:PRO:HD3	2.38	0.48
1:B:227:LEU:HD21	1:B:269:PHE:CE1	2.49	0.48
1:A:76:SER:HB2	4:A:984:HOH:O	2.14	0.48
1:B:64:GLU:OE1	1:B:102:ARG:NH1	2.47	0.48
1:A:482:LEU:HD11	1:C:179:SER:OG	2.14	0.48
1:B:56:THR:HA	1:B:59:LYS:HE3	1.96	0.48
1:B:348:ASN:N	1:B:446:GLN:HE22	2.12	0.48
1:C:250:GLU:HG2	1:C:289:LEU:HD12	1.95	0.48
1:B:350:THR:HA	4:B:1003:HOH:O	2.14	0.47
1:C:376:PHE:O	1:C:378:ASP:N	2.47	0.47
1:A:469:LEU:HD12	1:C:395:LEU:CD2	2.35	0.47
1:B:225:SER:O	1:B:226:ARG:C	2.56	0.47
1:C:146:TYR:CE2	1:C:150:LEU:HD11	2.48	0.47
1:A:235:VAL:O	1:A:237:MET:N	2.48	0.47
1:B:199:ASN:C	1:B:201:ARG:H	2.22	0.47
1:C:115:ILE:HG22	1:C:202:LEU:HD23	1.95	0.47
1:A:316:LEU:HD12	1:A:343:PHE:CE1	2.50	0.47
1:C:468:ARG:HH11	1:C:468:ARG:CG	2.28	0.47
1:A:454:LYS:HB3	1:A:454:LYS:HZ2	1.79	0.47
1:C:202:LEU:HD12	1:C:202:LEU:H	1.79	0.47
1:A:82:LEU:HB2	2:A:700:SAH:OXT	2.15	0.47
1:A:97:LEU:C	1:A:97:LEU:HD12	2.39	0.47
1:B:136:ARG:HD2	1:B:214:TRP:CZ3	2.49	0.47
1:B:364:LEU:HA	1:B:392:ASN:ND2	2.29	0.47
1:C:58:TRP:CZ2	1:C:74:LYS:HA	2.50	0.47
1:C:286:GLN:HG2	1:C:289:LEU:HG	1.96	0.47
1:A:193:GLN:HA	1:A:197:LEU:HD12	1.97	0.47
1:C:327:ASP:O	1:C:331:VAL:HG23	2.15	0.47
1:C:162:GLU:O	1:C:166:GLN:HG3	2.15	0.46
1:C:241:ILE:HD12	1:C:241:ILE:O	2.15	0.46
1:A:73:VAL:H	1:A:87:LEU:CD1	2.26	0.46
1:A:101:LYS:HA	1:A:104:TRP:CE3	2.50	0.46
1:A:157:THR:OG1	1:A:177:THR:HG21	2.16	0.46
1:B:96:ILE:HG22	1:B:97:LEU:HG	1.97	0.46
1:A:100:PRO:C	1:A:102:ARG:N	2.72	0.46
1:A:180:VAL:O	1:A:184:VAL:HG23	2.15	0.46
1:A:192:GLU:HA	1:A:196:ILE:HD12	1.98	0.46
1:B:222:ARG:NH1	1:B:239:ASP:CG	2.73	0.46
1:C:110:VAL:HG12	1:C:131:PHE:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:ASN:HB2	1:A:107:PRO:CD	2.44	0.46
1:A:98:GLN:HE21	1:A:270:SER:HB2	1.79	0.46
1:A:277:VAL:HG13	1:A:281:GLU:HB2	1.97	0.46
1:B:367:THR:CA	4:B:892:HOH:O	2.52	0.46
1:C:202:LEU:C	1:C:204:PRO:HD3	2.41	0.46
1:A:241:ILE:HD13	1:A:285:ILE:HD11	1.96	0.46
1:C:82:LEU:O	2:C:702:SAH:N	2.49	0.46
1:A:390:ARG:HG2	4:A:925:HOH:O	2.14	0.46
1:B:292:SER:OG	1:B:295:GLU:HG3	2.15	0.46
1:C:61:LEU:HD11	1:C:237:MET:HB2	1.96	0.46
1:A:231:ASN:C	1:A:232:LEU:HD12	2.40	0.46
1:B:401:ARG:O	1:B:405:LYS:HG3	2.15	0.46
1:C:98:GLN:HB3	1:C:268:LEU:HD13	1.98	0.46
1:B:101:LYS:HA	1:B:104:TRP:CE2	2.51	0.46
1:B:286:GLN:NE2	1:B:288:ASP:C	2.72	0.46
1:B:157:THR:OG1	1:B:177:THR:HG21	2.15	0.45
1:B:393:GLU:O	1:B:396:LEU:HG	2.16	0.45
1:A:73:VAL:HG13	1:A:73:VAL:O	2.16	0.45
1:B:106:ASN:HB2	1:B:107:PRO:CD	2.46	0.45
1:B:188:CYS:HB3	1:B:212:PHE:CD1	2.51	0.45
1:C:92:ARG:O	1:C:93:ASN:HB2	2.15	0.45
1:C:106:ASN:HB2	1:C:107:PRO:CD	2.46	0.45
1:A:298:LEU:C	1:A:298:LEU:HD23	2.41	0.45
1:B:437:ARG:O	1:B:441:LYS:HG3	2.17	0.45
1:C:143:TRP:O	1:C:147:PHE:CD1	2.70	0.45
1:A:425:ASN:HA	4:A:1017:HOH:O	2.16	0.45
1:B:78:VAL:CG1	1:B:79:THR:N	2.79	0.45
1:B:104:TRP:CZ2	1:B:269:PHE:HB2	2.52	0.45
1:C:438:GLU:HG2	1:C:442:MET:CE	2.46	0.45
1:A:104:TRP:N	1:A:104:TRP:HE3	2.15	0.45
1:A:133:ILE:HD11	1:A:212:PHE:HA	1.99	0.45
1:A:243:HIS:HA	1:A:285:ILE:O	2.16	0.45
1:A:254:TYR:CD2	1:A:255:GLU:N	2.85	0.45
1:C:110:VAL:HG12	1:C:131:PHE:CB	2.46	0.45
1:C:188:CYS:SG	1:C:212:PHE:CG	3.10	0.45
1:C:398:LYS:O	1:C:402:GLU:HG2	2.16	0.45
1:A:138:ARG:C	1:A:140:ASP:H	2.22	0.45
1:A:226:ARG:HG3	1:A:226:ARG:HH11	1.81	0.45
1:A:286:GLN:HE21	1:A:288:ASP:CA	2.30	0.45
1:A:302:PHE:CD1	1:A:302:PHE:C	2.95	0.45
1:C:101:LYS:HA	1:C:104:TRP:CE2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:104:TRP:CZ2	1:C:269:PHE:HB2	2.52	0.45
