



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 05:11 PM UTC

PDB ID : 5ZMD / pdb_00005zmd
Title : Crystal structure of FTO in complex with m6dA modified ssDNA
Authors : Zhang, X.; Wei, L.H.; Luo, J.; Xiao, Y.; Liu, J.; Zhang, W.; Zhang, L.; Jia, G.F.
Deposited on : 2018-04-02
Resolution : 3.30 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
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

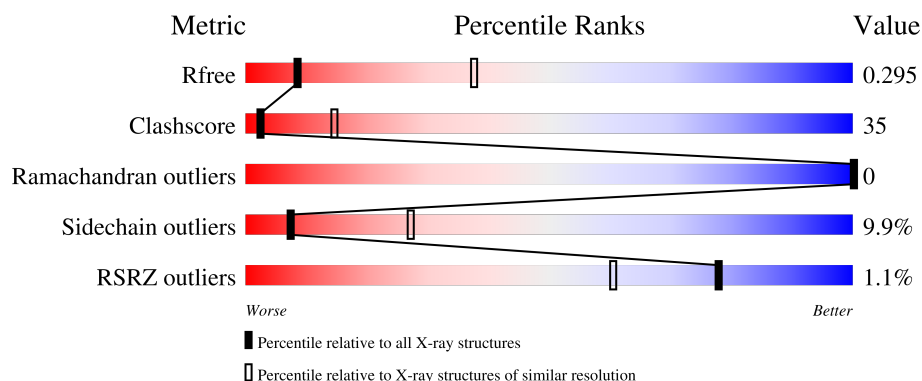
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	463	48% 30% 6% 13%
1	C	463	36% 38% 10% 15%
1	E	463	44% 36% 15%
1	G	463	44% 36% 5% 13%
2	B	9	11% 67% 22%

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Mol	Chain	Length	Quality of chain
2	D	9	
2	F	9	
2	H	9	

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
4	OGA	C	1002	-	-	X	-
4	OGA	G	1002	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13828 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 Alpha-ketoglutarate-dependent dioxygenase FTO.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	402	Total	C	N	O	S	0	0	0
			3282	2096	569	596	21			
1	C	395	Total	C	N	O	S	0	0	0
			3230	2063	559	588	20			
1	E	395	Total	C	N	O	S	0	0	0
			3228	2063	558	587	20			
1	G	403	Total	C	N	O	S	0	0	0
			3294	2101	573	600	20			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	86	LYS	GLN	engineered mutation	UNP Q9C0B1
A	306	LYS	GLN	engineered mutation	UNP Q9C0B1
C	86	LYS	GLN	engineered mutation	UNP Q9C0B1
C	306	LYS	GLN	engineered mutation	UNP Q9C0B1
E	86	LYS	GLN	engineered mutation	UNP Q9C0B1
E	306	LYS	GLN	engineered mutation	UNP Q9C0B1
G	86	LYS	GLN	engineered mutation	UNP Q9C0B1
G	306	LYS	GLN	engineered mutation	UNP Q9C0B1

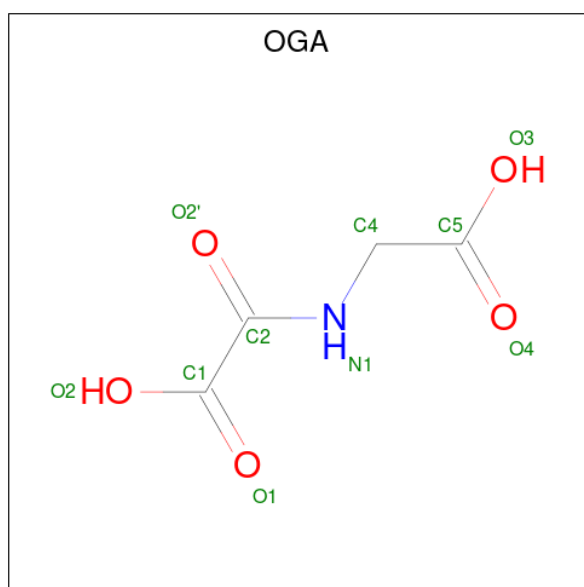
- Molecule 2 is a DNA chain called DNA (5'-D(P*TP*CP*TP*(6MA)P*TP*AP*TP*CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	9	Total	C	N	O	P	0	0	0
			183	89	29	56	9			
2	D	9	Total	C	N	O	P	0	0	0
			183	89	29	56	9			
2	F	9	Total	C	N	O	P	0	0	0
			183	89	29	56	9			
2	H	9	Total	C	N	O	P	0	0	0
			183	89	29	56	9			

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mn	0	0
			1	1		
3	C	1	Total	Mn	0	0
			1	1		
3	E	1	Total	Mn	0	0
			1	1		
3	G	1	Total	Mn	0	0
			1	1		

- Molecule 4 is N-OXALYLGLYCINE (CCD ID: OGA) (formula: C₄H₅NO₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			10	4	1	5		
4	C	1	Total	C	N	O	0	0
			10	4	1	5		
4	E	1	Total	C	N	O	0	0
			10	4	1	5		
4	G	1	Total	C	N	O	0	0
			10	4	1	5		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	10	Total	O	0	0
			10	10		

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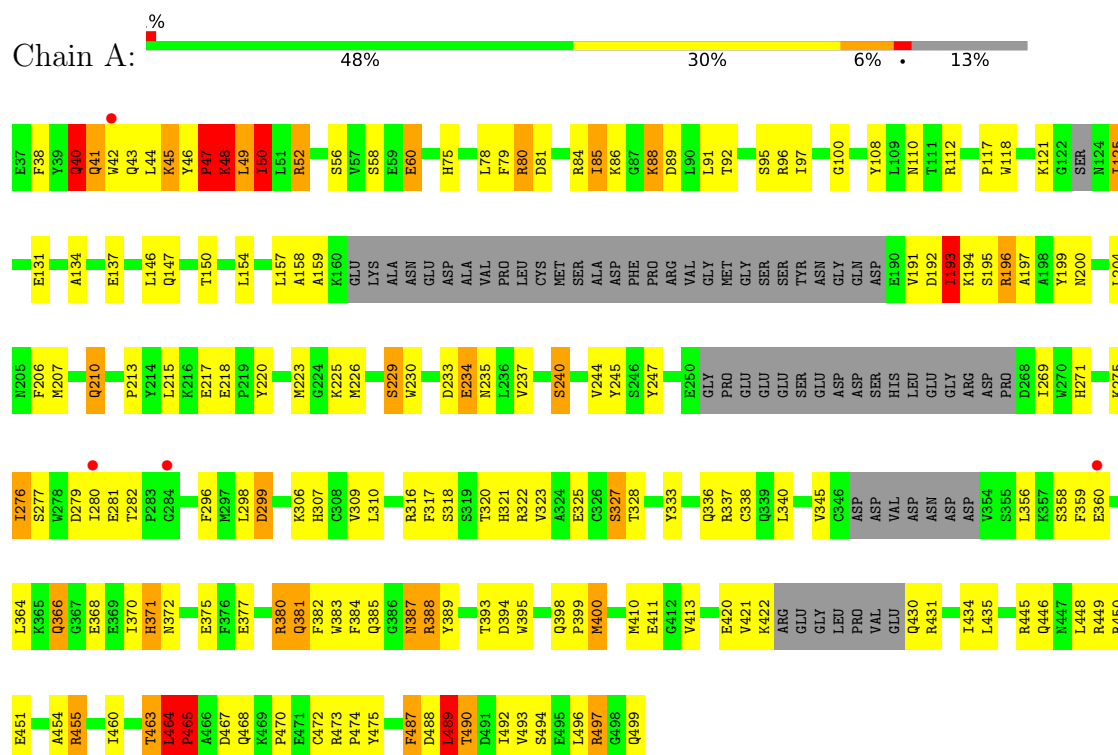
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	3	Total 3	O 3	0	0
5	D	2	Total 2	O 2	0	0
5	E	1	Total 1	O 1	0	0
5	G	2	Total 2	O 2	0	0

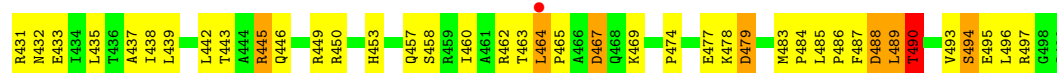
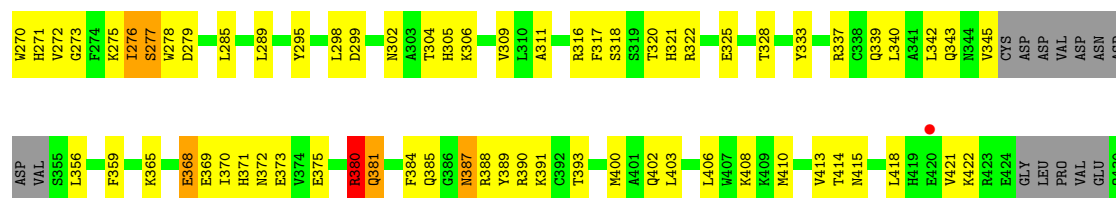
3 Residue-property plots

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.

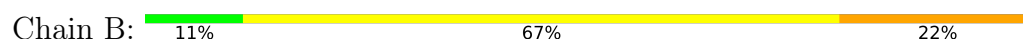
• Molecule 1: Alpha-ketoglutarate-dependent dioxygenase FTO







- Molecule 2: DNA (5'-D(P*TP*CP*TP*(6MA)P*TP*AP*TP*CP*G)-3')



- Molecule 2: DNA (5'-D(P*TP*CP*TP*(6MA)P*TP*AP*TP*CP*G)-3')



- Molecule 2: DNA (5'-D(P*TP*CP*TP*(6MA)P*TP*AP*TP*CP*G)-3')



- Molecule 2: DNA (5'-D(P*TP*CP*TP*(6MA)P*TP*AP*TP*CP*G)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	122.74Å 160.03Å 276.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.17 – 3.30 35.17 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.1 (35.17-3.30) 99.4 (35.17-3.30)	Depositor EDS
R_{merge}	0.29	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 3.32Å)	Xtrriage
Refinement program	PHENIX (1.10.1_2155)	Depositor
R, R_{free}	0.271 , 0.292 0.275 , 0.295	Depositor DCC
R_{free} test set	2063 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	75.6	Xtrriage
Anisotropy	0.578	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 27.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	13828	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.81 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.4472e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: MN, 6MA, OGA

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	1.14	13/3361 (0.4%)	1.36	31/4550 (0.7%)
1	C	1.18	18/3309 (0.5%)	1.24	25/4482 (0.6%)
1	E	0.83	9/3307 (0.3%)	1.16	25/4480 (0.6%)
1	G	1.00	9/3374 (0.3%)	1.24	30/4568 (0.7%)
2	B	1.19	1/177 (0.6%)	1.23	2/268 (0.7%)
2	D	0.25	0/177	0.54	0/268
2	F	0.46	0/177	0.57	0/268
2	H	0.24	0/177	0.51	0/268
All	All	1.03	50/14059 (0.4%)	1.23	113/19152 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1
1	G	0	1
All	All	0	2

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	43	GLN	C-N	14.10	1.52	1.33
1	A	47	PRO	CA-C	-11.38	1.42	1.52
2	B	8	DT	O3'-P	-10.59	1.45	1.61
1	G	50	ILE	C-O	-10.27	1.13	1.24
1	C	214	TYR	CA-C	-9.20	1.41	1.52
1	G	51	LEU	C-O	-8.94	1.13	1.24
1	E	62	HIS	N-CA	-7.47	1.37	1.46
1	G	90	LEU	C-O	-7.42	1.15	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	481	ALA	C-N	7.39	1.44	1.33
1	A	464	LEU	C-O	-7.31	1.18	1.24
1	C	324	ALA	C-O	-7.25	1.14	1.23
1	A	48	LYS	C-O	-7.20	1.15	1.24
1	C	214	TYR	C-O	-6.96	1.16	1.24
1	A	47	PRO	N-CA	-6.82	1.40	1.47
1	C	48	LYS	C-O	-6.74	1.15	1.24
1	C	50	ILE	C-O	-6.62	1.17	1.24
1	C	395	TRP	CA-C	-6.53	1.44	1.52
1	A	225	LYS	C-O	-6.44	1.15	1.23
1	G	490	THR	C-O	-6.42	1.16	1.24
1	G	59	GLU	C-O	-6.41	1.16	1.24
1	E	48	LYS	C-O	-6.40	1.15	1.24
1	G	494	SER	CA-C	-6.24	1.44	1.52
1	A	48	LYS	N-CA	-6.21	1.38	1.46
1	E	50	ILE	C-O	-6.00	1.18	1.24
1	E	384	PHE	C-O	-5.96	1.17	1.24
1	C	397	CYS	C-O	-5.88	1.17	1.24
1	G	488	ASP	CA-C	-5.87	1.45	1.52
1	A	465	PRO	C-O	-5.86	1.16	1.23
1	E	46	TYR	CA-C	5.85	1.60	1.52
1	C	85	ILE	N-CA	-5.84	1.40	1.46
1	C	46	TYR	CA-C	5.71	1.60	1.52
1	A	465	PRO	CA-C	-5.66	1.46	1.52
1	C	395	TRP	CA-CB	-5.58	1.44	1.53
1	A	50	ILE	C-O	-5.54	1.16	1.24
1	A	490	THR	C-O	-5.51	1.17	1.24
1	C	395	TRP	CB-CG	-5.46	1.33	1.50
1	E	62	HIS	C-O	-5.44	1.17	1.24
1	C	327	SER	CA-C	-5.36	1.45	1.52
1	G	43	GLN	C-O	-5.35	1.17	1.24
1	C	62	HIS	C-O	-5.33	1.18	1.24
1	C	324	ALA	CA-C	-5.25	1.46	1.52
1	C	331	LEU	C-N	-5.25	1.27	1.33
1	C	52	ARG	C-O	-5.25	1.18	1.24
1	E	108	TYR	CA-C	-5.21	1.46	1.52
1	E	460	ILE	C-O	-5.15	1.17	1.24
1	C	330	THR	C-O	-5.10	1.17	1.23
1	A	88	LYS	C-O	-5.07	1.17	1.23
1	G	50	ILE	CA-C	-5.04	1.46	1.52
1	A	465	PRO	CA-CB	-5.04	1.47	1.53
1	A	42	TRP	C-O	-5.01	1.17	1.24

