



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 04:49 AM UTC

PDB ID : 2H2E / pdb_00002h2e
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 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

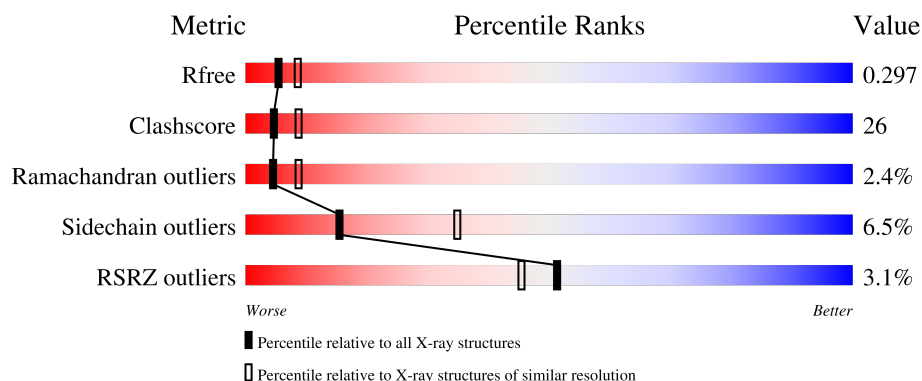
1 Overall quality at a glance

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	440	5% 52% 39% 5%
1	B	440	2% 55% 39% 5%
1	C	440	2% 57% 38% 5%

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.

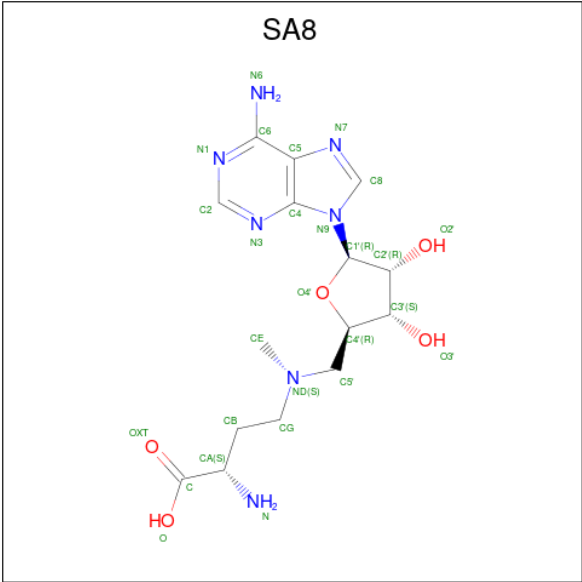
- Molecule 1 is a protein called Ribulose-1,5 bisphosphate carboxylase/oxygenase large subunit N-methyltransferase.

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:

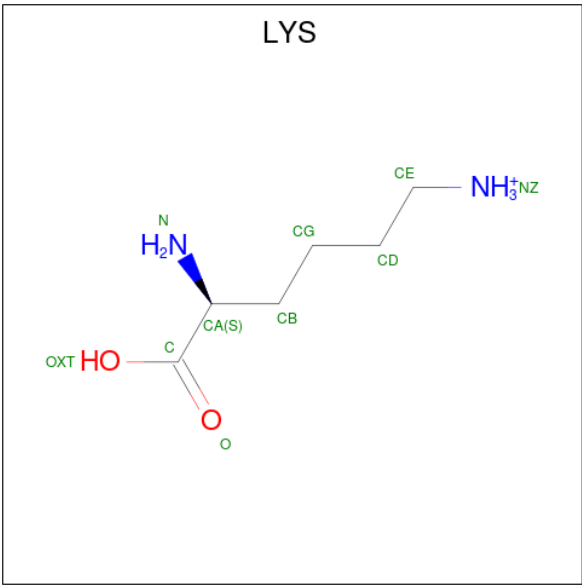
Chain	Residue	Modelled	Actual	Comment	Reference
A	483	GLU	-	cloning artifact	UNP Q43088
A	484	ASN	-	cloning artifact	UNP Q43088
A	485	LEU	-	cloning artifact	UNP Q43088
A	486	TYR	-	cloning artifact	UNP Q43088
A	487	PHE	-	cloning artifact	UNP Q43088
A	488	GLN	-	cloning artifact	UNP Q43088
B	483	GLU	-	cloning 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 (CCD ID: 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 (CCD ID: LYS) (formula: C₆H₁₅N₂O₂).



