



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2020 – 10:31 AM BST

PDB ID : 2H2E
Title : Structure of Rubisco LSMT bound to AzaAdoMet and Lysine
Authors : Couture, J.F.; Hauk, G.; Trievel, R.C.
Deposited on : 2006-05-18
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.14.4.dev1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.14.4.dev1

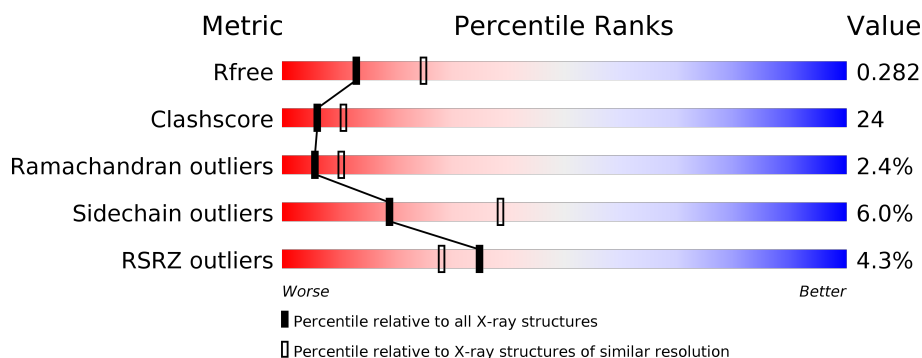
1 Overall quality at a glance

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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	440	<div> <div>6%</div> <div> <div></div> <div>53%</div> <div>38%</div> <div>5%</div> <div></div> </div> </div>
1	B	440	<div> <div>5%</div> <div> <div></div> <div>59%</div> <div>37%</div> <div></div> </div> </div>
1	C	440	<div> <div>3%</div> <div> <div></div> <div>58%</div> <div>38%</div> <div></div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10977 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.

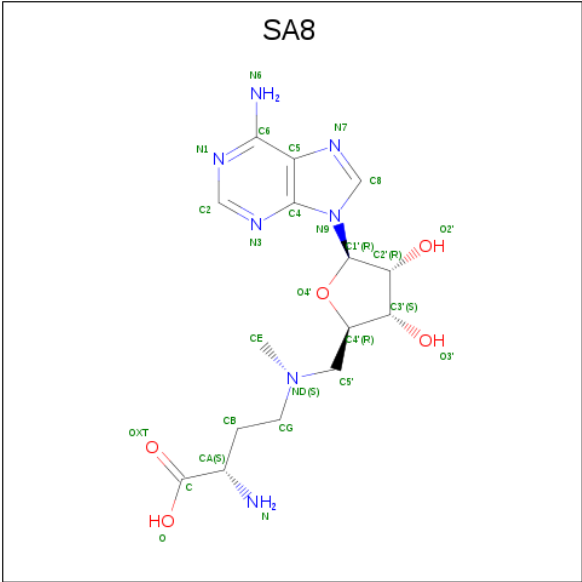
- Molecule 1 is a protein called Ribulose-1,5 bisphosphate carboxylase/oxygenase large subunit N-methyltransferase.

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 18 discrepancies between the modelled and reference sequences:

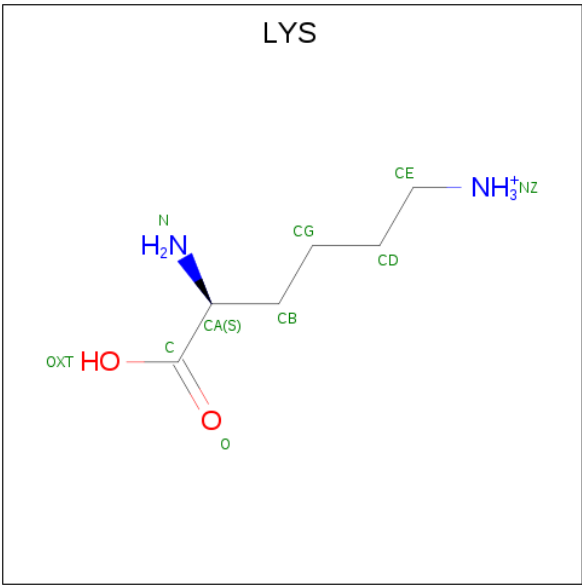
Chain	Residue	Modelled	Actual	Comment	Reference
A	483	GLU	-	CLONING ARTIFACT	UNP Q43088
A	484	ASN	-	CLONING ARTIFACT	UNP Q43088
A	485	LEU	-	CLONING ARTIFACT	UNP Q43088
A	486	TYR	-	CLONING ARTIFACT	UNP Q43088
A	487	PHE	-	CLONING ARTIFACT	UNP Q43088
A	488	GLN	-	CLONING ARTIFACT	UNP Q43088
B	483	GLU	-	CLONING ARTIFACT	UNP Q43088
B	484	ASN	-	CLONING ARTIFACT	UNP Q43088
B	485	LEU	-	CLONING ARTIFACT	UNP Q43088
B	486	TYR	-	CLONING ARTIFACT	UNP Q43088
B	487	PHE	-	CLONING ARTIFACT	UNP Q43088
B	488	GLN	-	CLONING ARTIFACT	UNP Q43088
C	483	GLU	-	CLONING ARTIFACT	UNP Q43088
C	484	ASN	-	CLONING ARTIFACT	UNP Q43088
C	485	LEU	-	CLONING ARTIFACT	UNP Q43088
C	486	TYR	-	CLONING ARTIFACT	UNP Q43088
C	487	PHE	-	CLONING ARTIFACT	UNP Q43088
C	488	GLN	-	CLONING ARTIFACT	UNP Q43088

- Molecule 2 is S-5'-AZAMETHIONINE-5'-DEOXYADENOSINE (three-letter code: SA8) (formula: C₁₅H₂₃N₇O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			27	15	7	5		
2	B	1	Total	C	N	O	0	0
			27	15	7	5		
2	C	1	Total	C	N	O	0	0
			27	15	7	5		

- Molecule 3 is LYSINE (three-letter code: LYS) (formula: C₆H₁₅N₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			10	6	2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			10	6	2	2		
3	C	1	Total	C	N	O	0	0
			10	6	2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	117	Total	O	0	0
			117	117		
4	B	127	Total	O	0	0
			127	127		
4	C	141	Total	O	0	0
			141	141		

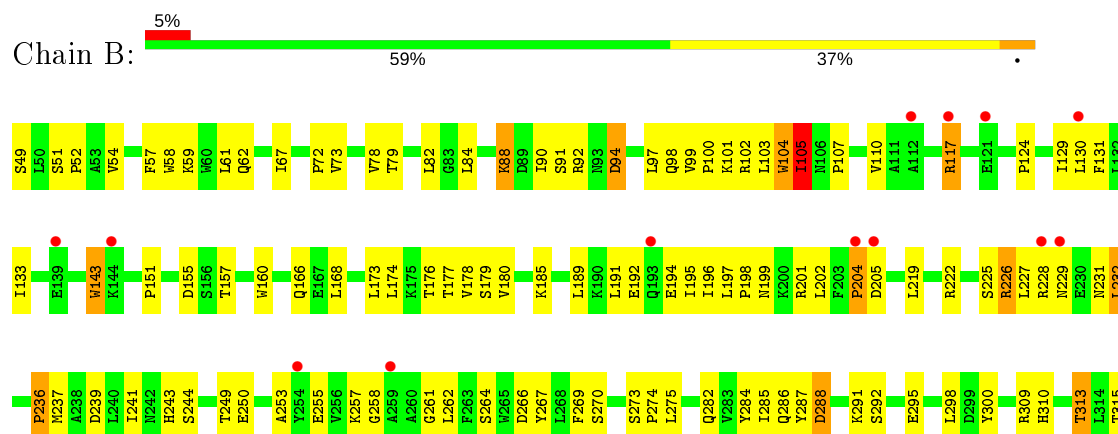
3 Residue-property plots

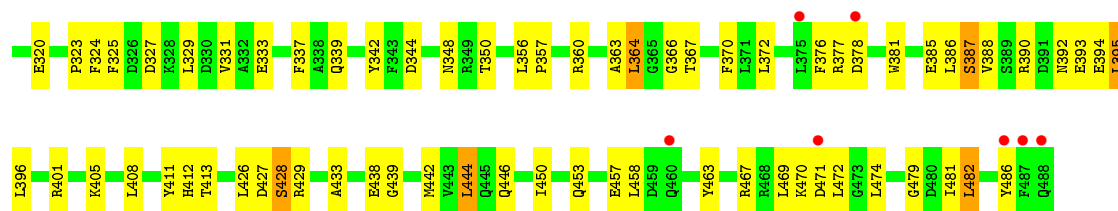
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