All (113) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	47	PRO	CB-CA-C	-32.02	84.98	111.87
1	A	47	PRO	N-CA-C	21.44	146.33	110.74
1	E	128	THR	N-CA-C	16.19	132.13	111.24
1	G	277	SER	N-CA-C	15.12	127.25	111.07
1	G	47	PRO	N-CA-C	14.16	132.76	113.65
2	B	8	DT	C2'-C3'-O3'	-12.67	92.50	111.50
1	A	47	PRO	O-C-N	12.64	131.70	122.73
1	C	47	PRO	N-CA-C	12.30	130.63	113.53
1	E	46	TYR	N-CA-C	12.29	136.97	109.81
1	E	46	TYR	CA-C-N	12.07	132.45	119.05
1	E	46	TYR	C-N-CA	12.07	132.45	119.05
1	C	46	TYR	CA-C-N	12.01	132.38	119.05
1	C	46	TYR	C-N-CA	12.01	132.38	119.05
1	A	48	LYS	N-CA-C	-11.97	85.31	110.80
1	G	46	TYR	CA-C-N	11.93	132.41	119.28
1	G	46	TYR	C-N-CA	11.93	132.41	119.28
1	C	116	VAL	N-CA-C	-11.93	98.37	108.63
1	C	46	TYR	N-CA-C	11.89	136.08	109.81
1	G	46	TYR	N-CA-C	11.68	135.62	109.81
1	E	47	PRO	N-CA-C	11.65	129.72	113.53
1	A	488	ASP	N-CA-C	11.62	123.63	110.97
1	E	485	LEU	CA-C-N	11.34	131.42	120.31
1	E	485	LEU	C-N-CA	11.34	131.42	120.31
1	C	43	GLN	O-C-N	11.15	136.88	122.39
1	A	40	GLN	N-CA-C	10.97	125.36	110.55
1	G	190	GLU	N-CA-C	-10.95	95.65	111.30
1	A	487	PHE	N-CA-C	-10.93	93.52	109.59
1	G	277	SER	CB-CA-C	-10.73	94.04	110.88
1	C	277	SER	N-CA-C	10.41	122.20	111.07
1	E	116	VAL	N-CA-C	-9.84	97.83	107.76
1	G	124	ASN	N-CA-C	9.72	124.86	111.74
1	G	121	LYS	N-CA-C	9.37	121.49	111.28
1	A	490	THR	N-CA-C	9.21	130.43	110.80
1	E	482	SER	CB-CA-C	-9.05	92.41	110.42
1	G	122	GLY	N-CA-C	-8.79	92.34	113.18
1	E	483	MET	N-CA-CB	8.63	125.73	110.37
1	E	128	THR	CB-CA-C	-8.53	96.79	110.86
1	G	50	ILE	CB-CA-C	-8.41	98.09	110.62
1	E	40	GLN	CA-C-N	-7.96	110.15	122.08
1	E	40	GLN	C-N-CA	-7.96	110.15	122.08
1	E	492	ILE	CB-CA-C	-7.94	101.81	111.97
1	C	43	GLN	CA-C-N	-7.87	109.42	122.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	43	GLN	C-N-CA	-7.87	109.42	122.17
1	A	42	TRP	N-CA-C	7.71	122.26	113.01
1	A	47	PRO	CA-C-N	7.65	136.15	121.54
1	A	47	PRO	C-N-CA	7.65	136.15	121.54
1	A	464	LEU	CA-C-N	7.40	127.44	119.89
1	A	464	LEU	C-N-CA	7.40	127.44	119.89
1	C	50	ILE	N-CA-C	7.29	118.62	108.12
1	A	193	ILE	CB-CA-C	-7.27	102.39	111.70
1	E	483	MET	N-CA-C	-7.25	93.80	109.81
1	C	125	ILE	N-CA-C	7.14	118.41	108.12
1	G	40	GLN	N-CA-C	7.08	120.18	109.41
1	G	432	ASN	N-CA-C	7.05	120.20	109.62
1	C	116	VAL	CB-CA-C	6.96	117.41	110.94
1	C	326	CYS	N-CA-C	6.96	121.03	112.54
1	C	48	LYS	N-CA-C	-6.79	104.98	112.72
1	A	380	ARG	CA-C-N	-6.78	111.62	120.44
1	A	380	ARG	C-N-CA	-6.78	111.62	120.44
1	C	490	THR	N-CA-C	6.73	117.96	108.00
1	C	398	GLN	CA-C-N	6.68	128.19	119.84
1	C	398	GLN	C-N-CA	6.68	128.19	119.84
1	A	490	THR	CB-CA-C	-6.65	97.19	110.42
1	G	489	LEU	N-CA-C	-6.63	96.69	110.80
1	A	277	SER	N-CA-C	6.51	118.38	111.28
1	E	48	LYS	N-CA-C	-6.45	104.99	112.92
1	E	41	GLN	CB-CA-C	6.41	120.91	111.88
1	A	492	ILE	N-CA-C	6.39	117.17	110.72
1	G	46	TYR	C-N-CD	-6.38	98.83	125.00
1	C	485	LEU	C-N-CD	-6.20	99.59	125.00
1	G	278	TRP	N-CA-C	-6.12	105.64	113.23
1	E	492	ILE	N-CA-C	6.10	116.27	110.42
1	C	50	ILE	N-CA-CB	-6.03	102.72	111.52
1	G	47	PRO	N-CA-CB	-5.99	96.92	103.39
1	A	234	GLU	N-CA-C	5.97	119.39	110.14
1	C	46	TYR	C-N-CD	-5.93	100.69	125.00
1	G	489	LEU	CB-CA-C	5.88	122.13	110.42
1	A	489	LEU	CA-C-N	5.82	132.66	121.54
1	A	489	LEU	C-N-CA	5.82	132.66	121.54
1	E	46	TYR	C-N-CD	-5.76	101.39	125.00
2	B	9	DC	C2'-C3'-O3'	5.75	120.13	111.50
1	A	375	GLU	N-CA-C	5.73	117.33	111.14
1	C	386	GLY	N-CA-C	5.68	120.04	112.77
1	G	479	ASP	CB-CA-C	-5.67	98.35	110.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	465	PRO	CA-C-O	5.60	127.70	121.43
1	E	497	ARG	CA-C-N	-5.56	111.69	121.70
1	E	497	ARG	C-N-CA	-5.56	111.69	121.70
1	A	420	GLU	CA-C-N	-5.56	112.61	121.34
1	A	420	GLU	C-N-CA	-5.56	112.61	121.34
1	C	213	PRO	N-CA-C	5.52	120.80	113.40
1	E	116	VAL	CA-C-O	5.51	122.40	119.15
1	C	358	SER	N-CA-C	5.45	116.69	108.46
1	G	276	ILE	N-CA-C	-5.42	101.84	109.21
1	G	51	LEU	CA-C-N	5.34	130.69	123.11
1	G	51	LEU	C-N-CA	5.34	130.69	123.11
1	E	385	GLN	N-CA-C	5.31	120.56	112.54
1	A	327	SER	N-CA-C	-5.28	103.05	110.50
1	A	380	ARG	O-C-N	-5.27	116.53	122.12
1	A	85	ILE	N-CA-C	5.27	114.85	107.37
1	A	60	GLU	N-CA-C	-5.25	105.73	111.82
1	C	50	ILE	CB-CA-C	-5.22	102.70	110.33
1	E	388	ARG	N-CA-C	-5.22	105.50	111.14
1	E	327	SER	N-CA-C	-5.21	103.15	110.50
1	A	86	LYS	N-CA-C	5.21	118.90	111.92
1	G	494	SER	CA-C-N	-5.15	113.33	120.38
1	G	494	SER	C-N-CA	-5.15	113.33	120.38
1	G	50	ILE	N-CA-C	5.14	115.89	108.48
1	G	110	ASN	CA-C-N	-5.10	115.53	122.93
1	G	110	ASN	C-N-CA	-5.10	115.53	122.93
1	G	380	ARG	CA-C-N	-5.07	113.55	120.44
1	G	380	ARG	C-N-CA	-5.07	113.55	120.44
1	G	226	MET	N-CA-C	5.01	117.07	108.90
1	C	390	ARG	N-CA-C	-5.01	106.27	112.38

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	45	LYS	Mainchain
1	G	45	LYS	Mainchain

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	3282	0	3226	192	1
1	C	3230	0	3164	289	0
1	E	3228	0	3161	217	0
1	G	3294	0	3237	244	1
2	B	183	0	106	8	0
2	D	183	0	106	7	0
2	F	183	0	106	11	0
2	H	183	0	106	10	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
4	A	10	0	3	3	0
4	C	10	0	3	4	0
4	E	10	0	3	0	0
4	G	10	0	3	5	0
5	A	10	0	0	1	0
5	C	3	0	0	1	0
5	D	2	0	0	0	0
5	E	1	0	0	0	0
5	G	2	0	0	0	0
All	All	13828	0	13224	941	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 35.

