



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 02:17 AM EDT

PDB ID : 1TUI / pdb_00001tui
Title : INTACT ELONGATION FACTOR TU IN COMPLEX WITH GDP
Authors : Polekhina, G.; Thirup, S.; Kjeldgaard, M.; Nissen, P.; Lippmann, C.; Nyborg, J.
Deposited on : 1996-05-23
Resolution : 2.70 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

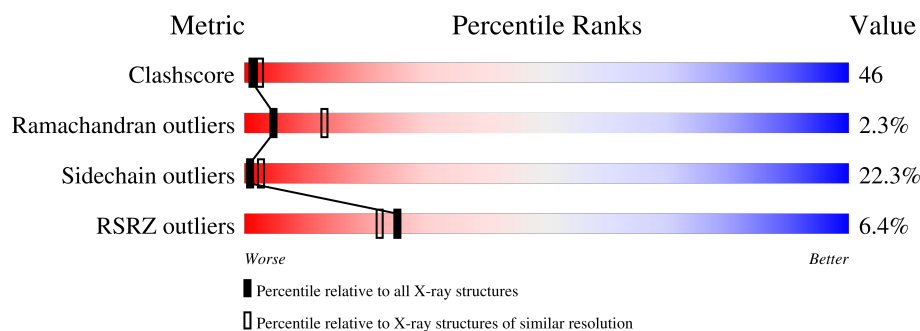
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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))
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	405	5% 30% 45% 19% . .
1	B	405	6% 27% 48% 18% 5% .
1	C	405	8% 29% 46% 18% 5% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9422 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.

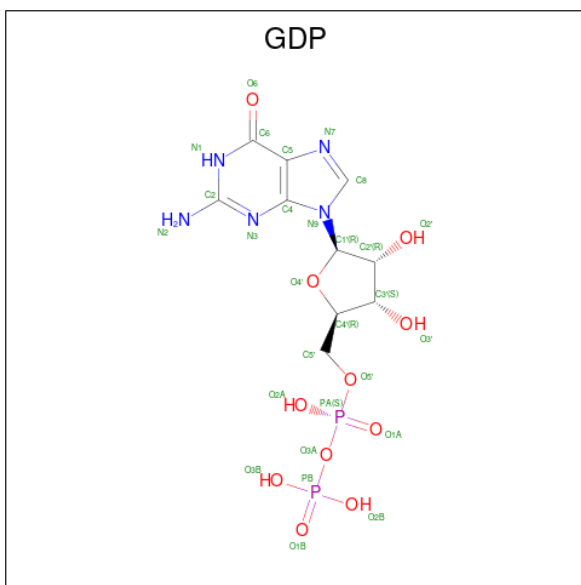
- Molecule 1 is a protein called ELONGATION FACTOR TU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	397	Total	C	N	O	S	0	0	0
			3080	1945	536	587	12			
1	B	397	Total	C	N	O	S	0	0	0
			3080	1945	536	587	12			
1	C	397	Total	C	N	O	S	0	0	0
			3080	1945	536	587	12			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 28	C 10	N 5	O 11	P 2	0	0
3	B	1	Total 28	C 10	N 5	O 11	P 2	0	0
3	C	1	Total 28	C 10	N 5	O 11	P 2	0	0

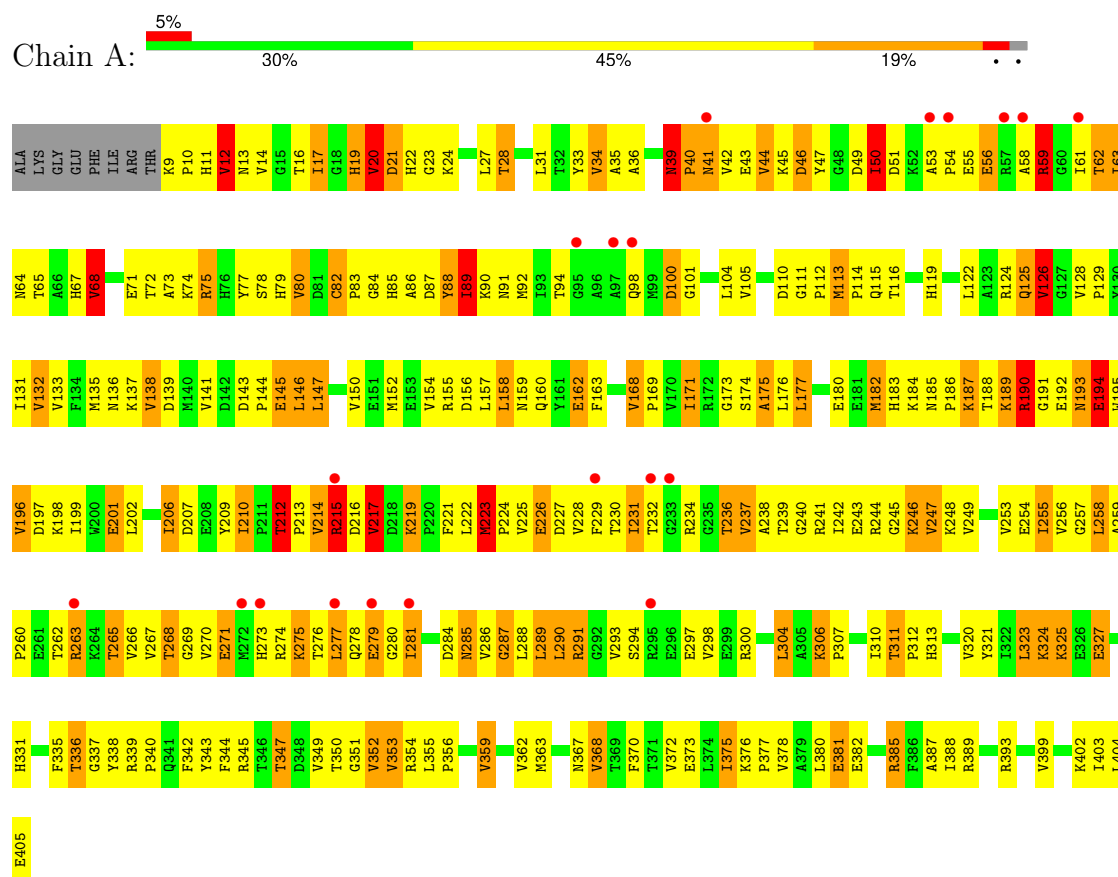
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	33	Total O 33 33	0	0
4	B	23	Total O 23 23	0	0
4	C	39	Total O 39 39	0	0

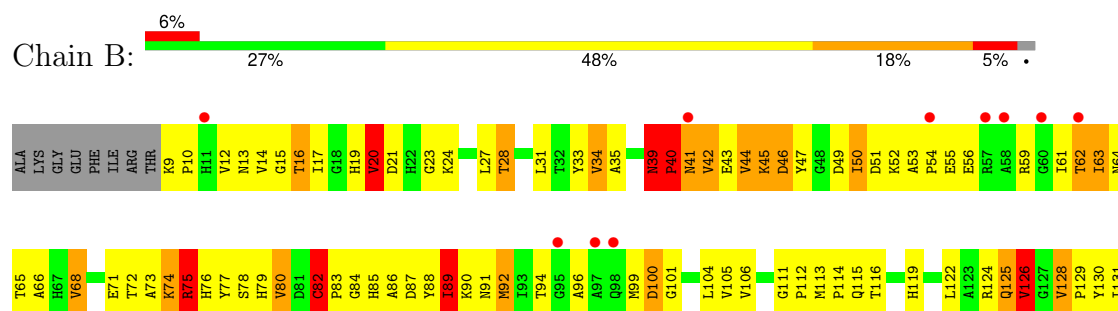
3 Residue-property plots

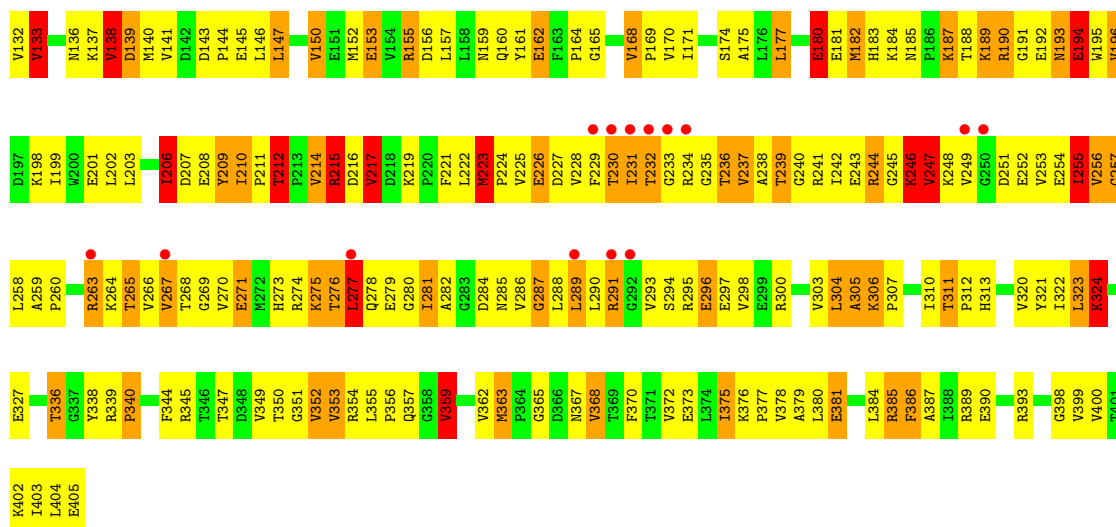
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

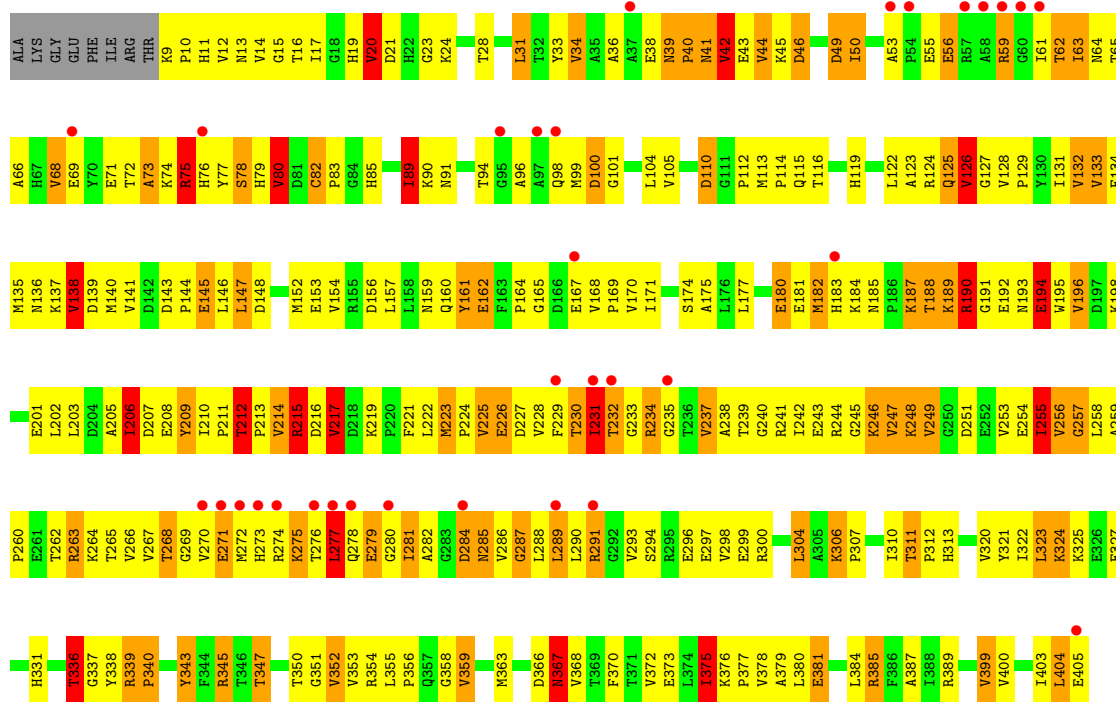


• Molecule 1: ELONGATION FACTOR TU





● Molecule 1: ELONGATION FACTOR TU



4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	175.90Å 175.90Å 223.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.70 20.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.70) 99.6 (20.00-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 2.59Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.235 , 0.300 0.219 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	51.0	Xtriage
Anisotropy	0.394	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 131.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9422	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.18% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

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

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	1.59	31/3139 (1.0%)	1.67	60/4259 (1.4%)
1	B	1.53	29/3139 (0.9%)	1.65	56/4259 (1.3%)
1	C	1.60	26/3139 (0.8%)	1.67	60/4259 (1.4%)
All	All	1.57	86/9417 (0.9%)	1.66	176/12777 (1.4%)

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	B	0	1
1	C	0	1
All	All	0	2

All (86) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	154	VAL	CA-CB	-11.45	1.41	1.54
1	B	214	VAL	CA-CB	-9.57	1.42	1.54
1	A	68	VAL	CA-CB	-9.45	1.45	1.55
1	A	349	VAL	CA-CB	-8.57	1.43	1.54
1	C	56	GLU	CA-C	-8.40	1.42	1.52
1	C	289	LEU	CA-C	-7.81	1.43	1.52
1	C	210	ILE	CA-CB	-7.72	1.46	1.53
1	B	150	VAL	CA-CB	-7.58	1.45	1.54
1	C	123	ALA	CA-CB	-7.57	1.41	1.53
1	B	20	VAL	CA-C	-7.45	1.44	1.52
1	A	196	VAL	CA-CB	-7.39	1.45	1.54
1	B	133	VAL	CA-C	-7.38	1.44	1.52
1	A	214	VAL	CA-CB	-7.30	1.45	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	140	MET	SD-CE	-7.28	1.61	1.79
1	A	133	VAL	CA-C	-7.24	1.44	1.52
1	A	110	ASP	CA-C	-7.23	1.43	1.52
1	B	196	VAL	CA-CB	-7.18	1.45	1.54
1	C	135	MET	SD-CE	-7.18	1.61	1.79
1	B	126	VAL	CA-CB	-7.11	1.46	1.54
1	A	135	MET	SD-CE	-6.94	1.62	1.79
1	A	154	VAL	CA-CB	-6.74	1.46	1.54
1	A	199	ILE	CA-CB	-6.70	1.46	1.54
1	A	126	VAL	CA-CB	-6.60	1.46	1.54
1	B	130	TYR	CA-C	-6.37	1.44	1.52
1	A	113	MET	SD-CE	-6.33	1.63	1.79
1	C	196	VAL	CA-CB	-6.33	1.46	1.54
1	A	217	VAL	CA-CB	-6.31	1.45	1.54
1	B	255	ILE	CA-CB	-6.29	1.46	1.53
1	B	56	GLU	CA-C	-6.24	1.45	1.52
1	C	343	TYR	CA-C	-6.23	1.45	1.53
1	B	106	VAL	CA-CB	-6.19	1.46	1.54
1	C	126	VAL	CA-CB	-6.18	1.47	1.54
1	A	11	HIS	CA-CB	-6.17	1.44	1.53
1	C	214	VAL	CA-CB	-6.15	1.46	1.54
1	C	80	VAL	CA-CB	-6.12	1.44	1.55
1	B	86	ALA	CA-CB	-6.12	1.43	1.53
1	A	403	ILE	CA-CB	-6.11	1.46	1.54
1	C	138	VAL	CA-CB	-6.09	1.46	1.54
1	B	303	VAL	CA-C	-6.08	1.45	1.52
1	C	375	ILE	CA-CB	-6.08	1.46	1.54
1	C	347	THR	CA-C	-6.05	1.45	1.52
1	A	183	HIS	CA-C	-6.02	1.45	1.52
1	A	50	ILE	CA-CB	-5.92	1.46	1.54
1	B	349	VAL	CA-CB	-5.87	1.46	1.54
1	B	92	MET	CA-C	-5.81	1.44	1.52
1	B	305	ALA	CA-C	-5.74	1.45	1.52
1	A	210	ILE	CA-CB	-5.72	1.46	1.54
1	A	289	LEU	CA-C	-5.70	1.45	1.52
1	C	237	VAL	CA-CB	-5.67	1.47	1.54
1	C	133	VAL	CA-C	-5.65	1.45	1.52
1	C	154	VAL	N-CA	-5.62	1.40	1.46
1	C	119	HIS	CA-CB	-5.57	1.44	1.53
1	B	210	ILE	CA-CB	-5.56	1.47	1.54
1	B	400	VAL	CA-CB	-5.44	1.47	1.54
1	B	223	MET	SD-CE	-5.42	1.66	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	138	VAL	CA-CB	-5.42	1.46	1.54
1	A	12	VAL	CA-CB	-5.41	1.45	1.55
1	A	382	GLU	CA-C	-5.40	1.46	1.52
1	B	217	VAL	CA-CB	-5.39	1.47	1.54
1	A	171	ILE	CA-CB	5.38	1.60	1.54
1	A	14	VAL	CA-CB	5.35	1.61	1.54
1	C	161	TYR	CA-C	-5.34	1.46	1.53
1	B	398	GLY	CA-C	5.33	1.57	1.52
1	C	282	ALA	CA-CB	-5.28	1.44	1.53
1	B	353	VAL	CA-CB	-5.26	1.48	1.54
1	A	119	HIS	CA-CB	-5.25	1.45	1.53
1	B	68	VAL	CA-CB	-5.25	1.50	1.55
1	C	20	VAL	CA-C	-5.24	1.45	1.52
1	C	368	VAL	CA-C	-5.24	1.46	1.52
1	B	357	GLN	CA-C	-5.23	1.45	1.52
1	A	342	PHE	CA-C	-5.23	1.46	1.52
1	B	128	VAL	CA-CB	-5.23	1.47	1.54
1	A	158	LEU	CA-C	-5.22	1.45	1.52
1	A	304	LEU	CA-C	-5.22	1.46	1.52
1	B	52	LYS	N-CA	-5.17	1.39	1.46
1	B	210	ILE	CA-C	-5.16	1.47	1.52
1	A	399	VAL	C-O	-5.14	1.18	1.24
1	A	197	ASP	CA-C	5.14	1.59	1.52
1	B	45	LYS	CA-C	-5.13	1.46	1.52
1	C	217	VAL	CA-CB	-5.13	1.47	1.54
1	A	335	PHE	CA-C	-5.12	1.46	1.53
1	C	56	GLU	C-O	5.11	1.29	1.23
1	A	86	ALA	CA-CB	-5.08	1.45	1.53
1	A	89	ILE	CA-CB	-5.07	1.48	1.54
1	C	366	ASP	CA-C	-5.05	1.46	1.53
1	B	359	VAL	CA-CB	-5.02	1.48	1.54