1:C:199:ASN:HB3	1:C:202:LEU:HD13	1.99	0.45
1:C:257:LYS:HD2	1:C:268:LEU:HD11	1.98	0.45
1:A:244:SER:HB2	1:A:284:TYR:CG	2.51	0.45
1:B:310:HIS:CD2	1:B:439:GLY:HA3	2.51	0.45
1:C:97:LEU:HD13	1:C:237:MET:HE3	1.99	0.45
1:A:241:ILE:HD13	1:A:285:ILE:CD1	2.46	0.45
1:A:376:PHE:O	1:A:378:ASP:N	2.49	0.45
1:A:485:LEU:O	1:A:486:TYR:HB3	2.16	0.45
1:B:318:ILE:O	1:B:339:GLN:NE2	2.49	0.45
1:A:101:LYS:HG3	1:A:104:TRP:CD1	2.52	0.45
1:A:146:TYR:CD1	1:A:236:PRO:HG3	2.52	0.45
1:C:73:VAL:HG22	1:C:74:LYS:N	2.32	0.44
1:C:260:ALA:O	1:C:262:LEU:HD22	2.16	0.44
1:A:176:THR:O	1:A:180:VAL:HG23	2.17	0.44
1:C:157:THR:OG1	1:C:177:THR:CG2	2.65	0.44
1:C:163:GLU:O	1:C:166:GLN:HB2	2.17	0.44
1:A:175:LYS:HD2	1:B:476:GLY:O	2.17	0.44
1:A:386:LEU:O	1:A:387:SER:HB3	2.17	0.44
1:A:293:ASN:HD22	1:A:310:HIS:CD2	2.35	0.44
1:B:199:ASN:C	1:B:201:ARG:N	2.75	0.44
1:C:346:PHE:HB2	1:C:349:ARG:HD2	1.99	0.44
1:A:103:LEU:HA	1:A:143:TRP:CH2	2.53	0.44
1:B:58:TRP:O	1:B:62:GLN:HG3	2.17	0.44
1:B:107:PRO:C	1:B:110:VAL:HG23	2.42	0.44
1:C:104:TRP:CH2	1:C:269:PHE:CB	2.99	0.44
1:B:54:VAL:HA	1:B:149:ILE:HD11	1.99	0.44
1:C:222:ARG:O	3:C:802:EPE:H32	2.18	0.44
1:A:70:LYS:HG3	4:A:913:HOH:O	2.16	0.44
1:A:99:VAL:HG21	1:A:237:MET:HB3	2.00	0.44
1:A:141:SER:HB3	4:A:806:HOH:O	2.17	0.44
1:A:315:THR:HG23	1:B:473:GLY:O	2.18	0.44
1:A:363:ALA:HB1	1:A:395:LEU:HD13	2.00	0.44
1:A:376:PHE:C	1:A:378:ASP:N	2.74	0.44
1:C:244:SER:HB2	1:C:284:TYR:CG	2.53	0.44
1:A:74:LYS:HG3	1:A:75:ALA:N	2.33	0.43
1:B:379:THR:HB	4:B:809:HOH:O	2.18	0.43
1:C:98:GLN:HA	1:C:269:PHE:O	2.18	0.43
1:A:486:TYR:HA	1:C:123:LYS:CD	2.48	0.43
1:B:105:ILE:HB	1:B:234:VAL:HB	1.98	0.43
1:B:167:GLU:HG3	1:B:437:ARG:HH12	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:356:LEU:N	1:B:357:PRO:HD2	2.33	0.43
1:B:110:VAL:HG13	1:B:131:PHE:CB	2.43	0.43
1:C:392:ASN:HA	4:C:927:HOH:O	2.18	0.43
1:A:103:LEU:HA	1:A:143:TRP:CZ3	2.54	0.43
1:B:483:GLU:C	1:B:485:LEU:H	2.24	0.43
1:C:110:VAL:HG23	1:C:111:ALA:N	2.32	0.43
1:C:197:LEU:HB2	1:C:198:PRO:CD	2.49	0.43
1:C:150:LEU:HA	1:C:151:PRO:HD3	1.85	0.43
1:A:98:GLN:HG2	1:A:270:SER:HA	2.01	0.43
1:A:99:VAL:HA	1:A:100:PRO:HD3	1.73	0.43
1:C:363:ALA:O	1:C:364:LEU:C	2.61	0.43
1:A:104:TRP:CE3	1:A:104:TRP:N	2.86	0.43
1:B:222:ARG:NH2	2:B:701:SAH:O	2.51	0.43
1:C:50:LEU:HD22	1:C:54:VAL:CG1	2.30	0.43
1:C:352:PRO:HA	1:C:353:PRO:HD3	1.93	0.43
1:C:163:GLU:CD	1:C:163:GLU:H	2.27	0.43
1:A:234:VAL:HG12	1:A:236:PRO:HD3	2.01	0.43
1:B:78:VAL:CG1	1:B:282:GLN:HE22	2.25	0.43
1:B:92:ARG:O	1:B:93:ASN:CB	2.67	0.43
1:A:163:GLU:CD	1:A:163:GLU:H	2.27	0.42
1:B:380:ILE:HG23	1:B:381:TRP:H	1.84	0.42
1:B:416:GLU:CD	1:B:416:GLU:H	2.26	0.42
1:C:438:GLU:CD	1:C:442:MET:HE2	2.43	0.42
1:A:143:TRP:NE1	4:A:802:HOH:O	2.28	0.42
1:B:468:ARG:HH11	1:B:468:ARG:CG	2.31	0.42
1:C:118:VAL:HG22	4:C:911:HOH:O	2.18	0.42
1:C:222:ARG:NH1	1:C:239:ASP:OD2	2.45	0.42
1:B:264:SER:HA	1:B:267:TYR:CE2	2.54	0.42
1:B:349:ARG:HG2	4:B:1015:HOH:O	2.18	0.42
1:A:78:VAL:CG2	1:A:80:GLU:HG2	2.49	0.42
1:A:277:VAL:CG1	1:A:281:GLU:HB2	2.49	0.42
1:A:451:PHE:O	1:A:455:GLU:HG3	2.20	0.42
1:A:351:LEU:HD23	1:A:351:LEU:HA	1.83	0.42
1:C:64:GLU:OE1	1:C:102:ARG:NH1	2.52	0.42
1:B:313:THR:HG21	1:C:478:ASN:ND2	2.34	0.42
1:C:390:ARG:HG2	1:C:390:ARG:HH11	1.85	0.42
1:A:157:THR:OG1	1:A:177:THR:CG2	2.68	0.42
1:B:366:GLY:H	1:C:465:GLN:HE22	1.68	0.42
1:B:126:LEU:HD22	1:B:191:LEU:HD11	2.02	0.42
