



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:11 AM UTC

PDB ID : 3V4T / pdb_00003v4t
Title : E. cloacae C115D MURA liganded with UNAG
Authors : Zhu, J.-Y.; Yang, Y.; Schonbrunn, E.
Deposited on : 2011-12-15
Resolution : 2.50 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

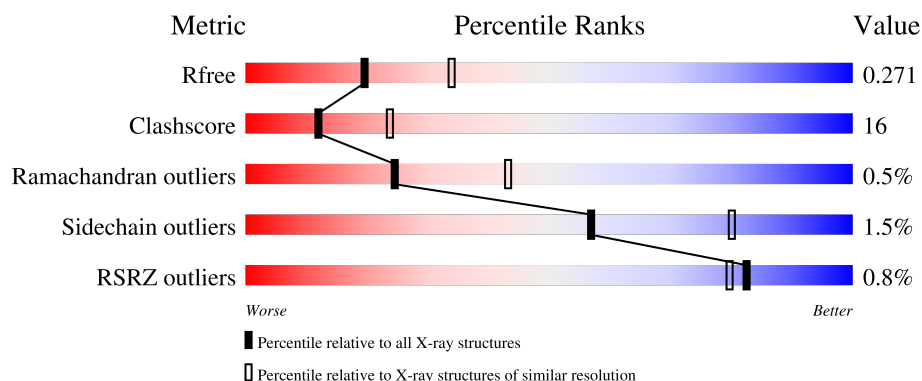
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

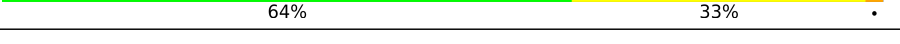
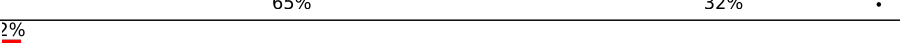
The reported resolution of this entry is 2.50 Å.

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	419	 68% 30% 2% 2%
1	B	419	 56% 40% 2% 2%
1	C	419	 64% 33% 2% 2%
1	D	419	 65% 32% 2% 2%
1	E	419	 63% 34% 2% 2%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	419	 71%27%•
1	G	419	 74%23%•
1	H	419	 70%27%•

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ACT	C	502	-	-	X	-
3	ACT	C	503	-	-	X	-
3	ACT	E	502	-	-	X	-
3	ACT	F	503	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 26190 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 UDP-N-acetylglucosamine 1-carboxyvinyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	419	Total	C	N	O	S	0	0	0
			3144	1977	554	600	13			
1	B	419	Total	C	N	O	S	0	0	0
			3144	1977	554	600	13			
1	C	419	Total	C	N	O	S	0	0	0
			3144	1977	554	600	13			
1	D	419	Total	C	N	O	S	0	0	0
			3144	1977	554	600	13			
1	E	419	Total	C	N	O	S	0	0	0
			3144	1977	554	600	13			
1	F	419	Total	C	N	O	S	0	0	0
			3144	1977	554	600	13			
1	G	419	Total	C	N	O	S	0	0	0
			3144	1977	554	600	13			
1	H	419	Total	C	N	O	S	0	0	0
			3144	1977	554	600	13			

There are 16 discrepancies between the modelled and reference sequences:

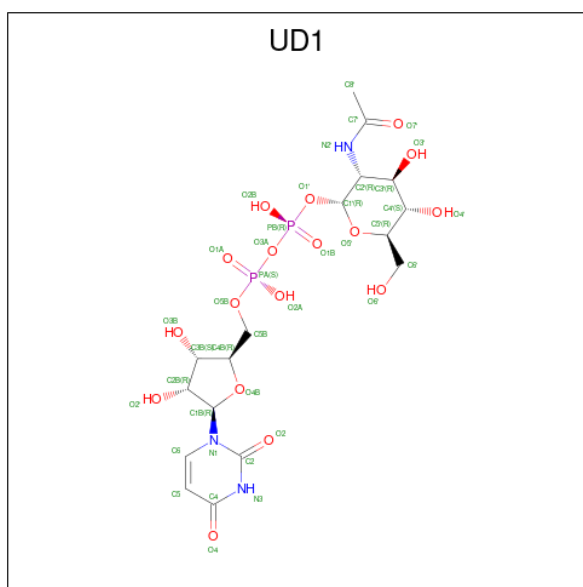
Chain	Residue	Modelled	Actual	Comment	Reference
A	67	IAS	ASN	SEE REMARK 999	UNP P33038
A	115	ASP	CYS	engineered mutation	UNP P33038
B	67	IAS	ASN	SEE REMARK 999	UNP P33038
B	115	ASP	CYS	engineered mutation	UNP P33038
C	67	IAS	ASN	SEE REMARK 999	UNP P33038
C	115	ASP	CYS	engineered mutation	UNP P33038
D	67	IAS	ASN	SEE REMARK 999	UNP P33038
D	115	ASP	CYS	engineered mutation	UNP P33038
E	67	IAS	ASN	SEE REMARK 999	UNP P33038
E	115	ASP	CYS	engineered mutation	UNP P33038
F	67	IAS	ASN	SEE REMARK 999	UNP P33038
F	115	ASP	CYS	engineered mutation	UNP P33038
G	67	IAS	ASN	SEE REMARK 999	UNP P33038

Continued on next page...

Continued from previous page...

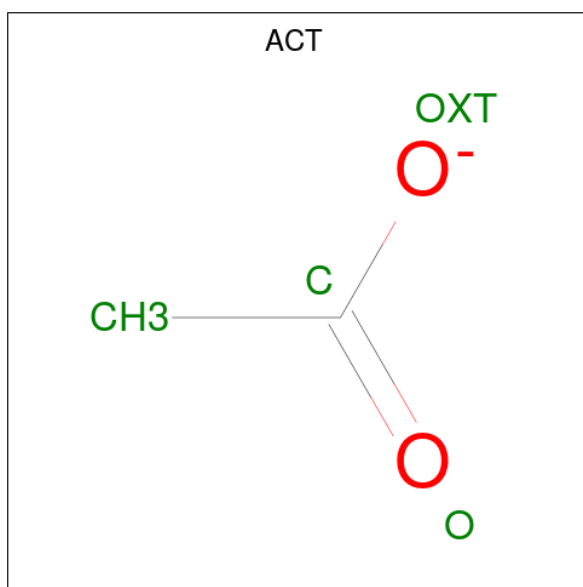
Chain	Residue	Modelled	Actual	Comment	Reference
G	115	ASP	CYS	engineered mutation	UNP P33038
H	67	IAS	ASN	SEE REMARK 999	UNP P33038
H	115	ASP	CYS	engineered mutation	UNP P33038

- Molecule 2 is URIDINE-DIPHOSPHATE-N-ACETYLGLUCOSAMINE (CCD ID: UD1) (formula: $\text{C}_{17}\text{H}_{27}\text{N}_3\text{O}_{17}\text{P}_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 39	C 17	N 3	O 17	P 2	0	0
2	B	1	Total 39	C 17	N 3	O 17	P 2	0	0
2	C	1	Total 39	C 17	N 3	O 17	P 2	0	0
2	D	1	Total 39	C 17	N 3	O 17	P 2	0	0
2	E	1	Total 39	C 17	N 3	O 17	P 2	0	0
2	F	1	Total 39	C 17	N 3	O 17	P 2	0	0
2	G	1	Total 39	C 17	N 3	O 17	P 2	0	0
2	H	1	Total 39	C 17	N 3	O 17	P 2	0	0

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: $\text{C}_2\text{H}_3\text{O}_2$).



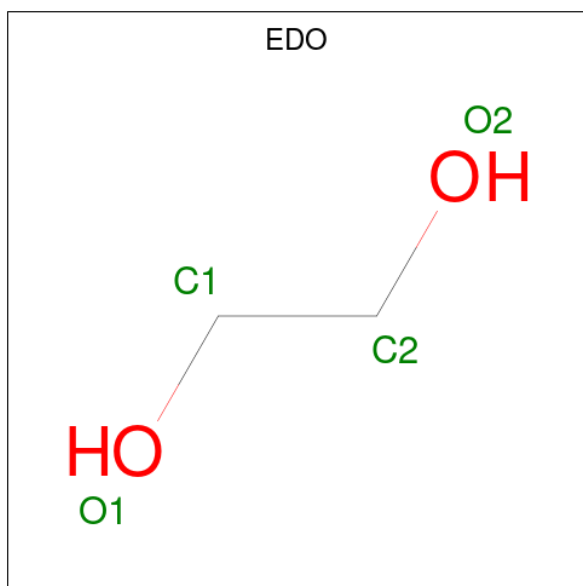
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	E	1	Total	C	O	0	0
			4	2	2		
3	E	1	Total	C	O	0	0
			4	2	2		
3	E	1	Total	C	O	0	0
			4	2	2		
3	F	1	Total	C	O	0	0
			4	2	2		
3	F	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	F	1	Total	C	O	0	0
			4	2	2		
3	H	1	Total	C	O	0	0
			4	2	2		
3	H	1	Total	C	O	0	0
			4	2	2		
3	H	1	Total	C	O	0	0
			4	2	2		
3	H	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	F	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0
4	G	1	Total C O 4 2 2	0	0
4	G	1	Total C O 4 2 2	0	0
4	G	1	Total C O 4 2 2	0	0
4	G	1	Total C O 4 2 2	0	0
4	G	1	Total C O 4 2 2	0	0
4	G	1	Total C O 4 2 2	0	0
4	G	1	Total C O 4 2 2	0	0
4	H	1	Total C O 4 2 2	0	0
4	H	1	Total C O 4 2 2	0	0
4	H	1	Total C O 4 2 2	0	0
4	H	1	Total C O 4 2 2	0	0
4	H	1	Total C O 4 2 2	0	0
4	H	1	Total C O 4 2 2	0	0
4	H	1	Total C O 4 2 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	67	Total O 67 67	0	0

Continued on next page...

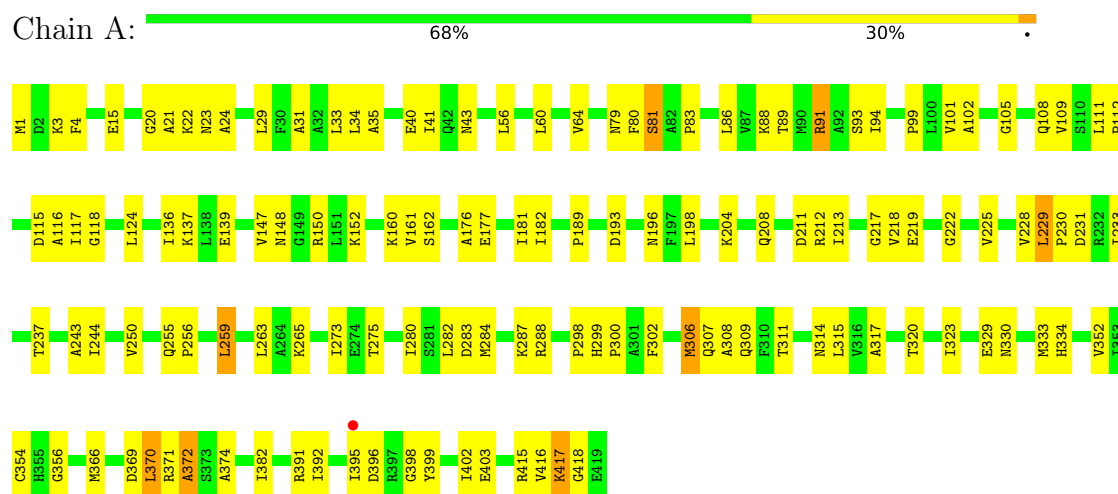
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	33	Total 33	O 33	0	0
5	C	53	Total 53	O 53	0	0
5	D	61	Total 61	O 61	0	0
5	E	66	Total 66	O 66	0	0
5	F	60	Total 60	O 60	0	0
5	G	67	Total 67	O 67	0	0
5	H	63	Total 63	O 63	0	0

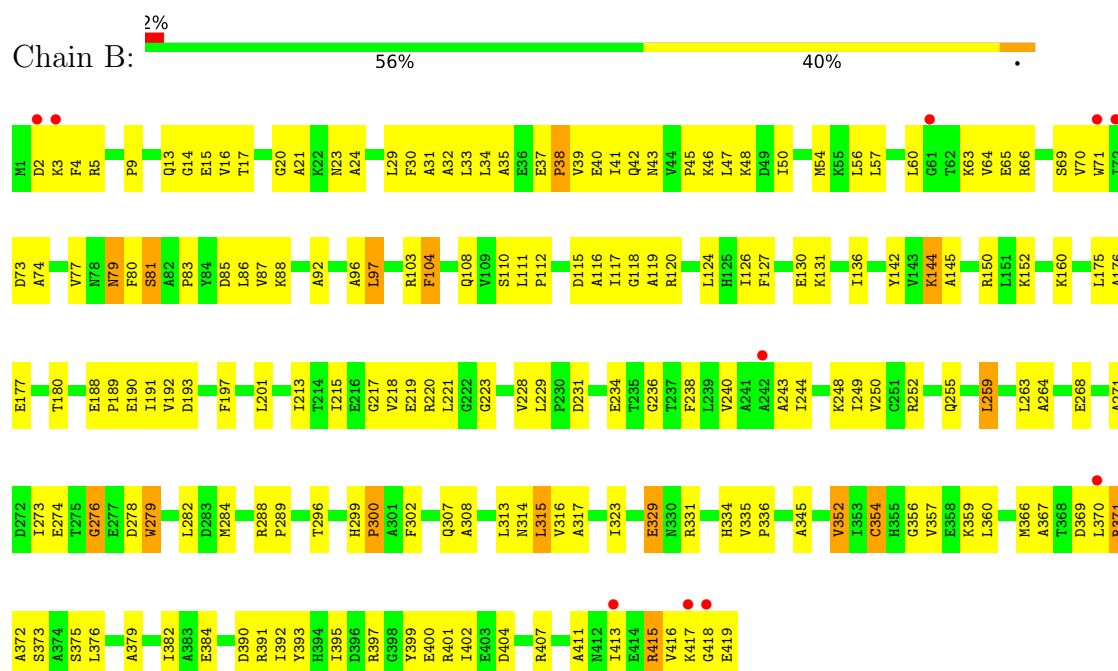
3 Residue-property plots

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

- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase

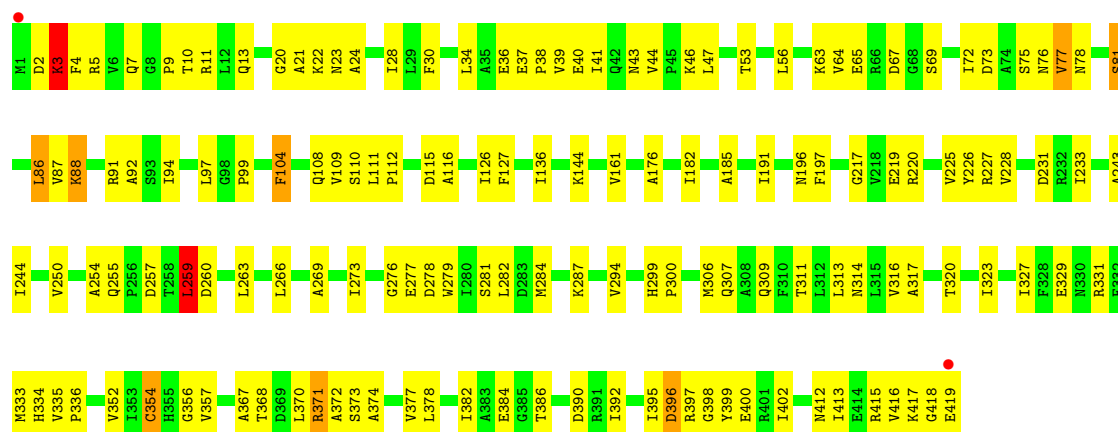


- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase



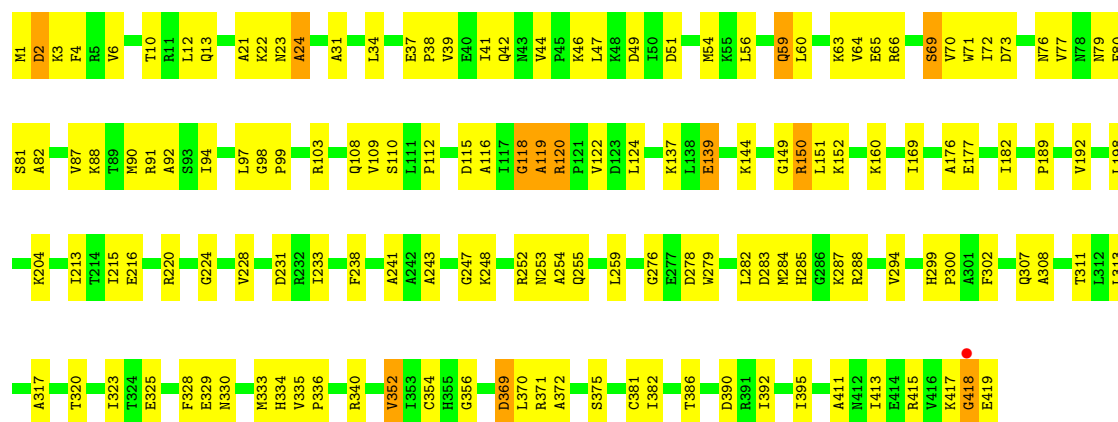
- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase

Chain C:  64% 33%



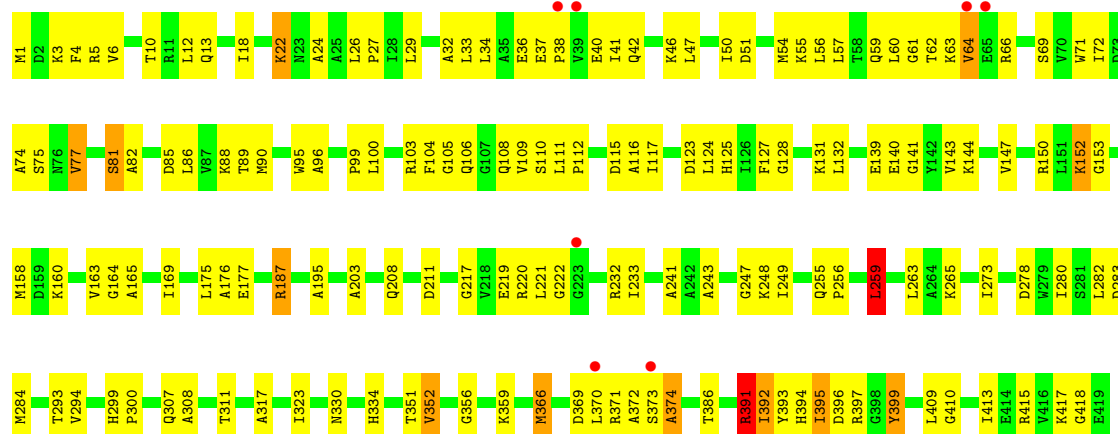
• Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase

Chain D:  65% 32%

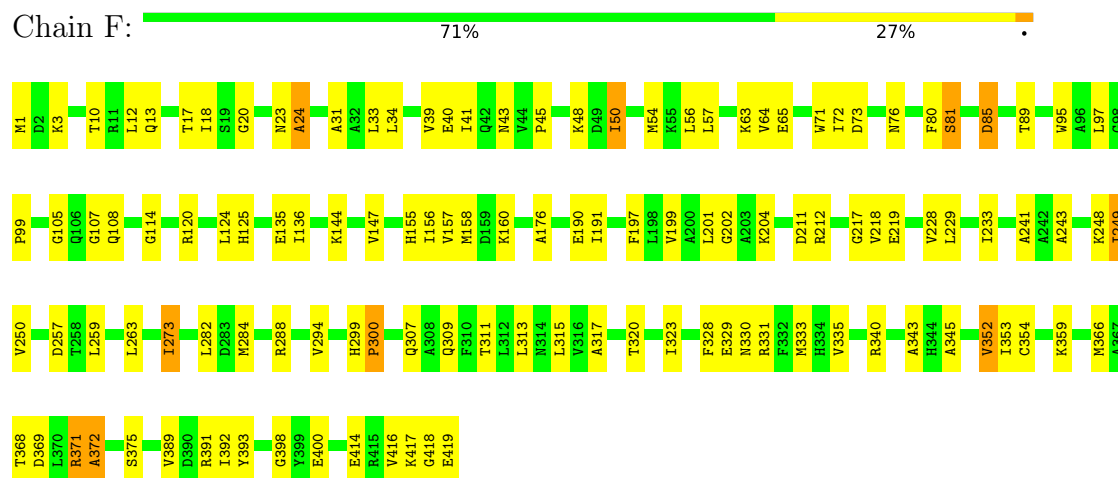


• Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase

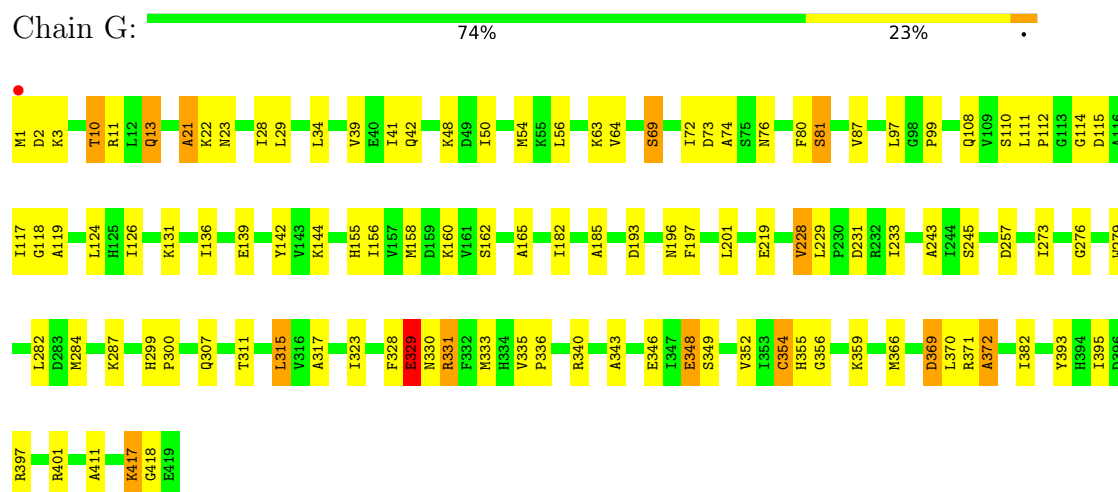
Chain E:  2% 63% 34%



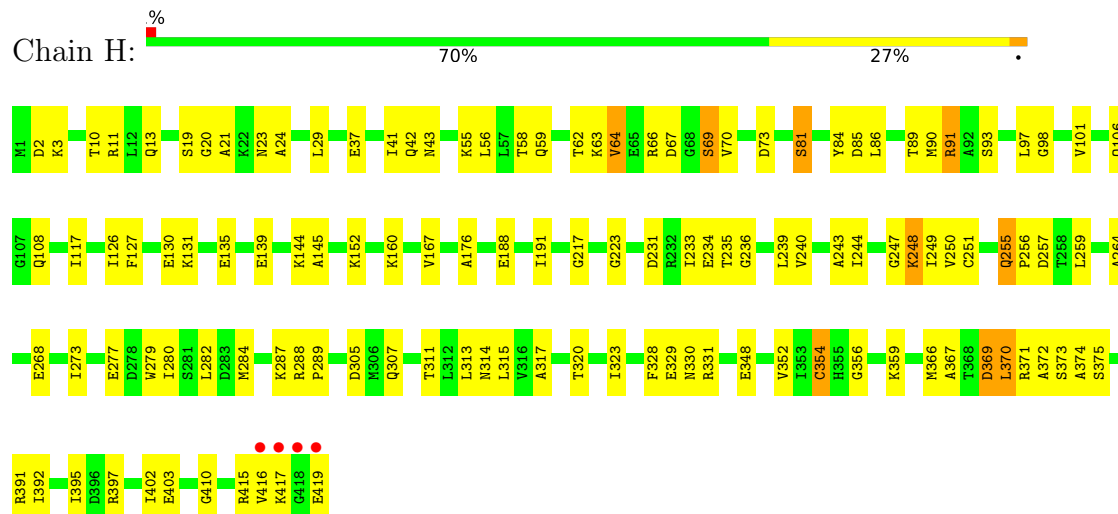
• Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase



• Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase



• Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	83.05Å 153.14Å 131.68Å 90.00° 102.36° 90.00°	Depositor
Resolution (Å)	19.77 – 2.50 19.77 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (19.77-2.50) 99.5 (19.77-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.46 (at 2.50Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.208 , 0.271 0.208 , 0.271	Depositor DCC
R_{free} test set	1216 reflections (1.10%)	wwPDB-VP
Wilson B-factor (Å ²)	39.3	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 45.3	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	26190	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.63% 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: ACT, EDO, IAS, UD1

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	0.69	2/3180 (0.1%)	1.27	22/4308 (0.5%)
1	B	0.66	5/3180 (0.2%)	1.30	30/4308 (0.7%)
1	C	0.65	1/3180 (0.0%)	1.28	23/4308 (0.5%)
1	D	0.65	2/3180 (0.1%)	1.29	30/4308 (0.7%)
1	E	0.64	2/3180 (0.1%)	1.27	27/4308 (0.6%)
1	F	0.63	5/3180 (0.2%)	1.27	26/4308 (0.6%)
1	G	0.69	6/3180 (0.2%)	1.28	27/4308 (0.6%)
1	H	0.61	0/3180	1.28	27/4308 (0.6%)
All	All	0.65	23/25440 (0.1%)	1.28	212/34464 (0.6%)

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	300	PRO	N-CD	-12.67	1.30	1.47
1	B	300	PRO	N-CD	-12.44	1.30	1.47
1	F	300	PRO	N-CD	-11.88	1.31	1.47
1	B	38	PRO	N-CD	-10.49	1.33	1.47
1	E	394	HIS	CG-ND1	-7.68	1.29	1.38
1	A	306	MET	SD-CE	-7.19	1.61	1.79
1	F	375	SER	C-O	-6.17	1.17	1.24
1	D	369	ASP	C-O	-5.98	1.16	1.24
1	F	335	VAL	CA-CB	5.95	1.57	1.54
1	E	394	HIS	CD2-NE2	-5.92	1.31	1.37
1	F	372	ALA	C-O	-5.92	1.17	1.24
1	B	279	TRP	NE1-CE2	-5.85	1.31	1.37
1	B	255	GLN	C-O	-5.85	1.19	1.24
1	G	372	ALA	C-O	-5.80	1.17	1.24
1	G	348	GLU	C-O	-5.79	1.17	1.24
1	G	155	HIS	CD2-NE2	-5.50	1.31	1.37
1	G	369	ASP	C-O	-5.46	1.17	1.24
1	D	375	SER	C-O	-5.34	1.17	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	352	VAL	CA-CB	5.31	1.61	1.54
1	G	3	LYS	C-O	-5.26	1.17	1.23
1	G	155	HIS	CG-ND1	-5.26	1.32	1.38
1	B	276	GLY	CA-C	-5.16	1.47	1.52
1	C	3	LYS	C-O	-5.01	1.17	1.23

All (212) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	287	LYS	N-CA-C	11.97	126.63	110.35
1	D	307	GLN	N-CA-C	11.04	124.50	111.02
1	B	81	SER	N-CA-C	10.91	126.74	109.50
1	E	307	GLN	N-CA-C	10.36	122.16	111.07
1	H	307	GLN	N-CA-C	9.99	123.21	111.02
1	C	81	SER	N-CA-C	9.45	125.02	109.24
1	H	81	SER	N-CA-C	9.30	124.77	109.24
1	G	417	LYS	N-CA-C	9.27	125.02	108.24
1	E	81	SER	N-CA-C	9.27	123.60	109.23
1	D	76	ASN	N-CA-C	9.26	123.27	112.72
1	H	287	LYS	N-CA-C	9.24	123.53	110.50
1	C	307	GLN	N-CA-C	9.22	122.17	111.11
1	G	76	ASN	N-CA-C	9.05	123.07	112.93
1	F	359	LYS	N-CA-C	8.92	124.14	109.24
1	G	80	PHE	N-CA-C	8.89	123.43	112.59
1	C	329	GLU	N-CA-C	8.85	120.70	111.14
1	G	23	ASN	N-CA-C	8.66	123.26	112.87
1	A	307	GLN	N-CA-C	8.57	121.39	111.11
1	F	418	GLY	N-CA-C	8.56	120.12	111.21
1	F	81	SER	N-CA-C	8.54	123.58	109.06
1	D	81	SER	N-CA-C	8.38	123.30	109.06
1	F	219	GLU	N-CA-C	8.29	120.31	111.28
1	C	76	ASN	N-CA-C	8.26	123.53	112.88
1	A	372	ALA	N-CA-C	-8.17	101.93	112.23
1	A	23	ASN	N-CA-C	8.00	122.61	113.01
1	E	374	ALA	N-CA-C	-7.97	102.65	112.38
1	B	219	GLU	N-CA-C	7.96	120.86	111.71
1	B	276	GLY	N-CA-C	-7.93	99.53	111.10
1	D	288	ARG	N-CA-C	-7.88	100.16	109.93
1	G	307	GLN	N-CA-C	7.87	120.56	111.11
1	B	97	LEU	N-CA-C	7.83	119.60	111.14
1	G	331	ARG	N-CA-C	7.78	121.22	112.97
1	B	103	ARG	N-CA-C	7.78	119.84	111.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	329	GLU	N-CA-C	7.70	122.35	112.34
1	D	287	LYS	N-CA-C	7.63	121.57	110.28
1	C	417	LYS	N-CA-C	-7.59	104.06	112.72
1	F	80	PHE	N-CA-C	7.58	121.84	112.59
1	B	80	PHE	N-CA-C	7.56	122.22	112.92
1	F	329	GLU	N-CA-C	7.55	120.57	111.82
1	A	81	SER	N-CA-C	7.51	121.79	109.24
1	B	23	ASN	N-CA-C	7.47	121.50	112.38
1	C	311	THR	N-CA-C	-7.47	103.08	111.07
1	H	259	LEU	N-CA-C	7.36	121.98	112.41
1	G	81	SER	N-CA-C	7.31	121.48	109.06
1	E	417	LYS	N-CA-C	7.27	120.79	109.96
1	B	307	GLN	N-CA-C	7.26	118.89	110.97
1	E	82	ALA	CA-C-N	7.26	127.18	119.85
1	E	82	ALA	C-N-CA	7.26	127.18	119.85
1	F	76	ASN	N-CA-C	7.21	121.79	112.92
1	B	359	LYS	N-CA-C	7.21	120.03	109.07
1	D	80	PHE	N-CA-C	7.19	120.70	112.57
1	G	273	ILE	N-CA-C	7.17	118.93	108.53
1	H	90	MET	N-CA-C	7.11	119.10	107.23
1	E	273	ILE	N-CA-C	6.96	118.51	108.48
1	A	211	ASP	N-CA-C	6.94	121.00	112.54
1	C	259	LEU	N-CA-C	6.91	121.10	111.56
1	A	273	ILE	N-CA-C	6.88	119.44	108.85
1	E	359	LYS	N-CA-C	6.84	119.57	108.76
1	C	23	ASN	N-CA-C	6.82	121.20	113.01
1	F	259	LEU	N-CA-C	6.73	120.84	111.56
1	B	315	LEU	N-CA-C	6.69	120.32	111.75
1	A	287	LYS	N-CA-C	6.67	119.90	110.50
1	H	273	ILE	N-CA-C	6.62	118.02	108.48
1	B	191	ILE	N-CA-C	-6.57	104.45	110.82
1	B	144	LYS	N-CA-C	6.55	119.94	107.75
1	C	354	CYS	N-CA-C	6.53	119.36	108.20
1	G	359	LYS	N-CA-C	6.51	119.04	108.76
1	F	311	THR	N-CA-C	-6.50	104.28	111.36
1	D	90	MET	N-CA-C	6.48	122.32	107.48
1	G	370	LEU	N-CA-C	6.45	118.31	111.28
1	E	399	TYR	N-CA-C	6.44	118.91	108.41
1	E	311	THR	N-CA-C	-6.42	104.36	111.36
1	F	273	ILE	N-CA-C	6.40	117.81	108.53
1	C	287	LYS	N-CA-C	6.36	118.24	110.41
1	G	3	LYS	N-CA-C	6.36	118.51	108.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	152	LYS	N-CA-C	6.34	118.86	108.52
1	F	85	ASP	N-CA-C	6.30	118.96	111.71
1	G	311	THR	N-CA-C	-6.24	104.48	111.28
1	D	311	THR	N-CA-C	-6.23	104.56	111.36
1	D	24	ALA	N-CA-C	-6.23	105.33	113.12
1	G	328	PHE	N-CA-C	6.19	119.56	109.59
1	F	24	ALA	N-CA-C	-6.18	104.71	112.93
1	B	136	ILE	N-CA-C	6.17	117.01	108.12
1	G	366	MET	N-CA-C	6.17	118.46	108.34
1	G	219	GLU	N-CA-C	6.16	117.99	111.28
1	D	98	GLY	CA-C-N	6.15	125.64	119.24
1	D	98	GLY	C-N-CA	6.15	125.64	119.24
1	D	103	ARG	N-CA-C	6.11	118.86	111.40
1	A	91	ARG	N-CA-C	6.10	119.56	111.75
1	G	97	LEU	N-CA-C	6.10	117.60	111.07
1	A	162	SER	N-CA-C	6.09	118.68	108.02
1	H	91	ARG	N-CA-C	6.09	118.70	111.33
1	B	399	TYR	N-CA-C	6.06	118.63	108.02
1	B	329	GLU	N-CA-C	6.06	117.56	111.07
1	H	24	ALA	N-CA-C	-6.05	105.56	113.12
1	E	255	GLN	CA-C-N	6.04	127.40	119.84
1	E	255	GLN	C-N-CA	6.04	127.40	119.84
1	E	211	ASP	N-CA-C	6.04	120.38	113.19
1	D	328	PHE	N-CA-C	6.03	120.66	113.12
1	C	273	ILE	N-CA-C	6.03	117.27	108.53
1	D	192	VAL	N-CA-C	-6.03	104.63	110.72
1	H	369	ASP	CA-C-N	6.02	128.34	120.28
1	H	369	ASP	C-N-CA	6.02	128.34	120.28
1	C	97	LEU	N-CA-C	5.99	118.33	111.02
1	B	366	MET	N-CA-C	5.98	118.27	108.52
1	H	64	VAL	N-CA-C	5.96	116.45	108.11
1	D	2	ASP	N-CA-C	5.96	123.49	110.80
1	F	257	ASP	N-CA-C	5.92	119.98	112.87
1	H	255	GLN	CA-C-N	5.91	127.23	119.84
1	H	255	GLN	C-N-CA	5.91	127.23	119.84
1	A	24	ALA	N-CA-C	-5.91	106.11	113.55
1	D	224	GLY	N-CA-C	5.90	118.12	110.45
1	G	329	GLU	N-CA-C	5.88	117.38	110.97
1	H	98	GLY	CA-C-N	5.87	125.34	119.24
1	H	98	GLY	C-N-CA	5.87	125.34	119.24
1	H	97	LEU	N-CA-C	5.87	118.17	111.02
1	F	13	GLN	N-CA-C	5.85	118.76	108.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	86	LEU	N-CA-C	5.85	117.45	111.14
1	A	288	ARG	N-CA-C	-5.84	102.69	109.93
1	A	403	GLU	N-CA-C	5.81	117.70	111.36
1	E	90	MET	N-CA-C	5.81	116.93	107.23
1	A	259	LEU	N-CA-C	5.80	119.48	111.71
1	D	150	ARG	N-CA-C	5.79	119.49	110.17
1	C	331	ARG	N-CA-C	5.75	120.08	112.25
1	B	331	ARG	N-CA-C	5.75	119.85	112.26
1	H	288	ARG	N-CA-C	-5.73	102.82	109.93
1	D	69	SER	N-CA-C	5.72	118.56	109.81
1	E	106	GLN	N-CA-C	5.70	118.06	109.23
1	H	23	ASN	N-CA-C	5.70	119.49	112.54
1	B	192	VAL	N-CA-C	-5.69	104.39	110.36
1	G	21	ALA	N-CA-C	5.65	118.38	109.96
1	E	64	VAL	N-CA-C	5.65	115.99	107.80
1	D	370	LEU	N-CA-C	5.63	118.19	111.71
1	E	366	MET	N-CA-C	5.63	118.28	108.76
1	E	259	LEU	N-CA-C	5.62	119.32	111.56
1	G	13	GLN	N-CA-C	5.62	117.94	109.23
1	F	328	PHE	N-CA-C	5.60	118.61	109.59
1	H	311	THR	N-CA-C	-5.56	105.14	111.14
1	E	18	ILE	N-CA-C	5.55	116.22	108.89
1	F	18	ILE	N-CA-C	5.54	116.22	109.30
1	G	315	LEU	N-CA-C	5.53	118.07	111.71
1	B	188	GLU	N-CA-C	5.52	115.95	109.60
1	H	191	ILE	N-CA-C	-5.51	105.35	110.53
1	B	150	ARG	N-CA-C	5.49	118.69	109.95
1	D	381	CYS	N-CA-C	5.48	117.96	111.33
1	E	3	LYS	N-CA-C	5.48	117.59	108.99
1	E	24	ALA	N-CA-C	-5.48	106.73	113.41
1	F	158	MET	N-CA-C	5.48	118.12	109.96
1	B	259	LEU	N-CA-C	5.47	120.80	112.54
1	F	156	ILE	N-CA-C	5.47	116.45	108.58
1	H	370	LEU	CA-CB-CG	5.45	135.39	116.30
1	E	95	TRP	N-CA-C	5.45	119.40	112.87
1	F	307	GLN	N-CA-C	5.44	117.66	111.02
1	E	247	GLY	N-CA-C	5.43	126.05	113.18
1	C	191	ILE	N-CA-C	-5.43	105.08	111.00
1	D	23	ASN	N-CA-C	5.41	119.36	112.87
1	C	396	ASP	N-CA-C	5.40	119.49	113.01
1	D	386	THR	N-CA-C	5.40	118.04	109.24
1	A	302	PHE	CA-C-N	5.36	125.53	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	302	PHE	C-N-CA	5.36	125.53	119.90
1	A	417	LYS	N-CA-C	5.35	122.20	110.80
1	G	162	SER	N-CA-C	5.35	117.11	108.34
1	F	95	TRP	N-CA-C	5.34	118.58	111.75
1	B	415	ARG	N-CA-C	5.33	117.86	109.39
1	G	354	CYS	N-CA-C	5.33	117.43	108.96
1	F	97	LEU	N-CA-C	5.32	116.76	111.07
1	B	142	TYR	N-CA-C	5.32	117.91	109.24
1	G	69	SER	N-CA-C	5.32	117.94	109.81
1	D	259	LEU	N-CA-C	5.31	118.89	111.56
1	H	354	CYS	N-CA-C	5.31	117.18	108.52
1	F	366	MET	N-CA-C	5.31	117.06	108.41
1	B	42	GLN	N-CA-C	5.28	118.61	110.42
1	C	219	GLU	N-CA-C	5.28	117.03	111.28
1	E	163	VAL	N-CA-C	-5.27	105.58	110.53
1	B	31	ALA	N-CA-C	-5.27	105.71	111.82
1	C	78	ASN	N-CA-C	5.27	120.19	113.55
1	B	104	PHE	N-CA-C	5.26	119.66	112.88
1	A	136	ILE	N-CA-C	5.25	115.84	108.17
1	A	3	LYS	N-CA-C	5.25	116.27	108.60
1	E	391	ARG	N-CA-C	5.25	118.63	111.39
1	D	120	ARG	N-CA-C	5.25	121.40	109.81
1	F	191	ILE	N-CA-C	-5.24	105.29	111.00
1	G	139	GLU	N-CA-C	5.23	116.84	107.80
1	C	413	ILE	N-CA-C	5.22	116.17	108.45
1	H	69	SER	N-CA-C	5.21	117.32	109.41
1	C	260	ASP	N-CA-C	5.20	117.36	111.11
1	H	374	ALA	N-CA-C	-5.20	106.04	112.38
1	D	302	PHE	CA-C-N	5.19	125.35	119.90
1	D	302	PHE	C-N-CA	5.19	125.35	119.90
1	B	354	CYS	N-CA-C	5.18	116.75	108.41
1	D	333	MET	N-CA-C	5.18	118.38	111.75
1	H	234	GLU	N-CA-C	-5.18	105.55	111.14
1	D	139	GLU	N-CA-C	5.14	116.70	107.80
1	H	58	THR	N-CA-C	-5.14	105.57	111.07
1	E	249	ILE	N-CA-C	5.13	114.96	107.88
1	B	79	ASN	N-CA-C	5.12	118.29	110.20
1	A	89	THR	N-CA-C	-5.11	107.17	113.41
1	A	311	THR	N-CA-C	-5.11	105.60	111.07
1	F	136	ILE	N-CA-C	5.10	115.32	107.77
1	B	390	ASP	N-CA-C	5.09	117.42	110.55
1	H	359	LYS	N-CA-C	5.09	117.45	108.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	255	GLN	CA-C-N	5.06	126.16	119.84
1	C	255	GLN	C-N-CA	5.06	126.16	119.84
1	D	255	GLN	CA-C-N	5.06	126.16	119.84
1	D	255	GLN	C-N-CA	5.06	126.16	119.84
1	G	142	TYR	N-CA-C	5.03	117.81	109.46
1	B	288	ARG	CB-CA-C	5.03	115.96	108.87
1	F	50	ILE	N-CA-C	-5.02	105.50	110.62
1	C	104	PHE	N-CA-C	5.02	119.55	113.38
1	A	80	PHE	N-CA-C	5.01	118.92	112.41
1	G	257	ASP	N-CA-C	5.01	118.49	112.38
1	F	249	ILE	N-CA-C	5.00	115.58	108.42

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3144	0	3215	98	0
1	B	3144	0	3215	142	1
1	C	3144	0	3215	113	0
1	D	3144	0	3215	96	0
1	E	3144	0	3215	120	0
1	F	3144	0	3215	79	0
1	G	3144	0	3215	79	0
1	H	3144	0	3215	100	1
2	A	39	0	25	1	0
2	B	39	0	25	0	0
2	C	39	0	25	0	0
2	D	39	0	25	0	0
2	E	39	0	25	0	0
2	F	39	0	25	0	0
2	G	39	0	25	0	0
2	H	39	0	25	0	0
3	A	16	0	12	0	0
3	B	4	0	3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	8	0	6	4	0
3	D	8	0	6	0	0
3	E	12	0	9	2	0
3	F	12	0	9	3	0
3	H	20	0	15	2	0
4	A	16	0	24	2	0
4	B	12	0	18	0	0
4	C	16	0	24	0	0
4	D	28	0	42	8	0
4	E	28	0	42	1	0
4	F	20	0	30	1	0
4	G	28	0	42	1	0
4	H	28	0	42	3	0
5	A	67	0	0	0	0
5	B	33	0	0	1	0
5	C	53	0	0	4	0
5	D	61	0	0	1	0
5	E	66	0	0	3	0
5	F	60	0	0	2	0
5	G	67	0	0	5	0
5	H	63	0	0	4	0
All	All	26190	0	26244	818	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (818) 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:G:1:MET:O	1:G:418:GLY:HA2	1.20	1.28
1:B:418:GLY:O	1:B:419:GLU:HG3	1.11	1.24
1:A:395:ILE:CD1	1:A:402:ILE:HG21	1.66	1.24
1:C:418:GLY:CA	1:C:419:GLU:O	1.83	1.24
1:A:395:ILE:HD11	1:A:402:ILE:CG2	1.69	1.23
1:C:392:ILE:O	1:C:395:ILE:HG22	1.11	1.22
1:C:418:GLY:HA3	1:C:419:GLU:O	1.40	1.21
1:G:1:MET:O	1:G:418:GLY:CA	1.90	1.20
1:B:418:GLY:O	1:B:419:GLU:CG	1.93	1.16
1:C:392:ILE:O	1:C:395:ILE:CG2	2.03	1.05
1:A:392:ILE:O	1:A:395:ILE:HG22	1.56	1.05
1:C:395:ILE:HD11	1:C:402:ILE:HG21	1.04	1.03