All (941) 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:46:TYR:HB3	1:G:47:PRO:CD	1.24	1.56
1:C:46:TYR:CB	1:C:47:PRO:HD3	1.15	1.45
1:G:46:TYR:CB	1:G:47:PRO:HD3	1.27	1.43
1:E:46:TYR:HB3	1:E:47:PRO:CD	1.04	1.41
1:E:46:TYR:CB	1:E:47:PRO:HD3	1.16	1.39
1:E:57:VAL:CG1	1:E:62:HIS:HE1	1.35	1.36
1:C:46:TYR:HB3	1:C:47:PRO:CD	1.07	1.34
1:G:218:GLU:HA	1:G:226:MET:CE	1.58	1.31
1:E:48:LYS:NZ	1:E:299:ASP:OD2	1.60	1.29
1:E:57:VAL:CG1	1:E:62:HIS:CE1	2.16	1.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:268:ASP:HB3	1:C:313:SER:OG	1.40	1.21
1:E:57:VAL:HG13	1:E:62:HIS:CE1	1.75	1.20
1:G:53:GLU:O	1:G:56:SER:OG	1.60	1.20
1:G:218:GLU:CA	1:G:226:MET:HE3	1.72	1.19
1:A:460:ILE:O	1:A:463:THR:HG22	1.42	1.19
1:C:77:CYS:SG	1:C:392:CYS:SG	1.18	1.18
1:G:445:ARG:CD	1:G:449:ARG:HH11	1.61	1.13
1:A:337:ARG:HH21	1:A:370:ILE:HG12	1.15	1.10
1:E:48:LYS:NZ	1:E:299:ASP:CG	2.11	1.09
1:E:46:TYR:HB3	1:E:47:PRO:HD2	1.34	1.08
1:C:81:ASP:OD1	1:C:388:ARG:NH2	1.87	1.08
1:G:333:TYR:OH	1:G:337:ARG:NH1	1.85	1.07
1:E:46:TYR:CG	1:E:47:PRO:HD3	1.92	1.05
1:A:237:VAL:O	1:A:240:SER:OG	1.75	1.04
1:C:483:MET:HE2	1:C:483:MET:HA	1.35	1.04
1:G:368:GLU:OE2	1:G:414:THR:OG1	1.76	1.03
1:G:309:VAL:CG2	4:G:1002:OGA:H4C1	1.88	1.03
1:G:218:GLU:HA	1:G:226:MET:HE3	1.03	1.02
1:E:462:ARG:HH21	1:E:462:ARG:HB2	1.21	1.01
1:E:458:SER:O	1:E:462:ARG:NH2	1.94	1.00
1:E:462:ARG:HB2	1:E:462:ARG:NH2	1.78	0.99
1:A:112:ARG:H	1:A:381:GLN:HE22	1.00	0.99
1:C:400:MET:HE3	1:C:403:LEU:HD12	1.43	0.98
1:C:121:LYS:H	1:C:121:LYS:HD2	1.28	0.98
1:C:105:THR:OG1	1:C:112:ARG:NH2	1.97	0.98
1:E:475:TYR:CE1	1:E:487:PHE:CD2	2.52	0.97
1:C:151:ILE:CD1	1:C:194:LYS:HE3	1.94	0.97
1:C:238:ASP:OD1	1:C:239:ARG:HG2	1.65	0.97
1:C:439:LEU:HD13	1:C:496:LEU:HD22	1.44	0.97
1:E:475:TYR:CE1	1:E:487:PHE:CE2	2.53	0.96
1:A:112:ARG:H	1:A:381:GLN:NE2	1.63	0.96
1:G:445:ARG:HG3	1:G:445:ARG:HH11	1.28	0.96
1:A:279:ASP:OD2	1:A:282:THR:HG23	1.65	0.95
1:C:62:HIS:O	1:C:66:GLN:HG3	1.65	0.95
1:G:309:VAL:HG21	4:G:1002:OGA:H4C1	1.48	0.95
1:G:445:ARG:HD2	1:G:449:ARG:HH11	1.30	0.95
1:G:445:ARG:HD3	1:G:449:ARG:HH11	1.29	0.95
1:A:446:GLN:HE22	1:A:490:THR:HG22	1.29	0.95
1:C:38:PHE:O	1:C:40:GLN:HG3	1.65	0.95
1:A:81:ASP:OD1	1:A:388:ARG:NH2	1.99	0.94
1:G:111:THR:HA	1:G:381:GLN:NE2	1.82	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:LEU:HD23	1:A:193:ILE:HG23	1.50	0.94
1:E:475:TYR:CD1	1:E:487:PHE:CE2	2.55	0.94
1:A:112:ARG:N	1:A:381:GLN:HE22	1.66	0.94
1:C:46:TYR:CG	1:C:47:PRO:HD3	2.02	0.93
1:C:46:TYR:HB3	1:C:47:PRO:HD2	1.49	0.93
1:C:135:ALA:O	1:C:138:THR:HG22	1.68	0.93
1:G:112:ARG:H	1:G:381:GLN:HE21	1.04	0.93
1:A:210:GLN:HE21	1:A:210:GLN:HA	1.33	0.93
1:E:485:LEU:HB3	1:E:486:PRO:CD	1.99	0.93
1:E:485:LEU:HB3	1:E:486:PRO:HD2	1.49	0.93
1:C:475:TYR:CD1	1:C:487:PHE:CE2	2.58	0.92
1:C:213:PRO:O	1:C:225:LYS:NZ	2.03	0.92
1:C:475:TYR:CD1	1:C:487:PHE:CD2	2.58	0.92
1:C:151:ILE:CD1	1:C:194:LYS:CE	2.47	0.92
1:C:57:VAL:CG2	1:C:62:HIS:CE1	2.53	0.91
1:G:112:ARG:H	1:G:381:GLN:NE2	1.67	0.91
1:G:464:LEU:HD13	1:G:464:LEU:H	1.36	0.91
1:E:40:GLN:O	1:E:41:GLN:OE1	1.89	0.91
1:C:151:ILE:HD11	1:C:194:LYS:CE	2.00	0.90
1:G:112:ARG:N	1:G:381:GLN:HE21	1.70	0.90
1:C:125:ILE:HD12	1:C:125:ILE:H	1.34	0.90
1:E:117:PRO:HD2	1:E:127:HIS:HE1	1.35	0.89
1:G:435:LEU:HD11	1:G:496:LEU:HG	1.53	0.89
1:C:309:VAL:CG2	4:C:1002:OGA:H4C1	2.03	0.89
1:A:393:THR:HG22	1:A:395:TRP:H	1.39	0.88
1:E:48:LYS:NZ	1:E:299:ASP:CB	2.37	0.88
1:G:400:MET:CE	1:G:403:LEU:HD12	2.04	0.87
1:G:40:GLN:O	1:G:40:GLN:NE2	2.08	0.87
1:E:37:GLU:N	1:E:37:GLU:OE1	2.08	0.87
1:G:387:ASN:O	1:G:387:ASN:ND2	2.07	0.87
1:G:400:MET:HE3	1:G:403:LEU:HD12	1.57	0.87
1:G:445:ARG:CD	1:G:449:ARG:NH1	2.36	0.87
1:E:112:ARG:HB3	1:E:381:GLN:HG2	1.54	0.87
1:G:445:ARG:HD3	1:G:449:ARG:NH1	1.89	0.86
1:C:458:SER:O	1:C:462:ARG:HG3	1.75	0.86
1:C:268:ASP:HB3	1:C:313:SER:CB	2.05	0.86
1:E:385:GLN:O	1:E:385:GLN:NE2	2.07	0.86
1:C:268:ASP:CB	1:C:313:SER:OG	2.24	0.86
1:E:57:VAL:HG11	1:E:62:HIS:HE1	1.41	0.86
1:E:57:VAL:HG12	1:E:62:HIS:HE1	1.38	0.86
1:G:443:THR:HG22	1:G:493:VAL:HG21	1.57	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:485:LEU:HB3	1:G:486:PRO:CD	2.05	0.85
1:A:193:ILE:O	1:A:194:LYS:C	2.15	0.85
1:A:337:ARG:HH21	1:A:370:ILE:CG1	1.89	0.85
1:A:497:ARG:HD3	1:C:41:GLN:NE2	1.92	0.85
1:E:119:PRO:O	1:E:140:LEU:HD22	1.77	0.84
1:C:337:ARG:HH21	1:C:370:ILE:CD1	1.89	0.84
1:C:112:ARG:O	1:C:385:GLN:NE2	2.09	0.84
1:E:458:SER:C	1:E:462:ARG:HH22	1.85	0.83
1:A:80:ARG:HG2	1:A:92:THR:O	1.78	0.83
1:C:475:TYR:CE1	1:C:487:PHE:HD2	1.96	0.83
1:C:316:ARG:HG2	1:C:317:PHE:N	1.92	0.83
1:A:279:ASP:OD2	1:A:282:THR:CG2	2.26	0.83
1:A:460:ILE:O	1:A:463:THR:CG2	2.27	0.83
1:G:121:LYS:HE3	1:G:121:LYS:O	1.77	0.83
1:E:80:ARG:HG2	1:E:80:ARG:HH21	1.41	0.83
1:G:48:LYS:NZ	1:G:299:ASP:HB3	1.92	0.83
1:A:84:ARG:NH2	1:A:89:ASP:OD1	2.13	0.82
1:E:46:TYR:CB	1:E:47:PRO:CD	1.95	0.82
1:A:464:LEU:HD12	1:A:464:LEU:H	1.43	0.82
1:E:100:GLY:C	1:E:118:TRP:NE1	2.38	0.82
1:A:40:GLN:O	1:A:40:GLN:NE2	2.12	0.81
1:G:112:ARG:N	1:G:381:GLN:NE2	2.27	0.81
1:E:475:TYR:CE1	1:E:487:PHE:HD2	1.99	0.81
1:C:475:TYR:CE1	1:C:487:PHE:CD2	2.69	0.81
1:G:218:GLU:CA	1:G:226:MET:CE	2.45	0.80
1:G:121:LYS:CE	1:G:121:LYS:HA	2.10	0.80
1:G:372:ASN:OD1	1:G:445:ARG:NH1	2.14	0.80
1:G:408:LYS:HE2	1:G:483:MET:SD	2.21	0.80
1:G:127:HIS:ND1	1:G:133:ALA:HB2	1.95	0.80
1:E:234:GLU:OE2	2:F:5:6MA:N6	2.12	0.80
1:C:151:ILE:HD11	1:C:194:LYS:NZ	1.97	0.79
1:C:189:ASP:CG	1:C:190:GLU:H	1.89	0.79
1:C:439:LEU:HD13	1:C:496:LEU:CD2	2.13	0.79
1:C:320:THR:CB	1:C:322:ARG:HH21	1.95	0.79
1:G:127:HIS:ND1	1:G:133:ALA:CB	2.46	0.79
1:A:382:PHE:HB2	1:A:400:MET:HE2	1.65	0.78
1:E:80:ARG:HH22	1:E:93:PRO:HA	1.49	0.78
1:A:213:PRO:HB2	2:B:9:DC:H3'	1.63	0.78
1:G:276:ILE:HG23	1:G:279:ASP:HB3	1.64	0.78
1:E:119:PRO:O	1:E:140:LEU:CD2	2.31	0.78
1:C:49:LEU:HD23	1:C:49:LEU:O	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:62:HIS:O	1:C:66:GLN:CG	2.31	0.78
1:C:237:VAL:HG12	1:C:240:SER:HB2	1.66	0.78
1:G:125:ILE:O	1:G:125:ILE:HD12	1.83	0.78
1:E:368:GLU:OE2	1:E:445:ARG:NH2	2.16	0.77
1:E:443:THR:HG22	1:E:493:VAL:HG11	1.66	0.77
1:G:237:VAL:HG23	1:G:240:SER:HB3	1.63	0.77
1:G:445:ARG:HG3	1:G:445:ARG:NH1	1.93	0.77
1:A:421:VAL:HG22	1:A:434:ILE:HD11	1.67	0.77
1:E:116:VAL:HG13	1:E:117:PRO:HD2	1.65	0.77
1:G:88:LYS:NZ	2:H:7:DA:OP2	2.16	0.77
1:C:337:ARG:HE	1:C:370:ILE:CD1	1.97	0.77
1:G:40:GLN:HG2	1:G:42:TRP:HB2	1.66	0.77
1:C:151:ILE:HD13	1:C:194:LYS:HE3	1.66	0.77
1:E:48:LYS:NZ	1:E:299:ASP:HB3	2.00	0.77
1:C:290:HIS:HB2	1:C:293:ASP:OD2	1.84	0.77
1:C:450:ARG:HG3	1:C:451:GLU:N	2.00	0.76
1:E:475:TYR:HE1	1:E:487:PHE:CE2	2.00	0.76
1:A:467:ASP:OD1	1:A:468:GLN:HG3	1.86	0.76
1:A:52:ARG:HG2	1:A:52:ARG:HH21	1.51	0.76
1:C:297:MET:HG2	1:C:301:LEU:HD23	1.67	0.76
1:C:449:ARG:HD2	1:C:487:PHE:HE1	1.51	0.76
1:A:446:GLN:HE22	1:A:490:THR:CG2	2.00	0.75
1:C:135:ALA:O	1:C:138:THR:CG2	2.34	0.75
1:C:483:MET:HA	1:C:483:MET:CE	2.15	0.75
1:G:485:LEU:HB3	1:G:486:PRO:HD2	1.68	0.75
1:C:309:VAL:HG22	4:C:1002:OGA:H4C1	1.67	0.75
1:A:84:ARG:O	1:A:110:ASN:ND2	2.19	0.75
1:C:445:ARG:O	1:C:449:ARG:HG2	1.87	0.75
2:F:9:DC:H5	2:H:10:DG:H1	1.35	0.75
1:A:147:GLN:NE2	5:A:1101:HOH:O	2.16	0.75
1:G:233:ASP:HB2	1:G:302:ASN:HD21	1.52	0.75
1:E:82:LEU:HD21	1:E:461:ALA:HB2	1.69	0.75
1:E:116:VAL:HG22	1:E:393:THR:HG21	1.69	0.75
1:E:475:TYR:HD1	1:E:487:PHE:CE2	2.02	0.74
1:E:274:PHE:HE1	1:E:297:MET:HE3	1.50	0.74
1:G:82:LEU:HD12	1:G:384:PHE:HZ	1.50	0.74
1:A:48:LYS:HE2	1:A:299:ASP:CB	2.17	0.74
1:C:138:THR:HG23	1:C:139:PHE:N	2.00	0.74
1:C:331:LEU:HD12	1:C:334:ILE:CG2	2.17	0.74
1:C:320:THR:OG1	1:C:322:ARG:NH2	2.18	0.74
1:A:207:MET:HE1	1:A:215:LEU:HD11	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:100:GLY:O	1:E:118:TRP:CD1	2.41	0.73
1:E:475:TYR:CD1	1:E:487:PHE:CD2	2.76	0.73
1:C:445:ARG:O	1:C:449:ARG:CG	2.36	0.73
1:A:125:ILE:HD12	1:A:125:ILE:O	1.89	0.73
1:G:333:TYR:CZ	1:G:337:ARG:NH1	2.55	0.73
1:E:475:TYR:CE1	1:E:487:PHE:HE2	2.03	0.73
1:E:100:GLY:HA2	1:E:118:TRP:CE2	2.23	0.73
1:G:215:LEU:HD22	1:G:226:MET:O	1.89	0.73
1:C:125:ILE:HD12	1:C:125:ILE:N	2.04	0.72
1:A:337:ARG:NH2	1:A:370:ILE:HG12	1.99	0.72
1:A:150:THR:HG21	1:A:199:TYR:OH	1.89	0.72
1:C:400:MET:HE3	1:C:403:LEU:CD1	2.19	0.72
1:A:233:ASP:OD1	1:A:307:HIS:CE1	2.43	0.72
1:G:40:GLN:HE21	1:G:40:GLN:C	1.98	0.71
1:G:445:ARG:HD2	1:G:449:ARG:NH1	2.03	0.71
1:C:400:MET:CE	1:C:403:LEU:HD12	2.20	0.71
1:E:207:MET:HE1	1:E:215:LEU:HD11	1.72	0.71
1:G:48:LYS:NZ	1:G:299:ASP:OD2	2.23	0.71
1:A:384:PHE:CZ	1:A:455:ARG:HD3	2.25	0.71
1:C:210:GLN:NE2	1:C:313:SER:O	2.23	0.71
1:G:121:LYS:HE3	1:G:121:LYS:HA	1.69	0.71
1:G:375:GLU:OE2	1:G:380:ARG:NH1	2.24	0.71
1:E:215:LEU:HB2	1:E:225:LYS:HD3	1.72	0.71
1:A:464:LEU:HD12	1:A:464:LEU:N	2.01	0.71
1:C:356:LEU:HD23	1:C:356:LEU:N	2.06	0.71
1:C:90:LEU:HD12	1:C:91:LEU:O	1.90	0.70
1:E:117:PRO:HD2	1:E:127:HIS:CE1	2.22	0.70
1:G:233:ASP:HB2	1:G:302:ASN:ND2	2.06	0.70
1:G:460:ILE:O	1:G:463:THR:OG1	2.08	0.70
1:E:117:PRO:CD	1:E:127:HIS:HE1	2.04	0.70
1:C:475:TYR:HD1	1:C:487:PHE:CD2	2.09	0.70
1:G:40:GLN:NE2	1:G:40:GLN:H	1.89	0.70
1:C:268:ASP:N	1:C:268:ASP:OD1	2.24	0.70
1:G:105:THR:OG1	1:G:112:ARG:NH1	2.23	0.70
1:E:108:TYR:HB2	1:E:234:GLU:OE1	1.91	0.70
1:E:404:GLU:OE1	1:E:473:ARG:NH1	2.18	0.70
1:C:57:VAL:HG22	1:C:62:HIS:CE1	2.25	0.70
1:C:431:ARG:HG3	1:C:431:ARG:HH11	1.55	0.70
1:E:46:TYR:CD2	1:E:47:PRO:HD3	2.27	0.70
1:G:483:MET:HG3	1:G:484:PRO:HD2	1.73	0.70
1:G:48:LYS:NZ	1:G:299:ASP:CB	2.54	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:81:ASP:OD1	1:G:388:ARG:NH2	2.25	0.69
1:C:337:ARG:HH21	1:C:370:ILE:HD11	1.56	0.69
1:E:118:TRP:CD1	1:E:118:TRP:H	2.08	0.69
1:E:88:LYS:HD2	2:F:6:DT:H1'	1.74	0.69
1:E:237:VAL:HG13	1:E:240:SER:HB3	1.74	0.69
1:A:79:PHE:HB2	1:A:388:ARG:NH1	2.07	0.69
1:A:371:HIS:CD2	1:A:445:ARG:NH2	2.60	0.69
1:C:300:ASP:O	1:C:303:ALA:N	2.23	0.69
1:E:341:ALA:HB2	1:E:370:ILE:HD13	1.74	0.69
1:A:237:VAL:HG23	1:A:240:SER:OG	1.92	0.69
1:C:154:LEU:HD23	1:C:193:ILE:HG23	1.75	0.68
1:G:309:VAL:HG22	4:G:1002:OGA:H4C1	1.76	0.68
1:C:121:LYS:HD2	1:C:121:LYS:N	2.07	0.68
1:G:159:ALA:O	1:G:160:LYS:HD2	1.94	0.68
1:A:422:LYS:NZ	1:A:422:LYS:HB3	2.07	0.68
1:G:483:MET:HG3	1:G:484:PRO:CD	2.24	0.68
1:A:112:ARG:O	1:A:385:GLN:NE2	2.27	0.68
