



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2023 – 03:05 AM EDT

PDB ID : 2G83
Title : Structure of activated G-alpha-i1 bound to a nucleotide-state-selective peptide: Minimal determinants for recognizing the active form of a G protein alpha subunit
Authors : Johnston, C.A.; Ramer, J.K.; Blaesius, R.; Kuhlman, B.; Arshavsky, V.Y.; Siderovski, D.P.
Deposited on : 2006-03-01
Resolution : 2.80 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](#) ①) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.35
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

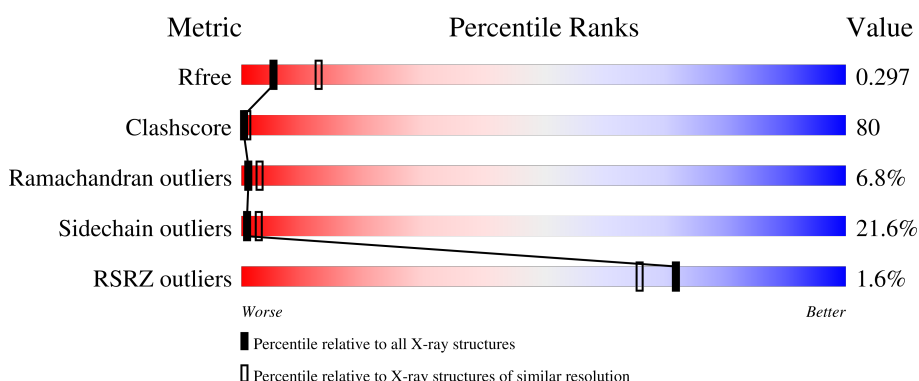
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	313	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">13%</div> <div style="text-align: center;">41%</div> <div style="text-align: left;">32%</div> <div style="text-align: right;">12%</div> </div>
1	B	313	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">11%</div> <div style="text-align: center;">36%</div> <div style="text-align: left;">33%</div> <div style="text-align: right;">17%</div> </div>
2	C	11	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">27%</div> <div style="text-align: center;">18%</div> <div style="text-align: left;">45%</div> <div style="text-align: right;">9%</div> </div>
2	D	11	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">18%</div> <div style="text-align: center;">27%</div> <div style="text-align: left;">55%</div> </div>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5190 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.

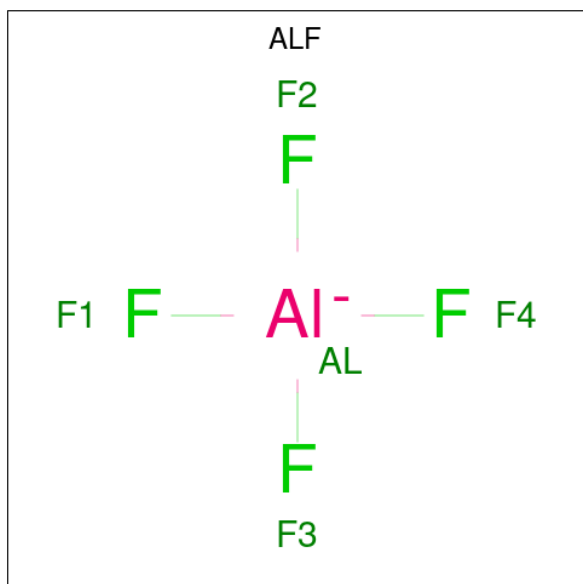
- Molecule 1 is a protein called Guanine nucleotide-binding protein G(i), alpha-1 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	303	Total 2450	C 1561	N 411	O 464	S 14	0	0	0
1	B	303	Total 2450	C 1561	N 411	O 464	S 14	0	0	0

- Molecule 2 is a protein called KB-1753 phage display peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	11	Total 96	C 63	N 17	O 16	0	0	0
2	D	11	Total 96	C 63	N 17	O 16	0	0	0

- Molecule 3 is TETRAFLUOROALUMINATE ION (three-letter code: ALF) (formula: AlF_4).

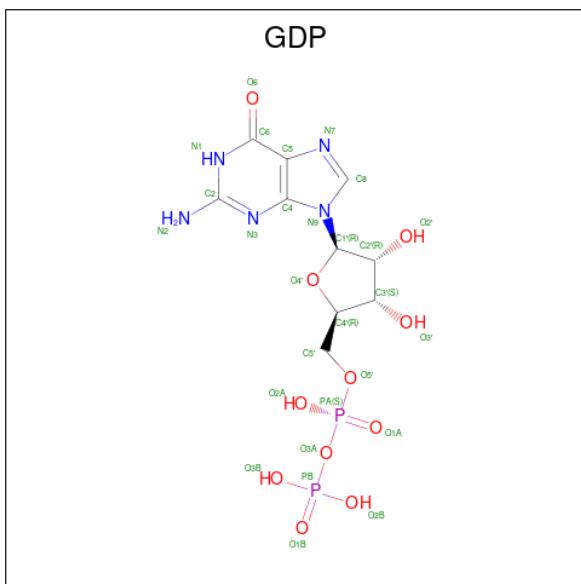


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Al	F	0	0
			5	1	4		
3	B	1	Total	Al	F	0	0
			5	1	4		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 5 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	17	Total	O	0	0
			17	17		

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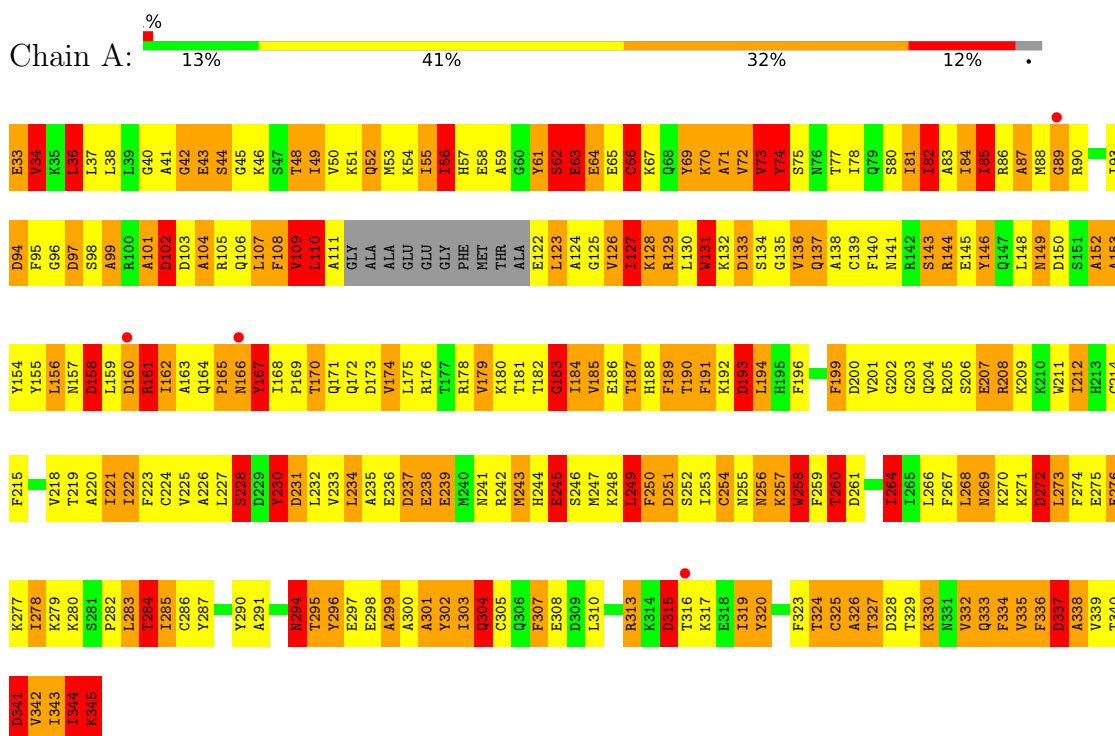
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	12	Total	O	0	0
			12	12		
6	C	1	Total	O	0	0
			1	1		

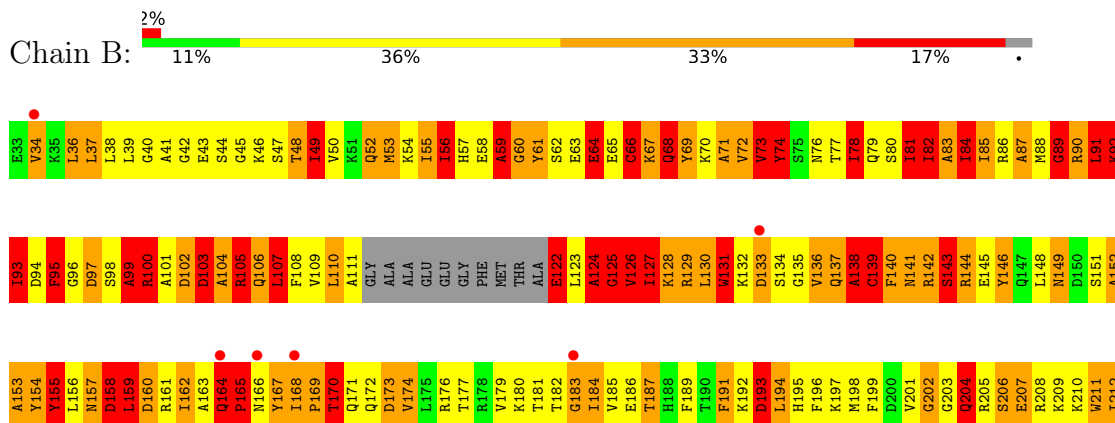
3 Residue-property plots

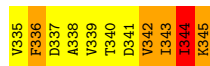
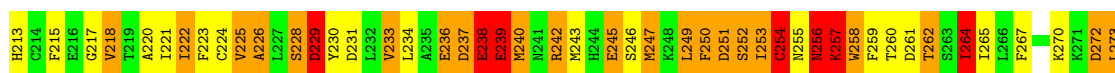
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Guanine nucleotide-binding protein G(i), alpha-1 subunit

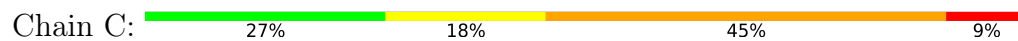


- Molecule 1: Guanine nucleotide-binding protein G(i), alpha-1 subunit

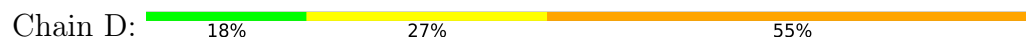




- Molecule 2: KB-1753 phage display peptide



- Molecule 2: KB-1753 phage display peptide



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	103.13Å 103.13Å 206.99Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.80 46.15 – 2.79	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.80) 87.8 (46.15-2.79)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.00 (at 2.81Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.269 , 0.300 0.269 , 0.297	Depositor DCC
R_{free} test set	3043 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	53.3	Xtrriage
Anisotropy	0.696	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 68.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	5190	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% 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, ALF, 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	3.81	372/2494 (14.9%)	2.22	70/3359 (2.1%)
1	B	3.44	272/2494 (10.9%)	1.89	74/3359 (2.2%)
2	C	3.38	14/100 (14.0%)	1.60	2/133 (1.5%)
2	D	3.86	19/100 (19.0%)	1.48	2/133 (1.5%)
All	All	3.63	677/5188 (13.0%)	2.04	148/6984 (2.1%)

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	A	0	18
1	B	0	29
2	D	0	1
All	All	0	48