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:SER:HB3	1:B:108:GLN:HG3	1.42	1.02
1:C:418:GLY:HA2	1:C:419:GLU:O	1.58	1.01
1:D:120:ARG:HH22	4:D:510:EDO:H12	1.26	1.01
1:C:395:ILE:CD1	1:C:402:ILE:HG21	1.92	0.98
1:B:15:GLU:HG2	1:B:250:VAL:HB	1.40	0.98
1:F:108:GLN:HG2	1:F:144:LYS:HG2	1.47	0.97
1:G:118:GLY:HA3	1:G:329:GLU:OE1	1.63	0.97
1:E:34:LEU:HD21	1:E:99:PRO:HA	1.46	0.96
1:C:56:LEU:HB2	1:C:86:LEU:HD13	1.48	0.95
1:D:233:ILE:HG21	1:D:371:ARG:HD2	1.48	0.94
1:C:395:ILE:HD11	1:C:402:ILE:CG2	1.97	0.93
1:G:108:GLN:HG2	1:G:144:LYS:HG2	1.51	0.93
1:H:108:GLN:HG2	1:H:144:LYS:HG2	1.51	0.93
1:C:4:PHE:HE2	1:C:395:ILE:HD13	1.34	0.92
1:H:370:LEU:HD12	1:H:397:ARG:HD3	1.51	0.91
1:H:2:ASP:HB3	1:H:392:ILE:HD11	1.53	0.90
1:H:370:LEU:CD1	1:H:397:ARG:HD3	2.03	0.89
1:C:63:LYS:HB3	1:C:73:ASP:HB3	1.55	0.88
1:A:333:MET:HA	1:A:333:MET:HE2	1.54	0.88
1:G:323:ILE:HB	1:G:352:VAL:HG12	1.54	0.87
1:D:369:ASP:HB3	1:D:372:ALA:HB3	1.55	0.87
1:D:94:ILE:HA	1:D:109:VAL:HG11	1.58	0.85
1:D:177:GLU:HG2	4:D:508:EDO:H21	1.58	0.84
1:G:2:ASP:OD1	1:G:417:LYS:HG2	1.78	0.83
1:C:233:ILE:HG23	1:C:306:MET:HE3	1.59	0.83
1:F:331:ARG:H	3:F:503:ACT:H2	1.43	0.83
1:A:259:LEU:HD12	1:A:263:LEU:HG	1.61	0.82
1:D:41:ILE:O	1:D:69:SER:HB2	1.79	0.82
1:F:369:ASP:HB3	1:F:372:ALA:HB3	1.62	0.82
1:G:1:MET:O	1:G:418:GLY:N	2.12	0.81
1:H:42:GLN:HA	1:H:69:SER:HB3	1.62	0.80
1:G:118:GLY:CA	1:G:329:GLU:OE1	2.28	0.80
1:C:367:ALA:HB1	1:C:373:SER:HB3	1.62	0.80
1:C:418:GLY:CA	1:C:419:GLU:C	2.52	0.79
1:B:64:VAL:O	1:B:65:GLU:HG3	1.84	0.77
1:G:243:ALA:HA	1:G:284:MET:HG3	1.67	0.77
1:G:81:SER:HB3	1:G:108:GLN:HB2	1.66	0.77
1:B:47:LEU:HB2	1:B:50:ILE:HG12	1.65	0.77
1:E:243:ALA:HA	1:E:284:MET:CG	2.14	0.77
1:G:48:LYS:HZ1	1:G:393:TYR:HB2	1.49	0.77
1:F:212:ARG:HD2	5:F:660:HOH:O	1.83	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:243:ALA:HA	1:H:284:MET:CG	2.15	0.76
1:B:4:PHE:CD1	1:B:392:ILE:HD13	2.20	0.76
1:C:4:PHE:CE2	1:C:395:ILE:HD13	2.20	0.76
1:D:108:GLN:HG2	1:D:144:LYS:HG2	1.69	0.75
1:E:366:MET:HE2	1:E:391:ARG:HD3	1.68	0.75
1:E:34:LEU:HD21	1:E:99:PRO:CA	2.17	0.75
1:H:108:GLN:CG	1:H:144:LYS:HG2	2.17	0.75
1:B:244:ILE:HD12	1:B:382:ILE:HD13	1.68	0.74
1:G:50:ILE:HG22	1:G:54:MET:HE2	1.68	0.74
1:E:55:LYS:HE3	1:E:86:LEU:HD21	1.69	0.74
1:C:370:LEU:HG	1:C:371:ARG:HG2	1.70	0.74
1:E:36:GLU:HG2	1:E:103:ARG:HH21	1.53	0.73
1:C:396:ASP:CG	1:C:415:ARG:HH22	1.95	0.73
1:E:36:GLU:O	1:E:75:SER:HB3	1.89	0.73
1:C:41:ILE:HG22	1:C:44:VAL:CG2	2.19	0.72
1:E:1:MET:N	1:E:418:GLY:HA2	2.04	0.72
1:G:233:ILE:HG21	1:G:371:ARG:HD2	1.71	0.72
1:F:48:LYS:NZ	1:F:393:TYR:HB2	2.03	0.72
1:C:257:ASP:HB3	3:C:502:ACT:H1	1.72	0.72
1:D:91:ARG:NH2	1:D:120:ARG:O	2.22	0.72
1:D:323:ILE:HB	1:D:352:VAL:CG1	2.20	0.72
1:B:37:GLU:HB2	1:B:223:GLY:H	1.55	0.71
1:G:323:ILE:HB	1:G:352:VAL:CG1	2.18	0.71
1:A:259:LEU:CD1	1:A:263:LEU:HG	2.20	0.71
1:C:3:LYS:HD3	1:C:390:ASP:OD1	1.89	0.71
1:G:48:LYS:NZ	1:G:393:TYR:HB2	2.06	0.71
1:B:259:LEU:HD12	1:B:263:LEU:HG	1.70	0.71
1:E:127:PHE:CZ	1:E:131:LYS:HE2	2.24	0.71
1:A:181:ILE:HG21	1:A:212:ARG:HD2	1.72	0.71
1:F:331:ARG:N	3:F:503:ACT:H2	2.05	0.71
1:B:63:LYS:HB3	1:B:73:ASP:HB3	1.72	0.71
1:F:33:LEU:HD21	1:F:57:LEU:HD22	1.73	0.71
1:H:243:ALA:HA	1:H:284:MET:HG2	1.73	0.70
1:A:29:LEU:HD23	1:A:41:ILE:CD1	2.21	0.70
1:C:9:PRO:HD3	1:C:384:GLU:HG3	1.73	0.70
1:H:315:LEU:HD23	1:H:354:CYS:HB3	1.72	0.70
1:A:334:HIS:HB3	1:A:372:ALA:HB1	1.73	0.70
1:C:108:GLN:HG2	1:C:144:LYS:HG2	1.74	0.70
1:C:327:ILE:HD12	3:C:503:ACT:H1	1.73	0.70
1:G:10:THR:HG21	1:G:411:ALA:HA	1.71	0.70
1:H:366:MET:HE3	1:H:391:ARG:HD2	1.74	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:ILE:HG23	1:A:306:MET:HE3	1.72	0.70
1:C:7:GLN:HB2	1:C:412:ASN:ND2	2.06	0.70
1:B:4:PHE:CE1	1:B:392:ILE:HD12	2.27	0.70
1:G:346:GLU:OE2	1:G:355:HIS:NE2	2.21	0.70
1:A:306:MET:HE2	1:A:309:GLN:NE2	2.06	0.69
1:A:395:ILE:CD1	1:A:402:ILE:CG2	2.49	0.69
1:B:21:ALA:HA	1:B:231:ASP:HB2	1.72	0.69
1:D:323:ILE:HB	1:D:352:VAL:HG13	1.73	0.69
1:E:370:LEU:HD23	1:E:370:LEU:H	1.58	0.69
1:A:176:ALA:O	1:A:217:GLY:HA3	1.91	0.69
1:G:315:LEU:HD13	1:G:343:ALA:HB1	1.75	0.68
1:G:333:MET:HG3	5:G:663:HOH:O	1.92	0.68
1:C:176:ALA:O	1:C:217:GLY:HA3	1.92	0.68
1:B:418:GLY:O	1:B:419:GLU:CB	2.41	0.68
1:A:229:LEU:HB2	1:A:230:PRO:HD2	1.75	0.68
1:E:22:LYS:HZ1	3:E:502:ACT:H2	1.58	0.68
1:B:417:LYS:HG2	1:B:418:GLY:N	2.09	0.68
1:C:81:SER:HB3	1:C:108:GLN:HB2	1.75	0.68
1:A:29:LEU:HD23	1:A:41:ILE:HD12	1.74	0.68
1:B:417:LYS:HG2	1:B:418:GLY:H	1.57	0.68
1:G:1:MET:C	1:G:418:GLY:HA2	2.14	0.68
1:C:306:MET:HE2	1:C:306:MET:HA	1.75	0.67
1:E:103:ARG:NH1	1:E:104:PHE:HZ	1.91	0.67
1:E:369:ASP:HB3	1:E:372:ALA:HB3	1.76	0.67
1:E:108:GLN:HG2	1:E:144:LYS:HG2	1.75	0.67
1:F:176:ALA:O	1:F:217:GLY:HA3	1.95	0.67
1:B:418:GLY:C	1:B:419:GLU:HG3	2.11	0.67
1:B:4:PHE:CD1	1:B:392:ILE:CD1	2.78	0.67
1:B:284:MET:HE2	1:B:289:PRO:HG3	1.77	0.67
1:G:243:ALA:HA	1:G:284:MET:CG	2.25	0.66
1:C:416:VAL:HG12	1:C:418:GLY:H	1.60	0.66
1:F:369:ASP:CB	1:F:372:ALA:HB3	2.25	0.66
1:D:42:GLN:HA	1:D:69:SER:HB3	1.78	0.66
1:D:149:GLY:O	1:D:150:ARG:HD3	1.96	0.66
1:E:36:GLU:HG2	1:E:103:ARG:NH2	2.11	0.66
1:E:282:LEU:C	1:E:282:LEU:HD23	2.20	0.66
1:A:323:ILE:HB	1:A:352:VAL:CG1	2.26	0.66
1:E:105:GLY:HA2	1:E:147:VAL:HG12	1.78	0.66
1:H:370:LEU:CD1	1:H:397:ARG:CD	2.74	0.66
1:A:229:LEU:HB2	1:A:230:PRO:CD	2.27	0.66
1:H:369:ASP:HB3	1:H:372:ALA:HB3	1.78	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:ILE:CG2	1:A:212:ARG:HD2	2.25	0.65
1:F:243:ALA:HA	1:F:284:MET:CG	2.26	0.65
1:A:317:ALA:O	1:A:356:GLY:HA3	1.96	0.65
1:B:176:ALA:O	1:B:217:GLY:HA3	1.95	0.65
1:A:370:LEU:O	1:A:371:ARG:HD2	1.96	0.65
1:B:401:ARG:HG2	5:B:616:HOH:O	1.96	0.65
1:D:137:LYS:HE3	1:D:139:GLU:OE1	1.97	0.65
1:G:126:ILE:HG23	1:G:136:ILE:HD13	1.77	0.65
1:A:306:MET:HE2	1:A:306:MET:HA	1.79	0.65
1:E:243:ALA:HA	1:E:284:MET:HG2	1.78	0.65
1:H:313:LEU:C	1:H:313:LEU:HD23	2.22	0.65
1:C:392:ILE:C	1:C:395:ILE:HG22	2.15	0.65
1:F:81:SER:HB3	1:F:108:GLN:HB2	1.79	0.65
1:H:395:ILE:HG21	1:H:402:ILE:HG21	1.79	0.64
1:A:369:ASP:C	1:A:371:ARG:H	2.05	0.64
1:C:227:ARG:HD2	5:C:637:HOH:O	1.97	0.64
1:C:396:ASP:OD2	1:C:415:ARG:NH2	2.21	0.64
1:E:393:TYR:O	1:E:397:ARG:HG3	1.97	0.64
1:H:63:LYS:HB3	1:H:73:ASP:HB3	1.80	0.64
1:A:243:ALA:HA	1:A:284:MET:CG	2.26	0.64
1:B:118:GLY:CA	1:B:329:GLU:OE2	2.46	0.64
1:E:128:GLY:HA3	1:E:169:ILE:HD11	1.79	0.64
1:E:243:ALA:HA	1:E:284:MET:HG3	1.78	0.64
1:F:243:ALA:HA	1:F:284:MET:HG3	1.77	0.64
1:A:111:LEU:HD12	1:A:112:PRO:HD2	1.80	0.64
1:F:3:LYS:HA	1:F:392:ILE:HG23	1.80	0.64
1:D:112:PRO:HA	4:D:509:EDO:H22	1.80	0.64
1:B:29:LEU:HD23	1:B:41:ILE:HD12	1.79	0.63
1:D:82:ALA:HB3	1:D:109:VAL:HG13	1.80	0.63
1:D:243:ALA:HA	1:D:284:MET:CG	2.27	0.63
1:B:74:ALA:O	1:B:77:VAL:HG23	1.97	0.63
1:H:108:GLN:NE2	1:H:144:LYS:HE2	2.13	0.63
1:H:41:ILE:O	1:H:69:SER:HB2	1.98	0.63
1:D:38:PRO:HG3	1:D:73:ASP:OD2	1.97	0.63
1:A:243:ALA:HA	1:A:284:MET:HG3	1.80	0.63
1:C:34:LEU:HD21	1:C:99:PRO:HA	1.81	0.63
1:G:41:ILE:O	1:G:69:SER:HB2	1.99	0.63
1:G:29:LEU:HD23	1:G:41:ILE:HD12	1.81	0.63
1:G:196:ASN:HB3	4:G:505:EDO:H12	1.80	0.63
1:C:24:ALA:HB3	1:C:228:VAL:HG13	1.81	0.62
1:A:306:MET:CE	1:A:309:GLN:NE2	2.61	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:10:THR:HG21	1:H:410:GLY:O	1.99	0.62
1:B:34:LEU:HD22	1:B:175:LEU:HD11	1.82	0.62
1:B:152:LYS:HD2	1:B:177:GLU:O	1.99	0.62
1:G:369:ASP:HB3	1:G:372:ALA:HB3	1.82	0.62
1:F:204:LYS:HE3	1:F:218:VAL:HG12	1.82	0.62
1:A:320:THR:HG21	1:C:320:THR:HG21	1.81	0.61
1:D:108:GLN:HG3	5:D:646:HOH:O	1.98	0.61
1:E:46:LYS:HG2	1:E:66:ARG:NH1	2.15	0.61
1:E:22:LYS:NZ	3:E:502:ACT:H2	2.16	0.61
1:B:2:ASP:OD2	1:B:415:ARG:HD3	2.01	0.61
1:F:63:LYS:HB3	1:F:73:ASP:HB3	1.81	0.61
1:G:335:VAL:HB	1:G:336:PRO:HD3	1.83	0.61
1:D:120:ARG:HH22	4:D:510:EDO:C1	2.07	0.61
1:F:3:LYS:NZ	1:F:419:GLU:C	2.58	0.61
1:D:92:ALA:HA	4:D:504:EDO:H12	1.82	0.61
1:F:323:ILE:HB	1:F:352:VAL:HG13	1.83	0.61
1:B:39:VAL:HG22	1:B:223:GLY:HA2	1.81	0.60
1:D:56:LEU:HD23	1:D:56:LEU:C	2.26	0.60
1:H:370:LEU:HD11	1:H:397:ARG:NE	2.16	0.60
1:B:3:LYS:O	1:B:3:LYS:HG3	2.02	0.60
1:B:334:HIS:HB3	1:B:372:ALA:HB1	1.83	0.60
1:B:367:ALA:HB1	1:B:373:SER:OG	2.01	0.60
1:D:124:LEU:HD11	1:D:160:LYS:HG2	1.84	0.60
1:B:4:PHE:CD2	1:B:413:ILE:HD11	2.36	0.60
1:B:373:SER:HB3	1:B:395:ILE:HG12	1.83	0.60
1:F:3:LYS:HB2	1:F:389:VAL:O	2.00	0.60
1:H:81:SER:HB3	1:H:108:GLN:HB2	1.83	0.60
1:H:176:ALA:O	1:H:217:GLY:HA3	2.02	0.59
1:D:313:LEU:C	1:D:313:LEU:HD23	2.27	0.59
1:E:5:ARG:NH1	1:E:386:THR:HG21	2.17	0.59
1:E:41:ILE:O	1:E:69:SER:HB2	2.03	0.59
1:A:150:ARG:HH12	1:A:219:GLU:HA	1.67	0.59
1:G:340:ARG:HG2	1:G:340:ARG:HH11	1.66	0.59
1:G:348:GLU:O	1:G:349:SER:HB3	2.03	0.59
1:E:150:ARG:HB2	1:E:177:GLU:CG	2.30	0.59
1:H:366:MET:CE	1:H:391:ARG:HD2	2.32	0.59
1:A:56:LEU:C	1:A:56:LEU:HD23	2.27	0.59
1:A:204:LYS:HE2	1:A:218:VAL:HG12	1.84	0.59
1:D:63:LYS:HB3	1:D:73:ASP:HB3	1.84	0.59
1:A:40:GLU:HB3	1:A:225:VAL:HG22	1.84	0.59
1:A:116:ALA:O	1:A:330:ASN:ND2	2.35	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:LYS:HE3	1:B:397:ARG:HG2	1.85	0.59
1:E:323:ILE:HB	1:E:352:VAL:HG13	1.85	0.59
1:H:56:LEU:C	1:H:56:LEU:HD23	2.28	0.59
1:E:152:LYS:HD2	1:E:153:GLY:N	2.18	0.59
1:F:56:LEU:C	1:F:56:LEU:HD23	2.27	0.59
1:G:317:ALA:O	1:G:356:GLY:HA3	2.03	0.59
1:B:4:PHE:CE1	1:B:392:ILE:CD1	2.85	0.58
1:C:4:PHE:HE2	1:C:395:ILE:CD1	2.12	0.58
1:A:259:LEU:HD12	1:A:263:LEU:CG	2.31	0.58
1:B:34:LEU:HD22	1:B:175:LEU:CD1	2.33	0.58
1:D:64:VAL:HG22	1:D:72:ILE:HD13	1.85	0.58
1:H:243:ALA:HA	1:H:284:MET:HG3	1.84	0.58
1:C:36:GLU:OE1	1:C:220:ARG:NE	2.35	0.58
1:F:48:LYS:HZ1	1:F:393:TYR:HB2	1.68	0.58
1:H:85:ASP:O	1:H:89:THR:HG23	2.03	0.58
1:A:370:LEU:O	1:A:370:LEU:HD12	2.03	0.58
1:H:152:LYS:HE3	5:H:627:HOH:O	2.03	0.58
1:B:4:PHE:H	1:B:392:ILE:HG21	1.68	0.57
1:C:334:HIS:HB3	1:C:372:ALA:HB1	1.85	0.57
1:F:197:PHE:CZ	1:F:201:LEU:HD11	2.40	0.57
1:G:124:LEU:HD11	1:G:160:LYS:HG2	1.85	0.57
1:B:56:LEU:HB2	1:B:86:LEU:HD13	1.84	0.57
1:B:118:GLY:HA3	1:B:329:GLU:OE2	2.03	0.57
1:C:259:LEU:HD12	1:C:263:LEU:HG	1.86	0.57
1:D:41:ILE:HG22	1:D:44:VAL:CG2	2.35	0.57
1:D:66:ARG:HB3	1:D:70:VAL:HG22	1.86	0.57
1:F:391:ARG:HB3	1:F:393:TYR:CE2	2.40	0.57
1:E:152:LYS:HD2	1:E:153:GLY:H	1.70	0.57
1:E:373:SER:HB2	1:E:395:ILE:CD1	2.35	0.57
1:E:40:GLU:OE2	1:E:71:TRP:NE1	2.38	0.57
1:F:315:LEU:HD21	1:F:345:ALA:HB2	1.85	0.57
1:A:15:GLU:HG2	1:A:250:VAL:HB	1.86	0.56
1:E:103:ARG:NH1	1:E:104:PHE:CZ	2.72	0.56
1:F:48:LYS:HZ3	1:F:393:TYR:HB2	1.70	0.56
1:E:105:GLY:HA2	1:E:147:VAL:CG1	2.33	0.56
1:E:330:ASN:CG	1:H:330:ASN:HB2	2.29	0.56
1:C:233:ILE:CG2	1:C:306:MET:HE3	2.33	0.56
1:E:127:PHE:CE2	1:E:131:LYS:HE2	2.41	0.56
1:A:395:ILE:HD11	1:A:402:ILE:HG21	0.75	0.56
1:D:243:ALA:HA	1:D:284:MET:HG3	1.88	0.56
1:A:233:ILE:CG2	1:A:306:MET:HE3	2.36	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:248:LYS:HD2	1:E:283:ASP:OD2	2.05	0.56
1:B:314:ASN:HB3	1:B:354:CYS:HB2	1.87	0.56
1:D:64:VAL:HG22	1:D:72:ILE:CD1	2.36	0.55
1:B:17:THR:HA	1:B:252:ARG:HB2	1.87	0.55
1:A:94:ILE:HA	1:A:109:VAL:HG11	1.88	0.55
1:B:29:LEU:HD23	1:B:41:ILE:CD1	2.37	0.55
1:B:417:LYS:CG	1:B:418:GLY:H	2.19	0.55
1:G:81:SER:HB3	1:G:108:GLN:CB	2.36	0.55
1:H:127:PHE:CE2	1:H:131:LYS:HD2	2.41	0.55
1:E:330:ASN:OD1	1:H:330:ASN:HB2	2.06	0.55
1:A:81:SER:HB3	1:A:108:GLN:HB2	1.89	0.55
1:B:372:ALA:O	1:B:375:SER:N	2.39	0.55
1:C:182:ILE:HG22	1:C:185:ALA:HB2	1.89	0.55
1:C:250:VAL:HG22	1:C:281:SER:HB2	1.88	0.55
1:H:282:LEU:C	1:H:282:LEU:HD23	2.32	0.55
1:E:36:GLU:OE1	1:E:220:ARG:HB2	2.07	0.55
1:H:323:ILE:HB	1:H:352:VAL:CG1	2.37	0.55
1:B:40:GLU:HG3	1:B:71:TRP:NE1	2.22	0.55
1:A:395:ILE:HG23	1:A:396:ASP:N	2.21	0.54
1:C:370:LEU:HD11	1:C:399:TYR:CD1	2.42	0.54
1:D:94:ILE:HD12	1:D:122:VAL:HG11	1.89	0.54
1:H:117:ILE:CG2	1:H:331:ARG:HG3	2.36	0.54
3:H:503:ACT:H2	5:H:606:HOH:O	2.07	0.54
1:B:21:ALA:HB2	1:B:231:ASP:HA	1.90	0.54
1:D:152:LYS:HD2	1:D:177:GLU:O	2.07	0.54
1:G:64:VAL:HG22	1:G:72:ILE:HD13	1.89	0.54
1:B:48:LYS:NZ	1:B:393:TYR:HB2	2.22	0.54
1:E:103:ARG:HH11	1:E:104:PHE:HZ	1.55	0.54
1:E:373:SER:HB2	1:E:395:ILE:HD11	1.89	0.54
1:H:248:LYS:NZ	1:H:248:LYS:HB3	2.23	0.54
1:C:77:VAL:HB	1:C:104:PHE:CZ	2.43	0.54
1:E:56:LEU:HD23	1:E:56:LEU:O	2.07	0.54
1:F:323:ILE:HB	1:F:352:VAL:CG1	2.38	0.54
1:B:9:PRO:HD3	1:B:384:GLU:HA	1.89	0.54
1:B:126:ILE:O	1:B:130:GLU:HG3	2.07	0.54
1:E:323:ILE:HB	1:E:352:VAL:CG1	2.37	0.54
1:F:120:ARG:HB3	5:F:622:HOH:O	2.07	0.54
1:B:97:LEU:HD12	1:B:97:LEU:O	2.08	0.53
1:H:188:GLU:OE1	1:H:188:GLU:N	2.41	0.53
1:B:244:ILE:HA	1:B:289:PRO:HG2	1.89	0.53
1:C:127:PHE:HB2	5:C:641:HOH:O	2.07	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:299:HIS:ND1	1:D:300:PRO:HA	2.24	0.53
1:E:124:LEU:HD11	1:E:160:LYS:HG3	1.90	0.53
1:G:56:LEU:HD23	1:G:56:LEU:O	2.08	0.53
1:A:31:ALA:HB1	1:A:198:LEU:HD21	1.90	0.53
1:A:115:ASP:HB3	1:A:118:GLY:O	2.08	0.53
1:C:317:ALA:O	1:C:356:GLY:HA3	2.08	0.53
1:A:282:LEU:C	1:A:282:LEU:HD23	2.34	0.53
1:E:150:ARG:HH12	1:E:219:GLU:HA	1.73	0.53
1:G:111:LEU:HD12	1:G:112:PRO:HD2	1.91	0.53
1:B:395:ILE:HG21	1:B:402:ILE:HG21	1.91	0.53
1:C:299:HIS:CG	1:C:300:PRO:HA	2.43	0.53
1:H:3:LYS:HB2	1:H:416:VAL:HB	1.91	0.53
1:H:62:THR:HG22	1:H:64:VAL:HG22	1.90	0.53
1:H:317:ALA:O	1:H:356:GLY:HA3	2.09	0.53
1:B:317:ALA:O	1:B:356:GLY:HA3	2.09	0.53
1:C:333:MET:HE2	1:C:368:THR:HB	1.91	0.53
1:B:45:PRO:O	1:B:50:ILE:HG13	2.09	0.53
1:D:49:ASP:OD2	4:D:505:EDO:O2	2.26	0.53
1:E:74:ALA:O	1:E:77:VAL:HG23	2.09	0.53
1:B:46:LYS:N	1:B:400:GLU:OE1	2.35	0.53
1:D:46:LYS:HG2	1:D:66:ARG:CZ	2.39	0.53
1:A:333:MET:HA	1:A:333:MET:CE	2.35	0.52
1:B:243:ALA:HA	1:B:284:MET:HG3	1.91	0.52
1:E:5:ARG:HH12	1:E:386:THR:HG21	1.73	0.52
1:A:181:ILE:HG23	1:A:212:ARG:CG	2.40	0.52
1:C:111:LEU:HD12	1:C:112:PRO:HD2	1.90	0.52
1:F:416:VAL:HG12	1:F:417:LYS:N	2.23	0.52
1:E:64:VAL:HG13	1:E:72:ILE:HD11	1.91	0.52
1:H:21:ALA:HA	1:H:231:ASP:HB2	1.91	0.52
1:A:152:LYS:HD2	1:A:177:GLU:O	2.09	0.52
1:C:316:VAL:HG23	1:C:316:VAL:O	2.08	0.52
1:F:3:LYS:HZ1	1:F:419:GLU:C	2.17	0.52
1:A:416:VAL:HG12	1:A:418:GLY:H	1.74	0.52
1:B:97:LEU:HD11	1:B:145:ALA:HB3	1.92	0.52
1:C:243:ALA:O	1:C:284:MET:HE2	2.09	0.52
1:E:150:ARG:HB2	1:E:177:GLU:HG3	1.91	0.52
1:B:213:ILE:HG22	1:B:215:ILE:HD11	1.91	0.52
1:C:40:GLU:HB3	1:C:225:VAL:HG22	1.92	0.52
1:C:243:ALA:HA	1:C:284:MET:HG3	1.92	0.52
1:E:125:HIS:CE1	1:E:164:GLY:C	2.88	0.52
1:B:108:GLN:NE2	1:B:144:LYS:HE2	2.24	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:ILE:HG12	1:B:250:VAL:N	2.24	0.52
1:E:299:HIS:CG	1:E:300:PRO:HA	2.45	0.52
1:C:41:ILE:HD11	1:C:197:PHE:CE1	2.45	0.52
1:E:56:LEU:HD23	1:E:56:LEU:C	2.34	0.52
1:F:33:LEU:HD21	1:F:57:LEU:CD2	2.38	0.52
1:A:1:MET:HE1	1:A:391:ARG:NE	2.25	0.52
1:B:87:VAL:HG21	1:B:110:SER:HB3	1.91	0.52
1:D:1:MET:N	1:D:418:GLY:O	2.43	0.52
1:H:37:GLU:HB2	1:H:223:GLY:N	2.25	0.52
1:H:370:LEU:HD11	1:H:397:ARG:CZ	2.40	0.52
1:A:34:LEU:HD21	1:A:99:PRO:HA	1.91	0.51
1:A:137:LYS:NZ	1:A:139:GLU:OE2	2.42	0.51
1:C:115:ASP:CG	1:C:116:ALA:H	2.17	0.51
1:C:126:ILE:HG23	1:C:136:ILE:HG21	1.92	0.51
1:B:119:ALA:N	1:B:329:GLU:OE2	2.44	0.51
1:D:118:GLY:O	1:D:119:ALA:HB3	2.09	0.51
1:E:111:LEU:HD13	1:E:143:VAL:CG2	2.40	0.51
1:E:330:ASN:HB2	1:H:330:ASN:OD1	2.10	0.51
1:F:105:GLY:HA2	1:F:147:VAL:HG12	1.92	0.51
1:A:275:THR:HG22	1:A:280:ILE:HG12	1.92	0.51
1:E:278:ASP:OD1	1:E:278:ASP:N	2.42	0.51
1:A:124:LEU:HD11	1:A:160:LYS:HG2	1.93	0.51
1:B:220:ARG:O	1:B:221:LEU:HD23	2.11	0.51
1:D:4:PHE:HE1	1:D:415:ARG:HB2	1.75	0.51
1:E:123:ASP:HA	4:E:508:EDO:H21	1.93	0.51
1:D:204:LYS:HB2	1:D:216:GLU:HB3	1.92	0.51
1:E:57:LEU:O	1:E:62:THR:HB	2.11	0.51
1:D:12:LEU:HD12	1:D:241:ALA:HB1	1.92	0.51
1:E:59:GLN:C	1:E:61:GLY:H	2.18	0.51
1:E:369:ASP:CB	1:E:372:ALA:HB3	2.40	0.51
1:B:282:LEU:C	1:B:282:LEU:HD23	2.35	0.51
1:D:369:ASP:CB	1:D:372:ALA:HB3	2.35	0.51
1:D:254:ALA:O	1:D:278:ASP:HA	2.11	0.51
1:D:417:LYS:C	1:D:419:GLU:H	2.18	0.51
1:G:193:ASP:CG	1:G:229:LEU:HD22	2.36	0.51
1:G:299:HIS:ND1	1:G:300:PRO:HA	2.26	0.51
1:H:108:GLN:CD	1:H:144:LYS:HE2	2.36	0.51
1:B:37:GLU:O	1:B:38:PRO:C	2.53	0.50
1:C:276:GLY:HA3	1:C:279:TRP:NE1	2.26	0.50
1:A:259:LEU:CD1	1:A:263:LEU:CG	2.88	0.50
1:D:299:HIS:CG	1:D:300:PRO:HA	2.46	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:115:ASP:OD2	1:E:117:ILE:HG12	2.12	0.50
1:G:21:ALA:HA	1:G:231:ASP:HB2	1.92	0.50
1:G:42:GLN:HA	1:G:69:SER:HB3	1.92	0.50
1:H:240:VAL:O	1:H:244:ILE:HG12	2.12	0.50
1:A:101:VAL:HG13	1:A:102:ALA:N	2.25	0.50
1:A:115:ASP:OD2	1:A:116:ALA:N	2.45	0.50
1:D:13:GLN:HA	1:D:248:LYS:O	2.10	0.50
1:F:340:ARG:HH11	1:F:340:ARG:HG2	1.74	0.50
1:G:131:LYS:HD3	1:G:156:ILE:HG23	1.94	0.50
1:B:5:ARG:NE	1:B:416:VAL:HG21	2.26	0.50
1:D:10:THR:HG21	1:D:411:ALA:HA	1.92	0.50
1:E:124:LEU:HD11	1:E:160:LYS:CG	2.42	0.50
1:E:176:ALA:O	1:E:217:GLY:HA3	2.12	0.50
1:F:313:LEU:C	1:F:313:LEU:HD23	2.37	0.50
1:C:36:GLU:O	1:C:75:SER:HB3	2.12	0.50
1:H:62:THR:HG22	1:H:64:VAL:CG2	2.42	0.50
1:B:21:ALA:HA	1:B:231:ASP:CB	2.42	0.49
1:A:81:SER:CB	1:A:108:GLN:HB2	2.42	0.49
1:C:294:VAL:HB	1:C:323:ILE:HD13	1.93	0.49
1:A:21:ALA:HA	1:A:231:ASP:HB2	1.94	0.49
1:B:37:GLU:HB2	1:B:223:GLY:N	2.23	0.49
1:B:180:THR:HB	1:B:215:ILE:HB	1.94	0.49
1:B:296:THR:HA	1:B:302:PHE:O	2.12	0.49
1:F:50:ILE:O	1:F:54:MET:HG3	2.11	0.49
1:G:108:GLN:CD	1:G:144:LYS:HE2	2.37	0.49
1:B:48:LYS:HZ3	1:B:393:TYR:HB2	1.76	0.49
1:E:152:LYS:CE	5:E:632:HOH:O	2.60	0.49
1:E:152:LYS:HE3	5:E:632:HOH:O	2.11	0.49
1:F:294:VAL:HB	1:F:323:ILE:HD13	1.94	0.49
1:H:329:GLU:HG2	1:H:330:ASN:H	1.76	0.49
1:B:35:ALA:O	1:B:74:ALA:HB3	2.13	0.49
1:C:94:ILE:HA	1:C:109:VAL:HG11	1.95	0.49
1:B:271:ALA:HB2	1:B:284:MET:SD	2.52	0.49
1:C:399:TYR:CD2	1:C:402:ILE:HD12	2.47	0.49