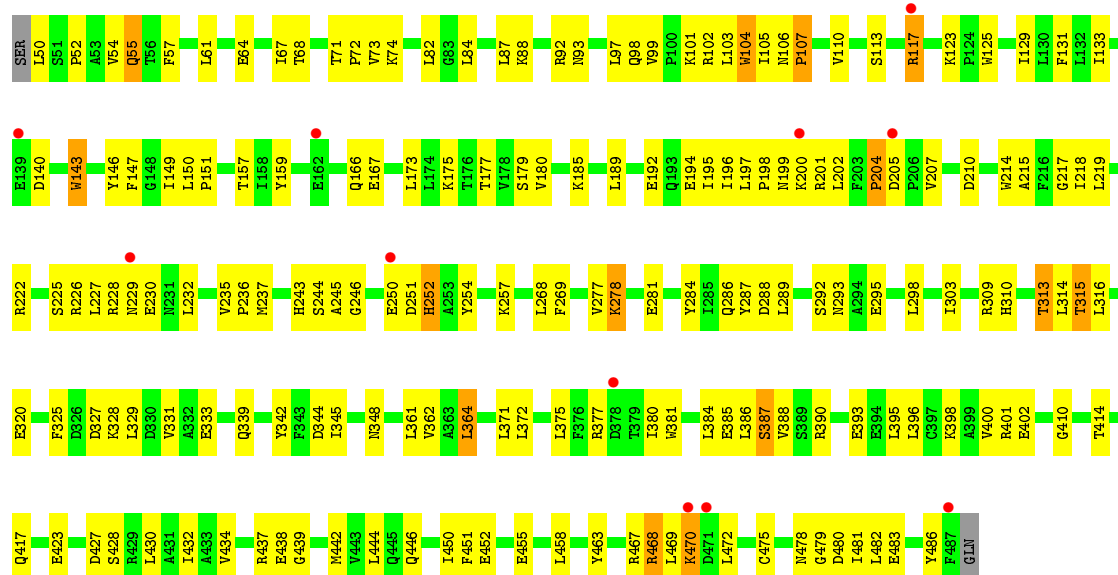


- Molecule 1: Ribulose-1,5 biphosphate carboxylase/oxygenase large subunit N-methyltransferase





- 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	132.63 Å 159.49 Å 267.51 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	16.73 – 2.60 16.73 – 2.59	Depositor EDS
% Data completeness (in resolution range)	98.2 (16.73-2.60) 97.6 (16.73-2.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 2.59 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.262 , 0.298 0.248 , 0.282	Depositor DCC
R_{free} test set	4320 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	57.3	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 56.7	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	10977	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% 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: SA8

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	0.40	0/3482	0.60	0/4723
1	B	0.40	0/3617	0.63	1/4906 (0.0%)
1	C	0.40	0/3601	0.62	0/4886
All	All	0.40	0/10700	0.61	1/14515 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	105	ILE	N-CA-C	-5.67	95.69	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3413	0	3384	189	0
1	B	3542	0	3501	165	0
1	C	3526	0	3488	171	0
2	A	27	0	22	7	0
2	B	27	0	22	5	0
2	C	27	0	22	6	0
3	A	10	0	12	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	10	0	12	0	0
3	C	10	0	12	5	0
4	A	117	0	0	14	0
4	B	127	0	0	12	0
4	C	141	0	0	21	0
All	All	10977	0	10475	513	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 24.