1:E:337:ARG:HG3	1:E:370:ILE:HG12	1.75	0.67
1:A:192:ASP:O	1:A:195:SER:HB3	1.94	0.67
1:C:492:ILE:HD12	1:C:492:ILE:N	2.09	0.67
1:C:289:LEU:HD13	1:C:316:ARG:HH11	1.58	0.67
1:A:48:LYS:HE2	1:A:299:ASP:HB3	1.76	0.67
1:A:52:ARG:HH21	1:A:52:ARG:CG	2.07	0.67
1:C:84:ARG:NH2	1:C:84:ARG:HG3	2.08	0.67
1:E:80:ARG:HH21	1:E:80:ARG:CG	2.07	0.67
1:A:497:ARG:NH1	1:A:497:ARG:HG3	2.09	0.67
1:C:151:ILE:CD1	1:C:194:LYS:CD	2.73	0.67
1:C:407:TRP:O	1:C:410:MET:N	2.27	0.66
1:C:489:LEU:HD23	1:C:489:LEU:O	1.95	0.66
1:A:382:PHE:CB	1:A:400:MET:HE2	2.26	0.66
1:E:458:SER:HB3	1:E:461:ALA:HB3	1.76	0.66
1:G:446:GLN:NE2	1:G:450:ARG:HH12	1.92	0.66
1:G:477:GLU:O	1:G:479:ASP:N	2.28	0.66
1:E:445:ARG:O	1:E:449:ARG:HG2	1.95	0.66
1:G:111:THR:HA	1:G:381:GLN:HE21	1.61	0.66
1:E:233:ASP:OD1	1:E:307:HIS:HE1	1.78	0.66
1:G:400:MET:HE3	1:G:400:MET:HA	1.78	0.66
1:C:69:PHE:HE1	1:C:204:LEU:HD22	1.59	0.65
1:E:117:PRO:HG2	1:E:127:HIS:CE1	2.31	0.65
1:G:269:ILE:HG12	1:G:271:HIS:HE1	1.62	0.65
1:A:279:ASP:OD1	1:A:280:ILE:N	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:ARG:HA	1:C:204:LEU:O	1.96	0.65
1:E:146:LEU:HD12	1:E:321:HIS:CD2	2.32	0.65
1:A:325:GLU:OE2	1:A:327:SER:OG	2.14	0.65
1:C:289:LEU:CD1	1:C:316:ARG:NH1	2.60	0.65
1:C:415:ASN:HA	1:C:418:LEU:CD2	2.25	0.65
2:F:3:DC:O2	1:G:306:LYS:HE3	1.97	0.65
1:G:121:LYS:HE3	1:G:121:LYS:CA	2.25	0.65
1:C:151:ILE:CD1	1:C:194:LYS:HD2	2.27	0.65
1:C:280:ILE:HG12	1:C:280:ILE:O	1.95	0.65
1:G:389:TYR:O	1:G:390:ARG:C	2.36	0.65
1:E:41:GLN:OE1	1:E:41:GLN:HA	1.96	0.65
1:C:340:LEU:HD13	1:C:340:LEU:O	1.97	0.65
1:C:45:LYS:CE	1:C:287:ILE:HD11	2.26	0.64
1:A:371:HIS:CD2	1:A:445:ARG:HH22	2.15	0.64
1:C:407:TRP:O	1:C:408:LYS:C	2.39	0.64
1:G:111:THR:CA	1:G:381:GLN:NE2	2.57	0.64
1:A:385:GLN:O	1:A:388:ARG:HG2	1.98	0.64
1:C:52:ARG:HG3	1:C:296:PHE:HE1	1.62	0.64
1:G:48:LYS:HZ1	1:G:299:ASP:HB3	1.61	0.64
1:C:268:ASP:HB3	1:C:313:SER:HG	1.58	0.64
1:C:337:ARG:HE	1:C:370:ILE:HD12	1.61	0.64
1:C:390:ARG:HA	1:C:393:THR:O	1.96	0.64
1:C:119:PRO:O	1:C:140:LEU:CD2	2.46	0.64
1:C:475:TYR:CD1	1:C:487:PHE:HE2	2.10	0.64
1:C:331:LEU:HD12	1:C:334:ILE:HG22	1.79	0.64
1:A:384:PHE:CD1	1:A:470:PRO:HB3	2.33	0.64
1:G:48:LYS:HZ2	1:G:299:ASP:CB	2.10	0.64
1:A:44:LEU:HD12	1:A:44:LEU:N	2.13	0.64
1:C:57:VAL:CG2	1:C:62:HIS:NE2	2.61	0.64
1:C:101:ASN:O	1:C:115:THR:HG21	1.98	0.64
1:C:138:THR:HG23	1:C:139:PHE:H	1.63	0.63
1:E:475:TYR:HE1	1:E:487:PHE:CD2	2.06	0.63
1:C:84:ARG:HG3	1:C:84:ARG:HH21	1.61	0.63
1:G:272:VAL:HG11	1:G:295:TYR:CE2	2.33	0.63
1:E:57:VAL:HG11	1:E:62:HIS:CE1	2.21	0.63
1:G:316:ARG:HH22	4:G:1002:OGA:C5	2.12	0.63
1:A:368:GLU:O	1:A:371:HIS:HB3	1.99	0.63
1:C:289:LEU:HD13	1:C:316:ARG:NH1	2.12	0.63
1:E:228:VAL:HB	1:E:309:VAL:HG22	1.81	0.63
1:C:91:LEU:HG	1:C:460:ILE:HD11	1.79	0.63
1:G:269:ILE:CG1	1:G:271:HIS:CE1	2.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:ARG:NH1	1:A:377:GLU:HG3	2.14	0.63
1:A:358:SER:OG	1:A:360:GLU:OE2	2.16	0.63
1:A:40:GLN:C	1:A:40:GLN:HE21	2.06	0.62
1:C:84:ARG:NH2	1:C:455:ARG:HG3	2.14	0.62
1:A:58:SER:C	1:A:60:GLU:H	2.06	0.62
1:C:446:GLN:OE1	1:C:488:ASP:HB3	1.98	0.62
1:E:101:ASN:N	1:E:118:TRP:NE1	2.48	0.62
1:E:80:ARG:HG2	1:E:80:ARG:NH2	2.09	0.62
1:C:338:CYS:O	1:C:341:ALA:HB3	1.98	0.62
1:E:402:GLN:O	1:E:406:LEU:HD13	1.98	0.62
1:C:340:LEU:HD13	1:C:340:LEU:C	2.25	0.62
1:C:151:ILE:HD11	1:C:194:LYS:CD	2.29	0.62
1:E:40:GLN:C	1:E:41:GLN:OE1	2.41	0.62
1:G:218:GLU:HG2	1:G:226:MET:HE2	1.82	0.62
1:C:341:ALA:HB2	1:C:370:ILE:HG21	1.82	0.62
1:C:57:VAL:HG22	1:C:62:HIS:NE2	2.15	0.62
1:E:91:LEU:HB2	1:E:460:ILE:HD11	1.82	0.62
1:G:218:GLU:N	1:G:226:MET:HE3	2.14	0.62
1:G:446:GLN:HE21	1:G:450:ARG:NH1	1.98	0.62
1:G:40:GLN:CG	1:G:42:TRP:HB2	2.30	0.61
1:G:131:GLU:O	1:G:134:ALA:N	2.33	0.61
1:A:49:LEU:O	1:A:49:LEU:HG	2.00	0.61
1:C:300:ASP:O	1:C:301:LEU:C	2.42	0.61
1:G:40:GLN:H	1:G:40:GLN:CD	2.07	0.61
1:C:189:ASP:OD1	1:C:190:GLU:N	2.33	0.61
1:C:415:ASN:HA	1:C:418:LEU:HD22	1.81	0.61
1:A:147:GLN:O	1:A:150:THR:OG1	2.13	0.61
1:G:85:ILE:HG23	1:G:85:ILE:O	1.99	0.61
1:G:309:VAL:HG21	4:G:1002:OGA:C4	2.27	0.61
1:C:205:ASN:HB2	1:C:318:SER:OG	2.00	0.61
1:G:125:ILE:HD12	1:G:125:ILE:C	2.25	0.61
1:C:45:LYS:CE	1:C:287:ILE:CD1	2.78	0.61
1:G:213:PRO:HG3	2:H:9:DC:P	2.41	0.61
1:G:477:GLU:O	1:G:478:LYS:C	2.42	0.61
1:E:94:VAL:HG11	1:E:205:ASN:HB3	1.82	0.61
1:G:48:LYS:HZ2	1:G:299:ASP:HB3	1.60	0.61
1:G:100:GLY:HA2	1:G:118:TRP:CE2	2.36	0.60
1:C:337:ARG:NH2	1:C:370:ILE:HD11	2.15	0.60
1:E:85:ILE:HG22	1:E:109:LEU:HD22	1.83	0.60
1:A:421:VAL:HG12	1:A:421:VAL:O	2.00	0.60
1:E:100:GLY:C	1:E:118:TRP:CD1	2.79	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:109:LEU:O	1:E:110:ASN:HB2	2.02	0.60
1:A:112:ARG:N	1:A:381:GLN:NE2	2.37	0.60
1:A:112:ARG:HB3	1:A:381:GLN:NE2	2.17	0.60
1:C:356:LEU:HB2	1:C:359:PHE:HE1	1.65	0.60
1:E:475:TYR:CD1	1:E:487:PHE:HE2	2.14	0.60
1:E:247:TYR:HB3	1:E:317:PHE:HB2	1.84	0.60
1:A:309:VAL:CG2	4:A:1002:OGA:H4C1	2.30	0.60
1:C:151:ILE:HD11	1:C:194:LYS:HD2	1.84	0.60
1:C:238:ASP:OD1	1:C:239:ARG:CG	2.47	0.60
1:E:411:GLU:O	1:E:414:THR:OG1	2.17	0.60
1:A:463:THR:O	1:A:463:THR:OG1	2.19	0.60
1:E:40:GLN:C	1:E:42:TRP:H	2.10	0.60
1:E:80:ARG:HG2	1:E:92:THR:O	2.02	0.60
1:G:49:LEU:HG	1:G:49:LEU:O	2.01	0.60
1:E:80:ARG:NH2	1:E:92:THR:O	2.35	0.59
1:A:279:ASP:OD1	1:A:281:GLU:N	2.27	0.59
1:A:384:PHE:CD1	1:A:470:PRO:CB	2.85	0.59
1:A:147:GLN:HG3	1:A:197:ALA:O	2.03	0.59
1:C:46:TYR:CB	1:C:47:PRO:CD	1.98	0.59
1:C:218:GLU:OE1	1:C:230:TRP:NE1	2.35	0.59
1:C:44:LEU:HD12	1:C:44:LEU:N	2.18	0.59
1:G:414:THR:O	1:G:418:LEU:HD13	2.02	0.59
1:C:337:ARG:HE	1:C:370:ILE:HD11	1.66	0.59
1:G:320:THR:OG1	1:G:322:ARG:NH1	2.36	0.59
1:A:497:ARG:CD	1:C:41:GLN:NE2	2.66	0.59
1:C:344:ASN:HA	1:C:357:LYS:HB2	1.84	0.59
1:G:410:MET:O	1:G:413:VAL:HG12	2.03	0.59
1:A:497:ARG:HG3	1:A:497:ARG:HH11	1.66	0.58
1:G:368:GLU:HG3	1:G:445:ARG:HH22	1.67	0.58
1:A:279:ASP:OD2	1:A:282:THR:OG1	2.20	0.58
1:C:366:GLN:NE2	5:C:1101:HOH:O	2.35	0.58
1:E:116:VAL:CG1	1:E:117:PRO:HD2	2.33	0.58
1:G:380:ARG:NH2	1:G:474:PRO:O	2.36	0.58
1:E:410:MET:O	1:E:413:VAL:HG22	2.03	0.58
1:C:52:ARG:HG3	1:C:296:PHE:CE1	2.38	0.58
1:E:192:ASP:O	1:E:196:ARG:HG3	2.03	0.58
1:G:433:GLU:C	1:G:435:LEU:H	2.11	0.58
1:E:280:ILE:HG12	1:E:280:ILE:O	2.03	0.58
1:G:189:ASP:HB3	1:G:191:VAL:HG23	1.86	0.58
1:C:475:TYR:HE1	1:C:487:PHE:HD2	1.49	0.58
1:E:44:LEU:HD12	1:E:44:LEU:N	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:GLN:O	1:A:388:ARG:CG	2.52	0.58
1:E:116:VAL:HG22	1:E:393:THR:CG2	2.34	0.58
1:G:46:TYR:CB	1:G:47:PRO:CD	2.12	0.58
1:A:422:LYS:HB3	1:A:422:LYS:HZ1	1.68	0.58
1:A:421:VAL:CG2	1:A:434:ILE:HD11	2.34	0.57
1:C:41:GLN:O	1:C:41:GLN:HG2	2.04	0.57
1:C:85:ILE:HG22	1:C:90:LEU:HD23	1.85	0.57
1:C:237:VAL:CG1	1:C:240:SER:HB2	2.34	0.57
1:G:400:MET:HE1	1:G:403:LEU:HD12	1.85	0.57
1:A:84:ARG:NH2	1:A:89:ASP:CG	2.62	0.57
1:A:337:ARG:O	1:A:338:CYS:C	2.47	0.57
1:A:193:ILE:O	1:A:195:SER:N	2.37	0.57
1:A:497:ARG:HE	1:C:41:GLN:HE22	1.50	0.57
1:C:492:ILE:HD12	1:C:492:ILE:H	1.68	0.57
1:G:111:THR:HA	1:G:381:GLN:HE22	1.66	0.57
1:G:159:ALA:O	1:G:160:LYS:CD	2.53	0.57
2:B:6:DT:H4'	2:B:7:DA:OP2	2.05	0.57
1:E:84:ARG:O	1:E:84:ARG:HG2	2.04	0.57
1:C:415:ASN:O	1:C:418:LEU:HD23	2.05	0.57
1:C:119:PRO:O	1:C:140:LEU:HD22	2.05	0.57
1:E:334:ILE:HD11	1:E:374:VAL:HG22	1.86	0.57
1:C:483:MET:HE2	1:C:483:MET:CA	2.22	0.56
1:G:356:LEU:HD13	1:G:359:PHE:CE2	2.40	0.56
1:G:94:VAL:HG11	1:G:205:ASN:HB3	1.87	0.56
1:G:449:ARG:HD3	1:G:487:PHE:CE1	2.41	0.56
1:A:146:LEU:HD12	1:A:321:HIS:CD2	2.40	0.56
1:A:497:ARG:HH11	1:A:497:ARG:CG	2.18	0.56
1:C:382:PHE:O	1:C:386:GLY:CA	2.53	0.56
1:C:398:GLN:N	1:C:399:PRO:HD2	2.19	0.56
1:E:37:GLU:HG3	1:E:42:TRP:HZ3	1.69	0.56
2:F:3:DC:C2	1:G:306:LYS:HE3	2.40	0.56
1:A:134:ALA:O	1:A:137:GLU:HB3	2.04	0.56
1:A:192:ASP:O	1:A:196:ARG:HD3	2.06	0.56
1:E:106:TYR:OH	1:E:322:ARG:NH1	2.39	0.56
1:G:192:ASP:O	1:G:196:ARG:HG3	2.05	0.56
1:A:448:LEU:HD11	1:C:281:GLU:HG2	1.87	0.56
1:G:464:LEU:HD13	1:G:464:LEU:N	2.12	0.56
1:A:97:ILE:HD12	1:A:389:TYR:CE1	2.40	0.56
1:C:337:ARG:NH2	1:C:370:ILE:CD1	2.64	0.56
1:C:356:LEU:HB2	1:C:359:PHE:CE1	2.41	0.56
1:C:469:LYS:HG3	1:C:469:LYS:O	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:151:ILE:O	1:E:193:ILE:HD11	2.06	0.56
1:A:322:ARG:HH12	4:A:1002:OGA:C1	2.19	0.55
1:A:337:ARG:O	1:A:340:LEU:N	2.39	0.55
1:A:380:ARG:NH2	1:A:474:PRO:O	2.39	0.55
1:A:383:TRP:NE1	1:A:473:ARG:HD3	2.20	0.55
1:C:475:TYR:CD1	1:C:487:PHE:HD2	2.09	0.55
1:C:492:ILE:H	1:C:492:ILE:CD1	2.19	0.55
1:C:382:PHE:O	1:C:386:GLY:N	2.39	0.55
1:C:400:MET:CE	1:C:403:LEU:CD1	2.80	0.55
1:E:146:LEU:HD12	1:E:321:HIS:HD2	1.71	0.55
1:G:90:LEU:HD21	2:H:7:DA:H2'	1.88	0.55
1:G:439:LEU:HD21	1:G:497:ARG:HD3	1.88	0.55
1:A:47:PRO:HA	1:A:49:LEU:H	1.72	0.55
1:E:82:LEU:CD2	1:E:461:ALA:HB2	2.36	0.55
1:E:96:ARG:HA	1:E:204:LEU:O	2.06	0.55
1:E:336:GLN:O	1:E:339:GLN:HG3	2.07	0.55
1:A:112:ARG:HH12	1:A:377:GLU:HG3	1.71	0.55
1:C:57:VAL:HG21	1:C:62:HIS:CE1	2.39	0.55
1:C:157:LEU:HD23	1:C:157:LEU:O	2.07	0.55
1:E:91:LEU:HB2	1:E:460:ILE:CD1	2.37	0.55
1:G:83:VAL:HG22	1:G:111:THR:HG21	1.88	0.55
1:A:328:THR:HA	1:A:333:TYR:CG	2.42	0.55
1:G:121:LYS:HE3	1:G:121:LYS:C	2.31	0.55
1:G:269:ILE:HG12	1:G:271:HIS:CE1	2.42	0.55
1:G:400:MET:CE	1:G:403:LEU:CD1	2.80	0.55
1:C:233:ASP:OD1	1:C:307:HIS:HE1	1.85	0.55
1:E:100:GLY:HA2	1:E:118:TRP:CZ2	2.42	0.55
1:E:235:ASN:O	1:E:235:ASN:ND2	2.39	0.55
2:F:3:DC:N3	1:G:306:LYS:CE	2.69	0.55
1:G:75:HIS:NE2	1:G:131:GLU:OE1	2.34	0.55
1:E:375:GLU:OE2	1:E:380:ARG:NH1	2.39	0.55
1:G:276:ILE:CG2	1:G:279:ASP:HB3	2.36	0.55
1:C:276:ILE:HB	1:C:279:ASP:HB3	1.89	0.54
1:C:459:ARG:O	1:C:463:THR:HG23	2.07	0.54
1:E:42:TRP:CD1	1:E:285:LEU:HD12	2.42	0.54
1:A:445:ARG:O	1:A:449:ARG:HG3	2.07	0.54
1:C:48:LYS:NZ	1:C:299:ASP:OD2	2.40	0.54
2:H:2:DT:H6	2:H:2:DT:H5'	1.73	0.54
1:E:345:VAL:HG23	1:E:355:SER:O	2.07	0.54
1:E:401:ALA:HA	1:E:404:GLU:HG2	1.89	0.54
1:G:131:GLU:O	1:G:132:ILE:C	2.48	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:111:THR:CA	1:G:381:GLN:HE21	2.20	0.54
1:G:464:LEU:H	1:G:464:LEU:CD1	2.13	0.54
1:A:85:ILE:O	1:A:85:ILE:HG23	2.08	0.54
1:A:157:LEU:O	1:A:158:ALA:C	2.50	0.54
1:A:381:GLN:O	1:A:382:PHE:C	2.48	0.54
1:C:84:ARG:HH21	1:C:84:ARG:CG	2.18	0.54
1:E:98:LEU:HD12	1:E:99:ILE:N	2.21	0.54