1:E:4:PHE:CD2	1:E:392:ILE:HG21	2.48	0.49
1:G:87:VAL:HG21	1:G:110:SER:HB3	1.95	0.49
1:C:357:VAL:HG13	5:C:606:HOH:O	2.11	0.49
1:F:24:ALA:HB3	1:F:228:VAL:HG13	1.93	0.49
1:B:372:ALA:O	1:B:373:SER:C	2.56	0.49
1:C:243:ALA:HA	1:C:284:MET:CG	2.43	0.49
1:E:46:LYS:HG2	1:E:66:ARG:CZ	2.43	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:367:ALA:HB1	1:H:373:SER:CB	2.43	0.49
1:C:87:VAL:HG21	1:C:110:SER:HB3	1.94	0.48
1:F:330:ASN:HB2	1:G:330:ASN:HB2	1.95	0.48
1:B:35:ALA:HB2	1:B:201:LEU:HD13	1.95	0.48
1:B:299:HIS:CG	1:B:300:PRO:HA	2.48	0.48
1:B:360:LEU:O	1:B:384:GLU:N	2.44	0.48
1:D:276:GLY:HA3	1:D:279:TRP:NE1	2.28	0.48
1:G:340:ARG:HH11	1:G:340:ARG:CG	2.26	0.48
1:C:220:ARG:HG3	1:C:220:ARG:HH11	1.78	0.48
1:E:294:VAL:HB	1:E:323:ILE:HD13	1.96	0.48
1:E:373:SER:CB	1:E:395:ILE:HD11	2.43	0.48
1:D:150:ARG:HG3	4:D:508:EDO:O1	2.14	0.48
1:F:369:ASP:CG	1:F:372:ALA:HB3	2.38	0.48
1:H:21:ALA:HA	1:H:231:ASP:CB	2.44	0.48
1:B:193:ASP:CG	1:B:229:LEU:HD22	2.38	0.48
1:B:234:GLU:HG3	1:B:238:PHE:CE2	2.49	0.48
1:D:22:LYS:HD3	1:D:371:ARG:NH1	2.28	0.48
1:F:45:PRO:HA	1:F:400:GLU:OE1	2.14	0.48
1:G:114:GLY:HA2	1:G:119:ALA:O	2.13	0.48
1:H:348:GLU:OE2	1:H:348:GLU:HA	2.13	0.48
1:A:83:PRO:HD2	1:A:86:LEU:HD12	1.96	0.48
1:B:117:ILE:HD11	1:B:120:ARG:NH1	2.28	0.48
1:F:331:ARG:H	3:F:503:ACT:CH3	2.22	0.48
1:G:160:LYS:HE3	5:G:655:HOH:O	2.13	0.48
1:C:91:ARG:HG3	5:C:646:HOH:O	2.13	0.48
1:F:330:ASN:CB	1:G:330:ASN:HB2	2.44	0.48
1:A:237:THR:OG1	1:A:306:MET:HE1	2.14	0.48
1:G:56:LEU:HD23	1:G:56:LEU:C	2.39	0.48
1:C:46:LYS:N	1:C:400:GLU:OE1	2.30	0.48
1:D:417:LYS:O	1:D:419:GLU:N	2.41	0.48
1:E:396:ASP:CG	1:E:415:ARG:HH22	2.22	0.48
1:B:220:ARG:HG3	1:B:220:ARG:HH11	1.79	0.47
1:B:234:GLU:OE2	1:B:238:PHE:HE2	1.97	0.47
1:B:407:ARG:HG3	1:B:411:ALA:O	2.13	0.47
1:C:309:GLN:OE1	1:C:309:GLN:N	2.44	0.47
1:C:373:SER:O	1:C:377:VAL:HG23	2.13	0.47
1:E:1:MET:C	1:E:418:GLY:HA2	2.39	0.47
1:E:308:ALA:HA	1:E:334:HIS:NE2	2.29	0.47
1:B:60:LEU:HD22	1:B:79:ASN:O	2.15	0.47
1:C:88:LYS:HB3	1:C:88:LYS:HE3	1.40	0.47
1:C:108:GLN:CG	1:C:144:LYS:HG2	2.43	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:233:ILE:HG23	1:C:306:MET:CE	2.39	0.47
1:D:115:ASP:OD2	1:D:116:ALA:N	2.48	0.47
1:F:320:THR:HG21	1:H:320:THR:HG21	1.96	0.47
1:B:30:PHE:CE1	1:B:96:ALA:HB2	2.49	0.47
1:B:276:GLY:HA3	1:B:279:TRP:NE1	2.29	0.47
1:C:37:GLU:HB3	1:C:38:PRO:CD	2.44	0.47
1:D:37:GLU:OE2	1:D:220:ARG:NH2	2.47	0.47
1:B:273:ILE:O	1:B:274:GLU:HG2	2.15	0.47
1:E:64:VAL:HG13	1:E:72:ILE:CD1	2.45	0.47
1:D:37:GLU:O	1:D:39:VAL:HG23	2.14	0.47
1:E:1:MET:H3	1:E:418:GLY:HA2	1.75	0.47
1:H:369:ASP:CB	1:H:372:ALA:HB3	2.43	0.47
1:C:276:GLY:HA3	1:C:279:TRP:CE2	2.48	0.47
1:C:282:LEU:C	1:C:282:LEU:HD23	2.40	0.47
1:E:6:VAL:HG22	1:E:413:ILE:HG13	1.96	0.47
1:A:282:LEU:HD23	1:A:283:ASP:N	2.30	0.47
1:B:13:GLN:HA	1:B:248:LYS:O	2.15	0.47
1:B:282:LEU:HD21	1:B:284:MET:HG2	1.95	0.47
1:B:299:HIS:ND1	1:B:300:PRO:HA	2.30	0.47
1:B:313:LEU:HD23	1:B:313:LEU:C	2.40	0.47
1:D:6:VAL:HG22	1:D:413:ILE:HG13	1.96	0.47
1:D:91:ARG:NH2	1:D:120:ARG:HB3	2.30	0.47
1:D:97:LEU:HB2	1:D:109:VAL:HG21	1.97	0.47
1:E:1:MET:H2	1:E:418:GLY:HA2	1.80	0.47
1:E:10:THR:HG21	1:E:410:GLY:O	2.15	0.47
1:E:42:GLN:HA	1:E:69:SER:CB	2.45	0.47
1:E:96:ALA:O	1:E:99:PRO:HD2	2.14	0.47
1:E:111:LEU:HD13	1:E:143:VAL:HG21	1.97	0.47
1:E:128:GLY:HA3	1:E:169:ILE:CD1	2.45	0.47
1:F:64:VAL:C	1:F:65:GLU:HG3	2.40	0.47
1:G:108:GLN:HG3	5:G:635:HOH:O	2.15	0.47
1:G:333:MET:O	1:G:336:PRO:HD2	2.15	0.47
1:H:248:LYS:NZ	1:H:248:LYS:CB	2.78	0.47
1:H:255:GLN:HG2	1:H:257:ASP:OD1	2.14	0.47
1:A:20:GLY:HA3	1:A:43:ASN:O	2.15	0.47
1:H:81:SER:CB	1:H:108:GLN:HB2	2.44	0.47
1:A:323:ILE:HB	1:A:352:VAL:HG13	1.97	0.47
1:C:299:HIS:ND1	1:C:300:PRO:HA	2.30	0.47
1:D:22:LYS:HB2	1:D:47:LEU:CD1	2.44	0.47
1:H:29:LEU:HD23	1:H:41:ILE:CD1	2.45	0.47
1:B:124:LEU:HD11	1:B:160:LYS:HG2	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:169:ILE:HG22	1:D:182:ILE:HD11	1.97	0.47
1:E:103:ARG:HB2	1:E:175:LEU:CD1	2.44	0.47
1:F:85:ASP:O	1:F:89:THR:HG23	2.15	0.47
1:F:248:LYS:HA	1:F:282:LEU:O	2.15	0.47
1:B:236:GLY:O	1:B:240:VAL:HG23	2.15	0.46
1:D:325:GLU:CG	1:D:329:GLU:H	2.28	0.46
1:G:74:ALA:HB3	5:G:637:HOH:O	2.15	0.46
1:H:91:ARG:C	1:H:93:SER:N	2.73	0.46
1:H:233:ILE:HD12	1:H:305:ASP:HB2	1.95	0.46
1:H:251:CYS:O	1:H:279:TRP:HA	2.15	0.46
1:H:370:LEU:HD11	1:H:397:ARG:CD	2.43	0.46
1:B:273:ILE:HG22	1:B:274:GLU:N	2.30	0.46
1:C:3:LYS:CD	1:C:390:ASP:OD1	2.62	0.46
1:C:277:GLU:HG3	3:C:502:ACT:O	2.15	0.46
1:D:325:GLU:HG3	1:D:329:GLU:H	1.80	0.46
1:F:233:ILE:HG21	1:F:371:ARG:CD	2.46	0.46
1:G:369:ASP:CB	1:G:372:ALA:HB3	2.45	0.46
1:H:91:ARG:C	1:H:93:SER:H	2.23	0.46
1:A:315:LEU:HD23	1:A:354:CYS:HB3	1.96	0.46
1:C:323:ILE:HB	1:C:352:VAL:HG12	1.97	0.46
1:F:249:ILE:HG12	1:F:250:VAL:N	2.30	0.46
1:H:2:ASP:C	1:H:392:ILE:HG12	2.41	0.46
1:B:369:ASP:C	1:B:371:ARG:H	2.23	0.46
1:D:243:ALA:HA	1:D:284:MET:HG2	1.96	0.46
1:F:157:VAL:O	4:F:509:EDO:H22	2.15	0.46
1:G:63:LYS:HB3	1:G:73:ASP:HB3	1.97	0.46
1:B:41:ILE:O	1:B:69:SER:HB2	2.16	0.46
1:C:266:LEU:O	1:C:269:ALA:HB3	2.16	0.46
1:D:60:LEU:O	1:D:77:VAL:HG13	2.16	0.46
1:D:116:ALA:O	1:D:330:ASN:ND2	2.38	0.46
1:F:41:ILE:HG23	1:F:228:VAL:HG23	1.97	0.46
1:F:282:LEU:C	1:F:282:LEU:HD23	2.40	0.46
1:F:288:ARG:NH2	1:F:317:ALA:O	2.48	0.46
1:H:84:TYR:CE1	4:H:507:EDO:H12	2.50	0.46
1:H:160:LYS:HA	5:H:653:HOH:O	2.16	0.46
1:A:369:ASP:C	1:A:371:ARG:N	2.74	0.46
1:D:21:ALA:HA	1:D:231:ASP:HB2	1.98	0.46
1:F:353:ILE:HD12	1:F:353:ILE:N	2.31	0.46
1:D:282:LEU:HD23	1:D:282:LEU:C	2.40	0.46
1:E:88:LYS:O	1:E:88:LYS:HG2	2.15	0.46
1:H:66:ARG:HB3	1:H:70:VAL:HG22	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:264:ALA:O	1:H:268:GLU:HG3	2.16	0.46
1:C:367:ALA:CB	1:C:373:SER:HB3	2.40	0.46
1:E:36:GLU:OE1	1:E:220:ARG:NE	2.49	0.46
1:G:331:ARG:NH2	1:G:371:ARG:HB2	2.30	0.46
1:A:147:VAL:HG13	1:A:147:VAL:O	2.16	0.46
1:B:213:ILE:HG22	1:B:215:ILE:CD1	2.45	0.46
1:G:315:LEU:HD23	1:G:354:CYS:HB3	1.98	0.46
1:H:320:THR:HA	1:H:354:CYS:O	2.16	0.46
1:B:14:GLY:O	1:B:249:ILE:HA	2.16	0.45
1:C:20:GLY:HA3	1:C:43:ASN:O	2.16	0.45
1:C:47:LEU:HB3	1:C:397:ARG:O	2.16	0.45
1:D:39:VAL:HG12	1:D:41:ILE:HD12	1.98	0.45
1:D:213:ILE:HG22	1:D:215:ILE:HD11	1.97	0.45
1:F:299:HIS:CG	1:F:300:PRO:HA	2.51	0.45
1:H:248:LYS:HB3	1:H:248:LYS:HZ3	1.80	0.45
1:D:51:ASP:HA	1:D:54:MET:CE	2.46	0.45
1:B:20:GLY:HA3	1:B:43:ASN:O	2.16	0.45
1:D:12:LEU:O	1:D:247:GLY:HA3	2.16	0.45
1:D:42:GLN:HA	1:D:69:SER:CB	2.46	0.45
1:F:416:VAL:CG1	1:F:417:LYS:N	2.79	0.45
1:H:126:ILE:O	1:H:130:GLU:HG3	2.16	0.45
1:A:4:PHE:HE2	1:A:395:ILE:HD13	1.80	0.45
1:B:85:ASP:HA	1:B:88:LYS:HE2	1.97	0.45
1:E:26:LEU:N	1:E:27:PRO:HD2	2.32	0.45
1:E:330:ASN:HB2	1:H:330:ASN:CG	2.42	0.45
1:F:34:LEU:HD21	1:F:99:PRO:HA	1.97	0.45
1:F:124:LEU:HD11	1:F:160:LYS:HG2	1.97	0.45
1:G:28:ILE:HD12	1:G:228:VAL:HG22	1.99	0.45
1:B:335:VAL:HB	1:B:336:PRO:CD	2.47	0.45
1:H:20:GLY:HA3	1:H:43:ASN:O	2.16	0.45
1:H:367:ALA:HB1	1:H:373:SER:HB2	1.97	0.45
1:B:376:LEU:O	1:B:379:ALA:HB3	2.17	0.45
1:D:59:GLN:OE1	1:D:79:ASN:ND2	2.49	0.45
1:E:51:ASP:HA	1:E:54:MET:HE2	1.98	0.45
1:F:40:GLU:CD	1:F:71:TRP:HE1	2.25	0.45
1:F:108:GLN:HG2	1:F:144:LYS:CG	2.34	0.45
1:H:249:ILE:HG12	1:H:250:VAL:N	2.31	0.45
1:G:115:ASP:OD2	1:G:117:ILE:HG12	2.17	0.45
1:G:299:HIS:CG	1:G:300:PRO:HA	2.51	0.45
1:A:105:GLY:HA2	1:A:147:VAL:CG1	2.47	0.45
1:B:111:LEU:HD12	1:B:112:PRO:HD2	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:VAL:O	1:B:316:VAL:HG23	2.17	0.45
1:C:22:LYS:HD2	1:C:398:GLY:HA2	1.97	0.45
1:F:309:GLN:OE1	1:F:309:GLN:N	2.39	0.45
1:E:5:ARG:NH1	5:E:641:HOH:O	2.40	0.45
1:G:11:ARG:HD3	1:G:13:GLN:OE1	2.17	0.45
1:G:197:PHE:CZ	1:G:201:LEU:HD11	2.52	0.45
1:G:401:ARG:HA	5:G:642:HOH:O	2.17	0.45
1:C:21:ALA:HA	1:C:231:ASP:HB2	1.98	0.44
1:D:31:ALA:HB1	1:D:198:LEU:HD21	1.98	0.44
1:F:299:HIS:ND1	1:F:300:PRO:HA	2.32	0.44
1:H:59:GLN:NE2	1:H:86:LEU:HD11	2.32	0.44
1:A:233:ILE:HG23	1:A:306:MET:CE	2.44	0.44
1:B:32:ALA:C	1:B:34:LEU:N	2.75	0.44
1:C:220:ARG:HG3	1:C:220:ARG:NH1	2.33	0.44
1:C:395:ILE:HG23	1:C:396:ASP:N	2.32	0.44
1:E:187:ARG:HD2	1:F:211:ASP:OD2	2.17	0.44
1:E:265:LYS:HE3	1:E:293:THR:O	2.17	0.44
1:E:374:ALA:HB2	1:E:399:TYR:CE1	2.52	0.44
1:F:12:LEU:CD1	1:F:241:ALA:HB1	2.46	0.44
1:G:276:GLY:HA3	1:G:279:TRP:CE2	2.53	0.44
1:B:115:ASP:HB3	1:B:120:ARG:HD3	2.00	0.44
1:F:64:VAL:HG13	1:F:72:ILE:HD13	2.00	0.44
1:G:34:LEU:HD21	1:G:99:PRO:HA	2.00	0.44
1:G:395:ILE:C	1:G:397:ARG:H	2.25	0.44
1:H:314:ASN:HD22	1:H:323:ILE:HD11	1.82	0.44
1:A:181:ILE:HG23	1:A:212:ARG:HG3	1.99	0.44
1:G:131:LYS:HE3	1:G:156:ILE:HG12	2.00	0.44
1:G:331:ARG:HG2	1:G:331:ARG:O	2.18	0.44
1:B:5:ARG:HE	1:B:416:VAL:HG21	1.81	0.44
1:B:87:VAL:HG11	1:B:110:SER:O	2.17	0.44
1:B:127:PHE:CZ	1:B:131:LYS:HE3	2.53	0.44
1:B:218:VAL:HG21	1:B:221:LEU:HD21	2.00	0.44
1:D:320:THR:HA	1:D:354:CYS:O	2.16	0.44
1:E:37:GLU:HB3	1:E:38:PRO:CD	2.48	0.44
1:E:50:ILE:O	1:E:54:MET:HG3	2.17	0.44
1:H:167:VAL:HG12	4:H:508:EDO:H22	1.98	0.44
1:A:366:MET:CE	1:D:88:LYS:HD2	2.48	0.44
1:B:81:SER:CB	1:B:108:GLN:HG3	2.30	0.44
1:D:124:LEU:HD11	1:D:160:LYS:CG	2.48	0.44
1:E:391:ARG:C	1:E:393:TYR:H	2.25	0.44
1:H:367:ALA:CB	1:H:373:SER:HB2	2.48	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:392:ILE:HD12	1:H:415:ARG:NH1	2.33	0.44
1:H:13:GLN:HA	1:H:248:LYS:O	2.18	0.44
1:E:109:VAL:HG12	1:E:110:SER:O	2.17	0.44
1:H:11:ARG:HD3	1:H:247:GLY:HA2	2.00	0.44
1:C:374:ALA:O	1:C:378:LEU:HG	2.18	0.44
1:E:233:ILE:HG21	1:E:371:ARG:HD3	2.00	0.44
1:E:12:LEU:HD12	1:E:241:ALA:HB1	2.00	0.43
1:G:193:ASP:CB	1:G:229:LEU:HD22	2.48	0.43
1:H:101:VAL:HG11	1:H:145:ALA:HB3	2.00	0.43
1:A:374:ALA:HB2	1:A:399:TYR:CE1	2.53	0.43
1:B:308:ALA:HA	1:B:334:HIS:NE2	2.32	0.43
1:F:39:VAL:HG12	1:F:40:GLU:N	2.32	0.43
1:F:107:GLY:C	1:F:108:GLN:HG3	2.43	0.43
1:G:64:VAL:HG22	1:G:72:ILE:CD1	2.49	0.43
1:H:67:IAS:CG	1:H:69:SER:N	2.81	0.43
1:B:24:ALA:HB3	1:B:228:VAL:HG13	1.99	0.43
1:D:3:LYS:HE2	1:D:390:ASP:OD1	2.18	0.43
1:A:323:ILE:HB	1:A:352:VAL:HG12	1.98	0.43
1:A:395:ILE:CG2	1:A:396:ASP:N	2.81	0.43
1:B:108:GLN:HB3	1:B:144:LYS:HG2	1.99	0.43
1:D:41:ILE:HG22	1:D:44:VAL:HG23	1.99	0.43
1:D:340:ARG:HG2	1:D:340:ARG:HH11	1.83	0.43
1:F:320:THR:HA	1:F:354:CYS:O	2.19	0.43
1:A:244:ILE:HD12	1:A:382:ILE:HD13	2.01	0.43
1:B:16:VAL:CG1	1:B:249:ILE:HD11	2.48	0.43
1:E:282:LEU:C	1:E:282:LEU:CD2	2.91	0.43
1:A:306:MET:HE2	1:A:309:GLN:HE22	1.81	0.43
1:B:220:ARG:HG3	1:B:220:ARG:NH1	2.33	0.43
1:D:87:VAL:HG11	1:D:110:SER:O	2.18	0.43
1:D:335:VAL:HB	1:D:336:PRO:CD	2.48	0.43
1:H:289:PRO:HD3	5:H:601:HOH:O	2.18	0.43
1:A:22:LYS:HD3	1:A:398:GLY:HA2	2.01	0.43
1:A:35:ALA:HB1	1:A:222:GLY:O	2.19	0.43
1:B:416:VAL:HG12	1:B:417:LYS:N	2.33	0.43
1:E:256:PRO:HG3	1:E:280:ILE:HG13	2.00	0.43
1:G:282:LEU:C	1:G:282:LEU:HD23	2.44	0.43
1:A:265:LYS:HD3	1:A:265:LYS:HA	1.78	0.43
1:D:151:LEU:O	1:D:176:ALA:HB1	2.19	0.43
1:D:189:PRO:HD3	1:D:299:HIS:CD2	2.54	0.43
1:D:317:ALA:O	1:D:356:GLY:HA3	2.18	0.43
1:G:371:ARG:HA	1:G:371:ARG:HD3	1.75	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:VAL:HG11	1:A:298:PRO:HB3	2.00	0.42
1:A:308:ALA:HA	1:A:334:HIS:NE2	2.34	0.42
1:B:32:ALA:O	1:B:34:LEU:N	2.52	0.42
1:C:64:VAL:HG13	1:C:72:ILE:CD1	2.49	0.42
1:C:115:ASP:CG	1:C:116:ALA:N	2.76	0.42
1:C:335:VAL:HB	1:C:336:PRO:CD	2.49	0.42
1:C:416:VAL:C	1:C:418:GLY:H	2.25	0.42
1:D:238:PHE:O	1:D:241:ALA:HB3	2.19	0.42
1:A:4:PHE:HE1	1:A:415:ARG:HB2	1.83	0.42
1:A:182:ILE:O	1:A:212:ARG:HA	2.19	0.42
1:B:302:PHE:CD1	1:B:302:PHE:C	2.97	0.42
1:B:315:LEU:O	1:B:357:VAL:HG22	2.18	0.42
1:D:2:ASP:HB3	1:D:392:ILE:HD11	2.01	0.42
1:E:63:LYS:O	1:E:72:ILE:HA	2.19	0.42
1:G:118:GLY:HA2	1:G:329:GLU:OE1	2.14	0.42
1:B:323:ILE:HB	1:B:352:VAL:HG13	2.01	0.42
1:C:254:ALA:O	1:C:278:ASP:HA	2.20	0.42
1:D:94:ILE:CD1	1:D:122:VAL:HG11	2.49	0.42
1:E:29:LEU:O	1:E:32:ALA:HB3	2.20	0.42
1:E:85:ASP:O	1:E:89:THR:HG23	2.19	0.42
1:E:259:LEU:HD12	1:E:263:LEU:HG	2.01	0.42
1:F:33:LEU:CD2	1:F:57:LEU:HD22	2.46	0.42
1:A:117:ILE:HG21	1:A:369:ASP:OD2	2.19	0.42
1:A:230:PRO:HG2	1:A:255:GLN:HB2	2.01	0.42
1:C:30:PHE:CZ	1:C:53:THR:HG23	2.54	0.42
1:D:308:ALA:HA	1:D:334:HIS:NE2	2.34	0.42
1:E:265:LYS:HA	1:E:265:LYS:HD3	1.84	0.42
1:E:323:ILE:O	1:E:351:THR:HA	2.20	0.42
1:H:235:THR:O	1:H:239:LEU:HG	2.19	0.42
1:A:306:MET:HE1	1:A:309:GLN:NE2	2.34	0.42
1:B:315:LEU:HD21	1:B:345:ALA:HB2	2.01	0.42
1:E:232:ARG:HB2	1:E:259:LEU:HD23	2.01	0.42
1:H:402:ILE:HG23	1:H:403:GLU:N	2.35	0.42
1:C:11:ARG:HD3	1:C:13:GLN:OE1	2.20	0.42
1:C:313:LEU:C	1:C:313:LEU:HD23	2.45	0.42
1:C:370:LEU:HD11	1:C:399:TYR:CE1	2.54	0.42
1:F:20:GLY:HA3	1:F:43:ASN:O	2.19	0.42
1:F:414:GLU:HG2	1:F:416:VAL:HG23	2.02	0.42
1:H:42:GLN:HA	1:H:69:SER:CB	2.41	0.42
1:A:21:ALA:HA	1:A:231:ASP:CB	2.49	0.42
1:C:136:ILE:HA	1:C:144:LYS:O	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:34:LEU:HD21	1:D:99:PRO:HA	2.00	0.42
1:B:77:VAL:HB	1:B:104:PHE:CZ	2.55	0.42
1:B:264:ALA:O	1:B:268:GLU:HG3	2.19	0.42
1:C:5:ARG:NH1	1:C:386:THR:HG21	2.35	0.42
1:E:139:GLU:C	1:E:141:GLY:H	2.27	0.42
1:F:114:GLY:C	1:G:333:MET:HE1	2.44	0.42
1:C:24:ALA:CB	1:C:228:VAL:HG13	2.48	0.42
1:C:28:ILE:HG23	1:C:197:PHE:CD2	2.54	0.42
1:C:244:ILE:HD12	1:C:382:ILE:HD13	2.01	0.42
1:D:213:ILE:HG22	1:D:215:ILE:CD1	2.50	0.42
1:E:111:LEU:HA	1:E:112:PRO:HD3	1.90	0.42
1:E:132:LEU:HD23	1:E:132:LEU:HA	1.87	0.42
1:E:317:ALA:O	1:E:356:GLY:HA3	2.20	0.42
1:G:182:ILE:HG22	1:G:185:ALA:HB2	2.00	0.42
1:H:2:ASP:HB3	1:H:392:ILE:CD1	2.38	0.42
1:H:370:LEU:HD12	1:H:397:ARG:CD	2.35	0.42
1:A:189:PRO:HD3	1:A:299:HIS:CD2	2.55	0.42
1:B:4:PHE:CE2	1:B:413:ILE:HD11	2.55	0.42
1:B:83:PRO:CG	1:B:86:LEU:HD12	2.50	0.42
1:D:294:VAL:HB	1:D:323:ILE:HD13	2.00	0.42
1:D:382:ILE:HD12	4:D:507:EDO:H22	2.01	0.42
1:H:55:LYS:HA	4:H:510:EDO:H22	2.02	0.42
1:B:197:PHE:O	1:B:201:LEU:HG	2.20	0.41
1:C:64:VAL:O	1:C:65:GLU:HG3	2.20	0.41
1:C:392:ILE:HB	1:C:395:ILE:HG21	2.01	0.41
1:E:115:ASP:CG	1:E:116:ALA:N	2.78	0.41
2:A:501:UD1:H5'2	4:A:507:EDO:O2	2.20	0.41
1:E:81:SER:HB3	1:E:108:GLN:HB2	2.02	0.41
1:E:103:ARG:HG2	1:E:104:PHE:CE1	2.54	0.41
1:H:66:ARG:CB	1:H:70:VAL:HG22	2.50	0.41
1:H:256:PRO:HG3	1:H:280:ILE:CG1	2.50	0.41
1:A:31:ALA:C	1:A:33:LEU:N	2.78	0.41
1:B:30:PHE:HE1	1:B:96:ALA:HB2	1.85	0.41
1:B:189:PRO:HD3	1:B:299:HIS:CD2	2.55	0.41
1:B:273:ILE:CG2	1:B:274:GLU:N	2.84	0.41
1:G:245:SER:HB3	1:G:382:ILE:HG22	2.01	0.41
1:H:56:LEU:HB2	1:H:86:LEU:HD13	2.02	0.41
1:H:117:ILE:HG22	1:H:331:ARG:HG3	2.01	0.41
1:A:81:SER:HA	1:A:108:GLN:O	2.20	0.41
1:A:298:PRO:HA	4:A:507:EDO:H11	2.03	0.41
1:B:391:ARG:C	1:B:393:TYR:H	2.28	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:203:ALA:HB2	1:E:221:LEU:HD21	2.03	0.41
1:C:37:GLU:HB3	1:C:38:PRO:HD2	2.02	0.41
1:E:195:ALA:HB3	1:E:208:GLN:HG3	2.02	0.41
1:G:22:LYS:HD3	1:G:371:ARG:NH2	2.35	0.41
1:G:50:ILE:O	1:G:54:MET:HG3	2.20	0.41
1:H:236:GLY:O	1:H:240:VAL:HG23	2.20	0.41
1:A:88:LYS:O	1:A:88:LYS:HG2	2.21	0.41
1:B:415:ARG:O	1:B:415:ARG:HG2	2.19	0.41
1:F:199:VAL:O	1:F:202:GLY:N	2.49	0.41
1:H:29:LEU:HD23	1:H:41:ILE:HD13	2.03	0.41
1:A:208:GLN:HA	1:A:213:ILE:HG12	2.03	0.41
1:B:54:MET:HG2	1:B:64:VAL:HG11	2.02	0.41
1:C:161:VAL:O	3:C:503:ACT:H2	2.21	0.41
1:D:252:ARG:O	1:D:253:ASN:HB2	2.21	0.41
1:E:59:GLN:C	1:E:61:GLY:N	2.78	0.41
1:E:96:ALA:C	1:E:99:PRO:HD2	2.45	0.41
1:E:158:MET:HE1	1:E:165:ALA:HB1	2.01	0.41
1:F:204:LYS:HG3	1:F:218:VAL:HG11	2.02	0.41
1:F:333:MET:HE2	1:F:368:THR:OG1	2.21	0.41
1:G:158:MET:HE1	1:G:165:ALA:HB1	2.03	0.41
1:A:60:LEU:HA	1:A:79:ASN:HB3	2.03	0.41
1:B:66:ARG:HD2	1:B:70:VAL:HG22	2.03	0.41
1:C:196:ASN:HB2	1:C:226:TYR:OH	2.20	0.41
1:D:12:LEU:CD1	1:D:241:ALA:HB1	2.51	0.41
1:D:65:GLU:HG3	1:D:71:TRP:HB2	2.02	0.41
1:H:370:LEU:HD12	1:H:397:ARG:HB2	2.03	0.41
1:A:256:PRO:HG3	1:A:280:ILE:HG12	2.02	0.41
1:B:373:SER:HB3	1:B:395:ILE:CG1	2.51	0.41
1:C:39:VAL:HG12	1:C:41:ILE:CD1	2.50	0.41
1:C:314:ASN:HB3	1:C:354:CYS:HB2	2.03	0.41
1:E:13:GLN:O	1:E:409:LEU:HA	2.21	0.41
1:E:42:GLN:HA	1:E:69:SER:HB2	2.02	0.41
1:F:371:ARG:NH2	1:F:398:GLY:O	2.54	0.41
1:G:131:LYS:HE3	1:G:131:LYS:HB3	1.94	0.41
1:H:369:ASP:CG	1:H:372:ALA:HB3	2.46	0.41
1:B:16:VAL:HG11	1:B:249:ILE:HD11	2.03	0.41
1:C:67:IAS:CG	1:C:69:SER:N	2.84	0.41
1:D:283:ASP:OD2	1:D:285:HIS:CE1	2.74	0.41
1:F:31:ALA:C	1:F:33:LEU:N	2.79	0.41
1:F:263:LEU:HD22	1:F:273:ILE:HD13	2.02	0.41
1:G:340:ARG:CG	1:G:340:ARG:NH1	2.83	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:370:LEU:CD1	1:H:397:ARG:CZ	2.99	0.41
1:B:57:LEU:HD23	1:B:57:LEU:HA	1.92	0.40
1:C:2:ASP:HB3	1:C:392:ILE:HD11	2.03	0.40
1:C:4:PHE:CD1	1:C:392:ILE:HD13	2.56	0.40
1:D:91:ARG:NH2	1:D:120:ARG:CB	2.84	0.40
1:E:57:LEU:O	1:E:62:THR:CB	2.69	0.40
1:H:56:LEU:HD23	1:H:56:LEU:O	2.20	0.40
1:H:117:ILE:HD12	1:H:328:PHE:CD2	2.56	0.40
1:A:196:ASN:OD1	1:A:208:GLN:NE2	2.55	0.40
1:E:33:LEU:HD13	1:E:100:LEU:HD21	2.03	0.40
1:F:315:LEU:HD22	1:F:343:ALA:HB1	2.01	0.40
1:H:63:LYS:HG2	3:H:504:ACT:H3	2.03	0.40
1:A:314:ASN:ND2	1:A:323:ILE:HD11	2.36	0.40
1:B:190:GLU:OE1	1:B:190:GLU:N	2.50	0.40
1:C:367:ALA:HB1	1:C:373:SER:CB	2.44	0.40
1:A:4:PHE:HD1	1:A:4:PHE:HA	1.79	0.40
1:A:91:ARG:C	1:A:93:SER:N	2.78	0.40
1:B:32:ALA:C	1:B:34:LEU:H	2.29	0.40
1:B:395:ILE:HG21	1:B:402:ILE:CG2	2.52	0.40
1:B:401:ARG:HB3	1:B:404:ASP:OD2	2.21	0.40
1:D:24:ALA:HB3	1:D:228:VAL:HG13	2.03	0.40
1:F:1:MET:CE	1:F:391:ARG:HG2	2.50	0.40
1:H:373:SER:C	1:H:375:SER:N	2.78	0.40
1:B:115:ASP:CG	1:B:116:ALA:N	2.80	0.40
1:C:4:PHE:CG	1:C:392:ILE:HG21	2.56	0.40
1:F:23:ASN:C	1:F:190:GLU:HG2	2.47	0.40
1:F:155:HIS:ND1	1:F:155:HIS:C	2.80	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:419:GLU:O	1:H:139:GLU:OE2[2_456]	1.89	0.31