All (513) 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:B:78:VAL:HG11	1:B:282:GLN:HE22	1.19	1.05
1:C:177:THR:HG22	1:C:298:LEU:HD13	1.43	0.96
1:C:50:LEU:HD22	1:C:54:VAL:HG11	1.46	0.96
1:B:367:THR:HA	4:B:905:HOH:O	1.66	0.94
1:A:395:LEU:HD22	1:B:469:LEU:HD12	1.49	0.93
1:B:286:GLN:HE21	1:B:288:ASP:H	0.97	0.91
1:A:238:ALA:HB1	1:A:271:LEU:HD22	1.50	0.91
1:C:219:LEU:HD11	1:C:232:LEU:HD21	1.56	0.86
1:A:226:ARG:O	1:A:227:LEU:HD13	1.80	0.82
1:C:482:LEU:HG	4:C:1016:HOH:O	1.80	0.81
1:B:472:LEU:HD13	1:B:474:LEU:HD21	1.61	0.81
1:C:102:ARG:HB2	4:C:906:HOH:O	1.81	0.80
1:A:192:GLU:HA	1:A:196:ILE:HB	1.62	0.79
1:A:130:LEU:HD11	1:A:191:LEU:HD22	1.66	0.78
1:B:78:VAL:HG11	1:B:282:GLN:NE2	1.99	0.77
1:C:315:THR:HG21	4:C:921:HOH:O	1.83	0.77
1:B:286:GLN:HE21	1:B:288:ASP:N	1.78	0.77
1:A:227:LEU:HD23	1:A:231:ASN:HA	1.67	0.77
1:A:73:VAL:HG21	1:A:84:LEU:HB3	1.66	0.77
1:B:395:LEU:HD22	1:C:469:LEU:HD12	1.68	0.76
1:C:227:LEU:HB2	4:C:917:HOH:O	1.86	0.75
1:A:238:ALA:CB	1:A:271:LEU:HD22	2.15	0.75
1:B:286:GLN:NE2	1:B:288:ASP:H	1.80	0.75
1:C:97:LEU:HB2	1:C:237:MET:HE1	1.67	0.75
1:C:73:VAL:HG21	1:C:84:LEU:HB3	1.67	0.74
1:A:117:ARG:H	1:A:117:ARG:HD2	1.51	0.74
1:A:98:GLN:HA	1:A:269:PHE:O	1.88	0.74
1:C:287:TYR:OH	2:C:802:SA8:HE3	1.88	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:ARG:HB2	1:B:92:ARG:NH1	2.04	0.73
1:B:202:LEU:H	1:B:202:LEU:HD12	1.54	0.73
1:A:97:LEU:HD22	1:A:237:MET:SD	2.29	0.73
1:A:286:GLN:HG2	1:A:289:LEU:HG	1.69	0.73
1:C:157:THR:OG1	1:C:177:THR:HG21	1.90	0.72
1:B:199:ASN:HB3	1:B:202:LEU:HD13	1.71	0.72
1:A:100:PRO:HD2	1:A:103:LEU:HD12	1.70	0.72
1:B:179:SER:OG	1:C:482:LEU:HD11	1.91	0.71
1:C:250:GLU:HA	4:C:907:HOH:O	1.89	0.71
1:B:107:PRO:O	1:B:110:VAL:HG22	1.91	0.70
1:A:482:LEU:HD21	1:C:180:VAL:HA	1.73	0.70
1:B:329:LEU:O	1:B:333:GLU:HG3	1.90	0.70
1:B:264:SER:HA	1:B:267:TYR:CZ	2.27	0.70
1:A:101:LYS:HA	1:A:104:TRP:CD2	2.27	0.70
1:C:286:GLN:HG2	1:C:289:LEU:HG	1.75	0.69
1:B:157:THR:OG1	1:B:177:THR:HG21	1.91	0.69
1:B:174:LEU:O	1:B:178:VAL:HG23	1.93	0.68
1:B:348:ASN:H	1:B:446:GLN:HE22	1.40	0.68
1:C:286:GLN:HE21	1:C:288:ASP:H	1.41	0.68
1:B:241:ILE:HG12	1:B:285:ILE:HG23	1.75	0.68
1:A:118:VAL:HG13	4:A:910:HOH:O	1.92	0.68
1:A:96:ILE:HD11	1:A:273:SER:HB2	1.75	0.68
1:B:97:LEU:HB2	1:B:237:MET:HE1	1.74	0.68
1:B:394:GLU:HB2	1:B:458:LEU:HD21	1.75	0.68
1:A:256:VAL:H	1:A:268:LEU:HD11	1.58	0.68
1:A:97:LEU:HD22	1:A:237:MET:CG	2.23	0.68
1:A:466:GLU:HB2	4:A:909:HOH:O	1.93	0.68
1:B:117:ARG:H	1:B:117:ARG:HD2	1.59	0.67
1:B:381:TRP:O	1:B:385:GLU:HG3	1.94	0.67
1:B:104:TRP:NE1	4:B:910:HOH:O	2.14	0.67
1:B:92:ARG:CB	1:B:92:ARG:HH11	2.08	0.67
1:C:398:LYS:O	1:C:402:GLU:HG2	1.95	0.67
1:A:314:LEU:HG	1:A:345:ILE:HD12	1.77	0.67
1:B:226:ARG:HD3	4:B:967:HOH:O	1.94	0.67
1:C:254:TYR:HH	3:C:901:LYS:N	1.93	0.67
1:B:197:LEU:HB2	1:B:198:PRO:HD3	1.77	0.66
1:C:92:ARG:O	1:C:93:ASN:HB2	1.95	0.66
1:A:104:TRP:CH2	1:A:269:PHE:HB2	2.31	0.66
1:B:73:VAL:HG21	1:B:84:LEU:HB3	1.76	0.66
1:A:107:PRO:O	1:A:110:VAL:HG22	1.96	0.66
1:B:101:LYS:HA	1:B:104:TRP:CD2	2.31	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:LYS:HA	1:B:104:TRP:CE2	2.31	0.66
1:B:226:ARG:HH22	1:B:288:ASP:HA	1.60	0.65
1:B:91:SER:HB2	1:B:94:ASP:OD1	1.97	0.65
1:C:99:VAL:O	1:C:104:TRP:HH2	1.79	0.65
1:C:97:LEU:HD13	1:C:237:MET:HE3	1.77	0.65
1:A:157:THR:OG1	1:A:177:THR:HG21	1.96	0.65
1:C:244:SER:C	1:C:246:GLY:H	2.00	0.65
1:B:67:ILE:HD11	1:B:237:MET:SD	2.37	0.65
1:C:201:ARG:HB3	1:C:201:ARG:HH11	1.62	0.65
1:A:219:LEU:HD11	1:A:232:LEU:HD21	1.79	0.64
1:A:54:VAL:HA	1:A:149:ILE:HD11	1.77	0.64
1:A:286:GLN:NE2	1:A:288:ASP:H	1.95	0.64
1:A:197:LEU:HB2	1:A:198:PRO:HD3	1.78	0.64
1:B:202:LEU:N	1:B:202:LEU:HD12	2.12	0.64
1:B:99:VAL:O	1:B:104:TRP:HH2	1.81	0.64
2:C:802:SA8:H3'	4:C:983:HOH:O	1.97	0.64
1:A:358:TYR:O	1:A:362:VAL:HG23	1.98	0.63
1:A:97:LEU:HD11	1:A:238:ALA:HB2	1.79	0.63
1:A:249:THR:HG22	4:A:904:HOH:O	1.98	0.63
1:C:479:GLY:O	1:C:483:GLU:HG2	1.99	0.63
1:C:117:ARG:H	1:C:117:ARG:HD2	1.63	0.63
1:C:320:GLU:HA	1:C:325:PHE:CD1	2.34	0.63
1:B:61:LEU:HB3	1:B:67:ILE:HG12	1.81	0.63
1:B:401:ARG:O	1:B:405:LYS:HG3	1.99	0.63
1:C:278:LYS:H	1:C:278:LYS:HE3	1.64	0.62
1:C:104:TRP:CH2	1:C:269:PHE:HB2	2.34	0.62
1:A:286:GLN:HE21	1:A:288:ASP:C	2.02	0.62
1:A:117:ARG:HG2	4:A:910:HOH:O	1.98	0.62
1:A:486:TYR:HB2	1:C:123:LYS:NZ	2.15	0.62
1:A:62:GLN:HA	1:A:67:ILE:HG23	1.82	0.62
1:C:99:VAL:O	1:C:104:TRP:CH2	2.53	0.62
1:B:110:VAL:HG12	1:B:131:PHE:CG	2.34	0.61
1:B:243:HIS:HB3	2:B:801:SA8:N7	2.16	0.61
1:B:59:LYS:HB2	1:B:59:LYS:NZ	2.14	0.61
1:B:73:VAL:CG2	1:B:84:LEU:HB3	2.31	0.61
1:A:287:TYR:OH	2:A:800:SA8:HE3	2.00	0.61
1:A:300:TYR:HB3	4:A:975:HOH:O	1.99	0.61
1:B:201:ARG:HB3	1:B:201:ARG:NH1	2.15	0.61
1:A:482:LEU:HD11	1:C:179:SER:OG	2.00	0.61
1:B:395:LEU:CD2	1:C:469:LEU:HD12	2.29	0.61
1:B:201:ARG:HB3	1:B:201:ARG:HH11	1.66	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:LEU:O	2:A:800:SA8:N	2.33	0.61
1:A:202:LEU:C	1:A:204:PRO:HD3	2.22	0.61
1:C:251:ASP:O	1:C:252:HIS:O	2.18	0.60
1:A:176:THR:O	1:A:180:VAL:HG23	2.01	0.60
1:C:103:LEU:O	1:C:143:TRP:CZ3	2.54	0.60
1:C:159:TYR:OH	1:C:217:GLY:HA3	2.02	0.60
1:B:408:LEU:HD21	1:B:444:LEU:HB3	1.82	0.60
1:C:286:GLN:HE21	1:C:288:ASP:N	1.99	0.60
1:C:313:THR:HB	1:C:344:ASP:OD1	2.02	0.60
1:C:74:LYS:HB3	1:C:87:LEU:HD21	1.83	0.60
1:B:176:THR:HG21	1:C:481:ILE:HD12	1.82	0.60
1:B:157:THR:OG1	1:B:177:THR:CG2	2.50	0.60
1:C:327:ASP:O	1:C:331:VAL:HG23	2.02	0.60
1:B:92:ARG:HB2	1:B:92:ARG:HH11	1.66	0.59
1:C:388:VAL:O	1:C:463:TYR:HB3	2.02	0.59
1:A:342:TYR:CZ	1:B:479:GLY:HA3	2.38	0.59
1:B:78:VAL:HG12	1:B:79:THR:N	2.18	0.59
1:C:97:LEU:HB2	1:C:237:MET:CE	2.33	0.59
1:A:60:TRP:O	1:A:64:GLU:HG2	2.02	0.59
1:A:176:THR:HG21	1:B:481:ILE:HD12	1.85	0.59
1:B:244:SER:HB2	1:B:284:TYR:CG	2.37	0.59
1:A:286:GLN:HE21	1:A:288:ASP:H	1.50	0.59
1:A:474:LEU:HD22	1:C:316:LEU:CD2	2.33	0.59
1:A:99:VAL:HG21	1:A:237:MET:HB3	1.85	0.58
1:A:252:HIS:NE2	1:A:285:ILE:HB	2.18	0.58
1:C:470:LYS:HA	1:C:470:LYS:HE2	1.85	0.58
1:A:370:PHE:HB3	4:A:923:HOH:O	2.03	0.58
1:C:129:ILE:O	1:C:133:ILE:HG13	2.04	0.58
1:C:225:SER:HA	4:C:917:HOH:O	2.02	0.58
1:B:262:LEU:HD23	4:B:911:HOH:O	2.02	0.58
1:C:199:ASN:HB3	1:C:202:LEU:HD13	1.86	0.58
1:A:99:VAL:CG2	1:A:237:MET:HB3	2.33	0.58
1:C:278:LYS:HE3	1:C:281:GLU:OE1	2.04	0.58
1:A:129:ILE:O	1:A:133:ILE:HG13	2.04	0.57
1:C:103:LEU:HA	1:C:143:TRP:CH2	2.39	0.57
1:B:393:GLU:O	1:B:396:LEU:HG	2.04	0.57
1:C:348:ASN:H	1:C:446:GLN:HE22	1.50	0.57
1:C:438:GLU:OE2	1:C:442:MET:HE2	2.05	0.57
1:A:157:THR:CB	1:A:177:THR:HG21	2.34	0.57
1:A:329:LEU:O	1:A:333:GLU:HG3	2.04	0.57
1:C:194:GLU:C	1:C:195:ILE:HD12	2.24	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:GLY:HA3	4:A:977:HOH:O	2.04	0.57
1:A:99:VAL:O	1:A:104:TRP:HH2	1.86	0.57
1:B:103:LEU:O	1:B:143:TRP:HZ3	1.87	0.57
1:B:323:PRO:HG2	1:B:324:PHE:CD1	2.39	0.57
1:B:348:ASN:N	1:B:446:GLN:HE22	2.02	0.57
1:A:99:VAL:O	1:A:104:TRP:CH2	2.58	0.57
1:B:438:GLU:HG2	1:B:442:MET:HE2	1.87	0.57
1:B:292:SER:OG	1:B:295:GLU:HG3	2.05	0.57
1:C:129:ILE:HG23	1:C:215:ALA:HB3	1.87	0.57
1:C:428:SER:O	1:C:432:ILE:HG13	2.04	0.57
1:A:177:THR:HG22	1:A:298:LEU:HG	1.86	0.56
1:A:320:GLU:HA	1:A:325:PHE:CD1	2.39	0.56
1:C:202:LEU:C	1:C:204:PRO:HD3	2.25	0.56
1:C:286:GLN:NE2	1:C:288:ASP:H	2.02	0.56
1:A:101:LYS:HA	1:A:104:TRP:CE2	2.40	0.56
1:C:235:VAL:HG12	4:C:902:HOH:O	2.06	0.56
1:C:104:TRP:CZ2	4:C:990:HOH:O	2.52	0.56
1:C:106:ASN:HB2	1:C:107:PRO:HD2	1.87	0.56
1:B:192:GLU:HA	1:B:196:ILE:HB	1.88	0.56
1:C:196:ILE:HD13	1:C:207:VAL:HG21	1.87	0.56
1:B:185:LYS:O	1:B:189:LEU:HG	2.05	0.56
