



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:25 PM UTC

PDB ID : 3VYW / pdb_00003vyw
Title : Crystal structure of MNMC2 from Aquifex Aeolicus
Authors : Shibata, R.; Bessho, Y.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2012-10-03
Resolution : 2.49 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

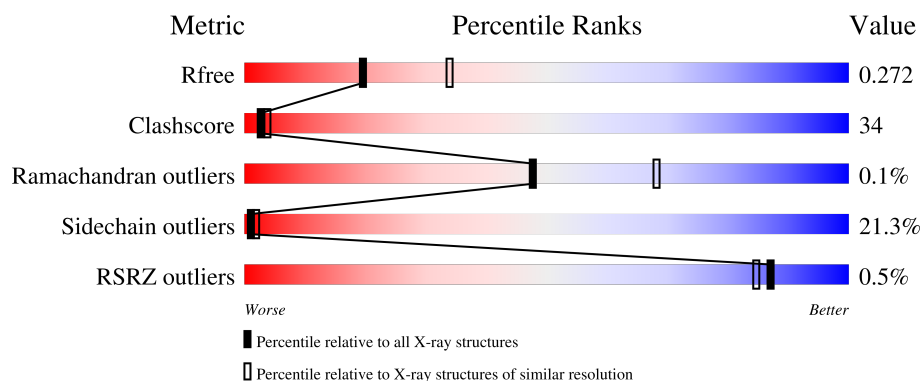
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.49 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	308	% 56% 28% 12% ..
1	B	308	42% 40% 16% ..
1	C	308	44% 38% 16% ..
1	D	308	% 42% 37% 19% ..

2 Entry composition [i](#)

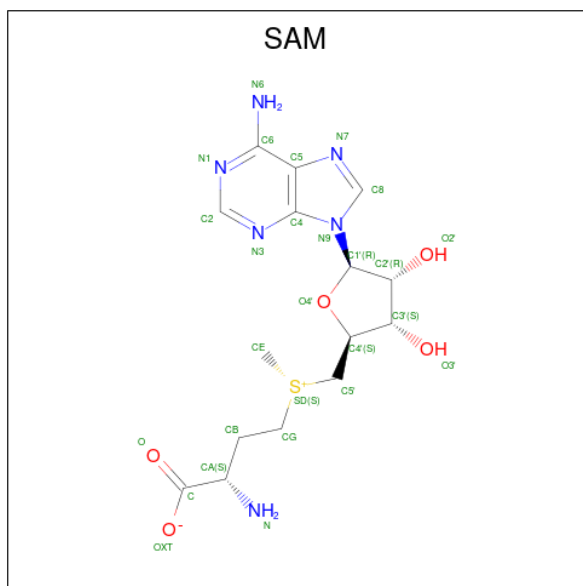
There are 4 unique types of molecules in this entry. The entry contains 10340 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 MNMC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	303	Total	C	N	O	Se	0	0	0
			2502	1623	419	458	2			
1	B	305	Total	C	N	O	Se	0	0	0
			2520	1634	425	459	2			
1	C	305	Total	C	N	O	Se	0	0	0
			2520	1634	425	459	2			
1	D	306	Total	C	N	O	Se	0	0	0
			2526	1637	426	461	2			

- Molecule 2 is S-ADENOSYLMETHIONINE (CCD ID: SAM) (formula: $C_{15}H_{22}N_6O_5S$).



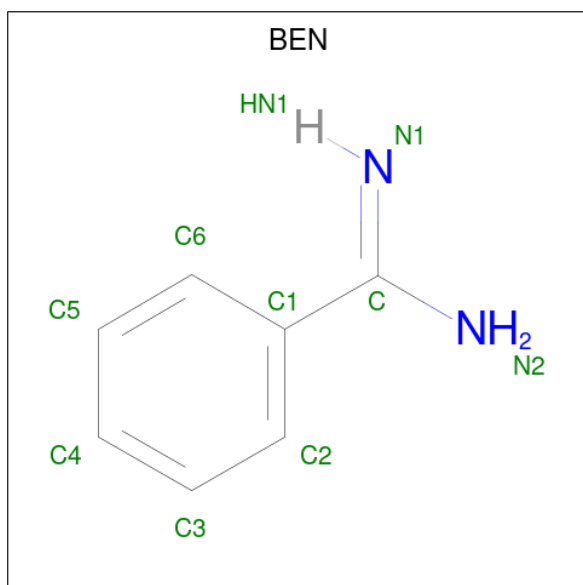
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
2	B	1	Total	C	N	O	S	0	0
			27	15	6	5	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
2	D	1	Total	C	N	O	S	0	0
			27	15	6	5	1		

- Molecule 3 is BENZAMIDINE (CCD ID: BEN) (formula: C₇H₈N₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	N	0	0
			9	7	2		
3	C	1	Total	C	N	0	0
			9	7	2		

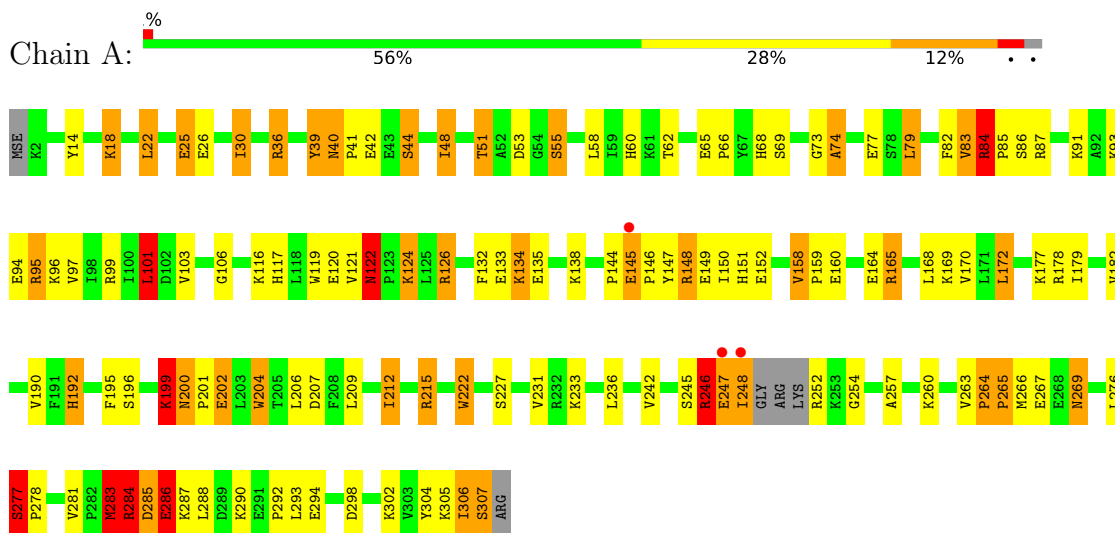
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	42	Total	O	0	0
			42	42		
4	B	32	Total	O	0	0
			32	32		
4	C	34	Total	O	0	0
			34	34		
4	D	38	Total	O	0	0
			38	38		

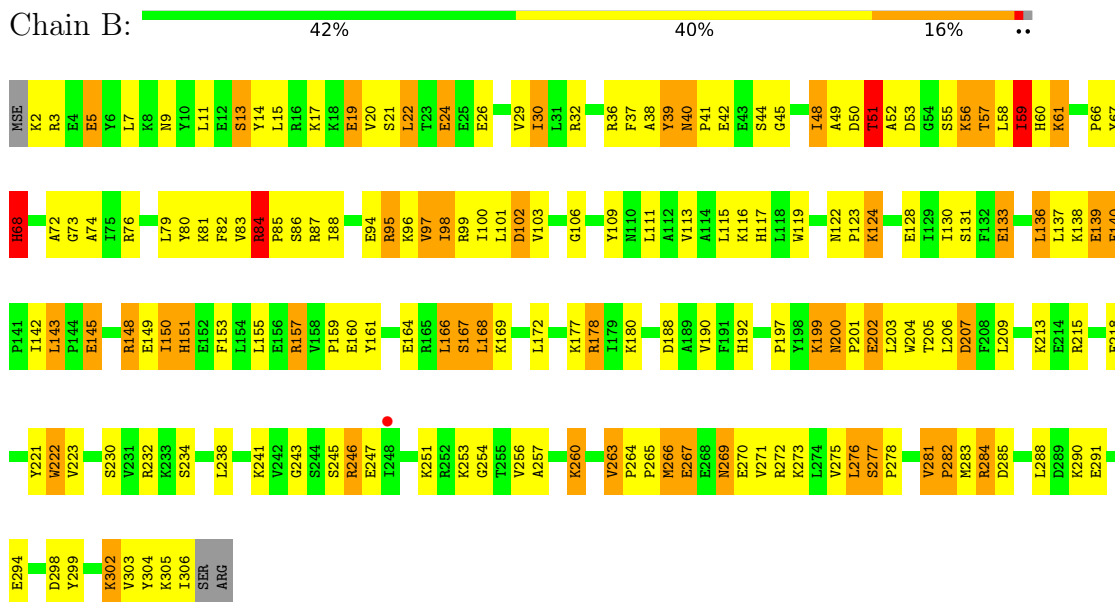
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

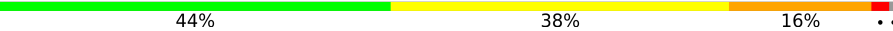
• Molecule 1: MNMC2

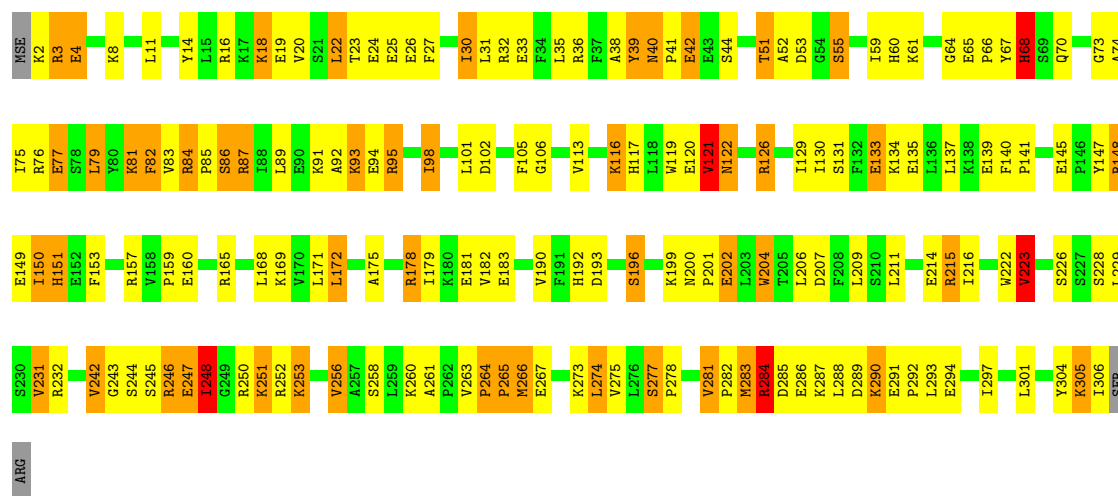


• Molecule 1: MNMC2



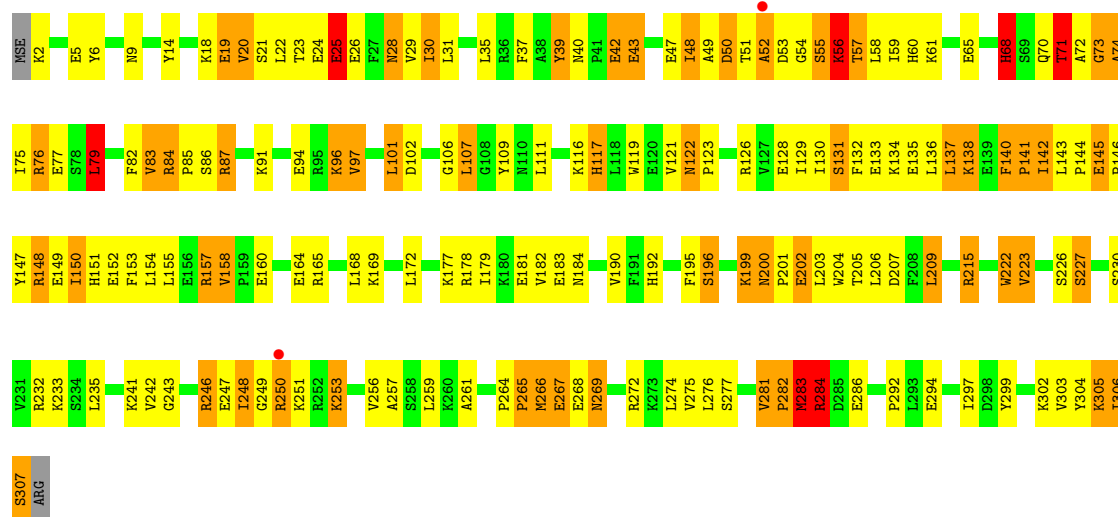
• Molecule 1: MNMC2

Chain C:  44% 38% 16% ..