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

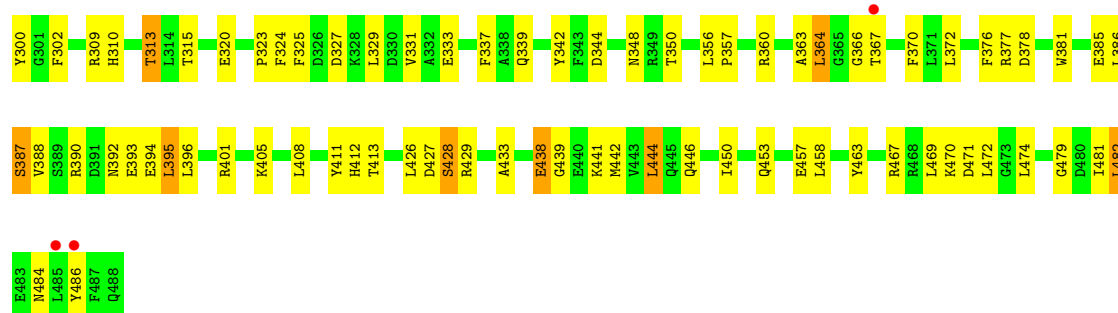
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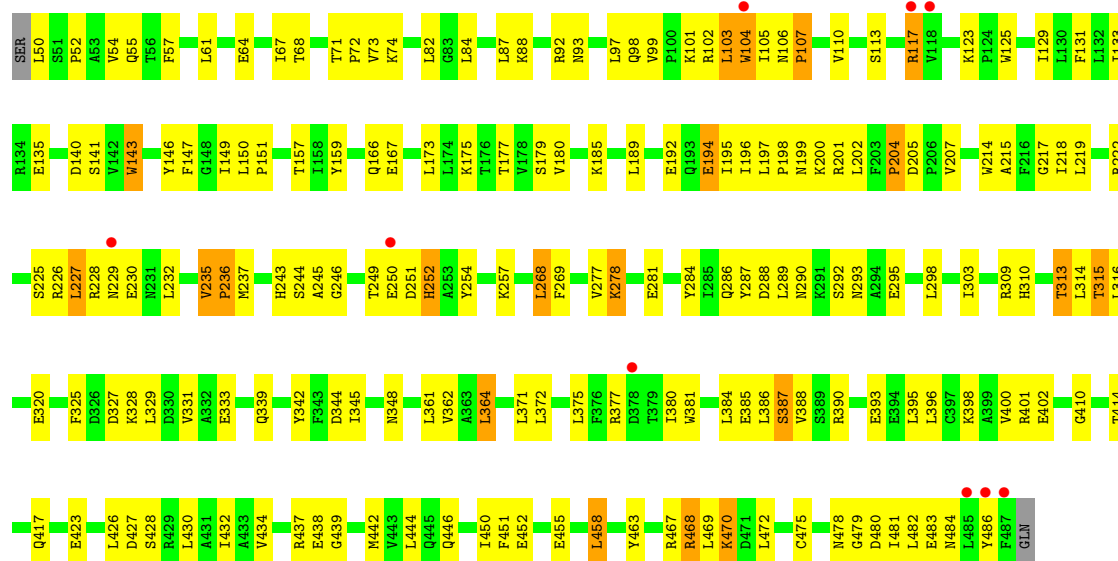
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			10	6	2	2		
3	C	1	Total	C	N	O	0	0
			10	6	2	2		

- 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		



- 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	132.63Å 159.49Å 267.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	16.73 – 2.60 16.73 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.2 (16.73-2.60) 97.8 (16.73-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 2.59Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.262 , 0.298 0.262 , 0.297	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 , 52.9	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	0.47	0/3482	0.91	2/4723 (0.0%)
1	B	0.48	0/3617	0.96	15/4906 (0.3%)
1	C	0.47	0/3601	0.94	8/4886 (0.2%)
All	All	0.47	0/10700	0.94	25/14515 (0.2%)

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	71	THR	CA-C-N	8.19	129.21	120.12
1	B	71	THR	C-N-CA	8.19	129.21	120.12
1	C	235	VAL	CA-C-N	7.57	129.30	119.84
1	C	235	VAL	C-N-CA	7.57	129.30	119.84
1	B	235	VAL	CA-C-N	6.78	128.32	119.84
1	B	235	VAL	C-N-CA	6.78	128.32	119.84
1	B	105	ILE	N-CA-C	-6.56	95.69	109.34
1	B	302	PHE	N-CA-C	6.50	117.15	108.38
1	C	339	GLN	N-CA-C	-6.34	104.42	111.71
1	B	438	GLU	N-CA-C	-6.25	104.39	111.14
1	B	484	ASN	N-CA-C	-6.07	106.03	113.50
1	B	268	LEU	N-CA-C	5.95	118.66	109.07
1	C	236	PRO	N-CA-C	5.94	124.70	112.47
1	C	268	LEU	N-CA-C	5.89	118.36	109.23
1	B	269	PHE	N-CA-C	-5.87	98.96	108.41
1	B	245	ALA	N-CA-C	-5.86	105.97	113.01
1	B	149	ILE	N-CA-C	-5.45	108.19	113.53
1	B	196	ILE	N-CA-C	5.39	115.60	110.42
1	A	420	GLU	N-CA-C	-5.36	105.48	112.23
1	C	290	ASN	N-CA-C	5.36	119.92	113.17
1	C	103	LEU	N-CA-C	5.22	119.34	112.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	194	GLU	N-CA-C	5.09	119.65	113.38
1	B	292	SER	N-CA-C	-5.04	103.01	110.46
1	A	290	ASN	N-CA-C	5.01	119.66	113.50
1	B	50	LEU	N-CA-C	5.01	117.70	111.24

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	200	0
1	B	3542	0	3501	177	0
1	C	3526	0	3488	180	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
3	B	10	0	12	0	0
3	C	10	0	12	4	0
4	A	117	0	0	14	0
4	B	127	0	0	13	0
4	C	141	0	0	21	0
All	All	10977	0	10475	545	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 26.