All (677) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	109	VAL	C-N	-26.49	0.73	1.34
1	A	110	LEU	C-N	-20.82	0.86	1.34
1	B	104	ALA	N-CA	19.89	1.86	1.46
1	B	60	GLY	N-CA	-17.34	1.20	1.46
1	B	290	TYR	CE2-CZ	-12.12	1.22	1.38
1	B	226	ALA	CA-CB	-12.06	1.27	1.52
1	B	220	ALA	CA-CB	-11.45	1.28	1.52
1	A	83	ALA	CA-CB	-11.10	1.29	1.52
1	A	230	TYR	CE2-CZ	-11.00	1.24	1.38
1	A	126	VAL	CB-CG1	-10.96	1.29	1.52
1	B	290	TYR	CD1-CE1	-10.94	1.23	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	185	VAL	CB-CG1	-10.91	1.29	1.52
1	A	274	PHE	CE2-CZ	-10.90	1.16	1.37
1	B	185	VAL	CB-CG1	-10.89	1.29	1.52
1	A	146	TYR	CD1-CE1	-10.60	1.23	1.39
1	B	290	TYR	CD2-CE2	-10.59	1.23	1.39
1	B	99	ALA	C-N	10.59	1.58	1.34
1	A	98	SER	C-O	-10.49	1.03	1.23
1	A	287	TYR	CE2-CZ	-10.47	1.25	1.38
1	A	230	TYR	CD1-CE1	-10.43	1.23	1.39
1	B	201	VAL	CB-CG2	-10.39	1.31	1.52
1	B	301	ALA	CA-CB	-10.33	1.30	1.52
1	A	302	TYR	CE2-CZ	-10.22	1.25	1.38
1	A	301	ALA	CA-CB	-10.21	1.31	1.52
1	A	69	TYR	CD2-CE2	-10.18	1.24	1.39
1	A	287	TYR	CD1-CE1	-10.18	1.24	1.39
1	B	82	ILE	N-CA	10.14	1.66	1.46
1	A	223	PHE	CD1-CE1	-10.11	1.19	1.39
1	A	302	TYR	CD1-CE1	-10.09	1.24	1.39
1	B	225	VAL	CB-CG1	-10.08	1.31	1.52
1	A	146	TYR	CD2-CE2	-10.07	1.24	1.39
1	A	69	TYR	CE1-CZ	-10.06	1.25	1.38
1	A	258	TRP	CE3-CZ3	-10.01	1.21	1.38
1	A	154	TYR	CE1-CZ	-9.98	1.25	1.38
1	B	338	ALA	CA-CB	-9.91	1.31	1.52
1	B	146	TYR	CD2-CE2	-9.90	1.24	1.39
1	A	226	ALA	CA-CB	-9.88	1.31	1.52
1	B	154	TYR	CE2-CZ	-9.81	1.25	1.38
1	B	50	VAL	CB-CG2	-9.80	1.32	1.52
1	B	55	ILE	CA-CB	-9.79	1.32	1.54
2	D	11	VAL	CB-CG2	-9.78	1.32	1.52
1	B	287	TYR	CD1-CE1	-9.73	1.24	1.39
1	B	308	GLU	CD-OE1	-9.71	1.15	1.25
1	A	199	PHE	CE1-CZ	-9.71	1.19	1.37
1	A	299	ALA	CA-CB	-9.70	1.32	1.52
1	B	290	TYR	CE1-CZ	-9.70	1.25	1.38
1	B	174	VAL	CB-CG2	-9.69	1.32	1.52
1	A	290	TYR	CE2-CZ	-9.63	1.26	1.38
1	A	291	ALA	CA-CB	-9.63	1.32	1.52
1	A	290	TYR	CE1-CZ	-9.62	1.26	1.38
1	B	230	TYR	CE2-CZ	-9.61	1.26	1.38
1	A	59	ALA	CA-CB	-9.60	1.32	1.52
1	B	296	TYR	CD2-CE2	-9.54	1.25	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	302	TYR	CD2-CE2	-9.49	1.25	1.39
1	A	69	TYR	CE2-CZ	-9.49	1.26	1.38
1	A	101	ALA	CA-CB	-9.48	1.32	1.52
1	A	302	TYR	CE1-CZ	-9.47	1.26	1.38
1	B	83	ALA	CA-CB	-9.45	1.32	1.52
1	A	287	TYR	CD2-CE2	-9.40	1.25	1.39
1	A	185	VAL	CB-CG2	-9.40	1.33	1.52
1	A	167	TYR	CE1-CZ	-9.37	1.26	1.38
1	A	230	TYR	CE1-CZ	-9.32	1.26	1.38
1	A	290	TYR	CD2-CE2	-9.25	1.25	1.39
1	B	191	PHE	CE2-CZ	-9.23	1.19	1.37
1	A	296	TYR	CE1-CZ	-9.23	1.26	1.38
1	A	124	ALA	CA-CB	-9.21	1.33	1.52
2	C	5	TYR	CE1-CZ	-9.21	1.26	1.38
1	B	287	TYR	CE2-CZ	-9.15	1.26	1.38
1	A	69	TYR	CD1-CE1	-9.14	1.25	1.39
1	B	342	VAL	CB-CG2	-9.14	1.33	1.52
1	B	230	TYR	CD1-CE1	-9.06	1.25	1.39
1	A	73	VAL	CB-CG1	-9.04	1.33	1.52
1	A	342	VAL	CB-CG1	-9.01	1.33	1.52
1	A	138	ALA	CA-CB	-8.96	1.33	1.52
1	A	307	PHE	CE1-CZ	-8.93	1.20	1.37
1	A	220	ALA	CA-CB	-8.93	1.33	1.52
1	B	50	VAL	CB-CG1	-8.90	1.34	1.52
1	A	338	ALA	CA-CB	-8.89	1.33	1.52
1	B	320	TYR	CE1-CZ	-8.87	1.27	1.38
1	B	225	VAL	CB-CG2	-8.84	1.34	1.52
1	B	287	TYR	CD2-CE2	-8.82	1.26	1.39
1	B	287	TYR	CE1-CZ	-8.82	1.27	1.38
1	B	139	CYS	N-CA	8.81	1.64	1.46
1	A	87	ALA	CA-CB	-8.80	1.33	1.52
1	A	104	ALA	CA-CB	-8.79	1.33	1.52
1	B	185	VAL	CB-CG2	-8.78	1.34	1.52
1	B	218	VAL	CB-CG1	-8.76	1.34	1.52
1	B	326	ALA	CA-CB	-8.76	1.34	1.52
1	B	296	TYR	CE2-CZ	-8.73	1.27	1.38
1	A	233	VAL	CB-CG2	-8.70	1.34	1.52
1	B	335	VAL	CB-CG1	-8.68	1.34	1.52
1	B	339	VAL	CB-CG2	-8.66	1.34	1.52
1	A	201	VAL	CB-CG2	-8.62	1.34	1.52
1	A	274	PHE	CE1-CZ	-8.61	1.21	1.37
1	B	302	TYR	CE2-CZ	-8.60	1.27	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	174	VAL	CB-CG2	-8.58	1.34	1.52
1	B	201	VAL	CB-CG1	-8.58	1.34	1.52
1	B	179	VAL	CB-CG1	-8.58	1.34	1.52
1	B	218	VAL	CB-CG2	-8.58	1.34	1.52
1	A	223	PHE	CE2-CZ	-8.55	1.21	1.37
1	B	233	VAL	CB-CG2	-8.55	1.34	1.52
1	A	302	TYR	CG-CD1	-8.53	1.28	1.39
1	A	111	ALA	CA-CB	-8.50	1.34	1.52
1	A	174	VAL	CB-CG1	-8.50	1.35	1.52
1	B	274	PHE	CE2-CZ	-8.50	1.21	1.37
1	A	155	TYR	CE2-CZ	-8.49	1.27	1.38
2	D	13	GLU	C-OXT	8.47	1.39	1.23
1	A	274	PHE	CG-CD1	-8.47	1.26	1.38
1	B	73	VAL	CA-CB	-8.46	1.36	1.54
1	A	50	VAL	CB-CG2	-8.45	1.35	1.52
2	D	6	TYR	CE2-CZ	-8.45	1.27	1.38
1	A	320	TYR	CD2-CE2	-8.43	1.26	1.39
1	B	41	ALA	CA-CB	-8.42	1.34	1.52
1	A	231	ASP	CB-CG	-8.36	1.34	1.51
1	B	323	PHE	CE1-CZ	-8.36	1.21	1.37
1	B	323	PHE	CE2-CZ	-8.36	1.21	1.37
1	A	320	TYR	CE2-CZ	-8.35	1.27	1.38
1	A	131	TRP	CE3-CZ3	-8.34	1.24	1.38
2	C	5	TYR	CE2-CZ	-8.33	1.27	1.38
1	B	290	TYR	CG-CD2	-8.32	1.28	1.39
1	A	146	TYR	CE1-CZ	-8.32	1.27	1.38
1	A	41	ALA	CA-CB	-8.31	1.35	1.52
2	D	5	TYR	CE1-CZ	-8.29	1.27	1.38
1	B	335	VAL	CB-CG2	-8.25	1.35	1.52
1	A	218	VAL	CB-CG2	-8.25	1.35	1.52
1	B	296	TYR	CE1-CZ	-8.24	1.27	1.38
1	B	155	TYR	CE1-CZ	-8.23	1.27	1.38
1	A	230	TYR	CD2-CE2	-8.22	1.27	1.39
1	B	285	ILE	CA-CB	-8.22	1.35	1.54
1	B	250	PHE	CE2-CZ	-8.19	1.21	1.37
1	A	332	VAL	CB-CG1	-8.19	1.35	1.52
1	B	302	TYR	CD2-CE2	-8.17	1.27	1.39
1	A	303	ILE	CA-CB	-8.17	1.36	1.54
1	B	146	TYR	CD1-CE1	-8.15	1.27	1.39
1	B	307	PHE	CE1-CZ	-8.14	1.21	1.37
1	A	50	VAL	CB-CG1	-8.14	1.35	1.52
1	A	274	PHE	CD2-CE2	-8.13	1.23	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	299	ALA	CA-CB	-8.13	1.35	1.52
1	B	146	TYR	CE2-CZ	-8.12	1.27	1.38
1	A	73	VAL	CB-CG2	-8.11	1.35	1.52
2	D	5	TYR	CD2-CE2	-8.10	1.27	1.39
1	A	296	TYR	CD2-CE2	-8.10	1.27	1.39
1	B	199	PHE	CE1-CZ	-8.09	1.22	1.37
1	A	267	PHE	CE2-CZ	-8.06	1.22	1.37
1	A	146	TYR	CE2-CZ	-8.05	1.28	1.38
1	A	218	VAL	CB-CG1	-8.03	1.35	1.52
1	A	344	ILE	C-N	-8.03	1.15	1.34
1	A	71	ALA	CA-CB	-8.03	1.35	1.52
1	B	56	ILE	CA-CB	-8.01	1.36	1.54
1	B	320	TYR	CD2-CE2	-8.00	1.27	1.39
1	B	250	PHE	CE1-CZ	-7.98	1.22	1.37
1	A	179	VAL	CB-CG1	-7.97	1.36	1.52
1	A	201	VAL	CB-CG1	-7.96	1.36	1.52
1	A	223	PHE	CE1-CZ	-7.95	1.22	1.37
1	A	225	VAL	CB-CG1	-7.94	1.36	1.52
1	A	230	TYR	CG-CD2	-7.93	1.28	1.39
1	A	167	TYR	CD1-CE1	-7.88	1.27	1.39
1	B	344	ILE	CA-CB	-7.87	1.36	1.54
1	A	223	PHE	CD2-CE2	-7.86	1.23	1.39
1	A	43	GLU	CD-OE1	-7.85	1.17	1.25
1	B	245	GLU	CD-OE2	-7.83	1.17	1.25
1	A	274	PHE	CD1-CE1	-7.83	1.23	1.39
1	A	223	PHE	CG-CD2	-7.83	1.27	1.38
1	B	191	PHE	CD1-CE1	-7.81	1.23	1.39
1	A	296	TYR	CE2-CZ	-7.79	1.28	1.38
1	B	165	PRO	N-CA	-7.79	1.34	1.47
1	A	34	VAL	CB-CG2	-7.79	1.36	1.52
1	B	290	TYR	CG-CD1	-7.79	1.29	1.39
1	A	168	ILE	CA-CB	-7.77	1.36	1.54
1	B	250	PHE	CD2-CE2	-7.76	1.23	1.39
1	A	126	VAL	CA-CB	-7.76	1.38	1.54
1	A	332	VAL	CA-CB	-7.76	1.38	1.54
1	A	155	TYR	CE1-CZ	-7.75	1.28	1.38
1	B	230	TYR	CE1-CZ	-7.73	1.28	1.38
1	A	61	TYR	CE1-CZ	-7.72	1.28	1.38
1	A	233	VAL	CB-CG1	-7.71	1.36	1.52
1	B	339	VAL	CB-CG1	-7.71	1.36	1.52
1	B	296	TYR	CG-CD2	-7.71	1.29	1.39
1	B	199	PHE	CE2-CZ	-7.70	1.22	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	342	VAL	CB-CG1	-7.70	1.36	1.52
1	A	199	PHE	CE2-CZ	-7.69	1.22	1.37
2	D	11	VAL	CB-CG1	-7.68	1.36	1.52
1	A	258	TRP	CE2-CZ2	-7.68	1.26	1.39
1	B	191	PHE	CG-CD1	-7.63	1.27	1.38
1	B	223	PHE	CD1-CE1	-7.62	1.24	1.39
1	B	245	GLU	CD-OE1	-7.62	1.17	1.25
1	B	230	TYR	CD2-CE2	-7.62	1.27	1.39
1	A	84	ILE	CA-CB	-7.61	1.37	1.54
1	A	95	PHE	CE2-CZ	-7.60	1.23	1.37
1	B	183	GLY	C-O	-7.59	1.11	1.23
1	A	95	PHE	CD1-CE1	-7.59	1.24	1.39
1	B	323	PHE	CD1-CE1	-7.58	1.24	1.39
1	A	284	THR	CB-CG2	-7.55	1.27	1.52
1	A	126	VAL	CB-CG2	-7.55	1.36	1.52
1	A	145	GLU	CD-OE1	-7.55	1.17	1.25
1	B	146	TYR	CE1-CZ	-7.54	1.28	1.38
1	A	290	TYR	CD1-CE1	-7.54	1.28	1.39
1	B	334	PHE	CD1-CE1	-7.51	1.24	1.39
1	B	174	VAL	CB-CG1	-7.51	1.37	1.52
1	B	274	PHE	CD1-CE1	-7.50	1.24	1.39
1	B	332	VAL	CB-CG1	-7.48	1.37	1.52
1	A	99	ALA	CA-CB	-7.48	1.36	1.52
2	C	11	VAL	CB-CG2	-7.46	1.37	1.52
1	B	336	PHE	CD1-CE1	-7.46	1.24	1.39
1	A	82	ILE	CA-CB	-7.43	1.37	1.54
1	B	267	PHE	CE2-CZ	-7.43	1.23	1.37
1	A	199	PHE	CD2-CE2	-7.42	1.24	1.39
1	A	335	VAL	CB-CG2	-7.42	1.37	1.52
1	A	287	TYR	CE1-CZ	-7.41	1.28	1.38
1	A	267	PHE	CE1-CZ	-7.40	1.23	1.37
1	A	320	TYR	CD1-CE1	-7.39	1.28	1.39
1	B	272	ASP	CB-CG	-7.39	1.36	1.51
1	B	320	TYR	CD1-CE1	-7.39	1.28	1.39
1	B	332	VAL	CB-CG2	-7.37	1.37	1.52
1	B	154	TYR	CD1-CE1	-7.34	1.28	1.39
1	B	174	VAL	CA-CB	-7.34	1.39	1.54
1	A	335	VAL	CB-CG1	-7.33	1.37	1.52
1	A	196	PHE	CG-CD1	-7.33	1.27	1.38
1	A	323	PHE	CE2-CZ	-7.32	1.23	1.37
1	B	155	TYR	CD1-CE1	-7.32	1.28	1.39
2	D	11	VAL	CA-CB	-7.29	1.39	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	61	TYR	CE2-CZ	-7.29	1.29	1.38
1	B	155	TYR	CE2-CZ	-7.28	1.29	1.38
1	A	320	TYR	CE1-CZ	-7.28	1.29	1.38
1	A	250	PHE	CE1-CZ	-7.27	1.23	1.37
1	A	181	THR	CB-CG2	-7.26	1.28	1.52
1	A	308	GLU	CD-OE1	-7.26	1.17	1.25
1	B	82	ILE	CA-CB	-7.26	1.38	1.54
1	B	154	TYR	CD2-CE2	-7.23	1.28	1.39
1	B	259	PHE	CE1-CZ	-7.23	1.23	1.37
1	B	250	PHE	CD1-CE1	-7.22	1.24	1.39
1	A	259	PHE	CE1-CZ	-7.21	1.23	1.37
1	B	154	TYR	CE1-CZ	-7.21	1.29	1.38
1	B	323	PHE	CD2-CE2	-7.21	1.24	1.39
2	D	5	TYR	CE2-CZ	-7.21	1.29	1.38
1	B	153	ALA	CA-CB	-7.20	1.37	1.52
1	B	282	PRO	CB-CG	-7.20	1.14	1.50
2	C	5	TYR	CD2-CE2	-7.19	1.28	1.39
1	A	95	PHE	CD2-CE2	-7.19	1.24	1.39
1	A	179	VAL	CB-CG2	-7.19	1.37	1.52
1	A	259	PHE	CG-CD1	-7.19	1.27	1.38
1	B	34	VAL	CB-CG1	-7.17	1.37	1.52
1	A	339	VAL	CB-CG2	-7.16	1.37	1.52
1	A	72	VAL	CB-CG2	-7.15	1.37	1.52
1	A	167	TYR	CE2-CZ	-7.14	1.29	1.38
1	A	287	TYR	CG-CD2	-7.13	1.29	1.39
2	C	11	VAL	CA-CB	-7.13	1.39	1.54
1	A	189	PHE	CD1-CE1	-7.12	1.25	1.39
1	A	167	TYR	CD2-CE2	-7.11	1.28	1.39
1	A	323	PHE	CE1-CZ	-7.11	1.23	1.37
1	A	136	VAL	CB-CG1	-7.11	1.38	1.52
1	A	300	ALA	CA-CB	-7.08	1.37	1.52
1	B	336	PHE	CD2-CE2	-7.07	1.25	1.39
1	A	109	VAL	CB-CG1	-7.07	1.38	1.52
1	B	45	GLY	C-O	-7.07	1.12	1.23
1	A	73	VAL	CA-CB	-7.06	1.40	1.54
1	A	221	ILE	CA-CB	-7.06	1.38	1.54
1	A	199	PHE	CG-CD2	-7.05	1.28	1.38
1	B	274	PHE	CD2-CE2	-7.05	1.25	1.39
1	B	252	SER	CB-OG	-7.04	1.33	1.42
1	B	61	TYR	CE1-CZ	-7.01	1.29	1.38
1	A	136	VAL	CB-CG2	-7.00	1.38	1.52
1	A	287	TYR	CG-CD1	-6.99	1.30	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	55	ILE	CB-CG2	-6.97	1.31	1.52
1	B	87	ALA	CA-CB	-6.97	1.37	1.52
1	A	108	PHE	CD1-CE1	-6.96	1.25	1.39
1	B	211	TRP	CZ3-CH2	-6.94	1.28	1.40
1	A	332	VAL	CB-CG2	-6.92	1.38	1.52
1	A	215	PHE	CE1-CZ	-6.92	1.24	1.37
1	B	302	TYR	CD1-CE1	-6.92	1.28	1.39
1	A	307	PHE	CD2-CE2	-6.91	1.25	1.39
1	A	223	PHE	CG-CD1	-6.91	1.28	1.38
2	D	10	TRP	CE3-CZ3	-6.91	1.26	1.38
1	B	223	PHE	CE1-CZ	-6.89	1.24	1.37
1	A	153	ALA	CA-CB	-6.89	1.38	1.52
2	C	10	TRP	CG-CD1	-6.89	1.27	1.36
1	A	208	ARG	NE-CZ	-6.88	1.24	1.33
1	B	259	PHE	CD1-CE1	-6.87	1.25	1.39
1	A	52	GLN	CB-CG	-6.87	1.33	1.52
1	A	278	ILE	CB-CG2	-6.86	1.31	1.52
1	A	308	GLU	CD-OE2	-6.86	1.18	1.25
1	A	34	VAL	CA-CB	-6.85	1.40	1.54
1	B	211	TRP	CE3-CZ3	-6.84	1.26	1.38
1	A	127	ILE	CA-CB	-6.84	1.39	1.54
1	A	215	PHE	CE2-CZ	-6.84	1.24	1.37
1	A	201	VAL	CA-CB	-6.82	1.40	1.54
1	B	250	PHE	CG-CD1	-6.82	1.28	1.38
1	A	259	PHE	CD2-CE2	-6.81	1.25	1.39
1	A	264	ILE	CA-CB	-6.81	1.39	1.54
1	A	218	VAL	CA-CB	-6.77	1.40	1.54
1	A	310	LEU	CG-CD2	-6.75	1.26	1.51
1	A	295	THR	CB-CG2	-6.75	1.30	1.52
1	A	155	TYR	CD2-CE2	-6.73	1.29	1.39
1	B	199	PHE	CD2-CE2	-6.73	1.25	1.39
1	B	69	TYR	CE2-CZ	-6.72	1.29	1.38
1	A	259	PHE	CE2-CZ	-6.72	1.24	1.37
1	A	191	PHE	CE1-CZ	-6.71	1.24	1.37
1	B	103	ASP	C-N	-6.71	1.18	1.34
1	A	230	TYR	CG-CD1	-6.70	1.30	1.39
1	B	199	PHE	CG-CD1	-6.70	1.28	1.38
1	A	336	PHE	CD2-CE2	-6.69	1.25	1.39
1	A	108	PHE	CB-CG	-6.69	1.40	1.51
1	B	127	ILE	CA-CB	-6.68	1.39	1.54
1	B	154	TYR	CG-CD2	-6.67	1.30	1.39
1	A	152	ALA	CA-CB	-6.65	1.38	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	211	TRP	CZ3-CH2	-6.65	1.29	1.40
1	B	230	TYR	CG-CD2	-6.64	1.30	1.39
1	A	155	TYR	CG-CD1	-6.63	1.30	1.39
1	A	191	PHE	CG-CD1	-6.62	1.28	1.38
1	A	53	MET	CG-SD	-6.61	1.64	1.81
1	A	154	TYR	CE2-CZ	-6.60	1.29	1.38
1	A	45	GLY	C-O	-6.59	1.13	1.23
1	A	140	PHE	CE1-CZ	-6.59	1.24	1.37
1	B	71	ALA	CA-CB	-6.57	1.38	1.52
1	B	221	ILE	CB-CG2	-6.57	1.32	1.52
2	D	5	TYR	CG-CD2	-6.57	1.30	1.39
1	B	225	VAL	CA-CB	-6.56	1.41	1.54
1	B	274	PHE	CG-CD1	-6.56	1.28	1.38
1	A	307	PHE	CG-CD2	-6.55	1.28	1.38
1	B	297	GLU	CD-OE1	-6.55	1.18	1.25
1	A	211	TRP	CE3-CZ3	-6.54	1.27	1.38
1	B	49	ILE	CA-CB	-6.54	1.39	1.54
1	B	201	VAL	CA-CB	-6.54	1.41	1.54
2	C	5	TYR	CD1-CE1	-6.54	1.29	1.39
1	A	69	TYR	CG-CD2	-6.53	1.30	1.39
1	A	190	THR	CB-CG2	-6.53	1.30	1.52
1	A	191	PHE	CE2-CZ	-6.52	1.25	1.37
1	A	323	PHE	CD2-CE2	-6.52	1.26	1.39
1	A	208	ARG	CZ-NH1	-6.51	1.24	1.33
1	A	146	TYR	CG-CD1	-6.51	1.30	1.39
1	A	211	TRP	CD2-CE2	-6.50	1.33	1.41
1	A	155	TYR	CD1-CE1	-6.50	1.29	1.39
1	B	296	TYR	CD1-CE1	-6.49	1.29	1.39
1	B	335	VAL	CA-CB	-6.49	1.41	1.54
1	B	223	PHE	CD2-CE2	-6.47	1.26	1.39
1	A	133	ASP	CB-CG	-6.47	1.38	1.51
1	A	267	PHE	CD2-CE2	-6.47	1.26	1.39
1	B	140	PHE	CE2-CZ	-6.47	1.25	1.37
2	C	9	ILE	CA-CB	-6.46	1.40	1.54
2	D	5	TYR	CG-CD1	-6.46	1.30	1.39
1	B	124	ALA	CA-CB	-6.44	1.39	1.52
1	A	211	TRP	CG-CD1	-6.44	1.27	1.36
1	B	173	ASP	CB-CG	-6.44	1.38	1.51
1	A	131	TRP	CZ3-CH2	-6.44	1.29	1.40
1	B	155	TYR	CD2-CE2	-6.43	1.29	1.39
1	A	297	GLU	CD-OE1	-6.43	1.18	1.25
1	A	250	PHE	CD2-CE2	-6.41	1.26	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	233	VAL	CB-CG1	-6.40	1.39	1.52
1	A	282	PRO	CB-CG	-6.40	1.18	1.50
1	A	74	TYR	CE2-CZ	-6.38	1.30	1.38
1	B	126	VAL	CA-CB	-6.38	1.41	1.54
1	A	191	PHE	CD1-CE1	-6.37	1.26	1.39
1	A	207	GLU	CD-OE1	-6.37	1.18	1.25
1	B	187	THR	CB-CG2	-6.37	1.31	1.52
1	A	136	VAL	CA-CB	-6.36	1.41	1.54
1	B	215	PHE	CG-CD1	-6.36	1.29	1.38
1	A	325	CYS	CB-SG	-6.36	1.71	1.82
1	B	336	PHE	CE2-CZ	-6.36	1.25	1.37
1	A	186	GLU	CD-OE1	-6.35	1.18	1.25
1	A	34	VAL	CB-CG1	-6.35	1.39	1.52
1	B	278	ILE	CA-CB	-6.34	1.40	1.54
1	A	127	ILE	CB-CG2	-6.34	1.33	1.52
1	A	334	PHE	CE1-CZ	-6.33	1.25	1.37
1	B	228	SER	CA-CB	-6.32	1.43	1.52
1	B	324	THR	CB-CG2	-6.31	1.31	1.52
1	A	56	ILE	CB-CG2	-6.30	1.33	1.52
1	B	52	GLN	CB-CG	-6.29	1.35	1.52
1	B	222	ILE	CA-CB	-6.29	1.40	1.54
1	A	55	ILE	CA-CB	-6.29	1.40	1.54
1	A	109	VAL	CB-CG2	-6.28	1.39	1.52
1	A	208	ARG	CG-CD	-6.27	1.36	1.51
1	B	34	VAL	CB-CG2	-6.26	1.39	1.52
1	A	187	THR	CB-CG2	-6.26	1.31	1.52
1	A	140	PHE	CE2-CZ	-6.26	1.25	1.37
1	B	302	TYR	CG-CD1	-6.25	1.31	1.39
1	B	202	GLY	C-O	-6.25	1.13	1.23
1	A	336	PHE	CD1-CE1	-6.24	1.26	1.39
1	B	191	PHE	CD2-CE2	-6.24	1.26	1.39
1	A	296	TYR	CG-CD2	-6.23	1.31	1.39
1	A	199	PHE	C-O	-6.23	1.11	1.23
1	A	324	THR	CB-CG2	-6.23	1.31	1.52
1	B	320	TYR	CE2-CZ	-6.23	1.30	1.38
1	B	302	TYR	CE1-CZ	-6.22	1.30	1.38
1	A	176	ARG	CZ-NH2	-6.21	1.25	1.33
1	A	250	PHE	CE2-CZ	-6.20	1.25	1.37
1	A	140	PHE	CD1-CE1	-6.20	1.26	1.39
1	B	69	TYR	CE1-CZ	-6.20	1.30	1.38
1	A	72	VAL	CA-CB	-6.18	1.41	1.54
1	B	155	TYR	CG-CD1	-6.17	1.31	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	131	TRP	CG-CD1	-6.16	1.28	1.36
1	B	259	PHE	CD2-CE2	-6.16	1.26	1.39
1	B	207	GLU	CD-OE1	-6.16	1.18	1.25
1	B	179	VAL	CA-CB	-6.16	1.41	1.54
1	A	225	VAL	CB-CG2	-6.15	1.40	1.52
1	B	310	LEU	CG-CD2	-6.15	1.29	1.51
1	A	307	PHE	CE2-CZ	-6.14	1.25	1.37
1	A	202	GLY	C-O	-6.13	1.13	1.23
1	B	85	ILE	CA-CB	-6.13	1.40	1.54
1	B	274	PHE	CE1-CZ	-6.13	1.25	1.37
1	B	240	MET	CG-SD	-6.13	1.65	1.81
1	A	264	ILE	CB-CG2	-6.12	1.33	1.52
1	B	211	TRP	CG-CD1	-6.12	1.28	1.36
1	A	85	ILE	CB-CG2	-6.12	1.33	1.52
1	B	334	PHE	CD2-CE2	-6.12	1.27	1.39
1	A	269	ASN	C-O	-6.12	1.11	1.23
1	B	215	PHE	CE2-CZ	-6.11	1.25	1.37
1	B	191	PHE	CE1-CZ	-6.10	1.25	1.37
1	B	270	LYS	CB-CG	-6.07	1.36	1.52
1	A	82	ILE	CB-CG2	-6.07	1.34	1.52
1	B	39	LEU	CG-CD1	-6.06	1.29	1.51
1	B	287	TYR	CG-CD2	-6.05	1.31	1.39
1	B	344	ILE	CB-CG2	-6.05	1.34	1.52
1	A	320	TYR	CG-CD1	-6.04	1.31	1.39
1	B	253	ILE	CB-CG2	-6.04	1.34	1.52
2	C	5	TYR	CG-CD1	-6.03	1.31	1.39
1	A	144	ARG	CB-CG	-6.03	1.36	1.52
1	A	140	PHE	CD2-CE2	-6.02	1.27	1.39
1	A	344	ILE	CB-CG2	-6.02	1.34	1.52
1	A	36	LEU	CG-CD2	-6.02	1.29	1.51
1	B	249	LEU	CG-CD1	-6.01	1.29	1.51
1	B	343	ILE	CA-CB	-6.01	1.41	1.54
1	A	84	ILE	CB-CG2	-6.01	1.34	1.52
1	A	335	VAL	CA-CB	-6.00	1.42	1.54
1	B	265	ILE	CB-CG2	-6.00	1.34	1.52
1	A	222	ILE	CA-CB	-6.00	1.41	1.54
1	B	278	ILE	CB-CG2	-5.99	1.34	1.52
1	A	250	PHE	CD1-CE1	-5.99	1.27	1.39
1	B	336	PHE	CE1-CZ	-5.99	1.25	1.37
1	A	48	THR	CB-CG2	-5.98	1.32	1.52
1	A	245	GLU	CD-OE2	-5.98	1.19	1.25
1	B	250	PHE	CG-CD2	-5.97	1.29	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	140	PHE	CE1-CZ	-5.96	1.26	1.37
1	A	344	ILE	CA-CB	-5.96	1.41	1.54
1	A	140	PHE	CG-CD2	-5.96	1.29	1.38
1	B	56	ILE	CB-CG2	-5.96	1.34	1.52
1	A	131	TRP	CE2-CZ2	-5.95	1.29	1.39
1	A	109	VAL	CA-CB	-5.95	1.42	1.54
1	A	319	ILE	CA-CB	-5.95	1.41	1.54
1	A	185	VAL	CA-CB	-5.94	1.42	1.54
1	A	302	TYR	CG-CD2	-5.94	1.31	1.39
1	B	320	TYR	CG-CD1	-5.93	1.31	1.39
1	B	72	VAL	CA-CB	-5.93	1.42	1.54
1	A	131	TRP	CD2-CE2	-5.93	1.34	1.41
1	A	154	TYR	CG-CD2	-5.92	1.31	1.39
1	A	189	PHE	CD2-CE2	-5.92	1.27	1.39
1	A	95	PHE	CE1-CZ	-5.91	1.26	1.37
1	B	222	ILE	CB-CG2	-5.91	1.34	1.52
1	B	323	PHE	CG-CD2	-5.90	1.29	1.38
1	A	56	ILE	CA-CB	-5.90	1.41	1.54
1	A	295	THR	N-CA	-5.90	1.34	1.46
1	A	182	THR	CA-CB	-5.89	1.38	1.53
1	A	40	GLY	C-O	-5.88	1.14	1.23
1	B	68	GLN	CB-CG	-5.88	1.36	1.52
1	A	95	PHE	CG-CD1	-5.88	1.29	1.38
1	A	176	ARG	C-O	-5.88	1.12	1.23
1	A	307	PHE	CD1-CE1	-5.88	1.27	1.39
1	B	211	TRP	CD2-CE2	-5.87	1.34	1.41
1	A	228	SER	CB-OG	-5.87	1.34	1.42
1	B	191	PHE	CG-CD2	-5.87	1.29	1.38
1	A	43	GLU	CD-OE2	-5.86	1.19	1.25
1	B	40	GLY	C-O	-5.84	1.14	1.23
1	B	43	GLU	CD-OE2	-5.84	1.19	1.25
1	B	223	PHE	CG-CD1	-5.83	1.29	1.38
1	A	108	PHE	CD2-CE2	-5.83	1.27	1.39
1	B	319	ILE	CA-CB	-5.82	1.41	1.54
1	A	227	LEU	CG-CD2	-5.82	1.30	1.51
1	B	215	PHE	CD2-CE2	-5.82	1.27	1.39
1	B	146	TYR	CG-CD1	-5.82	1.31	1.39
1	B	84	ILE	CA-CB	-5.81	1.41	1.54
1	B	206	SER	CA-CB	-5.81	1.44	1.52
2	D	6	TYR	CG-CD1	-5.80	1.31	1.39
1	A	298	GLU	CD-OE2	-5.80	1.19	1.25
1	A	285	ILE	CB-CG2	-5.80	1.34	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	72	VAL	CB-CG1	-5.79	1.40	1.52
1	A	191	PHE	CD2-CE2	-5.79	1.27	1.39
1	B	179	VAL	CB-CG2	-5.78	1.40	1.52
1	A	286	CYS	CB-SG	-5.78	1.72	1.81
1	B	332	VAL	CA-CB	-5.78	1.42	1.54
1	A	339	VAL	CB-CG1	-5.77	1.40	1.52
1	A	108	PHE	CG-CD1	-5.76	1.30	1.38
1	A	74	TYR	CD2-CE2	-5.75	1.30	1.39
1	A	69	TYR	CG-CD1	-5.75	1.31	1.39
1	A	215	PHE	CD2-CE2	-5.74	1.27	1.39
1	B	303	ILE	CB-CG2	-5.74	1.35	1.52
1	A	208	ARG	CZ-NH2	-5.74	1.25	1.33
1	A	267	PHE	CD1-CE1	-5.73	1.27	1.39
1	A	252	SER	CB-OG	-5.73	1.34	1.42
1	A	269	ASN	CB-CG	-5.72	1.37	1.51
1	B	211	TRP	CE2-CZ2	-5.72	1.30	1.39
1	B	300	ALA	CA-CB	-5.72	1.40	1.52
1	A	273	LEU	CG-CD2	-5.71	1.30	1.51
1	A	267	PHE	CG-CD2	-5.70	1.30	1.38
1	B	53	MET	CG-SD	-5.70	1.66	1.81
1	A	145	GLU	CD-OE2	-5.69	1.19	1.25
1	A	345	LYS	CB-CG	-5.69	1.37	1.52
1	B	224	CYS	CB-SG	-5.68	1.72	1.81
1	A	44	SER	CA-CB	-5.68	1.44	1.52
1	A	342	VAL	CB-CG2	-5.67	1.41	1.52
1	B	215	PHE	CD1-CE1	-5.67	1.27	1.39
1	A	74	TYR	CE1-CZ	-5.67	1.31	1.38
1	A	296	TYR	CD1-CE1	-5.67	1.30	1.39
1	A	53	MET	N-CA	-5.66	1.35	1.46
1	A	310	LEU	CG-CD1	-5.66	1.30	1.51
1	B	38	LEU	CG-CD2	-5.66	1.30	1.51
1	A	187	THR	CA-CB	-5.65	1.38	1.53
1	A	191	PHE	CG-CD2	-5.64	1.30	1.38
1	A	276	GLU	C-O	-5.64	1.12	1.23
1	B	218	VAL	CA-CB	-5.64	1.43	1.54
1	B	307	PHE	CG-CD2	-5.62	1.30	1.38
1	A	110	LEU	CG-CD1	-5.62	1.31	1.51
1	A	211	TRP	CE2-CZ2	-5.62	1.30	1.39
1	A	148	LEU	CG-CD1	-5.62	1.31	1.51
2	C	8	GLY	C-O	-5.61	1.14	1.23
2	D	10	TRP	CE2-CZ2	-5.61	1.30	1.39
1	B	298	GLU	CD-OE2	-5.60	1.19	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	221	ILE	CB-CG2	-5.60	1.35	1.52
1	A	236	GLU	CD-OE2	-5.60	1.19	1.25
1	A	125	GLY	C-O	-5.60	1.14	1.23
1	A	196	PHE	CE1-CZ	-5.60	1.26	1.37
1	A	222	ILE	CB-CG2	-5.60	1.35	1.52
2	D	10	TRP	CG-CD1	-5.60	1.28	1.36
1	B	199	PHE	CD1-CE1	-5.59	1.28	1.39
1	A	235	ALA	CA-CB	-5.59	1.40	1.52
1	B	181	THR	CB-CG2	-5.58	1.33	1.52
1	A	267	PHE	CG-CD1	-5.58	1.30	1.38
1	B	199	PHE	CG-CD2	-5.57	1.30	1.38
1	B	252	SER	CA-CB	-5.57	1.44	1.52
1	A	323	PHE	CD1-CE1	-5.57	1.28	1.39
1	A	138	ALA	C-O	-5.56	1.12	1.23
1	B	208	ARG	CZ-NH1	-5.56	1.25	1.33
1	B	287	TYR	CG-CD1	-5.56	1.31	1.39
1	B	196	PHE	CE2-CZ	-5.55	1.26	1.37
1	A	61	TYR	CG-CD2	-5.55	1.31	1.39
1	A	205	ARG	CZ-NH1	-5.55	1.25	1.33
1	B	74	TYR	CE2-CZ	-5.55	1.31	1.38
1	B	236	GLU	CD-OE2	-5.55	1.19	1.25
1	B	222	ILE	C-O	-5.54	1.12	1.23
1	A	196	PHE	CD1-CE1	-5.54	1.28	1.39
1	B	196	PHE	CD1-CE1	-5.53	1.28	1.39
1	A	207	GLU	CD-OE2	-5.52	1.19	1.25
1	B	176	ARG	NE-CZ	-5.52	1.25	1.33
1	B	69	TYR	CD2-CE2	-5.52	1.31	1.39
1	B	309	ASP	CB-CG	-5.52	1.40	1.51
1	A	184	ILE	CA-CB	-5.51	1.42	1.54
1	A	199	PHE	CD1-CE1	-5.51	1.28	1.39
2	D	9	ILE	CB-CG2	-5.49	1.35	1.52
1	B	46	LYS	CE-NZ	-5.48	1.35	1.49
1	B	215	PHE	CE1-CZ	-5.47	1.26	1.37
1	B	253	ILE	CA-CB	-5.47	1.42	1.54
1	A	336	PHE	CE2-CZ	-5.47	1.26	1.37
1	A	259	PHE	CG-CD2	-5.46	1.30	1.38
2	C	10	TRP	CE3-CZ3	-5.46	1.29	1.38
2	C	5	TYR	CG-CD2	-5.45	1.32	1.39
1	A	51	LYS	CD-CE	-5.45	1.37	1.51
1	A	189	PHE	CE1-CZ	-5.45	1.26	1.37
1	A	85	ILE	CA-CB	-5.45	1.42	1.54
1	B	136	VAL	CB-CG1	-5.44	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	196	PHE	CE2-CZ	-5.44	1.27	1.37
1	A	144	ARG	NE-CZ	-5.44	1.25	1.33
1	A	278	ILE	CA-CB	-5.43	1.42	1.54
1	A	77	THR	CB-CG2	-5.43	1.34	1.52
1	A	95	PHE	CG-CD2	-5.43	1.30	1.38
1	A	274	PHE	CG-CD2	-5.43	1.30	1.38
1	A	108	PHE	CG-CD2	-5.43	1.30	1.38
1	B	196	PHE	CD2-CE2	-5.43	1.28	1.39
1	A	303	ILE	CB-CG2	-5.42	1.36	1.52
1	A	300	ALA	CA-C	-5.42	1.38	1.52
1	B	146	TYR	CG-CD2	-5.42	1.32	1.39
1	B	180	LYS	CB-CG	-5.42	1.38	1.52
1	B	38	LEU	CG-CD1	-5.42	1.31	1.51
1	B	199	PHE	C-O	-5.42	1.13	1.23
1	B	334	PHE	CE1-CZ	-5.42	1.27	1.37
2	C	11	VAL	CB-CG1	-5.42	1.41	1.52
1	A	276	GLU	CA-C	-5.41	1.38	1.52
1	A	260	THR	CA-CB	-5.41	1.39	1.53
1	B	59	ALA	CA-CB	-5.41	1.41	1.52
1	A	233	VAL	CA-CB	-5.40	1.43	1.54
1	A	296	TYR	CG-CD1	-5.40	1.32	1.39
1	A	82	ILE	C-O	-5.40	1.13	1.23
1	B	170	THR	CB-CG2	-5.40	1.34	1.52
1	A	152	ALA	C-O	-5.39	1.13	1.23
1	A	170	THR	CB-CG2	-5.39	1.34	1.52
1	B	297	GLU	CG-CD	-5.39	1.43	1.51
1	B	189	PHE	CE2-CZ	-5.39	1.27	1.37
1	B	325	CYS	CB-SG	-5.38	1.73	1.81
1	B	316	THR	CB-CG2	-5.37	1.34	1.52
1	B	242	ARG	CZ-NH1	-5.36	1.26	1.33
1	A	179	VAL	CA-CB	-5.35	1.43	1.54
1	A	290	TYR	CG-CD2	-5.35	1.32	1.39
1	A	156	LEU	CG-CD1	-5.35	1.32	1.51
1	A	137	GLN	CB-CG	-5.34	1.38	1.52
1	A	236	GLU	CG-CD	-5.34	1.44	1.51
1	B	44	SER	CB-OG	-5.33	1.35	1.42
1	B	72	VAL	CB-CG1	-5.33	1.41	1.52
1	B	187	THR	CA-CB	-5.33	1.39	1.53
1	A	107	LEU	CG-CD1	-5.33	1.32	1.51
1	A	336	PHE	CG-CD2	-5.33	1.30	1.38
1	B	152	ALA	CA-CB	-5.32	1.41	1.52
1	B	154	TYR	CG-CD1	-5.32	1.32	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	36	LEU	C-O	-5.32	1.13	1.23
1	A	74	TYR	CD1-CE1	-5.32	1.31	1.39
1	B	182	THR	CB-CG2	-5.31	1.34	1.52
1	A	283	LEU	CG-CD1	-5.30	1.32	1.51
1	A	327	THR	CB-CG2	-5.29	1.34	1.52
1	A	165	PRO	CA-C	-5.28	1.42	1.52
1	B	320	TYR	CG-CD2	-5.28	1.32	1.39
1	A	170	THR	CA-CB	-5.27	1.39	1.53
1	B	285	ILE	CB-CG2	-5.27	1.36	1.52
1	A	236	GLU	CD-OE1	-5.26	1.19	1.25
1	B	207	GLU	C-O	-5.26	1.13	1.23
1	A	167	TYR	CG-CD1	-5.26	1.32	1.39
1	A	224	CYS	CB-SG	-5.25	1.73	1.81
1	A	234	LEU	CG-CD2	-5.25	1.32	1.51
1	B	185	VAL	CA-CB	-5.25	1.43	1.54
1	A	212	ILE	CA-CB	-5.25	1.42	1.54
1	A	176	ARG	CB-CG	-5.25	1.38	1.52
1	A	237	ASP	CB-CG	-5.24	1.40	1.51
1	B	48	THR	CB-CG2	-5.24	1.35	1.52
1	A	248	LYS	CB-CG	-5.24	1.38	1.52
1	A	268	LEU	CG-CD2	-5.23	1.32	1.51
1	A	51	LYS	CE-NZ	-5.22	1.35	1.49
1	A	66	CYS	CB-SG	-5.22	1.73	1.81
1	A	108	PHE	CA-CB	-5.22	1.42	1.53
1	B	323	PHE	CG-CD1	-5.22	1.30	1.38
1	A	266	LEU	CG-CD1	-5.20	1.32	1.51
1	A	36	LEU	CG-CD1	-5.19	1.32	1.51
1	A	48	THR	C-O	-5.19	1.13	1.23
1	A	137	GLN	CG-CD	-5.19	1.39	1.51
1	B	236	GLU	CD-OE1	-5.18	1.20	1.25
1	A	332	VAL	CA-C	-5.18	1.39	1.52
1	B	305	CYS	CB-SG	-5.18	1.73	1.81
1	B	320	TYR	C-O	-5.18	1.13	1.23
2	D	10	TRP	CD2-CE2	-5.18	1.35	1.41
1	A	42	GLY	C-O	-5.17	1.15	1.23
1	A	215	PHE	CG-CD1	-5.17	1.31	1.38
1	A	250	PHE	CG-CD1	-5.17	1.31	1.38
1	B	254	CYS	CB-SG	-5.16	1.73	1.81
1	A	250	PHE	CG-CD2	-5.15	1.31	1.38
1	A	269	ASN	CA-C	-5.15	1.39	1.52
1	A	334	PHE	CG-CD2	-5.15	1.31	1.38
1	B	196	PHE	CG-CD1	-5.15	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	285	ILE	CA-CB	-5.15	1.43	1.54
1	A	319	ILE	CB-CG2	-5.14	1.36	1.52
1	A	196	PHE	CB-CG	-5.14	1.42	1.51
1	A	272	ASP	CB-CG	-5.13	1.41	1.51
1	A	108	PHE	CE2-CZ	-5.12	1.27	1.37
2	D	8	GLY	C-O	-5.11	1.15	1.23
1	B	68	GLN	CG-CD	-5.10	1.39	1.51
1	A	336	PHE	CE1-CZ	-5.10	1.27	1.37
1	B	220	ALA	C-O	-5.09	1.13	1.23
1	B	288	PRO	CA-C	-5.09	1.42	1.52
1	B	186	GLU	CD-OE2	-5.08	1.20	1.25
1	A	323	PHE	CG-CD2	-5.08	1.31	1.38
2	D	10	TRP	CZ3-CH2	-5.08	1.31	1.40
1	A	268	LEU	CG-CD1	-5.08	1.33	1.51
1	A	140	PHE	CB-CG	-5.07	1.42	1.51
1	B	39	LEU	C-O	-5.07	1.13	1.23
1	A	219	THR	CB-CG2	-5.06	1.35	1.52
1	B	267	PHE	CD2-CE2	-5.06	1.29	1.39
1	B	49	ILE	CB-CG2	-5.05	1.37	1.52
1	B	73	VAL	CB-CG1	-5.05	1.42	1.52
1	A	81	ILE	C-O	-5.05	1.13	1.23
1	B	228	SER	CB-OG	-5.05	1.35	1.42
1	B	260	THR	CB-CG2	-5.05	1.35	1.52
1	A	83	ALA	N-CA	-5.05	1.36	1.46
2	D	5	TYR	CD1-CE1	-5.05	1.31	1.39
1	A	215	PHE	CD1-CE1	-5.04	1.29	1.39
1	A	154	TYR	CD2-CE2	-5.04	1.31	1.39
1	A	183	GLY	C-O	-5.04	1.15	1.23
1	A	215	PHE	CG-CD2	-5.03	1.31	1.38
1	B	217	GLY	C-O	-5.03	1.15	1.23
1	B	331	ASN	CA-C	-5.03	1.39	1.52
1	B	78	ILE	CA-CB	-5.03	1.43	1.54
1	B	264	ILE	CA-CB	-5.03	1.43	1.54
2	C	7	HIS	CA-C	-5.01	1.40	1.52
1	A	294	ASN	CB-CG	-5.01	1.39	1.51
1	A	290	TYR	CG-CD1	-5.00	1.32	1.39