• Molecule 1: MNMC2

Chain D:  42% 37% 19% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	55.49Å 107.58Å 117.71Å 90.00° 102.44° 90.00°	Depositor
Resolution (Å)	45.39 – 2.49 45.39 – 2.49	Depositor EDS
% Data completeness (in resolution range)	96.8 (45.39-2.49) 96.9 (45.39-2.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.53 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.191 , 0.255 (Not available) , 0.272	Depositor DCC
R_{free} test set	2346 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	47.9	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 38.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.025 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10340	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% 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 ⓘ

5.1 Standard geometry ⓘ

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

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	2.05	38/2554 (1.5%)	1.44	40/3437 (1.2%)
1	B	1.98	36/2573 (1.4%)	1.40	31/3462 (0.9%)
1	C	1.94	38/2573 (1.5%)	1.40	39/3462 (1.1%)
1	D	2.00	37/2579 (1.4%)	1.36	36/3470 (1.0%)
All	All	1.99	149/10279 (1.4%)	1.40	146/13831 (1.1%)

All (149) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	264	PRO	CA-C	-12.84	1.43	1.52
1	D	265	PRO	CA-C	-10.50	1.41	1.52
1	A	281	VAL	CA-C	-9.75	1.42	1.52
1	C	281	VAL	CA-C	-9.64	1.42	1.52
1	B	282	PRO	CA-C	8.94	1.62	1.52
1	B	284	ARG	N-CA	-8.94	1.34	1.46
1	A	82	PHE	C-N	-8.75	1.23	1.33
1	D	282	PRO	CA-C	-8.42	1.42	1.52
1	D	25	GLU	CA-C	-8.36	1.41	1.52
1	D	83	VAL	N-CA	-8.29	1.35	1.46
1	B	283	MSE	N-CA	-8.11	1.36	1.46
1	A	192	HIS	CG-ND1	-8.02	1.29	1.38
1	A	264	PRO	C-O	-7.88	1.18	1.24
1	D	281	VAL	C-N	7.82	1.43	1.33
1	C	267	GLU	C-N	-7.67	1.24	1.33
1	D	283	MSE	CA-C	-7.67	1.43	1.52
1	D	223	VAL	C-O	-7.58	1.16	1.24
1	B	283	MSE	C-N	7.31	1.44	1.33
1	B	82	PHE	C-O	-7.21	1.12	1.23
1	C	140	PHE	C-O	-7.14	1.14	1.24
1	C	264	PRO	C-N	-7.12	1.24	1.33
1	D	261	ALA	CA-C	7.11	1.62	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	246	ARG	C-N	7.05	1.43	1.33
1	A	264	PRO	CA-C	-7.01	1.47	1.52
1	B	51	THR	CA-C	-6.92	1.44	1.52
1	A	284	ARG	CA-C	6.91	1.61	1.52
1	D	192	HIS	CG-ND1	-6.88	1.30	1.38
1	B	223	VAL	C-O	-6.83	1.17	1.24
1	B	192	HIS	CG-ND1	-6.79	1.30	1.38
1	A	117	HIS	CG-ND1	-6.66	1.30	1.38
1	D	190	VAL	C-O	-6.61	1.17	1.24
1	D	266	MSE	CA-CB	-6.58	1.43	1.53
1	A	122	ASN	C-O	-6.57	1.19	1.25
1	B	267	GLU	CA-CB	-6.57	1.43	1.53
1	D	56	LYS	C-O	6.52	1.32	1.23
1	A	254	GLY	C-O	-6.48	1.17	1.23
1	B	117	HIS	CG-ND1	-6.47	1.31	1.38
1	B	100	ILE	C-O	-6.45	1.17	1.24
1	C	83	VAL	N-CA	6.43	1.55	1.46
1	D	284	ARG	N-CA	-6.41	1.37	1.45
1	A	283	MSE	C-N	6.41	1.44	1.33
1	D	151	HIS	CG-ND1	-6.37	1.31	1.38
1	B	256	VAL	C-O	-6.32	1.17	1.24
1	C	117	HIS	CG-ND1	-6.30	1.31	1.38
1	D	60	HIS	CG-ND1	-6.25	1.31	1.38
1	A	204	TRP	NE1-CE2	-6.25	1.30	1.37
1	D	256	VAL	C-O	-6.25	1.17	1.24
1	A	84	ARG	C-O	-6.20	1.19	1.24
1	C	266	MSE	N-CA	6.18	1.53	1.46
1	C	190	VAL	C-O	-6.09	1.17	1.24
1	C	192	HIS	CG-ND1	-6.08	1.31	1.38
1	A	117	HIS	CD2-NE2	-6.07	1.31	1.37
1	A	233	LYS	C-O	-6.06	1.16	1.24
1	B	97	VAL	C-O	-6.06	1.18	1.24
1	C	256	VAL	C-O	-6.03	1.17	1.24
1	C	60	HIS	CG-ND1	-6.02	1.31	1.38
1	C	151	HIS	CG-ND1	-5.99	1.31	1.38
1	A	151	HIS	CG-ND1	-5.99	1.31	1.38
1	C	192	HIS	CD2-NE2	-5.98	1.31	1.37
1	B	159	PRO	CA-C	-5.97	1.41	1.52
1	A	60	HIS	CG-ND1	-5.96	1.31	1.38
1	B	98	ILE	C-O	-5.92	1.18	1.24
1	A	190	VAL	C-O	-5.92	1.17	1.24
1	D	235	LEU	C-O	-5.86	1.17	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	283	MSE	CB-CG	-5.85	1.34	1.52
1	C	282	PRO	CA-C	-5.84	1.45	1.52
1	C	223	VAL	C-O	-5.84	1.18	1.24
1	D	132	PHE	C-O	-5.83	1.17	1.24
1	C	266	MSE	C-N	-5.81	1.25	1.33
1	D	68	HIS	CG-ND1	-5.80	1.31	1.38
1	A	151	HIS	CD2-NE2	-5.80	1.31	1.37
1	A	132	PHE	C-O	-5.77	1.17	1.24
1	B	222	TRP	NE1-CE2	-5.75	1.31	1.37
1	B	266	MSE	C-N	-5.74	1.25	1.33
1	C	266	MSE	CA-C	-5.74	1.45	1.52
1	B	60	HIS	CG-ND1	-5.71	1.31	1.38
1	B	103	VAL	C-O	-5.71	1.17	1.24
1	A	212	ILE	C-O	-5.71	1.17	1.24
1	A	222	TRP	NE1-CE2	-5.68	1.31	1.37
1	C	216	ILE	C-O	-5.65	1.18	1.24
1	B	130	ILE	C-O	-5.63	1.18	1.24
1	C	84	ARG	C-O	-5.61	1.19	1.24
1	D	128	GLU	C-O	-5.59	1.17	1.24
1	C	283	MSE	CG-SE	5.58	2.12	1.95
1	B	234	SER	C-O	-5.58	1.17	1.24
1	C	267	GLU	CA-C	-5.57	1.45	1.52
1	B	119	TRP	NE1-CE2	-5.55	1.31	1.37
1	D	266	MSE	N-CA	-5.53	1.38	1.45
1	D	52	ALA	CA-CB	-5.52	1.44	1.53
1	D	169	LYS	C-O	-5.52	1.17	1.24
1	B	84	ARG	C-O	-5.51	1.19	1.24
1	C	119	TRP	NE1-CE2	-5.48	1.31	1.37
1	C	130	ILE	C-O	-5.47	1.18	1.24
1	B	151	HIS	CG-ND1	-5.47	1.32	1.38
1	B	275	VAL	C-O	-5.46	1.17	1.24
1	D	25	GLU	CA-CB	-5.44	1.45	1.53
1	D	297	ILE	C-O	-5.42	1.17	1.24
1	D	281	VAL	C-O	-5.39	1.17	1.24
1	C	231	VAL	C-O	-5.39	1.17	1.24
1	D	56	LYS	CA-C	-5.38	1.45	1.53
1	D	117	HIS	CG-ND1	-5.37	1.32	1.38
1	A	144	PRO	C-N	5.35	1.41	1.33
1	A	200	ASN	C-O	-5.34	1.17	1.23
1	C	159	PRO	C-N	-5.34	1.26	1.33
1	B	276	LEU	N-CA	-5.34	1.39	1.46
1	C	283	MSE	CA-CB	-5.33	1.45	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	170	VAL	C-O	-5.30	1.18	1.24
1	D	60	HIS	CD2-NE2	-5.30	1.32	1.37
1	A	231	VAL	C-O	-5.29	1.18	1.24
1	A	236	LEU	C-O	-5.29	1.18	1.24
1	D	60	HIS	CA-C	-5.28	1.46	1.52
1	D	283	MSE	N-CA	-5.28	1.39	1.46
1	C	222	TRP	CA-C	-5.28	1.46	1.52
1	C	59	ILE	C-O	-5.27	1.18	1.24
1	A	77	GLU	C-O	-5.26	1.18	1.24
1	A	202	GLU	C-O	-5.26	1.17	1.24
1	A	65	GLU	C-O	-5.25	1.18	1.24
1	C	204	TRP	NE1-CE2	-5.25	1.31	1.37
1	A	267	GLU	CA-CB	-5.24	1.45	1.53
1	B	88	ILE	C-O	-5.23	1.17	1.24
1	B	128	GLU	C-O	-5.23	1.17	1.24
1	B	99	ARG	C-O	-5.22	1.17	1.24
1	D	222	TRP	NE1-CE2	-5.22	1.31	1.37
1	D	130	ILE	C-O	-5.21	1.18	1.24
1	B	24	GLU	C-O	-5.20	1.18	1.24
1	C	151	HIS	CD2-NE2	-5.19	1.32	1.37
1	D	230	SER	C-O	-5.18	1.18	1.24
1	C	117	HIS	CD2-NE2	-5.17	1.32	1.37
1	A	242	VAL	C-O	-5.17	1.18	1.24
1	C	129	ILE	C-O	-5.15	1.18	1.24
1	D	101	LEU	C-O	-5.15	1.17	1.24
1	A	101	LEU	C-O	-5.15	1.17	1.24
1	B	29	VAL	C-O	-5.14	1.18	1.24
1	B	52	ALA	CA-C	-5.13	1.45	1.52
1	C	242	VAL	C-O	-5.13	1.18	1.24
1	C	283	MSE	C-N	-5.11	1.26	1.33
1	A	119	TRP	NE1-CE2	-5.10	1.31	1.37
1	B	254	GLY	C-O	-5.09	1.19	1.23
1	B	68	HIS	CG-ND1	-5.07	1.32	1.38
1	C	75	ILE	C-O	-5.07	1.18	1.24
1	A	30	ILE	C-O	-5.06	1.18	1.24
1	A	292	PRO	C-O	-5.05	1.17	1.24
1	D	179	ILE	C-O	-5.04	1.18	1.24
1	A	44	SER	C-O	-5.03	1.17	1.23
1	B	221	TYR	C-O	-5.03	1.18	1.24
1	D	241	LYS	C-O	-5.03	1.18	1.24
1	A	286	GLU	N-CA	5.02	1.52	1.46
1	B	190	VAL	C-O	-5.01	1.18	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	68	HIS	CG-ND1	-5.00	1.32	1.38

All (146) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	283	MSE	O-C-N	-21.44	97.79	123.30
1	C	283	MSE	O-C-N	-21.16	99.36	123.06
1	B	266	MSE	CA-C-N	18.08	146.91	121.05
1	B	266	MSE	C-N-CA	18.08	146.91	121.05
1	B	283	MSE	CA-C-N	-16.68	97.92	122.94
1	B	283	MSE	C-N-CA	-16.68	97.92	122.94
1	A	266	MSE	O-C-N	16.00	143.87	122.59
1	B	83	VAL	N-CA-C	-15.23	97.20	111.67
1	A	266	MSE	CA-C-N	-14.22	97.60	123.05
1	A	266	MSE	C-N-CA	-14.22	97.60	123.05
1	C	266	MSE	O-C-N	14.07	139.65	123.19
1	A	283	MSE	CA-C-N	13.61	142.43	123.11
1	A	283	MSE	C-N-CA	13.61	142.43	123.11
1	C	283	MSE	CA-C-N	11.39	141.46	122.33
1	C	283	MSE	C-N-CA	11.39	141.46	122.33
1	A	82	PHE	N-CA-C	10.62	126.81	113.43
1	A	246	ARG	CA-C-N	-10.28	107.56	122.67
1	A	246	ARG	C-N-CA	-10.28	107.56	122.67
1	D	266	MSE	N-CA-C	-10.22	97.84	110.41
1	C	264	PRO	CB-CA-C	10.00	120.57	111.17
1	D	122	ASN	O-C-N	9.94	127.24	121.27
1	D	74	ALA	N-CA-C	-9.94	98.64	112.45
1	D	73	GLY	N-CA-C	-9.92	98.88	112.18
1	D	265	PRO	CA-C-O	9.60	134.29	122.19
1	D	82	PHE	CA-C-O	-9.59	108.64	119.67
1	A	284	ARG	N-CA-C	9.54	124.87	107.99
1	B	276	LEU	N-CA-C	9.16	124.58	113.41
1	C	281	VAL	O-C-N	-8.79	111.08	121.10
1	A	267	GLU	N-CA-C	-8.62	97.47	110.14
1	D	266	MSE	O-C-N	-8.50	112.28	122.65
1	C	281	VAL	CA-C-N	-8.46	110.85	119.99
1	C	281	VAL	C-N-CA	-8.46	110.85	119.99
1	C	265	PRO	N-CA-C	8.44	124.07	111.41
1	C	266	MSE	CA-C-N	8.20	132.43	120.95
1	C	266	MSE	C-N-CA	8.20	132.43	120.95
1	D	275	VAL	N-CA-C	8.07	118.87	110.72
1	A	276	LEU	N-CA-C	7.95	120.02	111.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	82	PHE	N-CA-C	7.85	123.44	113.55
1	C	82	PHE	CA-C-N	-7.67	110.31	121.65
1	C	82	PHE	C-N-CA	-7.67	110.31	121.65
1	B	140	PHE	O-C-N	7.16	129.55	121.53
1	C	94	GLU	N-CA-C	7.12	118.83	111.14
1	D	148	ARG	N-CA-C	7.12	119.04	111.28
1	B	266	MSE	CB-CA-C	7.03	121.28	109.48
1	C	282	PRO	CB-CA-C	-7.01	100.97	110.85
1	D	37	PHE	N-CA-C	6.96	119.89	111.82
1	A	283	MSE	O-C-N	6.87	131.12	123.16
1	A	284	ARG	CA-C-O	-6.86	113.12	120.46
1	C	207	ASP	N-CA-C	6.77	118.74	111.36
1	A	277	SER	N-CA-C	6.76	118.42	109.83
1	A	36	ARG	N-CA-C	6.74	118.70	111.36
1	B	267	GLU	CB-CA-C	6.71	119.90	109.84
1	A	281	VAL	CA-C-N	-6.59	112.88	119.99
1	A	281	VAL	C-N-CA	-6.59	112.88	119.99
1	A	74	ALA	N-CA-C	6.55	118.50	111.36
1	A	165	ARG	N-CA-C	6.55	118.50	111.36
1	D	261	ALA	O-C-N	6.55	128.86	121.53
1	C	265	PRO	CB-CA-C	6.53	119.51	110.95
1	D	25	GLU	CA-C-O	6.53	127.89	120.90
1	B	282	PRO	N-CA-C	-6.45	101.52	111.13
1	C	267	GLU	CA-C-O	-6.42	113.42	120.81
1	A	246	ARG	N-CA-C	6.41	119.94	109.24
1	B	148	ARG	N-CA-C	6.39	118.25	111.28
1	C	140	PHE	CA-C-N	-6.39	113.36	120.14
1	C	140	PHE	C-N-CA	-6.39	113.36	120.14
1	B	284	ARG	N-CA-C	6.39	119.81	109.40
1	D	71	THR	N-CA-C	6.38	118.03	111.14
1	D	282	PRO	CA-C-O	6.36	130.22	122.08
1	D	43	GLU	N-CA-C	6.34	118.71	110.53
1	B	267	GLU	N-CA-CB	6.32	119.28	109.48
1	B	145	GLU	N-CA-C	-6.28	101.11	109.84
1	B	277	SER	CA-C-N	6.25	126.16	119.28
1	B	277	SER	C-N-CA	6.25	126.16	119.28
1	D	281	VAL	CA-C-O	6.21	128.28	119.95
1	A	277	SER	CA-C-N	6.14	126.03	119.28
1	A	277	SER	C-N-CA	6.14	126.03	119.28
1	D	267	GLU	CA-C-N	-6.12	111.44	120.38
1	D	267	GLU	C-N-CA	-6.12	111.44	120.38
1	D	283	MSE	CA-C-O	-6.10	113.78	120.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	266	MSE	N-CA-CB	-6.07	100.50	110.52
1	B	266	MSE	N-CA-CB	5.96	120.35	110.52
1	D	207	ASP	N-CA-C	5.95	117.43	111.07
1	A	263	VAL	CA-C-N	5.91	123.92	119.66
1	A	263	VAL	C-N-CA	5.91	123.92	119.66
1	B	59	ILE	N-CA-C	-5.84	100.06	108.53
1	D	56	LYS	CA-C-O	-5.82	115.25	121.94
1	D	277	SER	CA-C-N	5.82	125.68	119.28
1	D	277	SER	C-N-CA	5.82	125.68	119.28
1	B	277	SER	N-CA-C	5.79	117.19	109.83
1	D	265	PRO	CB-CA-C	5.78	119.29	110.21
1	A	158	VAL	CA-C-O	-5.78	112.21	119.95
1	A	144	PRO	CA-C-N	-5.77	112.29	120.49
1	A	144	PRO	C-N-CA	-5.77	112.29	120.49
1	C	141	PRO	CA-C-N	-5.75	115.68	123.10
1	C	141	PRO	C-N-CA	-5.75	115.68	123.10
1	B	283	MSE	O-C-N	5.74	130.13	123.30
1	A	267	GLU	CB-CA-C	-5.73	100.16	110.36
1	C	70	GLN	N-CA-C	5.72	117.32	111.14
1	A	148	ARG	N-CA-C	5.68	117.55	111.36
1	D	20	VAL	CB-CA-C	-5.63	103.51	111.28
1	C	264	PRO	CA-C-O	5.63	125.18	120.73
1	C	247	GLU	N-CA-C	-5.58	102.02	110.28
1	D	122	ASN	CB-CA-C	-5.58	104.40	110.98
1	B	200	ASN	CA-C-N	5.57	125.09	119.19
1	B	200	ASN	C-N-CA	5.57	125.09	119.19
1	A	40	ASN	CA-C-N	5.57	125.41	119.28
1	A	40	ASN	C-N-CA	5.57	125.41	119.28
1	D	265	PRO	N-CA-C	-5.56	101.78	112.01
1	A	199	LYS	N-CA-C	5.55	117.42	111.36
1	A	83	VAL	N-CA-C	5.55	115.64	110.42
1	C	248	ILE	N-CA-C	5.54	116.27	110.62
1	D	283	MSE	N-CA-C	-5.52	99.91	108.90
1	A	285	ASP	CA-CB-CG	5.51	118.11	112.60
1	C	199	LYS	N-CA-C	5.50	117.36	111.36
1	A	134	LYS	N-CA-C	5.50	118.20	111.82
1	B	36	ARG	N-CA-C	5.47	117.32	111.36
1	B	40	ASN	CA-C-N	5.43	125.09	119.56
1	B	40	ASN	C-N-CA	5.43	125.09	119.56
1	C	283	MSE	CB-CA-C	5.39	118.73	109.51
1	C	148	ARG	N-CA-C	5.39	117.15	111.28
1	B	283	MSE	CA-C-O	-5.38	114.55	120.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	38	ALA	N-CA-C	5.37	117.80	110.55
1	C	277	SER	N-CA-C	5.35	116.63	109.83
1	B	266	MSE	N-CA-C	-5.33	101.02	109.76
1	D	73	GLY	CA-C-O	-5.28	117.76	121.88
1	C	121	VAL	CB-CA-C	-5.25	105.25	111.97
1	C	284	ARG	N-CA-CB	-5.25	101.99	110.81
1	D	121	VAL	N-CA-C	5.25	115.46	110.53
1	C	267	GLU	CB-CA-C	-5.24	101.50	109.89
1	A	95	ARG	N-CA-C	5.23	117.28	110.53
1	A	158	VAL	C-N-CD	-5.21	109.13	120.60
1	C	226	SER	N-CA-C	5.17	117.93	110.28
1	A	79	LEU	N-CA-C	5.16	116.71	111.14
1	D	141	PRO	CA-C-O	-5.13	115.50	121.34
1	C	79	LEU	N-CA-C	5.12	116.67	111.14
1	C	81	LYS	CA-C-O	5.10	125.18	119.41
1	B	266	MSE	CA-C-O	5.07	126.43	120.80
1	B	266	MSE	CG-SE-CE	5.07	110.08	98.92
1	D	79	LEU	N-CA-C	5.07	116.61	111.14
1	B	83	VAL	CB-CA-C	-5.04	105.85	111.80
1	D	199	LYS	N-CA-C	5.03	116.84	111.36
1	C	275	VAL	N-CA-C	5.03	115.80	110.72
1	D	259	LEU	N-CA-C	5.02	116.56	111.14
1	B	37	PHE	N-CA-C	5.01	117.63	111.82
1	A	30	ILE	CB-CA-C	-5.01	105.38	112.14
1	A	82	PHE	CB-CA-C	-5.01	101.24	109.65