All (545) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:97:LEU:HD22	1:B:237:MET:HE3	1.67	0.75
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: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
1:B:92:ARG:NH1	1:B:92:ARG:HB2	2.04	0.73
1:B:202:LEU:HD12	1:B:202:LEU:H	1.54	0.73
1:A:97:LEU:HD22	1:A:237:MET:SD	2.29	0.73
1:C:97:LEU:HD22	1:C:237:MET:HE3	1.68	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:C:438:GLU:HG2	1:C:442:MET:HE2	1.73	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:B:438:GLU:HG2	1:B:442:MET:HE2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:439:GLY:HA2	1:B:442:MET:HE3	1.74	0.69
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:C:244:SER:C	1:C:246:GLY:H	2.00	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:96:ILE:HD11	1:A:273:SER:HB2	1.75	0.68
1:A:118:VAL:HG13	4:A:910:HOH:O	1.92	0.68
1:B:394:GLU:HB2	1:B:458:LEU:HD21	1.75	0.68
1:A:97:LEU:HD22	1:A:237:MET:CG	2.23	0.68
1:A:256:VAL:H	1:A:268:LEU:HD11	1.58	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:A:286:GLN:HE21	1:A:288:ASP:C	2.02	0.67
1:B:92:ARG:CB	1:B:92:ARG:HH11	2.08	0.67
1:B:104:TRP:NE1	4:B:910:HOH:O	2.14	0.67
1:A:439:GLY:HA2	1:A:442:MET:HE3	1.74	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:B:197:LEU:HB2	1:B:198:PRO:HD3	1.77	0.66
1:A:104:TRP:CH2	1:A:269:PHE:HB2	2.31	0.66
1:C:92:ARG:O	1:C:93:ASN:HB2	1.95	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
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:A:202:LEU:C	1:A:204:PRO:HD3	2.22	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:A:157:THR:OG1	1:A:177:THR:HG21	1.96	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:54:VAL:HA	1:A:149:ILE:HD11	1.77	0.64
1:A:219:LEU:HD11	1:A:232:LEU:HD21	1.79	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:LEU:HD12	1:B:202:LEU:N	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:HE3	1:C:278:LYS:H	1.64	0.62
1:C:104:TRP:CH2	1:C:269:PHE:HB2	2.34	0.62
1:C:194:GLU:C	1:C:195:ILE:HD12	2.24	0.62
1:A:117:ARG:HG2	4:A:910:HOH:O	1.98	0.62
1:A:62:GLN:HA	1:A:67:ILE:HG23	1.82	0.62
1:A:486:TYR:HB2	1:C:123:LYS:NZ	2.15	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: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:B:243:HIS:HB3	2:B:801:SA8:N7	2.16	0.61
1:A:287:TYR:OH	2:A:800:SA8:HE3	2.00	0.61
1:C:202:LEU:C	1:C:204:PRO:HD3	2.25	0.61
1:A:300:TYR:HB3	4:A:975:HOH:O	1.99	0.61
1:A:482:LEU:HD11	1:C:179:SER:OG	2.00	0.61
1:B:201:ARG:HB3	1:B:201:ARG:NH1	2.15	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
1:A:82:LEU:O	2:A:800:SA8:N	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:TYR:HB2	1:C:123:LYS:HZ3	1.67	0.59
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:244:SER:C	1:C:246:GLY:N	2.59	0.58
1:C:470:LYS:HE2	1:C:470:LYS:HA	1.85	0.58
1:A:370:PHE:HB3	4:A:923:HOH:O	2.03	0.58
1:C:97:LEU:HD13	1:C:237:MET:HE3	1.85	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:97:LEU:HB2	1:C:237:MET:HE3	1.86	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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:143:TRP:CD1	1:B:143:TRP:H	2.22	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: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:394:GLU:HB2	1:A:458:LEU:HD21	1.89	0.55
1:A:418:ASP:O	1:A:422:LYS:HG3	2.06	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:50:LEU:HD22	1:C:54:VAL:CG1	2.28	0.55
1:B:97:LEU:HB2	1:B:237:MET:CE	2.37	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:202:LEU:HD12	1:C:202:LEU:H	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
1:B:202:LEU:C	1:B:204:PRO:HD3	2.32	0.54
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:A:167:GLU:HG3	1:A:437:ARG:NH1	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:439:GLY:HA2	1:C:442:MET:HE3	1.89	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:C:228:ARG:O	1:C:229:ASN:HB2	2.08	0.53
1:A:428:SER:HB2	4:A:936:HOH:O	2.09	0.53
1:B:226:ARG:NH2	1:B:250:GLU:CD	2.66	0.53
1:C:286:GLN:HE21	1:C:288:ASP:C	2.17	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: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:B:342:TYR:CZ	1:C:479:GLY:HA3	2.45	0.52
1:C:104:TRP:NE1	4:C:990:HOH:O	2.41	0.52
1:B:201:ARG:HH12	1:B:202:LEU:HD11	1.75	0.52
1:A:78:VAL:HG23	1:A:80:GLU:HG2	1.92	0.52
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: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:97:LEU:HB2	1:B:237:MET:HE3	1.92	0.51
1:B:104:TRP:O	1:B:105:ILE:HG13	2.10	0.51
1:B:194:GLU:C	1:B:195:ILE:HD12	2.35	0.51
1:C:54:VAL:HA	1:C:149:ILE:HD11	1.92	0.51
1:A:163:GLU:CD	1:A:163:GLU:H	2.17	0.51
1:C:201:ARG:HB3	1:C:201:ARG:NH1	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HG22	1:A:105:ILE:O	2.11	0.51
1:C:252:HIS:C	1:C:254:TYR:H	2.18	0.51
1:B:363:ALA:O	1:B:364:LEU:C	2.53	0.50
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: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:427:ASP:O	1:A:428:SER:C	2.55	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:HH11	1:A:201:ARG:HB3	1.77	0.49
1:A:428:SER:O	1:A:432:ILE:HG13	2.12	0.49
1:C:97:LEU:CD2	1:C:237:MET:HE3	2.38	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:100:PRO:C	1:A:102:ARG:N	2.70	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
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:98:GLN:HE21	1:A:270:SER:HG	1.57	0.48
1:A:159:TYR:OH	1:A:217:GLY:HA3	2.13	0.48
1:B:49:SER:O	1:B:52:PRO:HG2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:463:TYR:O	1:C:467:ARG:HG3	2.14	0.48
1:A:316:LEU:CD2	1:B:474:LEU:HD22	2.43	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: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:C:286:GLN:HE22	1:C:309:ARG:HH22	1.61	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:A:194:GLU:C	1:A:195:ILE:HD12	2.39	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:N	1:C:104:TRP:HE3	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:O	1:B:88:LYS:HD3	2.15	0.47
1:A:106:ASN:HB2	1:A:107:PRO:HD2	1.96	0.47
1:B:390:ARG:HG2	1:B:390:ARG:HH11	1.80	0.47
1:B:439:GLY:O	1:B:442:MET:HB2	2.14	0.47
1:C:64:GLU:OE1	1:C:102:ARG:NH1	2.48	0.47
