



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:55 PM UTC

PDB ID : 1BRL / pdb_00001brl
Title : THREE-DIMENSIONAL STRUCTURE OF BACTERIAL LUCIFERASE
FROM VIBRIO HARVEYI AT 2.4 ANGSTROMS RESOLUTION
Authors : Fisher, A.J.; Rayment, I.
Deposited on : 1995-03-20
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

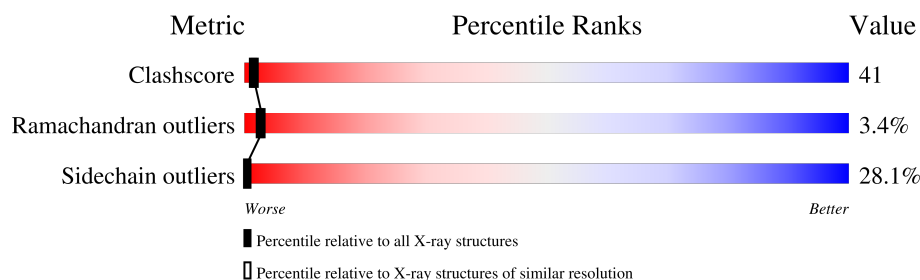
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	355	
1	C	355	
2	B	324	
2	D	324	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PO4	A	356	-	X	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 10432 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.

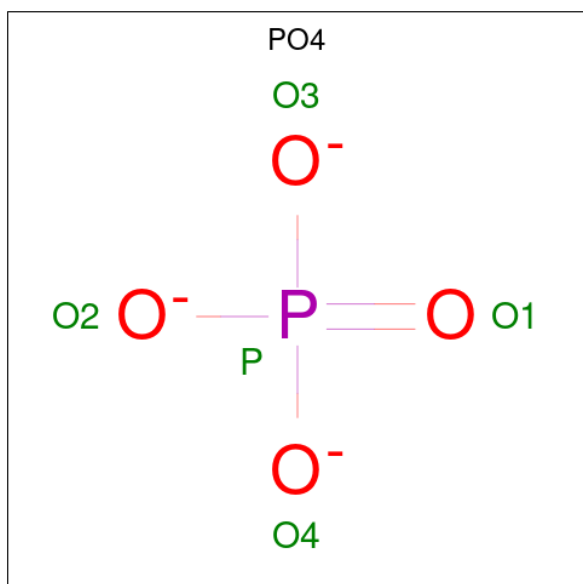
- Molecule 1 is a protein called BACTERIAL LUCIFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	0	0	0
			2679	1694	447	521	17			
1	C	340	Total	C	N	O	S	0	0	0
			2679	1694	447	521	17			

- Molecule 2 is a protein called BACTERIAL LUCIFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	319	Total	C	N	O	S	0	0	0
			2498	1572	427	484	15			
2	D	319	Total	C	N	O	S	0	0	0
			2498	1572	427	484	15			

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		

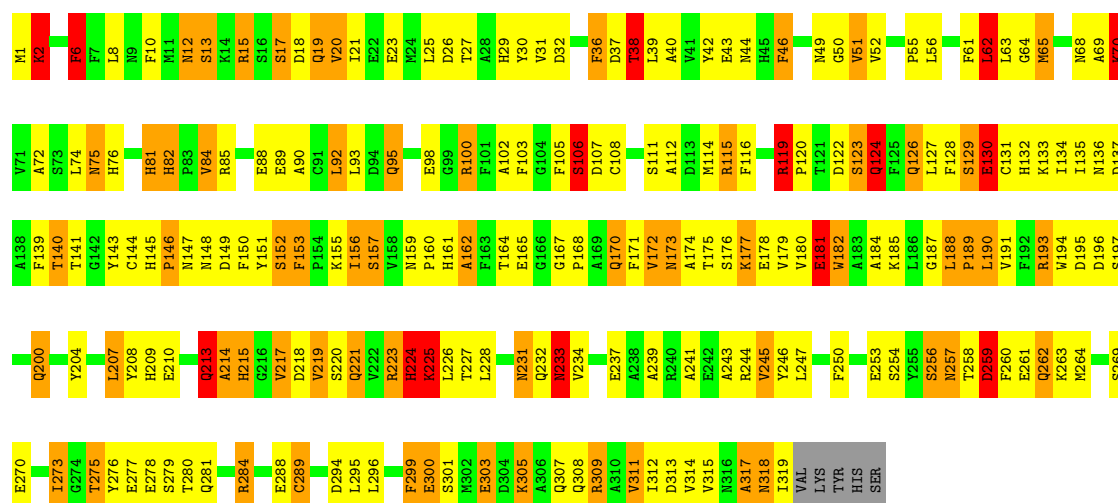
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	28	Total	O	0	0
			28	28		
4	B	45	Total	O	0	0
			45	45		