1:C:157:THR:HA	1:C:160:TRP:CD1	2.54	0.42
1:A:305:PRO:HA	4:A:859:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:PRO:HA	1:B:110:VAL:HG23	2.02	0.41
1:A:129:ILE:HG23	1:A:215:ALA:HB3	2.01	0.41
1:B:225:SER:O	1:B:227:LEU:HG	2.20	0.41
1:B:413:THR:O	1:B:441:LYS:HE2	2.20	0.41
1:C:115:ILE:HD13	1:C:134:ARG:HD3	2.02	0.41
1:C:377:ARG:HA	1:C:377:ARG:HD3	1.88	0.41
1:A:100:PRO:C	1:A:104:TRP:CZ3	2.98	0.41
1:A:101:LYS:HE3	4:A:846:HOH:O	2.20	0.41
1:A:205:ASP:N	1:A:205:ASP:OD1	2.53	0.41
1:B:239:ASP:O	3:B:801:EPE:O8	2.37	0.41
1:C:67:ILE:CD1	1:C:237:MET:SD	3.05	0.41
1:C:472:LEU:HD13	1:C:474:LEU:HD21	2.02	0.41
1:C:104:TRP:N	1:C:104:TRP:CE3	2.88	0.41
1:C:236:PRO:N	4:C:951:HOH:O	2.52	0.41
1:C:356:LEU:HD23	1:C:356:LEU:HA	1.85	0.41
1:B:218:ILE:O	1:B:222:ARG:HB2	2.21	0.41
1:C:316:LEU:HA	4:C:908:HOH:O	2.19	0.41
1:C:487:PHE:HB3	4:C:838:HOH:O	2.20	0.41
1:A:455:GLU:O	1:A:458:LEU:HB2	2.20	0.41
1:B:418:ASP:OD2	1:B:441:LYS:NZ	2.54	0.41
1:A:55:GLN:HE21	1:A:55:GLN:HB2	1.51	0.41
1:A:100:PRO:O	1:A:104:TRP:CZ3	2.74	0.41
1:B:241:ILE:HG13	1:B:241:ILE:H	1.66	0.41
1:C:61:LEU:HD13	1:C:237:MET:HB2	2.03	0.41
1:C:364:LEU:HD12	1:C:364:LEU:HA	1.85	0.41
1:C:376:PHE:C	1:C:378:ASP:N	2.77	0.41
1:A:57:PHE:CE1	1:A:146:TYR:HA	2.55	0.41
1:B:143:TRP:O	1:B:147:PHE:CD1	2.74	0.41
1:C:60:TRP:O	1:C:64:GLU:HG2	2.21	0.41
1:A:179:SER:OG	1:B:482:LEU:HD12	2.20	0.41
1:A:202:LEU:H	1:A:202:LEU:CD1	2.30	0.41
1:B:129:ILE:O	1:B:133:ILE:HG13	2.21	0.41
1:C:173:LEU:O	1:C:173:LEU:HD12	2.21	0.41
1:C:297:ALA:O	1:C:300:TYR:O	2.38	0.41
1:C:486:TYR:C	4:C:838:HOH:O	2.64	0.41
1:A:101:LYS:HA	1:A:104:TRP:CZ2	2.56	0.41
1:A:110:VAL:CG1	1:A:131:PHE:HB2	2.49	0.41
1:A:146:TYR:CE1	1:A:236:PRO:HA	2.56	0.41
1:A:377:ARG:HA	1:A:377:ARG:HD3	1.86	0.41
1:C:97:LEU:HD12	1:C:97:LEU:O	2.21	0.41
1:C:153:GLU:HG2	1:C:159:TYR:CG	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:174:LEU:O	1:C:175:LYS:C	2.64	0.41
1:C:241:ILE:HD12	1:C:241:ILE:N	2.36	0.41
1:A:59:LYS:HD3	1:A:59:LYS:HA	1.92	0.40
1:A:250:GLU:HG3	1:A:252:HIS:HE1	1.86	0.40
1:A:329:LEU:O	1:A:333:GLU:HG3	2.21	0.40
1:A:352:PRO:HA	1:A:353:PRO:HD3	1.96	0.40
1:A:408:LEU:HD21	1:A:444:LEU:HB3	2.03	0.40
1:B:115:ILE:HG22	1:B:202:LEU:HD23	2.03	0.40
1:B:315:THR:HG21	4:C:906:HOH:O	2.19	0.40
1:C:192:GLU:O	1:C:197:LEU:HG	2.21	0.40
1:C:250:GLU:HB3	1:C:286:GLN:CG	2.51	0.40
1:C:251:ASP:O	1:C:252:HIS:HB2	2.21	0.40
1:C:254:TYR:CD1	1:C:254:TYR:C	2.98	0.40
1:C:310:HIS:CD2	1:C:439:GLY:HA3	2.56	0.40
1:A:360:ARG:HD2	1:A:384:LEU:O	2.21	0.40
1:A:476:GLY:O	1:C:175:LYS:HD2	2.21	0.40
1:C:236:PRO:CA	4:C:951:HOH:O	2.69	0.40
1:C:286:GLN:HE21	1:C:288:ASP:CA	2.33	0.40
1:C:104:TRP:O	1:C:143:TRP:CH2	2.75	0.40
1:C:138:ARG:C	1:C:140:ASP:H	2.29	0.40
1:C:272:LYS:HD2	4:C:983:HOH:O	2.21	0.40
1:A:370:PHE:CD1	1:A:370:PHE:C	3.00	0.40
1:B:253:ALA:HA	1:B:270:SER:O	2.22	0.40
1:A:96:ILE:HD13	1:A:283:VAL:HG11	2.03	0.40
1:A:434:VAL:O	1:A:437:ARG:HG2	2.21	0.40
1:A:438:GLU:HG2	1:A:442:MET:HE2	2.03	0.40
1:A:478:ASN:CG	1:C:313:THR:HG21	2.47	0.40
1:B:146:TYR:CE1	1:B:236:PRO:HA	2.57	0.40
1:B:322:ASP:HA	1:B:323:PRO:HD2	1.95	0.40
1:B:323:PRO:CB	1:C:375:LEU:HD21	2.51	0.40
1:C:356:LEU:N	1:C:357:PRO:HD2	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	418/444 (94%)	369 (88%)	38 (9%)	11 (3%)	4	7
1	B	438/444 (99%)	404 (92%)	28 (6%)	6 (1%)	9	19
1	C	436/444 (98%)	396 (91%)	33 (8%)	7 (2%)	7	16
All	All	1292/1332 (97%)	1169 (90%)	99 (8%)	24 (2%)	6	13