All (176) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	39	ASN	C-N-CD	-14.23	66.66	125.00
1	B	39	ASN	C-N-CD	-14.05	67.40	125.00
1	A	39	ASN	C-N-CD	-13.96	67.75	125.00
1	A	75	ARG	N-CA-C	12.00	123.56	108.45
1	C	352	VAL	CB-CA-C	-10.47	94.89	110.81
1	C	75	ARG	N-CA-C	10.00	122.54	108.74
1	A	352	VAL	CB-CA-C	-9.87	95.81	110.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	94	THR	N-CA-C	-9.70	101.44	113.18
1	C	80	VAL	CB-CA-C	-9.70	97.80	111.38
1	C	212	THR	N-CA-C	-9.62	97.70	109.72
1	A	80	VAL	CB-CA-C	-9.47	98.42	111.49
1	B	75	ARG	N-CA-C	9.38	121.69	108.74
1	C	100	ASP	N-CA-C	-9.25	102.12	113.50
1	B	153	GLU	N-CA-C	-9.03	101.41	111.07
1	B	352	VAL	CB-CA-C	-8.93	98.70	110.84
1	B	237	VAL	N-CA-C	8.58	120.47	107.77
1	B	256	VAL	N-CA-C	8.32	119.81	108.17
1	A	94	THR	N-CA-C	-8.29	103.15	113.18
1	C	268	THR	N-CA-C	-8.26	101.30	112.94
1	B	80	VAL	CB-CA-C	-8.15	100.24	111.49
1	B	208	GLU	N-CA-C	8.04	119.82	111.14
1	C	257	GLY	N-CA-C	8.01	120.21	112.04
1	B	94	THR	N-CA-C	-8.00	103.50	113.18
1	A	236	THR	N-CA-C	7.90	122.68	110.20
1	A	72	THR	N-CA-C	-7.47	98.93	109.69
1	A	325	LYS	N-CA-C	-7.27	103.29	111.14
1	B	82	CYS	CA-C-N	7.26	126.76	118.85
1	B	82	CYS	C-N-CA	7.26	126.76	118.85
1	A	215	ARG	N-CA-C	-7.22	99.60	110.28
1	A	105	VAL	CB-CA-C	-7.09	101.19	110.84
1	C	20	VAL	CB-CA-C	-7.08	99.77	111.32
1	C	404	LEU	N-CA-C	-7.07	105.19	114.31
1	A	209	TYR	N-CA-C	7.05	120.36	111.69
1	C	105	VAL	CB-CA-C	-7.01	102.21	110.91
1	B	236	THR	N-CA-C	7.00	121.25	110.20
1	C	237	VAL	N-CA-C	6.98	118.10	107.77
1	C	399	VAL	CB-CA-C	-6.96	98.67	110.71
1	C	256	VAL	N-CA-C	6.92	117.86	108.17
1	B	168	VAL	C-N-CD	-6.90	96.70	125.00
1	B	267	VAL	N-CA-C	-6.88	100.70	109.30
1	A	145	GLU	N-CA-C	-6.86	103.89	111.36
1	B	255	ILE	CB-CA-C	-6.85	101.72	111.31
1	C	208	GLU	N-CA-C	6.78	119.67	111.40
1	B	72	THR	N-CA-C	-6.73	100.00	109.69
1	B	78	SER	N-CA-C	-6.71	98.26	109.07
1	B	177	LEU	N-CA-C	6.70	118.59	111.28
1	B	194	GLU	N-CA-C	6.67	118.20	111.07
1	C	212	THR	CA-C-N	6.62	126.79	120.31
1	C	212	THR	C-N-CA	6.62	126.79	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	133	VAL	CB-CA-C	-6.57	101.72	110.98
1	B	336	THR	N-CA-C	-6.56	100.56	110.28
1	A	268	THR	N-CA-C	-6.54	103.72	112.94
1	C	234	ARG	N-CA-C	6.46	119.63	111.69
1	A	304	LEU	N-CA-C	-6.46	99.20	109.59
1	C	168	VAL	C-N-CD	-6.33	99.04	125.00
1	A	256	VAL	N-CA-C	6.27	117.51	108.48
1	C	141	VAL	N-CA-C	6.24	117.08	107.78
1	B	100	ASP	N-CA-C	-6.24	104.73	112.90
1	B	196	VAL	CB-CA-C	-6.21	103.76	112.14
1	A	159	ASN	N-CA-C	-6.20	104.63	111.82
1	A	141	VAL	N-CA-C	6.19	117.00	107.78
1	B	209	TYR	N-CA-C	6.18	120.01	112.23
1	A	223	MET	CA-C-N	6.17	127.56	119.84
1	A	223	MET	C-N-CA	6.17	127.56	119.84
1	A	237	VAL	N-CA-C	6.14	116.86	107.77
1	A	186	PRO	CA-C-N	-6.03	112.59	122.54
1	A	186	PRO	C-N-CA	-6.03	112.59	122.54
1	A	20	VAL	CB-CA-C	-6.01	102.12	111.26
1	B	265	THR	CB-CA-C	-5.99	99.30	113.02
1	A	94	THR	CB-CA-C	-5.97	98.06	109.95
1	A	337	GLY	N-CA-C	-5.97	106.84	114.37
1	B	246	LYS	N-CA-C	5.96	117.91	108.79
1	C	110	ASP	N-CA-C	5.96	120.83	113.50
1	C	231	ILE	CB-CA-C	-5.95	105.07	112.45
1	C	72	THR	N-CA-C	-5.92	101.42	109.95
1	A	223	MET	CA-C-O	5.92	125.26	119.22
1	B	244	ARG	N-CA-C	5.91	118.10	108.76
1	B	386	PHE	N-CA-C	5.91	116.36	108.38
1	B	199	ILE	CB-CA-C	-5.89	104.19	112.14
1	C	89	ILE	CB-CA-C	-5.87	104.47	111.81
1	B	141	VAL	N-CA-C	5.84	116.48	107.78
1	B	89	ILE	CB-CA-C	-5.81	104.55	111.81
1	C	73	ALA	N-CA-C	-5.80	104.86	111.07
1	B	289	LEU	CA-CB-CG	-5.80	96.00	116.30
1	C	358	GLY	N-CA-C	-5.76	107.11	114.37
1	B	101	GLY	N-CA-C	-5.75	100.79	111.14
1	B	295	ARG	N-CA-C	-5.74	106.36	113.19
1	A	212	THR	O-C-N	5.73	127.49	121.42
1	A	98	GLN	N-CA-C	5.73	118.07	108.96
1	A	168	VAL	C-N-CD	-5.71	101.57	125.00
1	C	389	ARG	N-CA-C	5.71	118.86	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	215	ARG	N-CA-C	-5.70	101.85	110.28
1	B	155	ARG	N-CA-C	5.70	118.22	111.33
1	C	339	ARG	CB-CA-C	-5.69	103.56	111.41
1	A	89	ILE	CB-CA-C	-5.67	104.71	111.97
1	A	336	THR	N-CA-C	-5.67	101.89	110.28
1	A	353	VAL	N-CA-C	5.63	118.01	109.12
1	A	177	LEU	N-CA-C	5.60	117.39	111.28
1	A	59	ARG	N-CA-C	-5.60	106.40	113.23
1	B	52	LYS	CA-CB-CG	-5.60	102.91	114.10
1	B	206	ILE	CB-CA-C	-5.59	104.82	111.81
1	C	289	LEU	CA-CB-CG	-5.59	96.73	116.30
1	B	193	ASN	N-CA-C	5.58	118.49	109.40
1	C	167	GLU	N-CA-C	5.56	120.20	113.41
1	A	194	GLU	N-CA-C	5.56	117.02	111.07
1	C	209	TYR	N-CA-C	5.56	119.23	112.23
1	A	186	PRO	N-CA-C	-5.56	106.62	113.84
1	A	347	THR	N-CA-C	5.56	117.63	109.24
1	C	336	THR	N-CA-C	-5.56	102.17	110.23
1	A	39	ASN	CA-C-N	5.55	126.78	119.84
1	A	39	ASN	C-N-CA	5.55	126.78	119.84
1	B	212	THR	N-CA-C	-5.54	102.67	109.65
1	A	175	ALA	N-CA-C	-5.50	105.36	111.36
1	A	265	THR	CB-CA-C	-5.49	100.19	113.19
1	B	133	VAL	CB-CA-C	-5.48	102.48	110.81
1	B	363	MET	O-C-N	5.48	125.82	121.55
1	B	215	ARG	N-CA-C	-5.48	101.55	110.20
1	A	287	GLY	N-CA-C	-5.47	100.21	113.18
1	C	212	THR	CA-C-O	5.47	124.15	119.66
1	B	304	LEU	N-CA-C	-5.47	100.79	109.59
1	B	287	GLY	N-CA-C	-5.46	100.23	113.18
1	C	78	SER	N-CA-C	-5.46	100.29	109.07
1	A	56	GLU	N-CA-C	-5.45	99.42	108.75
1	C	368	VAL	CB-CA-C	-5.45	102.36	111.29
1	C	284	ASP	N-CA-C	5.44	118.11	109.96
1	A	78	SER	N-CA-C	-5.43	100.32	109.07
1	C	196	VAL	CB-CA-C	-5.43	104.81	112.14
1	A	135	MET	CG-SD-CE	-5.42	88.97	100.90
1	C	322	ILE	CB-CA-C	-5.38	103.10	110.96
1	C	98	GLN	N-CA-C	5.37	117.05	108.41
1	B	20	VAL	CB-CA-C	-5.36	103.12	111.26
1	B	74	LYS	N-CA-C	5.33	117.17	111.36
1	C	255	ILE	CB-CA-C	-5.33	103.85	111.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	287	GLY	N-CA-C	-5.33	100.56	113.18
1	A	213	PRO	N-CA-C	5.31	119.64	111.57
1	A	196	VAL	CB-CA-C	-5.31	104.97	112.14
1	A	368	VAL	CB-CA-C	-5.30	102.59	111.29
1	B	39	ASN	CA-C-N	5.30	126.47	119.84
1	B	39	ASN	C-N-CA	5.30	126.47	119.84
1	C	194	GLU	N-CA-C	5.29	116.73	111.07
1	C	225	VAL	N-CA-C	5.29	115.91	109.30
1	C	127	GLY	N-CA-C	5.28	122.87	115.43
1	B	139	ASP	CA-C-N	-5.28	113.84	122.54
1	B	139	ASP	C-N-CA	-5.28	113.84	122.54
1	A	59	ARG	CB-CA-C	5.26	120.05	111.26
1	B	105	VAL	CB-CA-C	-5.23	103.72	110.84
1	C	145	GLU	N-CA-C	-5.23	105.66	111.36
1	A	88	TYR	N-CA-C	5.21	116.65	111.07
1	C	101	GLY	N-CA-C	-5.19	103.17	110.91
1	C	188	THR	CB-CA-C	-5.18	101.12	109.72
1	B	347	THR	N-CA-C	5.18	117.06	109.24
1	A	290	LEU	CA-CB-CG	-5.17	98.21	116.30
1	A	146	LEU	CA-CB-CG	-5.15	98.27	116.30
1	A	327	GLU	CB-CA-C	-5.14	101.87	110.56
1	B	296	GLU	N-CA-C	-5.13	105.86	112.68
1	A	21	ASP	N-CA-CB	-5.13	108.32	114.17
1	C	337	GLY	N-CA-C	-5.12	107.92	114.37
1	C	94	THR	CB-CA-C	-5.11	99.78	109.95
1	C	206	ILE	CB-CA-C	-5.10	105.43	111.81
1	C	304	LEU	N-CA-C	-5.10	101.38	109.59
1	C	39	ASN	CA-C-N	5.10	126.22	119.84
1	C	39	ASN	C-N-CA	5.10	126.22	119.84
1	C	49	ASP	N-CA-CB	5.09	117.34	109.91
1	B	180	GLU	N-CA-CB	5.09	118.17	110.28
1	B	257	GLY	N-CA-C	5.08	116.78	111.95
1	A	199	ILE	CB-CA-C	-5.07	105.29	112.14
1	A	193	ASN	N-CA-C	5.06	117.65	109.40
1	B	324	LYS	N-CA-C	-5.05	104.01	110.53
1	C	248	LYS	N-CA-C	-5.04	101.54	109.50
1	A	59	ARG	NE-CZ-NH2	5.03	123.73	119.20
1	A	100	ASP	N-CA-C	-5.03	106.32	112.90
1	A	19	HIS	N-CA-C	5.02	116.81	110.33
1	C	299	GLU	N-CA-C	5.02	116.69	109.07
1	B	247	VAL	CB-CA-C	-5.01	102.78	110.50
1	A	132	VAL	N-CA-C	-5.01	101.04	108.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	153	GLU	N-CA-C	-5.00	105.72	111.07

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	133	VAL	Mainchain
1	C	367	ASN	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3080	0	3091	272	0
1	B	3080	0	3091	297	1
1	C	3080	0	3091	291	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	28	0	12	4	0
3	B	28	0	12	3	0
3	C	28	0	12	3	0
4	A	33	0	0	2	0
4	B	23	0	0	0	0
4	C	39	0	0	1	0
All	All	9422	0	9309	852	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 46.