1:B:97:LEU:HD22	1:B:237:MET:HE3	1.88	0.56
1:C:146:TYR:CE1	1:C:236:PRO:HA	2.41	0.56
1:B:327:ASP:O	1:B:331:VAL:HG23	2.06	0.56
1:C:310:HIS:CD2	1:C:439:GLY:HA3	2.41	0.56
1:A:418:ASP:O	1:A:422:LYS:HG3	2.06	0.55
1:A:394:GLU:HB2	1:A:458:LEU:HD21	1.89	0.55
1:B:313:THR:HB	1:B:344:ASP:OD1	2.06	0.55
1:B:241:ILE:HG12	1:B:285:ILE:CG2	2.35	0.55
1:C:73:VAL:CG2	1:C:84:LEU:HB3	2.37	0.55
1:B:227:LEU:HD22	1:B:255:GLU:OE1	2.06	0.55
1:C:104:TRP:HH2	1:C:269:PHE:H	1.55	0.55
1:C:244:SER:C	1:C:246:GLY:N	2.59	0.55
1:C:50:LEU:HD22	1:C:54:VAL:CG1	2.28	0.55
1:A:416:GLU:HB2	4:A:971:HOH:O	2.05	0.54
1:B:467:ARG:HA	1:B:470:LYS:HG3	1.88	0.54
1:C:228:ARG:O	1:C:229:ASN:HB2	2.08	0.54
1:C:97:LEU:HD22	1:C:237:MET:HE3	1.88	0.54
1:C:202:LEU:H	1:C:202:LEU:HD12	1.71	0.54
1:B:467:ARG:HA	1:B:470:LYS:CG	2.36	0.54
1:B:103:LEU:O	1:B:143:TRP:CZ3	2.60	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:LEU:HD22	1:A:237:MET:HG3	1.88	0.54
1:C:104:TRP:HZ2	4:C:990:HOH:O	1.89	0.54
1:A:199:ASN:HB3	1:A:202:LEU:HD13	1.88	0.54
1:B:239:ASP:HB3	4:B:907:HOH:O	2.08	0.54
1:A:243:HIS:HE1	1:A:286:GLN:OE1	1.90	0.54
1:A:313:THR:HB	1:A:344:ASP:OD1	2.08	0.54
1:B:286:GLN:HE22	1:B:309:ARG:HH22	1.54	0.53
1:A:155:ASP:OD2	1:A:428:SER:HB3	2.08	0.53
1:A:348:ASN:H	1:A:446:GLN:HE22	1.57	0.53
1:B:228:ARG:HA	4:B:923:HOH:O	2.08	0.53
1:B:264:SER:HA	1:B:267:TYR:CE2	2.43	0.53
1:B:288:ASP:HB3	1:B:291:LYS:HG3	1.88	0.53
1:C:329:LEU:O	1:C:333:GLU:HG3	2.08	0.53
1:B:97:LEU:HB2	1:B:237:MET:CE	2.37	0.53
1:A:167:GLU:HG3	1:A:437:ARG:NH1	2.22	0.53
1:C:110:VAL:HG12	1:C:131:PHE:CG	2.43	0.53
1:C:157:THR:OG1	1:C:177:THR:CG2	2.57	0.53
1:C:455:GLU:O	1:C:458:LEU:HB2	2.08	0.53
1:A:247:VAL:HG21	1:A:285:ILE:HA	1.91	0.53
1:A:325:PHE:CZ	1:A:329:LEU:HD22	2.44	0.53
1:A:360:ARG:HG2	1:A:392:ASN:OD1	2.08	0.53
1:A:428:SER:HB2	4:A:936:HOH:O	2.09	0.53
1:C:430:LEU:O	1:C:434:VAL:HG23	2.09	0.53
1:A:484:ASN:HB3	4:A:980:HOH:O	2.09	0.52
1:B:124:PRO:HG2	4:C:1009:HOH:O	2.07	0.52
1:B:264:SER:HA	1:B:267:TYR:CE1	2.44	0.52
1:A:286:GLN:HE22	1:A:309:ARG:HH22	1.57	0.52
1:B:411:TYR:HB3	4:B:903:HOH:O	2.08	0.52
1:A:103:LEU:HA	1:A:143:TRP:CH2	2.44	0.52
1:A:486:TYR:HB2	1:C:123:LYS:HZ2	1.75	0.52
1:B:287:TYR:O	1:B:288:ASP:HB2	2.09	0.52
1:C:293:ASN:OD1	1:C:303:ILE:HB	2.09	0.52
1:A:255:GLU:HB2	1:A:268:LEU:HD12	1.91	0.52
1:A:466:GLU:HG2	1:A:470:LYS:HE2	1.92	0.52
1:C:250:GLU:HG2	1:C:289:LEU:HD12	1.92	0.52
1:A:286:GLN:HE21	1:A:288:ASP:N	2.08	0.52
1:A:408:LEU:HD21	1:A:444:LEU:HB3	1.92	0.52
1:B:99:VAL:O	1:B:104:TRP:CH2	2.63	0.52
1:C:104:TRP:NE1	4:C:990:HOH:O	2.41	0.52
1:B:342:TYR:CZ	1:C:479:GLY:HA3	2.45	0.52
1:B:201:ARG:HH12	1:B:202:LEU:HD11	1.75	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:LEU:O	1:A:178:VAL:HG23	2.09	0.52
1:A:244:SER:HB2	1:A:284:TYR:CG	2.45	0.52
1:A:78:VAL:HG23	1:A:80:GLU:HG2	1.92	0.52
1:C:151:PRO:HD3	1:C:222:ARG:HH21	1.75	0.52
1:A:104:TRP:O	1:A:105:ILE:HG13	2.10	0.51
1:A:287:TYR:O	3:A:902:LYS:HA	2.11	0.51
1:B:104:TRP:O	1:B:105:ILE:HG13	2.10	0.51
1:C:54:VAL:HA	1:C:149:ILE:HD11	1.92	0.51
1:C:201:ARG:NH1	1:C:201:ARG:HB3	2.25	0.51
1:A:96:ILE:HD13	1:A:283:VAL:HG11	1.92	0.51
1:A:103:LEU:O	1:A:143:TRP:CZ3	2.64	0.51
1:A:60:TRP:CE3	1:A:61:LEU:HG	2.46	0.51
1:B:58:TRP:O	1:B:62:GLN:HG3	2.10	0.51
1:C:98:GLN:HA	1:C:269:PHE:O	2.10	0.51
1:A:105:ILE:O	1:A:105:ILE:HG22	2.11	0.51
1:C:192:GLU:HA	1:C:196:ILE:HB	1.93	0.50
1:A:386:LEU:O	1:A:387:SER:CB	2.59	0.50
1:B:241:ILE:CG1	1:B:285:ILE:HG23	2.39	0.50
1:C:97:LEU:HD22	1:C:237:MET:CE	2.42	0.50
1:A:277:VAL:HG13	1:A:281:GLU:HB2	1.92	0.50
1:A:114:GLU:OE1	1:A:134:ARG:NH2	2.45	0.50
1:A:119:CYS:HA	1:A:122:LEU:HD12	1.93	0.50
2:B:801:SA8:H3'	4:B:981:HOH:O	2.12	0.50
1:B:226:ARG:NH2	1:B:288:ASP:HA	2.26	0.50
1:A:101:LYS:HG3	1:A:104:TRP:CD1	2.47	0.50
2:A:800:SA8:HE2	3:A:902:LYS:NZ	2.27	0.50
2:A:800:SA8:H3'	4:A:975:HOH:O	2.10	0.50
1:B:228:ARG:O	1:B:229:ASN:HB2	2.12	0.50
1:C:167:GLU:HG3	1:C:437:ARG:NH1	2.27	0.50
1:A:157:THR:HA	1:A:160:TRP:CD1	2.47	0.50
1:A:118:VAL:HG22	4:A:910:HOH:O	2.11	0.49
1:B:360:ARG:HG2	1:B:392:ASN:OD1	2.12	0.49
1:C:82:LEU:O	2:C:802:SA8:N	2.45	0.49
1:A:201:ARG:HB3	1:A:201:ARG:HH11	1.77	0.49
1:A:428:SER:O	1:A:432:ILE:HG13	2.12	0.49
1:B:202:LEU:C	1:B:204:PRO:HD3	2.32	0.49
1:B:333:GLU:HA	1:B:337:PHE:O	2.12	0.49
1:C:446:GLN:O	1:C:450:ILE:HG13	2.12	0.49
1:A:110:VAL:HG12	1:A:131:PHE:CG	2.48	0.49
1:C:410:GLY:HA3	4:C:937:HOH:O	2.12	0.49
1:C:371:LEU:HB3	1:C:380:ILE:HD13	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:ASP:OD2	1:B:428:SER:HB3	2.13	0.49
1:B:176:THR:O	1:B:180:VAL:HG23	2.13	0.49
1:C:222:ARG:O	3:C:901:LYS:HE3	2.13	0.49
1:A:159:TYR:OH	1:A:217:GLY:HA3	2.13	0.48
1:A:98:GLN:HE21	1:A:270:SER:HG	1.57	0.48
1:B:160:TRP:CD1	1:B:429:ARG:HD3	2.48	0.48
1:B:323:PRO:HG2	1:B:324:PHE:HD1	1.78	0.48
1:B:49:SER:O	1:B:52:PRO:HG2	2.13	0.48
1:C:314:LEU:HG	1:C:345:ILE:HD12	1.95	0.48
1:C:481:ILE:HD11	4:C:1026:HOH:O	2.11	0.48
1:B:376:PHE:O	1:B:378:ASP:N	2.46	0.48
1:C:167:GLU:HG3	1:C:437:ARG:HH12	1.78	0.48
1:B:300:TYR:HA	4:B:981:HOH:O	2.12	0.48
1:C:483:GLU:HA	1:C:486:TYR:HD2	1.77	0.48
1:A:256:VAL:H	1:A:268:LEU:CD1	2.25	0.48
1:B:104:TRP:CH2	1:B:269:PHE:HB2	2.49	0.48
1:C:173:LEU:O	1:C:177:THR:HG23	2.14	0.48
1:C:469:LEU:HD22	1:C:472:LEU:HD21	1.96	0.48
1:A:476:GLY:O	1:C:175:LYS:HD2	2.13	0.48
1:C:103:LEU:HA	1:C:143:TRP:HH2	1.77	0.48
1:B:226:ARG:NH2	1:B:250:GLU:CD	2.66	0.48
1:C:463:TYR:O	1:C:467:ARG:HG3	2.14	0.48
1:A:401:ARG:NH1	1:A:452:GLU:HG3	2.29	0.48
1:B:388:VAL:O	1:B:463:TYR:HB3	2.14	0.48
1:A:316:LEU:CD2	1:B:474:LEU:HD22	2.43	0.48
1:C:286:GLN:HE21	1:C:288:ASP:C	2.17	0.48
1:C:286:GLN:HE22	1:C:309:ARG:HH22	1.61	0.48
1:C:57:PHE:CE2	1:C:61:LEU:HD11	2.49	0.48
1:C:73:VAL:HG22	1:C:74:LYS:N	2.28	0.48
1:B:100:PRO:O	1:B:104:TRP:CZ3	2.66	0.48
1:C:72:PRO:HB3	1:C:88:LYS:HE3	1.95	0.48
1:B:274:PRO:O	1:B:275:LEU:HD23	2.14	0.48
1:C:292:SER:OG	1:C:295:GLU:HG3	2.14	0.48
1:A:356:LEU:N	1:A:357:PRO:HD2	2.28	0.47
1:C:244:SER:O	1:C:246:GLY:N	2.46	0.47
1:A:167:GLU:HG2	1:A:430:LEU:CD1	2.44	0.47
1:C:104:TRP:HE3	1:C:104:TRP:N	2.12	0.47
1:C:390:ARG:HG2	1:C:390:ARG:HH11	1.78	0.47
1:C:468:ARG:HH11	1:C:468:ARG:HB3	1.79	0.47
1:B:88:LYS:HD3	1:B:88:LYS:O	2.15	0.47
1:C:64:GLU:OE1	1:C:102:ARG:NH1	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:ASN:HB2	1:A:107:PRO:HD2	1.96	0.47
1:B:390:ARG:HH11	1:B:390:ARG:HG2	1.80	0.47
1:B:439:GLY:O	1:B:442:MET:HB2	2.14	0.47
1:A:163:GLU:H	1:A:163:GLU:CD	2.17	0.47
1:B:194:GLU:C	1:B:195:ILE:HD12	2.35	0.47
1:B:482:LEU:HD22	1:B:486:TYR:CE2	2.50	0.47
1:C:113:SER:HB2	4:C:979:HOH:O	2.15	0.47
1:C:327:ASP:OD1	1:C:377:ARG:NH2	2.48	0.47
1:B:320:GLU:HA	1:B:325:PHE:CD1	2.49	0.47
1:A:348:ASN:N	1:A:446:GLN:HE22	2.14	0.46
1:C:50:LEU:N	4:C:933:HOH:O	2.48	0.46
1:A:115:ILE:HG22	1:A:202:LEU:HD22	1.98	0.46
1:A:188:CYS:HB3	1:A:212:PHE:CD1	2.49	0.46
1:B:88:LYS:O	1:B:90:ILE:HG13	2.15	0.46
1:A:136:ARG:HA	1:A:147:PHE:CD1	2.51	0.46
1:B:51:SER:N	1:B:52:PRO:HD2	2.30	0.46
1:A:310:HIS:CD2	1:A:439:GLY:HA3	2.51	0.46
1:B:92:ARG:CB	1:B:92:ARG:NH1	2.69	0.46
1:C:252:HIS:C	1:C:254:TYR:H	2.18	0.46
1:C:386:LEU:O	1:C:387:SER:CB	2.63	0.46
1:B:227:LEU:HB3	1:B:228:ARG:H	1.56	0.46
1:A:96:ILE:HD11	1:A:273:SER:CB	2.42	0.46
1:B:160:TRP:HA	1:B:429:ARG:NH1	2.31	0.46
1:C:67:ILE:CD1	1:C:71:THR:HG21	2.46	0.46
1:A:103:LEU:HA	1:A:143:TRP:HH2	1.81	0.46
1:B:117:ARG:N	1:B:117:ARG:HD2	2.30	0.46
1:B:273:SER:OG	1:B:275:LEU:O	2.33	0.46
1:B:363:ALA:O	1:B:364:LEU:C	2.53	0.46
1:A:199:ASN:HB3	1:A:202:LEU:CD1	2.45	0.46
1:B:226:ARG:NH2	1:B:250:GLU:OE2	2.49	0.46
1:B:394:GLU:CB	1:B:458:LEU:HD21	2.46	0.46