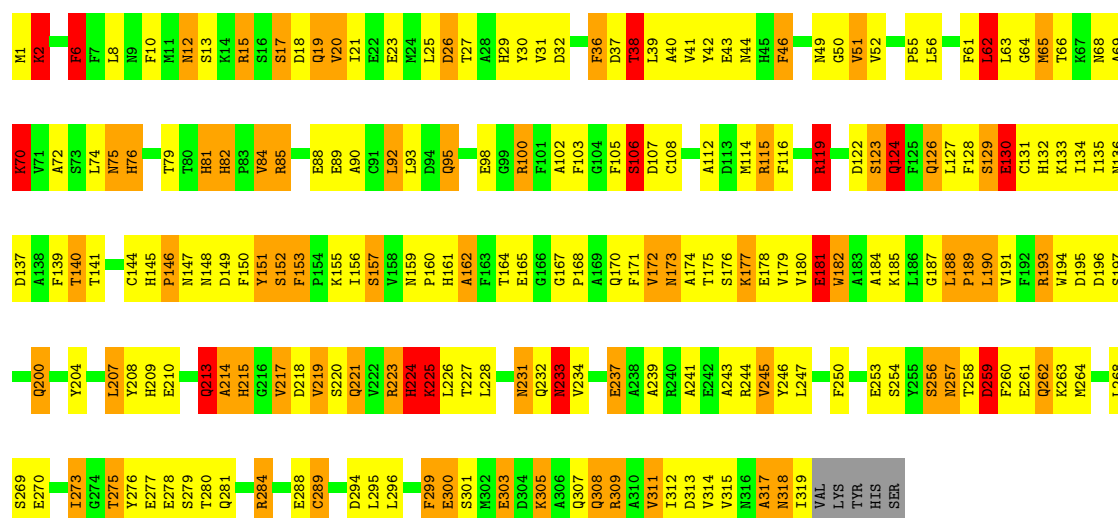
• Molecule 2: BACTERIAL LUCIFERASE

Chain B: 32% 42% 19% 5% .



• Molecule 2: BACTERIAL LUCIFERASE

Chain D: 32% 42% 20% 5% .



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	59.90Å 112.70Å 301.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (30.00-2.40)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.208 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10432	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.36	4/2740 (0.1%)	1.99	88/3716 (2.4%)
1	C	1.36	4/2740 (0.1%)	1.99	88/3716 (2.4%)
2	B	1.37	3/2552 (0.1%)	2.02	103/3457 (3.0%)
2	D	1.36	3/2552 (0.1%)	2.02	106/3457 (3.1%)
All	All	1.36	14/10584 (0.1%)	2.01	385/14346 (2.7%)

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
2	B	2	0
2	D	2	0
All	All	4	0

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	75	ALA	CA-C	-8.70	1.43	1.53
1	C	75	ALA	CA-C	-8.67	1.43	1.53
1	A	115	ARG	NE-CZ	6.94	1.40	1.33
1	C	115	ARG	NE-CZ	6.90	1.40	1.33
2	B	225	LYS	CA-C	-6.62	1.44	1.52
2	D	225	LYS	CA-C	-6.61	1.44	1.52
1	A	309	ALA	CA-C	-5.34	1.46	1.52
1	C	71	VAL	CA-C	-5.32	1.46	1.52
1	A	71	VAL	CA-C	-5.31	1.46	1.52
1	C	309	ALA	CA-C	-5.28	1.46	1.52
2	D	224	HIS	CA-C	-5.26	1.46	1.52
2	B	224	HIS	CA-C	-5.25	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	172	VAL	CA-C	-5.23	1.46	1.52
2	D	172	VAL	CA-C	-5.19	1.46	1.52