1:E:235:ASN:C	1:E:235:ASN:HD22	2.15	0.54
1:E:244:VAL:HG11	1:E:295:TYR:CZ	2.42	0.54
1:G:304:THR:OG1	1:G:305:HIS:HD2	1.91	0.54
1:G:469:LYS:O	1:G:469:LYS:HG3	2.07	0.54
1:G:494:SER:O	1:G:495:GLU:C	2.46	0.54
1:A:125:ILE:HD12	1:A:125:ILE:C	2.32	0.54
1:A:210:GLN:HA	1:A:210:GLN:NE2	2.13	0.54
1:E:101:ASN:HA	1:E:118:TRP:HE1	1.72	0.54
1:G:48:LYS:NZ	1:G:299:ASP:CG	2.66	0.54
1:A:193:ILE:O	1:A:196:ARG:N	2.41	0.54
1:E:68:ALA:O	1:E:72:LEU:HB2	2.08	0.54
1:E:117:PRO:O	1:E:127:HIS:CE1	2.61	0.54
1:E:382:PHE:O	1:E:386:GLY:N	2.40	0.54
1:E:462:ARG:HB2	1:E:462:ARG:CZ	2.38	0.54
1:C:44:LEU:N	1:C:44:LEU:CD1	2.71	0.54
1:C:400:MET:HE3	1:C:400:MET:HA	1.90	0.54
1:E:118:TRP:H	1:E:118:TRP:HD1	1.52	0.54
1:C:492:ILE:O	1:C:496:LEU:HB2	2.07	0.54
1:E:118:TRP:CD1	1:E:118:TRP:N	2.73	0.54
1:E:380:ARG:NH2	1:E:474:PRO:O	2.40	0.54
1:E:485:LEU:CB	1:E:486:PRO:CD	2.68	0.54
1:C:50:ILE:HD12	1:C:298:LEU:HD11	1.89	0.54
1:C:157:LEU:HD23	1:C:157:LEU:C	2.33	0.54
1:A:79:PHE:HB2	1:A:388:ARG:HH12	1.71	0.53
1:C:45:LYS:HE3	1:C:287:ILE:CD1	2.38	0.53
1:C:357:LYS:O	1:C:358:SER:HB3	2.08	0.53
1:C:62:HIS:C	1:C:66:GLN:HG3	2.30	0.53
1:E:57:VAL:HG12	1:E:62:HIS:CE1	2.21	0.53
1:G:218:GLU:CD	1:G:220:TYR:H	2.17	0.53
1:G:421:VAL:HG21	1:G:435:LEU:HD13	1.90	0.53
1:C:334:ILE:HD11	1:C:374:VAL:HG22	1.90	0.53
1:A:431:ARG:HG2	1:A:431:ARG:HH11	1.74	0.53
1:C:189:ASP:CG	1:C:190:GLU:N	2.59	0.53
1:A:50:ILE:HD13	1:A:298:LEU:HD11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:109:LEU:O	1:C:110:ASN:HB2	2.08	0.53
1:G:244:VAL:HG21	1:G:295:TYR:CZ	2.44	0.53
1:C:447:ASN:O	1:C:450:ARG:HG2	2.09	0.53
1:C:406:LEU:HA	1:C:409:LYS:HD3	1.91	0.53
1:A:44:LEU:N	1:A:44:LEU:CD1	2.72	0.53
1:E:44:LEU:N	1:E:44:LEU:CD1	2.71	0.53
1:E:148:ILE:O	1:E:151:ILE:HG13	2.08	0.53
1:G:372:ASN:OD1	1:G:445:ARG:HG3	2.09	0.53
1:C:450:ARG:HG3	1:C:451:GLU:H	1.74	0.53
1:C:461:ALA:HB1	1:C:470:PRO:HG3	1.90	0.53
1:E:101:ASN:N	1:E:118:TRP:HE1	2.05	0.53
1:G:80:ARG:HD3	1:G:92:THR:O	2.09	0.52
1:C:81:ASP:CG	1:C:388:ARG:HH22	2.14	0.52
1:C:68:ALA:HB2	1:C:138:THR:HG21	1.90	0.52
1:C:118:TRP:HD1	1:C:118:TRP:O	1.92	0.52
1:C:316:ARG:HG2	1:C:317:PHE:O	2.09	0.52
1:C:337:ARG:NE	1:C:370:ILE:HD11	2.24	0.52
1:C:339:GLN:NE2	1:C:343:GLN:OE1	2.43	0.52
1:A:233:ASP:OD1	1:A:307:HIS:HE1	1.91	0.52
1:A:446:GLN:NE2	1:A:490:THR:HG22	2.11	0.52
1:C:90:LEU:O	1:C:90:LEU:HG	2.10	0.52
1:C:135:ALA:C	1:C:138:THR:HG22	2.33	0.52
1:A:431:ARG:HG2	1:A:431:ARG:NH1	2.24	0.52
1:E:287:ILE:HG13	1:E:287:ILE:O	2.10	0.52
1:G:368:GLU:O	1:G:369:GLU:C	2.51	0.52
1:C:272:VAL:HG21	1:C:295:TYR:CE2	2.45	0.52
1:C:483:MET:CE	1:C:483:MET:CA	2.85	0.52
1:G:464:LEU:N	1:G:464:LEU:CD1	2.72	0.52
1:A:84:ARG:HH22	1:A:89:ASP:CG	2.18	0.52
1:A:384:PHE:CZ	1:A:455:ARG:CD	2.92	0.52
1:E:216:LYS:H	2:F:7:DA:H2	1.58	0.52
1:E:496:LEU:N	1:E:496:LEU:CD2	2.73	0.52
1:G:82:LEU:HD12	1:G:384:PHE:CZ	2.40	0.52
1:G:150:THR:O	1:G:154:LEU:HB2	2.09	0.52
1:C:97:ILE:HG22	1:C:204:LEU:HB2	1.91	0.51
1:C:309:VAL:HG21	4:C:1002:OGA:H4C1	1.87	0.51
1:A:333:TYR:O	1:A:337:ARG:HG2	2.11	0.51
1:A:435:LEU:HD11	1:A:496:LEU:HD22	1.93	0.51
1:C:203:LEU:HD12	1:C:322:ARG:CZ	2.40	0.51
1:G:443:THR:CG2	1:G:493:VAL:HG21	2.35	0.51
1:G:467:ASP:OD1	1:G:467:ASP:N	2.27	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:490:THR:O	1:G:490:THR:OG1	2.28	0.51
1:A:247:TYR:HB3	1:A:317:PHE:HB2	1.92	0.51
1:C:356:LEU:N	1:C:356:LEU:CD2	2.73	0.51
1:E:278:TRP:HB2	2:H:2:DT:H4'	1.93	0.51
2:F:5:6MA:H5'	2:F:6:DT:H72	1.91	0.51
1:G:139:PHE:CE2	1:G:204:LEU:HD21	2.45	0.51
1:C:406:LEU:O	1:C:409:LYS:HB2	2.11	0.51
1:C:415:ASN:N	1:C:485:LEU:HD11	2.26	0.51
1:A:410:MET:O	1:A:413:VAL:HG22	2.11	0.51
1:G:485:LEU:HB3	1:G:486:PRO:HD3	1.91	0.51
1:C:112:ARG:NH2	1:C:112:ARG:HG3	2.25	0.51
1:E:485:LEU:HB3	1:E:486:PRO:HD3	1.89	0.51
1:G:213:PRO:HB2	2:H:9:DC:H3'	1.93	0.51
1:C:85:ILE:O	1:C:85:ILE:HG23	2.11	0.51
1:C:377:GLU:O	1:C:377:GLU:HG3	2.11	0.51
1:E:94:VAL:CG1	1:E:205:ASN:HB3	2.41	0.51
1:E:101:ASN:CA	1:E:118:TRP:HE1	2.23	0.51
1:G:82:LEU:HD21	1:G:460:ILE:HG23	1.93	0.51
1:E:61:LEU:O	1:E:62:HIS:C	2.51	0.51
1:E:433:GLU:C	1:E:435:LEU:H	2.18	0.51
1:G:339:GLN:O	1:G:343:GLN:HG3	2.11	0.51
1:E:100:GLY:CA	1:E:118:TRP:CE2	2.94	0.50
1:G:431:ARG:HD3	1:G:433:GLU:HG3	1.93	0.50
1:C:82:LEU:HD12	1:C:460:ILE:HG12	1.93	0.50
1:E:48:LYS:HD2	1:E:299:ASP:HB3	1.92	0.50
1:A:48:LYS:HE2	1:A:299:ASP:HB2	1.94	0.50
1:C:216:LYS:HG3	2:D:7:DA:C2	2.47	0.50
1:E:460:ILE:HG13	1:E:460:ILE:O	2.11	0.50
1:G:77:CYS:O	1:G:97:ILE:HD13	2.11	0.50
1:A:449:ARG:HD3	1:A:487:PHE:CE1	2.46	0.50
1:C:492:ILE:N	1:C:492:ILE:CD1	2.73	0.50
1:C:151:ILE:HD12	1:C:194:LYS:HD2	1.93	0.50
1:G:80:ARG:HD2	1:G:91:LEU:HD22	1.94	0.50
1:G:273:GLY:HA2	1:G:285:LEU:O	2.11	0.50
1:G:337:ARG:HG3	1:G:370:ILE:HD13	1.94	0.50
1:A:497:ARG:NE	1:C:41:GLN:HE22	2.10	0.50
1:G:54:ALA:C	1:G:56:SER:H	2.20	0.50
1:G:269:ILE:HG13	1:G:271:HIS:CE1	2.47	0.50
1:A:78:LEU:HD23	1:A:97:ILE:HG22	1.94	0.50
1:C:100:GLY:HA2	1:C:118:TRP:CE2	2.47	0.50
1:C:414:THR:HG22	1:C:485:LEU:CD1	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:442:LEU:O	1:C:445:ARG:HB3	2.11	0.50
1:E:57:VAL:HG13	1:E:62:HIS:ND1	2.21	0.50
1:E:246:SER:OG	1:E:316:ARG:NH2	2.43	0.50
1:G:125:ILE:C	1:G:125:ILE:CD1	2.85	0.50
1:A:328:THR:HA	1:A:333:TYR:CD2	2.46	0.50
1:G:90:LEU:HD21	2:H:7:DA:H8	1.76	0.50
1:C:151:ILE:HD12	1:C:194:LYS:CD	2.40	0.49
1:G:421:VAL:HG13	1:G:422:LYS:HG3	1.94	0.49
1:C:340:LEU:C	1:C:340:LEU:CD1	2.85	0.49
1:C:414:THR:HG22	1:C:485:LEU:HD11	1.94	0.49
1:E:100:GLY:C	1:E:118:TRP:CE2	2.90	0.49
1:E:384:PHE:CD1	1:E:470:PRO:CB	2.96	0.49
1:C:439:LEU:CD1	1:C:496:LEU:HD22	2.30	0.49
1:E:209:PRO:HD3	1:E:315:PRO:HA	1.94	0.49
1:C:45:LYS:HE2	1:C:287:ILE:CD1	2.43	0.49
1:C:57:VAL:HG12	1:C:145:TYR:HE2	1.77	0.49
1:C:93:PRO:O	1:C:212:MET:CE	2.60	0.49
1:C:247:TYR:HB3	1:C:317:PHE:HB2	1.93	0.49
1:C:445:ARG:O	1:C:449:ARG:HG3	2.11	0.49
1:A:359:PHE:HA	1:A:364:LEU:HD11	1.93	0.49
1:A:385:GLN:O	1:A:388:ARG:NE	2.45	0.49
1:C:336:GLN:O	1:C:337:ARG:C	2.49	0.49
1:C:147:GLN:HG3	1:C:197:ALA:O	2.13	0.49
1:E:218:GLU:CD	1:E:220:TYR:H	2.21	0.49
1:E:306:LYS:NZ	1:G:86:LYS:NZ	2.61	0.49
1:G:446:GLN:NE2	1:G:450:ARG:NH1	2.56	0.49
1:A:410:MET:O	1:A:411:GLU:C	2.54	0.49
1:C:46:TYR:CD2	1:C:47:PRO:HD3	2.44	0.49
1:C:375:GLU:OE2	1:C:445:ARG:HD2	2.12	0.49
1:E:366:GLN:O	1:E:370:ILE:HD12	2.12	0.49
1:E:445:ARG:O	1:E:449:ARG:CG	2.60	0.49
1:G:246:SER:CB	1:G:289:LEU:HD13	2.43	0.49
1:C:268:ASP:HB3	1:C:313:SER:HB3	1.91	0.49
1:E:381:GLN:O	1:E:385:GLN:HG3	2.11	0.49
1:A:193:ILE:C	1:A:195:SER:N	2.70	0.49
1:C:40:GLN:N	1:C:40:GLN:CD	2.71	0.48
1:C:99:ILE:HG12	1:C:116:VAL:CG2	2.43	0.48
1:C:289:LEU:CD1	1:C:316:ARG:HH11	2.25	0.48
1:C:382:PHE:O	1:C:386:GLY:HA3	2.13	0.48
1:E:109:LEU:HD11	2:F:5:6MA:C8	2.43	0.48
1:A:309:VAL:HG21	4:A:1002:OGA:H4C1	1.93	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:215:LEU:O	1:C:225:LYS:HG2	2.12	0.48
1:G:127:HIS:ND1	1:G:133:ALA:HA	2.28	0.48
1:G:387:ASN:HD22	1:G:387:ASN:C	2.20	0.48
1:A:356:LEU:HD21	1:A:413:VAL:HB	1.94	0.48
1:G:237:VAL:HG12	1:G:325:GLU:HG2	1.95	0.48
1:G:365:LYS:HG3	1:G:437:ALA:O	2.13	0.48
1:A:38:PHE:O	1:A:40:GLN:HG3	2.13	0.48
1:C:69:PHE:CE1	1:C:204:LEU:HD22	2.44	0.48
1:E:458:SER:HB3	1:E:461:ALA:CB	2.43	0.48
1:G:415:ASN:C	1:G:415:ASN:HD22	2.18	0.48
1:G:439:LEU:O	1:G:443:THR:HG23	2.14	0.48
1:A:279:ASP:OD2	1:A:282:THR:CB	2.60	0.48
1:A:464:LEU:HB2	1:A:465:PRO:HD2	1.95	0.48
1:C:138:THR:CG2	1:C:139:PHE:N	2.72	0.48
1:G:246:SER:HB2	1:G:289:LEU:HD13	1.94	0.48
1:C:82:LEU:HD23	1:C:82:LEU:O	2.14	0.48
1:E:112:ARG:NH1	1:E:377:GLU:HG3	2.28	0.48
1:E:306:LYS:HZ1	1:G:86:LYS:NZ	2.11	0.48
1:A:235:ASN:C	1:A:235:ASN:HD22	2.21	0.48
1:G:272:VAL:HG11	1:G:295:TYR:CZ	2.48	0.48
1:A:213:PRO:HG3	2:B:9:DC:P	2.53	0.48
1:C:104:CYS:SG	1:C:326:CYS:HB3	2.54	0.48
1:C:237:VAL:O	1:C:240:SER:HB3	2.13	0.48
1:G:48:LYS:HZ1	1:G:299:ASP:CG	2.19	0.48
1:A:229:SER:O	1:A:230:TRP:C	2.54	0.48
1:C:328:THR:HA	1:C:333:TYR:CD2	2.48	0.48
1:C:337:ARG:NE	1:C:370:ILE:CD1	2.72	0.48
1:E:132:ILE:HD12	1:E:132:ILE:H	1.78	0.48
1:A:80:ARG:HB3	1:A:91:LEU:HD22	1.94	0.48
1:C:45:LYS:HD3	1:C:287:ILE:HD11	1.96	0.48
1:C:121:LYS:H	1:C:121:LYS:CD	2.07	0.48
1:C:379:LEU:HD21	1:C:404:GLU:HA	1.96	0.48
1:G:247:TYR:HB3	1:G:317:PHE:HB2	1.96	0.48
1:C:385:GLN:HG2	1:C:385:GLN:O	2.13	0.47
1:G:219:PRO:CD	1:G:226:MET:HE1	2.43	0.47
1:G:269:ILE:CG1	1:G:271:HIS:HE1	2.19	0.47
1:C:126:LYS:HB2	1:C:394:ASP:OD1	2.14	0.47
1:E:73:HIS:ND1	1:E:73:HIS:C	2.72	0.47
1:E:334:ILE:HD12	1:E:378:TRP:CD1	2.49	0.47
1:A:237:VAL:HG23	1:A:240:SER:CB	2.43	0.47
1:A:316:ARG:NH2	1:A:318:SER:HB3	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:5:6MA:O5'	2:B:5:6MA:H8	2.14	0.47
1:C:339:GLN:O	1:C:343:GLN:HG3	2.13	0.47
1:C:475:TYR:CE1	1:C:487:PHE:CE2	2.98	0.47
1:G:219:PRO:HD2	1:G:226:MET:HE1	1.96	0.47
1:G:368:GLU:O	1:G:371:HIS:N	2.46	0.47
1:G:387:ASN:ND2	1:G:387:ASN:C	2.73	0.47
1:A:125:ILE:C	1:A:125:ILE:CD1	2.87	0.47
1:C:340:LEU:HD22	1:C:340:LEU:HA	1.54	0.47
1:E:117:PRO:CG	1:E:127:HIS:HE1	2.28	0.47
1:C:245:TYR:HD1	1:C:294:CYS:SG	2.37	0.47
1:E:356:LEU:HD13	1:E:359:PHE:CE1	2.50	0.47
1:G:46:TYR:CG	1:G:47:PRO:HD3	2.30	0.47
1:G:489:LEU:HD12	1:G:489:LEU:N	2.30	0.47
1:C:65:VAL:HG21	1:C:142:LEU:HD22	1.96	0.47
1:E:390:ARG:HA	1:E:393:THR:O	2.15	0.47
1:A:96:ARG:HA	1:A:204:LEU:O	2.14	0.47
1:A:306:LYS:HE3	2:D:3:DC:N3	2.29	0.47
2:B:3:DC:H2''	2:B:4:DT:O4'	2.13	0.47
1:E:306:LYS:NZ	1:G:86:LYS:HZ1	2.11	0.47
1:E:496:LEU:N	1:E:496:LEU:HD22	2.30	0.47
1:G:216:LYS:H	2:H:7:DA:H2	1.61	0.47
1:G:270:TRP:CE3	1:G:311:ALA:HA	2.49	0.47
1:A:157:LEU:O	1:A:159:ALA:N	2.47	0.47
1:E:82:LEU:HD13	1:E:460:ILE:HG12	1.97	0.47
1:G:40:GLN:NE2	1:G:40:GLN:N	2.60	0.47
1:G:80:ARG:NH2	1:G:91:LEU:HD13	2.29	0.47
1:G:157:LEU:O	1:G:157:LEU:HG	2.12	0.47
1:A:235:ASN:O	1:A:235:ASN:ND2	2.47	0.47
1:C:45:LYS:HE2	1:C:287:ILE:HD13	1.97	0.47
1:E:404:GLU:CD	1:E:473:ARG:HH12	2.17	0.47
1:G:233:ASP:H	1:G:302:ASN:HD21	1.63	0.47
1:E:61:LEU:O	1:E:62:HIS:O	2.33	0.46
1:E:385:GLN:NE2	1:E:385:GLN:C	2.72	0.46
1:G:94:VAL:CG1	1:G:205:ASN:HB3	2.44	0.46
1:A:146:LEU:O	1:A:150:THR:HG23	2.14	0.46
1:E:338:CYS:O	1:E:342:LEU:HD23	2.16	0.46
1:E:382:PHE:CD2	1:E:400:MET:HG2	2.50	0.46
1:G:483:MET:HA	1:G:484:PRO:HD3	1.69	0.46
1:G:494:SER:OG	1:G:495:GLU:N	2.48	0.46
1:C:384:PHE:CE2	1:C:455:ARG:HB3	2.49	0.46