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	2502	0	2566	121	0
1	B	2520	0	2590	210	0
1	C	2520	0	2591	148	0
1	D	2526	0	2596	225	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	27	0	22	7	0
2	B	27	0	22	4	0
2	C	27	0	22	4	0
2	D	27	0	22	7	0
3	B	9	0	7	1	0
3	C	9	0	7	2	0
4	A	42	0	0	2	0
4	B	32	0	0	5	0
4	C	34	0	0	6	0
4	D	38	0	0	6	0
All	All	10340	0	10445	694	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 34.

All (694) 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:D:51:THR:CG2	1:D:73:GLY:HA2	1.31	1.55
1:B:143:LEU:HD11	1:B:151:HIS:CG	1.59	1.36
1:B:172:LEU:CD1	1:D:54:GLY:HA3	1.63	1.27
1:D:50:ASP:CB	1:D:56:LYS:HE2	1.65	1.23
1:C:44:SER:O	1:C:61:LYS:HE2	1.38	1.21
1:D:51:THR:CG2	1:D:73:GLY:CA	2.21	1.18
1:D:246:ARG:CG	1:D:246:ARG:HH11	1.56	1.17
1:B:19:GLU:O	1:B:19:GLU:HG2	1.42	1.16
1:B:143:LEU:CD1	1:B:151:HIS:CG	2.30	1.15
1:C:251:LYS:NZ	1:C:251:LYS:HB3	1.47	1.14
1:D:142:ILE:HD13	1:D:142:ILE:N	1.59	1.12
1:B:150:ILE:N	1:B:150:ILE:HD12	1.62	1.12
1:B:246:ARG:HH11	1:B:246:ARG:CB	1.63	1.12
1:B:22:LEU:HD12	1:B:22:LEU:N	1.51	1.11
1:B:150:ILE:CD1	1:B:150:ILE:H	1.61	1.11
1:B:246:ARG:HH11	1:B:246:ARG:CG	1.61	1.11
1:B:143:LEU:CD1	1:B:151:HIS:HB2	1.79	1.10
1:D:150:ILE:HD12	1:D:150:ILE:O	1.49	1.10
1:A:51:THR:HG23	1:A:73:GLY:HA2	1.24	1.10
1:D:247:GLU:OE1	1:D:250:ARG:HB2	1.49	1.10
1:A:246:ARG:H	1:A:246:ARG:CZ	1.65	1.09
1:B:143:LEU:CD1	1:B:151:HIS:CB	2.30	1.09
1:D:248:ILE:HD12	1:D:248:ILE:N	1.59	1.09