All (385) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	161	HIS	N-CA-C	10.41	123.60	111.11
2	D	161	HIS	N-CA-C	10.40	123.59	111.11
1	C	117	PHE	CA-CB-CG	-9.89	103.91	113.80
1	A	117	PHE	CA-CB-CG	-9.89	103.91	113.80
2	D	224	HIS	CA-C-N	-9.64	106.62	122.82
2	D	224	HIS	C-N-CA	-9.64	106.62	122.82
2	B	224	HIS	CA-C-N	-9.61	106.67	122.82
2	B	224	HIS	C-N-CA	-9.61	106.67	122.82
2	B	81	HIS	CA-CB-CG	9.26	123.06	113.80
2	D	81	HIS	CA-CB-CG	9.21	123.01	113.80
1	A	46	PHE	N-CA-C	9.12	124.06	113.38
1	C	46	PHE	N-CA-C	9.10	124.03	113.38
2	B	76	HIS	CA-CB-CG	-9.00	104.80	113.80
2	D	76	HIS	CA-CB-CG	-8.99	104.81	113.80
1	C	258	THR	CB-CA-C	8.82	127.98	110.42
1	A	258	THR	CB-CA-C	8.80	127.94	110.42
2	D	46	PHE	N-CA-C	8.67	123.33	112.24
2	B	46	PHE	N-CA-C	8.66	123.33	112.24
2	B	69	ALA	N-CA-C	8.57	123.17	110.48
2	D	69	ALA	N-CA-C	8.56	123.15	110.48
1	A	121	MET	N-CA-C	8.53	121.34	111.11
1	C	121	MET	N-CA-C	8.51	121.32	111.11
1	A	308	ILE	CB-CA-C	-8.40	101.03	112.04
1	C	308	ILE	CB-CA-C	-8.40	101.04	112.04
1	C	178	SER	N-CA-C	-8.07	102.42	111.71
2	D	259	ASP	N-CA-CB	8.07	124.14	110.49
1	A	178	SER	N-CA-C	-8.07	102.43	111.71
2	D	75	ASN	N-CA-CB	-8.06	99.30	111.64
2	B	259	ASP	N-CA-CB	8.06	124.11	110.49
2	D	284	ARG	CB-CA-C	7.94	123.93	110.74
2	B	284	ARG	CB-CA-C	7.94	123.92	110.74
1	C	174	ALA	CA-C-N	7.91	131.85	122.44
1	C	174	ALA	C-N-CA	7.91	131.85	122.44
1	A	174	ALA	CA-C-N	7.89	131.82	122.44
1	A	174	ALA	C-N-CA	7.89	131.82	122.44
2	B	141	THR	N-CA-CB	-7.87	100.12	110.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	141	THR	N-CA-CB	-7.85	100.15	110.59
1	A	74	ALA	CA-C-N	-7.76	104.19	122.20
1	A	74	ALA	C-N-CA	-7.76	104.19	122.20
1	C	74	ALA	CA-C-N	-7.74	104.24	122.20
1	C	74	ALA	C-N-CA	-7.74	104.24	122.20
2	B	70	LYS	N-CA-C	-7.64	100.44	110.53
2	D	70	LYS	N-CA-C	-7.64	100.44	110.53
2	B	103	PHE	N-CA-C	7.57	122.25	107.57
2	D	103	PHE	N-CA-C	7.56	122.24	107.57
1	C	75	ALA	CA-C-N	-7.54	111.25	121.66
1	C	75	ALA	C-N-CA	-7.54	111.25	121.66
2	B	132	HIS	CA-CB-CG	-7.54	106.26	113.80
1	C	11	GLN	CA-C-N	7.54	125.09	119.66
1	C	11	GLN	C-N-CA	7.54	125.09	119.66
1	A	11	GLN	CA-C-N	7.53	125.08	119.66
1	A	11	GLN	C-N-CA	7.53	125.08	119.66
1	A	75	ALA	CA-C-N	-7.52	111.28	121.66
1	A	75	ALA	C-N-CA	-7.52	111.28	121.66
2	D	132	HIS	CA-CB-CG	-7.51	106.29	113.80
1	A	230	THR	N-CA-C	7.50	121.72	109.72
1	C	230	THR	N-CA-C	7.49	121.69	109.72
1	C	151	ILE	N-CA-CB	7.46	122.23	112.60
2	D	90	ALA	N-CA-C	7.46	119.06	111.07