1:G:316:ARG:HG2	1:G:317:PHE:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:333:TYR:CE1	1:G:337:ARG:NH1	2.83	0.46
1:G:116:VAL:HG23	1:G:393:THR:HB	1.98	0.46
1:A:276:ILE:HG21	1:A:279:ASP:HB3	1.96	0.46
1:C:356:LEU:CB	1:C:359:PHE:HE1	2.27	0.46
1:E:117:PRO:HG2	1:E:127:HIS:HE1	1.80	0.46
1:E:384:PHE:CD1	1:E:470:PRO:HB3	2.50	0.46
1:E:430:GLN:O	1:E:432:ASN:N	2.46	0.46
1:G:127:HIS:ND1	1:G:133:ALA:CA	2.78	0.46
1:C:290:HIS:O	1:C:291:GLN:C	2.55	0.46
1:E:154:LEU:HD11	1:E:298:LEU:HD22	1.97	0.46
1:G:48:LYS:HZ1	1:G:299:ASP:CB	2.21	0.46
1:G:438:ILE:O	1:G:442:LEU:HD13	2.16	0.46
1:C:45:LYS:CE	1:C:287:ILE:HD13	2.46	0.46
1:C:118:TRP:O	1:C:118:TRP:CD1	2.69	0.46
1:E:99:ILE:HD13	1:E:116:VAL:HB	1.97	0.46
1:G:40:GLN:HG2	1:G:42:TRP:H	1.81	0.46
1:G:40:GLN:CD	1:G:40:GLN:N	2.71	0.46
1:A:269:ILE:HG23	1:A:271:HIS:CE1	2.51	0.46
1:C:125:ILE:N	1:C:125:ILE:CD1	2.72	0.46
1:G:478:LYS:HE2	1:G:478:LYS:HB3	1.68	0.46
1:E:112:ARG:HH11	1:E:377:GLU:HG3	1.81	0.46
1:G:453:HIS:CE1	1:G:457:GLN:NE2	2.84	0.46
1:G:458:SER:O	1:G:462:ARG:HG3	2.15	0.46
1:E:272:VAL:HG13	1:E:287:ILE:HG12	1.97	0.46
1:E:435:LEU:HD11	1:E:496:LEU:CD1	2.46	0.46
1:C:271:HIS:HB2	1:C:310:LEU:HB2	1.98	0.45
1:E:98:LEU:HD12	1:E:202:THR:O	2.16	0.45
1:G:218:GLU:HA	1:G:226:MET:HE1	1.76	0.45
1:A:496:LEU:HD23	1:A:496:LEU:HA	1.63	0.45
1:C:450:ARG:CG	1:C:451:GLU:N	2.77	0.45
1:E:46:TYR:O	1:E:49:LEU:O	2.33	0.45
1:E:117:PRO:CG	1:E:127:HIS:CE1	2.99	0.45
1:C:454:ALA:O	1:C:455:ARG:C	2.55	0.45
1:G:477:GLU:C	1:G:479:ASP:N	2.70	0.45
1:A:121:LYS:HD3	1:A:121:LYS:HA	1.41	0.45
1:A:472:CYS:O	1:A:475:TYR:HB2	2.16	0.45
1:C:364:LEU:HD23	1:C:364:LEU:HA	1.82	0.45
1:E:223:MET:HE2	1:E:286:ALA:HB2	1.97	0.45
1:A:58:SER:C	1:A:60:GLU:N	2.74	0.45
1:C:487:PHE:CD1	1:C:487:PHE:O	2.70	0.45
1:G:328:THR:HA	1:G:333:TYR:CD2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:408:LYS:HE3	1:C:408:LYS:HB3	1.47	0.45
1:E:481:ALA:O	1:E:482:SER:OG	2.32	0.45
1:E:487:PHE:O	1:E:487:PHE:CD1	2.70	0.45
1:A:40:GLN:CD	1:A:40:GLN:H	2.22	0.45
1:A:75:HIS:NE2	1:A:131:GLU:OE1	2.47	0.45
1:A:91:LEU:HD23	1:A:91:LEU:HA	1.86	0.45
1:C:192:ASP:O	1:C:193:ILE:C	2.58	0.45
1:G:61:LEU:HD12	1:G:61:LEU:HA	1.72	0.45
1:C:112:ARG:HG3	1:C:112:ARG:HH21	1.80	0.45
1:E:40:GLN:C	1:E:42:TRP:N	2.71	0.45
2:B:9:DC:H4'	2:B:10:DG:O5'	2.17	0.45
1:C:433:GLU:C	1:C:435:LEU:H	2.24	0.45
1:E:62:HIS:O	1:E:63:LYS:C	2.60	0.45
1:C:125:ILE:HD13	1:C:125:ILE:O	2.17	0.45
1:E:126:LYS:HG3	1:E:127:HIS:H	1.81	0.45
1:G:244:VAL:HG21	1:G:295:TYR:CE2	2.51	0.45
1:A:218:GLU:CD	1:A:220:TYR:H	2.25	0.44
1:A:276:ILE:CG2	1:A:279:ASP:HB3	2.47	0.44
1:E:338:CYS:SG	1:E:374:VAL:HG21	2.57	0.44
1:E:359:PHE:HA	1:E:364:LEU:HD11	1.99	0.44
1:A:245:TYR:O	1:A:318:SER:HA	2.17	0.44
1:C:231:HIS:HB3	2:D:5:6MA:O4'	2.16	0.44
1:C:415:ASN:CA	1:C:485:LEU:HD11	2.47	0.44
1:A:117:PRO:O	1:A:117:PRO:HG2	2.17	0.44
1:A:380:ARG:O	1:A:381:GLN:C	2.56	0.44
1:G:231:HIS:HB3	2:H:5:6MA:O4'	2.18	0.44
1:E:340:LEU:O	1:E:343:GLN:HG2	2.17	0.44
1:E:435:LEU:CG	1:E:496:LEU:HD12	2.48	0.44
1:A:473:ARG:HG2	1:A:474:PRO:HA	2.00	0.44
1:C:238:ASP:OD1	1:C:239:ARG:N	2.50	0.44
1:C:335:LEU:HD23	1:C:335:LEU:HA	1.65	0.44
1:E:48:LYS:CD	1:E:299:ASP:HB3	2.47	0.44
1:E:97:ILE:HD12	1:E:389:TYR:CZ	2.53	0.44
1:E:152:GLN:O	1:E:155:GLU:HG2	2.17	0.44
1:C:65:VAL:HG13	1:C:139:PHE:CE1	2.53	0.44
1:C:215:LEU:O	1:C:216:LYS:C	2.58	0.44
1:E:464:LEU:HD12	1:E:464:LEU:HA	1.73	0.44
1:C:88:LYS:HD3	2:D:6:DT:H1'	2.00	0.44
1:C:381:GLN:CD	1:C:452:TRP:HH2	2.26	0.44
1:E:391:LYS:HB3	1:E:391:LYS:HE3	1.86	0.44
1:G:80:ARG:HH21	1:G:91:LEU:HD13	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:196:ARG:HH22	1:G:239:ARG:HE	1.66	0.44
1:G:342:LEU:O	1:G:345:VAL:HG12	2.18	0.44
1:E:371:HIS:HE1	1:E:407:TRP:NE1	2.16	0.44
1:G:389:TYR:O	1:G:391:LYS:N	2.50	0.44
1:A:244:VAL:HG22	1:A:320:THR:HG22	2.00	0.44
1:C:84:ARG:HA	1:C:88:LYS:O	2.18	0.44
1:E:237:VAL:CG1	1:E:240:SER:HB3	2.44	0.44
1:G:154:LEU:HD12	1:G:154:LEU:HA	1.76	0.44
1:G:453:HIS:CE1	1:G:457:GLN:CD	2.95	0.44
1:C:215:LEU:HD12	1:C:225:LYS:HD3	2.00	0.43
1:G:400:MET:HE1	1:G:403:LEU:CD1	2.46	0.43
1:G:489:LEU:N	1:G:489:LEU:CD1	2.81	0.43
1:G:96:ARG:HA	1:G:204:LEU:O	2.18	0.43
1:A:499:GLN:O	1:A:499:GLN:HG2	2.17	0.43
1:G:385:GLN:HB2	1:G:388:ARG:NH1	2.32	0.43
1:E:46:TYR:HB3	1:E:47:PRO:HD3	0.44	0.43
1:G:207:MET:HE1	1:G:215:LEU:HD11	2.00	0.43
1:G:316:ARG:HG2	1:G:317:PHE:N	2.34	0.43
1:E:80:ARG:HH22	1:E:93:PRO:CA	2.24	0.43
1:E:207:MET:HG2	1:E:208:ASP:H	1.83	0.43
1:G:333:TYR:CE2	1:G:373:GLU:OE2	2.72	0.43
1:A:85:ILE:HD13	1:A:85:ILE:HG21	1.65	0.43
1:C:238:ASP:O	1:C:239:ARG:HB2	2.18	0.43
1:C:337:ARG:CZ	1:C:370:ILE:HD11	2.49	0.43
1:A:108:TYR:O	1:A:108:TYR:CG	2.72	0.43
1:A:372:ASN:OD1	1:A:445:ARG:HB2	2.19	0.43
1:E:310:LEU:H	1:E:310:LEU:HD22	1.84	0.43
1:G:61:LEU:O	1:G:62:HIS:C	2.58	0.43
1:G:218:GLU:CB	1:G:226:MET:CE	2.97	0.43
1:C:62:HIS:O	1:C:66:GLN:HG2	2.17	0.43
1:A:336:GLN:O	1:A:337:ARG:C	2.59	0.43
1:A:489:LEU:HD22	1:A:489:LEU:HA	1.79	0.43
2:B:3:DC:N4	1:C:277:SER:OG	2.52	0.43
1:C:475:TYR:HD1	1:C:487:PHE:CE2	2.27	0.43
1:E:226:MET:SD	1:E:229:SER:HA	2.59	0.43
1:E:289:LEU:HD23	1:E:289:LEU:HA	1.89	0.43
1:G:220:TYR:CD2	1:G:275:LYS:HE3	2.54	0.43
1:A:223:MET:HB3	1:A:310:LEU:HD13	2.01	0.43
1:A:280:ILE:O	1:A:280:ILE:HG12	2.19	0.43
1:A:340:LEU:HD22	1:A:366:GLN:OE1	2.19	0.43
1:A:450:ARG:HH22	1:C:222:GLY:N	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:246:SER:OG	1:C:316:ARG:NH1	2.50	0.43
1:A:464:LEU:C	1:A:464:LEU:CD1	2.90	0.42
1:C:355:SER:O	1:C:355:SER:OG	2.31	0.42
1:E:48:LYS:CE	1:E:299:ASP:HB3	2.49	0.42
1:E:485:LEU:CB	1:E:486:PRO:HD3	2.48	0.42
1:G:328:THR:HA	1:G:333:TYR:CG	2.54	0.42
1:C:96:ARG:CA	1:C:204:LEU:O	2.66	0.42
1:C:206:PHE:HA	1:C:316:ARG:O	2.19	0.42
1:E:384:PHE:CD1	1:E:470:PRO:HB2	2.53	0.42
1:G:196:ARG:NH2	1:G:239:ARG:HE	2.17	0.42
1:A:217:GLU:O	1:A:218:GLU:C	2.62	0.42
1:A:328:THR:HA	1:A:333:TYR:CD1	2.54	0.42
1:C:229:SER:H	2:D:7:DA:H61	1.67	0.42
1:C:431:ARG:HG3	1:C:431:ARG:NH1	2.28	0.42
1:G:111:THR:C	1:G:381:GLN:NE2	2.76	0.42
1:C:295:TYR:OH	4:C:1002:OGA:H4C2	2.20	0.42
1:E:439:LEU:O	1:E:443:THR:HG23	2.20	0.42
1:A:43:GLN:O	1:A:45:LYS:HG3	2.19	0.42
1:A:384:PHE:CD1	1:A:470:PRO:HB2	2.55	0.42
1:C:45:LYS:CD	1:C:287:ILE:HD11	2.49	0.42
1:C:103:GLY:O	1:C:330:THR:HA	2.19	0.42
1:E:112:ARG:O	1:E:385:GLN:OE1	2.37	0.42
1:E:414:THR:HG21	1:E:445:ARG:HH12	1.84	0.42
1:G:96:ARG:NH2	1:G:205:ASN:OD1	2.52	0.42
1:A:435:LEU:HD12	1:A:435:LEU:HA	1.85	0.42
1:C:300:ASP:OD1	1:C:301:LEU:N	2.53	0.42
1:C:475:TYR:CD1	1:C:476:TRP:N	2.88	0.42
1:G:99:ILE:HG12	1:G:116:VAL:CG1	2.48	0.42
1:G:143:ASN:OD1	1:G:321:HIS:ND1	2.37	0.42
1:G:245:TYR:O	1:G:318:SER:HA	2.19	0.42
1:G:439:LEU:CD1	1:G:493:VAL:HG23	2.50	0.42
1:A:387:ASN:ND2	1:A:387:ASN:O	2.52	0.42
1:C:331:LEU:HD12	1:C:331:LEU:HA	1.71	0.42
1:E:51:LEU:HD22	1:E:287:ILE:HD12	2.01	0.42
1:G:487:PHE:CG	1:G:487:PHE:O	2.73	0.42
1:A:333:TYR:CE1	1:A:337:ARG:HD3	2.55	0.42
1:A:50:ILE:HG12	1:A:296:PHE:HB2	2.02	0.41
1:A:206:PHE:CG	1:A:207:MET:N	2.88	0.41
1:C:43:GLN:O	1:C:45:LYS:HG2	2.19	0.41
1:E:40:GLN:H	1:E:40:GLN:HG2	1.63	0.41
1:C:106:TYR:CE1	1:C:235:ASN:HB3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:278:TRP:CD1	1:C:278:TRP:H	2.35	0.41
1:E:84:ARG:HA	1:E:88:LYS:O	2.20	0.41
1:E:398:GLN:N	1:E:399:PRO:HD2	2.35	0.41
1:A:269:ILE:HD12	1:A:269:ILE:HA	1.92	0.41
1:G:154:LEU:HD12	1:G:298:LEU:HD13	2.01	0.41
1:G:333:TYR:HE2	1:G:373:GLU:OE2	2.02	0.41
1:G:445:ARG:HH11	1:G:445:ARG:CG	2.11	0.41
1:A:52:ARG:CG	1:A:52:ARG:NH2	2.71	0.41
1:A:226:MET:CE	1:A:229:SER:HB3	2.51	0.41
2:D:9:DC:H6	2:D:9:DC:H2'	1.62	0.41
1:E:270:TRP:CE3	1:E:311:ALA:HA	2.54	0.41
1:G:289:LEU:HD11	1:G:295:TYR:HE2	1.84	0.41
1:A:489:LEU:HD13	1:A:489:LEU:O	2.20	0.41
1:C:109:LEU:HD11	2:D:5:6MA:C8	2.50	0.41
1:C:368:GLU:OE2	1:C:445:ARG:NH2	2.54	0.41
1:C:417:VAL:O	1:C:421:VAL:HG22	2.20	0.41
1:G:453:HIS:HE1	1:G:457:GLN:NE2	2.19	0.41
1:G:464:LEU:HB3	1:G:465:PRO:HD2	2.02	0.41
1:C:310:LEU:HD22	1:C:310:LEU:H	1.86	0.41
1:A:410:MET:HA	1:A:413:VAL:HG22	2.03	0.41
1:A:497:ARG:HD3	1:C:41:GLN:CD	2.45	0.41
1:C:100:GLY:HA2	1:C:118:TRP:CD2	2.56	0.41
1:C:360:GLU:O	1:C:363:VAL:HG12	2.21	0.41
1:A:450:ARG:NH2	1:C:222:GLY:N	2.69	0.41
1:A:454:ALA:O	1:A:455:ARG:C	2.60	0.41
1:E:268:ASP:OD1	1:E:268:ASP:N	2.53	0.41
1:E:489:LEU:HD12	1:E:489:LEU:HA	1.78	0.41
1:G:84:ARG:HH21	1:G:89:ASP:CG	2.29	0.41
1:G:85:ILE:O	1:G:86:LYS:C	2.61	0.41
1:G:389:TYR:C	1:G:391:LYS:N	2.78	0.41
1:A:41:GLN:O	1:A:41:GLN:CG	2.68	0.41
1:C:49:LEU:HD23	1:C:49:LEU:C	2.43	0.41
1:C:408:LYS:CG	1:C:483:MET:HE1	2.51	0.41
1:C:464:LEU:HD23	1:C:464:LEU:HA	1.79	0.41
1:E:41:GLN:OE1	1:E:41:GLN:CA	2.67	0.41
1:E:335:LEU:HD23	1:E:335:LEU:HA	1.89	0.41
1:G:100:GLY:HA2	1:G:118:TRP:CD2	2.56	0.41
1:A:52:ARG:HB3	1:A:52:ARG:CZ	2.51	0.41
1:C:233:ASP:HB2	1:C:302:ASN:OD1	2.21	0.41
1:C:320:THR:HB	1:C:322:ARG:HH21	1.83	0.41
1:E:232:HIS:CE1	1:E:306:LYS:HG2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:208:ASP:C	1:G:210:GLN:H	2.28	0.41
1:G:246:SER:OG	1:G:316:ARG:HD2	2.20	0.41
1:A:100:GLY:HA2	1:A:118:TRP:CE2	2.55	0.40
1:A:226:MET:HE3	1:A:229:SER:HB3	2.03	0.40
1:A:398:GLN:N	1:A:399:PRO:HD2	2.36	0.40
1:E:207:MET:HG2	1:E:208:ASP:N	2.35	0.40
1:E:360:GLU:O	1:E:363:VAL:HG12	2.20	0.40
2:F:7:DA:C8	2:F:7:DA:H5''	2.56	0.40
2:F:8:DT:O5'	2:F:8:DT:H6	2.04	0.40
1:G:98:LEU:O	1:G:116:VAL:HG12	2.21	0.40
1:A:40:GLN:NE2	1:A:40:GLN:C	2.71	0.40
1:A:52:ARG:NH2	1:A:52:ARG:CB	2.84	0.40
1:A:200:ASN:OD1	1:A:323:VAL:HA	2.21	0.40
1:C:157:LEU:O	1:C:157:LEU:CG	2.69	0.40
1:E:45:LYS:HB2	1:E:285:LEU:HD21	2.03	0.40
1:E:199:TYR:HA	1:E:323:VAL:HB	2.03	0.40
1:G:415:ASN:C	1:G:415:ASN:ND2	2.79	0.40
1:C:157:LEU:O	1:C:157:LEU:HG	2.21	0.40
1:A:213:PRO:HG3	2:B:9:DC:OP1	2.20	0.40
1:C:272:VAL:HG21	1:C:295:TYR:CZ	2.56	0.40
1:G:57:VAL:HG13	1:G:145:TYR:CE2	2.57	0.40
1:G:337:ARG:O	1:G:340:LEU:HB3	2.22	0.40
1:A:97:ILE:HD12	1:A:389:TYR:CZ	2.57	0.40
1:A:487:PHE:HD1	1:A:487:PHE:HA	1.72	0.40
1:E:200:ASN:OD1	1:E:324:ALA:N	2.55	0.40
1:G:402:GLN:O	1:G:406:LEU:HG	2.21	0.40
1:G:439:LEU:HD11	1:G:493:VAL:CG2	2.52	0.40
1:G:469:LYS:O	1:G:469:LYS:CG	2.70	0.40
1:G:477:GLU:C	1:G:479:ASP:H	2.30	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:A:56:SER:O	1:G:58:SER:OG[7_555]	2.01	0.19