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:THR:CG2	1:A:73:GLY:HA2	1.82	1.08
1:D:248:ILE:HD12	1:D:248:ILE:H	0.96	1.08
1:D:42:GLU:HA	1:D:42:GLU:OE1	1.50	1.08
1:B:51:THR:HG23	1:B:73:GLY:HA2	1.33	1.08
1:B:139:GLU:OE1	1:B:139:GLU:HA	1.53	1.08
1:B:22:LEU:HD12	1:B:22:LEU:H	0.95	1.07
1:D:25:GLU:OE2	1:D:25:GLU:HA	1.50	1.07
1:D:48:ILE:N	1:D:48:ILE:HD12	1.59	1.07
1:B:157:ARG:HH11	1:B:157:ARG:HG2	1.19	1.07
1:D:51:THR:HG21	1:D:73:GLY:HA2	1.37	1.06
1:D:246:ARG:HH11	1:D:246:ARG:HG3	1.11	1.06
1:A:22:LEU:HD23	1:A:22:LEU:H	1.20	1.06
1:B:51:THR:HB	1:B:55:SER:O	1.55	1.06
1:D:50:ASP:CA	1:D:56:LYS:HE2	1.86	1.05
1:B:246:ARG:HB2	1:B:246:ARG:NH1	1.71	1.05
1:B:150:ILE:HD12	1:B:150:ILE:H	1.11	1.04
1:B:172:LEU:HD13	1:D:54:GLY:CA	1.86	1.03
1:D:51:THR:HG22	1:D:73:GLY:CA	1.86	1.03
1:C:248:ILE:HD12	1:C:248:ILE:O	1.58	1.02
1:A:246:ARG:H	1:A:246:ARG:NE	1.56	1.02
1:B:246:ARG:HH11	1:B:246:ARG:HB2	1.22	1.01
1:C:251:LYS:HB3	1:C:251:LYS:HZ1	1.23	1.01
1:D:248:ILE:H	1:D:248:ILE:CD1	1.57	1.01
1:B:178:ARG:HG3	1:B:178:ARG:HH11	1.24	1.01
1:B:153:PHE:CD1	1:B:157:ARG:NH2	2.30	1.00
1:D:48:ILE:H	1:D:48:ILE:CD1	1.75	1.00
1:A:22:LEU:HD23	1:A:22:LEU:N	1.73	0.99
1:A:126:ARG:HG3	1:A:126:ARG:HH11	1.23	0.99
1:B:153:PHE:CE1	1:B:157:ARG:NH2	2.30	0.99
1:C:14:TYR:CE1	1:C:294:GLU:HG2	1.98	0.99
1:D:141:PRO:C	1:D:142:ILE:HD13	1.86	0.99
1:C:2:LYS:HG3	4:C:526:HOH:O	1.62	0.98
1:D:48:ILE:HD12	1:D:48:ILE:H	1.19	0.98
1:D:50:ASP:HA	1:D:56:LYS:HE2	1.43	0.98
1:D:50:ASP:HB3	1:D:56:LYS:HE2	1.44	0.98
1:B:145:GLU:HG2	1:B:148:ARG:NH2	1.79	0.98
1:B:136:LEU:HD22	1:B:172:LEU:CD2	1.93	0.98
1:D:57:THR:HG23	1:D:58:LEU:N	1.78	0.97
1:C:51:THR:HB	1:C:55:SER:O	1.63	0.96
1:A:106:GLY:HA3	2:A:501:SAM:HA	1.47	0.96
1:B:41:PRO:HD2	1:B:42:GLU:OE1	1.66	0.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:LEU:CD1	1:B:151:HIS:ND1	2.29	0.96
1:C:51:THR:HG23	1:C:73:GLY:HA2	1.47	0.96
1:C:22:LEU:C	1:C:22:LEU:HD12	1.91	0.95
1:B:269:ASN:ND2	1:B:269:ASN:H	1.64	0.95
1:A:306:ILE:N	1:A:306:ILE:CD1	2.30	0.95
1:B:136:LEU:HD22	1:B:172:LEU:HD22	1.47	0.95
1:B:246:ARG:HH11	1:B:246:ARG:HG3	1.30	0.94
1:B:22:LEU:N	1:B:22:LEU:CD1	2.30	0.94
1:B:145:GLU:CG	1:B:148:ARG:NH2	2.30	0.94
1:B:246:ARG:CB	1:B:246:ARG:NH1	2.30	0.94
1:B:56:LYS:HD3	4:B:517:HOH:O	1.67	0.94
1:A:145:GLU:HA	1:A:145:GLU:OE1	1.67	0.93
1:B:168:LEU:CD2	1:B:169:LYS:N	2.32	0.93
1:D:51:THR:HG22	1:D:73:GLY:HA2	0.93	0.92
1:C:42:GLU:HA	1:C:42:GLU:OE1	1.65	0.92
1:A:247:GLU:O	1:A:247:GLU:HG2	1.65	0.92
1:B:266:MSE:HE2	1:B:270:GLU:HB3	1.49	0.92
1:B:172:LEU:HD13	1:D:54:GLY:HA3	0.92	0.92
1:D:142:ILE:N	1:D:142:ILE:CD1	2.30	0.91
1:A:22:LEU:N	1:A:22:LEU:CD2	2.33	0.91
1:B:232:ARG:NH1	1:B:266:MSE:CE	2.34	0.91
1:B:157:ARG:HD3	1:B:161:TYR:CD1	2.05	0.91
1:C:251:LYS:NZ	1:C:251:LYS:CB	2.30	0.90
1:C:291:GLU:HB2	1:C:294:GLU:OE1	1.70	0.90
1:B:143:LEU:HD11	1:B:151:HIS:ND1	1.87	0.89
1:C:24:GLU:OE1	3:C:402:BEN:H6	1.72	0.89
1:B:143:LEU:HD12	1:B:151:HIS:CB	2.00	0.89
1:B:218:GLU:CD	1:B:260:LYS:HZ3	1.81	0.89
1:A:116:LYS:O	1:A:120:GLU:HG3	1.73	0.88
1:D:145:GLU:CD	1:D:148:ARG:CZ	2.46	0.88
1:D:286:GLU:HG3	4:D:529:HOH:O	1.72	0.88
1:B:269:ASN:H	1:B:269:ASN:HD22	1.21	0.87
1:B:137:LEU:O	1:B:140:PHE:CE1	2.28	0.87
1:B:168:LEU:CD2	1:B:168:LEU:C	2.46	0.86
1:B:168:LEU:HD22	1:B:169:LYS:N	1.90	0.86
1:C:251:LYS:HB3	1:C:251:LYS:HZ2	1.35	0.86
1:B:51:THR:CG2	1:B:73:GLY:HA2	2.04	0.86
1:A:306:ILE:N	1:A:306:ILE:HD12	1.89	0.86
1:B:168:LEU:C	1:B:168:LEU:HD22	2.00	0.85
1:D:52:ALA:HB2	1:D:71:THR:O	1.76	0.85
1:C:22:LEU:HD13	1:C:23:THR:O	1.77	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:136:LEU:HD21	1:D:158:VAL:CG1	2.06	0.85
1:D:49:ALA:O	1:D:56:LYS:HD3	1.77	0.84
1:B:291:GLU:HB2	1:B:294:GLU:OE1	1.77	0.84
1:B:218:GLU:CD	1:B:260:LYS:NZ	2.36	0.84
1:D:145:GLU:CD	1:D:148:ARG:NH2	2.36	0.84
1:A:79:LEU:O	1:A:84:ARG:HG2	1.77	0.84
1:B:22:LEU:H	1:B:22:LEU:CD1	1.86	0.84
1:B:44:SER:HB2	1:D:249:GLY:O	1.77	0.84
1:B:266:MSE:HG3	1:B:271:VAL:HG22	1.59	0.83
1:D:50:ASP:HA	1:D:56:LYS:CE	2.08	0.83
1:D:246:ARG:HG3	1:D:246:ARG:NH1	1.83	0.83
1:B:232:ARG:NH1	1:B:266:MSE:HE1	1.93	0.83
1:B:136:LEU:CD2	1:B:172:LEU:HD21	2.09	0.83
1:D:138:LYS:HD2	1:D:138:LYS:N	1.93	0.82
1:A:126:ARG:HH11	1:A:126:ARG:CG	1.92	0.82
1:A:246:ARG:NE	1:A:246:ARG:N	2.28	0.82
1:B:178:ARG:HG3	1:B:178:ARG:NH1	1.83	0.82
1:D:51:THR:HB	1:D:55:SER:O	1.79	0.82
1:C:41:PRO:HD2	4:C:512:HOH:O	1.79	0.81
1:D:52:ALA:CB	1:D:71:THR:O	2.27	0.81
1:B:157:ARG:HD3	1:B:161:TYR:CE1	2.15	0.81
1:D:140:PHE:O	1:D:142:ILE:CD1	2.29	0.81
1:B:145:GLU:CG	1:B:148:ARG:HH22	1.90	0.80
1:D:145:GLU:N	1:D:146:PRO:CD	2.44	0.80
1:D:75:ILE:HD11	1:D:144:PRO:HG2	1.62	0.80
1:A:172:LEU:N	1:A:172:LEU:HD23	1.97	0.80
1:B:168:LEU:HD23	1:B:169:LYS:N	1.96	0.80
1:D:49:ALA:O	1:D:56:LYS:CD	2.30	0.80
1:D:51:THR:HG21	1:D:73:GLY:CA	2.02	0.80
1:B:232:ARG:HH11	1:B:266:MSE:HE1	1.45	0.79
1:B:143:LEU:HD11	1:B:151:HIS:CB	2.01	0.79
1:C:22:LEU:CD1	1:C:23:THR:O	2.29	0.79
1:D:140:PHE:O	1:D:142:ILE:HD11	1.83	0.79
1:B:139:GLU:OE1	1:B:139:GLU:CA	2.30	0.79
1:C:23:THR:OG1	1:C:26:GLU:HG3	1.81	0.79
1:C:42:GLU:OE1	1:C:42:GLU:CA	2.30	0.79
1:A:51:THR:HG21	1:A:74:ALA:H	1.48	0.79
1:C:153:PHE:CE1	1:C:157:ARG:CZ	2.65	0.79
1:D:153:PHE:CE1	1:D:157:ARG:NH1	2.51	0.79
1:D:75:ILE:CD1	1:D:144:PRO:HG2	2.14	0.78
1:C:248:ILE:O	1:C:248:ILE:CD1	2.30	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:247:GLU:OE1	1:D:250:ARG:CB	2.30	0.78
1:D:42:GLU:OE1	1:D:42:GLU:CA	2.30	0.78
1:D:150:ILE:HD12	1:D:150:ILE:C	2.02	0.77
1:C:247:GLU:OE1	1:C:250:ARG:HD2	1.84	0.77
1:D:144:PRO:C	1:D:146:PRO:HD2	2.10	0.77
1:C:247:GLU:CD	1:C:250:ARG:HD3	2.09	0.77
1:B:106:GLY:HA3	2:B:401:SAM:HA	1.66	0.77
1:D:50:ASP:CG	1:D:56:LYS:HE2	2.09	0.77
1:B:136:LEU:CD2	1:B:172:LEU:CD2	2.63	0.77
1:D:57:THR:HG23	1:D:58:LEU:O	1.85	0.76
1:A:25:GLU:OE1	1:A:25:GLU:HA	1.85	0.76
1:B:157:ARG:HG2	1:B:157:ARG:NH1	1.92	0.76
1:D:50:ASP:HB3	1:D:56:LYS:CE	2.16	0.76
1:D:153:PHE:HE1	1:D:157:ARG:HH11	1.30	0.76
1:A:246:ARG:CZ	1:A:246:ARG:N	2.48	0.75
1:C:172:LEU:HD23	1:C:172:LEU:N	2.01	0.75
1:D:79:LEU:O	1:D:84:ARG:CG	2.34	0.75
1:A:304:TYR:O	1:A:306:ILE:CD1	2.34	0.75
1:D:153:PHE:HE1	1:D:157:ARG:NH1	1.85	0.75
1:D:306:ILE:CD1	1:D:306:ILE:N	2.49	0.75
1:A:306:ILE:HD13	1:A:306:ILE:H	1.52	0.75
1:B:157:ARG:CD	1:B:161:TYR:CD1	2.69	0.75
1:D:305:LYS:C	1:D:307:SER:H	1.93	0.75
1:D:136:LEU:HD21	1:D:158:VAL:HG11	1.67	0.75
1:A:179:ILE:O	1:A:215:ARG:NH1	2.20	0.75
1:B:172:LEU:CD1	1:D:54:GLY:CA	2.52	0.75
1:B:207:ASP:OD1	1:B:284:ARG:NH1	2.20	0.75
1:D:150:ILE:O	1:D:150:ILE:CD1	2.33	0.75
1:C:153:PHE:CE1	1:C:157:ARG:NE	2.55	0.74
1:D:96:LYS:HD2	1:D:126:ARG:HH12	1.51	0.74
1:D:49:ALA:HA	4:D:525:HOH:O	1.88	0.74
1:A:122:ASN:OD1	1:A:122:ASN:C	2.29	0.74
1:B:178:ARG:HH11	1:B:178:ARG:CG	1.97	0.73
1:D:246:ARG:HH11	1:D:246:ARG:HG2	1.49	0.73
1:B:157:ARG:NH1	1:B:157:ARG:CG	2.49	0.73
1:C:247:GLU:OE1	1:C:250:ARG:CD	2.37	0.73
1:A:306:ILE:HG22	1:A:306:ILE:O	1.89	0.73
1:D:141:PRO:C	1:D:142:ILE:CD1	2.60	0.73
1:C:287:LYS:O	1:C:288:LEU:HB2	1.87	0.73
1:D:122:ASN:OD1	1:D:122:ASN:C	2.31	0.73
1:D:53:ASP:OD1	1:D:53:ASP:C	2.30	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:PHE:HE1	1:B:157:ARG:HH21	1.29	0.72
1:C:122:ASN:C	1:C:122:ASN:OD1	2.30	0.72
1:D:79:LEU:O	1:D:84:ARG:HG3	1.89	0.72
1:A:304:TYR:C	1:A:306:ILE:CD1	2.63	0.72
1:D:248:ILE:N	1:D:248:ILE:CD1	2.30	0.72
1:A:306:ILE:CD1	1:A:306:ILE:H	1.99	0.71
1:C:51:THR:CG2	1:C:73:GLY:HA2	2.20	0.71
1:D:18:LYS:HB3	1:D:20:VAL:HG23	1.73	0.71
1:B:44:SER:CB	1:D:249:GLY:O	2.39	0.71
1:D:145:GLU:CD	1:D:148:ARG:NH1	2.47	0.71
1:C:193:ASP:OD2	2:C:401:SAM:N	2.24	0.71
1:C:175:ALA:O	1:C:179:ILE:HG22	1.91	0.71
1:D:246:ARG:CG	1:D:246:ARG:NH1	2.30	0.70
1:B:166:LEU:HD23	1:B:167:SER:N	2.07	0.70
1:C:76:ARG:NH2	1:C:247:GLU:OE1	2.24	0.70
1:D:138:LYS:HD2	1:D:138:LYS:H	1.54	0.70
1:B:143:LEU:HD13	1:B:151:HIS:HB2	1.72	0.70
1:D:135:GLU:O	1:D:135:GLU:HG2	1.92	0.70
1:C:248:ILE:HD12	1:C:248:ILE:C	2.16	0.69
1:D:49:ALA:HB3	1:D:57:THR:HG22	1.73	0.69
1:C:51:THR:CG2	1:C:53:ASP:OD1	2.41	0.69
1:B:272:ARG:HG2	1:B:276:LEU:HD12	1.75	0.69
1:D:28:ASN:N	1:D:28:ASN:HD22	1.90	0.69
1:A:164:GLU:HG3	1:A:165:ARG:H	1.57	0.69
1:B:272:ARG:HD2	4:B:521:HOH:O	1.92	0.69
1:A:207:ASP:OD1	1:A:284:ARG:NH1	2.25	0.68
1:C:64:GLY:C	1:C:65:GLU:HG2	2.18	0.68
1:B:2:LYS:HB2	1:B:5:GLU:CG	2.23	0.68
1:C:22:LEU:C	1:C:22:LEU:CD1	2.67	0.68
1:D:117:HIS:NE2	1:D:147:TYR:OH	2.21	0.68
1:D:135:GLU:O	1:D:135:GLU:CG	2.41	0.68
1:A:14:TYR:CE1	1:A:294:GLU:HG2	2.27	0.68
1:B:81:LYS:HE3	4:B:503:HOH:O	1.93	0.68
1:A:207:ASP:OD2	1:A:284:ARG:NH1	2.26	0.68
1:B:49:ALA:HB2	1:B:59:ILE:CD1	2.23	0.68
1:A:304:TYR:O	1:A:306:ILE:HD12	1.94	0.68
1:D:96:LYS:CD	1:D:126:ARG:NH1	2.57	0.68
1:D:134:LYS:HD3	2:D:401:SAM:C5	2.24	0.68
1:D:150:ILE:C	1:D:150:ILE:CD1	2.66	0.68
1:D:50:ASP:CB	1:D:56:LYS:CE	2.58	0.68
1:D:42:GLU:HB2	4:D:523:HOH:O	1.93	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:305:LYS:C	1:D:307:SER:N	2.51	0.67
1:D:91:LYS:HE3	4:D:514:HOH:O	1.94	0.67
1:A:207:ASP:CG	1:A:284:ARG:NH1	2.53	0.67
1:B:168:LEU:HD23	1:B:169:LYS:H	1.59	0.67
1:A:269:ASN:HD22	1:A:269:ASN:H	1.42	0.67
1:B:246:ARG:NH1	1:B:246:ARG:HG3	1.98	0.67
1:B:218:GLU:OE1	1:B:260:LYS:NZ	2.27	0.66
1:B:24:GLU:OE1	3:B:402:BEN:H2	1.95	0.66
1:D:24:GLU:O	1:D:28:ASN:ND2	2.29	0.65
1:D:306:ILE:HG22	1:D:306:ILE:O	1.96	0.65
1:C:251:LYS:HZ1	1:C:251:LYS:CB	2.01	0.65
1:A:91:LYS:O	1:A:95:ARG:HG3	1.97	0.65
1:D:145:GLU:OE2	1:D:148:ARG:NH1	2.30	0.65
1:D:306:ILE:N	1:D:306:ILE:HD12	2.11	0.65
1:B:290:LYS:NZ	1:B:298:ASP:OD2	2.30	0.65
1:D:145:GLU:OE2	1:D:148:ARG:NH2	2.30	0.65
1:D:145:GLU:OE1	1:D:148:ARG:NH1	2.30	0.65
1:A:66:PRO:HB2	1:A:68:HIS:O	1.95	0.65
1:C:51:THR:HG21	1:C:53:ASP:OD1	1.97	0.65
1:B:213:LYS:NZ	1:B:238:LEU:O	2.27	0.65
1:D:199:LYS:C	1:D:201:PRO:HD3	2.22	0.65
1:C:2:LYS:CG	4:C:526:HOH:O	2.32	0.65
1:C:145:GLU:OE1	1:C:148:ARG:NE	2.30	0.65
1:B:172:LEU:O	1:B:178:ARG:NH1	2.30	0.64
1:B:232:ARG:NH1	1:B:266:MSE:HE3	2.12	0.64
1:B:2:LYS:HB2	1:B:5:GLU:HG3	1.79	0.64
1:A:51:THR:HB	1:A:55:SER:O	1.98	0.64
1:B:281:VAL:HG11	1:B:302:LYS:HG2	1.79	0.64
1:D:145:GLU:OE1	1:D:145:GLU:HA	1.97	0.64
1:C:232:ARG:HG2	1:C:242:VAL:HG11	1.80	0.64
1:B:143:LEU:HD12	1:B:151:HIS:CG	2.26	0.64
1:D:79:LEU:O	1:D:84:ARG:HG2	1.97	0.64
1:D:149:GLU:OE2	1:D:149:GLU:HA	1.96	0.64
1:A:41:PRO:HD2	1:A:42:GLU:OE2	1.98	0.64
1:B:200:ASN:ND2	1:B:202:GLU:OE1	2.30	0.64
1:A:246:ARG:N	1:A:246:ARG:CD	2.61	0.64
1:B:157:ARG:CD	1:B:161:TYR:CE1	2.81	0.64
1:A:122:ASN:OD1	1:A:124:LYS:N	2.30	0.64
1:D:232:ARG:HH11	1:D:266:MSE:SE	2.30	0.64
1:A:304:TYR:C	1:A:306:ILE:HD13	2.23	0.63
1:C:126:ARG:HG3	1:C:126:ARG:HH11	1.62	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:145:GLU:N	1:D:146:PRO:HD3	2.11	0.63
1:C:22:LEU:HD12	1:C:22:LEU:O	1.99	0.63
1:C:248:ILE:CD1	1:C:248:ILE:C	2.71	0.63
1:C:246:ARG:HB3	1:C:253:LYS:HE3	1.80	0.63
1:C:89:LEU:O	1:C:93:LYS:HE3	1.99	0.63
1:A:84:ARG:HB2	1:A:85:PRO:HD3	1.80	0.62
1:C:148:ARG:NH2	1:C:149:GLU:HG3	2.14	0.62
1:B:76:ARG:NH2	1:B:247:GLU:CD	2.57	0.62
1:B:149:GLU:HB2	1:B:150:ILE:HD12	1.81	0.62
1:C:286:GLU:H	1:C:286:GLU:CD	2.07	0.62
1:D:25:GLU:O	1:D:29:VAL:HG23	1.99	0.62
1:B:200:ASN:N	1:B:201:PRO:HD3	2.14	0.62
1:C:76:ARG:NH1	1:C:247:GLU:OE1	2.31	0.62
1:A:246:ARG:H	1:A:246:ARG:CD	2.11	0.62
1:D:182:VAL:O	1:D:215:ARG:NH2	2.33	0.62
1:C:24:GLU:OE1	3:C:402:BEN:N1	2.33	0.61
1:D:253:LYS:HE3	1:D:267:GLU:OE1	2.00	0.61
1:B:123:PRO:HB2	1:B:124:LYS:HE2	1.82	0.61
1:B:79:LEU:O	1:B:84:ARG:HG2	1.99	0.61
1:D:96:LYS:HD2	1:D:126:ARG:NH1	2.14	0.61
1:A:195:PHE:CE1	2:A:501:SAM:H5'1	2.35	0.61
1:A:247:GLU:O	1:A:247:GLU:CG	2.43	0.61
1:A:172:LEU:O	1:A:178:ARG:NH1	2.34	0.61
1:B:269:ASN:HD22	1:B:269:ASN:N	1.97	0.61
1:C:82:PHE:O	1:C:86:SER:HB3	2.01	0.61
1:D:14:TYR:CE1	1:D:294:GLU:HG2	2.36	0.61
1:A:79:LEU:O	1:A:84:ARG:CG	2.49	0.61
1:B:45:GLY:O	1:B:61:LYS:HB2	2.01	0.61
1:D:137:LEU:O	1:D:140:PHE:CZ	2.53	0.60
1:B:49:ALA:HB2	1:B:59:ILE:HD12	1.82	0.60
1:D:138:LYS:H	1:D:138:LYS:CD	2.04	0.60
1:D:145:GLU:OE1	1:D:148:ARG:CZ	2.49	0.60
1:B:218:GLU:HB2	1:B:260:LYS:HD3	1.82	0.60
1:A:246:ARG:NE	1:A:246:ARG:O	2.29	0.60
1:C:66:PRO:HB2	1:C:68:HIS:O	2.01	0.60
1:B:266:MSE:HE2	1:B:270:GLU:CB	2.27	0.60
1:D:140:PHE:CD1	1:D:155:LEU:HD13	2.37	0.60
1:D:144:PRO:C	1:D:146:PRO:CD	2.74	0.60
1:B:143:LEU:HD12	1:B:151:HIS:ND1	2.15	0.59
1:D:96:LYS:CD	1:D:126:ARG:HH12	2.15	0.59
1:C:182:VAL:O	1:C:215:ARG:NH1	2.35	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:SER:O	1:A:87:ARG:HB2	2.01	0.59
1:D:304:TYR:C	1:D:305:LYS:CG	2.76	0.59
1:A:126:ARG:HG3	1:A:126:ARG:NH1	2.05	0.59
1:B:145:GLU:CD	1:B:148:ARG:HH22	2.10	0.59
1:C:82:PHE:HA	1:C:223:VAL:HG11	1.84	0.59
1:D:47:GLU:C	1:D:48:ILE:HD12	2.27	0.59
1:D:182:VAL:HB	1:D:215:ARG:HH21	1.68	0.58
1:B:166:LEU:CD2	1:B:168:LEU:HB2	2.32	0.58
1:B:153:PHE:CE1	1:B:157:ARG:CZ	2.87	0.58
1:B:166:LEU:HD21	1:B:168:LEU:HB2	1.84	0.58
1:D:51:THR:HG21	1:D:73:GLY:C	2.28	0.58
1:D:227:SER:HB3	1:D:232:ARG:HH21	1.68	0.58
1:A:164:GLU:HG3	1:A:165:ARG:N	2.18	0.58
1:B:19:GLU:O	1:B:19:GLU:CG	2.30	0.58
1:D:306:ILE:HD13	1:D:306:ILE:H	1.68	0.58
1:D:49:ALA:HB1	1:D:70:GLN:NE2	2.19	0.58
1:D:200:ASN:N	1:D:201:PRO:HD3	2.18	0.58
1:A:126:ARG:CG	1:A:126:ARG:NH1	2.56	0.58
1:A:287:LYS:O	1:A:288:LEU:HB2	2.02	0.57
1:B:84:ARG:N	1:B:85:PRO:HD2	2.19	0.57
1:C:33:GLU:OE1	1:C:304:TYR:OH	2.22	0.57
1:B:102:ASP:OD1	1:B:131:SER:OG	2.22	0.57
1:B:3:ARG:HG2	1:B:7:LEU:HD12	1.86	0.57
1:C:84:ARG:N	1:C:85:PRO:HD2	2.18	0.57
1:C:82:PHE:HA	1:C:223:VAL:CG1	2.34	0.57
1:B:42:GLU:OE1	1:B:42:GLU:N	2.30	0.57
1:B:243:GLY:HA3	1:B:264:PRO:O	2.04	0.57
1:D:30:ILE:HG22	1:D:31:LEU:N	2.18	0.57
1:D:243:GLY:HA2	1:D:266:MSE:HG3	1.84	0.57
1:C:11:LEU:HD23	1:C:31:LEU:HD13	1.87	0.57
1:D:138:LYS:N	1:D:138:LYS:CD	2.57	0.57
1:B:22:LEU:CB	1:B:26:GLU:OE1	2.53	0.57
1:D:76:ARG:NH2	1:D:247:GLU:OE2	2.37	0.57
1:C:39:TYR:C	1:C:39:TYR:CD2	2.76	0.57
1:B:50:ASP:OD1	1:B:56:LYS:CE	2.52	0.56
1:D:106:GLY:HA3	2:D:401:SAM:HA	1.87	0.56
1:D:155:LEU:N	1:D:155:LEU:HD23	2.19	0.56
1:B:133:GLU:OE2	2:B:401:SAM:O3'	2.23	0.56
1:C:304:TYR:C	1:C:305:LYS:HG2	2.29	0.56
1:D:227:SER:HB3	1:D:232:ARG:NH2	2.20	0.56
1:D:49:ALA:C	1:D:50:ASP:OD1	2.48	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:76:ARG:NH1	1:D:247:GLU:OE2	2.39	0.56
1:A:245:SER:HA	1:A:246:ARG:NH1	2.21	0.56
1:A:246:ARG:NE	1:A:246:ARG:CA	2.69	0.56
1:A:269:ASN:H	1:A:269:ASN:ND2	2.02	0.56
1:C:64:GLY:O	1:C:65:GLU:HG2	2.05	0.56
1:D:74:ALA:HB1	1:D:109:TYR:CD2	2.40	0.56
1:B:199:LYS:C	1:B:201:PRO:HD3	2.30	0.56
1:B:222:TRP:HB3	1:B:257:ALA:HB3	1.88	0.56
1:B:145:GLU:CD	1:B:148:ARG:NH2	2.64	0.55
1:D:267:GLU:O	1:D:268:GLU:C	2.46	0.55
1:B:95:ARG:NH2	1:B:188:ASP:OD1	2.37	0.55
1:D:222:TRP:HB3	1:D:257:ALA:HB3	1.89	0.55
1:B:51:THR:CG2	1:B:53:ASP:H	2.20	0.55
1:C:42:GLU:HB2	4:C:512:HOH:O	2.06	0.55
1:B:267:GLU:O	1:B:271:VAL:HG23	2.07	0.55
1:C:247:GLU:CD	1:C:250:ARG:CD	2.78	0.55
1:B:166:LEU:CD2	1:B:166:LEU:C	2.79	0.55
1:D:51:THR:CB	1:D:55:SER:O	2.54	0.55
1:D:140:PHE:CD1	1:D:140:PHE:N	2.75	0.55
1:B:2:LYS:HB2	1:B:5:GLU:OE2	2.06	0.55
1:C:22:LEU:HD11	1:C:27:PHE:HB2	1.89	0.55
1:D:306:ILE:CD1	1:D:306:ILE:H	2.19	0.55
1:A:305:LYS:C	1:A:307:SER:H	2.15	0.54
1:B:41:PRO:CD	1:B:42:GLU:OE1	2.47	0.54
1:B:153:PHE:CE1	1:B:157:ARG:NE	2.75	0.54
1:C:4:GLU:HB2	4:C:526:HOH:O	2.07	0.54
1:D:57:THR:HG23	1:D:58:LEU:C	2.31	0.54
1:D:76:ARG:NH1	1:D:76:ARG:HB3	2.22	0.54
1:D:144:PRO:O	1:D:146:PRO:HD2	2.07	0.54
1:B:86:SER:O	1:B:87:ARG:HB2	2.07	0.54
1:D:50:ASP:CG	1:D:56:LYS:CE	2.78	0.54
1:D:227:SER:CB	1:D:232:ARG:HH21	2.20	0.54
1:C:229:LEU:HD22	1:C:274:LEU:HD13	1.87	0.54
1:D:18:LYS:HB3	1:D:20:VAL:CG2	2.37	0.54
1:D:111:LEU:HD22	1:D:129:ILE:HD13	1.89	0.54
1:D:306:ILE:O	1:D:307:SER:CB	2.52	0.54
1:B:266:MSE:HG3	1:B:271:VAL:CG2	2.32	0.54
1:C:147:TYR:O	1:C:150:ILE:HG22	2.07	0.54
1:D:22:LEU:N	1:D:22:LEU:HD23	2.22	0.54
1:A:84:ARG:CZ	4:A:603:HOH:O	2.55	0.54
1:A:304:TYR:HB3	1:A:306:ILE:HD11	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:ARG:CZ	1:B:247:GLU:OE1	2.55	0.54
1:D:51:THR:HG21	1:D:74:ALA:N	2.22	0.54
1:D:133:GLU:OE2	2:D:401:SAM:O3'	2.23	0.54
1:C:51:THR:HG23	1:C:52:ALA:N	2.23	0.54
1:B:218:GLU:OE2	1:B:260:LYS:NZ	2.33	0.54
1:C:14:TYR:CD1	1:C:294:GLU:HG2	2.43	0.54
1:D:52:ALA:HB2	1:D:71:THR:C	2.32	0.54
1:C:51:THR:HG22	1:C:53:ASP:H	1.73	0.53
1:B:109:TYR:O	1:B:113:VAL:HG23	2.08	0.53
1:D:204:TRP:HB2	1:D:283:MSE:CE	2.39	0.53
1:D:227:SER:HA	1:D:232:ARG:HH21	1.74	0.53
2:D:401:SAM:N	4:D:504:HOH:O	2.34	0.53
1:A:99:ARG:HH11	1:A:99:ARG:HG3	1.73	0.53
1:A:199:LYS:HD3	1:A:199:LYS:N	2.16	0.53
1:B:59:ILE:HA	1:B:66:PRO:HA	1.89	0.53
1:D:195:PHE:CE1	2:D:401:SAM:H5'1	2.44	0.53
1:D:74:ALA:HB1	1:D:109:TYR:HD2	1.73	0.53
1:A:207:ASP:OD1	1:A:286:GLU:HA	2.08	0.53
1:D:5:GLU:O	1:D:9:ASN:ND2	2.41	0.53
1:C:14:TYR:CZ	1:C:294:GLU:HG2	2.41	0.53
1:C:67:TYR:O	2:C:401:SAM:HE2	2.09	0.53
1:C:68:HIS:HD2	1:C:77:GLU:OE1	1.91	0.53
1:D:51:THR:HG22	1:D:52:ALA:N	2.24	0.53
1:A:199:LYS:NZ	4:A:616:HOH:O	2.42	0.52
1:C:153:PHE:CE1	1:C:157:ARG:NH2	2.77	0.52
1:C:243:GLY:HA3	1:C:264:PRO:O	2.09	0.52
1:C:92:ALA:HB3	1:C:121:VAL:HG11	1.91	0.52
1:B:178:ARG:NH2	1:D:145:GLU:HB2	2.24	0.52
1:D:134:LYS:HD3	2:D:401:SAM:C6	2.39	0.52
1:A:134:LYS:HD3	2:A:501:SAM:C5	2.40	0.52
1:B:2:LYS:CB	1:B:5:GLU:HG3	2.39	0.52
1:B:11:LEU:HD11	1:B:15:LEU:HD11	1.90	0.52
1:B:218:GLU:CD	1:B:260:LYS:HZ2	2.17	0.52
1:A:158:VAL:HG12	1:A:159:PRO:HD3	1.90	0.52
1:C:150:ILE:HD12	1:C:150:ILE:O	2.09	0.52
1:D:76:ARG:CZ	1:D:247:GLU:OE2	2.58	0.52
1:C:211:LEU:HD11	1:C:288:LEU:HD11	1.90	0.52
1:B:51:THR:HG21	1:B:74:ALA:H	1.75	0.52
1:C:39:TYR:C	1:C:39:TYR:HD2	2.17	0.52
1:B:48:ILE:HG22	1:B:48:ILE:O	2.08	0.52
1:D:2:LYS:HE2	1:D:6:TYR:HB2	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:HIS:HE1	2:A:501:SAM:C	2.23	0.52
1:C:51:THR:CG2	1:C:53:ASP:H	2.23	0.52
1:B:57:THR:OG1	1:B:58:LEU:N	2.41	0.51
1:C:150:ILE:O	1:C:150:ILE:CD1	2.58	0.51
1:C:150:ILE:CG2	1:C:151:HIS:N	2.73	0.51
1:D:267:GLU:O	1:D:269:ASN:N	2.44	0.51
1:A:103:VAL:HB	1:A:192:HIS:HA	1.91	0.51
1:B:67:TYR:O	2:B:401:SAM:HE2	2.09	0.51
1:C:3:ARG:NH2	1:C:35:LEU:O	2.34	0.51
1:C:133:GLU:OE2	2:C:401:SAM:O3'	2.22	0.51
1:D:49:ALA:O	1:D:56:LYS:HD2	2.08	0.51
1:B:42:GLU:H	1:B:42:GLU:CD	2.18	0.51
1:B:50:ASP:OD1	1:B:56:LYS:HE3	2.10	0.51
1:D:75:ILE:HD11	1:D:144:PRO:CG	2.35	0.51
1:B:143:LEU:HD12	1:B:151:HIS:HB3	1.89	0.51
1:C:105:PHE:HB3	1:C:133:GLU:HG2	1.93	0.51
1:B:102:ASP:OD1	1:B:102:ASP:C	2.54	0.51
1:C:287:LYS:CB	1:C:289:ASP:OD2	2.59	0.51
1:D:153:PHE:CE1	1:D:157:ARG:HD3	2.46	0.50
1:A:204:TRP:HB2	1:A:283:MSE:CE	2.40	0.50
1:C:8:LYS:HG3	1:C:31:LEU:HD21	1.94	0.50
1:D:84:ARG:NH1	4:D:528:HOH:O	2.38	0.50
1:B:39:TYR:HB3	1:B:199:LYS:HD2	1.92	0.50
1:C:53:ASP:OD1	1:C:55:SER:OG	2.30	0.50
1:A:152:GLU:CD	1:B:80:TYR:HH	2.19	0.50
1:B:9:ASN:O	1:B:13:SER:OG	2.29	0.50
1:A:53:ASP:OD1	1:A:55:SER:OG	2.29	0.50
1:B:272:ARG:CD	4:B:521:HOH:O	2.54	0.50
1:C:26:GLU:HB3	1:C:306:ILE:CD1	2.42	0.50
1:D:18:LYS:C	1:D:19:GLU:HG2	2.36	0.50
1:D:133:GLU:O	1:D:172:LEU:HA	2.12	0.49
1:A:172:LEU:N	1:A:172:LEU:CD2	2.65	0.49
1:B:22:LEU:HB3	1:B:26:GLU:OE1	2.12	0.49
1:B:50:ASP:OD1	1:B:56:LYS:HE2	2.13	0.49
1:D:50:ASP:HA	1:D:56:LYS:CD	2.42	0.49
1:B:157:ARG:HD2	1:B:161:TYR:CD1	2.47	0.49
1:C:51:THR:CG2	1:C:52:ALA:N	2.70	0.49
1:A:39:TYR:C	1:A:39:TYR:CD2	2.89	0.49
1:C:122:ASN:OD1	1:C:122:ASN:O	2.30	0.49
1:A:122:ASN:OD1	1:A:122:ASN:O	2.30	0.49
1:B:50:ASP:HA	1:B:56:LYS:HD2	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:THR:HG21	1:A:74:ALA:N	2.23	0.49
1:B:157:ARG:HB3	1:B:161:TYR:HB2	1.94	0.49
1:C:204:TRP:HB2	1:C:283:MSE:HE3	1.94	0.49
1:A:26:GLU:O	1:A:30:ILE:HG12	2.13	0.49
1:B:96:LYS:HG2	1:B:97:VAL:HG23	1.95	0.49
1:B:39:TYR:C	1:B:39:TYR:CD2	2.89	0.49
1:B:66:PRO:HB2	1:B:68:HIS:O	2.12	0.49
1:C:169:LYS:HD3	1:C:171:LEU:HD21	1.94	0.49
1:A:83:VAL:O	1:A:86:SER:OG	2.29	0.49
1:A:91:LYS:O	1:A:95:ARG:CG	2.60	0.49
1:B:145:GLU:HG3	1:B:148:ARG:HH22	1.74	0.49
1:D:68:HIS:HD2	1:D:77:GLU:HB3	1.77	0.49
1:A:200:ASN:N	1:A:201:PRO:CD	2.75	0.49
1:C:51:THR:HG22	1:C:53:ASP:OD1	2.11	0.49
1:C:293:LEU:O	1:C:297:ILE:HG13	2.13	0.49
1:D:39:TYR:C	1:D:39:TYR:CD2	2.89	0.49
1:A:158:VAL:HG13	1:A:159:PRO:HA	1.95	0.48
1:B:166:LEU:HD23	1:B:166:LEU:C	2.37	0.48
1:C:84:ARG:HB2	1:C:85:PRO:HD3	1.94	0.48
1:A:133:GLU:O	1:A:172:LEU:HA	2.13	0.48
1:C:41:PRO:HD2	1:C:42:GLU:H	1.79	0.48
1:C:84:ARG:HB2	1:C:85:PRO:CD	2.44	0.48
1:D:84:ARG:N	1:D:85:PRO:CD	2.76	0.48
1:D:140:PHE:CG	1:D:155:LEU:HD13	2.48	0.48
1:D:204:TRP:HB2	1:D:283:MSE:HE1	1.95	0.48
1:C:153:PHE:HE1	1:C:157:ARG:NH2	2.11	0.48
1:D:53:ASP:OD1	1:D:55:SER:OG	2.29	0.48
1:A:96:LYS:C	1:A:97:VAL:HG23	2.38	0.48
1:B:3:ARG:NH2	1:B:38:ALA:O	2.46	0.48
1:C:26:GLU:HB3	1:C:306:ILE:HD13	1.95	0.48
1:D:83:VAL:O	1:D:86:SER:OG	2.30	0.48
1:D:202:GLU:CG	1:D:292:PRO:HG3	2.43	0.48
1:A:84:ARG:N	1:A:85:PRO:CD	2.77	0.48
1:B:87:ARG:HA	4:B:516:HOH:O	2.14	0.48
1:C:153:PHE:CD1	1:C:157:ARG:CZ	2.97	0.48
1:C:229:LEU:CD2	1:C:274:LEU:HD13	2.44	0.48
1:C:284:ARG:HD2	1:C:284:ARG:HA	1.47	0.48
1:B:109:TYR:CD1	1:B:143:LEU:HD21	2.48	0.48
1:D:50:ASP:OD1	1:D:56:LYS:CE	2.62	0.48
1:D:149:GLU:OE2	1:D:149:GLU:CA	2.62	0.48
1:A:145:GLU:OE1	1:A:148:ARG:N	2.42	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:ASP:OD1	1:C:131:SER:OG	2.21	0.48
1:D:75:ILE:CD1	1:D:144:PRO:CG	2.89	0.48
1:A:182:VAL:O	1:A:215:ARG:NH1	2.47	0.47
1:B:72:ALA:O	1:B:76:ARG:NE	2.39	0.47
1:C:200:ASN:ND2	1:C:202:GLU:OE1	2.47	0.47
1:C:285:ASP:OD1	1:C:290:LYS:HB2	2.14	0.47
1:A:145:GLU:OE1	1:A:146:PRO:C	2.56	0.47
1:B:49:ALA:CB	1:B:59:ILE:CD1	2.91	0.47
1:B:106:GLY:N	1:B:133:GLU:OE2	2.34	0.47
1:A:277:SER:HA	1:A:278:PRO:HD3	1.77	0.47
1:B:14:TYR:CD1	1:B:294:GLU:HG2	2.50	0.47
1:D:205:THR:O	1:D:209:LEU:HB2	2.14	0.47
1:B:51:THR:HG23	1:B:53:ASP:H	1.79	0.47
1:D:51:THR:CG2	1:D:52:ALA:N	2.78	0.47
1:A:147:TYR:O	1:A:150:ILE:HG22	2.15	0.47
1:C:76:ARG:CZ	1:C:247:GLU:OE1	2.63	0.47
1:C:81:LYS:O	1:C:223:VAL:HG13	2.15	0.47
1:A:152:GLU:CD	1:B:80:TYR:OH	2.58	0.47
1:A:126:ARG:HA	1:A:165:ARG:O	2.14	0.47
1:C:258:SER:OG	1:C:261:ALA:HB3	2.15	0.47
1:C:278:PRO:O	1:C:281:VAL:HG23	2.15	0.47
1:A:204:TRP:HB2	1:A:283:MSE:HE1	1.97	0.46
1:B:44:SER:HB3	1:D:249:GLY:C	2.40	0.46
1:B:136:LEU:HD21	1:B:172:LEU:HD21	1.94	0.46
1:C:65:GLU:OE1	1:C:196:SER:HB3	2.16	0.46
1:B:51:THR:CG2	1:B:53:ASP:OD1	2.64	0.46
1:B:272:ARG:O	1:B:276:LEU:HB2	2.15	0.46
1:D:102:ASP:OD1	1:D:131:SER:OG	2.32	0.46
1:A:18:LYS:HD2	1:A:18:LYS:HA	1.48	0.46
1:D:28:ASN:HD22	1:D:28:ASN:H	1.58	0.46
1:D:68:HIS:CD2	1:D:77:GLU:OE1	2.68	0.46
1:A:51:THR:CG2	1:A:73:GLY:CA	2.75	0.46
1:B:137:LEU:O	1:B:140:PHE:CZ	2.66	0.46
1:D:272:ARG:HG2	1:D:276:LEU:HD12	1.97	0.46
1:B:178:ARG:HD2	1:B:178:ARG:HA	1.64	0.46
1:C:150:ILE:CD1	1:C:150:ILE:C	2.89	0.46
1:D:58:LEU:HD12	1:D:107:LEU:HD21	1.97	0.46
1:B:76:ARG:NH2	1:B:247:GLU:OE1	2.49	0.46
1:D:233:LYS:HG2	1:D:282:PRO:HD3	1.96	0.46
1:C:116:LYS:HE3	1:C:120:GLU:OE2	2.16	0.46
1:D:145:GLU:OE2	1:D:148:ARG:CZ	2.57	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:ARG:HH22	1:B:247:GLU:CD	2.25	0.45
1:B:153:PHE:HE2	1:B:166:LEU:HD12	1.81	0.45
1:A:133:GLU:OE2	2:A:501:SAM:O3'	2.26	0.45
1:A:222:TRP:HB3	1:A:257:ALA:HB3	1.98	0.45
1:B:122:ASN:OD1	1:B:122:ASN:C	2.58	0.45
1:C:273:LYS:O	1:C:277:SER:HB3	2.16	0.45
1:A:247:GLU:O	1:A:248:ILE:C	2.60	0.45
1:B:2:LYS:HB2	1:B:5:GLU:CD	2.41	0.45
1:C:228:SER:HB3	1:C:231:VAL:HB	1.99	0.45
1:A:304:TYR:CB	1:A:306:ILE:HD11	2.47	0.45
1:B:143:LEU:CG	1:B:151:HIS:ND1	2.79	0.45
1:A:53:ASP:OD1	1:A:53:ASP:C	2.59	0.45
1:B:285:ASP:CG	1:B:288:LEU:HA	2.42	0.45
1:C:76:ARG:NH1	1:C:250:ARG:CZ	2.80	0.45
1:C:178:ARG:HD2	1:C:178:ARG:HA	1.78	0.45
1:D:203:LEU:HA	1:D:203:LEU:HD23	1.63	0.45
1:D:249:GLY:O	1:D:250:ARG:HD3	2.17	0.45
1:D:14:TYR:CD1	1:D:294:GLU:HG2	2.52	0.45
1:D:65:GLU:OE1	1:D:196:SER:HB3	2.16	0.45
1:D:299:TYR:O	1:D:303:VAL:HG23	2.16	0.45
1:A:106:GLY:HA3	2:A:501:SAM:HG2	1.99	0.45
1:C:287:LYS:HB3	1:C:289:ASP:OD2	2.17	0.45
1:D:304:TYR:O	1:D:306:ILE:CD1	2.65	0.45
1:A:25:GLU:OE1	1:A:25:GLU:CA	2.60	0.44
1:B:40:ASN:HB3	1:B:42:GLU:OE2	2.17	0.44
1:C:40:ASN:HA	1:C:41:PRO:HD3	1.70	0.44
1:C:202:GLU:HG2	1:C:292:PRO:HG3	1.97	0.44
1:D:243:GLY:HA3	1:D:264:PRO:O	2.17	0.44
1:B:44:SER:CB	1:D:249:GLY:C	2.90	0.44
1:B:230:SER:OG	1:B:281:VAL:O	2.29	0.44
1:B:267:GLU:HG2	1:B:269:ASN:HD21	1.83	0.44
1:C:86:SER:O	1:C:87:ARG:HB2	2.17	0.44
1:D:76:ARG:HB3	1:D:76:ARG:CZ	2.48	0.44
1:D:227:SER:CB	1:D:232:ARG:NH2	2.80	0.44
1:B:203:LEU:HD11	2:B:401:SAM:C5	2.47	0.44
1:A:306:ILE:O	1:A:306:ILE:CG2	2.60	0.44
1:D:304:TYR:C	1:D:306:ILE:HD13	2.43	0.44
1:A:290:LYS:HE2	1:A:298:ASP:OD2	2.18	0.44
1:B:277:SER:HA	1:B:278:PRO:HD3	1.79	0.44
1:D:150:ILE:HD13	1:D:150:ILE:HA	1.60	0.44
1:B:53:ASP:OD1	1:B:55:SER:OG	2.30	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:79:LEU:HD12	1:C:79:LEU:HA	1.83	0.44
1:D:6:TYR:CD2	1:D:6:TYR:C	2.95	0.44
1:B:264:PRO:HA	1:B:265:PRO:HD2	1.69	0.44
1:C:76:ARG:NH1	1:C:250:ARG:NH1	2.65	0.44
1:D:50:ASP:HA	1:D:56:LYS:HD3	2.00	0.44
1:D:50:ASP:OD1	1:D:56:LYS:HE2	2.17	0.44
1:B:84:ARG:HB2	1:B:85:PRO:HD3	2.00	0.44
1:D:242:VAL:HG12	1:D:266:MSE:HE2	1.98	0.44
1:C:287:LYS:HB2	1:C:289:ASP:OD2	2.18	0.44
1:D:306:ILE:O	1:D:306:ILE:CG2	2.64	0.43
1:B:281:VAL:CG1	1:B:302:LYS:HG2	2.48	0.43
1:B:304:TYR:O	1:B:306:ILE:HG13	2.18	0.43
1:C:91:LYS:O	1:C:95:ARG:HG3	2.18	0.43
1:C:116:LYS:CE	1:C:120:GLU:OE2	2.67	0.43
1:A:39:TYR:O	1:A:41:PRO:HD3	2.17	0.43
1:C:211:LEU:HD11	1:C:288:LEU:CD1	2.48	0.43
1:D:183:GLU:O	1:D:184:ASN:HB2	2.18	0.43
1:D:18:LYS:C	1:D:19:GLU:CG	2.91	0.43
1:A:305:LYS:C	1:A:306:ILE:HD12	2.42	0.43
1:C:30:ILE:HD12	1:C:301:LEU:HD23	1.99	0.43
1:C:304:TYR:C	1:C:305:LYS:CG	2.91	0.43
1:D:57:THR:HG23	1:D:58:LEU:CA	2.48	0.43
1:A:48:ILE:HG12	1:A:58:LEU:CD2	2.48	0.43
1:A:96:LYS:O	1:A:97:VAL:CG2	2.67	0.43
1:A:101:LEU:HD23	1:A:101:LEU:HA	1.81	0.43
1:A:248:ILE:H	1:A:248:ILE:HG12	1.30	0.43
1:D:145:GLU:OE1	1:D:145:GLU:CA	2.66	0.43
1:B:166:LEU:CD2	1:B:167:SER:N	2.79	0.43
1:C:289:ASP:C	1:C:289:ASP:OD1	2.60	0.43
1:D:56:LYS:HD3	1:D:56:LYS:HA	1.84	0.43
1:C:53:ASP:OD1	1:C:53:ASP:C	2.59	0.43
1:C:91:LYS:O	1:C:95:ARG:CG	2.67	0.43
1:D:178:ARG:O	1:D:181:GLU:HG3	2.19	0.43
1:A:44:SER:HA	1:A:62:THR:OG1	2.19	0.43
1:C:51:THR:HG21	1:C:74:ALA:H	1.83	0.43
1:D:195:PHE:CE2	2:D:401:SAM:HE1	2.54	0.43
1:B:285:ASP:OD2	1:B:288:LEU:HA	2.19	0.42
1:D:49:ALA:O	1:D:50:ASP:OD1	2.37	0.42
1:D:102:ASP:O	1:D:131:SER:HA	2.19	0.42
1:B:150:ILE:H	1:B:150:ILE:HD13	1.70	0.42
1:C:98:ILE:O	1:C:98:ILE:HG22	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:274:LEU:HD12	1:D:274:LEU:HA	1.80	0.42
1:B:102:ASP:OD1	1:B:102:ASP:O	2.38	0.42
1:D:246:ARG:NH1	1:D:246:ARG:HG2	2.18	0.42
1:B:111:LEU:HD23	1:B:111:LEU:HA	1.75	0.42
1:A:96:LYS:C	1:A:97:VAL:CG2	2.93	0.42
1:B:11:LEU:CD1	1:B:15:LEU:HD11	2.49	0.42
1:B:49:ALA:CB	1:B:59:ILE:HD12	2.46	0.42
1:C:76:ARG:CZ	1:C:76:ARG:HB3	2.50	0.42
1:C:121:VAL:HG12	1:C:122:ASN:N	2.30	0.42
1:C:264:PRO:HA	1:C:265:PRO:HD3	1.79	0.42
1:B:115:LEU:HD23	1:B:115:LEU:HA	1.84	0.42
1:D:119:TRP:O	1:D:123:PRO:HD3	2.19	0.42
1:D:202:GLU:HG2	1:D:292:PRO:HG3	2.02	0.42
1:A:305:LYS:C	1:A:307:SER:N	2.76	0.42
1:A:135:GLU:O	1:A:135:GLU:HG2	2.19	0.42
1:C:106:GLY:HA3	2:C:401:SAM:HG2	2.02	0.42
1:A:285:ASP:OD2	1:A:288:LEU:HA	2.20	0.41
1:B:281:VAL:HG12	1:B:282:PRO:O	2.20	0.41
1:B:243:GLY:HA3	1:B:263:VAL:HG13	2.02	0.41
1:C:18:LYS:HD2	1:C:18:LYS:HA	1.70	0.41
1:D:200:ASN:ND2	1:D:202:GLU:OE1	2.53	0.41
1:A:164:GLU:CG	1:A:165:ARG:H	2.30	0.41
1:A:264:PRO:HA	1:A:265:PRO:HD3	1.71	0.41
1:B:267:GLU:CB	1:B:270:GLU:OE1	2.69	0.41
1:D:31:LEU:O	1:D:35:LEU:HG	2.21	0.41
1:C:153:PHE:CZ	1:C:157:ARG:NE	2.89	0.41
1:C:200:ASN:N	1:C:201:PRO:HD3	2.34	0.41
1:A:200:ASN:N	1:A:201:PRO:HD3	2.35	0.41
1:C:135:GLU:O	1:C:135:GLU:HG2	2.19	0.41
1:D:153:PHE:CD1	1:D:157:ARG:NH1	2.86	0.41
1:A:84:ARG:HG2	1:A:84:ARG:H	1.62	0.41
1:A:14:TYR:CD1	1:A:294:GLU:HG2	2.54	0.41
1:B:197:PRO:HA	1:B:204:TRP:CD1	2.56	0.41
1:C:30:ILE:CD1	1:C:301:LEU:HD23	2.51	0.41
1:C:39:TYR:HD2	1:C:39:TYR:O	2.03	0.41
1:C:150:ILE:HA	1:C:150:ILE:HD13	1.82	0.41
1:D:96:LYS:HG3	1:D:97:VAL:HG23	2.03	0.41
1:D:264:PRO:HA	1:D:265:PRO:HD3	1.80	0.41
1:A:51:THR:HG21	1:A:73:GLY:HA2	1.89	0.41
1:B:30:ILE:CD1	1:B:306:ILE:HD12	2.50	0.41
1:B:84:ARG:N	1:B:85:PRO:CD	2.84	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:ARG:HD2	1:B:161:TYR:CG	2.56	0.41
1:B:205:THR:HG21	1:B:285:ASP:HB2	2.03	0.41
1:D:143:LEU:HD22	1:D:144:PRO:HD2	2.03	0.41
1:B:145:GLU:CD	1:B:148:ARG:HH12	2.29	0.40
1:B:155:LEU:HA	1:B:155:LEU:HD23	1.74	0.40
1:C:32:ARG:HH11	1:C:32:ARG:HD3	1.72	0.40
1:D:253:LYS:CE	1:D:267:GLU:OE1	2.69	0.40
1:A:134:LYS:HD3	2:A:501:SAM:C6	2.51	0.40
1:C:84:ARG:NH2	4:C:529:HOH:O	2.54	0.40
1:D:284:ARG:HD2	1:D:284:ARG:HA	1.61	0.40
1:D:87:ARG:O	1:D:91:LYS:HG3	2.21	0.40
1:A:293:LEU:HD23	1:A:293:LEU:HA	1.88	0.40
1:B:299:TYR:O	1:B:303:VAL:HG23	2.21	0.40
1:D:72:ALA:O	1:D:76:ARG:HG3	2.21	0.40
1:C:79:LEU:HD13	1:C:113:VAL:HG11	2.04	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	299/308 (97%)	291 (97%)	7 (2%)	1 (0%)	36	55
1	B	303/308 (98%)	298 (98%)	5 (2%)	0	100	100
1	C	303/308 (98%)	297 (98%)	6 (2%)	0	100	100
1	D	304/308 (99%)	298 (98%)	6 (2%)	0	100	100
All	All	1209/1232 (98%)	1184 (98%)	24 (2%)	1 (0%)	48	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	265	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	275/276 (100%)	228 (83%)	47 (17%)	2	4
1	B	276/276 (100%)	217 (79%)	59 (21%)	1	2
1	C	276/276 (100%)	215 (78%)	61 (22%)	1	2
1	D	277/276 (100%)	209 (76%)	68 (24%)	1	1
All	All	1104/1104 (100%)	869 (79%)	235 (21%)	1	2