1	A	322	ASN	CA-C-N	-7.45	113.38	123.14
1	A	322	ASN	C-N-CA	-7.45	113.38	123.14
2	B	90	ALA	N-CA-C	7.44	119.03	111.07
1	C	322	ASN	CA-C-N	-7.43	113.40	123.14
1	C	322	ASN	C-N-CA	-7.43	113.40	123.14
1	A	151	ILE	N-CA-CB	7.43	122.19	112.60
1	C	263	ASP	N-CA-C	7.39	126.54	110.80
1	A	263	ASP	N-CA-C	7.38	126.51	110.80
2	D	152	SER	N-CA-CB	7.30	122.66	110.77
2	B	152	SER	N-CA-CB	7.28	122.64	110.77
2	D	300	GLU	N-CA-C	7.26	119.82	111.11
2	B	300	GLU	N-CA-C	7.25	119.81	111.11
2	D	254	SER	N-CA-C	7.22	120.57	111.69
2	B	254	SER	N-CA-C	7.22	120.57	111.69
1	C	225	CYS	N-CA-C	7.20	121.31	109.06
1	A	225	CYS	N-CA-C	7.19	121.28	109.06
1	A	209	ASN	N-CA-C	7.16	118.73	111.07
1	C	209	ASN	N-CA-C	7.14	118.71	111.07
1	A	267	THR	N-CA-C	-7.13	103.68	112.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	267	THR	N-CA-C	-7.13	103.68	112.88
1	C	139	PHE	N-CA-C	7.11	121.06	112.38
1	A	139	PHE	N-CA-C	7.09	121.03	112.38
1	C	346	ASP	CA-C-N	-7.08	115.65	123.16
1	C	346	ASP	C-N-CA	-7.08	115.65	123.16
2	D	119	ARG	CB-CA-C	7.06	119.54	109.38
2	B	119	ARG	CB-CA-C	7.05	119.54	109.38
1	A	346	ASP	CA-C-N	-7.05	115.69	123.16
1	A	346	ASP	C-N-CA	-7.05	115.69	123.16
1	A	342	LEU	CA-C-O	6.93	127.89	120.55
1	C	190	MET	N-CA-C	6.92	119.59	109.07
1	C	342	LEU	CA-C-O	6.92	127.88	120.55
1	A	190	MET	N-CA-C	6.87	119.52	109.07
1	C	45	HIS	N-CA-C	6.82	120.95	109.76
1	A	45	HIS	N-CA-C	6.82	120.94	109.76
1	C	340	MET	N-CA-CB	6.80	120.12	110.67
1	A	263	ASP	CA-C-N	-6.80	113.68	122.79
1	A	263	ASP	C-N-CA	-6.80	113.68	122.79
1	C	263	ASP	CA-C-N	-6.79	113.69	122.79
1	C	263	ASP	C-N-CA	-6.79	113.69	122.79
1	A	340	MET	N-CA-CB	6.78	120.10	110.67
1	A	111	ASP	CA-CB-CG	-6.75	105.85	112.60
1	C	111	ASP	CA-CB-CG	-6.75	105.85	112.60
1	A	291	ARG	N-CA-C	6.69	120.55	110.64
1	C	291	ARG	N-CA-C	6.68	120.53	110.64
2	B	68	ASN	N-CA-C	6.68	121.81	112.93
2	B	6	PHE	CB-CA-C	6.67	120.47	109.72
2	B	171	PHE	CA-CB-CG	-6.67	107.13	113.80
2	D	68	ASN	N-CA-C	6.67	121.80	112.93
2	D	6	PHE	CB-CA-C	6.66	120.45	109.72
2	D	171	PHE	CA-CB-CG	-6.66	107.14	113.80
1	A	103	PHE	N-CA-C	6.62	119.55	109.62
2	D	245	VAL	N-CA-C	-6.59	104.33	110.53
2	B	245	VAL	N-CA-C	-6.58	104.34	110.53
1	C	103	PHE	N-CA-C	6.58	119.49	109.62
1	C	223	ASP	CA-CB-CG	-6.52	106.08	112.60
1	A	223	ASP	CA-CB-CG	-6.51	106.09	112.60
2	D	20	VAL	N-CA-CB	6.50	117.73	110.51
2	B	20	VAL	N-CA-CB	6.50	117.73	110.51
2	B	98	GLU	CB-CA-C	-6.49	103.17	111.86
2	D	98	GLU	CB-CA-C	-6.47	103.19	111.86