All (148) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	110	LEU	O-C-N	-51.45	40.38	122.70
1	A	109	VAL	C-N-CA	-44.44	10.61	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	109	VAL	CA-C-N	-39.37	30.58	117.20
1	B	95	PHE	CB-CA-C	-19.04	72.33	110.40
1	A	110	LEU	CA-C-N	18.78	158.52	117.20
1	A	341	ASP	CB-CA-C	-16.82	76.75	110.40
1	B	152	ALA	CB-CA-C	-16.09	85.97	110.10
1	B	99	ALA	CB-CA-C	-15.18	87.33	110.10
1	B	239	GLU	N-CA-CB	-15.04	83.53	110.60
1	B	105	ARG	CB-CA-C	-13.82	82.77	110.40
1	B	183	GLY	N-CA-C	13.53	146.93	113.10
1	B	105	ARG	N-CA-C	13.38	147.12	111.00
1	B	126	VAL	CB-CA-C	-12.99	86.72	111.40
1	B	107	LEU	CB-CA-C	-12.82	85.85	110.20
1	B	81	ILE	N-CA-CB	-12.40	82.28	110.80
1	A	341	ASP	C-N-CA	12.25	152.32	121.70
1	A	152	ALA	CB-CA-C	-11.78	92.43	110.10
1	A	110	LEU	C-N-CA	11.62	150.75	121.70
1	B	104	ALA	N-CA-CB	11.34	125.98	110.10
1	B	126	VAL	N-CA-C	10.98	140.65	111.00
1	A	109	VAL	O-C-N	-10.83	105.37	122.70
1	A	272	ASP	CB-CG-OD2	10.34	127.60	118.30
1	B	89	GLY	N-CA-C	10.31	138.87	113.10
1	B	95	PHE	N-CA-C	10.11	138.29	111.00
1	B	107	LEU	N-CA-C	9.97	137.93	111.00
1	B	59	ALA	N-CA-CB	9.92	123.98	110.10
1	A	337	ASP	CB-CG-OD2	9.84	127.15	118.30
1	B	81	ILE	C-N-CA	-9.81	97.16	121.70
1	B	152	ALA	N-CA-C	9.54	136.77	111.00
1	A	231	ASP	CB-CG-OD2	9.51	126.86	118.30
1	A	102	ASP	CB-CG-OD2	9.49	126.84	118.30
1	A	328	ASP	CB-CG-OD2	9.35	126.72	118.30
1	B	80	SER	CB-CA-C	-9.32	92.40	110.10
2	C	7	HIS	N-CA-C	-9.27	85.97	111.00
1	B	257	LYS	N-CA-CB	-8.94	94.52	110.60
1	A	193	ASP	CB-CG-OD2	8.86	126.27	118.30
1	B	82	ILE	CB-CA-C	-8.80	94.01	111.60
1	B	165	PRO	N-CD-CG	-8.74	90.09	103.20
1	B	265	ILE	CG1-CB-CG2	-8.74	92.18	111.40
1	A	231	ASP	N-CA-C	8.50	133.96	111.00
1	B	158	ASP	CB-CG-OD2	8.23	125.71	118.30
1	B	272	ASP	CB-CG-OD2	8.22	125.70	118.30
1	B	138	ALA	CB-CA-C	-8.20	97.79	110.10
1	B	237	ASP	CB-CG-OD2	8.21	125.68	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	291	ALA	CB-CA-C	-8.17	97.85	110.10
1	A	334	PHE	N-CA-C	8.08	132.81	111.00
1	A	237	ASP	CB-CG-OD2	7.92	125.42	118.30
1	A	231	ASP	N-CA-CB	-7.89	96.39	110.60
1	B	99	ALA	C-N-CA	-7.89	101.97	121.70
1	B	139	CYS	N-CA-CB	-7.87	96.43	110.60
1	A	344	ILE	O-C-N	-7.68	110.41	122.70
1	A	150	ASP	CB-CG-OD2	7.64	125.18	118.30
1	A	345	LYS	N-CA-C	7.59	131.50	111.00
1	B	100	ARG	N-CA-C	7.59	131.50	111.00
1	B	256	ASN	CB-CA-C	-7.52	95.36	110.40
2	D	9	ILE	CG1-CB-CG2	-7.34	95.26	111.40
1	A	133	ASP	CB-CG-OD2	7.32	124.89	118.30
1	B	100	ARG	N-CA-CB	-7.27	97.51	110.60
1	B	204	GLN	N-CA-C	-7.25	91.42	111.00
1	B	127	ILE	N-CA-CB	-7.18	94.29	110.80
1	B	138	ALA	N-CA-C	7.16	130.34	111.00
1	A	200	ASP	CB-CG-OD2	7.13	124.72	118.30
1	B	239	GLU	CB-CA-C	7.11	124.61	110.40
1	A	239	GLU	N-CA-CB	-7.09	97.84	110.60
1	B	231	ASP	CB-CG-OD2	7.00	124.61	118.30
1	A	334	PHE	CB-CA-C	-6.96	96.47	110.40
1	B	59	ALA	C-N-CA	6.86	136.71	122.30
1	A	344	ILE	CB-CA-C	6.85	125.30	111.60
1	A	249	LEU	CA-CB-CG	6.85	131.05	115.30
1	A	231	ASP	CB-CG-OD1	-6.83	112.16	118.30
1	A	341	ASP	CB-CG-OD2	6.83	124.44	118.30
1	A	144	ARG	NE-CZ-NH1	-6.80	116.90	120.30
1	B	99	ALA	CA-C-N	-6.80	102.25	117.20
1	A	160	ASP	CB-CG-OD2	6.78	124.40	118.30
1	A	181	THR	N-CA-C	-6.73	92.82	111.00
1	B	82	ILE	N-CA-C	6.69	129.07	111.00
1	A	34	VAL	CB-CA-C	6.56	123.86	111.40
1	B	337	ASP	CB-CG-OD2	6.49	124.14	118.30
1	A	234	LEU	CA-CB-CG	6.46	130.17	115.30
1	A	62	SER	N-CA-C	-6.42	93.66	111.00
1	B	152	ALA	C-N-CA	6.40	137.70	121.70
1	A	264	ILE	CB-CA-C	-6.34	98.92	111.60
1	A	282	PRO	N-CD-CG	-6.33	93.70	103.20
2	D	11	VAL	CB-CA-C	-6.32	99.38	111.40
1	A	89	GLY	C-N-CA	6.26	137.34	121.70
1	B	201	VAL	CB-CA-C	-6.22	99.58	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	315	ASP	CB-CG-OD2	6.16	123.84	118.30
1	B	64	GLU	N-CA-C	-6.11	94.51	111.00
1	A	152	ALA	N-CA-C	6.10	127.47	111.00
1	A	110	LEU	N-CA-CB	-6.09	98.21	110.40
1	B	229	ASP	CB-CG-OD2	6.09	123.78	118.30
1	B	91	LEU	CB-CG-CD2	-6.07	100.69	111.00
1	B	99	ALA	N-CA-C	5.97	127.11	111.00
2	C	11	VAL	CB-CA-C	-5.95	100.09	111.40
1	A	66	CYS	CB-CA-C	5.93	122.26	110.40
1	A	161	ARG	NE-CZ-NH2	5.93	123.27	120.30
1	B	184	ILE	N-CA-C	5.91	126.96	111.00
1	B	225	VAL	CB-CA-C	-5.89	100.22	111.40
1	A	158	ASP	CB-CG-OD2	5.88	123.59	118.30
1	B	99	ALA	O-C-N	5.86	132.08	122.70
1	A	335	VAL	N-CA-C	5.83	126.73	111.00
1	B	94	ASP	CB-CG-OD2	5.79	123.51	118.30
1	B	72	VAL	CB-CA-C	-5.77	100.43	111.40
1	B	97	ASP	N-CA-C	-5.77	95.41	111.00
1	A	310	LEU	CB-CG-CD2	-5.76	101.21	111.00
1	A	161	ARG	NE-CZ-NH1	-5.73	117.43	120.30
1	A	233	VAL	CB-CA-C	-5.73	100.52	111.40
1	A	341	ASP	N-CA-C	-5.70	95.61	111.00
1	A	59	ALA	N-CA-CB	-5.68	102.15	110.10
1	A	344	ILE	CA-C-N	5.67	129.69	117.20
1	B	103	ASP	O-C-N	-5.65	113.66	122.70
1	B	261	ASP	CB-CG-OD2	5.65	123.38	118.30
1	A	335	VAL	N-CA-CB	-5.64	99.09	111.50
1	A	315	ASP	CB-CG-OD2	5.60	123.34	118.30
1	A	190	THR	OG1-CB-CG2	-5.57	97.19	110.00
1	A	234	LEU	CB-CG-CD1	-5.57	101.53	111.00
1	A	261	ASP	CB-CG-OD2	5.54	123.29	118.30
1	A	97	ASP	CB-CG-OD2	5.53	123.27	118.30
1	A	38	LEU	CB-CG-CD1	-5.49	101.66	111.00
1	B	194	LEU	CB-CG-CD1	-5.41	101.80	111.00
1	A	98	SER	CA-C-N	-5.40	105.32	117.20
1	A	194	LEU	N-CA-CB	-5.40	99.61	110.40
1	B	282	PRO	N-CD-CG	-5.39	95.12	103.20
1	A	123	LEU	CA-CB-CG	5.37	127.64	115.30
1	B	38	LEU	CB-CG-CD1	-5.36	101.88	111.00
1	B	139	CYS	N-CA-C	5.35	125.44	111.00
1	A	232	LEU	CB-CG-CD1	-5.34	101.92	111.00
1	A	90	ARG	N-CA-CB	-5.34	100.99	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	34	VAL	CB-CA-C	-5.25	101.42	111.40
1	B	125	GLY	N-CA-C	-5.20	100.09	113.10
1	B	159	LEU	CA-CB-CG	-5.18	103.38	115.30
1	A	129	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	A	63	GLU	N-CA-CB	-5.16	101.31	110.60
1	B	104	ALA	N-CA-C	-5.16	97.08	111.00
1	B	328	ASP	CB-CG-OD2	5.16	122.94	118.30
1	B	316	THR	OG1-CB-CG2	-5.14	98.17	110.00
1	A	344	ILE	CG1-CB-CG2	-5.14	100.10	111.40
1	A	251	ASP	CB-CG-OD2	5.11	122.90	118.30
1	B	91	LEU	CA-CB-CG	-5.08	103.61	115.30
1	B	122	GLU	CB-CA-C	-5.07	100.25	110.40
1	B	59	ALA	N-CA-C	-5.07	97.31	111.00
1	A	82	ILE	CB-CA-C	-5.05	101.49	111.60
1	A	284	THR	OG1-CB-CG2	-5.05	98.38	110.00
1	A	221	ILE	CB-CA-C	-5.02	101.55	111.60
1	B	164	GLN	C-N-CD	-5.02	109.55	120.60
1	B	309	ASP	CB-CG-OD2	5.02	122.82	118.30
1	B	249	LEU	CA-CB-CG	5.01	126.82	115.30
1	B	179	VAL	CB-CA-C	-5.00	101.89	111.40