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	415/419 (99%)	398 (96%)	14 (3%)	3 (1%)	18	34
1	B	415/419 (99%)	386 (93%)	26 (6%)	3 (1%)	18	34
1	C	415/419 (99%)	404 (97%)	9 (2%)	2 (0%)	24	43
1	D	415/419 (99%)	398 (96%)	14 (3%)	3 (1%)	18	34
1	E	415/419 (99%)	389 (94%)	21 (5%)	5 (1%)	10	20
1	F	415/419 (99%)	399 (96%)	16 (4%)	0	100	100
1	G	415/419 (99%)	400 (96%)	15 (4%)	0	100	100
1	H	415/419 (99%)	397 (96%)	18 (4%)	0	100	100
All	All	3320/3352 (99%)	3171 (96%)	133 (4%)	16 (0%)	24	43

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	119	ALA
1	E	60	LEU
1	E	77	VAL
1	B	33	LEU
1	A	417	LYS
1	B	92	ALA
1	B	370	LEU
1	C	92	ALA
1	D	118	GLY
1	E	140	GLU
1	A	148	ASN
1	A	370	LEU
1	D	418	GLY
1	E	222	GLY
1	C	77	VAL
1	E	392	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	329/329 (100%)	325 (99%)	4 (1%)	63	83
1	B	329/329 (100%)	326 (99%)	3 (1%)	70	87
1	C	329/329 (100%)	324 (98%)	5 (2%)	57	80
1	D	329/329 (100%)	326 (99%)	3 (1%)	70	87
1	E	329/329 (100%)	322 (98%)	7 (2%)	47	74
1	F	329/329 (100%)	323 (98%)	6 (2%)	51	77
1	G	329/329 (100%)	325 (99%)	4 (1%)	63	83
1	H	329/329 (100%)	321 (98%)	8 (2%)	43	70
All	All	2632/2632 (100%)	2592 (98%)	40 (2%)	57	80

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	VAL
1	A	193	ASP
1	A	228	VAL
1	A	229	LEU
1	B	278	ASP
1	B	352	VAL
1	B	371	ARG
1	C	3	LYS
1	C	10	THR
1	C	88	LYS
1	C	259	LEU
1	C	371	ARG
1	D	59	GLN
1	D	352	VAL
1	D	395	ILE
1	E	22	LYS
1	E	47	LEU
1	E	187	ARG
1	E	259	LEU
1	E	352	VAL
1	E	391	ARG
1	E	395	ILE
1	F	10	THR
1	F	17	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	125	HIS
1	F	135	GLU
1	F	229	LEU
1	F	371	ARG
1	G	10	THR
1	G	39	VAL
1	G	228	VAL
1	G	329	GLU
1	H	19	SER
1	H	106	GLN
1	H	135	GLU
1	H	248	LYS
1	H	277	GLU
1	H	371	ARG
1	H	417	LYS
1	H	419	GLU

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

Mol	Chain	Res	Type
1	A	59	GLN
1	A	76	ASN
1	A	299	HIS
1	B	78	ASN
1	B	299	HIS
1	B	307	GLN
1	C	23	ASN
1	C	108	GLN
1	D	13	GLN
1	D	42	GLN
1	D	76	ASN
1	D	79	ASN
1	D	285	HIS
1	E	59	GLN
1	E	78	ASN
1	E	255	GLN
1	E	299	HIS
1	E	394	HIS
1	F	7	GLN
1	F	59	GLN
1	G	7	GLN
1	G	42	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	307	GLN
1	H	13	GLN
1	H	255	GLN
1	H	355	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	IAS	A	67	1	6,7,8	1.01	0	3,8,10	0.98	0
1	IAS	D	67	1	6,7,8	1.01	0	3,8,10	0.87	0
1	IAS	C	67	1	6,7,8	0.94	0	3,8,10	1.03	0
1	IAS	B	67	1	6,7,8	0.92	0	3,8,10	1.00	0
1	IAS	E	67	1	6,7,8	0.97	0	3,8,10	1.01	0
1	IAS	H	67	1	6,7,8	1.02	0	3,8,10	0.95	0
1	IAS	F	67	1	6,7,8	0.98	0	3,8,10	1.14	0
1	IAS	G	67	1	6,7,8	1.03	0	3,8,10	1.02	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
1	IAS	A	67	1	-	0/7/7/8	-
1	IAS	D	67	1	-	3/7/7/8	-
1	IAS	C	67	1	-	2/7/7/8	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	IAS	B	67	1	-	2/7/7/8	-
1	IAS	E	67	1	-	2/7/7/8	-
1	IAS	H	67	1	-	1/7/7/8	-
1	IAS	F	67	1	-	2/7/7/8	-
1	IAS	G	67	1	-	0/7/7/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	67	IAS	O-C-CA-N
1	D	67	IAS	OXT-C-CA-N
1	B	67	IAS	O-C-CA-CB
1	C	67	IAS	O-C-CA-CB
1	D	67	IAS	C-CA-CB-CG
1	B	67	IAS	OXT-C-CA-CB
1	C	67	IAS	OXT-C-CA-CB
1	F	67	IAS	OXT-C-CA-CB
1	E	67	IAS	OXT-C-CA-CB
1	H	67	IAS	OXT-C-CA-CB
1	F	67	IAS	O-C-CA-CB
1	E	67	IAS	O-C-CA-CB

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	67	IAS	1	0
1	H	67	IAS	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