2	B	156	ILE	CB-CA-C	-6.45	102.30	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	346	ASP	N-CA-C	6.44	121.30	113.38
1	C	346	ASP	N-CA-C	6.44	121.30	113.38
2	D	156	ILE	CB-CA-C	-6.44	102.32	111.40
2	D	318	ASN	CA-CB-CG	6.44	119.04	112.60
2	B	317	ALA	N-CA-CB	6.41	121.33	110.49
2	B	318	ASN	CA-CB-CG	6.40	119.00	112.60
2	B	233	ASN	CA-CB-CG	6.40	119.00	112.60
2	D	233	ASN	CA-CB-CG	6.40	119.00	112.60
1	A	228	TYR	CB-CA-C	-6.38	96.44	110.67
2	D	317	ALA	N-CA-CB	6.38	121.27	110.49
2	B	153	PHE	CA-C-N	-6.36	114.10	120.21
2	B	153	PHE	C-N-CA	-6.36	114.10	120.21
1	C	41	LEU	N-CA-C	6.36	119.30	109.07
1	C	228	TYR	CB-CA-C	-6.36	96.50	110.67
1	A	41	LEU	N-CA-C	6.35	119.29	109.07
2	D	153	PHE	CA-C-N	-6.32	114.15	120.21
2	D	153	PHE	C-N-CA	-6.32	114.15	120.21
2	D	299	PHE	CA-C-N	6.29	129.04	120.54
2	D	299	PHE	C-N-CA	6.29	129.04	120.54
2	B	299	PHE	CA-C-N	6.28	129.01	120.54
2	B	299	PHE	C-N-CA	6.28	129.01	120.54
2	D	250	PHE	CA-CB-CG	-6.28	107.53	113.80
2	B	250	PHE	CA-CB-CG	-6.26	107.54	113.80
2	D	128	PHE	CA-C-N	6.26	129.51	120.38
2	D	128	PHE	C-N-CA	6.26	129.51	120.38
2	B	128	PHE	CA-C-N	6.25	129.50	120.38
2	B	128	PHE	C-N-CA	6.25	129.50	120.38
2	B	13	SER	N-CA-C	-6.24	105.16	112.89
2	D	237	GLU	N-CA-CB	6.23	119.93	110.28
2	D	13	SER	N-CA-C	-6.22	105.18	112.89
1	A	197	ASN	CA-CB-CG	-6.21	106.39	112.60
2	B	237	GLU	N-CA-CB	6.21	119.91	110.28
1	C	197	ASN	CA-CB-CG	-6.21	106.39	112.60
2	D	81	HIS	N-CA-CB	-6.18	101.53	110.87
2	B	311	VAL	CB-CA-C	6.18	120.12	112.02
2	D	311	VAL	CB-CA-C	6.18	120.11	112.02
2	B	81	HIS	N-CA-CB	-6.16	101.58	110.87
1	A	258	THR	CA-C-O	6.15	129.30	120.51
1	A	350	TYR	N-CA-C	6.15	123.89	110.80
2	B	275	THR	N-CA-C	-6.13	100.63	110.14
1	C	350	TYR	N-CA-C	6.13	123.85	110.80
2	D	275	THR	N-CA-C	-6.13	100.64	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	258	THR	CA-C-O	6.12	129.26	120.51
1	A	328	GLU	N-CA-C	6.07	119.79	112.38
1	A	346	ASP	CA-CB-CG	-6.07	106.53	112.60
1	C	346	ASP	CA-CB-CG	-6.07	106.53	112.60
1	C	328	GLU	N-CA-C	6.04	119.75	112.38
1	A	237	ASN	CA-CB-CG	6.01	118.61	112.60
1	C	237	ASN	CA-CB-CG	6.00	118.60	112.60
2	B	221	GLN	N-CA-C	5.99	119.06	111.69
2	D	221	GLN	N-CA-C	5.96	119.02	111.69
1	C	258	THR	CA-C-N	5.90	132.81	121.54
1	C	258	THR	C-N-CA	5.90	132.81	121.54
1	A	258	THR	CA-C-N	5.89	132.80	121.54
1	A	258	THR	C-N-CA	5.89	132.80	121.54
2	D	284	ARG	N-CA-CB	5.89	119.39	109.78
2	B	284	ARG	N-CA-CB	5.89	119.38	109.78