All (235) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LYS
1	A	22	LEU
1	A	25	GLU
1	A	36	ARG
1	A	39	TYR
1	A	40	ASN
1	A	48	ILE
1	A	51	THR
1	A	55	SER
1	A	69	SER
1	A	84	ARG
1	A	93	LYS
1	A	94	GLU
1	A	101	LEU
1	A	121	VAL
1	A	122	ASN
1	A	124	LYS
1	A	126	ARG
1	A	138	LYS
1	A	145	GLU
1	A	149	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	160	GLU
1	A	168	LEU
1	A	169	LYS
1	A	172	LEU
1	A	177	LYS
1	A	196	SER
1	A	199	LYS
1	A	202	GLU
1	A	206	LEU
1	A	209	LEU
1	A	212	ILE
1	A	215	ARG
1	A	227	SER
1	A	246	ARG
1	A	247	GLU
1	A	248	ILE
1	A	252	ARG
1	A	260	LYS
1	A	269	ASN
1	A	277	SER
1	A	283	MSE
1	A	284	ARG
1	A	286	GLU
1	A	302	LYS
1	A	306	ILE
1	A	307	SER
1	B	5	GLU
1	B	13	SER
1	B	17	LYS
1	B	19	GLU
1	B	20	VAL
1	B	21	SER
1	B	22	LEU
1	B	30	ILE
1	B	32	ARG
1	B	39	TYR
1	B	48	ILE
1	B	51	THR
1	B	56	LYS
1	B	57	THR
1	B	59	ILE
1	B	61	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	68	HIS
1	B	84	ARG
1	B	94	GLU
1	B	95	ARG
1	B	98	ILE
1	B	101	LEU
1	B	102	ASP
1	B	116	LYS
1	B	124	LYS
1	B	133	GLU
1	B	136	LEU
1	B	138	LYS
1	B	139	GLU
1	B	142	ILE
1	B	143	LEU
1	B	150	ILE
1	B	157	ARG
1	B	160	GLU
1	B	164	GLU
1	B	166	LEU
1	B	167	SER
1	B	168	LEU
1	B	177	LYS
1	B	178	ARG
1	B	180	LYS
1	B	199	LYS
1	B	202	GLU
1	B	206	LEU
1	B	207	ASP
1	B	209	LEU
1	B	215	ARG
1	B	241	LYS
1	B	245	SER
1	B	246	ARG
1	B	251	LYS
1	B	253	LYS
1	B	260	LYS
1	B	263	VAL
1	B	269	ASN
1	B	273	LYS
1	B	281	VAL
1	B	302	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	305	LYS
1	C	3	ARG
1	C	4	GLU
1	C	16	ARG
1	C	18	LYS
1	C	19	GLU
1	C	20	VAL
1	C	22	LEU
1	C	25	GLU
1	C	30	ILE
1	C	36	ARG
1	C	39	TYR
1	C	40	ASN
1	C	42	GLU
1	C	51	THR
1	C	55	SER
1	C	68	HIS
1	C	77	GLU
1	C	86	SER
1	C	87	ARG
1	C	93	LYS
1	C	95	ARG
1	C	98	ILE
1	C	101	LEU
1	C	116	LYS
1	C	121	VAL
1	C	122	ASN
1	C	126	ARG
1	C	133	GLU
1	C	134	LYS
1	C	137	LEU
1	C	139	GLU
1	C	150	ILE
1	C	160	GLU
1	C	165	ARG
1	C	168	LEU
1	C	172	LEU
1	C	178	ARG
1	C	181	GLU
1	C	183	GLU
1	C	196	SER
1	C	202	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	206	LEU
1	C	209	LEU
1	C	214	GLU
1	C	215	ARG
1	C	223	VAL
1	C	244	SER
1	C	245	SER
1	C	246	ARG
1	C	248	ILE
1	C	251	LYS
1	C	252	ARG
1	C	253	LYS
1	C	256	VAL
1	C	260	LYS
1	C	263	VAL
1	C	266	MSE
1	C	274	LEU
1	C	284	ARG
1	C	290	LYS
1	C	305	LYS
1	D	19	GLU
1	D	21	SER
1	D	23	THR
1	D	25	GLU
1	D	26	GLU
1	D	28	ASN
1	D	30	ILE
1	D	39	TYR
1	D	40	ASN
1	D	42	GLU
1	D	43	GLU
1	D	48	ILE
1	D	50	ASP
1	D	55	SER
1	D	56	LYS
1	D	57	THR
1	D	59	ILE
1	D	61	LYS
1	D	68	HIS
1	D	71	THR
1	D	76	ARG
1	D	79	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	84	ARG
1	D	87	ARG
1	D	94	GLU
1	D	96	LYS
1	D	97	VAL
1	D	101	LEU
1	D	107	LEU
1	D	116	LYS
1	D	131	SER
1	D	137	LEU
1	D	138	LYS
1	D	140	PHE
1	D	142	ILE
1	D	145	GLU
1	D	150	ILE
1	D	152	GLU
1	D	154	LEU
1	D	157	ARG
1	D	158	VAL
1	D	160	GLU
1	D	164	GLU
1	D	165	ARG
1	D	168	LEU
1	D	177	LYS
1	D	196	SER
1	D	200	ASN
1	D	202	GLU
1	D	206	LEU
1	D	209	LEU
1	D	215	ARG
1	D	223	VAL
1	D	226	SER
1	D	227	SER
1	D	246	ARG
1	D	248	ILE
1	D	250	ARG
1	D	251	LYS
1	D	253	LYS
1	D	269	ASN
1	D	281	VAL
1	D	283	MSE
1	D	284	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	302	LYS
1	D	305	LYS
1	D	306	ILE
1	D	307	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	40	ASN
1	A	68	HIS
1	A	269	ASN
1	B	28	ASN
1	B	269	ASN
1	C	28	ASN
1	C	68	HIS
1	D	9	ASN
1	D	28	ASN
1	D	68	HIS
1	D	70	GLN
1	D	269	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	BEN	C	402	-	9,9,9	1.39	1 (11%)	7,11,11	1.33	0
3	BEN	B	402	-	9,9,9	0.79	0	7,11,11	0.47	0
2	SAM	D	401	-	27,29,29	1.76	6 (22%)	34,42,42	2.11	13 (38%)
2	SAM	B	401	-	27,29,29	1.86	6 (22%)	34,42,42	2.42	9 (26%)
2	SAM	C	401	-	27,29,29	1.77	5 (18%)	34,42,42	2.17	8 (23%)
2	SAM	A	501	-	27,29,29	1.88	7 (25%)	34,42,42	2.29	11 (32%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BEN	C	402	-	-	4/4/4/4	0/1/1/1
3	BEN	B	402	-	-	4/4/4/4	0/1/1/1
2	SAM	D	401	-	-	3/17/33/33	0/3/3/3
2	SAM	B	401	-	-	0/17/33/33	0/3/3/3
2	SAM	C	401	-	-	2/17/33/33	0/3/3/3
2	SAM	A	501	-	-	3/17/33/33	0/3/3/3