1:B:88:LYS:HD3	1:B:88:LYS:C	2.39	0.47
1:A:370:PHE:CD1	1:A:370:PHE:C	2.93	0.47
1:B:482:LEU:HD22	1:B:486:TYR:CE2	2.50	0.47
1:C:97:LEU:CB	1:C:237:MET:HE3	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:NH1	1:B:92:ARG:CB	2.69	0.46
1:C:315:THR:C	1:C:316:LEU:HD23	2.39	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:C:97:LEU:HD22	1:C:237:MET:CE	2.42	0.46
1:A:103:LEU:HA	1:A:143:TRP:HH2	1.81	0.46
1:B:117:ARG:HD2	1:B:117:ARG:N	2.30	0.46
1:B:273:SER:OG	1:B:275:LEU:O	2.33	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:313:THR:HG21	1:C:478:ASN:CG	2.41	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:B:370:PHE:CD1	1:B:370:PHE:C	2.94	0.45
1:A:96:ILE:HD11	1:A:273:SER:CA	2.46	0.45
1:B:376:PHE:C	1:B:378:ASP:H	2.25	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:A:226:ARG:C	1:A:227:LEU:HD13	2.41	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:HB3	1:A:201:ARG:NH1	2.31	0.45
1:B:202:LEU:O	1:B:204:PRO:HD3	2.17	0.45
1:B:97:LEU:CD2	1:B:237:MET:HE3	2.43	0.45
1:B:59:LYS:HB2	1:B:59:LYS:HZ2	1.77	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:GLU:OE1	1:C:141:SER:OG	2.32	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:228:ARG:C	1:C:230:GLU:H	2.24	0.45
1:C:396:LEU:HD12	1:C:396:LEU:C	2.42	0.45
1:C:438:GLU:CG	1:C:442:MET:HE2	2.45	0.45
1:A:106:ASN:O	1:A:107:PRO:C	2.59	0.45
1:B:225:SER:O	1:B:226:ARG:C	2.60	0.45
1:C:73:VAL:HG22	1:C:74:LYS:H	1.82	0.45
1:C:107:PRO:HB2	4:C:939:HOH:O	2.15	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:59:LYS:O	1:A:63:GLU:HG3	2.17	0.44
1:A:465:GLN:O	1:A:468:ARG:HB3	2.16	0.44
1:B:50:LEU:O	1:B:51:SER:C	2.60	0.44
1:B:104:TRP:CZ2	1:B:269:PHE:HB2	2.52	0.44
1:B:244:SER:C	1:B:246:GLY:N	2.73	0.44
1:C:97:LEU:CG	1:C:237:MET:HE3	2.46	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:B:101:LYS:C	1:B:103:LEU:N	2.75	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:96:ILE:CD1	1:A:283:VAL:HG11	2.47	0.44
1:A:255:GLU:HB3	1:A:268:LEU:O	2.17	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:N	1:A:104:TRP:HE3	2.16	0.44
1:A:390:ARG:HH11	1:A:390:ARG:HG2	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
2:A:800:SA8:HE2	3:A:902:LYS:HZ3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:138:ARG:C	1:A:140:ASP:H	2.26	0.43
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: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:58:TRP:CE2	1:A:67:ILE:HD12	2.54	0.43
1:A:100:PRO:C	1:A:102:ARG:H	2.24	0.43
1:A:302:PHE:CD1	1:A:302:PHE:C	2.96	0.43
1:A:466:GLU:O	1:A:470:LYS:HG2	2.19	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:226:ARG:HD2	3:C:901:LYS:N	2.33	0.43
1:C:293:ASN:ND2	1:C:309:ARG:HB2	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:50:LEU:HD23	1:A:50:LEU:C	2.43	0.43
1:A:243:HIS:CE1	1:A:286:GLN:OE1	2.71	0.43
1:B:244:SER:C	1:B:246:GLY:H	2.25	0.43
1:A:61:LEU:HB3	1:A:67:ILE:HG22	2.00	0.43
1:A:255:GLU:N	1:A:255:GLU:OE1	2.52	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:97:LEU:CB	1:A:237:MET:HE3	2.49	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:A:325:PHE:CD2	1:A:325:PHE:C	2.97	0.43
1:B:88:LYS:O	1:B:89:ASP:C	2.61	0.43
1:B:151:PRO:HD3	1:B:222:ARG:HH21	1.83	0.43
1:C:104:TRP:N	1:C:104:TRP:CE3	2.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:151:PRO:CD	1:C:222:ARG:HH21	2.32	0.42
1:C:185:LYS:O	1:C:189:LEU:HG	2.18	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:C:286:GLN:NE2	1:C:288:ASP:C	2.76	0.42
1:A:172:GLN:OE1	1:A:313:THR:HG23	2.19	0.42
1:A:240:LEU:O	1:A:241:ILE:C	2.63	0.42
1:B:313:THR:HG21	1:C:478:ASN:OD1	2.18	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:A:226:ARG:C	1:A:227:LEU:HD22	2.44	0.42
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: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:HD12	1:C:202:LEU:N	2.34	0.42
1:A:319:SER:O	1:A:325:PHE:HD1	2.02	0.42
1:C:106:ASN:HB2	1:C:107:PRO:CD	2.48	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:B:376:PHE:C	1:B:378:ASP:N	2.78	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:252:HIS:C	1:C:254:TYR:N	2.77	0.42
1:C:400:VAL:HG11	1:C:451:PHE:CD1	2.55	0.42
1:A:199:ASN:N	1:A:199:ASN:ND2	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:73:VAL:CG2	1:A:84:LEU:HB3	2.44	0.41
1:A:202:LEU:O	1:A:204:PRO:HD3	2.19	0.41
1:C:243:HIS:HB2	1:C:287:TYR:CD2	2.55	0.41
1:A:243:HIS:HE1	1:A:286:GLN:CD	2.28	0.41
1:A:377:ARG:HD3	1:A:377:ARG:HA	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:478:ASN:CG	1:C:313:THR:HG21	2.44	0.41
1:C:251:ASP:O	1:C:252:HIS:C	2.63	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:88:LYS:HD2	1:A:88:LYS:HA	1.89	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:227:LEU:HD22	1:A:227:LEU:N	2.35	0.41
1:A:316:LEU:HD23	1:B:474:LEU:HD22	2.03	0.41
1:B:364:LEU:HD12	1:B:364:LEU:HA	1.87	0.41
1:B:438:GLU:CG	1:B:442:MET:HE2	2.48	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:63:GLU:C	1:B:65:GLY:H	2.28	0.41
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:C:97:LEU:HB2	1:C:237:MET:HE1	2.02	0.41
1:A:62:GLN:CA	1:A:67:ILE:HG23	2.49	0.41
1:A:126:LEU:HD22	1:A:191:LEU:HD11	2.02	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:B:412:HIS:CD2	1:B:413:THR:HG23	2.55	0.41
1:B:446:GLN:O	1:B:450:ILE:HG13	2.21	0.41
1:C:390:ARG:HG2	1:C:390:ARG:NH1	2.36	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:97:LEU:CB	1:B:237:MET:HE3	2.50	0.40
1:B:441:LYS:NZ	4:B:903:HOH:O	2.53	0.40
1:C:146:TYR:CZ	1:C:150:LEU:HD21	2.56	0.40
1:A:237:MET:C	1:A:239:ASP:H	2.28	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:B:98:GLN:HA	1:B:269:PHE:O	2.21	0.40
1:B:310:HIS:CD2	1:B:439:GLY:HA3	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD23	1:C:482:LEU:HA	1.87	0.40
1:A:99:VAL:HA	1:A:100:PRO:HD3	1.89	0.40
1:A:480:ASP:O	1:A:484:ASN:HB2	2.22	0.40
1:C:52:PRO:O	1:C:55:GLN:HB3	2.21	0.40
1:C:310:HIS:HD2	4:C:984:HOH:O	2.05	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	418/440 (95%)	360 (86%)	47 (11%)	11 (3%)	4	7
1	B	438/440 (100%)	381 (87%)	45 (10%)	12 (3%)	4	7
1	C	436/440 (99%)	392 (90%)	36 (8%)	8 (2%)	6	14
All	All	1292/1320 (98%)	1133 (88%)	128 (10%)	31 (2%)	4	9