2	B	75	ASN	N-CA-CB	-5.89	99.29	111.36
2	D	82	HIS	CA-CB-CG	-5.88	107.92	113.80
1	A	299	ASN	CA-CB-CG	5.88	118.48	112.60
2	D	29	HIS	CA-CB-CG	-5.88	107.92	113.80
2	B	82	HIS	CA-CB-CG	-5.87	107.93	113.80
2	B	29	HIS	CA-CB-CG	-5.86	107.94	113.80
1	A	76	ILE	N-CA-CB	5.83	116.89	110.53
1	C	299	ASN	CA-CB-CG	5.83	118.44	112.60
1	A	220	THR	N-CA-CB	-5.83	101.53	110.16
2	D	38	THR	CA-C-O	-5.83	114.47	120.89
2	D	308	GLN	CB-CA-C	-5.83	101.11	110.79
2	B	308	GLN	CB-CA-C	-5.83	101.11	110.79
1	A	230	THR	N-CA-CB	-5.82	101.12	111.08
1	C	220	THR	N-CA-CB	-5.82	101.55	110.16
1	A	160	PRO	CA-C-N	-5.81	113.48	122.09
1	A	160	PRO	C-N-CA	-5.81	113.48	122.09
1	C	230	THR	N-CA-CB	-5.81	101.14	111.08
1	A	103	PHE	N-CA-CB	-5.81	103.44	110.53
2	B	38	THR	CA-C-O	-5.81	114.50	120.89
1	A	161	SER	CB-CA-C	5.80	119.11	109.53
1	C	161	SER	CB-CA-C	5.80	119.10	109.53
2	B	173	ASN	CA-C-N	5.80	130.86	122.16
2	B	173	ASN	C-N-CA	5.80	130.86	122.16
2	D	173	ASN	CA-C-N	5.80	130.86	122.16
2	D	173	ASN	C-N-CA	5.80	130.86	122.16
1	C	103	PHE	N-CA-CB	-5.79	103.46	110.53
1	C	160	PRO	CA-C-N	-5.79	113.52	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	160	PRO	C-N-CA	-5.79	113.52	122.09
1	C	49	PHE	CA-CB-CG	5.79	119.58	113.80
2	D	239	ALA	CA-C-O	5.79	126.64	120.10
2	B	239	ALA	CA-C-O	5.78	126.63	120.10
1	C	76	ILE	N-CA-CB	5.78	116.83	110.53
2	B	260	PHE	N-CA-C	-5.77	104.18	111.11
2	D	260	PHE	N-CA-C	-5.77	104.19	111.11
2	B	165	GLU	N-CA-CB	5.77	118.62	109.51
2	D	165	GLU	N-CA-CB	5.77	118.62	109.51
2	B	70	LYS	CA-C-N	-5.76	114.93	122.94
2	B	70	LYS	C-N-CA	-5.76	114.93	122.94
2	D	70	LYS	CA-C-N	-5.76	114.94	122.94
2	D	70	LYS	C-N-CA	-5.76	114.94	122.94
1	A	7	LEU	N-CA-C	5.75	117.78	108.41
1	C	7	LEU	N-CA-C	5.75	117.78	108.41
2	B	191	VAL	CB-CA-C	5.75	118.18	110.42
1	A	174	ALA	O-C-N	5.75	130.03	123.31
1	A	49	PHE	CA-CB-CG	5.74	119.54	113.80
2	D	278	GLU	CA-C-N	5.74	128.22	120.65
2	D	278	GLU	C-N-CA	5.74	128.22	120.65
2	B	278	GLU	CA-C-N	5.73	128.22	120.65
2	B	278	GLU	C-N-CA	5.73	128.22	120.65
2	D	191	VAL	CB-CA-C	5.73	118.16	110.42
1	C	174	ALA	O-C-N	5.71	129.99	123.31
2	B	32	ASP	CA-CB-CG	5.70	118.30	112.60
2	D	32	ASP	CA-CB-CG	5.70	118.30	112.60
2	D	189	PRO	CB-CA-C	-5.68	103.79	111.12
1	A	248	GLY	N-CA-C	-5.67	99.73	113.18
2	B	303	GLU	N-CA-C	5.66	117.13	111.07
1	C	248	GLY	N-CA-C	-5.66	99.76	113.18
2	D	303	GLU	N-CA-C	5.66	117.13	111.07
2	B	189	PRO	CB-CA-C	-5.65	103.84	111.12
2	D	189	PRO	N-CA-CB	5.62	108.68	103.39