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	SAM	C5-N7	-4.74	1.30	1.39
2	C	401	SAM	C5-N7	-4.66	1.30	1.39
2	D	401	SAM	C5-N7	-4.36	1.31	1.39
2	B	401	SAM	C5-N7	-4.29	1.31	1.39
2	B	401	SAM	C8-N9	-3.94	1.30	1.37
2	C	401	SAM	C4-N9	-3.67	1.30	1.37
2	D	401	SAM	C4-N9	-3.49	1.30	1.37
2	A	501	SAM	C8-N9	-3.48	1.31	1.37
2	D	401	SAM	C8-N9	-3.39	1.31	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	SAM	OXT-C	-3.35	1.20	1.30
2	B	401	SAM	C4-N9	-3.28	1.30	1.37
2	A	501	SAM	C4-N9	-3.27	1.30	1.37
2	C	401	SAM	C8-N9	-3.08	1.32	1.37
2	D	401	SAM	OXT-C	-2.90	1.21	1.30
2	C	401	SAM	OXT-C	-2.82	1.21	1.30
2	B	401	SAM	OXT-C	-2.77	1.21	1.30
2	B	401	SAM	C5-C4	2.60	1.43	1.39
2	D	401	SAM	CE-SD	-2.55	1.62	1.78
2	C	401	SAM	CE-SD	-2.51	1.63	1.78
2	D	401	SAM	C5-C4	2.50	1.43	1.39
3	C	402	BEN	C-N2	-2.48	1.27	1.33
2	A	501	SAM	CE-SD	-2.47	1.63	1.78
2	B	401	SAM	CE-SD	-2.39	1.63	1.78
2	A	501	SAM	C5-C4	2.17	1.43	1.39
2	A	501	SAM	C2-N3	-2.05	1.30	1.33