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	390/463 (84%)	353 (90%)	37 (10%)	0	100	100
1	C	383/463 (83%)	356 (93%)	27 (7%)	0	100	100
1	E	383/463 (83%)	349 (91%)	34 (9%)	0	100	100
1	G	393/463 (85%)	355 (90%)	38 (10%)	0	100	100
All	All	1549/1852 (84%)	1413 (91%)	136 (9%)	0	100	100

There are no Ramachandran outliers to report.

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	356/408 (87%)	315 (88%)	41 (12%)	5	21
1	C	350/408 (86%)	297 (85%)	53 (15%)	3	13
1	E	350/408 (86%)	328 (94%)	22 (6%)	16	44
1	G	357/408 (88%)	333 (93%)	24 (7%)	15	42
All	All	1413/1632 (87%)	1273 (90%)	140 (10%)	7	27

All (140) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	41	GLN

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Mol	Chain	Res	Type
1	A	45	LYS
1	A	46	TYR
1	A	47	PRO
1	A	48	LYS
1	A	49	LEU
1	A	50	ILE
1	A	52	ARG
1	A	80	ARG
1	A	88	LYS
1	A	95	SER
1	A	125	ILE
1	A	191	VAL
1	A	193	ILE
1	A	196	ARG
1	A	210	GLN
1	A	229	SER
1	A	234	GLU
1	A	240	SER
1	A	275	LYS
1	A	276	ILE
1	A	299	ASP
1	A	345	VAL
1	A	366	GLN
1	A	371	HIS
1	A	381	GLN
1	A	387	ASN
1	A	388	ARG
1	A	394	ASP
1	A	400	MET
1	A	430	GLN
1	A	451	GLU
1	A	455	ARG
1	A	463	THR
1	A	464	LEU
1	A	465	PRO
1	A	489	LEU
1	A	493	VAL
1	A	494	SER
1	A	497	ARG
1	C	40	GLN
1	C	41	GLN
1	C	49	LEU