There are no chirality outliers.

All (48) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	109	VAL	Mainchain,Peptide
1	A	110	LEU	Mainchain
1	A	183	GLY	Peptide
1	A	230	TYR	Mainchain
1	A	238	GLU	Mainchain
1	A	254	CYS	Peptide
1	A	256	ASN	Peptide
1	A	268	LEU	Peptide
1	A	272	ASP	Peptide
1	A	304	GLN	Peptide
1	A	33	GLU	Peptide
1	A	330	LYS	Peptide
1	A	333	GLN	Peptide
1	A	341	ASP	Mainchain,Peptide
1	A	88	MET	Peptide
1	A	89	GLY	Peptide
1	B	100	ARG	Peptide

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Mol	Chain	Res	Type	Group
1	B	102	ASP	Peptide
1	B	103	ASP	Peptide
1	B	105	ARG	Peptide
1	B	124	ALA	Peptide
1	B	125	GLY	Peptide
1	B	131	TRP	Peptide
1	B	137	GLN	Peptide
1	B	152	ALA	Peptide
1	B	158	ASP	Peptide
1	B	159	LEU	Peptide
1	B	164	GLN	Peptide
1	B	183	GLY	Peptide
1	B	251	ASP	Peptide
1	B	254	CYS	Peptide
1	B	256	ASN	Peptide
1	B	290	TYR	Peptide
1	B	296	TYR	Peptide
1	B	328	ASP	Peptide
1	B	330	LYS	Peptide
1	B	56	ILE	Peptide
1	B	59	ALA	Peptide
1	B	64	GLU	Peptide
1	B	66	CYS	Peptide
1	B	73	VAL	Peptide
1	B	78	ILE	Peptide
1	B	89	GLY	Peptide
1	B	92	LYS	Peptide
1	B	99	ALA	Mainchain
2	D	12	GLY	Peptide

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	2450	0	2428	273	3
1	B	2450	0	2429	521	0
2	C	96	0	82	11	0
2	D	96	0	82	10	3

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	5	0	0	0	0
3	B	5	0	0	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	28	0	9	1	0
5	B	28	0	8	2	0
6	A	17	0	0	1	0
6	B	12	0	0	0	0
6	C	1	0	0	0	0
All	All	5190	0	5038	815	3

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 80.