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

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Mol	Chain	Res	Type
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
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%)	349 (93%)	25 (7%)	15	33
1	B	386/386 (100%)	361 (94%)	25 (6%)	15	35
1	C	384/386 (100%)	360 (94%)	24 (6%)	16	36
All	All	1144/1158 (99%)	1070 (94%)	74 (6%)	15	35

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	ILE
1	A	80	GLU
1	A	89	ASP
1	A	99	VAL
1	A	104	TRP
1	A	107	PRO
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	252	HIS
1	A	267	TYR
1	A	268	LEU
1	A	298	LEU
1	A	313	THR
1	A	315	THR
1	A	321	SER
1	A	395	LEU
1	A	426	LEU
1	A	427	ASP
1	A	444	LEU
1	A	445	GLN
1	A	486	TYR
1	B	55	GLN
1	B	59	LYS
1	B	68	THR
1	B	72	PRO
1	B	79	THR
1	B	80	GLU
1	B	88	LYS
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

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Mol	Chain	Res	Type
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	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	227	LEU
1	C	249	THR
1	C	257	LYS
1	C	268	LEU
1	C	278	LYS
1	C	313	THR
1	C	315	THR
1	C	395	LEU
1	C	423	GLU
1	C	426	LEU
1	C	427	ASP
1	C	444	LEU
1	C	458	LEU
1	C	468	ARG
1	C	470	LYS
1	C	480	ASP
1	C	484	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) 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	242	ASN
1	A	243	HIS

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Mol	Chain	Res	Type
1	A	282	GLN
1	A	286	GLN
1	A	348	ASN
1	A	446	GLN
1	B	62	GLN
1	B	145	HIS
1	B	152	GLN
1	B	169	GLN
1	B	286	GLN
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	252	HIS
1	C	286	GLN
1	C	308	ASN
1	C	310	HIS
1	C	339	GLN
1	C	412	HIS
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 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	$\# Z > 2$
2	SA8	C	802	-	28,29,29	1.31	3 (10%)	37,42,42	1.29	3 (8%)
3	LYS	B	900	-	8,9,9	0.79	0	7,10,10	0.34	0
2	SA8	B	801	-	28,29,29	1.50	4 (14%)	37,42,42	1.22	3 (8%)
2	SA8	A	800	-	28,29,29	1.50	3 (10%)	37,42,42	1.15	4 (10%)
3	LYS	C	901	-	8,9,9	0.63	0	7,10,10	0.34	0
3	LYS	A	902	-	8,9,9	0.73	0	7,10,10	0.40	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	C	802	-	-	6/17/33/33	0/3/3/3
3	LYS	B	900	-	-	2/9/9/9	-
2	SA8	B	801	-	-	5/17/33/33	0/3/3/3
2	SA8	A	800	-	-	6/17/33/33	0/3/3/3
3	LYS	C	901	-	-	5/9/9/9	-
3	LYS	A	902	-	-	5/9/9/9	-