1:A:214:TRP:O	1:A:218:ILE:HG12	2.15	0.46
1:B:250:GLU:OE2	1:B:288:ASP:HA	2.16	0.45
1:A:96:ILE:HD11	1:A:273:SER:CA	2.46	0.45
1:C:361:LEU:HD13	1:C:384:LEU:HD11	1.97	0.45
2:C:802:SA8:HE2	3:C:901:LYS:NZ	2.31	0.45
1:B:386:LEU:O	1:B:387:SER:CB	2.63	0.45
1:C:244:SER:HB2	1:C:284:TYR:CG	2.51	0.45
1:A:146:TYR:CE1	1:A:236:PRO:HA	2.52	0.45
1:A:201:ARG:NH1	1:A:201:ARG:HB3	2.31	0.45
1:B:202:LEU:O	1:B:204:PRO:HD3	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:ASP:O	1:A:428:SER:C	2.55	0.45
1:B:59:LYS:HZ2	1:B:59:LYS:HB2	1.77	0.45
1:A:100:PRO:C	1:A:102:ARG:N	2.70	0.45
1:A:101:LYS:HA	1:A:104:TRP:CE3	2.51	0.45
1:A:472:LEU:HD21	1:C:362:VAL:HG11	1.99	0.45
1:C:107:PRO:HB2	4:C:939:HOH:O	2.15	0.45
1:C:73:VAL:HG22	1:C:74:LYS:H	1.82	0.45
1:A:310:HIS:HE1	4:A:919:HOH:O	2.00	0.45
1:B:82:LEU:O	2:B:801:SA8:N	2.48	0.45
1:A:465:GLN:O	1:A:468:ARG:HB3	2.16	0.44
1:A:59:LYS:O	1:A:63:GLU:HG3	2.17	0.44
1:B:104:TRP:CZ2	1:B:269:PHE:HB2	2.52	0.44
1:C:364:LEU:HD23	1:C:372:LEU:HD11	1.99	0.44
1:A:243:HIS:HB3	2:A:800:SA8:N7	2.32	0.44
1:A:78:VAL:CG2	1:A:80:GLU:HG2	2.47	0.44
1:B:103:LEU:HA	1:B:143:TRP:CH2	2.52	0.44
1:C:381:TRP:O	1:C:385:GLU:HG3	2.17	0.44
1:A:222:ARG:O	3:A:902:LYS:HE3	2.18	0.44
1:C:386:LEU:O	1:C:387:SER:HB3	2.17	0.44
1:A:209:LEU:O	1:A:212:PHE:HB2	2.18	0.44
1:B:104:TRP:O	1:B:143:TRP:CH2	2.69	0.44
3:C:901:LYS:N	4:C:948:HOH:O	2.50	0.44
1:A:255:GLU:HB3	1:A:268:LEU:O	2.17	0.44
1:A:96:ILE:CD1	1:A:283:VAL:HG11	2.47	0.44
1:B:129:ILE:O	1:B:133:ILE:HG13	2.18	0.44
1:B:177:THR:HG22	1:B:298:LEU:HD13	1.98	0.44
1:A:104:TRP:HE3	1:A:104:TRP:N	2.16	0.44
1:A:390:ARG:HG2	1:A:390:ARG:HH11	1.83	0.44
1:B:363:ALA:HB1	1:B:395:LEU:HD13	1.99	0.44
1:C:401:ARG:NH1	1:C:452:GLU:HG3	2.33	0.44
1:A:167:GLU:HG3	1:A:437:ARG:HH12	1.83	0.44
1:B:219:LEU:HD11	1:B:232:LEU:CD2	2.48	0.44
1:C:377:ARG:HA	1:C:377:ARG:HD3	1.82	0.44
1:C:475:CYS:HB2	4:C:1020:HOH:O	2.17	0.44
1:A:202:LEU:H	1:A:202:LEU:HD12	1.81	0.44
1:A:238:ALA:O	1:A:241:ILE:HG22	2.18	0.44
1:B:54:VAL:O	1:B:57:PHE:HB3	2.18	0.44
1:A:311:ALA:HB2	1:A:346:PHE:CD2	2.53	0.43
1:A:315:THR:HB	1:A:342:TYR:CD2	2.53	0.43
1:A:388:VAL:O	1:A:463:TYR:HB3	2.18	0.43
1:B:97:LEU:HD22	1:B:237:MET:CE	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:SER:N	4:B:1005:HOH:O	2.51	0.43
1:B:243:HIS:H	2:B:801:SA8:C8	2.31	0.43
1:A:150:LEU:HA	1:A:151:PRO:HD3	1.86	0.43
1:B:253:ALA:HA	1:B:270:SER:O	2.17	0.43
1:C:104:TRP:CE2	4:C:990:HOH:O	2.71	0.43
1:A:157:THR:OG1	1:A:177:THR:CG2	2.65	0.43
1:B:173:LEU:HD12	1:B:177:THR:HG23	2.00	0.43
1:C:107:PRO:O	1:C:110:VAL:HG22	2.18	0.43
1:C:214:TRP:O	1:C:218:ILE:HG12	2.19	0.43
1:A:466:GLU:O	1:A:470:LYS:HG2	2.19	0.43
1:A:58:TRP:CE2	1:A:67:ILE:HD12	2.54	0.43
1:B:356:LEU:N	1:B:357:PRO:HD2	2.33	0.43
1:C:125:TRP:O	1:C:129:ILE:HG13	2.19	0.43
1:C:293:ASN:ND2	1:C:309:ARG:HB2	2.33	0.43
1:C:226:ARG:HD2	3:C:901:LYS:N	2.33	0.43
1:B:78:VAL:CG1	1:B:79:THR:N	2.80	0.43
1:C:67:ILE:HD11	1:C:237:MET:SD	2.59	0.43
1:A:243:HIS:CE1	1:A:286:GLN:OE1	2.71	0.43
1:A:194:GLU:C	1:A:195:ILE:HD12	2.39	0.43
1:A:255:GLU:N	1:A:255:GLU:OE1	2.52	0.43
1:A:61:LEU:HB3	1:A:67:ILE:HG22	2.00	0.43
1:A:104:TRP:O	1:A:105:ILE:CG1	2.67	0.43
1:A:221:SER:O	2:A:800:SA8:HE1	2.18	0.43
1:A:99:VAL:HG21	1:A:235:VAL:HG12	2.01	0.43
1:A:235:VAL:HG21	1:A:269:PHE:CD1	2.53	0.43
1:B:151:PRO:HD3	1:B:222:ARG:HH21	1.83	0.43
1:C:104:TRP:CE3	1:C:104:TRP:N	2.86	0.43
1:B:168:LEU:HD21	1:B:433:ALA:HA	2.00	0.42
1:B:262:LEU:HD22	1:B:266:ASP:HB2	2.01	0.42
1:C:185:LYS:O	1:C:189:LEU:HG	2.18	0.42
1:C:151:PRO:CD	1:C:222:ARG:HH21	2.32	0.42
1:A:104:TRP:CE3	1:A:104:TRP:N	2.87	0.42
1:A:247:VAL:HG21	1:A:285:ILE:CA	2.49	0.42
1:B:364:LEU:HD23	1:B:372:LEU:HD11	2.01	0.42
1:C:226:ARG:HD3	1:C:252:HIS:CD2	2.54	0.42
1:C:226:ARG:HB3	1:C:252:HIS:CE1	2.54	0.42
1:A:172:GLN:OE1	1:A:313:THR:HG23	2.19	0.42
1:C:147:PHE:HD2	1:C:150:LEU:HD12	1.84	0.42
1:C:364:LEU:HD12	1:C:364:LEU:HA	1.84	0.42
1:B:313:THR:HG21	1:C:478:ASN:OD1	2.18	0.42
1:B:88:LYS:HD3	1:B:88:LYS:C	2.39	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:453:GLN:O	1:B:457:GLU:HG3	2.20	0.42
1:B:192:GLU:O	1:B:197:LEU:HG	2.19	0.42
1:B:97:LEU:CB	1:B:237:MET:HE1	2.47	0.42
1:B:323:PRO:HB3	1:C:375:LEU:HD21	2.01	0.42
1:B:482:LEU:HB2	4:B:975:HOH:O	2.19	0.42
1:C:202:LEU:N	1:C:202:LEU:HD12	2.34	0.42
1:A:319:SER:O	1:A:325:PHE:HD1	2.02	0.42
1:A:370:PHE:CD1	1:A:370:PHE:C	2.93	0.42
1:C:106:ASN:HB2	1:C:107:PRO:CD	2.48	0.42
1:C:315:THR:C	1:C:316:LEU:HD23	2.39	0.42
1:C:458:LEU:HD12	1:C:458:LEU:HA	1.74	0.42
1:A:57:PHE:CD1	1:A:146:TYR:HA	2.54	0.42
1:A:337:PHE:HB3	1:A:358:TYR:HE1	1.85	0.42
1:B:257:LYS:HB3	1:B:258:GLY:H	1.60	0.42
1:C:243:HIS:HB3	2:C:802:SA8:N7	2.35	0.42
1:A:222:ARG:HD3	1:A:239:ASP:OD2	2.20	0.42
1:B:101:LYS:HG3	1:B:104:TRP:CD1	2.55	0.42
1:C:400:VAL:HG11	1:C:451:PHE:CD1	2.55	0.42
1:A:199:ASN:ND2	1:A:199:ASN:N	2.68	0.42
1:B:350:THR:HG23	4:B:1019:HOH:O	2.19	0.42
1:C:277:VAL:HG13	1:C:281:GLU:HB2	2.02	0.42
1:A:202:LEU:O	1:A:204:PRO:HD3	2.19	0.41
1:A:486:TYR:HB2	1:C:123:LYS:HZ3	1.85	0.41
1:A:73:VAL:CG2	1:A:84:LEU:HB3	2.44	0.41
1:C:243:HIS:HB2	1:C:287:TYR:CD2	2.55	0.41
1:A:377:ARG:HA	1:A:377:ARG:HD3	1.90	0.41
1:A:199:ASN:N	1:A:199:ASN:HD22	2.18	0.41
1:A:220:ARG:HG3	4:A:994:HOH:O	2.21	0.41
1:B:130:LEU:HD21	1:B:191:LEU:HD13	2.02	0.41
1:C:315:THR:HB	1:C:342:TYR:CD2	2.55	0.41
1:C:414:THR:OG1	1:C:417:GLN:HG3	2.20	0.41
1:A:151:PRO:CD	1:A:222:ARG:HH21	2.33	0.41
1:A:384:LEU:HD23	1:A:384:LEU:HA	1.85	0.41
1:A:88:LYS:HA	1:A:88:LYS:HD2	1.89	0.41
1:A:227:LEU:HD22	1:A:227:LEU:N	2.35	0.41
1:B:364:LEU:HD12	1:B:364:LEU:HA	1.87	0.41
1:A:316:LEU:HD23	1:B:474:LEU:HD22	2.03	0.41
1:A:105:ILE:HD11	1:A:143:TRP:CD2	2.55	0.41
1:A:404:CYS:O	1:A:408:LEU:HG	2.20	0.41
1:A:219:LEU:HD11	1:A:232:LEU:CD2	2.49	0.41
1:B:313:THR:HG21	1:C:478:ASN:CG	2.41	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:103:LEU:O	1:C:143:TRP:HZ3	1.99	0.41
1:C:328:LYS:HE2	1:C:364:LEU:HB3	2.02	0.41
1:A:126:LEU:HD22	1:A:191:LEU:HD11	2.02	0.41
1:B:412:HIS:CD2	1:B:413:THR:HG23	2.55	0.41
1:C:390:ARG:HG2	1:C:390:ARG:NH1	2.36	0.41
1:A:157:THR:HB	1:A:177:THR:HG21	2.03	0.41
1:A:225:SER:OG	1:A:231:ASN:HB3	2.21	0.41
1:A:62:GLN:CA	1:A:67:ILE:HG23	2.49	0.41
1:B:370:PHE:C	1:B:370:PHE:CD1	2.94	0.41
1:B:446:GLN:O	1:B:450:ILE:HG13	2.21	0.41
1:A:226:ARG:C	1:A:227:LEU:HD13	2.41	0.41
1:A:472:LEU:HD23	1:A:472:LEU:HA	1.94	0.41
1:B:225:SER:HB2	1:B:226:ARG:H	1.64	0.41
2:C:802:SA8:HB1	2:C:802:SA8:H4'	2.03	0.41
1:A:380:ILE:HG23	1:A:381:TRP:N	2.36	0.40
1:B:376:PHE:C	1:B:378:ASP:H	2.25	0.40
1:C:146:TYR:CZ	1:C:150:LEU:HD21	2.56	0.40
2:A:800:SA8:HE2	3:A:902:LYS:HZ3	1.84	0.40
2:B:801:SA8:H4'	2:B:801:SA8:HA	2.03	0.40
1:C:101:LYS:HA	1:C:104:TRP:CD2	2.56	0.40
1:C:393:GLU:O	1:C:396:LEU:HG	2.20	0.40
1:A:100:PRO:C	1:A:102:ARG:H	2.24	0.40
1:B:310:HIS:CD2	1:B:439:GLY:HA3	2.55	0.40
1:B:98:GLN:HA	1:B:269:PHE:O	2.21	0.40
1:C:143:TRP:O	1:C:147:PHE:CD1	2.75	0.40
1:C:197:LEU:HB2	1:C:198:PRO:CD	2.51	0.40
1:A:106:ASN:HB2	1:A:107:PRO:CD	2.51	0.40
1:C:482:LEU:HA	1:C:482:LEU:HD23	1.87	0.40
1:A:480:ASP:O	1:A:484:ASN:HB2	2.22	0.40
1:A:99:VAL:HA	1:A:100:PRO:HD3	1.89	0.40
1:C:228:ARG:C	1:C:230:GLU:H	2.24	0.40
1:C:310:HIS:HD2	4:C:984:HOH:O	2.05	0.40
1:C:396:LEU:C	1:C:396:LEU:HD12	2.42	0.40
1:C:52:PRO:O	1:C:55:GLN:HB3	2.21	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	418/440 (95%)	360 (86%)	47 (11%)	11 (3%)	5	9
1	B	438/440 (100%)	381 (87%)	45 (10%)	12 (3%)	5	8
1	C	436/440 (99%)	392 (90%)	36 (8%)	8 (2%)	8	16
All	All	1292/1320 (98%)	1133 (88%)	128 (10%)	31 (2%)	6	10