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	66	VAL
1	A	73	VAL
1	A	236	PRO
1	A	387	SER
1	B	364	LEU
1	B	377	ARG
1	B	387	SER
1	C	364	LEU
1	C	387	SER
1	A	104	TRP
1	A	105	ILE
1	B	226	ARG
1	C	377	ARG
1	A	377	ARG
1	B	288	ASP
1	C	105	ILE
1	C	236	PRO
1	A	204	PRO
1	A	364	LEU
1	C	204	PRO
1	A	200	LYS
1	C	198	PRO
1	A	52	PRO
1	B	479	GLY

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	374/390 (96%)	357 (96%)	17 (4%)	24	50
1	B	386/390 (99%)	366 (95%)	20 (5%)	21	44
1	C	384/390 (98%)	360 (94%)	24 (6%)	16	36
All	All	1144/1170 (98%)	1083 (95%)	61 (5%)	20	43

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	GLN
1	A	67	ILE
1	A	104	TRP
1	A	143	TRP
1	A	202	LEU
1	A	218	ILE
1	A	236	PRO
1	A	237	MET
1	A	241	ILE
1	A	315	THR
1	A	373	GLU
1	A	378	ASP
1	A	385	GLU
1	A	395	LEU
1	A	426	LEU
1	A	444	LEU
1	A	453	GLN
1	B	55	GLN
1	B	73	VAL
1	B	80	GLU
1	B	88	LYS
1	B	93	ASN
1	B	104	TRP
1	B	110	VAL
1	B	143	TRP
1	B	236	PRO
1	B	241	ILE
1	B	313	THR
1	B	315	THR
1	B	373	GLU
1	B	378	ASP

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Mol	Chain	Res	Type
1	B	385	GLU
1	B	395	LEU
1	B	426	LEU
1	B	444	LEU
1	B	453	GLN
1	B	468	ARG
1	C	55	GLN
1	C	74	LYS
1	C	104	TRP
1	C	107	PRO
1	C	143	TRP
1	C	152	GLN
1	C	218	ILE
1	C	236	PRO
1	C	237	MET
1	C	241	ILE
1	C	249	THR
1	C	250	GLU
1	C	255	GLU
1	C	257	LYS
1	C	298	LEU
1	C	313	THR
1	C	315	THR
1	C	378	ASP
1	C	385	GLU
1	C	395	LEU
1	C	444	LEU
1	C	453	GLN
1	C	468	ARG
1	C	482	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	GLN
1	A	93	ASN
1	A	98	GLN
1	A	169	GLN
1	A	286	GLN
1	A	310	HIS
1	A	392	ASN
1	B	55	GLN