All (10) 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	CG-ND	3.46	1.56	1.46
2	A	800	SA8	C4-N3	3.37	1.40	1.34
2	B	801	SA8	CG-ND	3.36	1.56	1.46
2	C	802	SA8	CG-ND	3.03	1.55	1.46
2	B	801	SA8	C4-N3	2.88	1.39	1.34
2	C	802	SA8	C4-N3	2.67	1.39	1.34
2	B	801	SA8	C4-N9	2.13	1.42	1.37

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	SA8	O4'-C4'-C5'	4.61	116.43	108.88
2	C	802	SA8	CE-ND-C5'	-3.86	105.01	111.32
2	C	802	SA8	O4'-C4'-C5'	3.85	115.18	108.88
2	A	800	SA8	O4'-C4'-C5'	3.69	114.92	108.88
2	A	800	SA8	CE-ND-C5'	-2.67	106.95	111.32
2	A	800	SA8	N9-C8-N7	2.30	117.20	113.94
2	B	801	SA8	N9-C8-N7	2.25	117.13	113.94
2	B	801	SA8	CE-ND-C5'	-2.23	107.67	111.32
2	C	802	SA8	N9-C8-N7	2.14	116.98	113.94
2	A	800	SA8	C4-N9-C8	-2.13	103.50	105.74

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	800	SA8	OXT-C-CA-N
2	A	800	SA8	C4'-C5'-ND-CG
2	B	801	SA8	CA-CB-CG-ND
2	C	802	SA8	OXT-C-CA-N
2	C	802	SA8	C4'-C5'-ND-CG
3	A	902	LYS	O-C-CA-N
3	C	901	LYS	OXT-C-CA-CB
2	A	800	SA8	O-C-CA-N
2	C	802	SA8	O-C-CA-N
2	B	801	SA8	C4'-C5'-ND-CG
3	A	902	LYS	OXT-C-CA-N
3	C	901	LYS	OXT-C-CA-N
3	C	901	LYS	O-C-CA-CB
3	C	901	LYS	O-C-CA-N
2	A	800	SA8	C-CA-CB-CG
2	B	801	SA8	C-CA-CB-CG
2	C	802	SA8	C-CA-CB-CG
2	A	800	SA8	CA-CB-CG-ND
2	C	802	SA8	CA-CB-CG-ND
3	B	900	LYS	OXT-C-CA-CB
3	B	900	LYS	O-C-CA-CB
2	A	800	SA8	C4'-C5'-ND-CE
2	C	802	SA8	C4'-C5'-ND-CE
2	B	801	SA8	C4'-C5'-ND-CE
3	A	902	LYS	OXT-C-CA-CB
3	A	902	LYS	O-C-CA-CB

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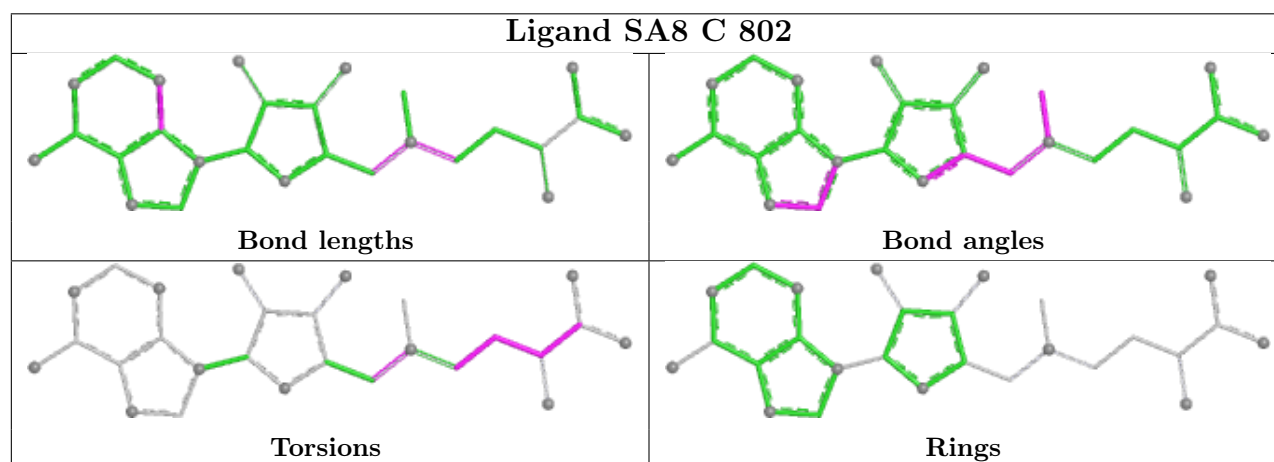
Mol	Chain	Res	Type	Atoms
3	C	901	LYS	CA-CB-CG-CD
3	A	902	LYS	N-CA-CB-CG
2	B	801	SA8	O-C-CA-N