All (852) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:GLY:HA3	1:C:69:GLU:HG3	1.15	1.08
1:A:75:ARG:HH21	1:A:212:THR:HG23	1.20	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:227:ASP:HB3	1:C:229:PHE:HE1	1.24	1.00
1:A:276:THR:HG22	1:A:277:LEU:H	1.28	0.97
1:C:144:PRO:HA	1:C:147:LEU:HD12	1.44	0.97
1:C:311:THR:HG22	1:C:312:PRO:HD2	1.47	0.96
1:A:324:LYS:HB2	1:A:327:GLU:HG3	1.49	0.94
1:C:276:THR:HG22	1:C:277:LEU:H	1.28	0.94
1:C:324:LYS:HB2	1:C:327:GLU:HG3	1.48	0.94
1:A:350:THR:H	1:A:375:ILE:HD11	1.30	0.93
1:A:144:PRO:HA	1:A:147:LEU:HD12	1.49	0.93
1:B:227:ASP:HB3	1:B:229:PHE:HE1	1.33	0.93
1:A:311:THR:HG22	1:A:312:PRO:HD2	1.51	0.93
1:C:311:THR:HB	1:C:313:HIS:CE1	2.05	0.92
1:A:227:ASP:HB3	1:A:229:PHE:HE1	1.33	0.92
1:A:350:THR:N	1:A:375:ILE:HD11	1.84	0.92
1:C:350:THR:N	1:C:375:ILE:HD11	1.83	0.91
1:B:276:THR:HG22	1:B:277:LEU:H	1.34	0.91
1:B:350:THR:N	1:B:375:ILE:HD11	1.87	0.90
1:C:113:MET:HB3	1:C:114:PRO:HD2	1.54	0.90
1:A:33:TYR:CE1	1:A:44:VAL:HG13	2.07	0.89
1:B:263:ARG:NH1	1:B:297:GLU:HG2	1.86	0.88
1:B:324:LYS:HB2	1:B:327:GLU:HG3	1.55	0.88
1:B:33:TYR:CE1	1:B:44:VAL:HG13	2.08	0.87
1:B:75:ARG:HH21	1:B:212:THR:HG23	1.39	0.87
1:B:74:LYS:HG2	1:B:75:ARG:HG3	1.55	0.87
1:B:311:THR:HB	1:B:313:HIS:CE1	2.11	0.86
1:B:144:PRO:HA	1:B:147:LEU:HD12	1.56	0.86
1:B:311:THR:HG22	1:B:312:PRO:HD2	1.56	0.86
1:B:350:THR:H	1:B:375:ILE:HD11	1.39	0.86
1:B:350:THR:HB	1:B:375:ILE:HG12	1.58	0.86
1:A:113:MET:HB3	1:A:114:PRO:HD2	1.56	0.85
1:A:286:VAL:HG21	1:A:288:LEU:HD21	1.57	0.85
1:C:33:TYR:CE1	1:C:44:VAL:HG13	2.11	0.85
1:C:227:ASP:HB3	1:C:229:PHE:CE1	2.11	0.85
1:C:350:THR:H	1:C:375:ILE:HD11	1.41	0.85
1:A:291:ARG:HG2	1:A:291:ARG:HH11	1.41	0.85
1:B:311:THR:HB	1:B:313:HIS:HE1	1.39	0.85
1:C:74:LYS:HG2	1:C:75:ARG:HG3	1.56	0.85
1:B:231:ILE:CG2	1:B:234:ARG:HB2	2.06	0.85
1:A:263:ARG:NH1	1:A:297:GLU:HG2	1.92	0.85
1:A:277:LEU:HD12	1:A:278:GLN:N	1.93	0.84
1:B:270:VAL:HG12	1:B:271:GLU:H	1.43	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:PRO:HG2	1:A:359:VAL:HG23	1.59	0.83
1:C:248:LYS:HB3	1:C:279:GLU:HG3	1.60	0.82
1:B:231:ILE:HG22	1:B:234:ARG:HB2	1.61	0.82
1:C:136:ASN:ND2	1:C:137:LYS:H	1.76	0.82
1:A:311:THR:CG2	1:A:312:PRO:HD2	2.09	0.81
1:A:231:ILE:HG22	1:A:234:ARG:HG3	1.62	0.81
1:B:277:LEU:HD12	1:B:278:GLN:N	1.94	0.81
1:C:263:ARG:NH1	1:C:297:GLU:HG2	1.95	0.81
1:A:311:THR:HB	1:A:313:HIS:CE1	2.15	0.81
1:C:246:LYS:HB3	1:C:281:ILE:HG12	1.63	0.81
1:A:74:LYS:HG2	1:A:75:ARG:HG3	1.62	0.81
1:B:231:ILE:HD12	1:B:234:ARG:HD3	1.63	0.81
1:C:356:PRO:HG2	1:C:359:VAL:HG23	1.63	0.81
1:B:287:GLY:C	1:B:288:LEU:HD23	2.05	0.80
1:B:356:PRO:HG2	1:B:359:VAL:HG23	1.62	0.80
1:A:122:LEU:HA	1:A:125:GLN:HG3	1.63	0.80
1:B:248:LYS:HB3	1:B:279:GLU:HG3	1.64	0.80
1:B:113:MET:HB3	1:B:114:PRO:HD2	1.64	0.80
1:B:350:THR:HB	1:B:375:ILE:CG1	2.13	0.79
1:C:270:VAL:HG12	1:C:271:GLU:H	1.48	0.79
1:C:223:MET:HE3	1:C:240:GLY:O	1.82	0.79
1:A:59:ARG:HE	1:A:387:ALA:HB2	1.48	0.78
1:A:248:LYS:HB3	1:A:279:GLU:HG3	1.63	0.78
1:C:217:VAL:CG1	1:C:281:ILE:HD13	2.13	0.78
1:C:217:VAL:HG12	1:C:281:ILE:HD13	1.65	0.78
1:A:223:MET:HE3	1:A:240:GLY:O	1.84	0.78
1:C:350:THR:HB	1:C:375:ILE:HG12	1.66	0.78
1:B:33:TYR:HA	1:B:44:VAL:CG2	2.14	0.77
1:A:350:THR:HB	1:A:375:ILE:HG12	1.64	0.77
1:B:291:ARG:HH11	1:B:291:ARG:HG2	1.49	0.77
1:A:217:VAL:CG1	1:A:281:ILE:HD13	2.15	0.77
1:B:233:GLY:HA3	1:C:69:GLU:CG	2.07	0.77
1:C:198:LYS:HA	1:C:201:GLU:HG3	1.67	0.77
1:B:233:GLY:CA	1:C:69:GLU:HG3	2.09	0.76
1:C:291:ARG:HG2	1:C:291:ARG:HH11	1.51	0.76
1:C:338:TYR:CE2	1:C:340:PRO:HG3	2.20	0.76
1:A:136:ASN:ND2	1:A:175:ALA:H	1.84	0.76
1:B:59:ARG:HE	1:B:387:ALA:HB2	1.50	0.76
1:C:311:THR:HB	1:C:313:HIS:HE1	1.51	0.76
1:C:311:THR:CG2	1:C:312:PRO:HD2	2.14	0.76
1:C:171:ILE:HD13	1:C:202:LEU:HA	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:286:VAL:HG21	1:C:288:LEU:HD21	1.67	0.76
1:B:227:ASP:HB3	1:B:229:PHE:CE1	2.21	0.75
1:A:270:VAL:HG12	1:A:271:GLU:H	1.52	0.75
1:B:273:HIS:O	1:B:275:LYS:HE3	1.87	0.75
1:A:350:THR:HB	1:A:375:ILE:CG1	2.16	0.75
1:B:217:VAL:CG1	1:B:281:ILE:HD13	2.17	0.74
1:B:268:THR:CG2	1:B:291:ARG:HB2	2.17	0.74
1:A:75:ARG:NH2	1:A:212:THR:HG23	1.99	0.74
1:A:286:VAL:CG2	1:A:288:LEU:HD21	2.17	0.74
1:B:193:ASN:HD21	1:B:195:TRP:H	1.37	0.73
1:B:273:HIS:O	1:B:275:LYS:HG2	1.88	0.73
1:C:75:ARG:HH21	1:C:212:THR:HG23	1.52	0.73
1:A:356:PRO:HG2	1:A:359:VAL:CG2	2.19	0.73
1:A:227:ASP:HB3	1:A:229:PHE:CE1	2.21	0.72
1:C:277:LEU:HD12	1:C:278:GLN:N	2.04	0.72
1:A:216:ASP:HA	1:A:219:LYS:HD2	1.72	0.72
1:B:356:PRO:HG2	1:B:359:VAL:CG2	2.18	0.72
1:C:259:ALA:HB1	1:C:260:PRO:HD2	1.70	0.72
1:A:33:TYR:HA	1:A:44:VAL:CG2	2.19	0.72
1:B:311:THR:CG2	1:B:312:PRO:HD2	2.19	0.72
1:C:246:LYS:HG2	1:C:281:ILE:HG12	1.70	0.72
1:B:156:ASP:O	1:B:160:GLN:HG3	1.89	0.71
1:C:225:VAL:HG12	1:C:300:ARG:HA	1.72	0.71
1:C:193:ASN:HD21	1:C:195:TRP:H	1.39	0.71
1:B:286:VAL:HG21	1:B:288:LEU:HD21	1.73	0.71
1:B:231:ILE:CD1	1:B:234:ARG:HH11	2.04	0.71
1:B:287:GLY:O	1:B:288:LEU:HD23	1.90	0.71
1:B:233:GLY:N	1:C:69:GLU:OE2	2.24	0.70
1:A:287:GLY:C	1:A:288:LEU:HD23	2.15	0.70
1:B:190:ARG:O	1:B:192:GLU:N	2.22	0.70
1:C:39:ASN:O	1:C:41:ASN:N	2.24	0.70
1:C:171:ILE:CD1	1:C:202:LEU:HA	2.21	0.70
1:C:253:VAL:HA	1:C:307:PRO:HD3	1.73	0.70
1:C:356:PRO:HD2	1:C:359:VAL:HB	1.73	0.70
1:A:101:GLY:HA3	1:A:210:ILE:HD13	1.74	0.70
1:A:39:ASN:O	1:A:41:ASN:N	2.25	0.70
1:C:287:GLY:C	1:C:288:LEU:HD23	2.17	0.70
1:B:270:VAL:HG12	1:B:271:GLU:N	2.07	0.70
1:C:267:VAL:HG12	1:C:269:GLY:H	1.56	0.70
1:A:311:THR:HB	1:A:313:HIS:HE1	1.57	0.69
1:A:246:LYS:HG2	1:A:281:ILE:HG12	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:268:THR:HG23	1:B:291:ARG:HB2	1.75	0.69
1:B:246:LYS:HB3	1:B:281:ILE:HG12	1.74	0.69
1:A:23:GLY:HA2	3:A:407:GDP:PA	2.33	0.69
1:A:246:LYS:HG2	1:A:281:ILE:CG1	2.22	0.69
1:B:23:GLY:HA2	3:B:407:GDP:PA	2.32	0.69
1:B:136:ASN:ND2	1:B:175:ALA:H	1.91	0.69
1:B:231:ILE:HD12	1:B:234:ARG:HH11	1.56	0.69
1:C:246:LYS:HG2	1:C:281:ILE:CG1	2.22	0.69
1:C:85:HIS:O	1:C:89:ILE:HG12	1.93	0.69
1:C:273:HIS:O	1:C:275:LYS:HE3	1.92	0.69
1:C:350:THR:HB	1:C:375:ILE:CG1	2.23	0.69
1:B:258:LEU:N	1:B:258:LEU:HD23	2.09	0.68
1:C:291:ARG:HG2	1:C:291:ARG:NH1	2.07	0.68
1:C:356:PRO:HG2	1:C:359:VAL:CG2	2.23	0.68
1:A:223:MET:HG2	1:A:224:PRO:HD2	1.75	0.68
1:A:291:ARG:HG2	1:A:291:ARG:NH1	2.05	0.68
1:A:92:MET:O	1:A:385:ARG:NH2	2.27	0.68
1:A:339:ARG:HD2	4:A:436:HOH:O	1.93	0.68
1:C:246:LYS:CG	1:C:281:ILE:HG12	2.23	0.68
1:B:245:GLY:C	1:B:246:LYS:HG3	2.16	0.68
1:C:241:ARG:HA	1:C:285:ASN:HA	1.76	0.68
1:B:221:PHE:HA	1:B:244:ARG:O	1.93	0.67
1:C:246:LYS:CB	1:C:281:ILE:HG12	2.25	0.67
1:A:9:LYS:HE2	1:A:73:ALA:O	1.94	0.67
1:A:113:MET:O	1:A:116:THR:HB	1.93	0.67
1:B:230:THR:HA	1:B:235:GLY:O	1.95	0.67
1:C:270:VAL:HG12	1:C:271:GLU:N	2.09	0.67
1:A:217:VAL:O	1:A:245:GLY:HA2	1.93	0.67
1:A:226:GLU:O	1:A:300:ARG:NH1	2.28	0.67
1:A:268:THR:HG21	1:A:291:ARG:HB2	1.76	0.67
1:B:225:VAL:HG12	1:B:300:ARG:HA	1.76	0.67
1:C:190:ARG:O	1:C:192:GLU:N	2.25	0.67
1:A:193:ASN:HD22	1:A:196:VAL:HG23	1.60	0.67
1:C:23:GLY:HA2	3:C:407:GDP:PA	2.35	0.67
1:C:61:ILE:CG2	1:C:90:LYS:HD3	2.25	0.67
1:C:258:LEU:HD23	1:C:258:LEU:N	2.10	0.67
1:A:206:ILE:HG22	1:A:207:ASP:N	2.10	0.67
1:C:33:TYR:HA	1:C:44:VAL:CG2	2.24	0.67
1:A:259:ALA:HB1	1:A:260:PRO:HD2	1.76	0.67
1:B:214:VAL:HG12	1:B:215:ARG:O	1.94	0.66
1:A:276:THR:HG22	1:A:277:LEU:N	2.07	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:323:LEU:CD1	1:C:327:GLU:HB2	2.25	0.66
1:B:88:TYR:O	1:B:92:MET:HG3	1.96	0.66
1:C:59:ARG:HE	1:C:387:ALA:HB2	1.60	0.66
1:B:223:MET:HE3	1:B:240:GLY:O	1.96	0.66
1:B:113:MET:O	1:B:116:THR:HB	1.96	0.66
1:B:85:HIS:O	1:B:89:ILE:HG12	1.94	0.66
1:A:190:ARG:O	1:A:192:GLU:N	2.29	0.66
1:C:255:ILE:HD13	1:C:298:VAL:HG22	1.78	0.66
1:C:9:LYS:HE2	1:C:73:ALA:O	1.95	0.66
1:B:39:ASN:O	1:B:41:ASN:N	2.29	0.65
1:B:231:ILE:O	1:B:234:ARG:N	2.28	0.65
1:C:74:LYS:C	1:C:75:ARG:HG3	2.21	0.65
1:A:258:LEU:N	1:A:258:LEU:HD23	2.10	0.65
1:B:291:ARG:HG2	1:B:291:ARG:NH1	2.07	0.65
1:A:225:VAL:HG12	1:A:300:ARG:HA	1.77	0.65
1:B:226:GLU:O	1:B:300:ARG:NH1	2.28	0.65
1:A:231:ILE:CG2	1:A:234:ARG:HG3	2.26	0.65
1:A:245:GLY:C	1:A:246:LYS:HG3	2.21	0.65
1:B:74:LYS:C	1:B:75:ARG:HG3	2.22	0.65
1:B:313:HIS:O	1:B:377:PRO:HA	1.97	0.65
1:A:61:ILE:HG21	1:A:90:LYS:HD3	1.78	0.65
1:A:74:LYS:C	1:A:75:ARG:HG3	2.21	0.65
1:A:194:GLU:HG2	1:A:195:TRP:N	2.12	0.65
1:B:46:ASP:OD1	1:B:46:ASP:N	2.28	0.65
1:B:293:VAL:HG11	1:B:298:VAL:HG23	1.77	0.65
1:C:122:LEU:HA	1:C:125:GLN:HG3	1.79	0.65
1:B:13:ASN:HB2	1:B:100:ASP:OD2	1.96	0.65
1:B:216:ASP:HA	1:B:219:LYS:HD2	1.78	0.65
1:A:33:TYR:CZ	1:A:44:VAL:HG13	2.32	0.64
1:B:266:VAL:HG12	1:B:267:VAL:O	1.96	0.64
1:B:23:GLY:HA2	3:B:407:GDP:O2A	1.98	0.64
1:C:266:VAL:HG12	1:C:267:VAL:O	1.96	0.64
1:A:223:MET:HG2	1:A:224:PRO:CD	2.28	0.64
1:C:320:VAL:HG12	1:C:321:TYR:N	2.11	0.64
1:C:216:ASP:HA	1:C:219:LYS:HD2	1.80	0.64
1:C:323:LEU:HD12	1:C:327:GLU:HB2	1.80	0.64
1:A:55:GLU:HB3	1:A:62:THR:HG22	1.80	0.64
1:C:231:ILE:HD12	1:C:234:ARG:NH1	2.13	0.64
1:A:171:ILE:HD13	1:A:202:LEU:HA	1.80	0.64
1:B:259:ALA:HB1	1:B:260:PRO:HD2	1.78	0.64
1:A:257:GLY:O	1:A:259:ALA:N	2.29	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:LYS:HA	1:A:201:GLU:HG3	1.80	0.63
1:B:33:TYR:CZ	1:B:44:VAL:HG13	2.32	0.63