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Mol	Chain	Res	Type
1	B	145	HIS
1	B	152	GLN
1	B	169	GLN
1	B	286	GLN
1	B	310	HIS
1	B	412	HIS
1	B	446	GLN
1	B	484	ASN
1	B	488	GLN
1	C	55	GLN
1	C	98	GLN
1	C	145	HIS
1	C	152	GLN
1	C	166	GLN
1	C	169	GLN
1	C	286	GLN
1	C	310	HIS
1	C	478	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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	$\# Z > 2$
3	EPE	A	800	-	15,15,15	1.75	3 (20%)	19,20,20	1.27	3 (15%)
2	SAH	B	701	-	27,28,28	0.85	2 (7%)	36,40,40	0.65	0
2	SAH	C	702	-	27,28,28	0.86	0	36,40,40	0.65	0
3	EPE	C	802	-	15,15,15	1.69	2 (13%)	19,20,20	1.43	5 (26%)
3	EPE	B	801	-	15,15,15	1.73	3 (20%)	19,20,20	1.30	4 (21%)
2	SAH	A	700	-	27,28,28	0.90	1 (3%)	36,40,40	0.71	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EPE	A	800	-	-	0/9/19/19	0/1/1/1
2	SAH	B	701	-	-	4/15/31/31	0/3/3/3
2	SAH	C	702	-	-	3/15/31/31	0/3/3/3
3	EPE	C	802	-	-	2/9/19/19	0/1/1/1
3	EPE	B	801	-	-	1/9/19/19	0/1/1/1
2	SAH	A	700	-	-	3/15/31/31	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	800	EPE	O3S-S	5.14	1.66	1.47
3	B	801	EPE	O3S-S	5.10	1.66	1.47
3	C	802	EPE	O3S-S	5.02	1.66	1.47
3	B	801	EPE	C5-N4	2.38	1.53	1.46
2	A	700	SAH	C4-N3	2.27	1.38	1.34
3	A	800	EPE	C5-N4	2.27	1.53	1.46
3	C	802	EPE	C3-N4	2.16	1.52	1.46
2	B	701	SAH	C4-N3	2.15	1.38	1.34
3	A	800	EPE	C3-N4	2.07	1.52	1.46
2	B	701	SAH	OXT-C	-2.07	1.24	1.30
3	B	801	EPE	C3-N4	2.02	1.52	1.46

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	802	EPE	C6-N1-C2	2.67	114.60	108.84
3	C	802	EPE	O1S-S-C10	-2.67	102.69	106.73
3	A	800	EPE	O2S-S-C10	2.51	110.53	106.73
3	B	801	EPE	O1S-S-C10	-2.49	102.96	106.73
3	B	801	EPE	C6-N1-C2	2.44	114.09	108.84
3	C	802	EPE	O3S-S-O1S	-2.41	105.37	111.40
3	C	802	EPE	O2S-S-C10	2.37	110.31	106.73
3	A	800	EPE	O3S-S-O1S	-2.28	105.71	111.40
3	B	801	EPE	O2S-S-C10	2.26	110.15	106.73
3	B	801	EPE	O3S-S-O1S	-2.11	106.12	111.40
3	C	802	EPE	C10-C9-N1	-2.09	104.44	112.36
3	A	800	EPE	C6-N1-C2	2.04	113.23	108.84

There are no chirality outliers.

All (13) torsion outliers are listed below:

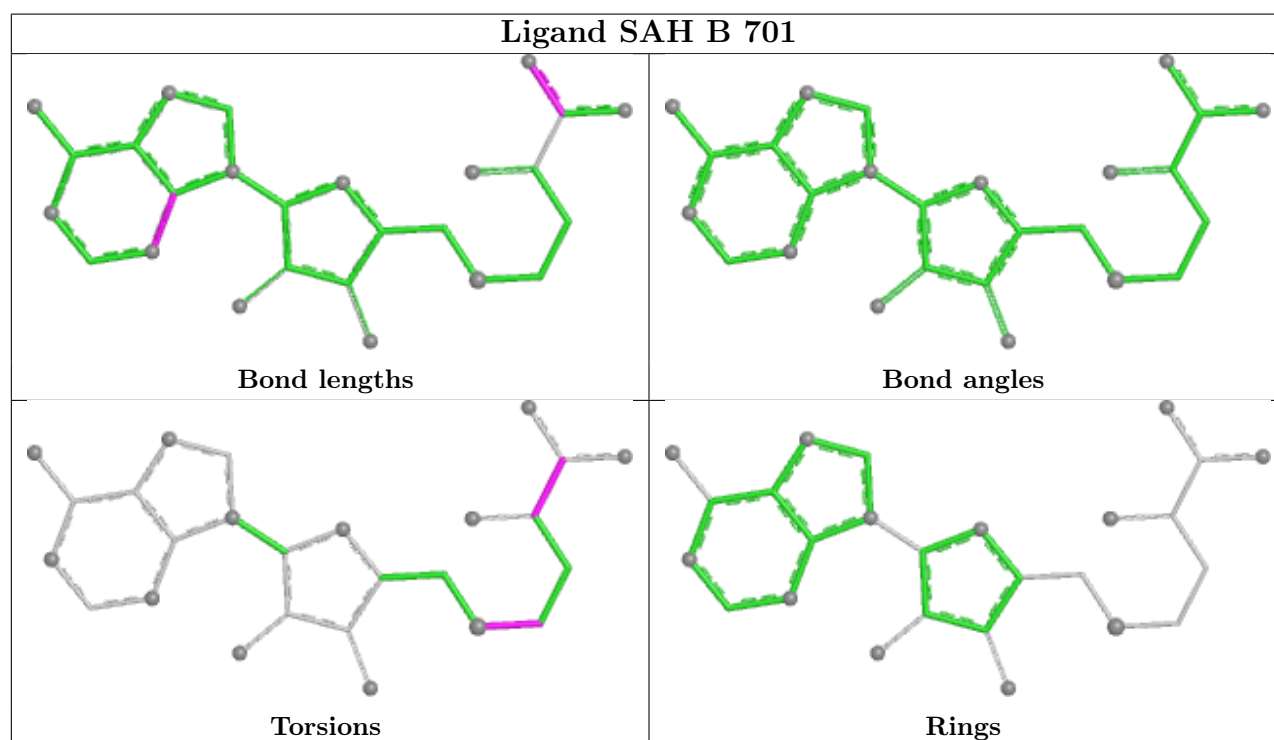
Mol	Chain	Res	Type	Atoms
3	B	801	EPE	N4-C7-C8-O8
3	C	802	EPE	C10-C9-N1-C6
2	B	701	SAH	OXT-C-CA-CB
2	A	700	SAH	C3'-C4'-C5'-SD
2	B	701	SAH	O-C-CA-CB
3	C	802	EPE	C10-C9-N1-C2
2	C	702	SAH	CB-CG-SD-C5'
2	A	700	SAH	CB-CG-SD-C5'
2	B	701	SAH	CB-CG-SD-C5'
2	C	702	SAH	C-CA-CB-CG
2	A	700	SAH	O-C-CA-N
2	C	702	SAH	O-C-CA-N
2	B	701	SAH	OXT-C-CA-N