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Mol	Chain	Res	Type
1	C	52	ARG
1	C	58	SER
1	C	66	GLN
1	C	77	CYS
1	C	84	ARG
1	C	85	ILE
1	C	90	LEU
1	C	97	ILE
1	C	121	LYS
1	C	124	ASN
1	C	125	ILE
1	C	126	LYS
1	C	128	THR
1	C	129	GLU
1	C	149	GLU
1	C	156	GLU
1	C	192	ASP
1	C	203	LEU
1	C	210	GLN
1	C	212	MET
1	C	234	GLU
1	C	268	ASP
1	C	275	LYS
1	C	276	ILE
1	C	277	SER
1	C	280	ILE
1	C	316	ARG
1	C	326	CYS
1	C	328	THR
1	C	336	GLN
1	C	356	LEU
1	C	385	GLN
1	C	388	ARG
1	C	398	GLN
1	C	414	THR
1	C	445	ARG
1	C	449	ARG
1	C	455	ARG
1	C	457	GLN
1	C	469	LYS
1	C	477	GLU
1	C	479	ASP

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Mol	Chain	Res	Type
1	C	483	MET
1	C	488	ASP
1	C	490	THR
1	C	493	VAL
1	C	494	SER
1	C	495	GLU
1	C	496	LEU
1	C	497	ARG
1	E	41	GLN
1	E	45	LYS
1	E	50	ILE
1	E	53	GLU
1	E	73	HIS
1	E	80	ARG
1	E	108	TYR
1	E	116	VAL
1	E	118	TRP
1	E	121	LYS
1	E	234	GLU
1	E	385	GLN
1	E	457	GLN
1	E	459	ARG
1	E	460	ILE
1	E	462	ARG
1	E	464	LEU
1	E	467	ASP
1	E	489	LEU
1	E	490	THR
1	E	493	VAL
1	E	497	ARG
1	G	40	GLN
1	G	42	TRP
1	G	45	LYS
1	G	47	PRO
1	G	49	LEU
1	G	50	ILE
1	G	51	LEU
1	G	56	SER
1	G	80	ARG
1	G	90	LEU
1	G	149	GLU
1	G	210	GLN

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Mol	Chain	Res	Type
1	G	268	ASP
1	G	269	ILE
1	G	277	SER
1	G	368	GLU
1	G	380	ARG
1	G	381	GLN
1	G	387	ASN
1	G	445	ARG
1	G	464	LEU
1	G	467	ASP
1	G	488	ASP
1	G	490	THR

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

Mol	Chain	Res	Type
1	A	40	GLN
1	A	73	HIS
1	A	210	GLN
1	A	381	GLN
1	A	430	GLN
1	A	446	GLN
1	C	339	GLN
1	C	343	GLN
1	C	344	ASN
1	C	366	GLN
1	C	415	ASN
1	C	457	GLN
1	E	62	HIS
1	E	127	HIS
1	E	385	GLN
1	G	40	GLN
1	G	210	GLN
1	G	302	ASN
1	G	305	HIS
1	G	307	HIS
1	G	314	GLN
1	G	371	HIS
1	G	381	GLN
1	G	415	ASN
1	G	446	GLN
1	G	453	HIS

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Mol	Chain	Res	Type
1	G	468	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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$
2	6MA	F	5	2	21,24,25	1.58	4 (19%)	27,34,37	2.24	9 (33%)
2	6MA	B	5	2	21,24,25	1.56	4 (19%)	27,34,37	2.25	9 (33%)
2	6MA	D	5	2	21,24,25	1.57	4 (19%)	27,34,37	2.31	9 (33%)
2	6MA	H	5	2	21,24,25	1.56	4 (19%)	27,34,37	2.29	10 (37%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	6MA	F	5	2	-	2/9/23/24	0/3/3/3
2	6MA	B	5	2	-	0/9/23/24	0/3/3/3
2	6MA	D	5	2	-	0/9/23/24	0/3/3/3
2	6MA	H	5	2	-	0/9/23/24	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	5	6MA	C5-C4	4.77	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	5	6MA	C5-C4	4.71	1.47	1.39
2	B	5	6MA	C5-C4	4.66	1.47	1.39
2	H	5	6MA	C5-C4	4.63	1.47	1.39
2	D	5	6MA	C5-C6	2.86	1.48	1.41
2	H	5	6MA	C5-C6	2.77	1.48	1.41
2	F	5	6MA	C5-C6	2.73	1.48	1.41
2	B	5	6MA	C5-C6	2.72	1.48	1.41
2	H	5	6MA	C8-N7	2.37	1.36	1.31
2	D	5	6MA	C8-N7	2.36	1.36	1.31
2	B	5	6MA	C8-N7	2.36	1.36	1.31
2	F	5	6MA	C8-N7	2.30	1.36	1.31
2	F	5	6MA	C5-N7	-2.29	1.34	1.39
2	B	5	6MA	C5-N7	-2.28	1.34	1.39
2	H	5	6MA	C5-N7	-2.24	1.35	1.39
2	D	5	6MA	C5-N7	-2.17	1.35	1.39

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	5	6MA	C5-C4-N3	-5.92	118.57	126.72
2	F	5	6MA	C5-C4-N3	-5.90	118.60	126.72
2	B	5	6MA	C5-C4-N3	-5.83	118.69	126.72
2	H	5	6MA	C5-C4-N3	-5.76	118.78	126.72
2	B	5	6MA	N3-C4-N9	4.68	135.13	127.17
2	F	5	6MA	N3-C4-N9	4.61	135.01	127.17
2	D	5	6MA	N3-C4-N9	4.61	135.01	127.17
2	H	5	6MA	N3-C4-N9	4.52	134.85	127.17
2	D	5	6MA	C2-N3-C4	3.79	121.09	111.83
2	H	5	6MA	C2-N3-C4	3.73	120.95	111.83
2	F	5	6MA	C2-N3-C4	3.72	120.92	111.83
2	B	5	6MA	C2-N3-C4	3.71	120.90	111.83
2	H	5	6MA	C6-C5-N7	3.65	136.40	132.43
2	H	5	6MA	C4-C5-N7	-3.56	106.51	110.58
2	D	5	6MA	C4-C5-N7	-3.53	106.54	110.58
2	D	5	6MA	C6-C5-N7	3.47	136.21	132.43
2	F	5	6MA	C4-C5-N7	-3.44	106.65	110.58
2	D	5	6MA	C1-N6-C6	-3.32	119.77	122.85
2	B	5	6MA	C4-C5-N7	-3.30	106.81	110.58
2	H	5	6MA	N3-C2-N1	-3.30	123.59	128.58
2	F	5	6MA	C6-C5-N7	3.28	136.01	132.43
2	D	5	6MA	N3-C2-N1	-3.28	123.61	128.58
2	B	5	6MA	N3-C2-N1	-3.27	123.64	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	5	6MA	N3-C2-N1	-3.21	123.72	128.58
2	B	5	6MA	C6-C5-N7	3.14	135.85	132.43
2	B	5	6MA	C1-N6-C6	-3.12	119.95	122.85
2	H	5	6MA	C1-N6-C6	-3.12	119.96	122.85
2	F	5	6MA	C1-N6-C6	-3.05	120.02	122.85
2	H	5	6MA	C4-N9-C8	2.74	108.62	105.74
2	B	5	6MA	C4-N9-C8	2.66	108.53	105.74
2	H	5	6MA	C5-N7-C8	2.64	107.60	103.45
2	D	5	6MA	C5-N7-C8	2.54	107.45	103.45
2	D	5	6MA	C4-N9-C8	2.50	108.36	105.74
2	B	5	6MA	C5-N7-C8	2.45	107.31	103.45
2	F	5	6MA	C5-N7-C8	2.45	107.29	103.45
2	F	5	6MA	C4-N9-C8	2.38	108.24	105.74
2	H	5	6MA	N9-C8-N7	-2.13	110.91	113.94

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	5	6MA	C2'-C1'-N9-C4
2	F	5	6MA	O4'-C1'-N9-C4

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	5	6MA	3	0
2	B	5	6MA	1	0
2	D	5	6MA	2	0
2	H	5	6MA	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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$
4	OGA	G	1002	3	9,9,9	4.62	3 (33%)	8,11,11	2.59	3 (37%)
4	OGA	A	1002	3	9,9,9	4.62	3 (33%)	8,11,11	2.60	3 (37%)
4	OGA	E	1002	3	9,9,9	4.59	3 (33%)	8,11,11	2.45	2 (25%)
4	OGA	C	1002	3	9,9,9	4.63	3 (33%)	8,11,11	2.46	2 (25%)

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	OGA	G	1002	3	-	0/8/9/9	-
4	OGA	A	1002	3	-	0/8/9/9	-
4	OGA	E	1002	3	-	0/8/9/9	-
4	OGA	C	1002	3	-	0/8/9/9	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1002	OGA	C2-N1	11.29	1.52	1.33
4	C	1002	OGA	C2-N1	11.28	1.52	1.33
4	G	1002	OGA	C2-N1	11.27	1.52	1.33
4	E	1002	OGA	C2-N1	11.21	1.52	1.33
4	G	1002	OGA	C2-C1	-6.92	1.46	1.54
4	C	1002	OGA	C2-C1	-6.85	1.46	1.54
4	A	1002	OGA	C2-C1	-6.84	1.46	1.54
4	E	1002	OGA	C2-C1	-6.72	1.46	1.54
4	A	1002	OGA	C4-N1	3.08	1.53	1.45
4	E	1002	OGA	C4-N1	3.07	1.53	1.45
4	G	1002	OGA	C4-N1	3.06	1.53	1.45
4	C	1002	OGA	C4-N1	3.06	1.53	1.45

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1002	OGA	C4-N1-C2	-6.36	111.47	121.29
4	A	1002	OGA	C4-N1-C2	-6.36	111.47	121.29
4	E	1002	OGA	C4-N1-C2	-6.35	111.49	121.29
4	G	1002	OGA	C4-N1-C2	-6.33	111.52	121.29
4	E	1002	OGA	O2'-C2-C1	-2.19	118.48	121.36
4	G	1002	OGA	O2'-C2-C1	-2.19	118.48	121.36
4	C	1002	OGA	O2'-C2-C1	-2.16	118.52	121.36
4	A	1002	OGA	O2'-C2-C1	-2.15	118.53	121.36
4	A	1002	OGA	O3-C5-C4	2.05	120.60	112.81
4	G	1002	OGA	O3-C5-C4	2.04	120.57	112.81

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	1002	OGA	5	0
4	A	1002	OGA	3	0
4	C	1002	OGA	4	0

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	402/463 (86%)	0.05	4 (0%) 79 63	13, 27, 52, 64	0
1	C	395/463 (85%)	0.12	6 (1%) 72 53	14, 31, 57, 70	0
1	E	395/463 (85%)	0.17	3 (0%) 82 68	17, 34, 54, 80	0
1	G	403/463 (87%)	0.12	5 (1%) 76 58	11, 26, 52, 75	0
2	B	8/9 (88%)	-0.15	0 100 100	13, 22, 29, 43	0
2	D	8/9 (88%)	-0.01	0 100 100	13, 24, 31, 51	0
2	F	8/9 (88%)	0.06	0 100 100	13, 24, 27, 45	0
2	H	8/9 (88%)	0.10	0 100 100	13, 18, 30, 45	0
All	All	1627/1888 (86%)	0.11	18 (1%) 78 60	11, 29, 54, 80	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	498	GLY	3.7
1	G	124	ASN	3.5
1	C	379	LEU	3.4
1	G	128	THR	3.4
1	C	434	ILE	2.5
1	A	280	ILE	2.5
1	A	42	TRP	2.4
1	E	434	ILE	2.3
1	G	41	GLN	2.3
1	G	464	LEU	2.3
1	E	392	CYS	2.3
1	C	375	GLU	2.2
1	C	280	ILE	2.2
1	A	284	GLY	2.2
1	G	420	GLU	2.1
1	C	159	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	421	VAL	2.1
1	A	360	GLU	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
2	6MA	F	5	22/23	0.90	0.12	6,21,33,40	0
2	6MA	B	5	22/23	0.95	0.10	8,14,21,23	0
2	6MA	H	5	22/23	0.95	0.11	5,12,15,17	0
2	6MA	D	5	22/23	0.96	0.10	8,16,24,30	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(Å ²)	Q<0.9
4	OGA	C	1002	10/10	0.88	0.19	12,18,26,29	0
4	OGA	G	1002	10/10	0.88	0.18	10,12,20,30	0
3	MN	G	1001	1/1	0.90	0.12	13,13,13,13	0
3	MN	C	1001	1/1	0.92	0.08	17,17,17,17	0
4	OGA	E	1002	10/10	0.93	0.13	14,22,24,29	0
4	OGA	A	1002	10/10	0.96	0.09	8,16,21,32	0
3	MN	E	1001	1/1	0.97	0.07	20,20,20,20	0
3	MN	A	1001	1/1	0.99	0.06	12,12,12,12	0

6.5 Other polymers [i](#)

There are no such residues in this entry.