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	105	ILE
1	A	387	SER
1	B	226	ARG
1	B	364	LEU
1	C	252	HIS
1	C	387	SER
1	A	104	TRP
1	A	232	LEU
1	A	236	PRO
1	B	204	PRO
1	B	288	ASP
1	B	366	GLY
1	B	387	SER
1	C	140	ASP
1	A	204	PRO
1	A	428	SER
1	B	377	ARG
1	B	428	SER
1	C	200	LYS
1	C	364	LEU
1	B	105	ILE
1	C	245	ALA
1	A	469	LEU
1	C	204	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	241	ILE
1	B	231	ASN
1	B	236	PRO
1	A	479	GLY
1	B	261	GLY
1	A	365	GLY
1	C	105	ILE

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	374/386 (97%)	348 (93%)	26 (7%)	15	30
1	B	386/386 (100%)	365 (95%)	21 (5%)	22	44
1	C	384/386 (100%)	362 (94%)	22 (6%)	20	41
All	All	1144/1158 (99%)	1075 (94%)	69 (6%)	19	39

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	TRP
1	A	89	ASP
1	A	94	ASP
1	A	104	TRP
1	A	117	ARG
1	A	143	TRP
1	A	157	THR
1	A	199	ASN
1	A	205	ASP
1	A	236	PRO
1	A	237	MET
1	A	252	HIS
1	A	267	TYR
1	A	268	LEU
1	A	298	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	299	ASP
1	A	300	TYR
1	A	313	THR
1	A	315	THR
1	A	321	SER
1	A	339	GLN
1	A	395	LEU
1	A	426	LEU
1	A	427	ASP
1	A	444	LEU
1	A	486	TYR
1	B	72	PRO
1	B	88	LYS
1	B	94	ASP
1	B	102	ARG
1	B	104	TRP
1	B	117	ARG
1	B	143	TRP
1	B	166	GLN
1	B	205	ASP
1	B	232	LEU
1	B	236	PRO
1	B	249	THR
1	B	313	THR
1	B	315	THR
1	B	339	GLN
1	B	395	LEU
1	B	426	LEU
1	B	427	ASP
1	B	444	LEU
1	B	471	ASP
1	B	482	LEU
1	C	55	GLN
1	C	68	THR
1	C	104	TRP
1	C	107	PRO
1	C	117	ARG
1	C	143	TRP
1	C	166	GLN
1	C	205	ASP
1	C	210	ASP
1	C	257	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	268	LEU
1	C	278	LYS
1	C	313	THR
1	C	315	THR
1	C	339	GLN
1	C	395	LEU
1	C	423	GLU
1	C	427	ASP
1	C	444	LEU
1	C	468	ARG
1	C	470	LYS
1	C	480	ASP