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	SAM	C5-C4-N3	-7.61	116.24	126.72
2	A	501	SAM	C5-C4-N3	-6.82	117.33	126.72
2	C	401	SAM	C5-C4-N3	-6.45	117.83	126.72
2	D	401	SAM	C5-C4-N3	-5.41	119.26	126.72
2	B	401	SAM	N3-C4-N9	5.19	136.00	127.17
2	C	401	SAM	N3-C4-N9	5.15	135.93	127.17
2	A	501	SAM	N3-C4-N9	4.81	135.35	127.17
2	A	501	SAM	C2-N3-C4	4.35	122.45	111.83
2	B	401	SAM	C4-C5-N7	-4.29	105.68	110.58
2	C	401	SAM	C2-N3-C4	4.21	122.12	111.83
2	B	401	SAM	C2-N3-C4	4.16	121.99	111.83
2	D	401	SAM	N3-C4-N9	4.14	134.21	127.17
2	D	401	SAM	C4-C5-N7	-3.89	106.13	110.58
2	C	401	SAM	N3-C2-N1	-3.84	122.78	128.58
2	D	401	SAM	C2-N3-C4	3.62	120.67	111.83
2	A	501	SAM	C4-C5-N7	-3.60	106.47	110.58
2	A	501	SAM	N3-C2-N1	-3.50	123.28	128.58
2	A	501	SAM	CB-CA-C	3.31	119.23	110.45
2	D	401	SAM	N3-C2-N1	-3.29	123.60	128.58
2	B	401	SAM	O4'-C1'-C2'	-3.25	99.66	106.62
2	A	501	SAM	CG-SD-C5'	3.24	111.36	103.43
2	B	401	SAM	CG-SD-C5'	3.21	111.29	103.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	SAM	CG-SD-C5'	3.09	110.98	103.43
2	B	401	SAM	O3'-C3'-C4'	-3.04	102.36	111.08
2	D	401	SAM	C5-N7-C8	3.03	108.22	103.45
2	B	401	SAM	N3-C2-N1	-2.91	124.18	128.58
2	A	501	SAM	O4'-C1'-N9	2.70	113.28	108.09
2	B	401	SAM	C5-N7-C8	2.59	107.52	103.45
2	D	401	SAM	C4-N9-C8	2.55	108.41	105.74
2	D	401	SAM	CG-SD-C5'	2.53	109.61	103.43
2	A	501	SAM	C5-N7-C8	2.49	107.36	103.45
2	C	401	SAM	O4'-C1'-C2'	-2.44	101.39	106.62
2	D	401	SAM	C6-C5-N7	2.40	136.72	132.09
2	D	401	SAM	O4'-C1'-N9	2.38	112.66	108.09
2	D	401	SAM	C2-N1-C6	2.32	122.55	118.73
2	D	401	SAM	N9-C8-N7	-2.28	110.71	113.94
2	C	401	SAM	O4'-C1'-N9	2.27	112.45	108.09
2	D	401	SAM	O4'-C1'-C2'	-2.22	101.87	106.62
2	A	501	SAM	OXT-C-O	-2.19	119.10	124.08
2	A	501	SAM	C6-C5-N7	2.16	136.26	132.09
2	C	401	SAM	C4-C5-N7	-2.02	108.28	110.58

There are no chirality outliers.