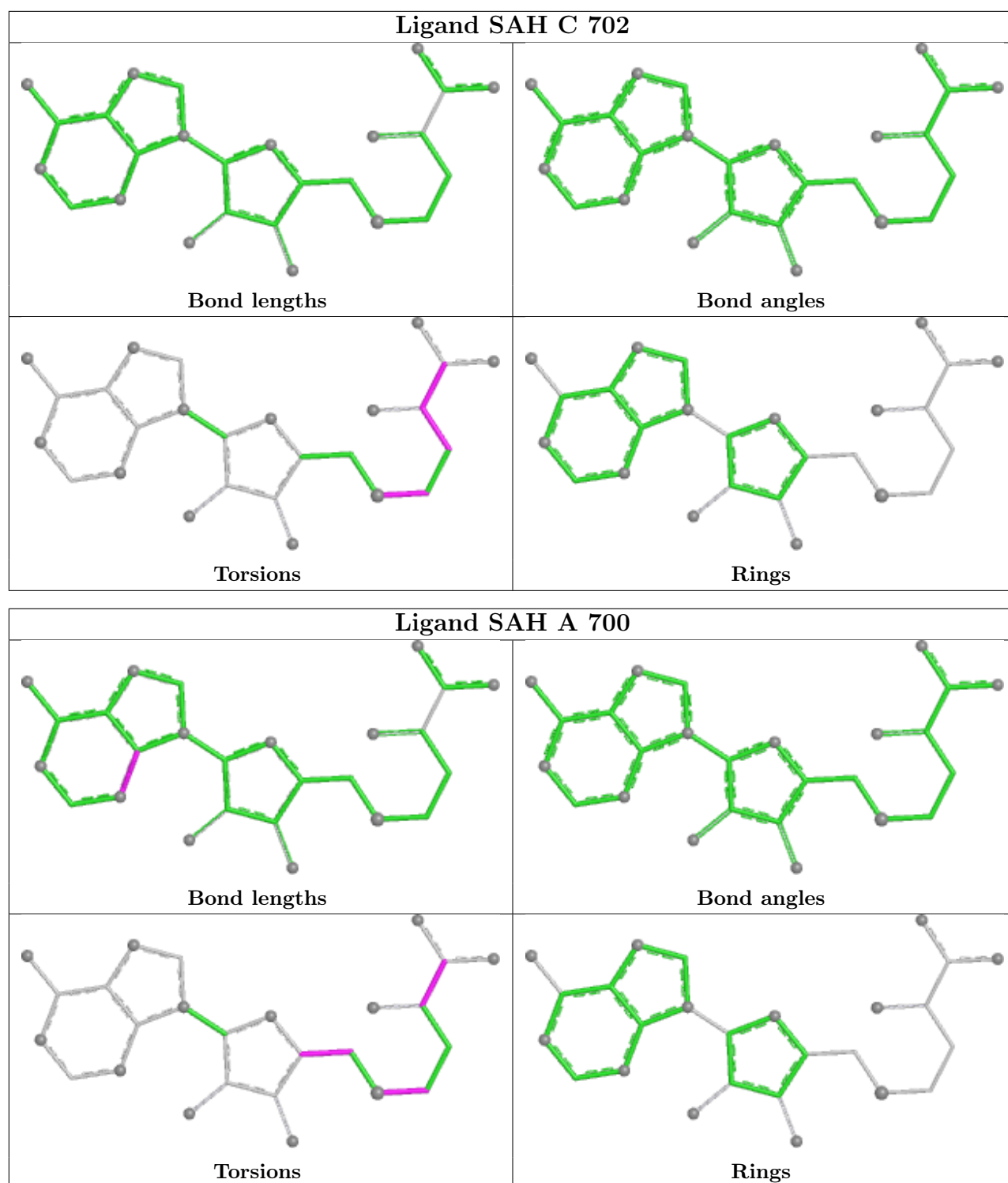
There are no ring outliers.