72 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	ACT	H	505	-	3,3,3	1.12	0	3,3,3	0.86	0
4	EDO	C	507	-	3,3,3	0.47	0	2,2,2	0.35	0
2	UD1	E	501	-	40,41,41	2.09	11 (27%)	59,62,62	1.44	9 (15%)
4	EDO	C	504	-	3,3,3	0.40	0	2,2,2	0.35	0
4	EDO	E	509	-	3,3,3	0.32	0	2,2,2	0.39	0
4	EDO	G	506	-	3,3,3	0.50	0	2,2,2	0.32	0
2	UD1	G	501	-	40,41,41	2.01	9 (22%)	59,62,62	1.45	9 (15%)
3	ACT	H	506	-	3,3,3	1.11	0	3,3,3	0.77	0
4	EDO	D	504	-	3,3,3	0.37	0	2,2,2	0.45	0
4	EDO	E	508	-	3,3,3	0.51	0	2,2,2	0.29	0
3	ACT	A	503	-	3,3,3	1.06	0	3,3,3	0.89	0
3	ACT	H	504	-	3,3,3	1.07	0	3,3,3	0.81	0
4	EDO	H	507	-	3,3,3	0.43	0	2,2,2	0.33	0
4	EDO	A	508	-	3,3,3	0.47	0	2,2,2	0.35	0
4	EDO	E	506	-	3,3,3	0.53	0	2,2,2	0.30	0
4	EDO	A	509	-	3,3,3	0.50	0	2,2,2	0.37	0
4	EDO	C	505	-	3,3,3	0.56	0	2,2,2	0.29	0
4	EDO	D	507	-	3,3,3	0.41	0	2,2,2	0.37	0
4	EDO	E	511	-	3,3,3	0.49	0	2,2,2	0.33	0
4	EDO	F	506	-	3,3,3	0.44	0	2,2,2	0.38	0
4	EDO	D	508	-	3,3,3	0.53	0	2,2,2	0.28	0
2	UD1	F	501	-	40,41,41	2.06	10 (25%)	59,62,62	1.40	9 (15%)
2	UD1	H	501	-	40,41,41	2.20	13 (32%)	59,62,62	1.39	8 (13%)
3	ACT	A	502	-	3,3,3	1.21	0	3,3,3	0.83	0
3	ACT	C	502	-	3,3,3	0.99	0	3,3,3	0.88	0
4	EDO	G	504	-	3,3,3	0.55	0	2,2,2	0.29	0
4	EDO	D	505	-	3,3,3	0.32	0	2,2,2	0.43	0
4	EDO	H	509	-	3,3,3	0.47	0	2,2,2	0.34	0
3	ACT	D	502	-	3,3,3	1.06	0	3,3,3	0.84	0
4	EDO	D	506	-	3,3,3	0.62	0	2,2,2	0.25	0
4	EDO	F	505	-	3,3,3	0.41	0	2,2,2	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	ACT	E	503	-	3,3,3	1.06	0	3,3,3	0.88	0
4	EDO	F	508	-	3,3,3	0.45	0	2,2,2	0.36	0
3	ACT	E	504	-	3,3,3	1.09	0	3,3,3	0.86	0
4	EDO	E	510	-	3,3,3	0.56	0	2,2,2	0.25	0
4	EDO	G	505	-	3,3,3	0.44	0	2,2,2	0.36	0
4	EDO	A	506	-	3,3,3	0.50	0	2,2,2	0.38	0
4	EDO	G	503	-	3,3,3	0.45	0	2,2,2	0.39	0
2	UD1	A	501	-	40,41,41	1.95	10 (25%)	59,62,62	1.41	7 (11%)
3	ACT	F	503	-	3,3,3	1.05	0	3,3,3	0.79	0
4	EDO	B	504	-	3,3,3	0.40	0	2,2,2	0.39	0
4	EDO	B	503	-	3,3,3	0.32	0	2,2,2	0.48	0
3	ACT	A	504	-	3,3,3	1.14	0	3,3,3	0.78	0
4	EDO	H	511	-	3,3,3	0.47	0	2,2,2	0.37	0
4	EDO	D	509	-	3,3,3	0.41	0	2,2,2	0.37	0
4	EDO	E	505	-	3,3,3	0.48	0	2,2,2	0.36	0
2	UD1	D	501	-	40,41,41	2.17	11 (27%)	59,62,62	1.47	8 (13%)
3	ACT	B	502	-	3,3,3	1.06	0	3,3,3	0.83	0
4	EDO	A	507	-	3,3,3	0.42	0	2,2,2	0.41	0
4	EDO	H	510	-	3,3,3	0.47	0	2,2,2	0.35	0
4	EDO	F	507	-	3,3,3	0.45	0	2,2,2	0.32	0
3	ACT	H	503	-	3,3,3	1.13	0	3,3,3	0.78	0
3	ACT	F	504	-	3,3,3	1.05	0	3,3,3	0.86	0
4	EDO	D	510	-	3,3,3	0.50	0	2,2,2	0.39	0
4	EDO	H	513	-	3,3,3	0.50	0	2,2,2	0.34	0
4	EDO	C	506	-	3,3,3	0.49	0	2,2,2	0.32	0
3	ACT	A	505	-	3,3,3	1.06	0	3,3,3	0.82	0
2	UD1	C	501	-	40,41,41	1.81	10 (25%)	59,62,62	1.38	8 (13%)
3	ACT	H	502	-	3,3,3	1.09	0	3,3,3	0.87	0
4	EDO	G	502	-	3,3,3	0.40	0	2,2,2	0.36	0
3	ACT	F	502	-	3,3,3	1.10	0	3,3,3	0.84	0
4	EDO	B	505	-	3,3,3	0.38	0	2,2,2	0.40	0
4	EDO	G	507	-	3,3,3	0.54	0	2,2,2	0.28	0
3	ACT	C	503	-	3,3,3	0.89	0	3,3,3	0.96	0
4	EDO	E	507	-	3,3,3	0.60	0	2,2,2	0.29	0
4	EDO	F	509	-	3,3,3	0.52	0	2,2,2	0.37	0
4	EDO	G	508	-	3,3,3	0.87	0	2,2,2	0.34	0
4	EDO	H	512	-	3,3,3	0.49	0	2,2,2	0.37	0
3	ACT	D	503	-	3,3,3	1.14	0	3,3,3	0.76	0
2	UD1	B	501	-	40,41,41	2.05	12 (30%)	59,62,62	1.40	9 (15%)
4	EDO	H	508	-	3,3,3	0.54	0	2,2,2	0.31	0
3	ACT	E	502	-	3,3,3	1.05	0	3,3,3	0.75	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
4	EDO	C	507	-	-	0/1/1/1	-
2	UD1	E	501	-	-	6/26/63/63	0/3/3/3
4	EDO	C	504	-	-	0/1/1/1	-
4	EDO	E	509	-	-	0/1/1/1	-
4	EDO	G	506	-	-	1/1/1/1	-
2	UD1	G	501	-	-	5/26/63/63	0/3/3/3
4	EDO	D	504	-	-	1/1/1/1	-
4	EDO	E	508	-	-	1/1/1/1	-
4	EDO	H	507	-	-	0/1/1/1	-
4	EDO	A	508	-	-	1/1/1/1	-
4	EDO	E	506	-	-	1/1/1/1	-
4	EDO	A	509	-	-	0/1/1/1	-
4	EDO	C	505	-	-	1/1/1/1	-
4	EDO	D	507	-	-	1/1/1/1	-
4	EDO	E	511	-	-	1/1/1/1	-
4	EDO	F	506	-	-	1/1/1/1	-
4	EDO	D	508	-	-	1/1/1/1	-
2	UD1	F	501	-	-	5/26/63/63	0/3/3/3
2	UD1	H	501	-	-	5/26/63/63	0/3/3/3
4	EDO	H	509	-	-	0/1/1/1	-
4	EDO	G	504	-	-	0/1/1/1	-
4	EDO	D	505	-	-	0/1/1/1	-
4	EDO	F	505	-	-	0/1/1/1	-
4	EDO	F	508	-	-	1/1/1/1	-
4	EDO	E	510	-	-	0/1/1/1	-
4	EDO	G	505	-	-	1/1/1/1	-
4	EDO	A	506	-	-	0/1/1/1	-
4	EDO	G	503	-	-	0/1/1/1	-
2	UD1	A	501	-	-	5/26/63/63	0/3/3/3
4	EDO	B	504	-	-	0/1/1/1	-
4	EDO	B	503	-	-	0/1/1/1	-
4	EDO	H	511	-	-	1/1/1/1	-
4	EDO	D	509	-	-	0/1/1/1	-
4	EDO	E	505	-	-	1/1/1/1	-
2	UD1	D	501	-	-	5/26/63/63	0/3/3/3
4	EDO	A	507	-	-	1/1/1/1	-
4	EDO	H	510	-	-	1/1/1/1	-
4	EDO	F	507	-	-	0/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	D	510	-	-	1/1/1/1	-
4	EDO	H	513	-	-	0/1/1/1	-
4	EDO	C	506	-	-	0/1/1/1	-
2	UD1	C	501	-	-	5/26/63/63	0/3/3/3
4	EDO	G	502	-	-	1/1/1/1	-
4	EDO	B	505	-	-	1/1/1/1	-
4	EDO	G	507	-	-	0/1/1/1	-
4	EDO	F	509	-	-	0/1/1/1	-
4	EDO	E	507	-	-	1/1/1/1	-
4	EDO	G	508	-	-	1/1/1/1	-
4	EDO	H	512	-	-	0/1/1/1	-
2	UD1	B	501	-	-	6/26/63/63	0/3/3/3
4	EDO	H	508	-	-	0/1/1/1	-
4	EDO	D	506	-	-	1/1/1/1	-

All (86) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	UD1	PA-O3A	-9.23	1.49	1.59
2	H	501	UD1	PA-O3A	-9.08	1.49	1.59
2	F	501	UD1	PA-O3A	-8.64	1.50	1.59
2	E	501	UD1	PA-O3A	-8.36	1.50	1.59
2	G	501	UD1	PA-O3A	-8.27	1.50	1.59
2	B	501	UD1	PA-O3A	-7.95	1.50	1.59
2	A	501	UD1	PA-O3A	-7.37	1.51	1.59
2	C	501	UD1	PA-O3A	-5.81	1.53	1.59
2	A	501	UD1	O5'-C5'	3.36	1.52	1.44
2	D	501	UD1	O5'-C5'	3.36	1.52	1.44
2	D	501	UD1	C2-N1	2.95	1.43	1.38
2	E	501	UD1	O3B-C3B	2.89	1.50	1.43
2	E	501	UD1	C2-N1	2.88	1.43	1.38
2	G	501	UD1	O5'-C5'	2.80	1.51	1.44
2	H	501	UD1	PB-O1B	-2.79	1.41	1.50
2	E	501	UD1	O5'-C5'	2.75	1.51	1.44
2	C	501	UD1	PB-O2B	-2.74	1.42	1.55
2	H	501	UD1	C2-N1	2.74	1.42	1.38
2	A	501	UD1	O2'-C2B	2.69	1.49	1.43
2	A	501	UD1	O2-C2	2.68	1.27	1.23
2	H	501	UD1	O3'-C3'	2.67	1.49	1.43
2	F	501	UD1	O2'-C2B	2.67	1.49	1.43
2	H	501	UD1	C1'-C2'	2.66	1.57	1.53
2	B	501	UD1	O5'-C5'	2.65	1.50	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	501	UD1	PB-O2B	-2.60	1.43	1.55
2	B	501	UD1	O3B-C3B	2.57	1.49	1.43
2	H	501	UD1	O5'-C5'	2.55	1.50	1.44
2	F	501	UD1	PB-O3A	-2.53	1.56	1.59
2	B	501	UD1	PB-O3A	-2.52	1.56	1.59
2	C	501	UD1	O3B-C3B	2.51	1.49	1.43
2	A	501	UD1	O4'-C4'	2.51	1.49	1.43
2	D	501	UD1	C8'-C7'	2.47	1.55	1.50
2	G	501	UD1	C8'-C7'	2.46	1.55	1.50
2	G	501	UD1	C2-N1	2.46	1.42	1.38
2	G	501	UD1	O2'-C2B	2.46	1.49	1.43
2	C	501	UD1	O2'-C2B	2.46	1.49	1.43
2	A	501	UD1	PB-O2B	-2.44	1.44	1.55
2	C	501	UD1	C8'-C7'	2.43	1.55	1.50
2	C	501	UD1	O5'-C5'	2.42	1.50	1.44
2	A	501	UD1	C8'-C7'	2.41	1.55	1.50
2	E	501	UD1	PB-O2B	-2.41	1.44	1.55
2	F	501	UD1	PB-O2B	-2.41	1.44	1.55
2	F	501	UD1	PB-O1B	-2.40	1.42	1.50
2	H	501	UD1	O2-C2	2.40	1.27	1.23
2	G	501	UD1	PB-O1B	-2.39	1.42	1.50
2	A	501	UD1	O3B-C3B	2.39	1.48	1.43
2	B	501	UD1	C4'-C5'	2.38	1.58	1.53
2	E	501	UD1	O2'-C2B	2.38	1.48	1.43
2	D	501	UD1	O2'-C2B	2.36	1.48	1.43
2	F	501	UD1	O5'-C5'	2.36	1.50	1.44
2	H	501	UD1	O2'-C2B	2.35	1.48	1.43
2	D	501	UD1	O2-C2	2.35	1.27	1.23
2	D	501	UD1	O3'-C3'	2.34	1.48	1.43
2	A	501	UD1	C2'-N2'	2.34	1.49	1.45
2	E	501	UD1	C8'-C7'	2.33	1.55	1.50
2	C	501	UD1	PB-O1B	-2.31	1.42	1.50
2	B	501	UD1	C1'-C2'	2.29	1.56	1.53
2	H	501	UD1	O3B-C3B	2.29	1.48	1.43
2	D	501	UD1	PB-O2B	-2.29	1.44	1.55
2	F	501	UD1	O3B-C3B	2.28	1.48	1.43
2	D	501	UD1	C3B-C4B	2.24	1.58	1.53
2	B	501	UD1	PB-O2B	-2.22	1.45	1.55
2	H	501	UD1	PB-O2B	-2.22	1.45	1.55
2	F	501	UD1	PA-O2A	-2.22	1.45	1.55
2	B	501	UD1	C3B-C4B	2.21	1.58	1.53
2	H	501	UD1	C6-N1	2.21	1.43	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	UD1	C8'-C7'	2.19	1.55	1.50
2	H	501	UD1	C8'-C7'	2.17	1.55	1.50
2	C	501	UD1	C6-N1	2.16	1.43	1.38
2	E	501	UD1	O3'-C3'	2.16	1.48	1.43
2	D	501	UD1	PB-O1B	-2.15	1.43	1.50
2	E	501	UD1	PB-O1B	-2.14	1.43	1.50
2	B	501	UD1	O2'-C2B	2.13	1.48	1.43
2	H	501	UD1	C3B-C4B	2.13	1.58	1.53
2	D	501	UD1	O5'-C1'	2.13	1.47	1.41
2	B	501	UD1	O4'-C4'	2.12	1.48	1.43
2	B	501	UD1	O3'-C3'	2.11	1.48	1.43
2	E	501	UD1	O5'-C1'	2.10	1.47	1.41
2	G	501	UD1	O3'-C3'	2.08	1.48	1.43
2	F	501	UD1	O2-C2	2.07	1.26	1.23
2	C	501	UD1	O2-C2	2.05	1.26	1.23
2	G	501	UD1	C1B-N1	2.04	1.53	1.47
2	C	501	UD1	C2-N1	2.02	1.41	1.38
2	F	501	UD1	C8'-C7'	2.02	1.54	1.50
2	E	501	UD1	C1B-N1	2.02	1.53	1.47
2	A	501	UD1	PA-O2A	-2.01	1.46	1.55

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	UD1	O3A-PA-O1A	-4.02	98.61	110.70
2	A	501	UD1	O3A-PA-O1A	-3.68	99.64	110.70
2	E	501	UD1	O3A-PA-O1A	-3.60	99.87	110.70
2	B	501	UD1	O3A-PA-O1A	-3.56	100.00	110.70
2	F	501	UD1	O3A-PA-O1A	-3.52	100.11	110.70
2	G	501	UD1	O3A-PA-O1A	-3.49	100.21	110.70
2	G	501	UD1	O2'-C2B-C1B	3.49	122.11	110.10
2	H	501	UD1	O3B-C3B-C4B	3.47	121.06	111.08
2	B	501	UD1	O3B-C3B-C4B	3.45	121.00	111.08
2	H	501	UD1	O3A-PA-O1A	-3.42	100.42	110.70
2	D	501	UD1	O2'-C2B-C1B	3.40	121.82	110.10
2	G	501	UD1	O2A-PA-O3A	3.36	116.35	107.27
2	B	501	UD1	O2A-PA-O3A	3.35	116.34	107.27
2	E	501	UD1	O2'-C2B-C1B	3.27	121.36	110.10
2	E	501	UD1	O2A-PA-O3A	3.25	116.05	107.27
2	G	501	UD1	O3B-C3B-C4B	3.16	120.17	111.08
2	A	501	UD1	O2A-PA-O3A	3.15	115.78	107.27
2	D	501	UD1	O3B-C3B-C4B	3.12	120.05	111.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	UD1	O2B-PB-O3A	3.11	115.67	107.27
2	D	501	UD1	O2A-PA-O3A	3.07	115.56	107.27
2	E	501	UD1	O3B-C3B-C4B	3.06	119.87	111.08
2	C	501	UD1	O3B-C3B-C4B	3.06	119.86	111.08
2	H	501	UD1	O2'-C2B-C1B	3.05	120.60	110.10
2	A	501	UD1	O3B-C3B-C4B	3.02	119.77	111.08
2	B	501	UD1	N3-C2-N1	3.01	118.82	114.89
2	C	501	UD1	O2'-C2B-C1B	3.01	120.48	110.10
2	F	501	UD1	O2'-C2B-C1B	3.00	120.43	110.10
2	A	501	UD1	O2'-C2B-C3B	3.00	121.42	111.82
2	F	501	UD1	O2A-PA-O3A	2.98	115.32	107.27
2	F	501	UD1	O2'-C2B-C3B	2.96	121.30	111.82
2	A	501	UD1	O2'-C2B-C1B	2.96	120.28	110.10
2	B	501	UD1	O2'-C2B-C3B	2.96	121.29	111.82
2	A	501	UD1	O2B-PB-O3A	2.95	115.26	107.27
2	H	501	UD1	O2A-PA-O3A	2.89	115.08	107.27
2	E	501	UD1	O2'-C2B-C3B	2.89	121.08	111.82
2	C	501	UD1	O3A-PA-O1A	-2.88	102.03	110.70
2	F	501	UD1	O3B-C3B-C4B	2.85	119.25	111.08
2	H	501	UD1	O2'-C2B-C3B	2.84	120.93	111.82
2	C	501	UD1	O2'-C2B-C3B	2.84	120.92	111.82
2	G	501	UD1	O2B-PB-O3A	2.81	114.87	107.27
2	E	501	UD1	O2B-PB-O3A	2.79	114.80	107.27
2	D	501	UD1	O2'-C2B-C3B	2.78	120.74	111.82
2	D	501	UD1	O2B-PB-O3A	2.74	114.68	107.27
2	C	501	UD1	O2A-PA-O3A	2.69	114.54	107.27
2	G	501	UD1	O2'-C2B-C3B	2.67	120.37	111.82
2	H	501	UD1	O2B-PB-O3A	2.66	114.46	107.27
2	B	501	UD1	O2'-C2B-C1B	2.64	119.20	110.10
2	E	501	UD1	N3-C2-N1	2.62	118.30	114.89
2	B	501	UD1	O2B-PB-O3A	2.56	114.19	107.27
2	G	501	UD1	N3-C2-N1	2.52	118.18	114.89
2	C	501	UD1	N3-C2-N1	2.46	118.10	114.89
2	H	501	UD1	N3-C2-N1	2.42	118.04	114.89
2	A	501	UD1	N3-C2-N1	2.42	118.04	114.89
2	G	501	UD1	C1B-N1-C2	2.39	121.88	117.59
2	D	501	UD1	N3-C2-N1	2.35	117.95	114.89
2	F	501	UD1	N3-C2-N1	2.33	117.93	114.89
2	F	501	UD1	O2B-PB-O3A	2.33	113.56	107.27
2	E	501	UD1	O1'-PB-O1B	-2.31	102.41	109.81
2	F	501	UD1	C1B-N1-C2	2.29	121.70	117.59
2	E	501	UD1	C1B-N1-C2	2.21	121.56	117.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	501	UD1	C4'-C3'-C2'	-2.20	107.20	110.40
2	B	501	UD1	C2B-C3B-C4B	-2.17	98.41	102.61
2	F	501	UD1	O1'-PB-O1B	-2.15	102.92	109.81
2	B	501	UD1	O1'-PB-O1B	-2.12	103.02	109.81
2	D	501	UD1	C1B-N1-C2	2.02	121.22	117.59
2	C	501	UD1	O4-C4-N3	2.02	122.20	119.27
2	G	501	UD1	C6-N1-C2	-2.00	118.56	121.00

There are no chirality outliers.

All (64) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	UD1	C5B-O5B-PA-O1A
2	A	501	UD1	C5B-O5B-PA-O2A
2	A	501	UD1	C5B-O5B-PA-O3A
2	B	501	UD1	C5B-O5B-PA-O1A
2	B	501	UD1	C5B-O5B-PA-O2A
2	B	501	UD1	C5B-O5B-PA-O3A
2	C	501	UD1	C5B-O5B-PA-O1A
2	C	501	UD1	C5B-O5B-PA-O2A
2	C	501	UD1	C5B-O5B-PA-O3A
2	D	501	UD1	C5B-O5B-PA-O1A
2	D	501	UD1	C5B-O5B-PA-O2A
2	D	501	UD1	C5B-O5B-PA-O3A
2	E	501	UD1	C5B-O5B-PA-O1A
2	E	501	UD1	C5B-O5B-PA-O2A
2	E	501	UD1	C5B-O5B-PA-O3A
2	F	501	UD1	C5B-O5B-PA-O1A
2	F	501	UD1	C5B-O5B-PA-O2A
2	F	501	UD1	C5B-O5B-PA-O3A
2	G	501	UD1	C5B-O5B-PA-O1A
2	G	501	UD1	C5B-O5B-PA-O2A
2	G	501	UD1	C5B-O5B-PA-O3A
2	H	501	UD1	C5B-O5B-PA-O1A
2	H	501	UD1	C5B-O5B-PA-O2A
2	H	501	UD1	C5B-O5B-PA-O3A
4	D	507	EDO	O1-C1-C2-O2
4	E	507	EDO	O1-C1-C2-O2
4	E	508	EDO	O1-C1-C2-O2
4	F	506	EDO	O1-C1-C2-O2
4	G	505	EDO	O1-C1-C2-O2
4	G	508	EDO	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	H	510	EDO	O1-C1-C2-O2
4	E	506	EDO	O1-C1-C2-O2
4	G	506	EDO	O1-C1-C2-O2
2	C	501	UD1	PB-O3A-PA-O1A
4	C	505	EDO	O1-C1-C2-O2
4	E	511	EDO	O1-C1-C2-O2
4	H	511	EDO	O1-C1-C2-O2
2	A	501	UD1	PB-O3A-PA-O1A
2	B	501	UD1	PB-O3A-PA-O1A
2	D	501	UD1	PB-O3A-PA-O1A
4	D	508	EDO	O1-C1-C2-O2
4	D	510	EDO	O1-C1-C2-O2
4	A	508	EDO	O1-C1-C2-O2
2	B	501	UD1	C3'-C2'-N2'-C7'
2	E	501	UD1	PB-O3A-PA-O2A
2	F	501	UD1	PB-O3A-PA-O1A
2	G	501	UD1	PB-O3A-PA-O1A
4	A	507	EDO	O1-C1-C2-O2
4	B	505	EDO	O1-C1-C2-O2
4	F	508	EDO	O1-C1-C2-O2
2	E	501	UD1	C3'-C2'-N2'-C7'
4	D	506	EDO	O1-C1-C2-O2
4	G	502	EDO	O1-C1-C2-O2
2	A	501	UD1	PB-O3A-PA-O2A
2	D	501	UD1	PB-O3A-PA-O2A
2	E	501	UD1	PB-O3A-PA-O1A
2	F	501	UD1	PB-O3A-PA-O2A
2	G	501	UD1	PB-O3A-PA-O2A
2	H	501	UD1	PB-O3A-PA-O1A
2	H	501	UD1	PB-O3A-PA-O2A
2	C	501	UD1	C3'-C2'-N2'-C7'
4	D	504	EDO	O1-C1-C2-O2
4	E	505	EDO	O1-C1-C2-O2
2	B	501	UD1	PB-O3A-PA-O2A

There are no ring outliers.

20 monomers are involved in 27 short contacts:

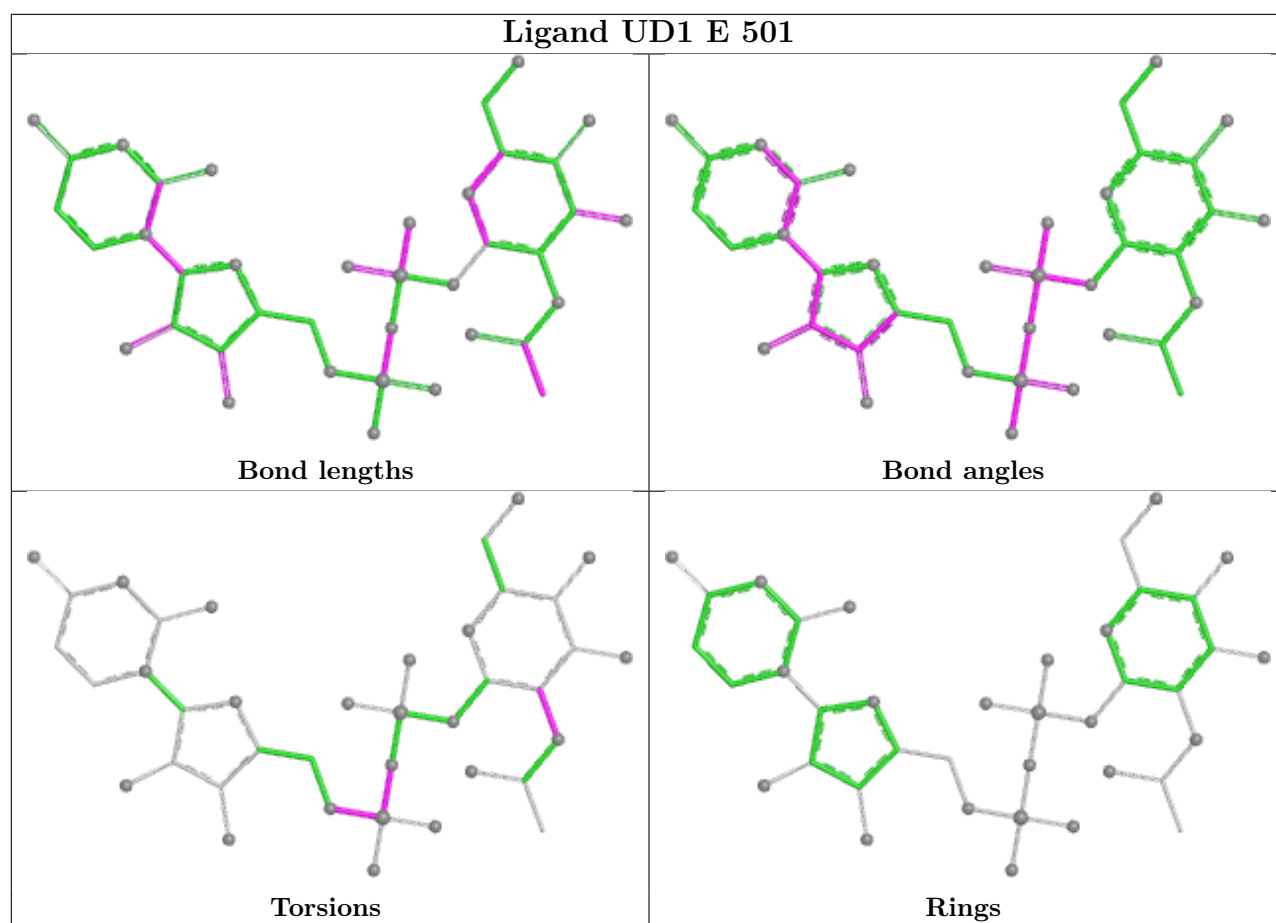
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	504	EDO	1	0
4	E	508	EDO	1	0
3	H	504	ACT	1	0

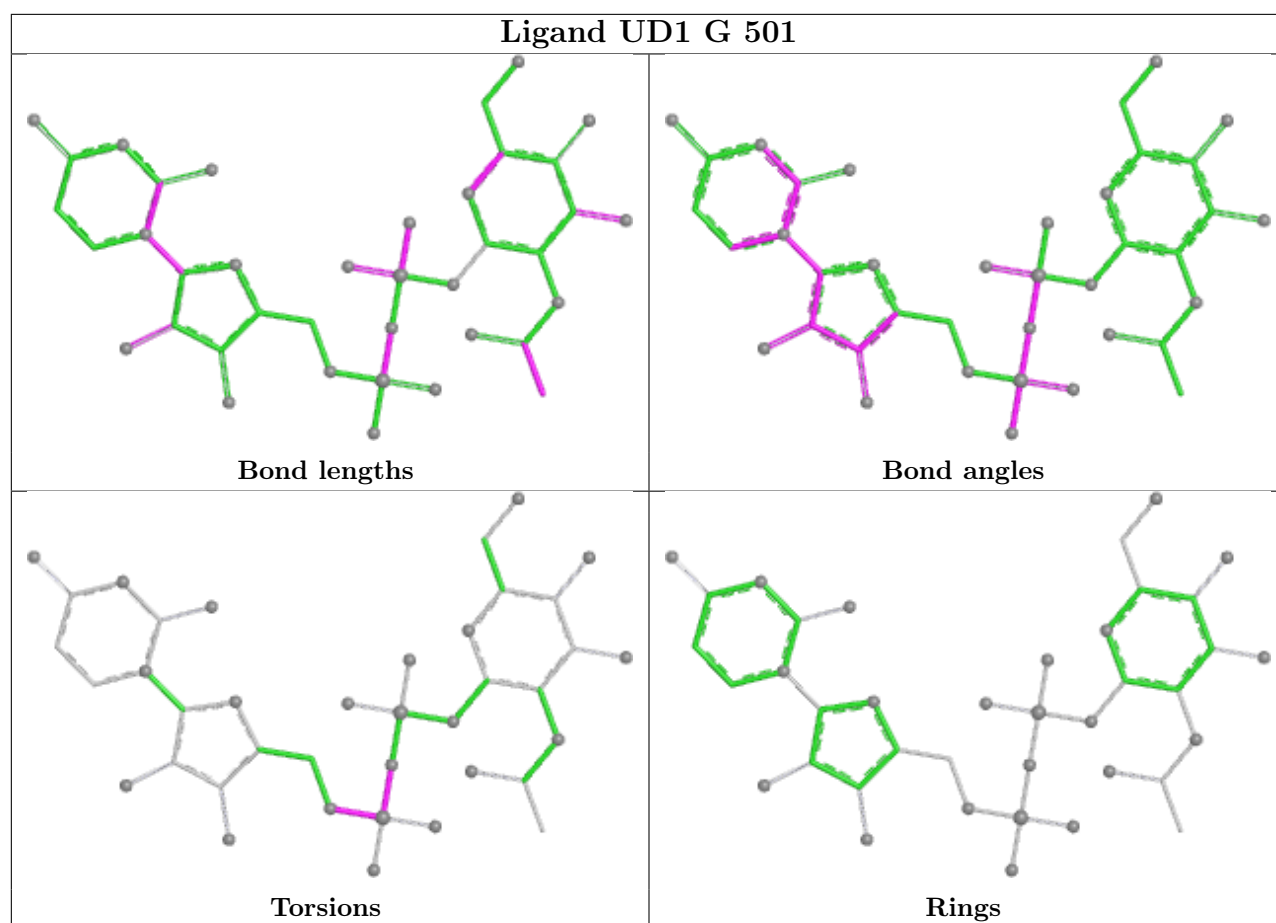
Continued on next page...