1:C:270:VAL:O	1:C:271:GLU:HB2	1.97	0.63
1:B:55:GLU:HB3	1:B:62:THR:HG22	1.79	0.63
1:A:136:ASN:HD21	1:A:175:ALA:H	1.46	0.63
1:C:245:GLY:C	1:C:246:LYS:HG3	2.22	0.63
1:A:270:VAL:HG12	1:A:271:GLU:N	2.13	0.63
1:C:380:LEU:HD23	1:C:384:LEU:HD23	1.79	0.63
1:A:355:LEU:CD1	1:A:362:VAL:HG23	2.29	0.63
1:C:33:TYR:HB3	1:C:182:MET:HB3	1.81	0.63
1:B:122:LEU:HA	1:B:125:GLN:HG3	1.80	0.62
1:C:313:HIS:O	1:C:377:PRO:HA	1.99	0.62
1:A:277:LEU:HD12	1:A:278:GLN:H	1.64	0.62
1:B:293:VAL:HG11	1:B:298:VAL:CG2	2.29	0.62
1:B:350:THR:O	1:B:375:ILE:HG13	2.00	0.62
1:C:61:ILE:HG21	1:C:90:LYS:HD3	1.82	0.62
1:A:273:HIS:O	1:A:275:LYS:HE3	1.98	0.62
1:B:270:VAL:O	1:B:271:GLU:HB2	1.99	0.62
1:A:217:VAL:HG12	1:A:281:ILE:HD13	1.80	0.62
1:A:246:LYS:CG	1:A:281:ILE:HG12	2.30	0.62
1:C:226:GLU:O	1:C:300:ARG:NH1	2.33	0.62
1:B:246:LYS:HG2	1:B:281:ILE:CG1	2.29	0.62
1:B:246:LYS:HG2	1:B:281:ILE:HG12	1.80	0.62
1:B:193:ASN:HD22	1:B:196:VAL:H	1.46	0.62
1:A:19:HIS:HD2	1:A:115:GLN:H	1.48	0.62
1:A:266:VAL:HG12	1:A:267:VAL:O	1.99	0.62
1:A:310:ILE:CD1	1:A:381:GLU:HG2	2.29	0.62
1:B:198:LYS:HA	1:B:201:GLU:HG3	1.82	0.62
1:B:217:VAL:HG12	1:B:281:ILE:HD13	1.81	0.62
1:C:257:GLY:O	1:C:259:ALA:N	2.30	0.62
1:C:268:THR:CG2	1:C:291:ARG:HB2	2.29	0.62
1:C:113:MET:HB3	1:C:114:PRO:CD	2.28	0.62
1:A:61:ILE:CG2	1:A:90:LYS:HD3	2.30	0.61
1:A:46:ASP:N	1:A:46:ASP:OD1	2.33	0.61
1:B:238:ALA:HB2	1:B:290:LEU:HD11	1.82	0.61
1:B:320:VAL:HG12	1:B:321:TYR:N	2.14	0.61
1:C:193:ASN:HD22	1:C:196:VAL:HG23	1.64	0.61
1:A:19:HIS:CD2	1:A:115:GLN:H	2.18	0.61
1:C:231:ILE:HG21	1:C:234:ARG:HD3	1.81	0.61
1:A:268:THR:CG2	1:A:291:ARG:HB2	2.30	0.61
1:B:136:ASN:ND2	1:B:137:LYS:H	1.97	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:VAL:O	1:B:245:GLY:HA2	2.00	0.60
1:B:277:LEU:HD12	1:B:278:GLN:H	1.66	0.60
1:C:286:VAL:CG2	1:C:288:LEU:HD21	2.31	0.60
1:C:46:ASP:N	1:C:46:ASP:OD1	2.30	0.60
1:B:28:THR:HG22	1:B:50:ILE:HD12	1.83	0.60
1:B:323:LEU:HD13	1:B:327:GLU:HB2	1.83	0.60
1:B:33:TYR:HA	1:B:44:VAL:HG22	1.83	0.60
1:B:75:ARG:NH2	1:B:212:THR:HG23	2.11	0.60
1:C:255:ILE:HD13	1:C:298:VAL:CG2	2.31	0.60
1:B:291:ARG:HH11	1:B:291:ARG:CG	2.15	0.60
1:C:113:MET:O	1:C:116:THR:HB	2.02	0.60
1:B:19:HIS:CD2	1:B:115:GLN:H	2.19	0.60
1:C:265:THR:HG21	1:C:293:VAL:CG2	2.31	0.60
1:B:150:VAL:HA	1:B:153:GLU:HG3	1.84	0.60
1:A:311:THR:HG22	1:A:312:PRO:CD	2.28	0.60
1:A:189:LYS:N	1:A:192:GLU:OE2	2.30	0.60
1:B:14:VAL:O	1:B:79:HIS:HA	2.02	0.60
1:A:12:VAL:O	1:A:77:TYR:HA	2.02	0.59
1:C:343:TYR:CE1	1:C:347:THR:HA	2.37	0.59
1:A:113:MET:HB3	1:A:114:PRO:CD	2.27	0.59
1:C:188:THR:HG22	1:C:189:LYS:N	2.17	0.59
1:C:268:THR:HG21	1:C:291:ARG:HB2	1.84	0.59
1:A:356:PRO:HD2	1:A:359:VAL:HB	1.84	0.59
1:B:253:VAL:HA	1:B:307:PRO:HD3	1.84	0.59
1:A:350:THR:O	1:A:375:ILE:HG13	2.03	0.59
1:A:75:ARG:NH1	1:A:77:TYR:OH	2.29	0.59
1:B:350:THR:CB	1:B:375:ILE:HD11	2.33	0.59
1:C:33:TYR:CZ	1:C:44:VAL:HG13	2.37	0.59
1:B:265:THR:CG2	1:B:293:VAL:HG23	2.33	0.59
1:C:36:ALA:O	1:C:39:ASN:N	2.35	0.59
1:B:9:LYS:HE2	1:B:73:ALA:O	2.03	0.59
1:C:19:HIS:HD2	1:C:115:GLN:H	1.51	0.59
1:C:136:ASN:ND2	1:C:137:LYS:N	2.50	0.59
1:B:61:ILE:CG2	1:B:90:LYS:HD3	2.33	0.58
1:B:61:ILE:HG21	1:B:90:LYS:HD3	1.85	0.58
1:B:257:GLY:O	1:B:259:ALA:N	2.34	0.58
1:C:19:HIS:CD2	1:C:115:GLN:H	2.20	0.58
1:A:28:THR:HG22	1:A:50:ILE:HD12	1.83	0.58
1:A:372:VAL:HG12	1:A:373:GLU:N	2.16	0.58
1:B:33:TYR:HB3	1:B:182:MET:HB3	1.85	0.58
1:C:16:THR:HB	1:C:24:LYS:HB3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:GLY:O	1:A:288:LEU:HD23	2.03	0.58
1:B:9:LYS:NZ	1:B:71:GLU:OE2	2.29	0.58
1:B:171:ILE:HD13	1:B:202:LEU:HA	1.86	0.58
1:B:286:VAL:CG2	1:B:288:LEU:HD21	2.32	0.58
1:C:193:ASN:ND2	1:C:195:TRP:H	2.02	0.58
1:C:231:ILE:HD12	1:C:234:ARG:HH11	1.68	0.58
1:B:263:ARG:HH12	1:B:297:GLU:HG2	1.67	0.58
1:C:246:LYS:HB3	1:C:281:ILE:CG1	2.31	0.58
1:A:9:LYS:NZ	1:A:71:GLU:OE2	2.28	0.57
1:B:267:VAL:HG12	1:B:269:GLY:H	1.69	0.57
1:C:55:GLU:HB3	1:C:62:THR:HG22	1.86	0.57
1:A:33:TYR:CD1	1:A:44:VAL:HG22	2.38	0.57
1:A:231:ILE:HG21	1:A:234:ARG:HD3	1.86	0.57
1:B:246:LYS:CG	1:B:281:ILE:HG12	2.34	0.57
1:B:276:THR:HG22	1:B:277:LEU:N	2.13	0.57
1:C:53:ALA:HB1	1:C:65:THR:C	2.30	0.57
1:C:227:ASP:CB	1:C:229:PHE:HE1	2.09	0.57
1:A:253:VAL:HA	1:A:307:PRO:HD3	1.87	0.57
1:B:34:VAL:HG12	1:B:35:ALA:N	2.19	0.57
1:C:265:THR:HG21	1:C:293:VAL:HG23	1.86	0.57
1:A:246:LYS:HB3	1:A:281:ILE:HG12	1.86	0.57
1:A:34:VAL:HG22	1:A:196:VAL:HG13	1.86	0.57
1:B:171:ILE:CD1	1:B:202:LEU:HA	2.35	0.57
1:B:206:ILE:HG22	1:B:207:ASP:N	2.18	0.57
1:C:350:THR:O	1:C:375:ILE:HG13	2.05	0.57
1:C:10:PRO:O	1:C:75:ARG:HB3	2.05	0.56
1:C:193:ASN:HD22	1:C:196:VAL:H	1.53	0.56
1:C:206:ILE:HG22	1:C:207:ASP:N	2.20	0.56
1:A:23:GLY:HA2	3:A:407:GDP:O3A	2.04	0.56
1:A:113:MET:H	1:A:116:THR:CB	2.18	0.56
1:C:230:THR:HA	1:C:235:GLY:O	2.05	0.56
1:A:214:VAL:HG12	1:A:215:ARG:O	2.06	0.56
1:A:40:PRO:HD2	1:A:41:ASN:ND2	2.21	0.56
1:A:156:ASP:O	1:A:160:GLN:HG3	2.05	0.56
1:C:138:VAL:HG12	1:C:139:ASP:N	2.20	0.56
1:C:143:ASP:HB3	1:C:146:LEU:HD12	1.87	0.56
1:C:291:ARG:HH11	1:C:291:ARG:CG	2.17	0.56
1:B:288:LEU:HD23	1:B:288:LEU:N	2.14	0.56
1:C:17:ILE:C	1:C:24:LYS:HD3	2.30	0.56
1:C:273:HIS:O	1:C:275:LYS:HG2	2.06	0.56
1:A:136:ASN:ND2	1:A:137:LYS:H	2.03	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:PRO:CA	1:C:147:LEU:HD12	2.28	0.56
1:C:238:ALA:HB2	1:C:290:LEU:HD11	1.87	0.56
1:A:36:ALA:O	1:A:39:ASN:N	2.38	0.56
1:B:232:THR:OG1	1:C:78:SER:HB3	2.06	0.56
1:C:23:GLY:HA2	3:C:407:GDP:O2A	2.06	0.56
1:C:223:MET:HE3	1:C:240:GLY:C	2.31	0.56
1:B:372:VAL:HG12	1:B:373:GLU:N	2.20	0.56
1:A:320:VAL:HG12	1:A:321:TYR:N	2.22	0.55
1:A:353:VAL:HG12	1:A:354:ARG:N	2.21	0.55
1:C:64:ASN:O	1:C:82:CYS:HB3	2.07	0.55
1:A:344:PHE:O	1:A:345:ARG:HB2	2.07	0.55
1:C:133:VAL:HB	1:C:170:VAL:HA	1.88	0.55
1:C:171:ILE:HD13	1:C:202:LEU:CA	2.35	0.55
1:B:113:MET:HB3	1:B:114:PRO:CD	2.35	0.55
1:C:343:TYR:HE1	1:C:347:THR:HA	1.72	0.55
1:B:350:THR:HB	1:B:375:ILE:CD1	2.36	0.55
1:A:217:VAL:HG11	1:A:281:ILE:HD13	1.87	0.55
1:A:182:MET:HE1	1:A:188:THR:HB	1.89	0.55
1:B:268:THR:HG21	1:B:291:ARG:HB2	1.87	0.55
1:C:13:ASN:HB2	1:C:100:ASP:OD2	2.07	0.55
1:A:171:ILE:CD1	1:A:202:LEU:HA	2.36	0.54
1:B:193:ASN:HD21	1:B:195:TRP:N	2.05	0.54
1:C:193:ASN:HD21	1:C:195:TRP:N	2.04	0.54
1:A:223:MET:HE3	1:A:240:GLY:C	2.32	0.54
1:B:193:ASN:ND2	1:B:195:TRP:H	2.01	0.54
1:B:246:LYS:CB	1:B:281:ILE:HG12	2.37	0.54
1:C:193:ASN:ND2	1:C:196:VAL:H	2.05	0.54
1:A:174:SER:OG	1:A:177:LEU:HG	2.08	0.54
1:A:193:ASN:HD22	1:A:196:VAL:H	1.56	0.54
1:A:254:GLU:O	1:A:304:LEU:HA	2.07	0.54
1:C:33:TYR:HA	1:C:44:VAL:HG22	1.89	0.54
1:A:68:VAL:HG12	1:A:79:HIS:HB3	1.89	0.54
1:B:223:MET:HE3	1:B:240:GLY:CA	2.38	0.54
1:B:350:THR:CA	1:B:375:ILE:HD11	2.38	0.54
1:C:238:ALA:CB	1:C:290:LEU:HD11	2.38	0.54
1:A:112:PRO:C	1:A:113:MET:HG2	2.33	0.54
1:A:187:LYS:O	1:A:189:LYS:HG2	2.08	0.54
1:A:193:ASN:HD21	1:A:195:TRP:H	1.55	0.54
1:B:137:LYS:HA	3:B:407:GDP:N1	2.23	0.54
1:B:231:ILE:HD12	1:B:234:ARG:NH1	2.23	0.54
1:B:246:LYS:HB3	1:B:281:ILE:CG1	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:GLU:HB3	1:A:62:THR:CG2	2.37	0.53
1:A:355:LEU:HD13	1:A:362:VAL:HG23	1.89	0.53
1:B:223:MET:HE3	1:B:240:GLY:C	2.33	0.53
1:B:265:THR:HG22	1:B:291:ARG:O	2.09	0.53
1:B:188:THR:HG22	1:B:189:LYS:N	2.23	0.53
1:C:75:ARG:HD2	1:C:77:TYR:OH	2.08	0.53
1:C:231:ILE:O	1:C:234:ARG:N	2.41	0.53
1:A:33:TYR:CG	1:A:44:VAL:HG22	2.43	0.53
1:A:122:LEU:O	1:A:125:GLN:N	2.42	0.53
1:B:180:GLU:O	1:B:183:HIS:HB2	2.07	0.53
1:B:189:LYS:N	1:B:192:GLU:OE1	2.39	0.53
1:C:311:THR:HG22	1:C:312:PRO:CD	2.30	0.53
1:A:221:PHE:HA	1:A:244:ARG:O	2.08	0.53
1:A:247:VAL:N	1:A:280:GLY:O	2.34	0.53
1:C:136:ASN:ND2	1:C:175:ALA:H	2.05	0.53
1:C:189:LYS:N	1:C:192:GLU:OE2	2.41	0.53
1:B:17:ILE:C	1:B:24:LYS:HD3	2.34	0.53
1:B:311:THR:HG22	1:B:312:PRO:CD	2.33	0.53
1:B:112:PRO:C	1:B:113:MET:HG2	2.33	0.53
1:B:238:ALA:CB	1:B:290:LEU:HD11	2.38	0.53
1:C:231:ILE:CG2	1:C:234:ARG:HB2	2.39	0.53
1:A:263:ARG:HH12	1:A:297:GLU:HG2	1.69	0.53
1:A:270:VAL:O	1:A:271:GLU:HB2	2.07	0.53
1:A:350:THR:CA	1:A:375:ILE:HD11	2.37	0.53
1:B:310:ILE:HD12	1:B:381:GLU:HG2	1.91	0.53
1:C:28:THR:HG22	1:C:50:ILE:HD12	1.91	0.53
1:B:254:GLU:O	1:B:304:LEU:HA	2.08	0.52
1:C:277:LEU:HD12	1:C:278:GLN:H	1.73	0.52
1:A:193:ASN:ND2	1:A:196:VAL:H	2.07	0.52
1:A:338:TYR:CE2	1:A:340:PRO:HG3	2.44	0.52
1:B:306:LYS:HG3	1:B:307:PRO:N	2.14	0.52
1:B:234:ARG:NH1	1:C:76:HIS:CE1	2.78	0.52
1:C:75:ARG:NH1	1:C:207:ASP:HA	2.23	0.52
1:A:33:TYR:HA	1:A:44:VAL:HG22	1.90	0.52
1:A:277:LEU:HD12	1:A:277:LEU:C	2.35	0.52
1:B:174:SER:OG	1:B:177:LEU:HG	2.09	0.52
1:C:350:THR:CA	1:C:375:ILE:HD11	2.40	0.52
1:A:77:TYR:OH	1:A:206:ILE:HG22	2.09	0.52
1:B:241:ARG:HA	1:B:285:ASN:HA	1.91	0.52
1:C:214:VAL:HG12	1:C:215:ARG:O	2.10	0.52
1:B:124:ARG:HH21	1:B:162:GLU:C	2.18	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:404:LEU:O	1:C:405:GLU:HG3	2.09	0.52
1:A:85:HIS:O	1:A:89:ILE:HG12	2.09	0.52
1:B:277:LEU:HD12	1:B:277:LEU:C	2.33	0.52
1:C:350:THR:HB	1:C:375:ILE:CD1	2.40	0.52
1:A:350:THR:HB	1:A:375:ILE:CD1	2.40	0.52
1:C:77:TYR:OH	1:C:206:ILE:HG22	2.10	0.52
1:A:13:ASN:HB2	1:A:100:ASP:OD2	2.10	0.52
1:B:161:TYR:O	1:B:162:GLU:HB2	2.10	0.52
1:B:380:LEU:HD23	1:B:384:LEU:HD23	1.90	0.52
1:C:180:GLU:O	1:C:183:HIS:HB2	2.09	0.52
1:A:313:HIS:O	1:A:377:PRO:HA	2.09	0.52