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

Mol	Chain	Res	Type
1	A	55	GLN
1	A	145	HIS
1	A	169	GLN
1	A	193	GLN
1	A	199	ASN
1	A	243	HIS
1	A	286	GLN
1	A	348	ASN
1	A	446	GLN
1	B	98	GLN
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	145	HIS
1	C	152	GLN
1	C	169	GLN
1	C	193	GLN
1	C	252	HIS
1	C	286	GLN
1	C	310	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	446	GLN

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 monosaccharides 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$
2	SA8	A	800	-	22,29,29	1.73	5 (22%)	21,42,42	1.36	3 (14%)
2	SA8	B	801	-	22,29,29	1.69	4 (18%)	21,42,42	1.42	3 (14%)
3	LYS	A	902	-	5,9,9	0.54	0	4,10,10	0.50	0
2	SA8	C	802	-	22,29,29	1.52	5 (22%)	21,42,42	1.54	3 (14%)
3	LYS	B	900	-	5,9,9	0.72	0	4,10,10	0.36	0
3	LYS	C	901	-	5,9,9	0.62	0	4,10,10	0.44	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	SA8	A	800	-	-	3/9/33/33	0/3/3/3
2	SA8	B	801	-	-	3/9/33/33	0/3/3/3
3	LYS	A	902	-	-	1/5/9/9	-
2	SA8	C	802	-	-	3/9/33/33	0/3/3/3
3	LYS	B	900	-	-	0/5/9/9	-
3	LYS	C	901	-	-	1/5/9/9	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	SA8	C5'-ND	4.42	1.57	1.47
2	A	800	SA8	C5'-ND	4.27	1.57	1.47
2	C	802	SA8	C5'-ND	3.98	1.56	1.47
2	A	800	SA8	C4-N3	3.67	1.40	1.35
2	A	800	SA8	CG-ND	3.65	1.56	1.46
2	B	801	SA8	CG-ND	3.56	1.56	1.46
2	C	802	SA8	CG-ND	3.21	1.55	1.46
2	B	801	SA8	C4-N3	3.00	1.39	1.35
2	C	802	SA8	C4-N3	2.73	1.39	1.35
2	B	801	SA8	C8-N7	-2.53	1.30	1.34
2	A	800	SA8	C8-N7	-2.43	1.30	1.34
2	C	802	SA8	C8-N7	-2.39	1.30	1.34
2	A	800	SA8	C2-N3	2.34	1.35	1.32
2	C	802	SA8	C2-N3	2.04	1.35	1.32

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	SA8	O4'-C4'-C5'	4.56	116.43	108.90
2	C	802	SA8	CE-ND-C5'	-3.86	105.01	111.32
2	C	802	SA8	O4'-C4'-C5'	3.80	115.18	108.90
2	A	800	SA8	O4'-C4'-C5'	3.64	114.92	108.90
2	A	800	SA8	CE-ND-C5'	-2.67	106.95	111.32
2	C	802	SA8	C3'-C2'-C1'	2.40	104.59	100.98
2	A	800	SA8	C3'-C2'-C1'	2.31	104.45	100.98
2	B	801	SA8	CE-ND-C5'	-2.23	107.67	111.32
2	B	801	SA8	C5-C6-N6	2.08	123.51	120.35

There are no chirality outliers.

All (11) torsion outliers are listed below:

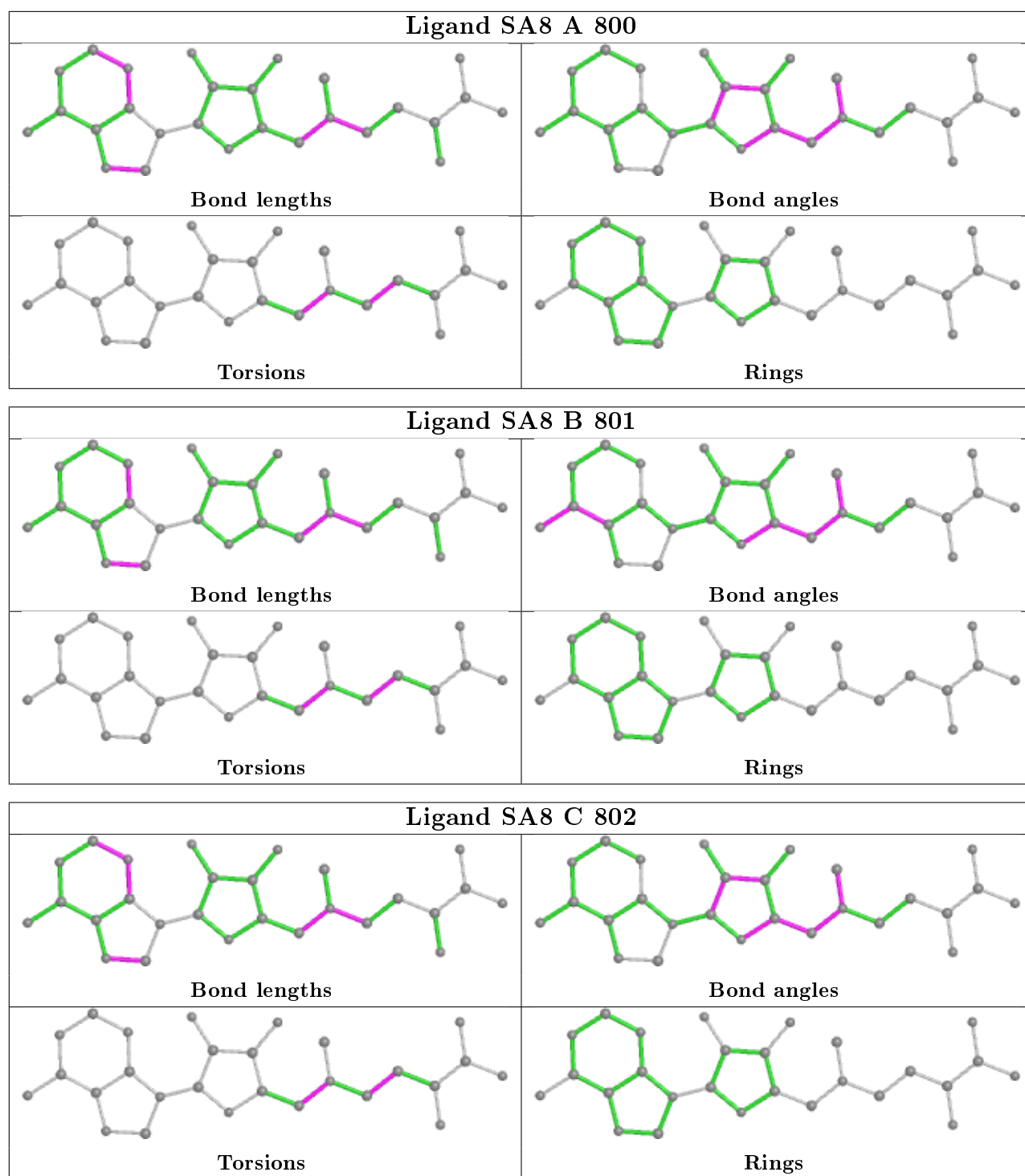
Mol	Chain	Res	Type	Atoms
2	A	800	SA8	CA-CB-CG-ND
2	A	800	SA8	C4'-C5'-ND-CG
2	B	801	SA8	CA-CB-CG-ND
2	C	802	SA8	C4'-C5'-ND-CG
2	B	801	SA8	C4'-C5'-ND-CG
2	A	800	SA8	C4'-C5'-ND-CE
2	C	802	SA8	C4'-C5'-ND-CE
2	C	802	SA8	CA-CB-CG-ND
2	B	801	SA8	C4'-C5'-ND-CE
3	C	901	LYS	CA-CB-CG-CD
3	A	902	LYS	N-CA-CB-CG

There are no ring outliers.