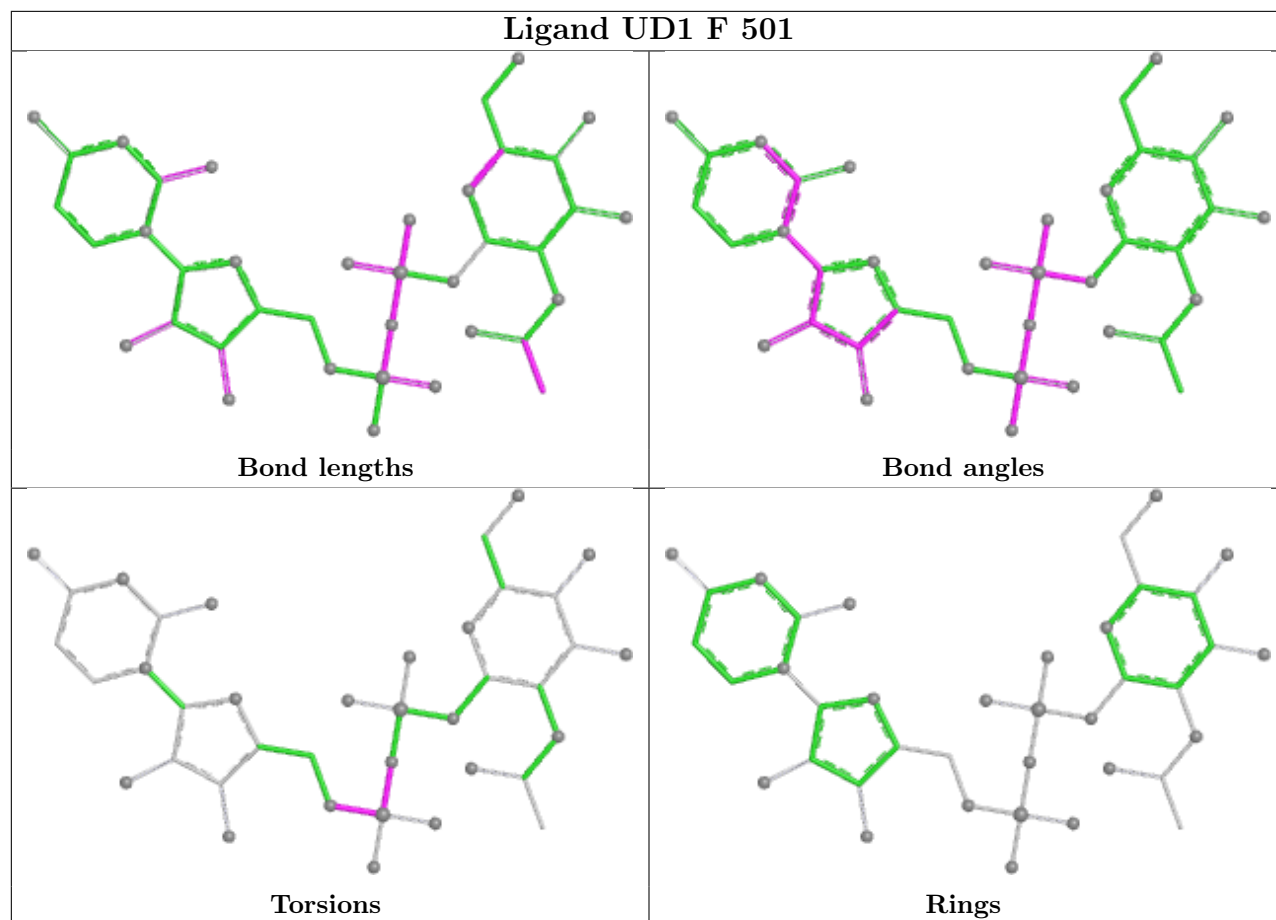
Continued from previous page...

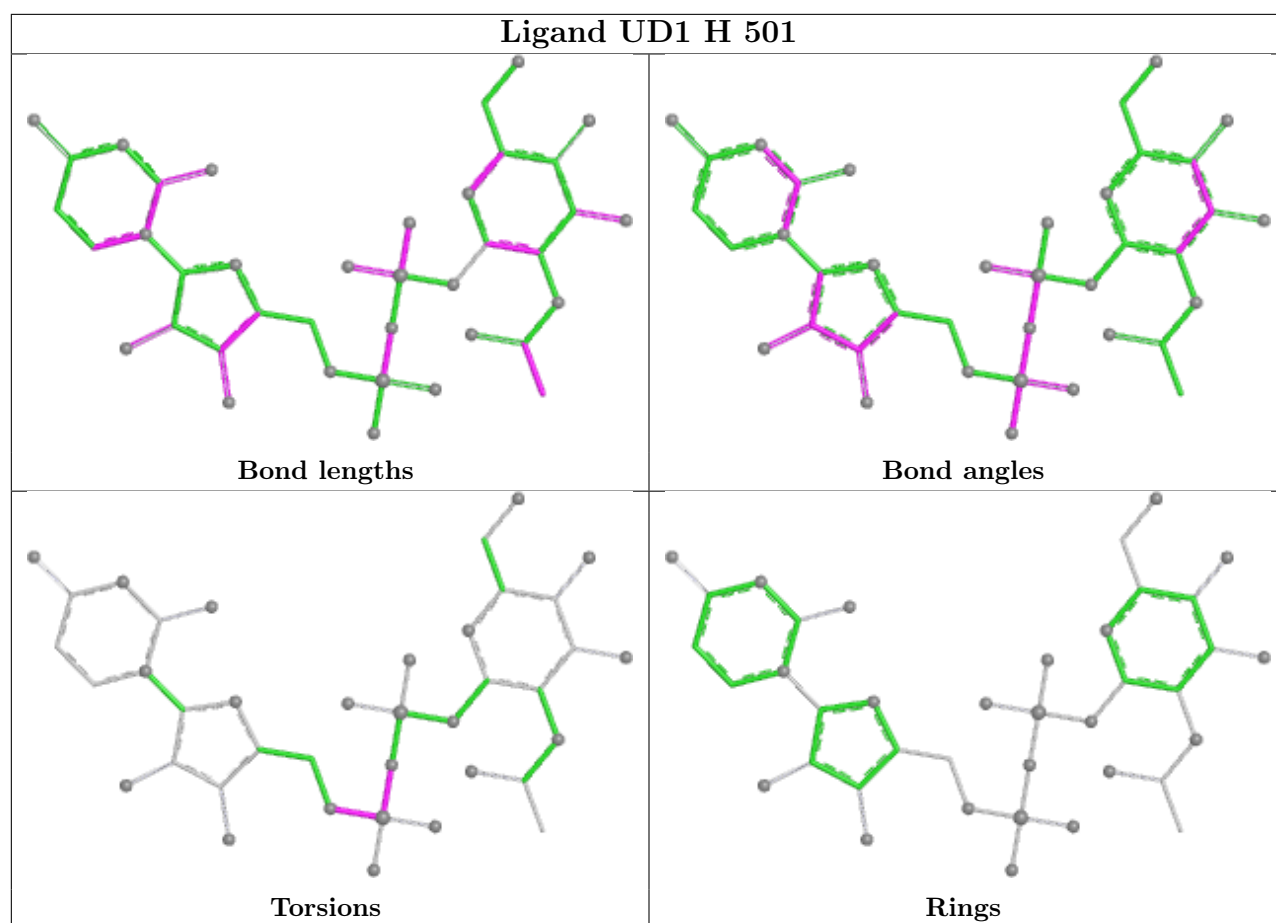
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	507	EDO	1	0
4	D	507	EDO	1	0
4	D	508	EDO	2	0
3	C	502	ACT	2	0
4	D	505	EDO	1	0
4	G	505	EDO	1	0
2	A	501	UD1	1	0
3	F	503	ACT	3	0
4	D	509	EDO	1	0
4	A	507	EDO	2	0
4	H	510	EDO	1	0
3	H	503	ACT	1	0
4	D	510	EDO	2	0
3	C	503	ACT	2	0
4	F	509	EDO	1	0
4	H	508	EDO	1	0
3	E	502	ACT	2	0

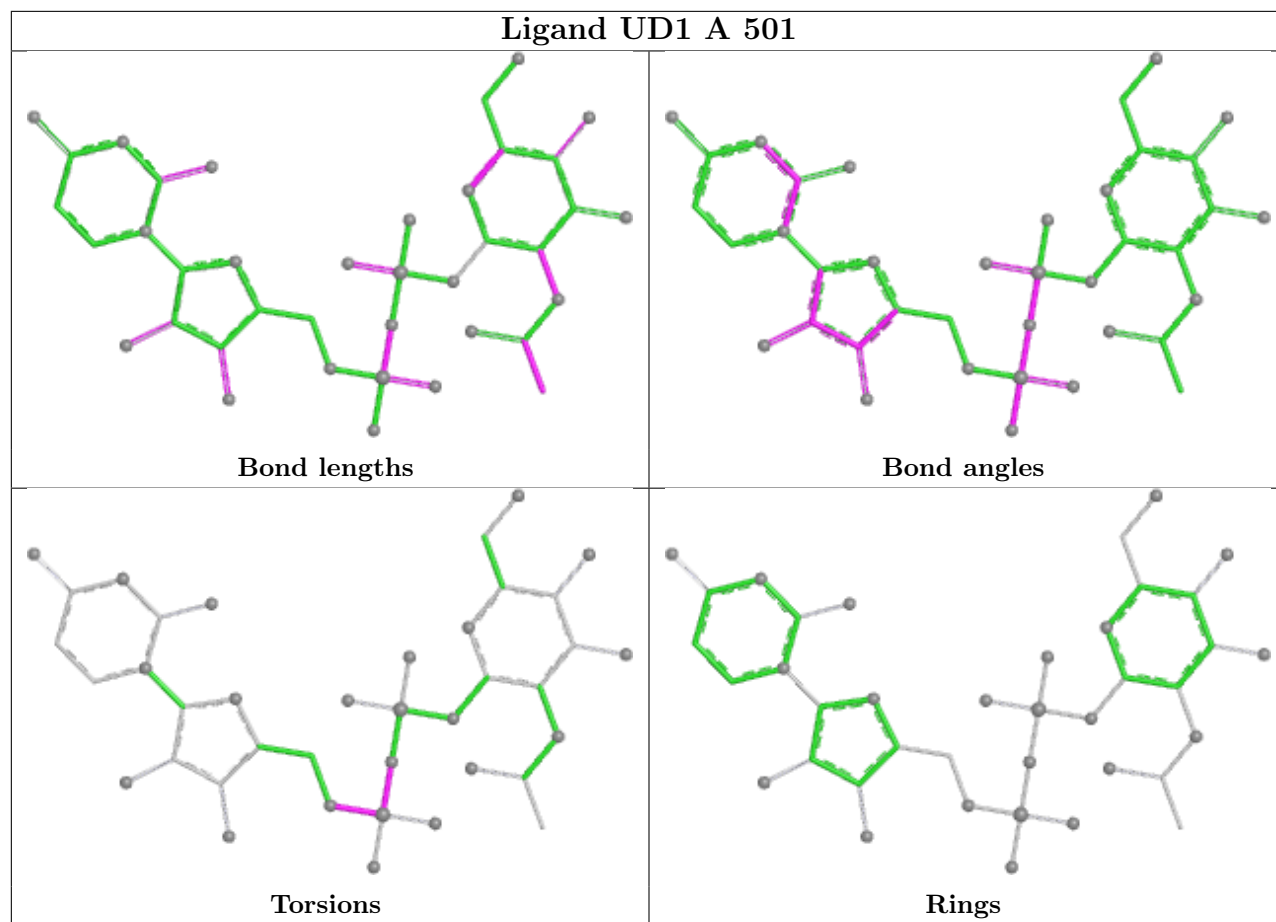
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