1:B:19:HIS:HD2	1:B:115:GLN:H	1.56	0.52
1:B:64:ASN:O	1:B:82:CYS:HB3	2.10	0.52
1:B:65:THR:HG22	1:B:66:ALA:N	2.25	0.52
1:B:34:VAL:HG22	1:B:196:VAL:HG13	1.91	0.51
1:B:193:ASN:HD21	1:B:195:TRP:HB2	1.74	0.51
1:B:193:ASN:ND2	1:B:196:VAL:H	2.09	0.51
1:C:293:VAL:HG11	1:C:298:VAL:HG23	1.91	0.51
1:C:15:GLY:HA3	1:C:99:MET:CE	2.40	0.51
1:B:10:PRO:O	1:B:75:ARG:HB3	2.09	0.51
1:B:33:TYR:CD1	1:B:44:VAL:HG22	2.46	0.51
1:C:209:TYR:O	1:C:211:PRO:HD3	2.11	0.51
1:C:223:MET:CE	1:C:240:GLY:N	2.73	0.51
1:C:287:GLY:O	1:C:288:LEU:HD23	2.09	0.51
1:A:22:HIS:ND1	4:A:420:HOH:O	2.31	0.51
1:B:356:PRO:HD2	1:B:359:VAL:HB	1.93	0.51
1:C:124:ARG:HH21	1:C:162:GLU:C	2.19	0.51
1:C:174:SER:OG	1:C:177:LEU:HG	2.10	0.51
1:A:276:THR:CG2	1:A:277:LEU:H	2.12	0.51
1:B:203:LEU:O	1:B:206:ILE:HB	2.11	0.51
1:C:265:THR:CG2	1:C:293:VAL:HG23	2.39	0.51
1:A:255:ILE:HD13	1:A:298:VAL:HG22	1.92	0.51
1:A:350:THR:CB	1:A:375:ILE:HD11	2.40	0.51
1:A:377:PRO:C	1:A:378:VAL:HG23	2.35	0.51
1:B:185:ASN:HB2	1:B:188:THR:OG1	2.11	0.51
1:B:231:ILE:HD12	1:B:234:ARG:CD	2.38	0.51
1:C:255:ILE:HG21	1:C:298:VAL:HG22	1.93	0.51
1:B:323:LEU:CD1	1:B:327:GLU:HB2	2.41	0.51
1:B:338:TYR:CE2	1:B:340:PRO:HG3	2.46	0.51
1:A:258:LEU:HD23	1:A:258:LEU:H	1.76	0.50
1:C:246:LYS:HG2	1:C:281:ILE:CD1	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:TYR:OH	1:A:46:ASP:OD1	2.28	0.50
1:C:33:TYR:HB3	1:C:182:MET:CB	2.41	0.50
1:C:68:VAL:HG12	1:C:79:HIS:HB3	1.94	0.50
1:B:193:ASN:ND2	1:B:195:TRP:N	2.60	0.50
1:B:246:LYS:HB3	1:B:280:GLY:O	2.11	0.50
1:C:156:ASP:O	1:C:160:GLN:HG3	2.11	0.50
1:B:355:LEU:HD11	1:B:362:VAL:HG23	1.93	0.50
1:C:187:LYS:O	1:C:189:LYS:HG2	2.12	0.50
1:A:355:LEU:HD11	1:A:362:VAL:HG23	1.92	0.50
1:B:258:LEU:HD23	1:B:377:PRO:O	2.11	0.50
1:C:231:ILE:CD1	1:C:234:ARG:HH11	2.25	0.50
1:C:246:LYS:HG2	1:C:281:ILE:HD11	1.94	0.50
1:B:194:GLU:HG2	1:B:195:TRP:N	2.25	0.50
1:A:136:ASN:O	1:A:137:LYS:HB2	2.11	0.50
1:A:404:LEU:O	1:A:405:GLU:HG3	2.11	0.49
1:B:223:MET:CE	1:B:240:GLY:N	2.75	0.49
1:B:234:ARG:NH2	1:B:271:GLU:OE1	2.36	0.49
1:C:399:VAL:HG12	1:C:400:VAL:N	2.23	0.49
1:A:258:LEU:HD23	1:A:377:PRO:O	2.12	0.49
1:C:353:VAL:HG12	1:C:354:ARG:N	2.25	0.49
1:B:41:ASN:H	1:B:41:ASN:ND2	2.09	0.49
1:C:377:PRO:C	1:C:378:VAL:HG23	2.37	0.49
1:A:19:HIS:CD2	1:A:115:GLN:HB2	2.47	0.49
1:A:223:MET:CE	1:A:240:GLY:N	2.75	0.49
1:A:312:PRO:HA	1:A:378:VAL:O	2.12	0.49
1:B:84:GLY:O	1:B:87:ASP:HB2	2.12	0.49
1:C:164:PRO:O	1:C:164:PRO:HG2	2.11	0.49
1:C:203:LEU:O	1:C:206:ILE:HB	2.11	0.49
1:C:258:LEU:HD23	1:C:377:PRO:O	2.13	0.49
1:B:126:VAL:HG22	1:B:385:ARG:NH2	2.27	0.49
1:B:228:VAL:HA	1:B:237:VAL:O	2.12	0.49
1:B:389:ARG:HB3	1:B:393:ARG:O	2.13	0.49
1:A:33:TYR:HE1	1:A:45:LYS:O	1.96	0.49
1:C:193:ASN:ND2	1:C:195:TRP:N	2.61	0.49
1:B:231:ILE:HG21	1:B:234:ARG:CD	2.42	0.49
1:B:255:ILE:HG13	1:B:263:ARG:O	2.13	0.49
1:C:148:ASP:O	1:C:152:MET:HG2	2.12	0.49
1:A:339:ARG:HA	1:A:351:GLY:O	2.13	0.49
1:C:55:GLU:HB3	1:C:62:THR:CG2	2.43	0.48
1:C:63:ILE:HD13	1:C:91:ASN:N	2.28	0.48
1:C:276:THR:HG22	1:C:277:LEU:N	2.08	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:ARG:HD2	1:A:77:TYR:OH	2.13	0.48
1:A:246:LYS:CB	1:A:281:ILE:HG12	2.43	0.48
1:B:137:LYS:O	1:B:140:MET:HG3	2.14	0.48
1:B:214:VAL:HG12	1:B:215:ARG:N	2.27	0.48
1:C:221:PHE:O	1:C:306:LYS:N	2.39	0.48
1:A:27:LEU:HD21	1:A:202:LEU:HD21	1.94	0.48
1:B:40:PRO:HD2	1:B:41:ASN:ND2	2.29	0.48
1:C:190:ARG:C	1:C:192:GLU:H	2.20	0.48
1:C:231:ILE:O	1:C:231:ILE:HG22	2.13	0.48
1:C:372:VAL:HG12	1:C:373:GLU:N	2.29	0.48
1:A:23:GLY:HA2	3:A:407:GDP:O2A	2.13	0.48
1:B:404:LEU:O	1:B:405:GLU:HG3	2.13	0.48
1:B:187:LYS:O	1:B:189:LYS:HG2	2.14	0.48
1:C:384:LEU:HD12	1:C:385:ARG:N	2.28	0.48
1:A:17:ILE:C	1:A:24:LYS:HD3	2.39	0.48
1:B:133:VAL:HB	1:B:170:VAL:HA	1.94	0.48
1:B:136:ASN:O	1:B:137:LYS:HB2	2.13	0.48
1:B:353:VAL:HG12	1:B:354:ARG:N	2.28	0.48
1:C:126:VAL:HG22	1:C:385:ARG:NH2	2.29	0.48
1:A:19:HIS:HD2	1:A:115:GLN:N	2.12	0.48
1:B:82:CYS:HA	1:B:83:PRO:HD3	1.55	0.48
1:C:133:VAL:HG12	1:C:134:PHE:N	2.27	0.48
1:C:136:ASN:CG	1:C:137:LYS:N	2.72	0.48
1:C:323:LEU:HD13	1:C:327:GLU:HB2	1.96	0.48
1:B:350:THR:HB	1:B:375:ILE:HD11	1.95	0.47
1:C:217:VAL:HG12	1:C:281:ILE:CD1	2.40	0.47
1:B:54:PRO:O	1:B:64:ASN:HA	2.14	0.47
1:B:126:VAL:HG22	1:B:385:ARG:HH22	1.79	0.47
1:B:339:ARG:HA	1:B:351:GLY:O	2.14	0.47
1:B:350:THR:HG22	1:B:351:GLY:N	2.29	0.47
1:C:254:GLU:O	1:C:304:LEU:HA	2.14	0.47
1:C:256:VAL:HG12	1:C:379:ALA:HB2	1.96	0.47
1:C:258:LEU:HD23	1:C:258:LEU:H	1.79	0.47
1:A:124:ARG:HH21	1:A:162:GLU:C	2.22	0.47
1:A:350:THR:HB	1:A:375:ILE:HD11	1.97	0.47
1:B:281:ILE:O	1:B:284:ASP:HB2	2.15	0.47
1:B:74:LYS:HG2	1:B:75:ARG:CG	2.36	0.47
1:C:112:PRO:C	1:C:113:MET:HG2	2.39	0.47
1:B:128:VAL:HA	1:B:129:PRO:HD3	1.52	0.47
1:B:217:VAL:HG11	1:B:281:ILE:HD13	1.92	0.47
1:A:158:LEU:HB3	1:A:163:PHE:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:ILE:HG22	1:A:231:ILE:O	2.13	0.47
1:B:16:THR:HB	1:B:24:LYS:HB3	1.96	0.47
1:B:33:TYR:CZ	1:B:44:VAL:CG1	2.98	0.47
1:B:217:VAL:HG13	1:B:282:ALA:HB3	1.95	0.47
1:B:293:VAL:CG1	1:B:298:VAL:HG23	2.43	0.47
1:B:375:ILE:HG13	1:B:375:ILE:H	1.32	0.47
1:C:74:LYS:HG2	1:C:75:ARG:CG	2.37	0.47
1:C:273:HIS:C	1:C:274:ARG:HG3	2.40	0.47
1:C:281:ILE:O	1:C:284:ASP:HB2	2.15	0.47
1:A:113:MET:H	1:A:116:THR:HB	1.78	0.47
1:B:53:ALA:HA	1:B:54:PRO:HD3	1.74	0.47
1:B:363:MET:HE3	1:B:363:MET:HB3	1.87	0.47
1:C:189:LYS:O	1:C:192:GLU:HB2	2.15	0.47
1:C:320:VAL:CG1	1:C:321:TYR:N	2.78	0.47
1:A:111:GLY:HA2	1:A:150:VAL:HG13	1.97	0.47
1:A:236:THR:HG22	1:A:237:VAL:N	2.29	0.47
1:A:255:ILE:HD13	1:A:298:VAL:CG2	2.45	0.47
1:A:294:SER:OG	1:A:297:GLU:HG3	2.15	0.47
1:B:255:ILE:HD13	1:B:298:VAL:HG22	1.97	0.47
1:C:293:VAL:HG11	1:C:298:VAL:CG2	2.45	0.47
1:C:353:VAL:CG1	1:C:354:ARG:N	2.78	0.47
1:A:246:LYS:HB3	1:A:281:ILE:CG1	2.44	0.47
1:A:372:VAL:CG1	1:A:373:GLU:N	2.78	0.47
1:A:41:ASN:ND2	1:A:41:ASN:H	2.13	0.46
1:A:58:ALA:O	1:A:59:ARG:HB3	2.15	0.46
1:A:190:ARG:C	1:A:192:GLU:H	2.21	0.46
1:B:275:LYS:HG2	1:B:275:LYS:H	1.25	0.46
1:B:367:ASN:C	1:B:368:VAL:HG13	2.39	0.46
1:A:273:HIS:C	1:A:274:ARG:HG3	2.40	0.46
1:B:53:ALA:HB1	1:B:65:THR:C	2.40	0.46
1:B:274:ARG:HA	1:C:9:LYS:N	2.30	0.46
1:C:71:GLU:HG3	1:C:76:HIS:CD2	2.50	0.46
1:C:122:LEU:O	1:C:125:GLN:N	2.48	0.46
1:B:31:LEU:HA	1:B:31:LEU:HD23	1.63	0.46
1:B:33:TYR:CA	1:B:44:VAL:HG22	2.45	0.46
1:B:248:LYS:O	1:B:251:ASP:HB2	2.15	0.46
1:B:305:ALA:O	1:B:307:PRO:HD3	2.14	0.46
1:A:265:THR:CG2	1:A:293:VAL:HG23	2.45	0.46
1:A:273:HIS:O	1:A:275:LYS:HG2	2.15	0.46
1:B:215:ARG:HD2	1:B:215:ARG:HA	1.54	0.46
1:A:176:LEU:HD23	1:A:177:LEU:HD23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:HIS:HB2	1:A:380:LEU:HD12	1.97	0.46
1:A:228:VAL:C	1:A:229:PHE:CD1	2.93	0.46
1:C:269:GLY:O	1:C:288:LEU:HA	2.16	0.46
1:B:320:VAL:CG1	1:B:321:TYR:N	2.79	0.46
1:C:65:THR:HG22	1:C:66:ALA:N	2.31	0.46
1:C:188:THR:CG2	1:C:189:LYS:N	2.78	0.46
1:C:265:THR:HG21	1:C:293:VAL:HG21	1.97	0.46
1:A:54:PRO:O	1:A:64:ASN:HA	2.15	0.46
1:A:353:VAL:CG1	1:A:354:ARG:N	2.79	0.46
1:B:217:VAL:HG12	1:B:281:ILE:CD1	2.46	0.46
1:B:344:PHE:O	1:B:345:ARG:HB2	2.16	0.46
1:C:310:ILE:CD1	1:C:381:GLU:HG2	2.46	0.46
1:B:188:THR:CG2	1:B:189:LYS:N	2.79	0.45
1:B:229:PHE:O	1:B:237:VAL:N	2.39	0.45
1:C:56:GLU:O	1:C:62:THR:HA	2.15	0.45
1:A:20:VAL:CG2	1:A:115:GLN:HE22	2.29	0.45
1:B:19:HIS:HD2	1:B:115:GLN:N	2.14	0.45
1:B:230:THR:HG22	1:B:235:GLY:C	2.41	0.45
1:C:41:ASN:HB2	1:C:42:VAL:H	1.56	0.45
1:A:33:TYR:CA	1:A:44:VAL:HG22	2.46	0.45
1:A:128:VAL:HA	1:A:129:PRO:HD3	1.56	0.45
1:B:20:VAL:CG2	1:B:115:GLN:HE22	2.29	0.45
1:C:34:VAL:HG22	1:C:196:VAL:HG13	1.98	0.45
1:A:56:GLU:OE2	1:A:65:THR:HB	2.17	0.45
1:A:193:ASN:HD21	1:A:195:TRP:N	2.13	0.45
1:A:267:VAL:HG12	1:A:269:GLY:H	1.81	0.45
1:A:310:ILE:HD12	1:A:381:GLU:HG2	1.98	0.45
1:B:190:ARG:C	1:B:192:GLU:H	2.20	0.45
1:B:370:PHE:CD1	1:B:370:PHE:C	2.95	0.45
1:C:185:ASN:HB2	1:C:188:THR:OG1	2.16	0.45
1:C:246:LYS:HB3	1:C:280:GLY:O	2.17	0.45
1:C:276:THR:CG2	1:C:277:LEU:H	2.11	0.45
1:C:40:PRO:HD2	1:C:41:ASN:ND2	2.31	0.45
1:C:273:HIS:O	1:C:274:ARG:HG3	2.17	0.45
1:C:343:TYR:CE1	1:C:347:THR:CA	3.00	0.45
1:A:217:VAL:HG12	1:A:281:ILE:CD1	2.47	0.45
1:B:33:TYR:HE1	1:B:45:LYS:O	1.99	0.45
1:B:77:TYR:OH	1:B:206:ILE:HG22	2.16	0.45
1:B:91:ASN:ND2	1:B:96:ALA:HB3	2.32	0.45
1:C:193:ASN:CG	1:C:194:GLU:N	2.73	0.45
1:C:268:THR:HG23	1:C:291:ARG:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:339:ARG:HA	1:C:351:GLY:O	2.17	0.45
1:A:227:ASP:CB	1:A:229:PHE:HE1	2.17	0.45
1:B:214:VAL:CG1	1:B:215:ARG:N	2.80	0.45
1:C:177:LEU:HD13	1:C:195:TRP:CE2	2.51	0.45
1:C:384:LEU:HD12	1:C:384:LEU:C	2.40	0.45
1:A:323:LEU:HD13	1:A:327:GLU:HB2	1.99	0.45
1:B:71:GLU:HA	1:B:75:ARG:O	2.17	0.45
1:C:232:THR:OG1	1:C:233:GLY:N	2.50	0.45
1:C:266:VAL:O	1:C:268:THR:HG23	2.17	0.45
1:A:33:TYR:CZ	1:A:44:VAL:CG1	2.99	0.44
1:A:189:LYS:H	1:A:192:GLU:CD	2.22	0.44
1:A:389:ARG:HB3	1:A:393:ARG:O	2.16	0.44
1:A:269:GLY:O	1:A:288:LEU:HA	2.17	0.44
1:B:384:LEU:HD12	1:B:385:ARG:N	2.32	0.44
1:C:17:ILE:HG13	1:C:104:LEU:CD1	2.47	0.44
1:C:161:TYR:O	1:C:162:GLU:HB2	2.17	0.44
1:A:144:PRO:CA	1:A:147:LEU:HD12	2.34	0.44
1:B:144:PRO:CA	1:B:147:LEU:HD12	2.39	0.44
1:C:403:ILE:C	1:C:404:LEU:HG	2.39	0.44
1:A:67:HIS:O	1:A:68:VAL:HG23	2.17	0.44
1:B:143:ASP:HB3	1:B:146:LEU:HD12	1.98	0.44