6 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	800	EPE	3	0
2	B	701	SAH	1	0
2	C	702	SAH	2	0
3	C	802	EPE	3	0
3	B	801	EPE	5	0
2	A	700	SAH	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.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	424/444 (95%)	0.62	63 (14%) 5 4	47, 69, 122, 135	0
1	B	440/444 (99%)	0.05	11 (2%) 58 52	38, 63, 95, 115	0
1	C	438/444 (98%)	0.05	6 (1%) 73 69	44, 65, 95, 112	0
All	All	1302/1332 (97%)	0.24	80 (6%) 27 22	38, 65, 103, 135	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	256	VAL	5.5
1	A	110	VAL	5.1
1	B	365	GLY	5.1
1	A	253	ALA	5.0
1	C	487	PHE	5.0
1	A	486	TYR	4.4
1	A	189	LEU	4.3
1	A	111	ALA	3.9
1	A	143	TRP	3.8
1	A	146	TYR	3.8
1	A	202	LEU	3.7
1	A	138	ARG	3.5
1	A	254	TYR	3.4
1	A	206	PRO	3.4
1	A	268	LEU	3.3
1	A	207	VAL	3.2
1	A	107	PRO	3.2
1	A	227	LEU	3.2
1	A	232	LEU	3.1
1	A	56	THR	3.1
1	A	183	TYR	3.0
1	A	237	MET	3.0
1	A	196	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	234	VAL	3.0
1	A	190	LYS	2.9
1	B	143	TRP	2.8
1	A	209	LEU	2.8
1	B	366	GLY	2.8
1	A	140	ASP	2.8
1	A	53	ALA	2.8
1	A	114	GLU	2.8
1	A	137	SER	2.7
1	A	57	PHE	2.7
1	A	60	TRP	2.6
1	A	193	GLN	2.6
1	A	252	HIS	2.6
1	A	71	THR	2.6
1	A	126	LEU	2.6
1	A	203	PHE	2.5
1	A	96	ILE	2.5
1	A	130	LEU	2.5
1	A	50	LEU	2.5
1	A	198	PRO	2.5
1	A	66	VAL	2.5
1	A	377	ARG	2.4
1	A	70	LYS	2.4
1	A	204	PRO	2.4
1	A	235	VAL	2.4
1	A	212	PHE	2.4
1	B	201	ARG	2.4
1	B	482	LEU	2.3
1	A	118	VAL	2.3
1	A	471	ASP	2.3
1	A	104	TRP	2.3
1	C	143	TRP	2.3
1	C	193	GLN	2.3
1	A	178	VAL	2.3
1	A	197	LEU	2.3
1	A	267	TYR	2.2
1	C	206	PRO	2.2
1	A	205	ASP	2.2
1	B	114	GLU	2.2
1	A	61	LEU	2.2
1	A	150	LEU	2.2
1	A	364	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	133	ILE	2.2
1	A	195	ILE	2.2
1	B	367	THR	2.1
1	A	72	PRO	2.1
1	B	425	ASN	2.1
1	A	117	ARG	2.1
1	A	134	ARG	2.1
1	C	96	ILE	2.1
1	A	69	ALA	2.1
1	B	202	LEU	2.1
1	B	209	LEU	2.1
1	A	105	ILE	2.1
1	C	471	ASP	2.0
1	A	147	PHE	2.0
1	B	104	TRP	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.

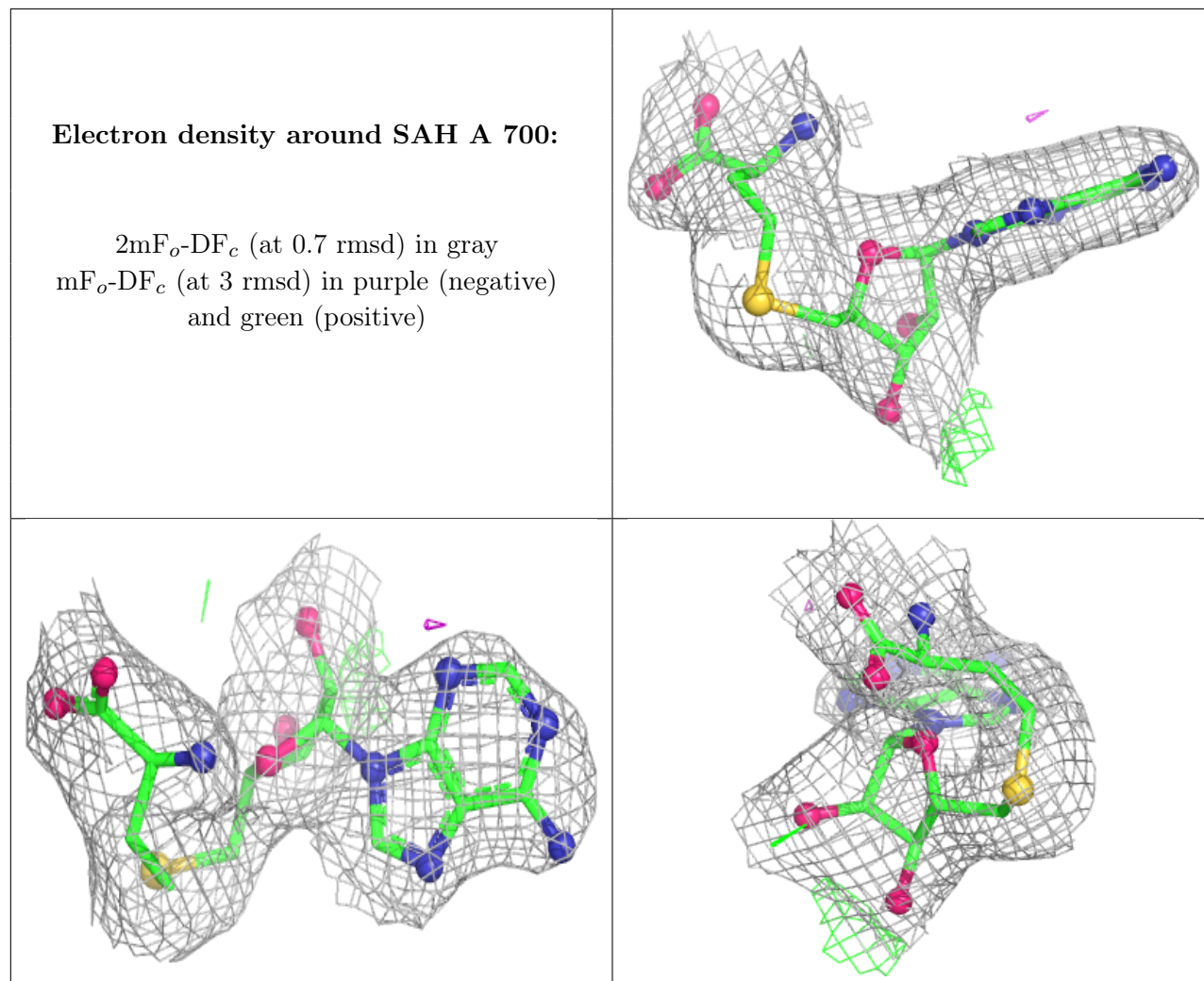
6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	EPE	A	800	15/15	0.89	0.15	80,82,95,96	0
3	EPE	B	801	15/15	0.89	0.18	71,73,85,86	0
3	EPE	C	802	15/15	0.89	0.16	66,68,73,73	0
2	SAH	A	700	26/26	0.95	0.09	67,71,77,78	0
2	SAH	C	702	26/26	0.97	0.07	57,63,66,66	0
2	SAH	B	701	26/26	0.97	0.07	46,48,52,53	0