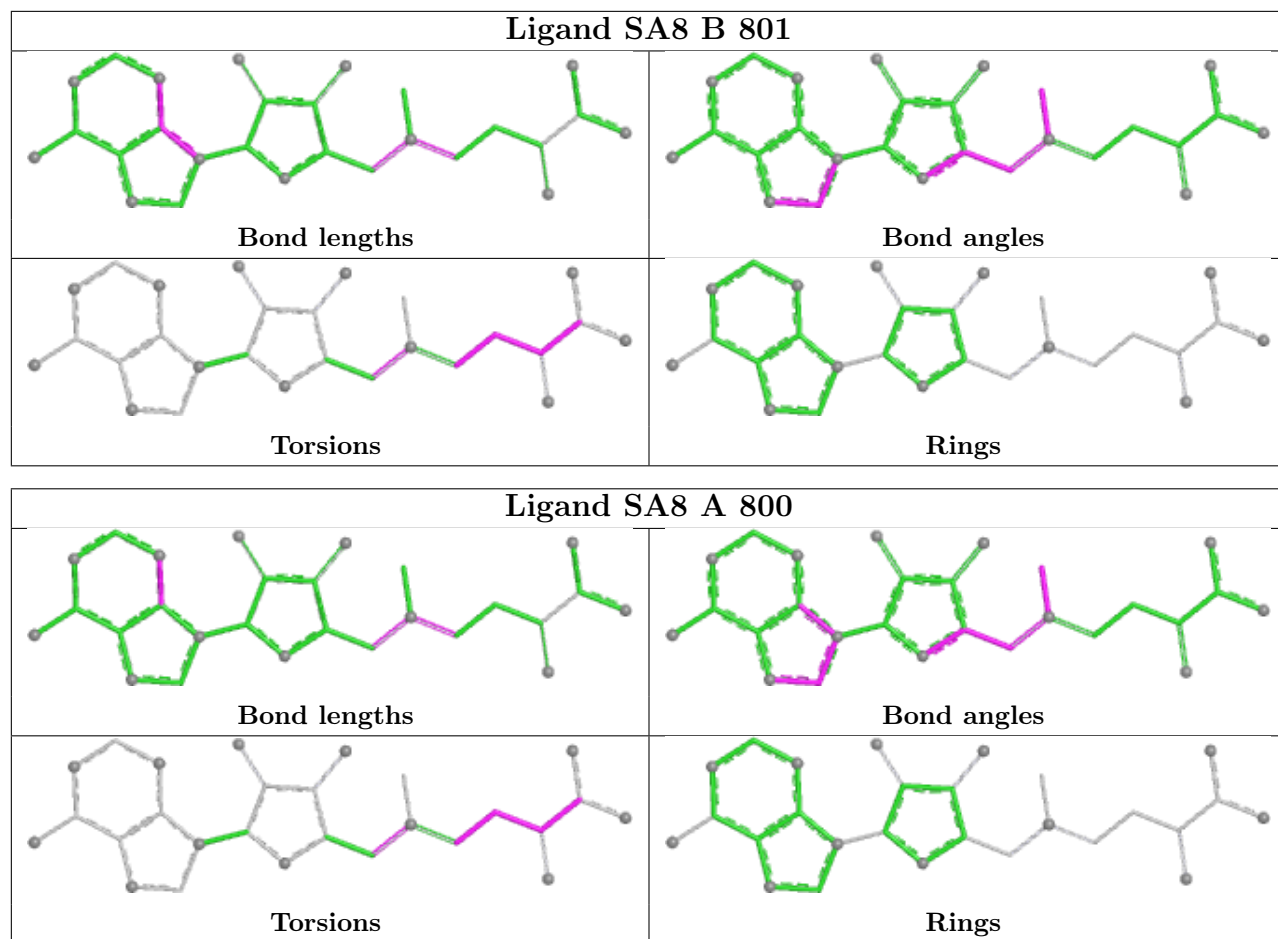
There are no ring outliers.

5 monomers are involved in 23 short contacts:

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

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	424/440 (96%)	0.29	23 (5%) 31 26	47, 71, 110, 127	0
1	B	440/440 (100%)	0.06	8 (1%) 67 63	39, 66, 103, 129	0
1	C	438/440 (99%)	-0.02	9 (2%) 63 58	44, 66, 99, 112	0
All	All	1302/1320 (98%)	0.11	40 (3%) 51 45	39, 68, 105, 129	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	256	VAL	6.1
1	B	486	TYR	4.6
1	A	486	TYR	4.4
1	C	486	TYR	4.4
1	A	253	ALA	4.2
1	A	267	TYR	3.6
1	C	250	GLU	3.4
1	C	487	PHE	3.2
1	B	258	GLY	3.1
1	C	117	ARG	3.0
1	B	193	GLN	3.0
1	C	229	ASN	2.9
1	A	67	ILE	2.8
1	A	112	ALA	2.8
1	A	70	LYS	2.7
1	A	254	TYR	2.7
1	B	260	ALA	2.7
1	B	485	LEU	2.6
1	A	202	LEU	2.6
1	A	145	HIS	2.6
1	B	367	THR	2.5
1	A	268	LEU	2.4
1	C	378	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	100	PRO	2.4
1	A	142	VAL	2.4
1	C	118	VAL	2.4
1	C	104	TRP	2.3
1	A	144	LYS	2.3
1	A	227	LEU	2.3
1	A	188	CYS	2.2
1	A	68	THR	2.2
1	B	111	ALA	2.2
1	A	111	ALA	2.2
1	B	139	GLU	2.1
1	A	203	PHE	2.1
1	A	124	PRO	2.1
1	A	198	PRO	2.1
1	A	199	ASN	2.1
1	A	140	ASP	2.0
1	C	485	LEU	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 oligosaccharides in this entry.