All (815) 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:100:ARG:CZ	1:B:129:ARG:HD2	1.19	1.55
1:B:167:TYR:CE1	1:B:169:PRO:HG3	1.51	1.46
1:B:126:VAL:C	1:B:130:LEU:CD1	1.89	1.41
1:B:104:ALA:N	1:B:104:ALA:CA	1.86	1.39
1:B:126:VAL:C	1:B:130:LEU:HD12	1.40	1.36
1:A:110:LEU:O	1:A:110:LEU:HD23	1.24	1.34
1:B:108:PHE:O	1:B:111:ALA:HB2	1.28	1.33
1:B:100:ARG:HH22	1:B:129:ARG:CG	1.40	1.32
1:B:100:ARG:NH2	1:B:129:ARG:NE	1.79	1.29
1:B:64:GLU:O	1:B:67:LYS:HB2	1.34	1.28
1:A:345:LYS:HD3	1:A:345:LYS:N	1.39	1.25
1:B:162:ILE:HB	1:B:167:TYR:CE2	1.72	1.24
1:A:342:VAL:O	1:A:345:LYS:HG2	1.37	1.23
1:A:33:GLU:C	1:A:34:VAL:HG23	1.51	1.22
1:A:63:GLU:HB3	1:A:64:GLU:OE2	1.41	1.20
1:B:167:TYR:HD1	1:B:168:ILE:N	1.38	1.19
1:B:168:ILE:N	1:B:168:ILE:HD12	1.56	1.19
1:B:159:LEU:C	1:B:159:LEU:HD12	1.62	1.17
1:B:159:LEU:HD12	1:B:159:LEU:O	1.41	1.16
1:B:167:TYR:CZ	1:B:169:PRO:HG3	1.81	1.16
1:B:212:ILE:HD12	1:B:212:ILE:N	1.48	1.15
1:A:103:ASP:OD1	1:A:129:ARG:NH2	1.78	1.15
1:B:344:ILE:HG22	1:B:345:LYS:N	1.49	1.15
1:B:110:LEU:H	1:B:110:LEU:CD1	1.44	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:ARG:NH2	1:B:129:ARG:CG	2.04	1.14
1:B:162:ILE:CB	1:B:167:TYR:CE2	2.30	1.14
1:A:345:LYS:N	1:A:345:LYS:CD	1.96	1.14
1:B:126:VAL:O	1:B:130:LEU:HD11	1.44	1.14
1:B:162:ILE:CG2	1:B:167:TYR:CE2	2.30	1.14
1:B:63:GLU:HG2	1:B:64:GLU:OE2	1.47	1.12
1:A:165:PRO:O	1:A:166:ASN:HB2	1.50	1.10
1:B:129:ARG:HG3	1:B:129:ARG:HH11	1.00	1.10
1:B:124:ALA:C	1:B:126:VAL:HG23	1.70	1.10
1:B:126:VAL:O	1:B:130:LEU:CD1	0.81	1.10
1:B:86:ARG:HH11	1:B:86:ARG:HB3	1.04	1.10
1:B:110:LEU:N	1:B:110:LEU:HD12	1.67	1.10
1:A:338:ALA:O	1:A:341:ASP:O	1.69	1.08
1:B:162:ILE:HG22	1:B:167:TYR:CE2	1.86	1.08
1:B:100:ARG:CZ	1:B:129:ARG:CD	1.95	1.07
1:B:81:ILE:HG23	1:B:82:ILE:N	1.60	1.07
1:B:108:PHE:C	1:B:111:ALA:HB2	1.73	1.07
1:B:167:TYR:CE1	1:B:169:PRO:CG	2.36	1.07
1:B:122:GLU:O	1:B:122:GLU:HG3	1.52	1.06
1:A:110:LEU:O	1:A:110:LEU:CD2	2.04	1.06
1:B:159:LEU:HG	1:B:160:ASP:H	1.15	1.06
1:B:97:ASP:OD2	1:B:99:ALA:HB3	1.55	1.05
1:B:86:ARG:HB3	1:B:86:ARG:NH1	1.73	1.04
1:B:78:ILE:HG22	1:B:79:GLN:N	1.68	1.04
1:B:54:LYS:O	1:B:58:GLU:O	1.75	1.04
1:B:108:PHE:O	1:B:111:ALA:CB	2.06	1.04
1:B:168:ILE:HD12	1:B:168:ILE:H	1.05	1.03
1:B:110:LEU:H	1:B:110:LEU:HD12	0.88	1.03
1:B:63:GLU:O	1:B:67:LYS:HG3	1.56	1.02
1:B:162:ILE:HB	1:B:167:TYR:HE2	1.09	1.02
1:B:159:LEU:C	1:B:161:ARG:H	1.62	1.02
1:B:212:ILE:H	1:B:212:ILE:CD1	1.59	1.02
1:B:167:TYR:CE1	1:B:168:ILE:C	2.34	1.01
1:B:100:ARG:O	1:B:103:ASP:HB2	1.61	1.01
1:B:81:ILE:CG2	1:B:82:ILE:H	1.71	1.00
1:A:137:GLN:O	1:A:141:ASN:ND2	1.94	1.00
1:B:105:ARG:O	1:B:109:VAL:CG2	2.09	1.00
1:B:167:TYR:CD1	1:B:168:ILE:N	2.30	1.00
1:A:52:GLN:O	1:A:56:ILE:HG13	1.62	0.99
1:B:71:ALA:O	1:B:74:TYR:HB2	1.63	0.99
1:B:81:ILE:HG23	1:B:82:ILE:H	0.85	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:GLN:HE21	1:B:68:GLN:N	1.60	0.98
1:B:100:ARG:HA	1:B:103:ASP:OD2	1.62	0.98
1:A:269:ASN:O	1:A:270:LYS:HB2	1.62	0.98
1:A:96:GLY:N	1:A:133:ASP:OD2	1.96	0.97
1:A:74:TYR:O	1:A:78:ILE:HG13	1.64	0.97
1:A:33:GLU:C	1:A:34:VAL:CG2	2.30	0.97
1:A:228:SER:O	1:A:277:LYS:NZ	1.97	0.96
1:B:124:ALA:O	1:B:127:ILE:N	1.98	0.96
1:B:78:ILE:HG22	1:B:79:GLN:CA	1.96	0.95
1:B:86:ARG:NH1	1:B:86:ARG:CB	2.29	0.95
1:A:344:ILE:C	1:A:345:LYS:HD3	1.87	0.95
1:B:100:ARG:NH2	1:B:129:ARG:HD3	1.38	0.95
1:B:126:VAL:O	1:B:130:LEU:CG	2.15	0.94
1:B:159:LEU:HG	1:B:160:ASP:N	1.72	0.94
1:B:124:ALA:O	1:B:126:VAL:HG23	1.64	0.94
1:A:245:GLU:O	1:A:245:GLU:HG3	1.65	0.94
1:A:62:SER:OG	1:A:65:GLU:HB2	1.68	0.94
1:B:86:ARG:HH11	1:B:86:ARG:CB	1.81	0.94
1:B:131:TRP:NE1	1:B:157:ASN:OD1	2.01	0.94
1:B:344:ILE:HG22	1:B:345:LYS:H	1.24	0.93
1:B:82:ILE:O	1:B:82:ILE:HG22	1.68	0.93
1:B:167:TYR:CD1	1:B:167:TYR:C	2.38	0.93
1:B:167:TYR:HE1	1:B:168:ILE:C	1.71	0.92
1:A:62:SER:H	1:A:65:GLU:HB2	1.35	0.92
1:B:85:ILE:HA	1:B:88:MET:HG3	1.49	0.91
1:A:70:LYS:HE3	1:A:167:TYR:O	1.71	0.91
1:A:108:PHE:O	1:A:109:VAL:O	1.87	0.91
1:B:332:VAL:O	1:B:332:VAL:HG12	1.69	0.90
1:A:139:CYS:O	1:A:146:TYR:OH	1.88	0.90
2:D:6:TYR:CE2	2:D:7:HIS:ND1	2.39	0.90
1:A:103:ASP:CG	1:A:129:ARG:HH21	1.75	0.90
1:B:100:ARG:HH21	1:B:129:ARG:NE	1.51	0.89
1:B:100:ARG:HH22	1:B:129:ARG:HD3	0.90	0.89
1:A:52:GLN:C	1:A:54:LYS:H	1.76	0.88
1:A:57:HIS:O	1:A:58:GLU:HG2	1.73	0.87
1:B:162:ILE:HG22	1:B:167:TYR:CZ	2.07	0.87
1:A:33:GLU:O	1:A:34:VAL:HG23	1.73	0.87
1:B:93:ILE:O	1:B:93:ILE:HG22	1.73	0.87
1:B:102:ASP:O	1:B:105:ARG:HB2	1.75	0.87
1:B:170:THR:O	1:B:173:ASP:N	2.07	0.86
1:B:159:LEU:CG	1:B:160:ASP:N	2.33	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:ARG:HG3	1:B:129:ARG:NH1	1.76	0.86
1:B:174:VAL:HG12	1:B:174:VAL:O	1.75	0.86
1:B:78:ILE:HG22	1:B:79:GLN:HA	1.58	0.86
1:B:256:ASN:OD1	1:B:257:LYS:N	2.08	0.85
1:A:63:GLU:O	1:A:67:LYS:HG3	1.75	0.85
1:A:278:ILE:O	1:A:278:ILE:HG13	1.75	0.85
2:D:11:VAL:HG23	2:D:12:GLY:O	1.77	0.85
1:B:73:VAL:HG12	1:B:73:VAL:O	1.74	0.85
1:B:159:LEU:C	1:B:161:ARG:N	2.28	0.85
1:B:52:GLN:O	1:B:56:ILE:CG1	2.25	0.85
1:B:257:LYS:HG2	1:B:258:TRP:N	1.92	0.85
1:B:36:LEU:HD23	1:B:198:MET:HG3	1.59	0.85
1:B:87:ALA:O	1:B:91:LEU:HB2	1.77	0.85
1:B:167:TYR:HD1	1:B:167:TYR:C	1.76	0.85
1:B:81:ILE:CG2	1:B:82:ILE:N	2.30	0.84
1:A:299:ALA:O	1:A:303:ILE:HG13	1.77	0.84
1:A:49:ILE:HG22	1:A:49:ILE:O	1.77	0.84
1:A:192:LYS:O	1:A:193:ASP:HB2	1.77	0.84
1:B:134:SER:O	1:B:138:ALA:CB	2.26	0.83
1:B:167:TYR:CE1	1:B:168:ILE:O	2.30	0.83
1:B:228:SER:O	1:B:277:LYS:NZ	2.10	0.83
1:B:99:ALA:HB3	1:B:100:ARG:HD2	1.58	0.83
1:B:104:ALA:O	1:B:107:LEU:HB2	1.78	0.83
1:B:97:ASP:OD2	1:B:100:ARG:HD2	1.77	0.83
1:A:283:LEU:C	1:A:285:ILE:H	1.82	0.83
1:B:168:ILE:H	1:B:168:ILE:CD1	1.85	0.83
1:B:62:SER:O	1:B:65:GLU:HB2	1.79	0.82
1:B:100:ARG:HD2	1:B:100:ARG:N	1.95	0.82
1:B:142:ARG:HH21	1:B:145:GLU:CD	1.82	0.82
1:B:282:PRO:O	1:B:285:ILE:HG13	1.80	0.82
1:B:57:HIS:O	1:B:58:GLU:HG2	1.79	0.82
1:B:102:ASP:O	1:B:104:ALA:HB3	1.80	0.81
1:B:126:VAL:O	1:B:130:LEU:HD12	1.03	0.81
1:B:123:LEU:O	1:B:126:VAL:CG2	2.29	0.81
1:B:343:ILE:HG22	1:B:343:ILE:O	1.81	0.81
1:B:247:MET:HE1	1:B:287:TYR:CE1	2.16	0.81
2:D:11:VAL:HG23	2:D:11:VAL:O	1.76	0.81
1:B:105:ARG:O	1:B:109:VAL:HG23	1.81	0.80
1:B:162:ILE:CB	1:B:167:TYR:HE2	1.78	0.80
1:B:162:ILE:HA	1:B:167:TYR:CD2	2.17	0.80
1:B:52:GLN:O	1:B:56:ILE:HG13	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:TYR:CD1	1:B:168:ILE:C	2.55	0.80
1:B:162:ILE:HB	1:B:167:TYR:CD2	2.16	0.80
1:B:247:MET:HE1	1:B:287:TYR:HE1	1.47	0.80
1:B:57:HIS:O	1:B:58:GLU:CG	2.29	0.80
1:A:283:LEU:O	1:A:285:ILE:N	2.14	0.80
1:B:97:ASP:OD2	1:B:99:ALA:CB	2.30	0.80
1:B:100:ARG:O	1:B:103:ASP:CB	2.30	0.80
1:B:124:ALA:HA	1:B:127:ILE:HG13	1.63	0.80
1:A:62:SER:OG	1:A:65:GLU:CG	2.30	0.80
1:B:59:ALA:CB	1:B:60:GLY:O	2.30	0.80
1:B:66:CYS:O	1:B:169:PRO:HD2	1.82	0.80
1:A:109:VAL:HG12	1:A:110:LEU:CA	2.12	0.80
1:B:59:ALA:HB1	1:B:60:GLY:O	1.80	0.79
1:A:33:GLU:O	1:A:34:VAL:CG2	2.30	0.79
1:B:100:ARG:HH22	1:B:129:ARG:CD	0.21	0.79
1:B:124:ALA:O	1:B:126:VAL:CG2	2.30	0.79
1:B:100:ARG:CA	1:B:103:ASP:OD2	2.29	0.79
1:A:122:GLU:O	1:A:122:GLU:HG2	1.79	0.79
1:B:167:TYR:HE1	1:B:169:PRO:N	1.81	0.79
1:B:97:ASP:OD2	1:B:100:ARG:CD	2.30	0.79
1:A:62:SER:OG	1:A:65:GLU:CB	2.30	0.79
1:A:303:ILE:C	1:A:305:CYS:H	1.86	0.79
1:B:124:ALA:O	1:B:126:VAL:CB	2.30	0.79
1:A:57:HIS:O	1:A:58:GLU:CG	2.30	0.79
1:B:124:ALA:O	1:B:127:ILE:CG1	2.30	0.79
1:B:343:ILE:O	1:B:343:ILE:CG2	2.30	0.78
1:A:122:GLU:O	1:A:122:GLU:CG	2.30	0.78
1:B:73:VAL:O	1:B:73:VAL:CG1	2.31	0.78
1:B:68:GLN:N	1:B:68:GLN:NE2	2.30	0.78
1:B:124:ALA:O	1:B:126:VAL:CA	2.30	0.78
1:B:130:LEU:O	1:B:136:VAL:HG21	1.84	0.78
1:B:332:VAL:O	1:B:332:VAL:CG1	2.30	0.78
1:B:134:SER:O	1:B:138:ALA:HB2	1.83	0.78
1:B:61:TYR:HB2	1:B:171:GLN:NE2	1.99	0.77
1:B:307:PHE:C	1:B:309:ASP:H	1.87	0.77
1:A:63:GLU:CB	1:A:64:GLU:OE2	2.29	0.77
1:B:97:ASP:CG	1:B:99:ALA:HB3	2.04	0.77
1:B:167:TYR:HE1	1:B:169:PRO:CG	1.92	0.77
1:B:63:GLU:CG	1:B:64:GLU:OE2	2.30	0.77
1:B:126:VAL:C	1:B:130:LEU:HD13	1.77	0.77
1:B:104:ALA:O	1:B:107:LEU:CB	2.33	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:ASP:C	1:B:104:ALA:CA	2.52	0.77
1:B:107:LEU:O	1:B:111:ALA:HA	1.85	0.77
1:A:97:ASP:C	1:A:99:ALA:H	1.87	0.77
1:A:101:ALA:O	1:A:105:ARG:HG3	1.85	0.77
2:C:6:TYR:HD2	2:C:6:TYR:O	1.68	0.76
1:A:93:ILE:HG22	1:A:94:ASP:H	1.49	0.76
1:B:103:ASP:N	1:B:106:GLN:HG3	1.99	0.76
1:B:167:TYR:HE1	1:B:169:PRO:CA	1.98	0.76
1:A:123:LEU:O	1:A:127:ILE:HG13	1.84	0.76
1:B:162:ILE:CA	1:B:167:TYR:CD2	2.69	0.76
1:B:124:ALA:O	1:B:127:ILE:HG13	1.85	0.76
1:B:123:LEU:O	1:B:126:VAL:HG23	1.86	0.76
1:B:282:PRO:O	1:B:282:PRO:HG2	1.85	0.76
1:B:174:VAL:O	1:B:174:VAL:CG1	2.33	0.75
1:A:52:GLN:C	1:A:54:LYS:N	2.34	0.75
1:B:63:GLU:O	1:B:67:LYS:CG	2.33	0.75
1:B:192:LYS:O	1:B:193:ASP:HB2	1.86	0.75
1:A:313:ARG:C	1:A:315:ASP:H	1.87	0.75
1:B:49:ILE:O	1:B:49:ILE:HG22	1.85	0.75
1:B:86:ARG:HH12	1:B:90:ARG:NH1	1.84	0.75
1:A:260:THR:O	1:A:260:THR:CG2	2.29	0.74
1:B:68:GLN:HE21	1:B:68:GLN:H	1.35	0.74
1:B:97:ASP:HB3	1:B:100:ARG:HG2	1.67	0.74
1:B:311:ASN:O	1:B:314:LYS:HE3	1.87	0.74
1:B:162:ILE:CB	1:B:167:TYR:CD2	2.70	0.74
1:B:234:LEU:HD23	1:B:242:ARG:HG2	1.69	0.74
1:A:234:LEU:HD23	1:A:242:ARG:HG2	1.69	0.74
1:A:343:ILE:O	1:A:344:ILE:C	2.23	0.74
1:A:52:GLN:O	1:A:56:ILE:CG1	2.35	0.74
1:A:82:ILE:HG22	1:A:82:ILE:O	1.80	0.73
1:B:49:ILE:O	1:B:49:ILE:CG2	2.34	0.73
1:B:72:VAL:C	1:B:74:TYR:H	1.89	0.73
1:B:167:TYR:HD1	1:B:168:ILE:CA	2.00	0.73
1:B:125:GLY:O	1:B:129:ARG:HB2	1.87	0.73
1:B:212:ILE:HD12	1:B:212:ILE:H	0.67	0.73
1:B:100:ARG:NH2	1:B:129:ARG:CD	0.80	0.73
1:A:332:VAL:HG12	1:A:332:VAL:O	1.85	0.72
1:B:342:VAL:C	1:B:344:ILE:H	1.91	0.72
1:B:134:SER:C	1:B:136:VAL:H	1.89	0.72
1:B:167:TYR:CD1	1:B:168:ILE:O	2.42	0.72
1:A:165:PRO:O	1:A:166:ASN:CB	2.30	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:GLY:N	1:B:126:VAL:HG23	2.05	0.71
1:A:126:VAL:CG1	1:A:126:VAL:O	2.34	0.71
1:B:61:TYR:HA	1:B:65:GLU:OE1	1.90	0.71
1:B:97:ASP:HB3	1:B:100:ARG:CG	2.20	0.71
1:A:269:ASN:O	1:A:270:LYS:CB	2.30	0.71
1:B:283:LEU:HG	1:B:283:LEU:O	1.88	0.71
1:B:52:GLN:O	1:B:56:ILE:HG12	1.89	0.71
1:B:88:MET:HE3	1:B:93:ILE:CG2	2.21	0.71
1:B:103:ASP:O	1:B:104:ALA:O	2.08	0.71
1:B:58:GLU:O	1:B:59:ALA:C	2.26	0.71
1:B:108:PHE:CA	1:B:111:ALA:HB2	2.19	0.71
1:A:272:ASP:OD2	5:A:355:GDP:N2	2.15	0.71
1:B:63:GLU:C	1:B:64:GLU:OE2	2.29	0.71
1:B:77:THR:O	1:B:78:ILE:C	2.29	0.70
1:B:124:ALA:CA	1:B:127:ILE:HG13	2.21	0.70
1:A:126:VAL:O	1:A:126:VAL:HG12	1.85	0.70
1:B:91:LEU:O	1:B:92:LYS:HB2	1.91	0.70
1:A:343:ILE:O	1:A:345:LYS:N	2.25	0.70
1:B:34:VAL:HG12	1:B:34:VAL:O	1.90	0.70
1:B:61:TYR:HB2	1:B:171:GLN:HE22	1.56	0.70
1:A:207:GLU:C	1:A:209:LYS:H	1.95	0.70
1:A:82:ILE:O	1:A:82:ILE:CG2	2.33	0.70
1:B:62:SER:C	1:B:64:GLU:H	1.94	0.70
1:B:110:LEU:CD1	1:B:110:LEU:N	2.29	0.70
1:B:167:TYR:CD1	1:B:168:ILE:CA	2.74	0.70
2:C:6:TYR:O	2:C:6:TYR:CD2	2.44	0.69
1:B:103:ASP:O	1:B:104:ALA:C	2.31	0.69
1:B:52:GLN:NE2	1:B:326:ALA:O	2.23	0.69
1:B:110:LEU:O	1:B:111:ALA:C	2.30	0.69
1:B:159:LEU:O	1:B:161:ARG:N	2.24	0.69
1:B:47:SER:OG	5:B:355:GDP:O3B	2.10	0.69
1:A:49:ILE:O	1:A:49:ILE:CG2	2.37	0.69
1:B:100:ARG:C	1:B:102:ASP:H	1.93	0.69
1:B:294:ASN:CG	1:B:294:ASN:O	2.30	0.69
1:B:97:ASP:HB3	1:B:100:ARG:CD	2.24	0.68
1:B:251:ASP:O	1:B:255:ASN:HB2	1.92	0.68
1:A:333:GLN:HG2	1:A:334:PHE:N	2.04	0.68
1:B:329:THR:HG22	1:B:329:THR:O	1.93	0.68
1:B:85:ILE:C	1:B:87:ALA:N	2.37	0.68
1:B:100:ARG:HH21	1:B:129:ARG:CD	1.33	0.68
1:B:97:ASP:O	1:B:100:ARG:HG2	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:ASP:OD1	1:B:237:ASP:C	2.30	0.68
1:B:54:LYS:O	1:B:58:GLU:C	2.32	0.68
1:A:260:THR:O	1:A:260:THR:HG22	1.90	0.67
1:B:85:ILE:O	1:B:86:ARG:C	2.30	0.67
1:B:87:ALA:O	1:B:88:MET:C	2.30	0.67
1:B:191:PHE:C	1:B:193:ASP:H	1.98	0.67
1:B:307:PHE:O	1:B:309:ASP:N	2.28	0.67
1:A:294:ASN:C	1:A:295:THR:HG23	2.14	0.67
1:B:57:HIS:C	1:B:58:GLU:HG3	2.14	0.67
1:B:69:TYR:O	1:B:70:LYS:C	2.31	0.67
1:B:82:ILE:O	1:B:82:ILE:CG2	2.36	0.67
1:A:93:ILE:HG22	1:A:94:ASP:N	2.09	0.67
1:B:167:TYR:OH	1:B:169:PRO:HB3	1.94	0.67
1:B:314:LYS:O	1:B:315:ASP:C	2.30	0.67
1:A:54:LYS:HG3	1:A:54:LYS:O	1.95	0.66
1:B:86:ARG:HH12	1:B:90:ARG:HH12	1.40	0.66
1:B:126:VAL:CA	1:B:130:LEU:HD12	2.25	0.66
1:B:140:PHE:CG	1:B:140:PHE:O	2.48	0.66
1:B:85:ILE:O	1:B:87:ALA:N	2.28	0.66
1:B:105:ARG:O	1:B:109:VAL:HG21	1.92	0.66
1:A:64:GLU:OE2	1:A:64:GLU:N	2.29	0.66
1:B:124:ALA:O	1:B:126:VAL:N	2.29	0.66
1:B:127:ILE:O	1:B:130:LEU:N	2.29	0.66
1:B:64:GLU:OE2	1:B:64:GLU:N	2.29	0.66
1:B:109:VAL:HB	1:B:110:LEU:HD12	1.78	0.66
1:B:156:LEU:O	1:B:158:ASP:N	2.29	0.66
1:B:342:VAL:C	1:B:344:ILE:N	2.46	0.66
1:B:53:MET:O	1:B:57:HIS:HB2	1.95	0.65
1:B:64:GLU:HA	1:B:67:LYS:HG3	1.78	0.65
1:B:301:ALA:O	1:B:302:TYR:C	2.29	0.65
1:A:303:ILE:C	1:A:305:CYS:N	2.45	0.65
1:B:101:ALA:O	1:B:104:ALA:CB	2.45	0.65
1:B:142:ARG:NH2	1:B:145:GLU:OE2	2.29	0.65
1:B:159:LEU:C	1:B:159:LEU:CD1	2.28	0.65
1:B:289:GLU:C	1:B:290:TYR:O	2.29	0.65
1:B:311:ASN:OD1	1:B:312:LYS:N	2.29	0.65
1:A:207:GLU:C	1:A:209:LYS:N	2.46	0.65
1:B:62:SER:O	1:B:64:GLU:N	2.30	0.65
1:B:139:CYS:O	1:B:141:ASN:N	2.29	0.65
1:B:142:ARG:O	1:B:144:ARG:N	2.29	0.65
1:B:159:LEU:O	1:B:162:ILE:N	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:ASP:OD1	1:B:105:ARG:NH1	2.30	0.65
1:A:85:ILE:O	1:A:87:ALA:N	2.30	0.65
1:A:130:LEU:O	1:A:132:LYS:N	2.30	0.65
1:A:313:ARG:O	1:A:315:ASP:N	2.30	0.65
1:B:63:GLU:N	1:B:64:GLU:OE2	2.30	0.65
1:B:65:GLU:O	1:B:67:LYS:N	2.28	0.65
1:B:191:PHE:O	1:B:193:ASP:N	2.30	0.65
1:B:142:ARG:NH2	1:B:145:GLU:OE1	2.30	0.64
1:B:342:VAL:O	1:B:344:ILE:N	2.30	0.64
1:B:57:HIS:C	1:B:58:GLU:CG	2.64	0.64
1:A:52:GLN:O	1:A:54:LYS:N	2.30	0.64
1:A:303:ILE:O	1:A:305:CYS:N	2.30	0.64
1:B:64:GLU:O	1:B:68:GLN:NE2	2.31	0.64
1:A:329:THR:HG22	1:A:329:THR:O	1.98	0.64
1:A:65:GLU:O	1:A:67:LYS:N	2.29	0.64
1:B:85:ILE:O	1:B:88:MET:N	2.30	0.64
1:B:123:LEU:O	1:B:124:ALA:C	2.33	0.64
1:B:104:ALA:N	1:B:104:ALA:C	2.49	0.64
1:B:134:SER:O	1:B:136:VAL:N	2.30	0.64
1:A:72:VAL:O	1:A:74:TYR:N	2.30	0.64
1:A:160:ASP:O	1:A:164:GLN:HG3	1.97	0.64
1:B:48:THR:HG22	1:B:48:THR:O	1.98	0.64
1:B:148:LEU:O	1:B:149:ASN:C	2.30	0.64
1:B:158:ASP:OD2	1:B:161:ARG:NH2	2.30	0.64
1:B:162:ILE:CG2	1:B:167:TYR:CZ	2.76	0.64
1:B:277:LYS:O	1:B:279:LYS:N	2.31	0.64
1:A:72:VAL:O	1:A:73:VAL:C	2.30	0.63
1:A:313:ARG:C	1:A:315:ASP:N	2.51	0.63
1:A:343:ILE:C	1:A:345:LYS:N	2.51	0.63
1:B:78:ILE:HG23	1:B:82:ILE:HG13	1.79	0.63
1:B:225:VAL:HG12	1:B:226:ALA:N	2.09	0.63
1:B:100:ARG:O	1:B:102:ASP:N	2.32	0.63
1:B:109:VAL:HB	1:B:110:LEU:CD1	2.29	0.63
2:C:6:TYR:HD2	2:C:7:HIS:HD1	1.45	0.63
1:A:253:ILE:C	1:A:255:ASN:H	2.00	0.63
1:A:340:THR:OG1	1:A:341:ASP:N	2.30	0.63
1:B:100:ARG:N	1:B:100:ARG:CD	2.50	0.63
1:A:161:ARG:HH11	1:A:161:ARG:CG	2.12	0.63
1:B:158:ASP:OD2	1:B:161:ARG:NE	2.30	0.63
1:B:167:TYR:CZ	1:B:169:PRO:CG	2.70	0.63
1:B:293:SER:OG	1:B:294:ASN:N	2.30	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:GLN:NE2	1:A:326:ALA:O	2.30	0.63
1:B:96:GLY:O	1:B:98:SER:N	2.32	0.63
1:B:331:ASN:O	1:B:333:GLN:N	2.32	0.63
1:B:134:SER:O	1:B:138:ALA:HB3	1.97	0.62
1:B:143:SER:O	1:B:145:GLU:N	2.31	0.62
1:A:294:ASN:OD1	1:A:294:ASN:N	2.29	0.62
1:B:81:ILE:O	1:B:82:ILE:C	2.32	0.62
1:B:100:ARG:NH1	1:B:129:ARG:CD	2.58	0.62
1:A:302:TYR:O	1:A:305:CYS:HB3	1.99	0.62
1:A:272:ASP:OD1	1:A:272:ASP:N	2.31	0.62
1:A:136:VAL:HG12	1:A:136:VAL:O	1.99	0.62
1:A:332:VAL:O	1:A:332:VAL:CG1	2.46	0.62
1:B:142:ARG:O	1:B:143:SER:C	2.36	0.62
1:B:153:ALA:O	1:B:154:TYR:C	2.29	0.62
1:B:253:ILE:O	1:B:254:CYS:C	2.30	0.62
1:B:127:ILE:O	1:B:130:LEU:HB2	2.00	0.62
1:B:207:GLU:OE1	1:B:210:LYS:NZ	2.30	0.62
1:A:109:VAL:CG1	1:A:110:LEU:CA	2.74	0.62
1:B:42:GLY:N	1:B:203:GLY:O	2.32	0.62
1:B:134:SER:C	1:B:136:VAL:N	2.45	0.62
1:B:88:MET:HE3	1:B:93:ILE:HG21	1.81	0.61
1:B:63:GLU:O	1:B:63:GLU:HG3	2.01	0.61
1:B:72:VAL:C	1:B:74:TYR:N	2.43	0.61
1:B:225:VAL:CG1	1:B:226:ALA:N	2.59	0.61
1:A:62:SER:OG	1:A:65:GLU:HG3	1.99	0.61
1:A:264:ILE:HD13	1:A:264:ILE:N	2.14	0.61
1:A:264:ILE:HG22	1:A:264:ILE:O	1.88	0.61
1:B:135:GLY:C	1:B:138:ALA:HB3	2.21	0.61
1:A:33:GLU:CA	1:A:34:VAL:HG23	2.28	0.61
1:A:84:ILE:O	1:A:85:ILE:C	2.30	0.61
1:A:161:ARG:NH2	1:A:173:ASP:OD1	2.33	0.61
1:A:277:LYS:C	1:A:279:LYS:H	2.04	0.61
1:A:302:TYR:O	1:A:305:CYS:CB	2.48	0.61
1:B:126:VAL:HG12	1:B:130:LEU:HD11	1.83	0.61
1:B:127:ILE:O	1:B:131:TRP:N	2.30	0.61
1:B:191:PHE:C	1:B:193:ASP:N	2.52	0.61
1:A:57:HIS:C	1:A:58:GLU:CG	2.65	0.61
1:B:129:ARG:CG	1:B:129:ARG:NH1	2.53	0.61
1:B:278:ILE:O	1:B:278:ILE:HG13	1.98	0.61
1:A:149:ASN:N	1:A:149:ASN:OD1	2.29	0.61
1:A:325:CYS:O	1:A:327:THR:N	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:ILE:C	1:B:87:ALA:H	2.03	0.61
1:B:308:GLU:HG3	1:B:319:ILE:HB	1.83	0.61
1:B:124:ALA:O	1:B:127:ILE:HG12	2.00	0.60
1:A:97:ASP:C	1:A:99:ALA:N	2.53	0.60
1:A:277:LYS:O	1:A:279:LYS:N	2.34	0.60
1:A:241:ASN:HB3	1:A:244:HIS:HB2	1.82	0.60
1:B:95:PHE:O	1:B:96:GLY:C	2.36	0.60
1:A:109:VAL:HG12	1:A:110:LEU:HA	1.79	0.60
1:B:91:LEU:O	1:B:92:LYS:CB	2.49	0.60
1:A:65:GLU:O	1:A:66:CYS:C	2.40	0.60
1:A:109:VAL:HG12	1:A:110:LEU:CB	2.30	0.60
1:A:221:ILE:HG22	1:A:222:ILE:N	2.17	0.60
1:A:249:LEU:O	1:A:250:PHE:C	2.36	0.60