1:B:169:PRO:HG3	1:B:209:TYR:CE2	2.53	0.44
1:B:338:TYR:OH	1:B:390:GLU:OE2	2.28	0.44
1:C:11:HIS:HA	1:C:76:HIS:O	2.17	0.44
1:C:181:GLU:C	1:C:183:HIS:N	2.75	0.44
1:C:312:PRO:HA	1:C:378:VAL:O	2.18	0.44
1:C:350:THR:HB	1:C:375:ILE:HD11	1.98	0.44
1:A:263:ARG:CZ	1:A:297:GLU:HB3	2.47	0.44
1:B:63:ILE:HD13	1:B:91:ASN:N	2.33	0.44
1:B:312:PRO:C	1:B:313:HIS:CG	2.96	0.44
1:C:159:ASN:OD1	1:C:165:GLY:N	2.50	0.44
1:A:82:CYS:HA	1:A:83:PRO:HD3	1.63	0.44
1:A:138:VAL:HB	1:A:173:GLY:O	2.18	0.44
1:A:268:THR:HA	1:B:273:HIS:CE1	2.53	0.44
1:C:19:HIS:HD2	1:C:115:GLN:N	2.12	0.44
1:C:41:ASN:ND2	1:C:41:ASN:H	2.15	0.44
1:C:194:GLU:HG2	1:C:195:TRP:N	2.32	0.44
1:C:228:VAL:C	1:C:229:PHE:CD1	2.95	0.44
1:C:253:VAL:HA	1:C:307:PRO:CD	2.46	0.44
1:A:9:LYS:HA	1:A:10:PRO:HD3	1.86	0.44
1:A:46:ASP:O	1:A:50:ILE:HG13	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:LEU:HD23	1:A:146:LEU:HA	1.66	0.44
1:A:185:ASN:HB2	1:A:188:THR:OG1	2.17	0.44
1:A:246:LYS:HB3	1:A:280:GLY:O	2.17	0.44
1:A:310:ILE:HD11	1:A:381:GLU:HG2	2.00	0.44
1:C:363:MET:HE3	1:C:363:MET:HB3	1.84	0.44
1:B:267:VAL:HG13	1:B:288:LEU:HB3	2.00	0.44
1:C:77:TYR:CZ	1:C:206:ILE:CG2	3.00	0.44
1:A:9:LYS:HZ3	1:A:71:GLU:HG2	1.83	0.44
1:A:31:LEU:HD23	1:A:31:LEU:HA	1.66	0.44
1:A:124:ARG:NH2	1:A:163:PHE:CD1	2.86	0.44
1:B:74:LYS:O	1:B:75:ARG:HG3	2.17	0.44
1:B:152:MET:HE3	1:B:152:MET:HB3	1.89	0.44
1:C:193:ASN:HD21	1:C:195:TRP:HB2	1.82	0.44
1:C:202:LEU:O	1:C:205:ALA:HB3	2.18	0.44
1:C:215:ARG:HD2	1:C:215:ARG:HA	1.25	0.44
1:A:47:TYR:O	1:A:51:ASP:N	2.41	0.43
1:A:293:VAL:HG11	1:A:298:VAL:HG23	2.00	0.43
1:A:312:PRO:C	1:A:313:HIS:CG	2.96	0.43
1:C:294:SER:OG	1:C:297:GLU:HG3	2.18	0.43
1:A:171:ILE:HD13	1:A:202:LEU:CA	2.47	0.43
1:B:33:TYR:HB3	1:B:182:MET:CB	2.49	0.43
1:C:231:ILE:HG21	1:C:234:ARG:HB2	2.00	0.43
1:C:350:THR:CB	1:C:375:ILE:HD11	2.47	0.43
1:A:77:TYR:CZ	1:A:206:ILE:CG2	3.01	0.43
1:A:84:GLY:O	1:A:87:ASP:HB2	2.19	0.43
1:B:146:LEU:HA	1:B:146:LEU:HD23	1.69	0.43
1:C:31:LEU:HD23	1:C:31:LEU:HA	1.68	0.43
1:C:74:LYS:O	1:C:75:ARG:HG3	2.18	0.43
1:C:248:LYS:O	1:C:251:ASP:HB2	2.18	0.43
1:A:215:ARG:HA	1:A:215:ARG:HD2	1.45	0.43
1:B:55:GLU:HB3	1:B:62:THR:CG2	2.45	0.43
1:B:294:SER:C	1:B:296:GLU:H	2.25	0.43
1:C:17:ILE:HG13	1:C:104:LEU:HD13	2.01	0.43
1:C:221:PHE:HA	1:C:244:ARG:O	2.18	0.43
1:B:20:VAL:HG23	1:B:115:GLN:OE1	2.19	0.43
1:B:228:VAL:C	1:B:229:PHE:CD1	2.96	0.43
1:B:355:LEU:CD1	1:B:362:VAL:HG23	2.48	0.43
1:C:75:ARG:NH1	1:C:77:TYR:OH	2.29	0.43
1:C:363:MET:HE1	4:C:417:HOH:O	2.19	0.43
1:A:53:ALA:HB1	1:A:65:THR:C	2.44	0.43
1:A:124:ARG:HH21	1:A:163:PHE:N	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:ASN:CG	1:A:194:GLU:N	2.76	0.43
1:B:223:MET:HA	1:B:224:PRO:HD3	1.44	0.43
1:B:138:VAL:HG12	1:B:139:ASP:N	2.33	0.43
1:B:193:ASN:CG	1:B:194:GLU:N	2.76	0.43
1:B:238:ALA:HB2	1:B:290:LEU:CD1	2.49	0.43
1:B:258:LEU:HD23	1:B:258:LEU:H	1.81	0.43
1:B:310:ILE:CD1	1:B:381:GLU:HG2	2.48	0.43
1:C:33:TYR:CD1	1:C:44:VAL:HG22	2.53	0.43
1:A:198:LYS:HD3	1:A:201:GLU:OE2	2.18	0.43
1:A:281:ILE:O	1:A:284:ASP:HB2	2.18	0.43
1:B:265:THR:HG21	1:B:293:VAL:HG23	2.00	0.43
1:C:53:ALA:HB2	1:C:66:ALA:HB2	2.01	0.43
1:C:223:MET:HG2	1:C:224:PRO:CD	2.49	0.43
1:A:40:PRO:HD2	1:A:41:ASN:HD22	1.81	0.43
1:C:275:LYS:HG2	1:C:275:LYS:H	1.25	0.43
1:A:265:THR:HG21	1:A:293:VAL:CG2	2.49	0.43
1:A:270:VAL:CG1	1:A:271:GLU:N	2.82	0.43
1:A:325:LYS:HD2	1:A:331:HIS:HB3	2.01	0.43
1:B:285:ASN:N	1:B:285:ASN:ND2	2.66	0.43
1:C:137:LYS:HA	3:C:407:GDP:N1	2.33	0.43
1:C:272:MET:HG2	1:C:273:HIS:N	2.34	0.43
1:C:370:PHE:CD1	1:C:370:PHE:C	2.97	0.43
1:A:136:ASN:CG	1:A:137:LYS:N	2.77	0.42
1:A:143:ASP:HB3	1:A:146:LEU:HD12	1.99	0.42
1:B:47:TYR:O	1:B:51:ASP:N	2.40	0.42
1:A:74:LYS:HG2	1:A:75:ARG:CG	2.43	0.42
1:B:276:THR:O	1:B:277:LEU:HB2	2.17	0.42
1:C:294:SER:C	1:C:296:GLU:H	2.28	0.42
1:A:56:GLU:O	1:A:62:THR:HA	2.19	0.42
1:A:343:TYR:CE1	1:A:347:THR:HA	2.54	0.42
1:A:375:ILE:HG13	1:A:375:ILE:H	1.40	0.42
1:B:71:GLU:HG3	1:B:76:HIS:CD2	2.55	0.42
1:B:223:MET:HE3	1:B:240:GLY:N	2.34	0.42
1:B:256:VAL:HG12	1:B:379:ALA:HB2	2.02	0.42
1:C:270:VAL:CG1	1:C:271:GLU:N	2.80	0.42
1:B:136:ASN:CG	1:B:137:LYS:N	2.76	0.42
1:B:322:ILE:O	1:B:365:GLY:N	2.49	0.42
1:B:355:LEU:HB3	1:B:356:PRO:HD2	2.00	0.42
1:C:223:MET:HA	1:C:224:PRO:HD3	1.36	0.42
1:C:345:ARG:HH11	1:C:345:ARG:HD2	1.66	0.42
1:A:313:HIS:HD2	1:A:405:GLU:C	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:LEU:O	1:A:160:GLN:N	2.50	0.42
1:A:185:ASN:C	1:A:187:LYS:N	2.76	0.42
1:A:345:ARG:HH11	1:A:345:ARG:HD2	1.68	0.42
1:B:19:HIS:ND1	1:B:20:VAL:N	2.68	0.42
1:B:265:THR:CG2	1:B:293:VAL:CG2	2.98	0.42
1:A:16:THR:HB	1:A:24:LYS:HB3	2.02	0.42
1:A:17:ILE:HG13	1:A:104:LEU:HD13	2.01	0.42
1:A:246:LYS:HG2	1:A:281:ILE:HD11	2.02	0.42
1:B:136:ASN:ND2	1:B:137:LYS:N	2.67	0.42
1:B:265:THR:HG21	1:B:293:VAL:CG2	2.50	0.42
1:B:294:SER:OG	1:B:296:GLU:HB2	2.19	0.42
1:C:20:VAL:CG2	1:C:115:GLN:HE22	2.32	0.42
1:C:343:TYR:CD1	1:C:347:THR:C	2.98	0.42
1:A:34:VAL:HG12	1:A:35:ALA:N	2.33	0.42
1:A:325:LYS:HD2	1:A:331:HIS:CB	2.50	0.42
1:B:16:THR:O	1:B:88:TYR:HE2	2.03	0.42
1:B:181:GLU:C	1:B:183:HIS:N	2.76	0.42
1:C:146:LEU:HA	1:C:146:LEU:HD23	1.71	0.42
1:C:249:VAL:C	1:C:251:ASP:H	2.28	0.42
1:A:152:MET:HE3	1:A:152:MET:HB3	1.84	0.42
1:B:111:GLY:HA2	1:B:150:VAL:HG13	2.01	0.42
1:B:313:HIS:HD2	1:B:405:GLU:C	2.28	0.42
1:B:386:PHE:CD1	1:B:386:PHE:C	2.98	0.42
1:C:33:TYR:CZ	1:C:44:VAL:CG1	3.02	0.42
1:C:33:TYR:HE1	1:C:45:LYS:O	2.03	0.42
1:C:113:MET:CB	1:C:114:PRO:CD	2.94	0.42
1:C:128:VAL:HA	1:C:129:PRO:HD3	1.54	0.42
1:A:262:THR:HG22	1:A:263:ARG:N	2.32	0.41
1:B:294:SER:OG	1:B:297:GLU:N	2.47	0.41
1:B:403:ILE:HD12	1:B:403:ILE:HG23	1.75	0.41
1:A:63:ILE:HD13	1:A:91:ASN:N	2.34	0.41
1:A:241:ARG:HA	1:A:285:ASN:HA	2.02	0.41
1:A:246:LYS:HG2	1:A:281:ILE:CD1	2.50	0.41
1:A:363:MET:HB3	1:A:363:MET:HE3	1.73	0.41
1:A:370:PHE:CD1	1:A:370:PHE:C	2.98	0.41
1:B:17:ILE:HG13	1:B:104:LEU:HD13	2.02	0.41
1:B:231:ILE:CB	1:B:234:ARG:HB2	2.49	0.41
1:C:265:THR:CG2	1:C:293:VAL:CG2	2.96	0.41
1:C:267:VAL:HG12	1:C:269:GLY:N	2.31	0.41
1:C:270:VAL:CG1	1:C:271:GLU:H	2.25	0.41
1:A:27:LEU:HD21	1:A:202:LEU:CD2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:ASN:HD21	1:A:195:TRP:HB2	1.84	0.41
1:A:223:MET:CE	1:A:240:GLY:CA	2.98	0.41
1:A:285:ASN:HD22	1:A:285:ASN:N	2.18	0.41
1:C:77:TYR:OH	1:C:207:ASP:HA	2.21	0.41
1:C:288:LEU:HD23	1:C:288:LEU:N	2.33	0.41
1:A:89:ILE:HG12	1:A:89:ILE:H	1.57	0.41
1:A:238:ALA:CB	1:A:290:LEU:HD11	2.51	0.41
1:A:265:THR:CG2	1:A:293:VAL:CG2	2.99	0.41
1:B:143:ASP:HA	1:B:144:PRO:HD2	1.88	0.41
1:C:75:ARG:NH2	1:C:212:THR:HG23	2.28	0.41
1:C:277:LEU:HD12	1:C:277:LEU:C	2.43	0.41
1:A:157:LEU:HD23	1:A:157:LEU:HA	1.80	0.41
1:B:136:ASN:ND2	1:B:174:SER:HA	2.36	0.41
1:A:247:VAL:HG23	1:A:280:GLY:HA3	2.03	0.41
1:A:306:LYS:HA	1:A:307:PRO:HD2	1.88	0.41
1:B:312:PRO:O	1:B:313:HIS:CG	2.74	0.41
1:C:336:THR:OG1	1:C:355:LEU:N	2.50	0.41
1:A:273:HIS:O	1:A:274:ARG:HG3	2.21	0.41
1:B:27:LEU:HA	1:B:175:ALA:HB1	2.03	0.41
1:C:14:VAL:O	1:C:80:VAL:HG23	2.21	0.41
1:C:157:LEU:HA	1:C:157:LEU:HD23	1.80	0.41
1:A:389:ARG:HA	1:A:393:ARG:O	2.21	0.41
1:B:164:PRO:O	1:B:164:PRO:HG2	2.19	0.41
1:C:89:ILE:HG12	1:C:89:ILE:H	1.67	0.41
1:C:247:VAL:O	1:C:280:GLY:N	2.27	0.41
1:A:88:TYR:O	1:A:92:MET:HG3	2.20	0.41
1:A:137:LYS:C	1:A:139:ASP:N	2.78	0.41
1:A:388:ILE:C	1:A:389:ARG:HG2	2.46	0.41
1:B:210:ILE:HA	1:B:211:PRO:HD3	1.89	0.41
1:B:263:ARG:CZ	1:B:297:GLU:HG2	2.48	0.41
1:B:294:SER:C	1:B:296:GLU:N	2.78	0.41
1:C:82:CYS:CB	1:C:83:PRO:CD	2.98	0.41
1:C:91:ASN:ND2	1:C:96:ALA:HB3	2.35	0.41
1:C:223:MET:CE	1:C:240:GLY:CA	2.99	0.41
1:C:262:THR:HG22	1:C:263:ARG:N	2.34	0.41
1:A:92:MET:O	1:A:126:VAL:HG21	2.21	0.41
1:B:119:HIS:CD2	1:B:119:HIS:N	2.87	0.41
1:B:294:SER:OG	1:B:297:GLU:HG3	2.20	0.41
1:C:228:VAL:HA	1:C:237:VAL:O	2.21	0.41
1:C:265:THR:HB	1:C:266:VAL:H	1.74	0.41
1:B:9:LYS:HZ2	1:B:71:GLU:CD	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:PRO:HD2	1:B:41:ASN:HD22	1.85	0.40
1:B:385:ARG:HG3	1:B:399:VAL:HG22	2.03	0.40
1:C:320:VAL:O	1:C:367:ASN:HA	2.20	0.40
1:A:19:HIS:HB2	1:A:116:THR:OG1	2.21	0.40
1:B:159:ASN:OD1	1:B:165:GLY:N	2.53	0.40
1:C:19:HIS:CD2	1:C:115:GLN:HB2	2.56	0.40
1:C:110:ASP:OD1	1:C:110:ASP:N	2.49	0.40
1:C:132:VAL:HG22	1:C:169:PRO:HG2	2.03	0.40
1:C:325:LYS:HD2	1:C:331:HIS:CB	2.52	0.40
1:A:137:LYS:HA	3:A:407:GDP:N1	2.36	0.40
1:A:293:VAL:HG11	1:A:298:VAL:CG2	2.51	0.40
1:B:46:ASP:O	1:B:50:ILE:HG13	2.20	0.40
1:B:157:LEU:HA	1:B:157:LEU:HD23	1.81	0.40
1:B:247:VAL:N	1:B:280:GLY:O	2.48	0.40
1:C:16:THR:HG23	1:C:79:HIS:CE1	2.57	0.40
1:C:38:GLU:HG2	1:C:189:LYS:NZ	2.37	0.40
1:C:212:THR:HA	1:C:213:PRO:HD2	1.63	0.40
1:A:223:MET:HE3	1:A:240:GLY:CA	2.52	0.40
1:B:15:GLY:HA3	1:B:99:MET:CE	2.51	0.40
1:B:223:MET:CE	1:B:239:THR:C	2.95	0.40
1:B:230:THR:HG22	1:B:235:GLY:O	2.22	0.40
1:C:56:GLU:OE2	1:C:65:THR:HB	2.22	0.40
1:A:168:VAL:HA	1:A:169:PRO:HD2	1.84	0.40
1:A:255:ILE:HG21	1:A:298:VAL:HG22	2.02	0.40
1:A:263:ARG:CZ	1:A:297:GLU:HG2	2.50	0.40
1:A:356:PRO:CG	1:A:359:VAL:CG2	2.97	0.40
1:B:89:ILE:HG12	1:B:89:ILE:H	1.60	0.40
1:B:323:LEU:HD13	1:B:327:GLU:CB	2.50	0.40
1:B:377:PRO:C	1:B:378:VAL:HG23	2.47	0.40
1:C:206:ILE:HG21	1:C:206:ILE:HD13	1.68	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:194:GLU:OE2	1:C:232:THR:O[2_665]	2.19	0.01