2	B	189	PRO	N-CA-CB	5.61	108.67	103.39
2	B	173	ASN	CA-CB-CG	5.58	118.18	112.60
2	B	171	PHE	N-CA-CB	5.58	121.16	111.39
2	D	171	PHE	N-CA-CB	5.57	121.14	111.39
2	D	173	ASN	CA-CB-CG	5.57	118.17	112.60
2	B	181	GLU	CB-CG-CD	5.56	122.05	112.60
1	C	151	ILE	CB-CA-C	-5.56	103.58	111.19
1	A	232	VAL	N-CA-C	5.55	115.78	107.51
2	D	181	GLU	CB-CG-CD	5.55	122.03	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	26	ASN	CA-CB-CG	-5.55	107.05	112.60
2	B	62	LEU	CB-CA-C	-5.54	101.43	110.85
2	D	62	LEU	CB-CA-C	-5.54	101.43	110.85
1	A	151	ILE	CB-CA-C	-5.54	103.60	111.19
2	D	2	LYS	N-CA-C	5.54	118.85	109.76
1	C	26	ASN	CA-CB-CG	-5.53	107.07	112.60
1	C	232	VAL	N-CA-C	5.53	115.75	107.51
1	C	37	ASP	N-CA-C	5.53	119.72	112.92
2	B	2	LYS	N-CA-C	5.53	118.83	109.76
1	A	37	ASP	N-CA-C	5.49	119.68	112.92
1	A	328	GLU	CA-C-N	5.48	128.17	120.28
1	A	328	GLU	C-N-CA	5.48	128.17	120.28
1	C	328	GLU	CA-C-N	5.47	128.15	120.28
1	C	328	GLU	C-N-CA	5.47	128.15	120.28
2	D	81	HIS	N-CA-C	5.41	117.47	109.69
2	B	174	ALA	CB-CA-C	-5.40	103.60	112.03
1	A	226	LEU	CB-CA-C	-5.38	101.93	110.81
2	D	174	ALA	CB-CA-C	-5.38	103.64	112.03
2	D	74	LEU	N-CA-C	5.38	116.94	111.14
2	B	81	HIS	N-CA-C	5.37	117.42	109.69
2	B	74	LEU	N-CA-C	5.37	116.94	111.14
1	C	226	LEU	CB-CA-C	-5.37	101.95	110.81
2	D	130	GLU	CB-CG-CD	5.37	121.72	112.60
2	B	312	ILE	N-CA-C	5.36	115.99	110.36
2	D	312	ILE	N-CA-C	5.36	115.99	110.36
2	B	130	GLU	CB-CG-CD	5.36	121.70	112.60
1	C	78	LEU	N-CA-C	5.35	121.63	109.81
1	A	78	LEU	N-CA-C	5.34	121.62	109.81
1	C	229	ILE	N-CA-C	-5.34	100.79	108.48
1	A	80	THR	N-CA-C	5.34	122.17	110.80
1	A	168	ALA	CA-C-N	5.34	125.59	119.83
1	A	168	ALA	C-N-CA	5.34	125.59	119.83
2	D	182	TRP	N-CA-CB	-5.34	101.99	109.94
1	C	168	ALA	CA-C-N	5.33	125.59	119.83
1	C	168	ALA	C-N-CA	5.33	125.59	119.83
1	A	229	ILE	N-CA-C	-5.33	100.80	108.48
2	D	188	LEU	CA-C-N	5.33	125.62	119.92
2	D	188	LEU	C-N-CA	5.33	125.62	119.92
1	C	80	THR	N-CA-C	5.32	122.14	110.80
2	B	188	LEU	CA-C-N	5.31	125.61	119.92
2	B	188	LEU	C-N-CA	5.31	125.61	119.92
2	B	182	TRP	N-CA-CB	-5.30	102.04	109.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	193	ARG	N-CA-C	5.29	117.37	109.59
2	B	193	ARG	N-CA-C	5.27	117.34	109.59
2	B	215	HIS	CA-CB-CG	-5.27	108.53	113.80
2	D	215	HIS	CA-CB-CG	-5.27	108.53	113.80
2	B	92	LEU	CA-C-N	5.26	127.33	120.28
2	B	92	LEU	C-N-CA	5.26	127.33	120.28
2	D	92	LEU	CA-C-N	5.26	127.33	120.28
2	D	92	LEU	C-N-CA	5.26	127.33	120.28