1:B:65:GLU:C	1:B:67:LYS:H	2.03	0.60
1:B:311:ASN:OD1	1:B:311:ASN:C	2.33	0.60
1:A:81:ILE:HG13	1:A:81:ILE:O	2.02	0.60
1:B:336:PHE:O	1:B:340:THR:OG1	2.19	0.60
1:B:212:ILE:N	1:B:212:ILE:CD1	2.29	0.59
1:A:294:ASN:C	1:A:295:THR:CG2	2.66	0.59
1:A:36:LEU:HD22	1:A:37:LEU:N	2.18	0.59
1:A:61:TYR:HB2	1:A:171:GLN:NE2	2.18	0.59
1:B:78:ILE:CG2	1:B:82:ILE:HG13	2.31	0.59
1:B:163:ALA:O	1:B:165:PRO:CD	2.51	0.59
1:A:275:GLU:HB2	1:A:296:TYR:CD1	2.38	0.59
1:B:81:ILE:HA	1:B:84:ILE:HG13	1.84	0.59
1:B:272:ASP:CG	1:B:273:LEU:H	2.05	0.59
1:B:344:ILE:O	1:B:345:LYS:C	2.30	0.59
1:B:97:ASP:OD2	1:B:100:ARG:HD3	2.02	0.58
1:A:70:LYS:CE	1:A:167:TYR:O	2.50	0.58
1:B:86:ARG:NH1	1:B:86:ARG:HB2	2.18	0.58
1:B:100:ARG:C	1:B:102:ASP:N	2.55	0.58
2:C:7:HIS:O	2:C:9:ILE:HG13	2.03	0.58
1:A:62:SER:HG	1:A:65:GLU:CD	2.06	0.58
1:B:164:GLN:C	1:B:165:PRO:O	2.39	0.58
1:B:170:THR:O	1:B:171:GLN:C	2.40	0.58
1:A:37:LEU:HD12	1:A:199:PHE:HB2	1.85	0.58
1:B:59:ALA:HB3	1:B:60:GLY:O	2.02	0.58
1:B:88:MET:HB3	1:B:93:ILE:HG21	1.84	0.58
1:B:123:LEU:O	1:B:123:LEU:HD12	2.03	0.58
1:B:163:ALA:O	1:B:164:GLN:C	2.39	0.58
1:A:336:PHE:O	1:A:340:THR:HG23	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:LEU:C	1:B:132:LYS:H	2.07	0.58
1:B:139:CYS:C	1:B:141:ASN:H	2.05	0.58
1:B:102:ASP:C	1:B:104:ALA:HB3	2.24	0.58
1:B:156:LEU:C	1:B:158:ASP:H	2.06	0.58
1:B:71:ALA:HA	1:B:74:TYR:HD2	1.69	0.58
1:A:191:PHE:C	1:A:193:ASP:H	2.06	0.57
1:B:54:LYS:O	1:B:58:GLU:N	2.36	0.57
1:B:88:MET:HB3	1:B:93:ILE:CG2	2.35	0.57
2:D:13:GLU:OE2	2:D:13:GLU:N	2.30	0.57
1:B:102:ASP:O	1:B:105:ARG:CB	2.52	0.57
1:A:61:TYR:H	1:A:171:GLN:HE22	1.53	0.57
1:B:100:ARG:HH21	1:B:129:ARG:HD2	0.94	0.57
1:B:107:LEU:O	1:B:107:LEU:HD12	2.04	0.57
1:A:190:THR:HA	1:A:194:LEU:O	2.04	0.57
1:B:139:CYS:C	1:B:141:ASN:N	2.54	0.57
1:A:130:LEU:O	1:A:131:TRP:C	2.37	0.57
1:A:203:GLY:O	1:A:208:ARG:NE	2.37	0.57
1:A:42:GLY:O	1:A:43:GLU:HB2	2.04	0.57
1:B:62:SER:C	1:B:64:GLU:N	2.57	0.57
1:B:63:GLU:CA	1:B:64:GLU:OE2	2.52	0.57
1:B:126:VAL:HB	1:B:127:ILE:HG12	1.87	0.57
1:A:301:ALA:O	1:A:305:CYS:HB2	2.05	0.56
1:A:234:LEU:O	1:A:237:ASP:C	2.43	0.56
1:A:48:THR:O	1:A:48:THR:HG22	2.06	0.56
1:A:57:HIS:C	1:A:58:GLU:HG3	2.25	0.56
1:A:253:ILE:O	1:A:255:ASN:N	2.37	0.56
1:B:127:ILE:CA	1:B:130:LEU:HB2	2.35	0.56
1:A:133:ASP:C	1:A:135:GLY:H	2.09	0.56
2:C:11:VAL:HG23	2:C:12:GLY:N	2.21	0.56
1:B:131:TRP:HE3	1:B:131:TRP:HA	1.70	0.56
1:A:283:LEU:C	1:A:285:ILE:N	2.41	0.56
1:B:54:LYS:NZ	1:B:59:ALA:CB	2.68	0.56
1:B:123:LEU:O	1:B:126:VAL:HG21	2.03	0.56
1:B:142:ARG:NE	1:B:145:GLU:OE2	2.36	0.56
1:B:191:PHE:O	1:B:192:LYS:C	2.44	0.56
1:B:96:GLY:O	1:B:97:ASP:C	2.41	0.55
1:B:59:ALA:HB1	1:B:60:GLY:C	2.25	0.55
1:B:62:SER:N	1:B:65:GLU:OE1	2.40	0.55
1:B:100:ARG:HH21	1:B:129:ARG:HE	1.47	0.55
1:B:123:LEU:C	1:B:126:VAL:HG23	2.27	0.55
1:A:342:VAL:HG12	1:A:343:ILE:N	2.19	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:ASP:CG	1:B:99:ALA:CB	2.74	0.55
1:B:131:TRP:HA	1:B:131:TRP:CE3	2.39	0.55
1:B:100:ARG:CZ	1:B:129:ARG:HD3	2.01	0.55
1:B:124:ALA:C	1:B:127:ILE:HG13	2.27	0.55
1:A:203:GLY:O	1:A:204:GLN:C	2.39	0.55
1:B:100:ARG:C	1:B:103:ASP:OD2	2.45	0.55
1:B:218:VAL:O	1:B:262:THR:OG1	2.23	0.55
1:A:130:LEU:C	1:A:132:LYS:N	2.59	0.55
1:A:133:ASP:C	1:A:135:GLY:N	2.52	0.55
1:A:133:ASP:O	1:A:134:SER:C	2.40	0.55
1:B:100:ARG:NH2	1:B:129:ARG:CB	2.70	0.55
1:B:253:ILE:O	1:B:255:ASN:N	2.40	0.55
1:A:54:LYS:HG2	1:A:55:ILE:N	2.20	0.54
1:A:191:PHE:C	1:A:193:ASP:N	2.57	0.54
1:B:108:PHE:HA	1:B:111:ALA:HB2	1.89	0.54
1:A:203:GLY:C	1:A:204:GLN:O	2.35	0.54
1:B:84:ILE:O	1:B:87:ALA:HB3	2.06	0.54
1:B:127:ILE:HA	1:B:130:LEU:HB2	1.88	0.54
1:A:69:TYR:O	1:A:71:ALA:N	2.41	0.54
1:B:142:ARG:NH2	1:B:145:GLU:CD	2.59	0.54
1:A:153:ALA:O	1:A:157:ASN:HB2	2.08	0.54
1:B:102:ASP:O	1:B:103:ASP:O	2.26	0.54
1:B:167:TYR:CE1	1:B:169:PRO:CA	2.87	0.54
1:B:64:GLU:CA	1:B:67:LYS:HG3	2.37	0.54
1:B:155:TYR:OH	1:B:173:ASP:O	2.25	0.54
1:B:250:PHE:O	1:B:251:ASP:C	2.41	0.54
1:B:67:LYS:C	1:B:68:GLN:HE21	2.11	0.54
1:B:69:TYR:O	1:B:71:ALA:N	2.41	0.54
1:B:97:ASP:HB3	1:B:100:ARG:HD3	1.90	0.54
1:B:272:ASP:CG	1:B:273:LEU:N	2.61	0.54
1:A:340:THR:O	1:A:342:VAL:N	2.41	0.53
1:B:329:THR:O	1:B:329:THR:CG2	2.55	0.53
1:A:66:CYS:HB3	1:A:169:PRO:O	2.07	0.53
1:A:178:ARG:C	1:A:179:VAL:HG23	2.28	0.53
1:B:57:HIS:O	1:B:58:GLU:HG3	2.05	0.53
1:B:67:LYS:O	1:B:70:LYS:HB2	2.07	0.53
1:A:192:LYS:O	1:A:193:ASP:CB	2.49	0.53
1:B:82:ILE:O	1:B:86:ARG:HG3	2.09	0.53
1:B:143:SER:C	1:B:145:GLU:H	2.11	0.53
1:B:162:ILE:CG2	1:B:167:TYR:HE2	1.99	0.53
1:A:73:VAL:O	1:A:73:VAL:HG12	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:PHE:O	1:B:97:ASP:O	2.26	0.53
1:B:126:VAL:CA	1:B:130:LEU:CD1	2.82	0.53
1:B:164:GLN:OE1	1:B:164:GLN:N	2.30	0.53
1:B:36:LEU:CD2	1:B:198:MET:HG3	2.37	0.53
1:B:328:ASP:C	1:B:328:ASP:OD1	2.41	0.53
1:A:80:SER:O	1:A:84:ILE:HG13	2.09	0.53
1:A:62:SER:O	1:A:66:CYS:SG	2.66	0.53
1:A:104:ALA:C	1:A:106:GLN:H	2.12	0.53
1:B:86:ARG:CB	1:B:86:ARG:CZ	2.86	0.53
1:B:167:TYR:CE1	1:B:169:PRO:CD	2.91	0.53
1:A:163:ALA:O	1:A:164:GLN:C	2.46	0.53
1:A:329:THR:O	1:A:329:THR:CG2	2.55	0.53
1:B:250:PHE:C	1:B:252:SER:N	2.59	0.52
1:B:135:GLY:O	1:B:138:ALA:HB3	2.09	0.52
1:B:137:GLN:N	1:B:138:ALA:HB3	2.23	0.52
1:A:69:TYR:O	1:A:70:LYS:C	2.44	0.52
1:B:128:LYS:O	1:B:129:ARG:C	2.43	0.52
1:B:344:ILE:CG2	1:B:345:LYS:H	2.01	0.52
1:B:192:LYS:O	1:B:193:ASP:CB	2.55	0.52
1:A:62:SER:HG	1:A:65:GLU:CG	2.22	0.52
1:B:65:GLU:C	1:B:67:LYS:N	2.63	0.52
1:B:167:TYR:C	1:B:168:ILE:HD12	2.28	0.52
1:B:92:LYS:O	1:B:93:ILE:HG12	2.10	0.52
1:B:167:TYR:OH	1:B:169:PRO:CB	2.58	0.52
1:B:142:ARG:O	1:B:145:GLU:HG3	2.10	0.52
1:B:222:ILE:O	1:B:222:ILE:HG22	2.02	0.52
1:B:272:ASP:OD1	1:B:272:ASP:N	2.30	0.51
1:A:104:ALA:C	1:A:106:GLN:N	2.60	0.51
1:B:101:ALA:C	1:B:104:ALA:CB	2.78	0.51
1:A:245:GLU:O	1:A:245:GLU:CG	2.45	0.51
1:B:170:THR:OG1	1:B:173:ASP:CG	2.48	0.51
1:B:170:THR:H	1:B:173:ASP:HB2	1.76	0.51
1:B:308:GLU:OE2	1:B:319:ILE:O	2.27	0.51
1:A:36:LEU:CD2	1:A:37:LEU:H	2.24	0.51
1:A:260:THR:O	1:A:260:THR:HG23	2.07	0.51
1:B:156:LEU:C	1:B:158:ASP:N	2.61	0.51
1:B:134:SER:O	1:B:135:GLY:C	2.46	0.51
1:A:36:LEU:HD22	1:A:37:LEU:H	1.75	0.51
1:A:158:ASP:OD2	1:A:161:ARG:NE	2.43	0.51
1:B:63:GLU:HG2	1:B:64:GLU:CD	2.26	0.51
1:B:100:ARG:O	1:B:103:ASP:OD2	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:ILE:O	1:A:128:LYS:C	2.46	0.50
1:A:133:ASP:O	1:A:135:GLY:N	2.44	0.50
1:A:193:ASP:O	1:A:194:LEU:HD23	2.11	0.50
1:B:309:ASP:OD1	1:B:309:ASP:O	2.29	0.50
1:B:253:ILE:C	1:B:255:ASN:H	2.14	0.50
1:A:102:ASP:OD1	1:A:102:ASP:O	2.30	0.50
1:B:307:PHE:C	1:B:309:ASP:N	2.53	0.50
1:A:85:ILE:O	1:A:86:ARG:C	2.49	0.50
1:A:128:LYS:O	1:A:129:ARG:C	2.46	0.50
1:A:161:ARG:CG	1:A:161:ARG:NH1	2.72	0.50
1:A:162:ILE:HB	1:A:167:TYR:CZ	2.46	0.50
1:B:148:LEU:O	1:B:149:ASN:O	2.30	0.50
1:B:163:ALA:O	1:B:165:PRO:N	2.45	0.50
1:A:161:ARG:HH22	1:A:173:ASP:CG	2.14	0.50
1:A:188:HIS:O	1:A:189:PHE:HB3	2.10	0.50
1:A:191:PHE:O	1:A:193:ASP:N	2.45	0.50
1:B:124:ALA:O	1:B:126:VAL:C	2.49	0.50
1:B:237:ASP:OD1	1:B:237:ASP:O	2.30	0.50
1:A:136:VAL:O	1:A:136:VAL:CG1	2.58	0.50
1:A:207:GLU:O	1:A:209:LYS:N	2.45	0.50
1:A:72:VAL:C	1:A:74:TYR:N	2.62	0.50
1:B:296:TYR:O	1:B:300:ALA:HB2	2.11	0.50
1:A:161:ARG:NH1	1:A:161:ARG:HG2	2.27	0.50
1:B:134:SER:OG	1:B:135:GLY:N	2.43	0.50
1:B:284:THR:HA	1:B:287:TYR:O	2.12	0.50
1:A:237:ASP:C	1:A:237:ASP:OD1	2.46	0.49
1:B:77:THR:O	1:B:78:ILE:O	2.30	0.49
1:B:250:PHE:C	1:B:252:SER:H	2.14	0.49
1:A:57:HIS:O	1:A:58:GLU:HG3	2.12	0.49
1:A:143:SER:O	1:A:146:TYR:O	2.30	0.49
1:A:243:MET:CE	1:A:303:ILE:HD13	2.42	0.49
1:B:72:VAL:O	1:B:73:VAL:C	2.42	0.49
1:B:294:ASN:O	1:B:294:ASN:OD1	2.29	0.49
1:A:203:GLY:O	1:A:204:GLN:O	2.29	0.49
1:A:72:VAL:C	1:A:74:TYR:H	2.16	0.49
1:A:109:VAL:CG1	1:A:110:LEU:HA	2.40	0.49
1:A:178:ARG:C	1:A:179:VAL:CG2	2.80	0.49
1:B:125:GLY:O	1:B:129:ARG:N	2.30	0.49
1:B:159:LEU:O	1:B:163:ALA:N	2.44	0.49
1:A:109:VAL:CB	1:A:110:LEU:HB2	2.43	0.49
1:B:110:LEU:O	1:B:111:ALA:O	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:344:ILE:O	1:B:345:LYS:O	2.30	0.49
2:D:11:VAL:O	2:D:12:GLY:O	2.29	0.49
1:A:97:ASP:OD2	1:A:99:ALA:HB2	2.13	0.49
1:A:81:ILE:O	1:A:85:ILE:HG12	2.12	0.49
1:A:253:ILE:C	1:A:255:ASN:N	2.56	0.49
1:A:276:GLU:O	1:A:279:LYS:HB2	2.13	0.49
1:B:102:ASP:N	1:B:103:ASP:HB2	2.28	0.49
1:B:123:LEU:O	1:B:124:ALA:O	2.29	0.49
1:B:277:LYS:C	1:B:279:LYS:N	2.64	0.49
1:B:81:ILE:O	1:B:83:ALA:N	2.46	0.48
1:A:33:GLU:O	1:A:34:VAL:HG22	2.11	0.48
1:A:85:ILE:C	1:A:87:ALA:H	2.16	0.48
1:A:187:THR:C	1:A:188:HIS:HD2	2.16	0.48
1:B:52:GLN:C	1:B:54:LYS:H	2.15	0.48
1:B:87:ALA:O	1:B:88:MET:O	2.30	0.48
1:B:126:VAL:O	1:B:130:LEU:HD13	0.67	0.48
1:A:84:ILE:O	1:A:85:ILE:O	2.31	0.48
1:B:81:ILE:O	1:B:84:ILE:N	2.45	0.48
1:B:158:ASP:OD2	1:B:158:ASP:O	2.30	0.48
1:B:162:ILE:O	1:B:167:TYR:HD2	1.96	0.48
1:B:311:ASN:O	1:B:314:LYS:CE	2.60	0.48
1:B:253:ILE:C	1:B:255:ASN:N	2.60	0.48
1:A:165:PRO:O	1:A:165:PRO:HG2	2.13	0.48
1:B:86:ARG:NH1	1:B:90:ARG:HH12	2.11	0.48
1:B:142:ARG:C	1:B:144:ARG:N	2.66	0.48
1:B:130:LEU:C	1:B:132:LYS:N	2.67	0.48
1:A:128:LYS:O	1:A:130:LEU:N	2.47	0.48
1:B:72:VAL:O	1:B:74:TYR:N	2.46	0.48
1:B:167:TYR:OH	1:B:169:PRO:HG3	2.09	0.48
1:A:304:GLN:O	1:A:304:GLN:HG2	2.14	0.47
1:B:127:ILE:O	1:B:128:LYS:C	2.50	0.47
1:A:62:SER:N	1:A:65:GLU:HB2	2.17	0.47
1:B:146:TYR:N	1:B:146:TYR:CD1	2.82	0.47
2:D:11:VAL:C	2:D:12:GLY:O	2.46	0.47
1:B:164:GLN:HA	1:B:165:PRO:HD2	1.24	0.47
1:A:93:ILE:CG2	1:A:94:ASP:N	2.76	0.47
1:B:101:ALA:O	1:B:104:ALA:HB3	2.14	0.47
1:B:167:TYR:CE1	1:B:169:PRO:CB	2.95	0.47
1:B:243:MET:HG3	1:B:243:MET:O	2.14	0.47
1:B:72:VAL:O	1:B:72:VAL:HG12	2.15	0.47
1:B:140:PHE:O	1:B:140:PHE:CD1	2.67	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:LEU:CD2	1:A:37:LEU:N	2.78	0.47
1:B:170:THR:C	1:B:172:GLN:N	2.67	0.47
1:A:256:ASN:OD1	1:A:257:LYS:N	2.48	0.47
1:B:78:ILE:HD12	1:B:78:ILE:HA	1.50	0.46
1:B:104:ALA:O	1:B:107:LEU:HB3	2.14	0.46
1:B:342:VAL:O	1:B:343:ILE:C	2.52	0.46
1:A:159:LEU:O	1:A:160:ASP:C	2.51	0.46
1:A:184:ILE:HG22	1:A:185:VAL:N	2.30	0.46
1:B:247:MET:CE	1:B:287:TYR:OH	2.63	0.46
1:A:69:TYR:C	1:A:71:ALA:N	2.64	0.46
1:B:167:TYR:OH	1:B:169:PRO:CG	2.63	0.46
1:A:106:GLN:O	1:A:106:GLN:HG3	2.16	0.46
1:B:57:HIS:NE2	1:B:191:PHE:CD1	2.80	0.46
1:B:102:ASP:O	1:B:105:ARG:N	2.48	0.46
1:B:164:GLN:O	1:B:165:PRO:C	2.53	0.46
1:B:289:GLU:O	1:B:290:TYR:C	2.50	0.46
1:A:97:ASP:O	1:A:99:ALA:N	2.49	0.46
1:A:231:ASP:N	1:A:231:ASP:OD1	2.38	0.46
1:A:85:ILE:C	1:A:87:ALA:N	2.67	0.46
1:B:86:ARG:O	1:B:89:GLY:C	2.54	0.46
1:B:86:ARG:HH12	1:B:90:ARG:CZ	2.28	0.46
1:A:109:VAL:HG12	1:A:110:LEU:HB2	1.98	0.45
1:A:222:ILE:O	1:A:222:ILE:HG22	2.14	0.45
1:A:335:VAL:O	1:A:338:ALA:HB3	2.16	0.45
1:B:124:ALA:O	1:B:126:VAL:HB	2.16	0.45
1:B:124:ALA:C	1:B:126:VAL:N	2.60	0.45
1:B:128:LYS:C	1:B:130:LEU:N	2.66	0.45
1:B:158:ASP:OD2	1:B:161:ARG:CZ	2.64	0.45
2:D:13:GLU:H	2:D:13:GLU:CD	2.08	0.45
1:A:131:TRP:CE3	1:A:156:LEU:HD13	2.51	0.45
1:A:278:ILE:O	1:A:278:ILE:CG1	2.52	0.45
1:B:62:SER:O	1:B:65:GLU:CB	2.60	0.45
1:A:172:GLN:HA	1:A:175:LEU:HD12	1.98	0.45
1:A:191:PHE:O	1:A:192:LYS:C	2.52	0.45
1:A:304:GLN:O	1:A:304:GLN:CG	2.65	0.45
1:B:153:ALA:C	1:B:155:TYR:N	2.66	0.45
1:B:277:LYS:C	1:B:279:LYS:H	2.19	0.45
1:A:156:LEU:HA	1:A:156:LEU:HD23	1.66	0.45
1:B:107:LEU:O	1:B:111:ALA:CA	2.61	0.45
1:A:64:GLU:N	1:A:64:GLU:CD	2.70	0.45
1:B:68:GLN:NE2	1:B:68:GLN:H	2.04	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:ASP:CB	1:B:100:ARG:CD	2.94	0.45
1:B:245:GLU:C	1:B:247:MET:H	2.19	0.45
1:B:132:LYS:C	1:B:133:ASP:O	2.50	0.45
1:B:295:THR:O	1:B:296:TYR:C	2.55	0.45
1:B:341:ASP:O	1:B:344:ILE:HB	2.16	0.45
1:B:56:ILE:HD13	1:B:56:ILE:HG23	1.65	0.45
1:B:84:ILE:HG23	1:B:84:ILE:HD13	1.63	0.45
1:B:101:ALA:C	1:B:104:ALA:HB2	2.37	0.45
1:B:164:GLN:O	1:B:167:TYR:HB2	2.17	0.45
1:B:171:GLN:H	1:B:171:GLN:HG2	1.55	0.45
1:B:264:ILE:O	1:B:264:ILE:HG22	2.17	0.45
1:A:241:ASN:HB3	1:A:244:HIS:CG	2.52	0.45
1:B:233:VAL:HB	1:B:238:GLU:O	2.17	0.45
1:A:243:MET:HE1	1:A:303:ILE:HD13	1.99	0.44
1:B:123:LEU:C	1:B:126:VAL:CG2	2.84	0.44
1:A:93:ILE:CG2	1:A:94:ASP:H	2.25	0.44
1:A:139:CYS:O	1:A:139:CYS:SG	2.75	0.44
1:B:97:ASP:CB	1:B:100:ARG:HD3	2.45	0.44
1:B:100:ARG:NH1	1:B:129:ARG:HD3	2.26	0.44
1:A:330:LYS:HB3	1:A:330:LYS:HE2	1.75	0.44
2:C:5:TYR:HA	2:C:9:ILE:O	2.17	0.44
1:B:167:TYR:HE1	1:B:169:PRO:CD	2.27	0.44
1:A:170:THR:O	1:A:174:VAL:HG23	2.17	0.44
1:B:330:LYS:CG	1:B:331:ASN:N	2.76	0.44
1:B:103:ASP:C	1:B:104:ALA:C	2.75	0.44
1:B:164:GLN:O	1:B:167:TYR:CB	2.66	0.44
1:B:226:ALA:O	1:B:229:ASP:HB2	2.18	0.44
1:B:250:PHE:O	1:B:252:SER:N	2.51	0.44
1:B:49:ILE:HG23	1:B:49:ILE:HD13	1.59	0.44
1:A:54:LYS:O	1:A:58:GLU:HB2	2.18	0.44
1:B:88:MET:CE	1:B:95:PHE:CE1	3.00	0.44
1:A:63:GLU:C	1:A:64:GLU:OE2	2.56	0.43
1:A:69:TYR:C	1:A:71:ALA:H	2.21	0.43
1:A:130:LEU:C	1:A:132:LYS:H	2.20	0.43
1:B:168:ILE:N	1:B:168:ILE:CD1	2.29	0.43
1:B:168:ILE:HA	1:B:169:PRO:HD3	1.56	0.43
1:B:170:THR:OG1	1:B:173:ASP:OD2	2.36	0.43
1:B:195:HIS:CE1	1:B:197:LYS:HE2	2.53	0.43
1:A:133:ASP:HB3	1:A:136:VAL:H	1.83	0.43
1:A:284:THR:H	1:A:284:THR:HG23	1.50	0.43
1:B:37:LEU:HD12	1:B:37:LEU:HA	1.73	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:GLU:O	1:A:122:GLU:HG3	2.16	0.43
1:A:253:ILE:O	1:A:254:CYS:C	2.53	0.43
1:A:337:ASP:O	1:A:338:ALA:C	2.50	0.43
1:A:271:LYS:HG2	1:A:324:THR:O	2.19	0.43
1:B:48:THR:OG1	5:B:355:GDP:O1A	2.25	0.43
1:A:343:ILE:HD13	1:A:343:ILE:HG21	1.77	0.43
1:B:127:ILE:C	1:B:130:LEU:HB2	2.39	0.43
1:A:107:LEU:O	1:A:110:LEU:HB3	2.18	0.43
1:B:100:ARG:NH2	1:B:129:ARG:HD2	0.26	0.43
1:A:172:GLN:HE21	1:A:172:GLN:HB2	1.59	0.43
1:B:165:PRO:O	1:B:166:ASN:C	2.56	0.43
1:B:301:ALA:C	1:B:303:ILE:N	2.65	0.43
1:A:65:GLU:C	1:A:67:LYS:H	2.21	0.43
1:B:264:ILE:HG21	1:B:264:ILE:HD12	1.65	0.43
1:A:65:GLU:C	1:A:67:LYS:N	2.71	0.42
1:A:253:ILE:HG23	1:A:253:ILE:HD12	1.66	0.42
1:B:154:TYR:CE2	1:B:173:ASP:OD1	2.72	0.42
1:A:319:ILE:HG21	1:A:319:ILE:HD13	1.69	0.42
1:B:243:MET:HG2	1:B:286:CYS:SG	2.60	0.42
1:B:328:ASP:OD1	1:B:329:THR:N	2.52	0.42
1:A:238:GLU:HG2	1:A:239:GLU:HG2	2.01	0.42
1:B:88:MET:CB	1:B:93:ILE:HG21	2.49	0.42
1:B:102:ASP:O	1:B:103:ASP:C	2.57	0.42
1:B:137:GLN:H	1:B:138:ALA:HB3	1.84	0.42
1:B:209:LYS:O	1:B:212:ILE:HD11	2.19	0.42
1:B:211:TRP:C	1:B:213:HIS:H	2.20	0.42
1:B:247:MET:HE2	1:B:287:TYR:OH	2.19	0.42
1:A:221:ILE:HG21	1:A:221:ILE:HD13	1.50	0.42
1:B:149:ASN:OD1	1:B:149:ASN:N	2.29	0.42
1:A:159:LEU:C	1:A:161:ARG:N	2.69	0.42
1:B:68:GLN:H	1:B:68:GLN:HG2	1.54	0.42
1:B:245:GLU:C	1:B:247:MET:N	2.73	0.42
1:B:164:GLN:H	1:B:164:GLN:CD	2.11	0.42
1:B:303:ILE:O	1:B:304:GLN:C	2.56	0.42
1:A:56:ILE:HG23	1:A:56:ILE:HD13	1.57	0.42
1:A:73:VAL:O	1:A:73:VAL:CG1	2.63	0.42
1:B:162:ILE:HG21	1:B:162:ILE:HD12	1.80	0.42
1:B:187:THR:O	1:B:187:THR:HG22	2.05	0.42
1:A:251:ASP:O	1:A:255:ASN:HB2	2.20	0.42
1:A:303:ILE:HD13	1:A:303:ILE:HG23	1.78	0.42
1:B:103:ASP:O	1:B:106:GLN:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:ARG:NH2	1:A:180:LYS:HG3	2.34	0.41
1:B:127:ILE:C	1:B:130:LEU:H	2.21	0.41
2:C:5:TYR:CD1	2:C:5:TYR:N	2.88	0.41
1:A:188:HIS:CD2	1:A:188:HIS:N	2.83	0.41
1:A:257:LYS:H	1:A:257:LYS:HG3	1.38	0.41
2:C:7:HIS:H	2:C:9:ILE:H	1.66	0.41
1:B:102:ASP:O	1:B:104:ALA:C	2.59	0.41
1:B:64:GLU:O	1:B:67:LYS:CB	2.30	0.41
1:B:127:ILE:HB	1:B:128:LYS:H	1.44	0.41
2:D:9:ILE:HD13	2:D:9:ILE:HG21	1.50	0.41
1:A:273:LEU:HD23	1:A:273:LEU:HA	1.81	0.41
1:A:342:VAL:O	1:A:343:ILE:C	2.57	0.41
1:B:52:GLN:C	1:B:54:LYS:N	2.74	0.41
1:B:126:VAL:HG12	1:B:130:LEU:CD1	2.48	0.41
1:B:331:ASN:O	1:B:332:VAL:C	2.56	0.41
2:D:11:VAL:H	2:D:11:VAL:HG22	1.61	0.41
1:B:204:GLN:O	1:B:205:ARG:C	2.55	0.41
1:B:319:ILE:HG21	1:B:319:ILE:HD13	1.65	0.41
2:C:9:ILE:HG22	2:C:10:TRP:N	2.35	0.41
1:A:172:GLN:O	1:A:173:ASP:C	2.58	0.41
2:C:6:TYR:CD2	2:C:6:TYR:C	2.92	0.41
1:A:49:ILE:HD13	1:A:49:ILE:HG23	1.69	0.41
1:A:122:GLU:N	6:A:3:HOH:O	2.53	0.41
1:B:88:MET:HE3	1:B:88:MET:HB3	1.82	0.41
1:B:98:SER:O	1:B:100:ARG:N	2.54	0.41
1:B:102:ASP:H	1:B:103:ASP:HB2	1.84	0.41
1:B:211:TRP:C	1:B:213:HIS:N	2.71	0.41
1:B:238:GLU:C	1:B:239:GLU:HG2	2.13	0.41
1:A:49:ILE:HG21	1:A:49:ILE:HD12	1.68	0.41
1:A:144:ARG:HH11	1:A:144:ARG:HD3	1.55	0.41
1:A:276:GLU:O	1:A:277:LYS:C	2.55	0.41
1:A:305:CYS:C	1:A:307:PHE:N	2.71	0.41
1:A:325:CYS:O	1:A:326:ALA:C	2.56	0.41
1:B:202:GLY:HA2	3:B:359:ALF:F3	2.10	0.41
1:A:102:ASP:C	1:A:104:ALA:N	2.66	0.40
1:A:319:ILE:HG22	1:A:320:TYR:N	2.33	0.40
1:A:56:ILE:HG21	1:A:56:ILE:HD12	1.69	0.40
1:A:143:SER:HA	1:A:146:TYR:CE1	2.55	0.40
1:A:162:ILE:O	1:A:162:ILE:HG13	2.21	0.40
2:D:6:TYR:CD2	2:D:7:HIS:ND1	2.81	0.40
1:A:85:ILE:HD12	1:A:85:ILE:HG23	1.88	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:LYS:C	1:A:279:LYS:N	2.64	0.40
1:A:303:ILE:O	1:A:304:GLN:C	2.57	0.40
1:B:55:ILE:HD13	1:B:55:ILE:HG21	1.52	0.40
1:B:142:ARG:CZ	1:B:145:GLU:OE2	2.70	0.40
1:A:256:ASN:C	1:A:258:TRP:H	2.23	0.40
1:B:76:ASN:HD22	1:B:76:ASN:HA	1.65	0.40
1:B:88:MET:HE1	1:B:95:PHE:CD1	2.56	0.40
1:B:91:LEU:HA	1:B:91:LEU:HD23	0.95	0.40
1:A:78:ILE:HD12	1:A:78:ILE:HG21	1.86	0.40
1:B:247:MET:HE1	1:B:287:TYR:CZ	2.54	0.40
1:B:319:ILE:HG22	1:B:320:TYR:N	2.35	0.40
2:C:11:VAL:H	2:C:11:VAL:HG22	1.53	0.40