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	395/405 (98%)	358 (91%)	29 (7%)	8 (2%)	6	16
1	B	395/405 (98%)	354 (90%)	31 (8%)	10 (2%)	4	11
1	C	395/405 (98%)	360 (91%)	26 (7%)	9 (2%)	5	13
All	All	1185/1215 (98%)	1072 (90%)	86 (7%)	27 (2%)	5	13

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	PRO
1	A	42	VAL
1	A	232	THR
1	B	40	PRO
1	B	42	VAL
1	B	232	THR
1	C	40	PRO
1	C	42	VAL
1	A	190	ARG
1	A	191	GLY
1	B	191	GLY
1	C	190	ARG
1	C	191	GLY
1	C	232	THR
1	C	271	GLU
1	A	271	GLU
1	B	190	ARG
1	B	271	GLU
1	B	276	THR
1	A	258	LEU
1	B	277	LEU
1	C	277	LEU
1	C	345	ARG
1	B	368	VAL

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Mol	Chain	Res	Type
1	C	340	PRO
1	B	340	PRO
1	A	368	VAL

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	332/338 (98%)	257 (77%)	75 (23%)	1	3
1	B	332/338 (98%)	257 (77%)	75 (23%)	1	3
1	C	332/338 (98%)	260 (78%)	72 (22%)	1	3
All	All	996/1014 (98%)	774 (78%)	222 (22%)	1	3

All (222) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	VAL
1	A	17	ILE
1	A	20	VAL
1	A	21	ASP
1	A	28	THR
1	A	34	VAL
1	A	39	ASN
1	A	41	ASN
1	A	43	GLU
1	A	44	VAL
1	A	46	ASP
1	A	49	ASP
1	A	50	ILE
1	A	59	ARG
1	A	62	THR
1	A	63	ILE
1	A	68	VAL
1	A	80	VAL
1	A	82	CYS

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Mol	Chain	Res	Type
1	A	89	ILE
1	A	125	GLN
1	A	126	VAL
1	A	131	ILE
1	A	132	VAL
1	A	138	VAL
1	A	145	GLU
1	A	147	LEU
1	A	155	ARG
1	A	162	GLU
1	A	180	GLU
1	A	182	MET
1	A	184	LYS
1	A	187	LYS
1	A	189	LYS
1	A	190	ARG
1	A	194	GLU
1	A	201	GLU
1	A	206	ILE
1	A	212	THR
1	A	215	ARG
1	A	217	VAL
1	A	219	LYS
1	A	222	LEU
1	A	223	MET
1	A	226	GLU
1	A	230	THR
1	A	231	ILE
1	A	239	THR
1	A	242	ILE
1	A	243	GLU
1	A	246	LYS
1	A	247	VAL
1	A	249	VAL
1	A	255	ILE
1	A	263	ARG
1	A	275	LYS
1	A	277	LEU
1	A	279	GLU
1	A	281	ILE
1	A	285	ASN
1	A	289	LEU

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Mol	Chain	Res	Type
1	A	291	ARG
1	A	306	LYS
1	A	311	THR
1	A	323	LEU
1	A	324	LYS
1	A	336	THR
1	A	352	VAL
1	A	359	VAL
1	A	367	ASN
1	A	375	ILE
1	A	376	LYS
1	A	381	GLU
1	A	385	ARG
1	A	402	LYS
1	B	12	VAL
1	B	16	THR
1	B	20	VAL
1	B	21	ASP
1	B	28	THR
1	B	34	VAL
1	B	39	ASN
1	B	40	PRO
1	B	41	ASN
1	B	42	VAL
1	B	43	GLU
1	B	44	VAL
1	B	46	ASP
1	B	49	ASP
1	B	50	ILE
1	B	62	THR
1	B	63	ILE
1	B	68	VAL
1	B	75	ARG
1	B	80	VAL
1	B	82	CYS
1	B	89	ILE
1	B	125	GLN
1	B	126	VAL
1	B	131	ILE
1	B	132	VAL
1	B	138	VAL
1	B	145	GLU

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Mol	Chain	Res	Type
1	B	147	LEU
1	B	155	ARG
1	B	162	GLU
1	B	168	VAL
1	B	180	GLU
1	B	182	MET
1	B	184	LYS
1	B	187	LYS
1	B	189	LYS
1	B	194	GLU
1	B	206	ILE
1	B	212	THR
1	B	215	ARG
1	B	217	VAL
1	B	222	LEU
1	B	223	MET
1	B	226	GLU
1	B	230	THR
1	B	231	ILE
1	B	236	THR
1	B	239	THR
1	B	242	ILE
1	B	243	GLU
1	B	246	LYS
1	B	247	VAL
1	B	249	VAL
1	B	252	GLU
1	B	255	ILE
1	B	263	ARG
1	B	264	LYS
1	B	275	LYS
1	B	277	LEU
1	B	281	ILE
1	B	289	LEU
1	B	291	ARG
1	B	306	LYS
1	B	311	THR
1	B	323	LEU
1	B	324	LYS
1	B	336	THR
1	B	352	VAL
1	B	359	VAL

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Mol	Chain	Res	Type
1	B	375	ILE
1	B	376	LYS
1	B	381	GLU
1	B	385	ARG
1	B	402	LYS
1	C	12	VAL
1	C	20	VAL
1	C	21	ASP
1	C	31	LEU
1	C	34	VAL
1	C	41	ASN
1	C	42	VAL
1	C	43	GLU
1	C	44	VAL
1	C	46	ASP
1	C	49	ASP
1	C	50	ILE
1	C	59	ARG
1	C	62	THR
1	C	63	ILE
1	C	68	VAL
1	C	75	ARG
1	C	80	VAL
1	C	82	CYS
1	C	89	ILE
1	C	125	GLN
1	C	126	VAL
1	C	131	ILE
1	C	132	VAL
1	C	138	VAL
1	C	145	GLU
1	C	147	LEU
1	C	162	GLU
1	C	180	GLU
1	C	182	MET
1	C	184	LYS
1	C	187	LYS
1	C	189	LYS
1	C	190	ARG
1	C	194	GLU
1	C	206	ILE
1	C	212	THR

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Mol	Chain	Res	Type
1	C	215	ARG
1	C	217	VAL
1	C	222	LEU
1	C	223	MET
1	C	226	GLU
1	C	230	THR
1	C	231	ILE
1	C	239	THR
1	C	242	ILE
1	C	243	GLU
1	C	246	LYS
1	C	247	VAL
1	C	249	VAL
1	C	255	ILE
1	C	263	ARG
1	C	264	LYS
1	C	275	LYS
1	C	277	LEU
1	C	279	GLU
1	C	281	ILE
1	C	285	ASN
1	C	289	LEU
1	C	291	ARG
1	C	306	LYS
1	C	311	THR
1	C	323	LEU
1	C	324	LYS
1	C	336	THR
1	C	352	VAL
1	C	359	VAL
1	C	367	ASN
1	C	375	ILE
1	C	376	LYS
1	C	381	GLU
1	C	385	ARG

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	19	HIS
1	A	41	ASN
1	A	91	ASN

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Mol	Chain	Res	Type
1	A	136	ASN
1	A	193	ASN
1	A	273	HIS
1	A	285	ASN
1	A	313	HIS
1	A	367	ASN
1	B	19	HIS
1	B	41	ASN
1	B	91	ASN
1	B	136	ASN
1	B	193	ASN
1	B	285	ASN
1	C	11	HIS
1	C	19	HIS
1	C	41	ASN
1	C	76	HIS
1	C	91	ASN
1	C	136	ASN
1	C	193	ASN
1	C	273	HIS
1	C	285	ASN
1	C	313	HIS
1	C	367	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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$
3	GDP	A	407	2	29,30,30	1.70	2 (6%)	45,47,47	1.60	10 (22%)
3	GDP	B	407	2	29,30,30	1.96	3 (10%)	45,47,47	1.32	6 (13%)
3	GDP	C	407	2	29,30,30	1.48	1 (3%)	45,47,47	1.71	6 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GDP	A	407	2	-	1/16/32/32	0/3/3/3
3	GDP	B	407	2	-	2/16/32/32	0/3/3/3
3	GDP	C	407	2	-	3/16/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	407	GDP	PA-O3A	-8.37	1.50	1.59
3	A	407	GDP	PA-O3A	-8.31	1.50	1.59
3	C	407	GDP	PA-O3A	-6.87	1.52	1.59
3	B	407	GDP	PB-O2B	-4.53	1.38	1.54
3	B	407	GDP	O3'-C3'	-2.28	1.37	1.43
3	A	407	GDP	O3'-C3'	-2.09	1.37	1.43

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	407	GDP	C1'-N9-C4	5.54	142.85	126.49
3	C	407	GDP	C1'-N9-C8	-4.50	113.95	126.73
3	C	407	GDP	O2B-PB-O1B	4.20	127.21	110.83
3	A	407	GDP	C1'-N9-C4	4.14	138.71	126.49
3	C	407	GDP	C2'-C1'-N9	3.89	124.06	113.25
3	A	407	GDP	O2B-PB-O1B	3.36	123.92	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	407	GDP	O3B-PB-O2B	-3.14	96.01	107.80
3	B	407	GDP	C1'-N9-C4	3.02	135.39	126.49
3	A	407	GDP	O4'-C1'-C2'	-2.93	100.34	106.62
3	A	407	GDP	C8-N9-C4	-2.84	100.70	106.03
3	B	407	GDP	O2B-PB-O1B	2.77	121.62	110.83
3	A	407	GDP	C6-C5-C4	2.59	122.73	118.83
3	A	407	GDP	C1'-N9-C8	-2.48	119.70	126.73
3	A	407	GDP	O2'-C2'-C1'	2.44	118.52	110.10
3	A	407	GDP	C2'-C1'-N9	2.30	119.66	113.25
3	B	407	GDP	O3A-PA-O1A	-2.22	104.04	110.70
3	C	407	GDP	C5-C4-N3	-2.17	124.94	128.39
3	B	407	GDP	C1'-N9-C8	-2.16	120.60	126.73
3	A	407	GDP	N2-C2-N3	-2.10	115.58	119.67
3	C	407	GDP	O3B-PB-O3A	2.07	111.59	104.64
3	B	407	GDP	C5-C4-N3	-2.02	125.18	128.39
3	A	407	GDP	O3B-PB-O2B	-2.01	100.27	107.80

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	407	GDP	PA-O3A-PB-O2B
3	C	407	GDP	PA-O3A-PB-O2B
3	C	407	GDP	C5'-O5'-PA-O3A
3	B	407	GDP	PA-O3A-PB-O1B
3	C	407	GDP	C5'-O5'-PA-O1A
3	A	407	GDP	O4'-C4'-C5'-O5'