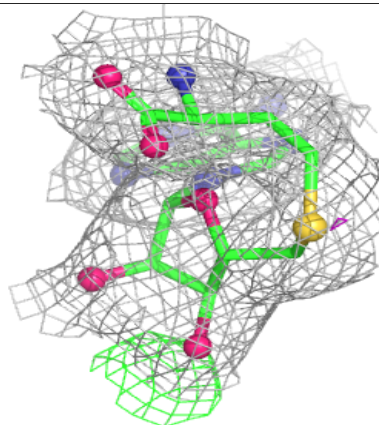
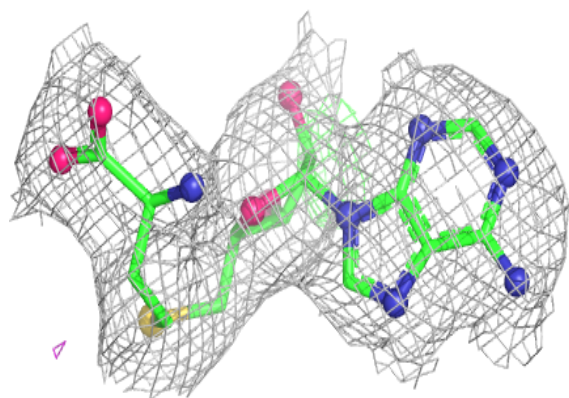
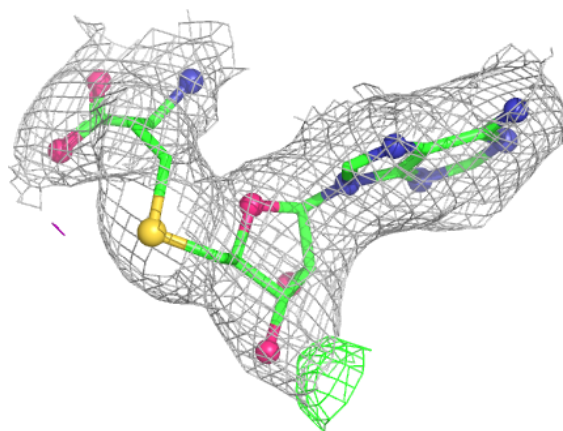
The following is a graphical depiction of the model fit to experimental electron density of all

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.

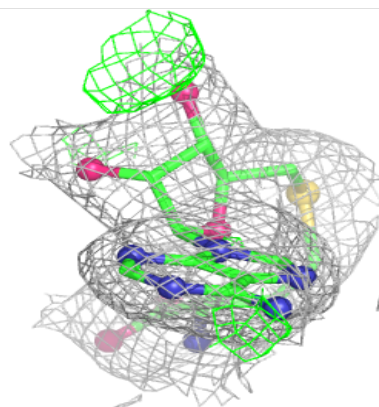
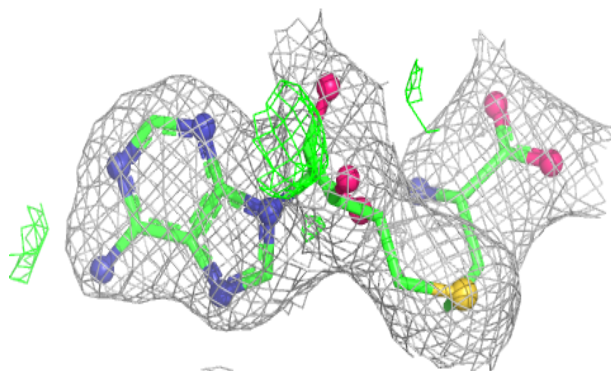
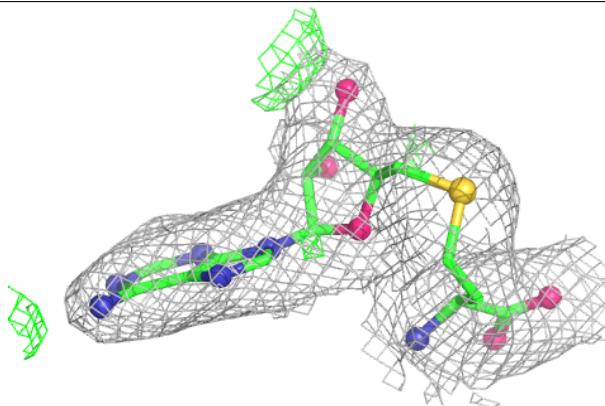


Electron density around SAH C 702:

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

**Electron density around SAH B 701:**

$2mF_o-DF_c$ (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.