All (3) 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:97:ASP:OD2	2:D:6:TYR:O[2_455]	1.40	0.80
1:A:97:ASP:CG	2:D:6:TYR:O[2_455]	2.07	0.13
1:A:97:ASP:OD1	2:D:6:TYR:O[2_455]	2.15	0.05

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	299/313 (96%)	240 (80%)	43 (14%)	16 (5%)	2	5
1	B	299/313 (96%)	232 (78%)	41 (14%)	26 (9%)	1	1
2	C	9/11 (82%)	8 (89%)	1 (11%)	0	100	100
2	D	9/11 (82%)	5 (56%)	4 (44%)	0	100	100
All	All	616/648 (95%)	485 (79%)	89 (14%)	42 (7%)	1	3

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	183	GLY
1	B	93	ILE
1	B	105	ARG
1	B	138	ALA
1	B	160	ASP
1	B	165	PRO
1	B	184	ILE
1	B	291	ALA
1	A	66	CYS
1	A	131	TRP
1	A	230	TYR
1	A	284	THR
1	A	326	ALA
1	A	344	ILE
1	B	82	ILE
1	B	92	LYS
1	B	99	ALA
1	B	126	VAL
1	B	143	SER
1	B	157	ASN
1	B	169	PRO
1	B	238	GLU
1	A	152	ALA
1	A	304	GLN
1	B	273	LEU
1	A	166	ASN
1	B	66	CYS
1	B	193	ASP
1	A	193	ASP
1	B	124	ALA
1	B	164	GLN
1	B	290	TYR
1	B	331	ASN
1	A	34	VAL
1	A	85	ILE
1	B	95	PHE
1	B	131	TRP
1	A	73	VAL
1	A	109	VAL
1	B	78	ILE
1	A	343	ILE
1	B	278	ILE

5.3.2 Protein sidechains [i](#)

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	267/272 (98%)	223 (84%)	44 (16%)	2	7
1	B	267/272 (98%)	195 (73%)	72 (27%)	0	1
2	C	8/8 (100%)	6 (75%)	2 (25%)	0	2
2	D	8/8 (100%)	7 (88%)	1 (12%)	4	14
All	All	550/560 (98%)	431 (78%)	119 (22%)	1	3

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	LEU
1	A	44	SER
1	A	46	LYS
1	A	49	ILE
1	A	56	ILE
1	A	62	SER
1	A	63	GLU
1	A	64	GLU
1	A	70	LYS
1	A	74	TYR
1	A	75	SER
1	A	82	ILE
1	A	94	ASP
1	A	102	ASP
1	A	127	ILE
1	A	128	LYS
1	A	143	SER
1	A	149	ASN
1	A	158	ASP
1	A	161	ARG
1	A	162	ILE
1	A	167	TYR
1	A	193	ASP
1	A	206	SER

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Mol	Chain	Res	Type
1	A	212	ILE
1	A	214	CYS
1	A	228	SER
1	A	243	MET
1	A	245	GLU
1	A	246	SER
1	A	247	MET
1	A	249	LEU
1	A	257	LYS
1	A	258	TRP
1	A	260	THR
1	A	264	ILE
1	A	280	LYS
1	A	294	ASN
1	A	313	ARG
1	A	315	ASP
1	A	316	THR
1	A	317	LYS
1	A	337	ASP
1	A	345	LYS
1	B	36	LEU
1	B	37	LEU
1	B	49	ILE
1	B	64	GLU
1	B	67	LYS
1	B	68	GLN
1	B	74	TYR
1	B	78	ILE
1	B	81	ILE
1	B	84	ILE
1	B	90	ARG
1	B	91	LEU
1	B	93	ILE
1	B	100	ARG
1	B	106	GLN
1	B	107	LEU
1	B	110	LEU
1	B	122	GLU
1	B	126	VAL
1	B	127	ILE
1	B	128	LYS
1	B	129	ARG