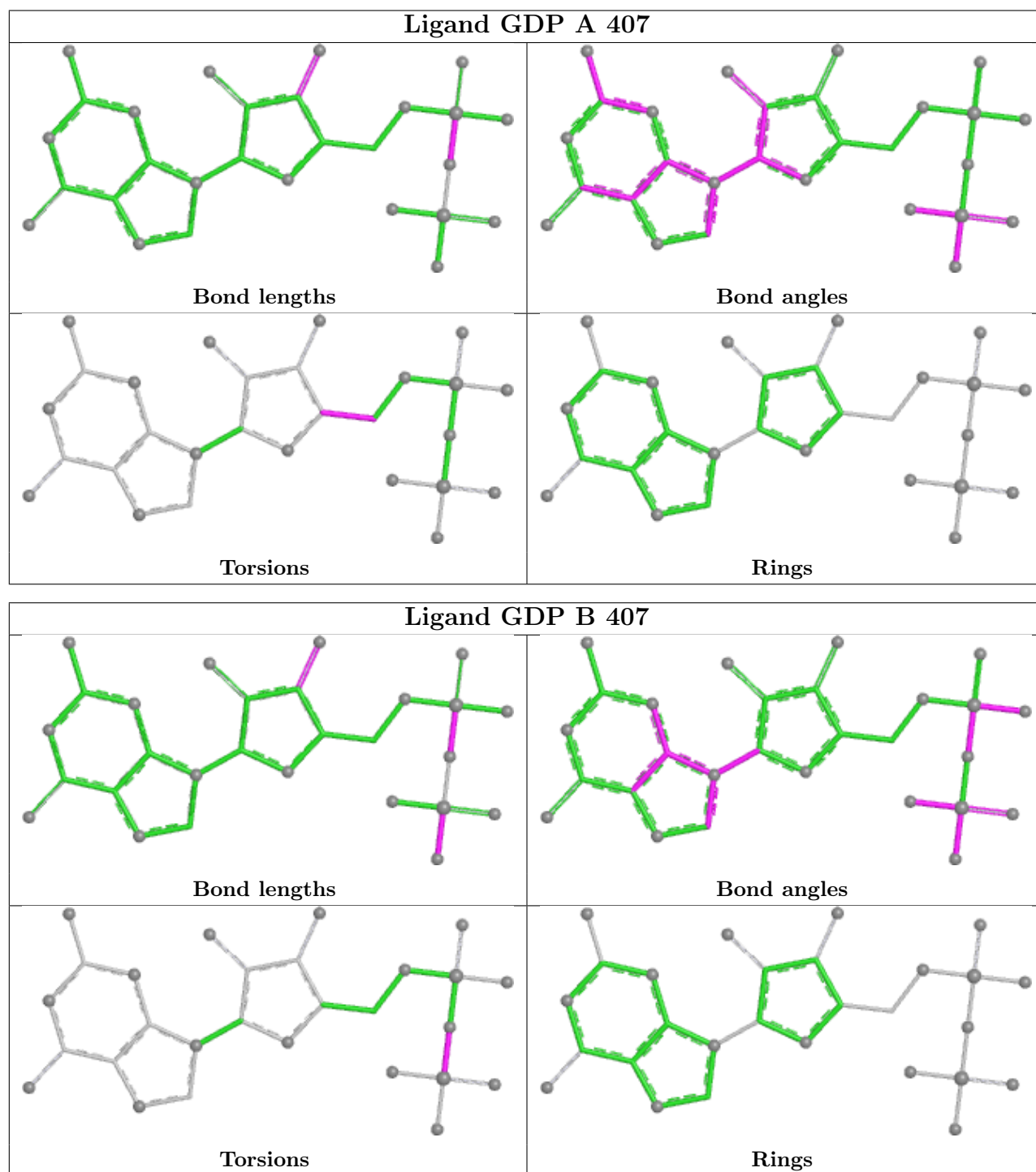
There are no ring outliers.

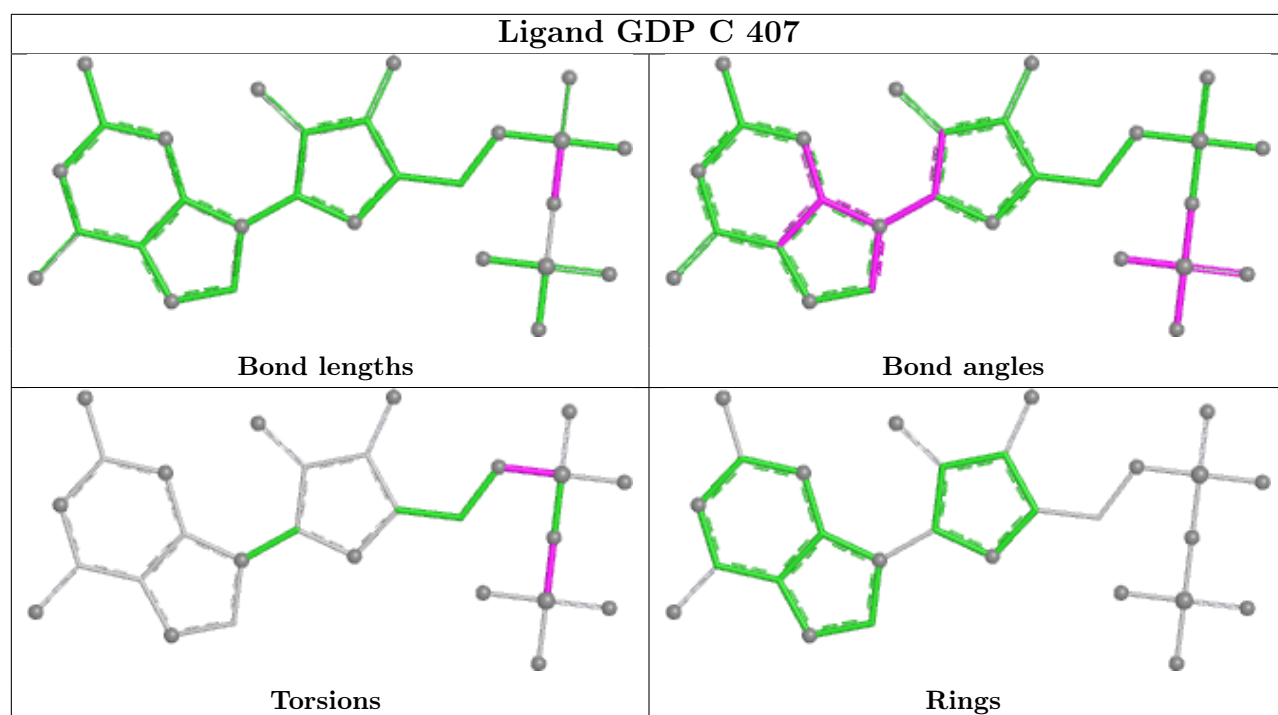
3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	407	GDP	4	0
3	B	407	GDP	3	0
3	C	407	GDP	3	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	397/405 (98%)	0.15	20 (5%) 34 30	15, 37, 82, 100	0
1	B	397/405 (98%)	0.20	24 (6%) 27 24	16, 40, 86, 100	0
1	C	397/405 (98%)	0.23	32 (8%) 18 15	9, 38, 80, 99	0
All	All	1191/1215 (98%)	0.19	76 (6%) 25 22	9, 39, 84, 100	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	58	ALA	5.4
1	B	234	ARG	5.4
1	B	229	PHE	5.3
1	C	232	THR	4.9
1	B	97	ALA	4.8
1	B	233	GLY	4.6
1	C	58	ALA	4.3
1	A	273	HIS	4.2
1	B	95	GLY	4.2
1	A	95	GLY	4.1
1	A	229	PHE	4.1
1	A	97	ALA	4.0
1	A	281	ILE	3.9
1	C	97	ALA	3.9
1	B	57	ARG	3.8
1	A	41	ASN	3.7
1	A	61	ILE	3.5
1	C	274	ARG	3.4
1	B	231	ILE	3.4
1	B	62	THR	3.3
1	C	291	ARG	3.2
1	C	57	ARG	3.2
1	C	53	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	289	LEU	3.1
1	C	273	HIS	3.1
1	A	277	LEU	3.1
1	B	232	THR	3.1
1	A	272	MET	3.1
1	C	54	PRO	3.0
1	B	58	ALA	3.0
1	B	11	HIS	2.8
1	C	59	ARG	2.8
1	C	37	ALA	2.7
1	B	54	PRO	2.6
1	B	277	LEU	2.6
1	A	263	ARG	2.6
1	C	183	HIS	2.6
1	A	53	ALA	2.6
1	B	263	ARG	2.6
1	A	57	ARG	2.6
1	C	231	ILE	2.5
1	B	292	GLY	2.5
1	C	60	GLY	2.5
1	C	229	PHE	2.5
1	B	41	ASN	2.5
1	C	280	GLY	2.4
1	C	61	ILE	2.4
1	C	277	LEU	2.4
1	A	233	GLY	2.4
1	C	278	GLN	2.4
1	C	271	GLU	2.3
1	B	60	GLY	2.3
1	A	279	GLU	2.3
1	C	276	THR	2.3
1	C	95	GLY	2.3
1	B	249	VAL	2.3
1	A	54	PRO	2.3
1	B	98	GLN	2.3
1	C	76	HIS	2.2
1	B	267	VAL	2.2
1	B	230	THR	2.2
1	C	69	GLU	2.2
1	C	270	VAL	2.2
1	A	232	THR	2.2
1	C	98	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	272	MET	2.2
1	C	405	GLU	2.2
1	C	284	ASP	2.1
1	C	167	GLU	2.1
1	A	98	GLN	2.1
1	B	250	GLY	2.1
1	C	289	LEU	2.1
1	C	235	GLY	2.1
1	A	215	ARG	2.0
1	A	295	ARG	2.0
1	B	291	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

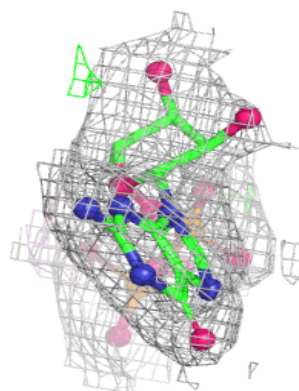
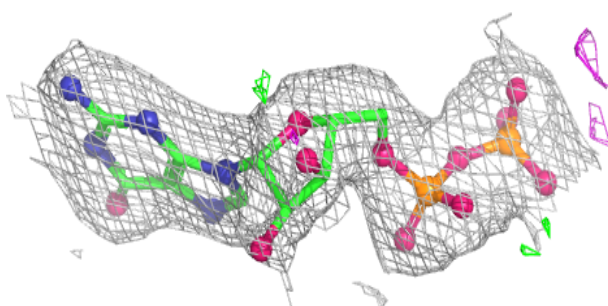
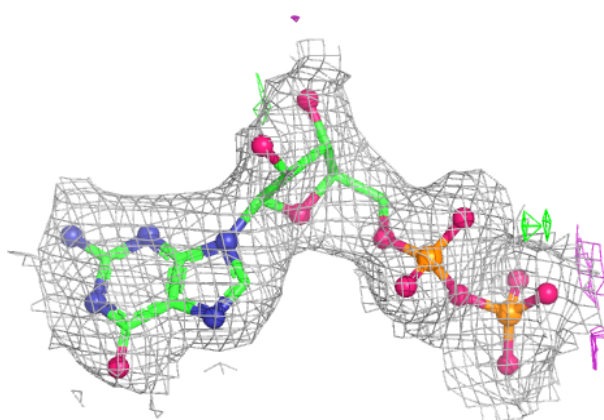
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MG	B	408	1/1	0.95	0.07	22,22,22,22	0
2	MG	A	408	1/1	0.96	0.09	24,24,24,24	0
2	MG	C	408	1/1	0.97	0.13	26,26,26,26	0
3	GDP	A	407	28/28	0.98	0.06	2,20,65,67	0
3	GDP	B	407	28/28	0.98	0.06	1,20,44,58	0
3	GDP	C	407	28/28	0.98	0.05	4,21,42,44	0

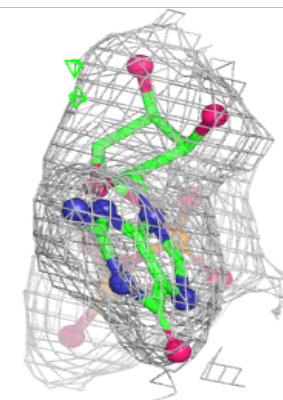
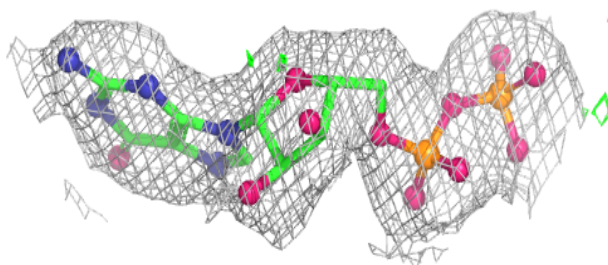
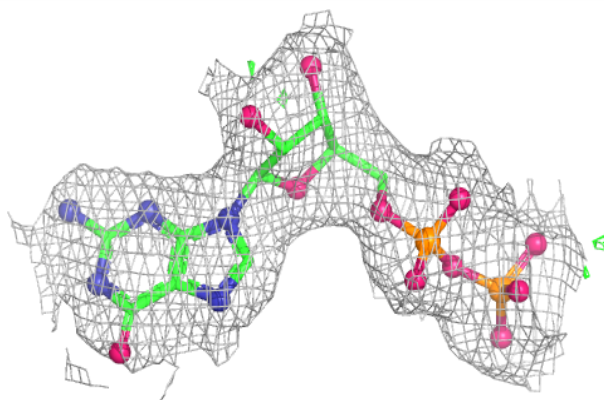
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

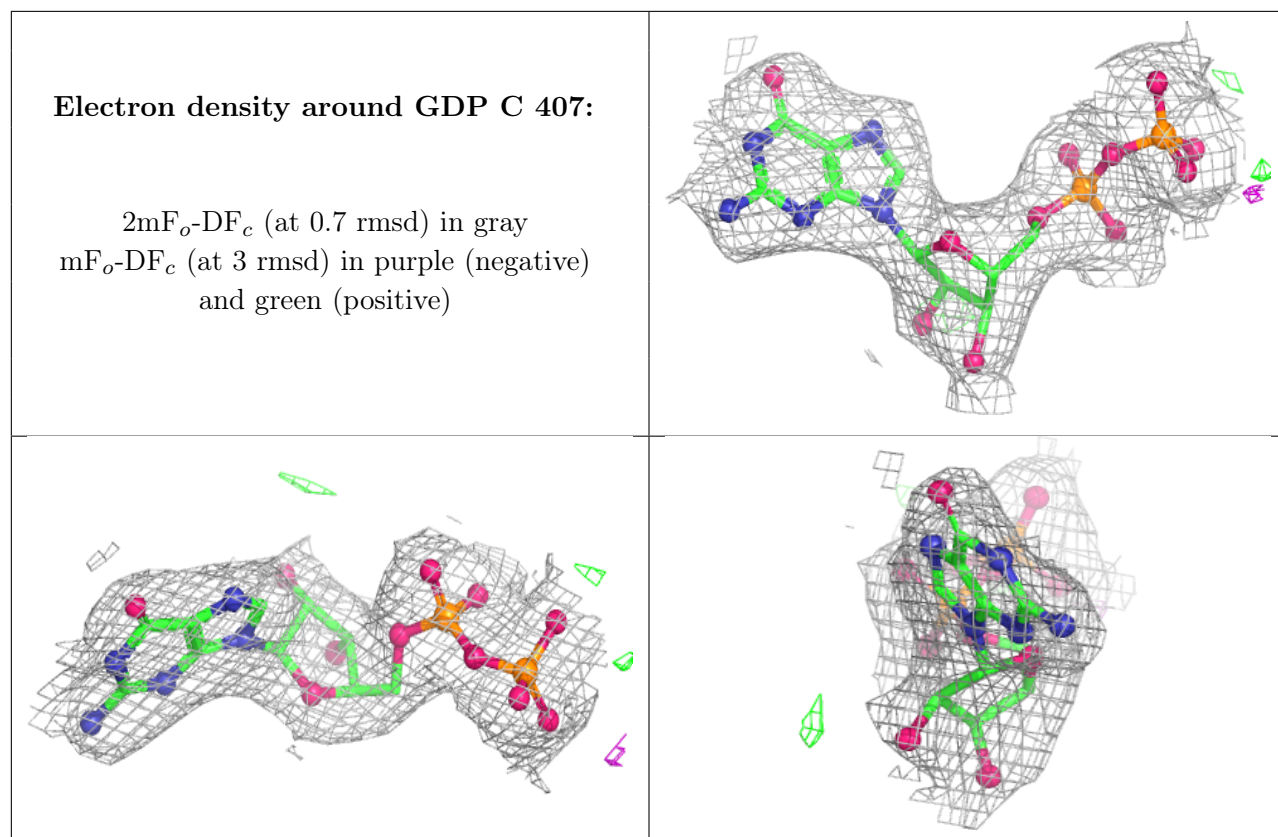
Electron density around GDP A 407:

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

**Electron density around GDP B 407:**

$2mF_o-DF_c$ (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.