5 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	800	SA8	7	0
2	B	801	SA8	5	0
3	A	902	LYS	4	0
2	C	802	SA8	6	0
3	C	901	LYS	5	0

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



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	424/440 (96%)	0.21	25 (5%)	22 17	47, 71, 110, 127	0
1	B	440/440 (100%)	0.09	20 (4%)	33 26	39, 66, 103, 129	0
1	C	438/440 (99%)	-0.01	11 (2%)	57 51	44, 66, 99, 112	0
All	All	1302/1320 (98%)	0.09	56 (4%)	35 28	39, 68, 105, 129	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	140	ASP	5.9
1	A	267	TYR	5.1
1	A	256	VAL	5.1
1	C	250	GLU	5.0
1	B	486	TYR	4.8
1	A	254	TYR	4.8
1	A	117	ARG	4.7
1	C	487	PHE	4.2
1	B	139	GLU	3.9
1	A	144	LYS	3.9
1	A	59	LYS	3.8
1	B	488	GLN	3.7
1	A	112	ALA	3.6
1	C	117	ARG	3.6
1	A	139	GLU	3.6
1	A	70	LYS	3.5
1	B	229	ASN	3.3
1	B	375	LEU	3.3
1	C	200	LYS	3.2
1	B	121	GLU	3.1
1	A	486	TYR	3.1
1	A	137	SER	3.1
1	A	226	ARG	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	378	ASP	2.9
1	B	205	ASP	2.9
1	C	205	ASP	2.9
1	C	229	ASN	2.9
1	C	139	GLU	2.8
1	A	50	LEU	2.8
1	B	117	ARG	2.8
1	B	378	ASP	2.8
1	A	250	GLU	2.7
1	C	471	ASP	2.7
1	A	145	HIS	2.7
1	A	253	ALA	2.6
1	A	111	ALA	2.6
1	B	471	ASP	2.6
1	A	138	ARG	2.5
1	C	470	LYS	2.5
1	A	197	LEU	2.5
1	B	144	LYS	2.5
1	A	121	GLU	2.5
1	B	112	ALA	2.4
1	B	259	ALA	2.4
1	B	254	TYR	2.4
1	B	193	GLN	2.3
1	B	130	LEU	2.3
1	A	201	ARG	2.3
1	A	471	ASP	2.3
1	B	204	PRO	2.2
1	B	228	ARG	2.2
1	B	460	GLN	2.2
1	A	65	GLY	2.1
1	A	69	ALA	2.1
1	C	162	GLU	2.1
1	B	487	PHE	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

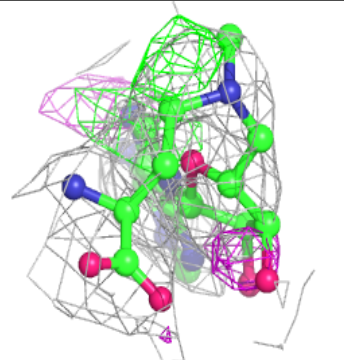
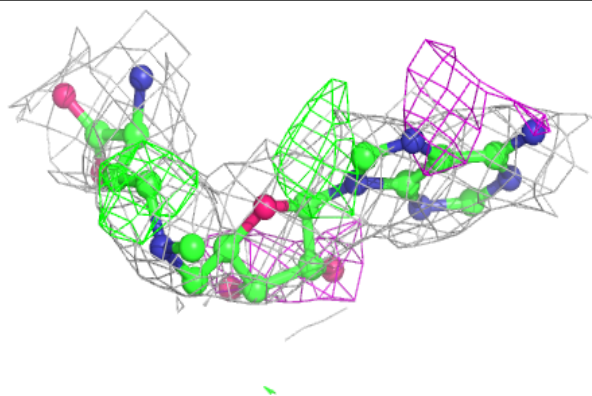
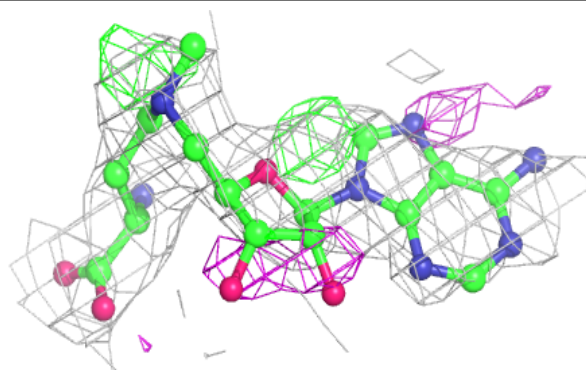
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SA8	B	801	27/27	0.75	0.32	85,97,100,103	0
3	LYS	A	902	10/10	0.77	0.27	81,91,96,96	0
2	SA8	A	800	27/27	0.79	0.26	100,103,107,107	0
3	LYS	B	900	10/10	0.83	0.26	69,79,84,84	0
2	SA8	C	802	27/27	0.85	0.26	90,98,102,105	0
3	LYS	C	901	10/10	0.91	0.15	52,61,64,64	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.

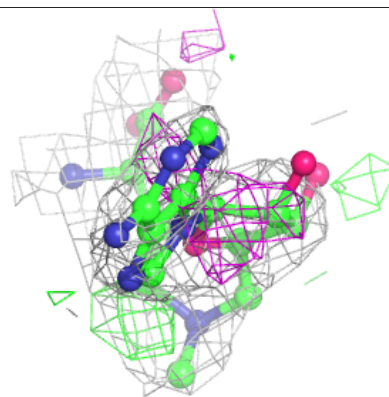
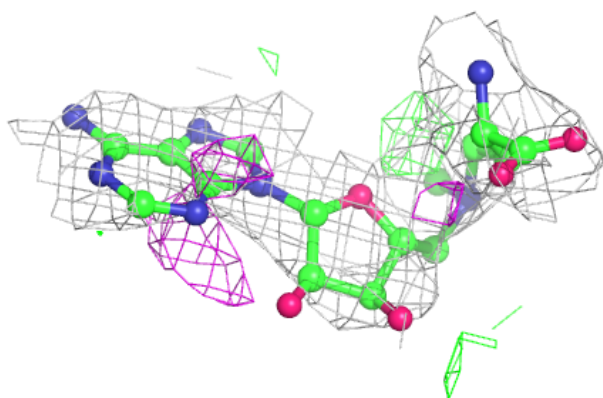
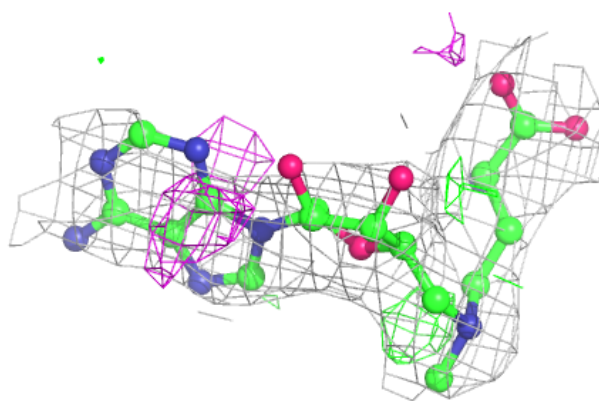
Electron density around SA8 B 801:

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

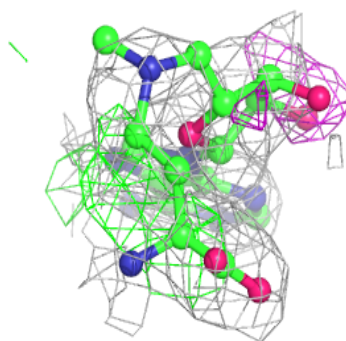
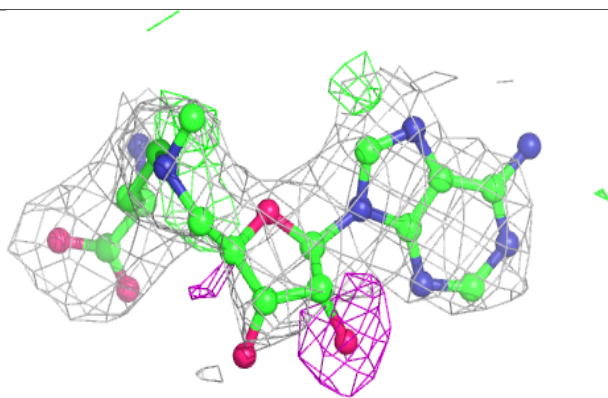
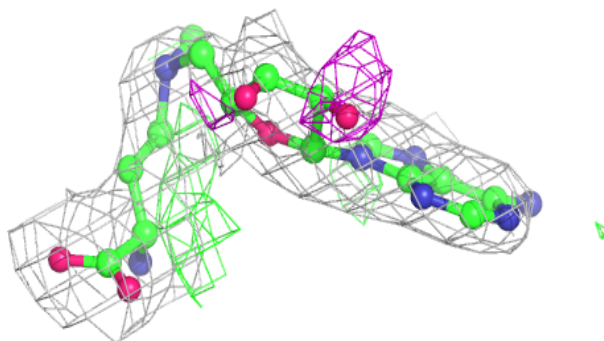


Electron density around SA8 A 800:

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

**Electron density around SA8 C 802:**

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



6.5 Other polymers

There are no such residues in this entry.