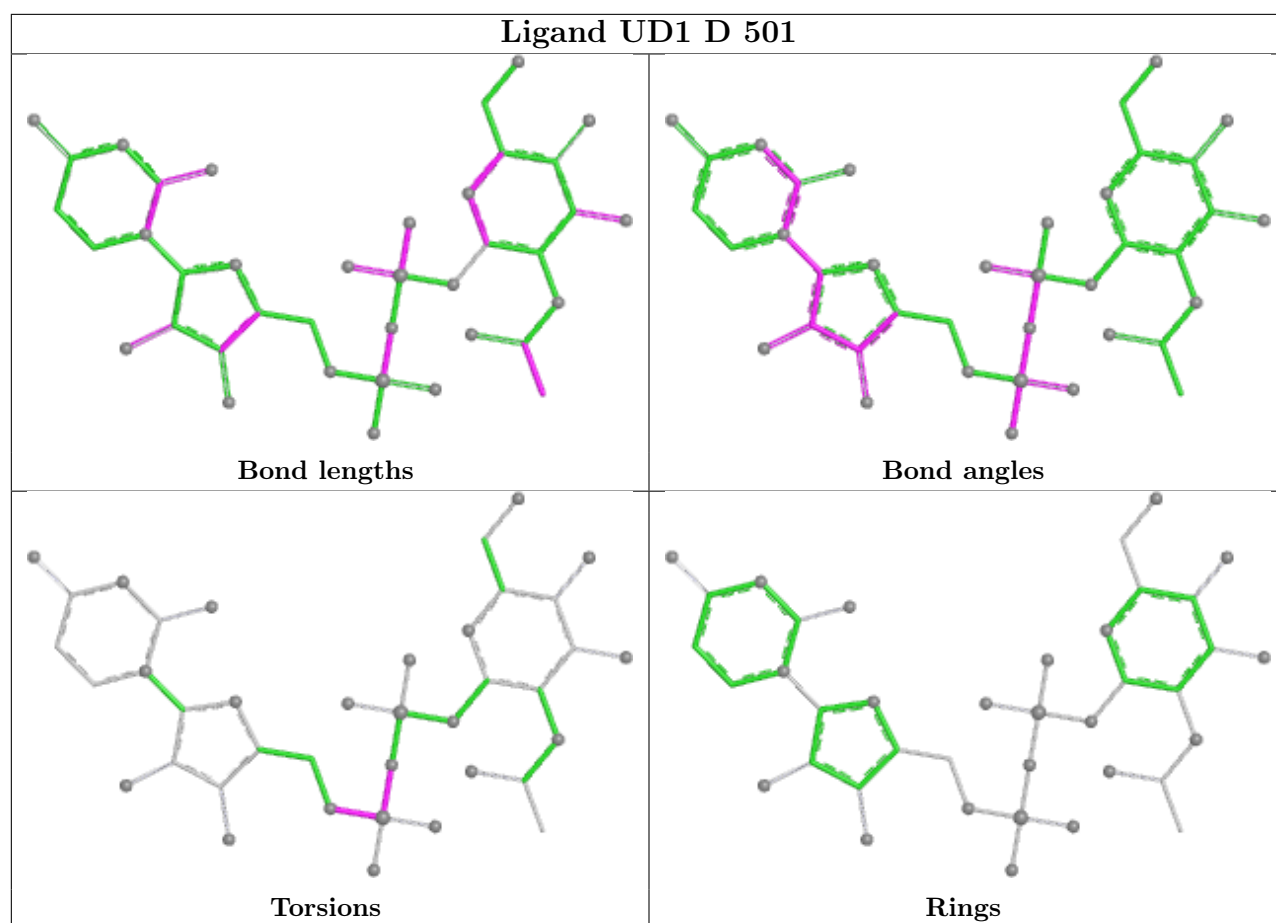


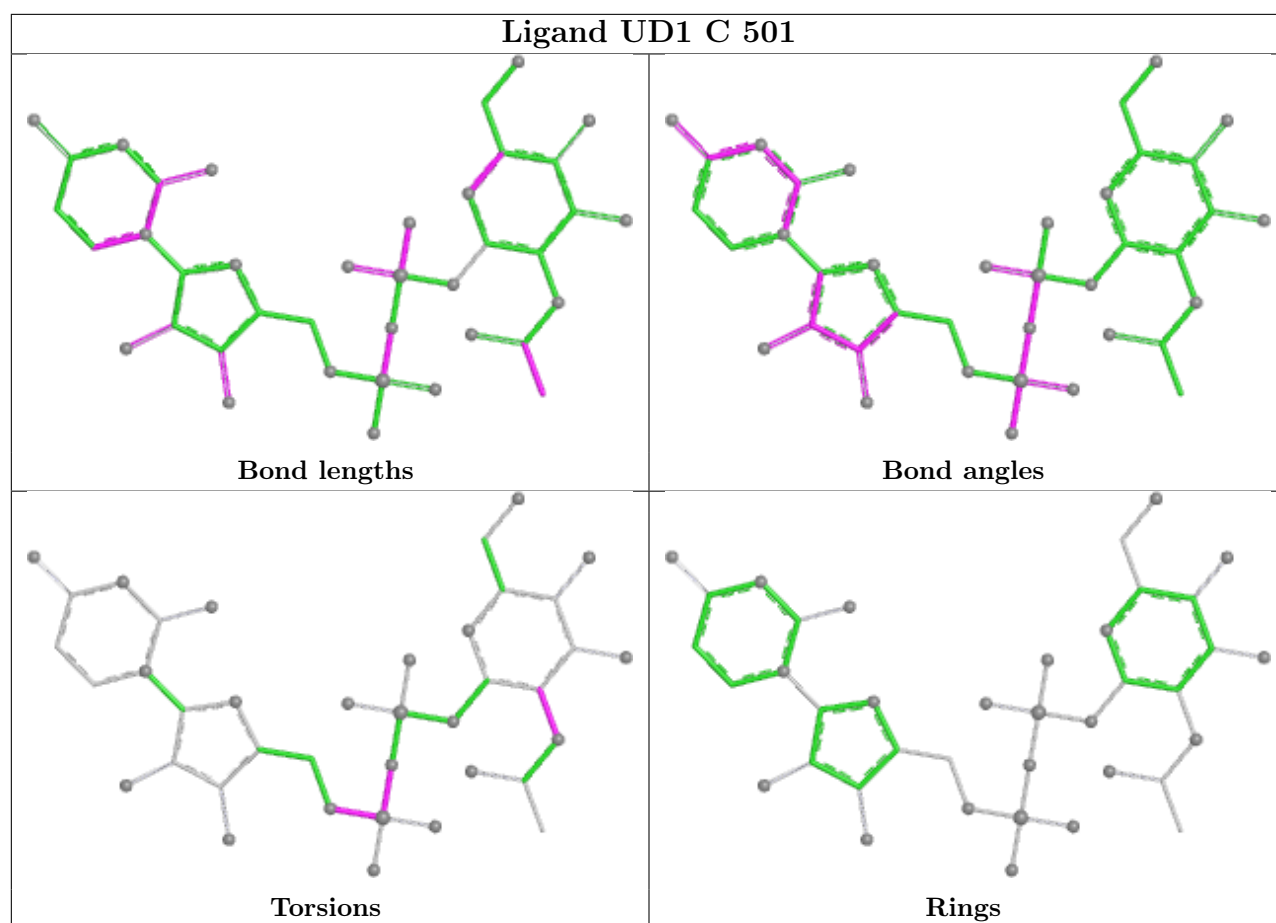


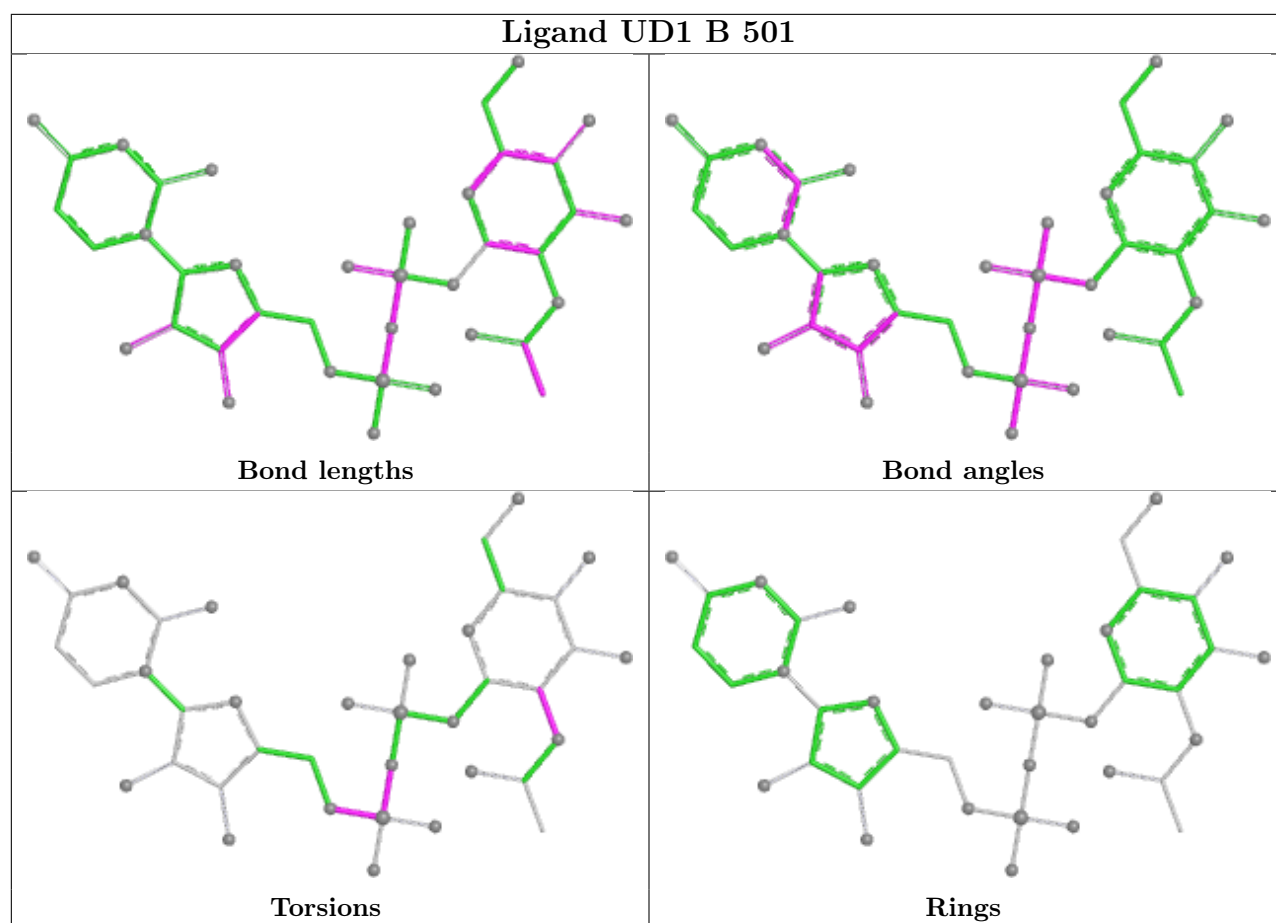












5.7 Other polymers [i](#)

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	418/419 (99%)	-0.28	1 (0%) 91 89	22, 36, 52, 87	0
1	B	418/419 (99%)	0.37	10 (2%) 59 55	30, 53, 75, 94	0
1	C	418/419 (99%)	-0.16	2 (0%) 87 85	24, 42, 58, 81	0
1	D	418/419 (99%)	-0.21	1 (0%) 91 89	22, 39, 58, 83	0
1	E	418/419 (99%)	0.02	7 (1%) 69 65	19, 42, 71, 92	0
1	F	418/419 (99%)	-0.17	0 100 100	24, 40, 58, 84	0
1	G	418/419 (99%)	-0.24	1 (0%) 91 89	22, 39, 56, 93	0
1	H	418/419 (99%)	-0.23	4 (0%) 79 76	19, 36, 52, 89	0
All	All	3344/3352 (99%)	-0.11	26 (0%) 82 80	19, 40, 64, 94	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	417	LYS	4.5
1	C	419	GLU	4.4
1	E	39	VAL	3.6
1	H	419	GLU	3.6
1	B	418	GLY	3.6
1	B	2	ASP	3.4
1	H	418	GLY	3.2
1	A	395	ILE	3.2
1	B	370	LEU	2.9
1	E	64	VAL	2.5
1	B	72	ILE	2.4
1	B	413	ILE	2.4
1	E	38	PRO	2.4
1	E	223	GLY	2.3
1	B	417	LYS	2.3
1	H	416	VAL	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	370	LEU	2.2
1	B	61	GLY	2.2
1	B	242	ALA	2.1
1	B	3	LYS	2.1
1	G	1	MET	2.1
1	D	418	GLY	2.1
1	E	65	GLU	2.1
1	C	1	MET	2.0
1	E	373	SER	2.0
1	B	71	TRP	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	IAS	F	67	8/9	0.81	0.11	59,60,62,64	0
1	IAS	E	67	8/9	0.82	0.10	68,70,71,72	0
1	IAS	B	67	8/9	0.84	0.08	73,74,76,76	0
1	IAS	D	67	8/9	0.87	0.09	56,57,61,62	0
1	IAS	C	67	8/9	0.90	0.08	49,52,52,53	0
1	IAS	G	67	8/9	0.90	0.07	36,38,41,42	0
1	IAS	A	67	8/9	0.92	0.06	34,36,37,37	0
1	IAS	H	67	8/9	0.95	0.05	34,35,37,38	0

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	ACT	F	502	4/4	0.54	0.13	69,69,70,70	0
3	ACT	F	504	4/4	0.54	0.20	68,70,70,70	0
3	ACT	A	505	4/4	0.57	0.18	72,72,73,73	0
3	ACT	A	503	4/4	0.58	0.17	67,68,68,69	0
3	ACT	E	504	4/4	0.60	0.16	81,81,82,82	0
3	ACT	A	502	4/4	0.63	0.18	47,51,51,51	0
3	ACT	H	502	4/4	0.65	0.19	55,57,58,58	0
3	ACT	D	502	4/4	0.70	0.14	52,54,55,56	0
3	ACT	F	503	4/4	0.71	0.21	49,52,52,52	0
4	EDO	A	509	4/4	0.71	0.15	55,56,56,56	0
4	EDO	E	510	4/4	0.73	0.14	59,62,63,63	0
3	ACT	B	502	4/4	0.76	0.15	69,71,71,71	0
4	EDO	E	505	4/4	0.76	0.16	51,55,55,57	0
3	ACT	C	502	4/4	0.76	0.16	74,75,75,76	0
4	EDO	E	511	4/4	0.76	0.14	62,64,65,65	0
3	ACT	E	503	4/4	0.78	0.17	74,75,75,75	0
4	EDO	F	507	4/4	0.78	0.21	60,63,63,64	0
4	EDO	D	508	4/4	0.80	0.19	58,59,60,60	0
3	ACT	H	505	4/4	0.81	0.18	57,58,59,60	0
4	EDO	C	505	4/4	0.82	0.12	51,54,55,56	0
3	ACT	D	503	4/4	0.82	0.17	68,68,69,69	0
4	EDO	B	505	4/4	0.83	0.13	59,59,59,60	0
4	EDO	E	508	4/4	0.84	0.09	54,54,55,55	0
4	EDO	F	508	4/4	0.84	0.15	59,62,62,63	0
4	EDO	F	509	4/4	0.84	0.12	44,45,47,49	0
4	EDO	G	506	4/4	0.84	0.13	57,58,58,58	0
4	EDO	H	513	4/4	0.84	0.12	56,56,56,57	0
4	EDO	F	506	4/4	0.85	0.13	59,59,61,61	0
4	EDO	C	507	4/4	0.85	0.10	54,54,54,54	0
3	ACT	H	503	4/4	0.86	0.11	42,45,46,47	0
3	ACT	E	502	4/4	0.86	0.12	63,64,64,65	0
4	EDO	E	507	4/4	0.86	0.12	45,46,47,47	0
4	EDO	D	507	4/4	0.86	0.12	58,59,59,61	0
4	EDO	G	505	4/4	0.87	0.11	62,63,64,64	0
4	EDO	D	506	4/4	0.87	0.15	48,50,52,53	0
4	EDO	H	510	4/4	0.87	0.10	56,58,59,60	0
4	EDO	H	511	4/4	0.87	0.09	54,56,57,58	0
3	ACT	C	503	4/4	0.87	0.17	52,53,55,56	0
4	EDO	G	504	4/4	0.88	0.09	45,45,46,47	0
4	EDO	C	506	4/4	0.88	0.13	55,57,57,58	0
3	ACT	H	504	4/4	0.88	0.14	58,58,58,59	0
3	ACT	H	506	4/4	0.89	0.10	57,57,58,58	0
4	EDO	G	507	4/4	0.89	0.10	48,49,50,51	0

Continued on next page...

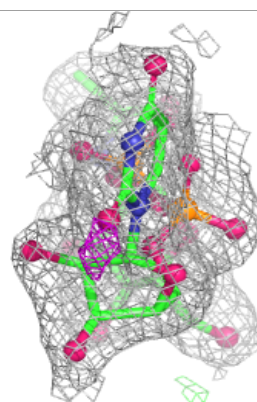
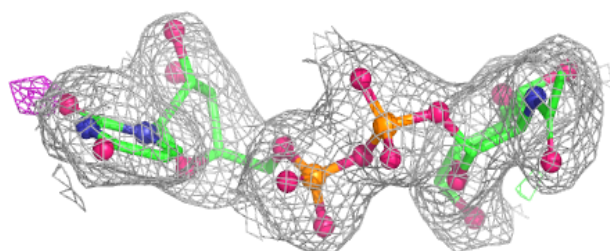
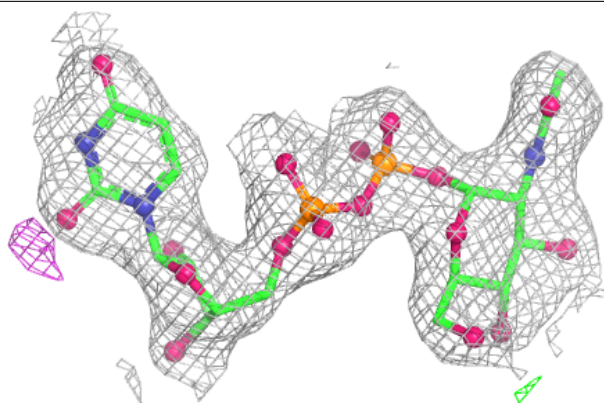
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	D	505	4/4	0.89	0.11	48,49,49,51	0
4	EDO	B	503	4/4	0.89	0.11	44,44,44,48	0
4	EDO	B	504	4/4	0.89	0.11	59,60,61,61	0
4	EDO	E	506	4/4	0.90	0.10	48,48,50,52	0
3	ACT	A	504	4/4	0.90	0.12	52,54,54,56	0
4	EDO	D	510	4/4	0.91	0.08	44,47,48,51	0
4	EDO	G	503	4/4	0.91	0.10	51,51,51,53	0
4	EDO	A	507	4/4	0.91	0.21	35,35,37,40	0
4	EDO	D	504	4/4	0.92	0.10	39,40,41,43	0
4	EDO	A	506	4/4	0.92	0.08	32,34,35,39	0
4	EDO	G	508	4/4	0.93	0.08	46,47,48,49	0
4	EDO	H	507	4/4	0.93	0.08	42,42,43,44	0
4	EDO	H	512	4/4	0.93	0.12	34,36,36,39	0
4	EDO	H	509	4/4	0.93	0.08	58,58,59,61	0
4	EDO	A	508	4/4	0.94	0.09	53,53,54,54	0
4	EDO	E	509	4/4	0.95	0.07	45,46,47,49	0
4	EDO	D	509	4/4	0.95	0.09	61,62,62,62	0
4	EDO	H	508	4/4	0.95	0.08	50,52,52,52	0
2	UD1	B	501	39/39	0.95	0.08	31,38,42,44	0
4	EDO	F	505	4/4	0.96	0.06	43,44,44,45	0
2	UD1	H	501	39/39	0.96	0.07	27,32,39,40	0
2	UD1	A	501	39/39	0.96	0.07	18,29,37,41	0
2	UD1	D	501	39/39	0.96	0.07	18,28,37,37	0
2	UD1	E	501	39/39	0.96	0.06	23,30,35,35	0
2	UD1	G	501	39/39	0.96	0.07	25,30,42,44	0
4	EDO	C	504	4/4	0.97	0.05	37,37,37,37	0
2	UD1	F	501	39/39	0.97	0.06	24,32,37,40	0
4	EDO	G	502	4/4	0.97	0.06	35,36,37,39	0
2	UD1	C	501	39/39	0.97	0.06	24,29,37,40	0

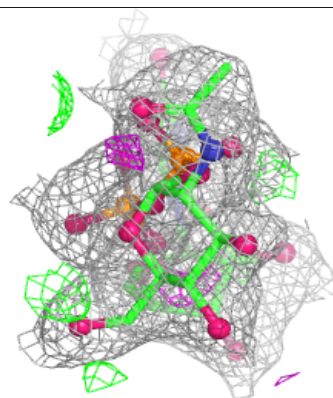
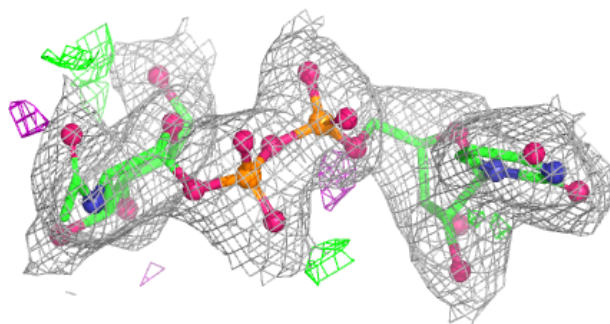
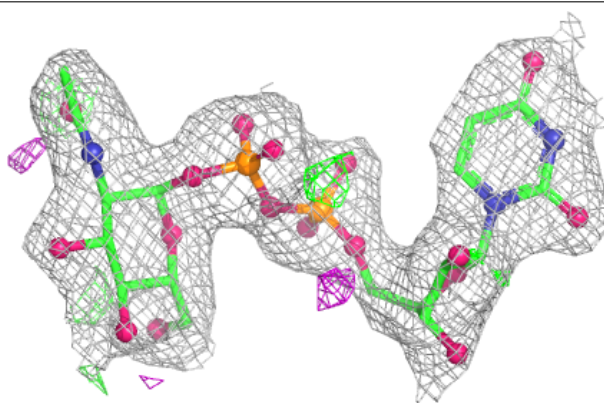
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around UD1 B 501:

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

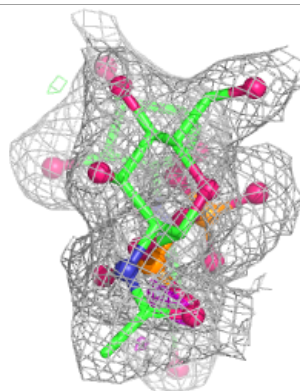
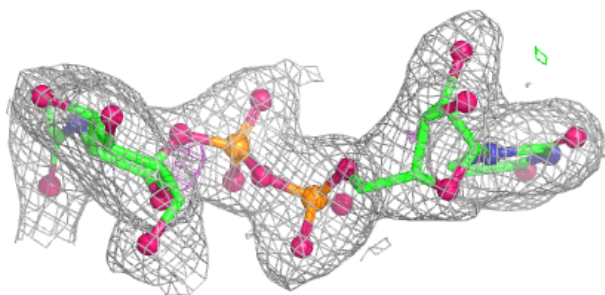
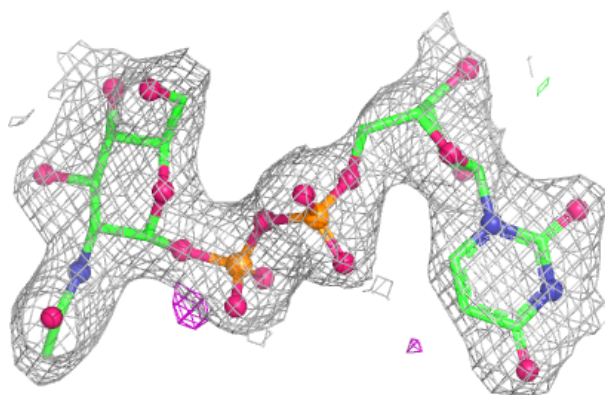
**Electron density around UD1 H 501:**

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

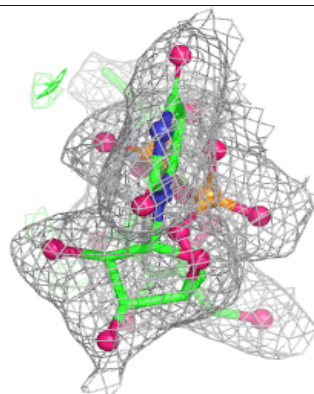
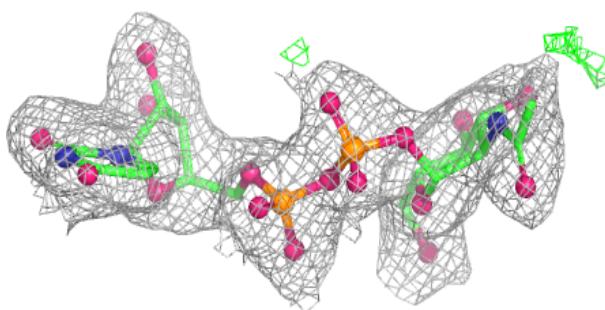
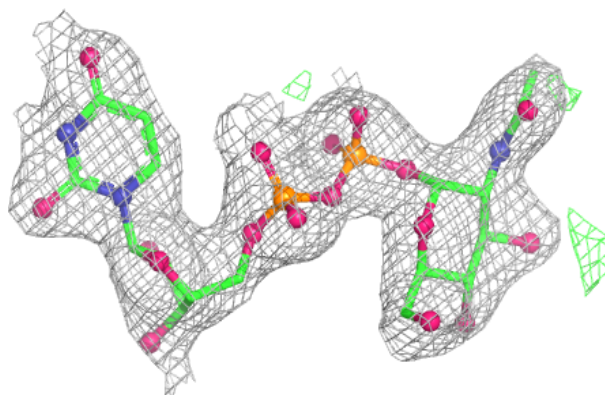


Electron density around UD1 A 501:

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

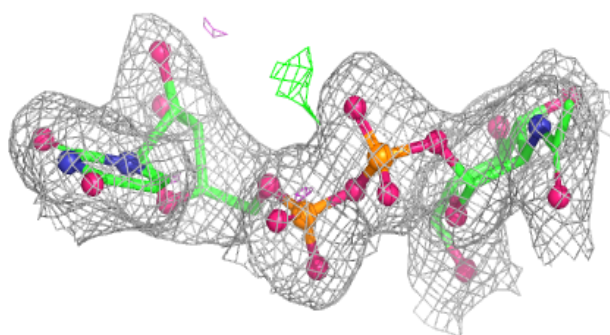
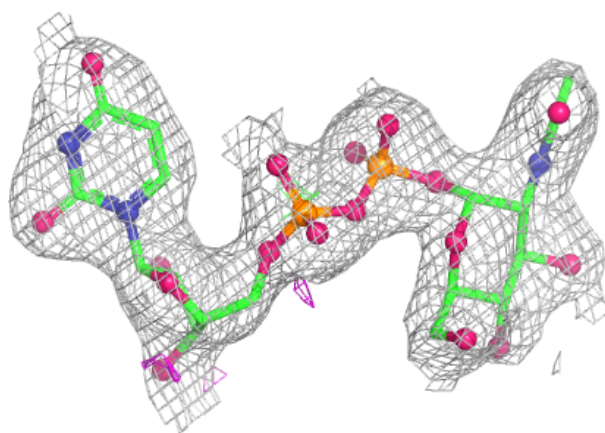
**Electron density around UD1 D 501:**

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

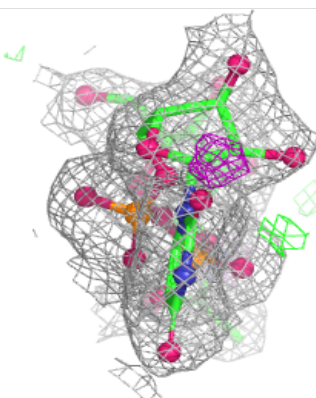
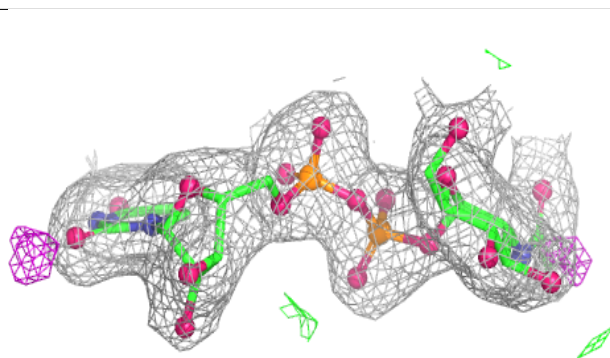
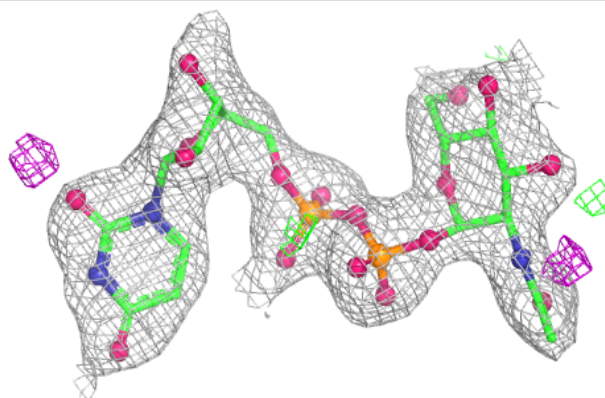


Electron density around UD1 E 501:

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

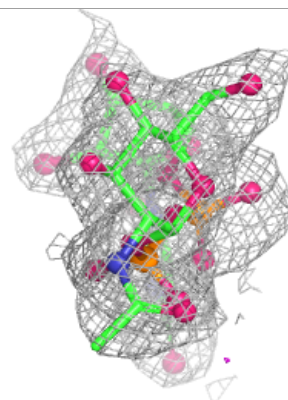
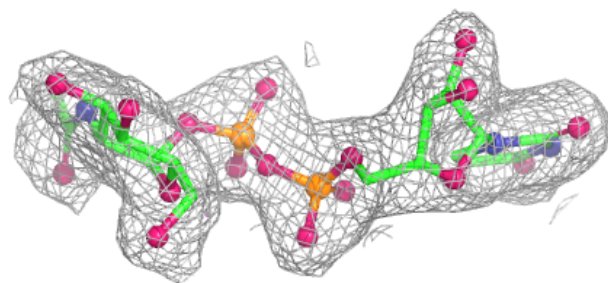
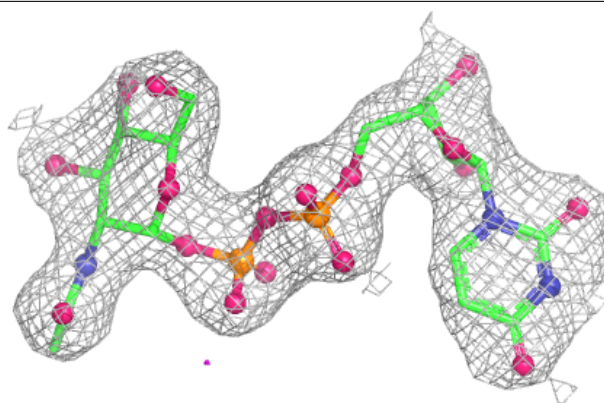
**Electron density around UD1 G 501:**

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

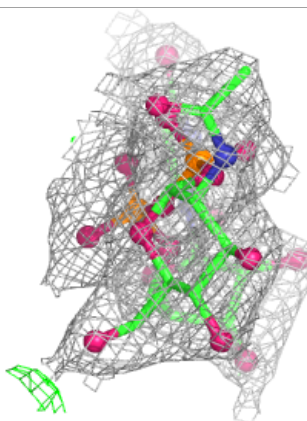
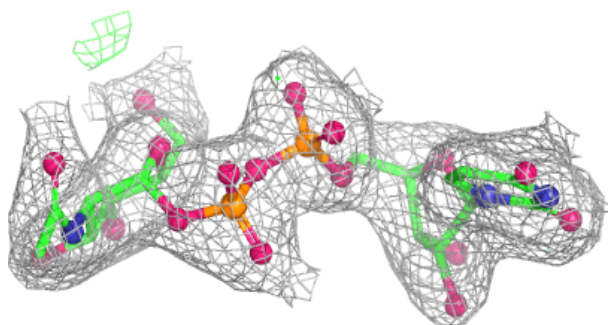
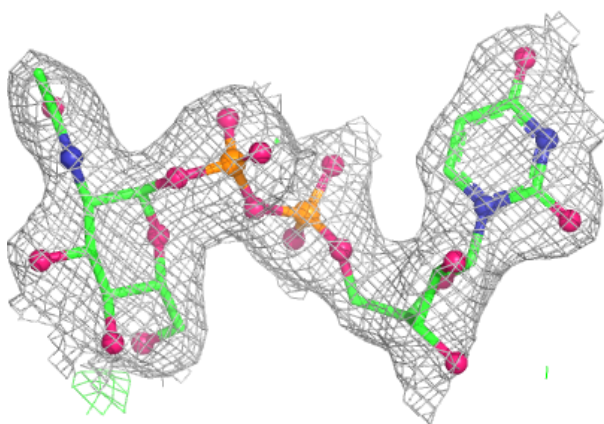


Electron density around UD1 F 501:

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

**Electron density around UD1 C 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.