6.4 Ligands ⓘ

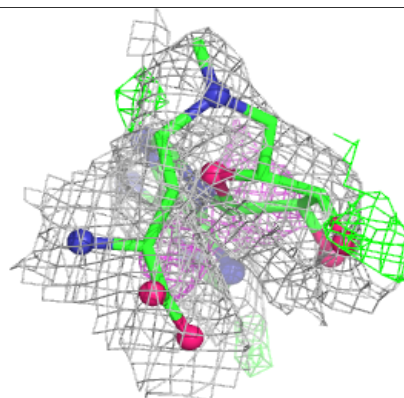
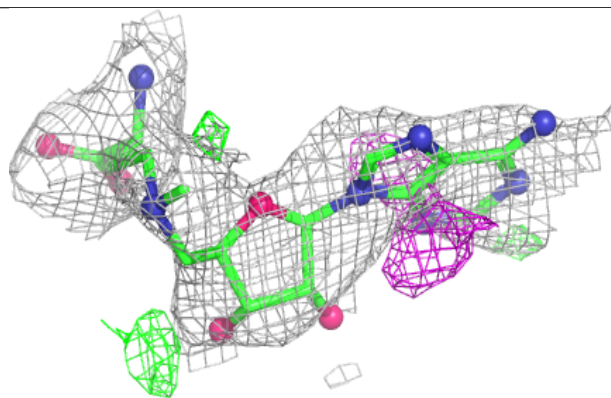
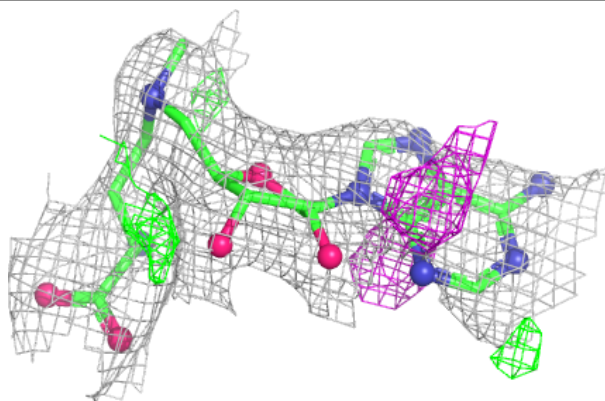
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SA8	A	800	27/27	0.78	0.18	100,103,107,107	0
2	SA8	B	801	27/27	0.80	0.18	85,97,100,103	0
3	LYS	A	902	10/10	0.84	0.14	81,91,96,96	0
2	SA8	C	802	27/27	0.86	0.17	90,98,102,105	0
3	LYS	B	900	10/10	0.86	0.17	69,79,84,84	0
3	LYS	C	901	10/10	0.92	0.11	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.

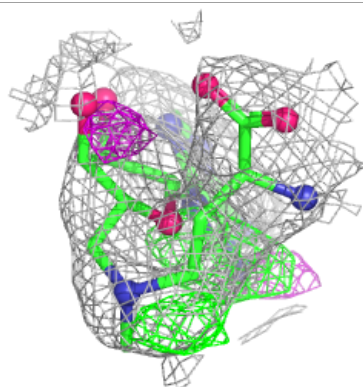
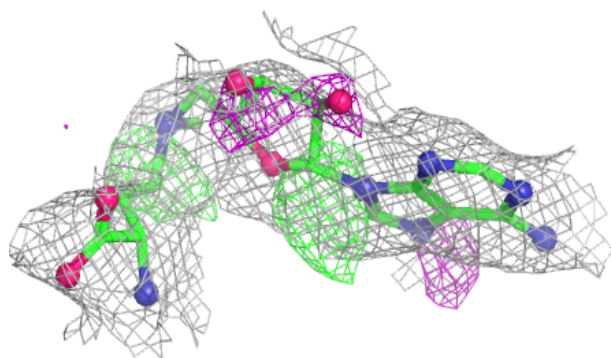
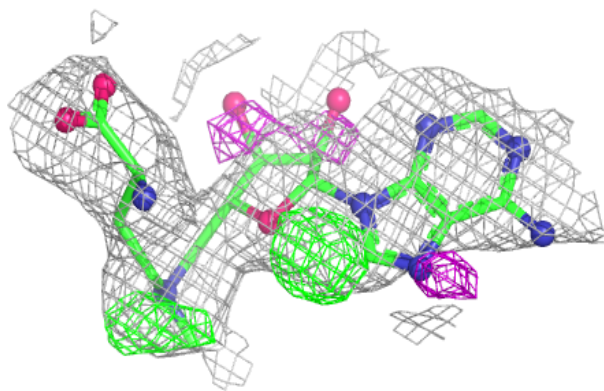
Electron density around SA8 A 800:

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

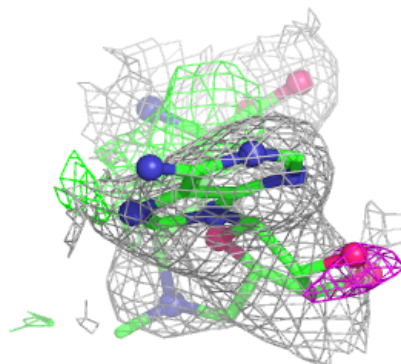
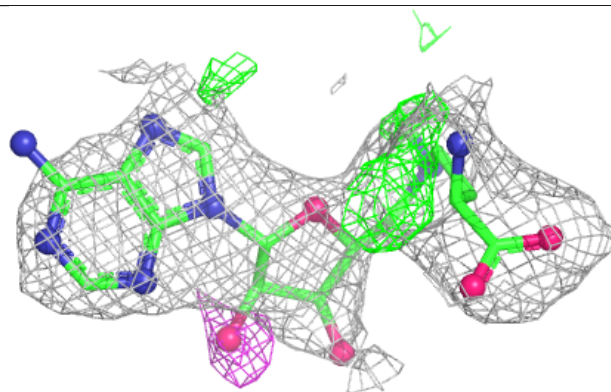
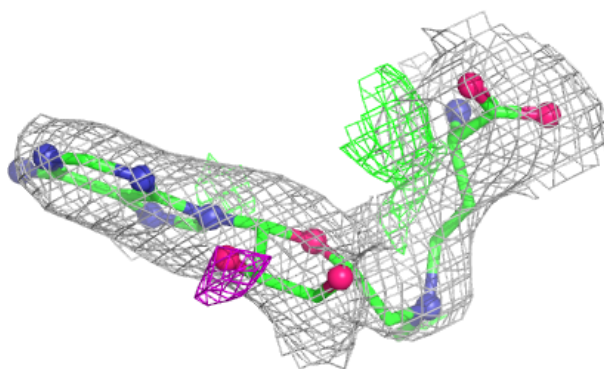


Electron density around SA8 B 801:

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

**Electron density around SA8 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 [i](#)

There are no such residues in this entry.