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Mol	Chain	Res	Type
1	B	130	LEU
1	B	131	TRP
1	B	133	ASP
1	B	139	CYS
1	B	141	ASN
1	B	142	ARG
1	B	143	SER
1	B	144	ARG
1	B	149	ASN
1	B	151	SER
1	B	155	TYR
1	B	159	LEU
1	B	162	ILE
1	B	164	GLN
1	B	167	TYR
1	B	168	ILE
1	B	170	THR
1	B	177	THR
1	B	193	ASP
1	B	194	LEU
1	B	204	GLN
1	B	206	SER
1	B	212	ILE
1	B	229	ASP
1	B	236	GLU
1	B	238	GLU
1	B	239	GLU
1	B	240	MET
1	B	246	SER
1	B	247	MET
1	B	249	LEU
1	B	257	LYS
1	B	258	TRP
1	B	262	THR
1	B	264	ILE
1	B	276	GLU
1	B	279	LYS
1	B	280	LYS
1	B	282	PRO
1	B	285	ILE
1	B	289	GLU
1	B	294	ASN

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Mol	Chain	Res	Type
1	B	297	GLU
1	B	304	GLN
1	B	316	THR
1	B	317	LYS
1	B	329	THR
1	B	331	ASN
1	B	344	ILE
1	B	345	LYS
2	C	6	TYR
2	C	7	HIS
2	D	7	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	164	GLN
1	A	171	GLN
1	A	188	HIS
1	A	269	ASN
1	A	304	GLN
1	B	68	GLN
1	B	171	GLN
1	B	172	GLN
1	B	195	HIS
1	B	304	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 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
3	ALF	B	359	1,4,5	0,4,4	-	-	-		
3	ALF	A	357	5,4,1	0,4,4	-	-	-		
5	GDP	A	355	3,4,1	24,30,30	4.27	22 (91%)	30,47,47	2.90	17 (56%)
5	GDP	B	355	3,4	24,30,30	3.83	18 (75%)	30,47,47	2.66	13 (43%)

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
5	GDP	A	355	3,4,1	-	4/12/32/32	0/3/3/3
5	GDP	B	355	3,4	-	1/12/32/32	0/3/3/3

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	355	GDP	C6-N1	-10.23	1.22	1.37
5	A	355	GDP	C6-N1	-9.67	1.23	1.37
5	A	355	GDP	C2'-C1'	-7.61	1.42	1.53
5	B	355	GDP	C2'-C1'	-5.82	1.44	1.53
5	A	355	GDP	PB-O2B	-5.48	1.33	1.54
5	A	355	GDP	C2-N1	-5.01	1.25	1.37
5	A	355	GDP	PB-O1B	-4.88	1.34	1.50
5	B	355	GDP	C8-N7	-4.67	1.27	1.35
5	B	355	GDP	PB-O2B	-4.66	1.36	1.54
5	A	355	GDP	C8-N7	-4.64	1.27	1.35
5	A	355	GDP	PA-O1A	-4.52	1.34	1.50
5	A	355	GDP	PA-O2A	-4.50	1.34	1.55
5	B	355	GDP	C2-N1	-4.36	1.26	1.37
5	A	355	GDP	O4'-C1'	-4.33	1.35	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	355	GDP	O2'-C2'	-4.32	1.32	1.43
5	A	355	GDP	C2'-C3'	-4.00	1.42	1.53
5	B	355	GDP	PB-O3B	-3.91	1.39	1.54
5	B	355	GDP	PA-O2A	-3.82	1.37	1.55
5	B	355	GDP	PA-O1A	-3.69	1.37	1.50
5	B	355	GDP	O3'-C3'	-3.60	1.34	1.43
5	A	355	GDP	O3'-C3'	-3.52	1.34	1.43
5	B	355	GDP	PA-O5'	-3.50	1.45	1.59
5	B	355	GDP	C2'-C3'	-3.44	1.43	1.53
5	A	355	GDP	C3'-C4'	-3.36	1.44	1.53
5	B	355	GDP	C5-C6	-3.35	1.40	1.47
5	A	355	GDP	O4'-C4'	-3.34	1.37	1.45
5	A	355	GDP	C5-C6	-3.32	1.40	1.47
5	A	355	GDP	PA-O5'	-3.29	1.46	1.59
5	B	355	GDP	C4-N3	-3.19	1.29	1.37
5	B	355	GDP	O2'-C2'	-3.18	1.35	1.43
5	A	355	GDP	C4-N3	-3.09	1.29	1.37
5	B	355	GDP	O4'-C4'	-2.86	1.38	1.45
5	B	355	GDP	C2-N2	-2.81	1.27	1.34
5	B	355	GDP	C3'-C4'	-2.76	1.45	1.53
5	A	355	GDP	O5'-C5'	-2.35	1.35	1.44
5	A	355	GDP	O6-C6	-2.34	1.18	1.23
5	A	355	GDP	C2-N3	-2.26	1.27	1.33
5	A	355	GDP	C5-C4	-2.26	1.37	1.43
5	A	355	GDP	C2-N2	-2.06	1.29	1.34
5	B	355	GDP	O6-C6	-2.01	1.19	1.23

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	355	GDP	O4'-C1'-C2'	-7.31	96.24	106.93
5	A	355	GDP	O3B-PB-O3A	6.10	125.11	104.64
5	B	355	GDP	O2B-PB-O3A	-5.38	86.59	104.64
5	A	355	GDP	O6-C6-N1	-5.35	114.33	120.65
5	B	355	GDP	O5'-PA-O1A	-5.26	88.50	109.07
5	B	355	GDP	O4'-C1'-C2'	-4.53	100.30	106.93
5	B	355	GDP	O3'-C3'-C4'	-4.02	99.42	111.05
5	A	355	GDP	O2B-PB-O1B	-4.00	95.03	110.68
5	B	355	GDP	O2A-PA-O5'	-3.66	90.75	107.75
5	A	355	GDP	O5'-C5'-C4'	3.66	121.58	108.99
5	B	355	GDP	O5'-C5'-C4'	3.65	121.55	108.99
5	B	355	GDP	O4'-C4'-C5'	3.63	121.30	109.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	355	GDP	O4'-C4'-C3'	-3.62	97.94	105.11
5	A	355	GDP	C5-C6-N1	3.55	120.22	113.95
5	A	355	GDP	C3'-C2'-C1'	3.52	106.28	100.98
5	B	355	GDP	C8-N7-C5	3.47	109.61	102.99
5	B	355	GDP	O3'-C3'-C2'	-3.28	101.20	111.82
5	A	355	GDP	O4'-C4'-C5'	3.13	119.67	109.37
5	B	355	GDP	O2'-C2'-C3'	-3.09	101.84	111.82
5	A	355	GDP	O2'-C2'-C3'	-2.82	102.71	111.82
5	A	355	GDP	O5'-PA-O1A	-2.78	98.19	109.07
5	A	355	GDP	O3A-PB-O1B	-2.67	96.36	111.19
5	A	355	GDP	O3B-PB-O1B	2.60	120.87	110.68
5	B	355	GDP	N1-C2-N3	2.40	127.80	123.32
5	A	355	GDP	C2-N1-C6	-2.18	121.07	125.10
5	A	355	GDP	C2'-C3'-C4'	-2.06	98.65	102.64
5	A	355	GDP	O3B-PB-O2B	2.05	115.46	107.64
5	A	355	GDP	O2B-PB-O3A	-2.04	97.81	104.64
5	B	355	GDP	O3A-PB-O1B	2.01	122.32	111.19
5	A	355	GDP	C8-N7-C5	2.01	106.81	102.99

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	355	GDP	C5'-O5'-PA-O1A
5	A	355	GDP	C5'-O5'-PA-O2A
5	A	355	GDP	PB-O3A-PA-O2A
5	B	355	GDP	PA-O3A-PB-O2B
5	A	355	GDP	C5'-O5'-PA-O3A

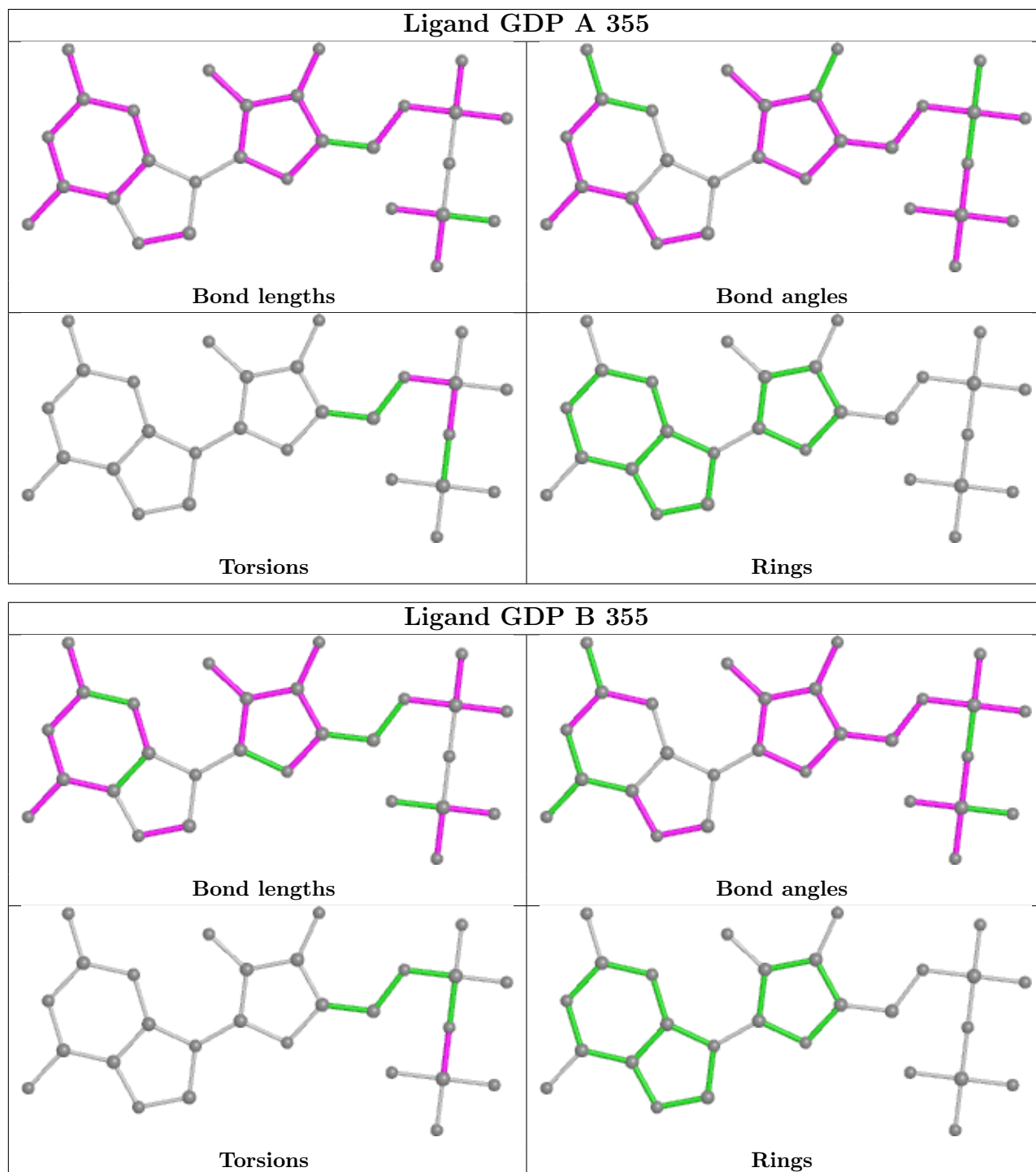
There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	359	ALF	1	0
5	A	355	GDP	1	0
5	B	355	GDP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	3
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	103:ASP	C	104:ALA	N	1.18
1	A	344:ILE	C	345:LYS	N	1.15
1	A	110:LEU	C	111:ALA	N	0.86
1	A	109:VAL	C	110:LEU	N	0.73

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	303/313 (96%)	-0.34	4 (1%) 77 72	27, 50, 84, 124	0
1	B	303/313 (96%)	-0.16	6 (1%) 65 56	29, 57, 110, 151	0
2	C	11/11 (100%)	-0.12	0 100 100	47, 66, 107, 109	0
2	D	11/11 (100%)	-0.50	0 100 100	45, 53, 80, 103	0
All	All	628/648 (96%)	-0.25	10 (1%) 72 66	27, 53, 104, 151	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	183	GLY	3.5
1	B	166	ASN	3.3
1	A	166	ASN	3.2
1	A	160	ASP	2.6
1	A	316	THR	2.4
1	B	133	ASP	2.4
1	B	168	ILE	2.4
1	B	34	VAL	2.2
1	A	89	GLY	2.1
1	B	164	GLN	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](#)

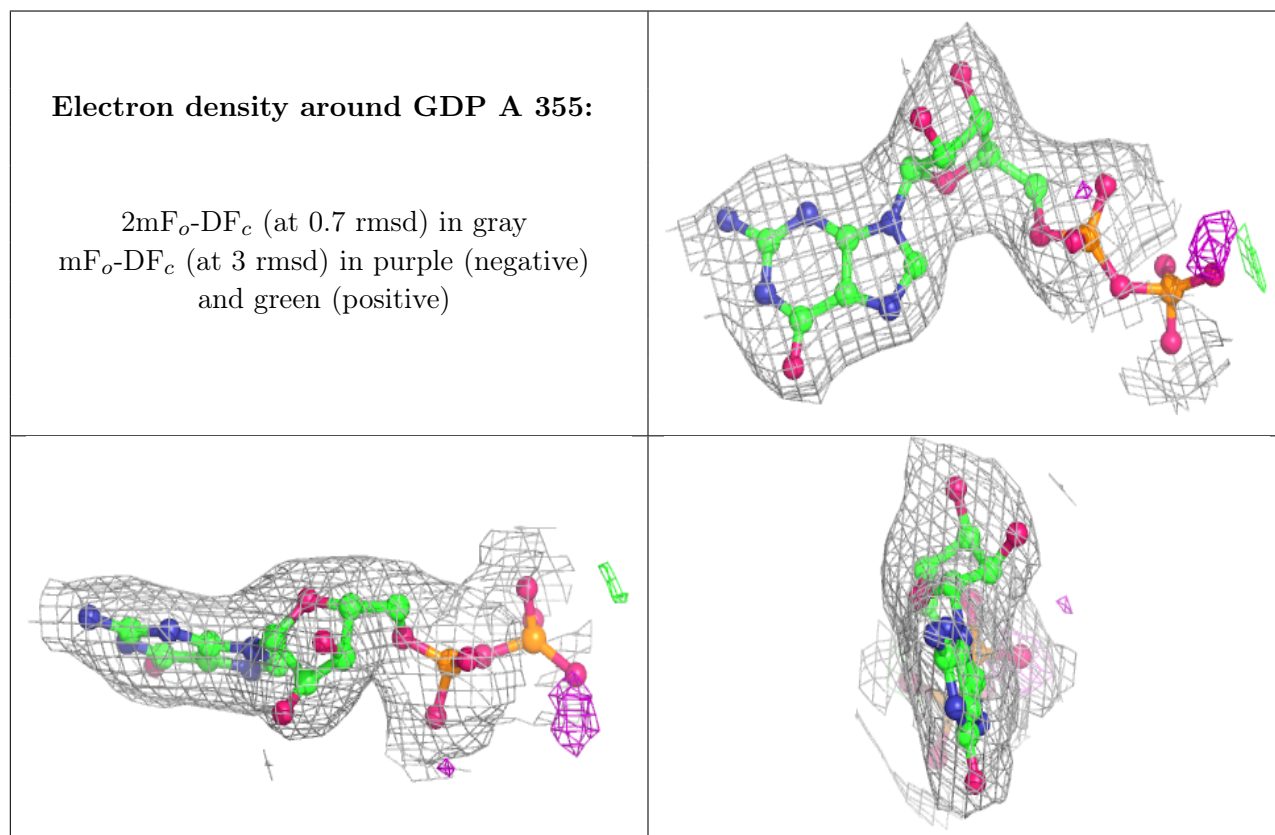
There are no monosaccharides in this entry.

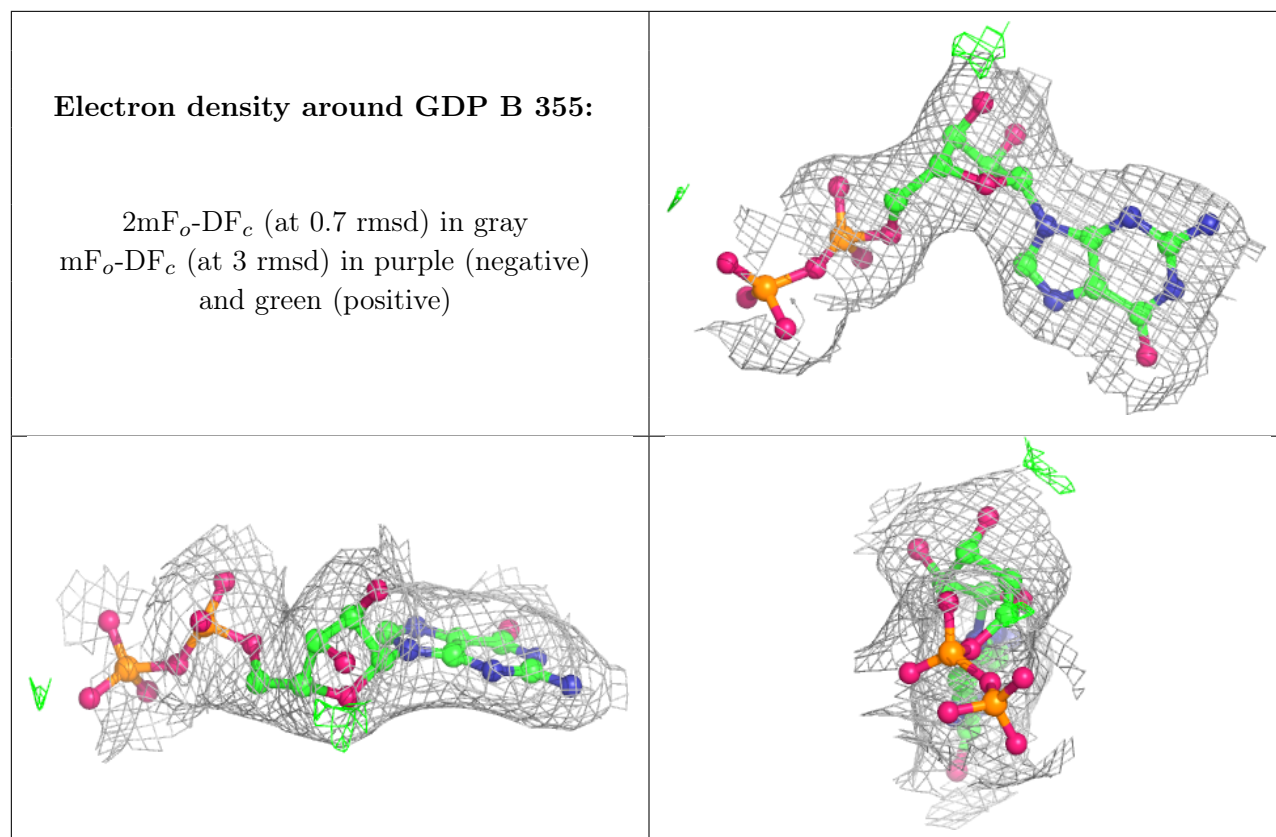
6.4 Ligands [i](#)

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	MG	B	358	1/1	0.94	0.26	45,45,45,45	0
3	ALF	B	359	5/5	0.96	0.24	59,61,63,65	0
5	GDP	A	355	28/28	0.96	0.18	30,33,39,40	0
3	ALF	A	357	5/5	0.97	0.36	53,53,55,56	0
4	MG	A	356	1/1	0.97	0.10	29,29,29,29	0
5	GDP	B	355	28/28	0.98	0.22	38,42,45,48	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.