All (16) torsion outliers are listed below:

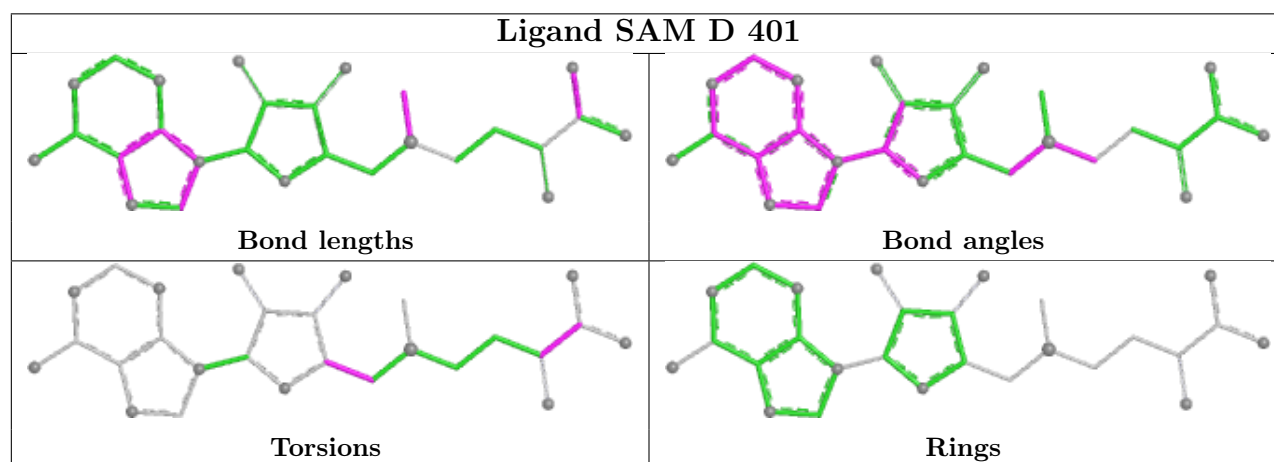
Mol	Chain	Res	Type	Atoms
2	A	501	SAM	C4'-C5'-SD-CG
2	C	401	SAM	OXT-C-CA-CB
2	A	501	SAM	O4'-C4'-C5'-SD
2	D	401	SAM	O4'-C4'-C5'-SD
2	A	501	SAM	C3'-C4'-C5'-SD
2	D	401	SAM	C3'-C4'-C5'-SD
2	C	401	SAM	O-C-CA-CB
3	B	402	BEN	N2-C-C1-C2
3	B	402	BEN	N2-C-C1-C6
3	C	402	BEN	N2-C-C1-C2
3	C	402	BEN	N2-C-C1-C6
2	D	401	SAM	O-C-CA-N
3	B	402	BEN	N1-C-C1-C2
3	B	402	BEN	N1-C-C1-C6
3	C	402	BEN	N1-C-C1-C2
3	C	402	BEN	N1-C-C1-C6

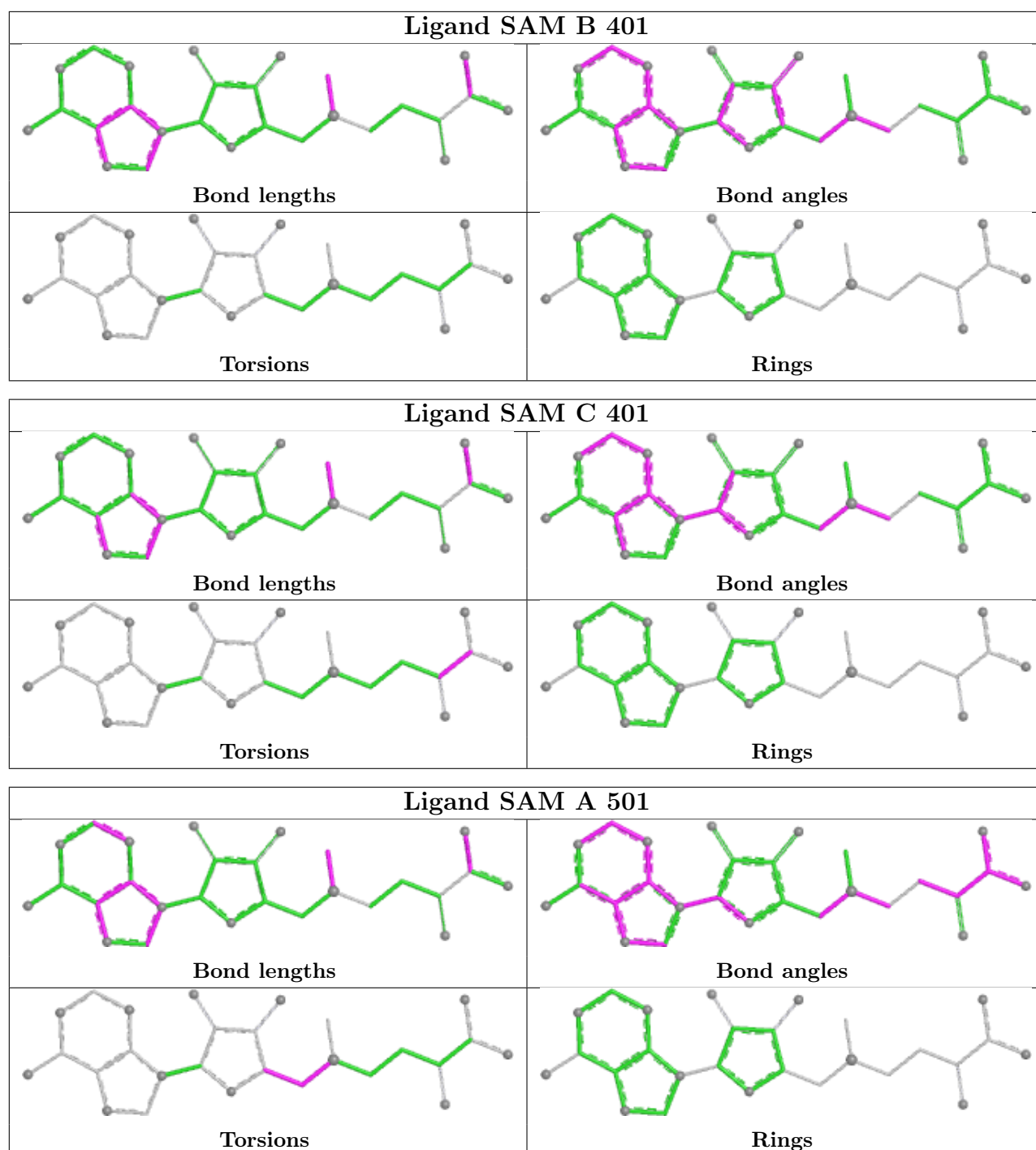
There are no ring outliers.

6 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	402	BEN	2	0
3	B	402	BEN	1	0
2	D	401	SAM	7	0
2	B	401	SAM	4	0
2	C	401	SAM	4	0
2	A	501	SAM	7	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	301/308 (97%)	-0.37	3 (0%) 79 76	25, 42, 71, 144	0
1	B	303/308 (98%)	-0.17	1 (0%) 90 87	23, 48, 83, 107	0
1	C	303/308 (98%)	-0.19	0 100 100	26, 51, 79, 119	0
1	D	304/308 (98%)	-0.14	2 (0%) 84 81	27, 49, 84, 114	0
All	All	1211/1232 (98%)	-0.22	6 (0%) 87 85	23, 47, 81, 144	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	248	ILE	5.7
1	D	52	ALA	4.0
1	A	247	GLU	2.9
1	A	145	GLU	2.8
1	B	248	ILE	2.4
1	D	250	ARG	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

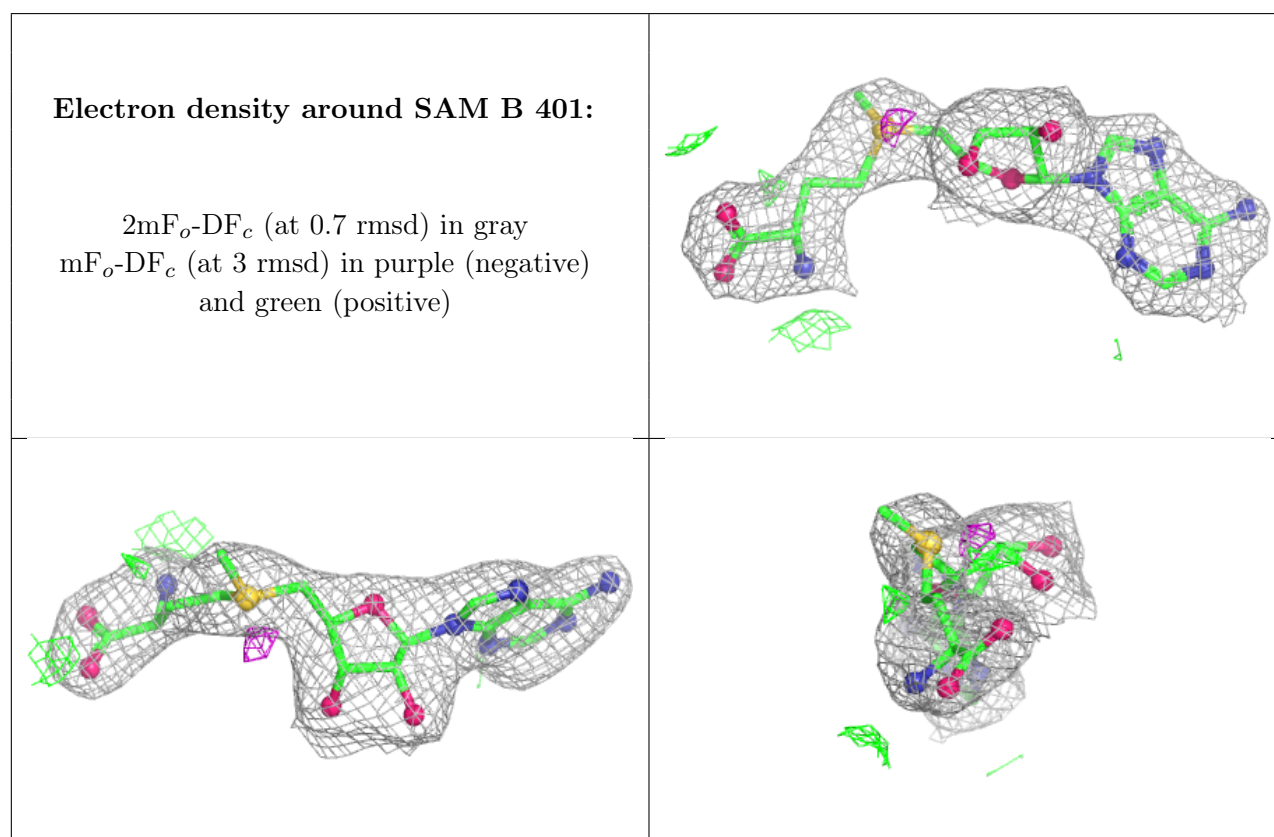
6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

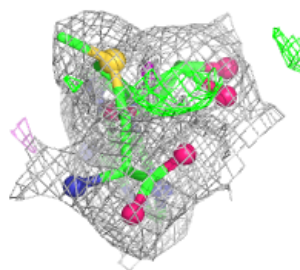
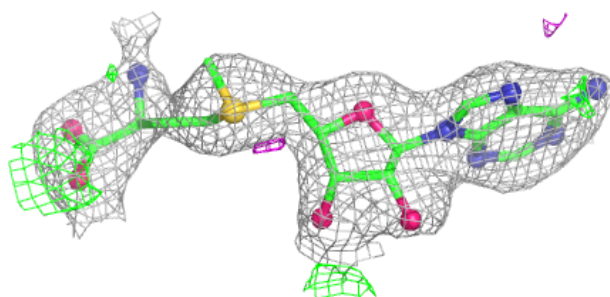
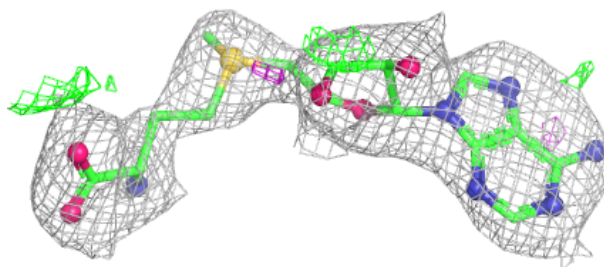
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	BEN	C	402	9/9	0.87	0.12	39,44,54,70	0
3	BEN	B	402	9/9	0.91	0.10	53,57,62,62	0
2	SAM	B	401	27/27	0.92	0.10	43,54,63,71	0
2	SAM	C	401	27/27	0.92	0.10	47,55,64,69	0
2	SAM	D	401	27/27	0.94	0.08	37,50,65,66	0
2	SAM	A	501	27/27	0.96	0.07	29,39,49,50	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.

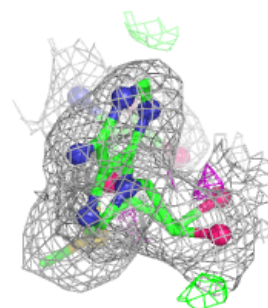
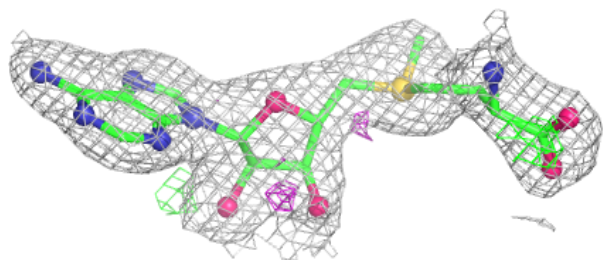
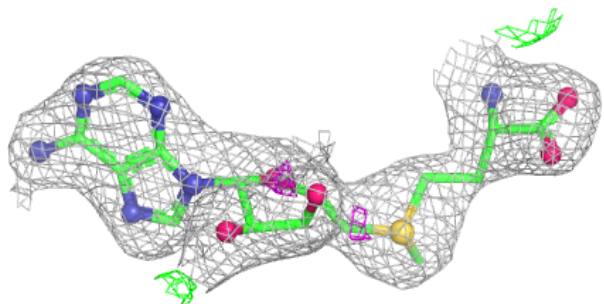


Electron density around SAM C 401:

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

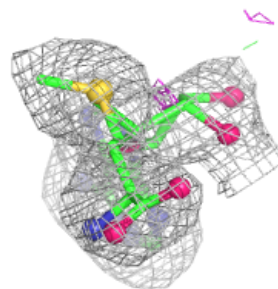
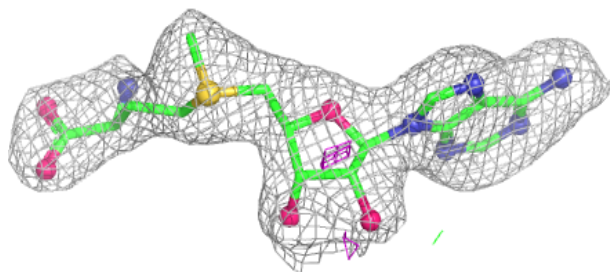
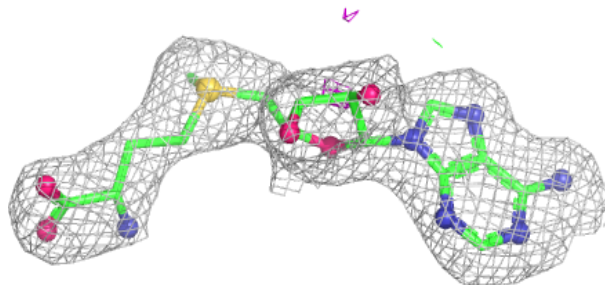
**Electron density around SAM D 401:**

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



Electron density around SAM A 501:

$2mF_o-DF_c$ (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.