2	D	52	VAL	N-CA-C	5.25	115.69	108.12
2	B	52	VAL	N-CA-C	5.24	115.67	108.12
2	B	170	GLN	CB-CA-C	-5.23	100.29	109.71
2	B	82	HIS	CB-CA-C	-5.23	105.73	110.44
2	D	288	GLU	N-CA-CB	5.23	117.73	109.94
2	D	82	HIS	CB-CA-C	-5.22	105.74	110.44
1	C	225	CYS	O-C-N	5.22	129.64	123.33
2	B	288	GLU	N-CA-CB	5.21	117.71	109.94
1	A	225	CYS	O-C-N	5.21	129.64	123.33
2	B	289	CYS	N-CA-C	5.21	117.70	111.71
2	D	170	GLN	CB-CA-C	-5.21	100.33	109.71
2	D	289	CYS	N-CA-C	5.21	117.70	111.71
1	C	154	PRO	CB-CA-C	-5.20	103.42	110.60
1	A	296	TYR	CA-C-O	5.20	125.77	119.11
1	C	296	TYR	CA-C-O	5.20	125.77	119.11
1	A	154	PRO	CB-CA-C	-5.20	103.43	110.60
1	A	172	VAL	CA-C-N	-5.20	116.50	122.95
1	A	172	VAL	C-N-CA	-5.20	116.50	122.95
2	D	26	ASP	CA-C-N	5.20	127.51	120.44
2	D	26	ASP	C-N-CA	5.20	127.51	120.44
2	B	26	ASP	CA-C-N	5.20	127.51	120.44
2	B	26	ASP	C-N-CA	5.20	127.51	120.44
2	B	106	SER	N-CA-C	5.19	116.33	108.07
1	C	191	ILE	N-CA-CB	5.19	118.31	111.25
1	C	68	THR	N-CA-CB	-5.19	104.00	110.90
1	C	163	TYR	CB-CA-C	-5.19	101.07	110.56
1	C	264	SER	N-CA-CB	5.19	118.26	110.11
2	D	106	SER	N-CA-C	5.19	116.32	108.07
2	B	237	GLU	CA-C-N	5.18	127.49	120.44
2	B	237	GLU	C-N-CA	5.18	127.49	120.44
1	A	163	TYR	CB-CA-C	-5.18	101.08	110.56
1	C	172	VAL	CA-C-N	-5.18	116.53	122.95
1	C	172	VAL	C-N-CA	-5.18	116.53	122.95
2	D	38	THR	O-C-N	5.17	129.27	123.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	237	GLU	CA-C-N	5.17	127.47	120.44
2	D	237	GLU	C-N-CA	5.17	127.47	120.44
1	A	68	THR	N-CA-CB	-5.17	104.03	110.90
1	A	264	SER	N-CA-CB	5.16	118.21	110.11
1	A	191	ILE	N-CA-CB	5.16	118.26	111.25
1	C	153	PHE	CA-C-N	5.15	125.36	120.31
1	C	153	PHE	C-N-CA	5.15	125.36	120.31
2	B	38	THR	O-C-N	5.14	129.24	123.48
2	B	313	ASP	CA-CB-CG	-5.12	107.47	112.60
2	D	313	ASP	CA-CB-CG	-5.12	107.48	112.60
1	A	153	PHE	CA-C-N	5.11	125.32	120.31
1	A	153	PHE	C-N-CA	5.11	125.32	120.31
2	B	162	ALA	N-CA-CB	5.11	119.13	110.49
2	D	259	ASP	CA-CB-CG	-5.11	107.49	112.60
1	A	320	ILE	CB-CA-C	-5.11	103.26	111.59
1	C	126	ALA	O-C-N	5.11	127.34	122.03
2	D	162	ALA	N-CA-CB	5.11	119.12	110.49
1	C	347	VAL	N-CA-C	-5.10	107.59	111.62
2	B	157	SER	N-CA-C	-5.10	101.96	110.17
1	A	178	SER	CA-C-O	5.10	125.86	120.10
2	B	258	THR	CA-C-O	5.10	125.68	119.05
2	B	237	GLU	O-C-N	5.10	128.54	122.27
1	C	320	ILE	CB-CA-C	-5.10	103.28	111.59
2	D	237	GLU	O-C-N	5.10	128.54	122.27
1	C	216	GLY	N-CA-C	5.10	122.75	114.90
1	A	126	ALA	O-C-N	5.09	127.33	122.03
2	D	157	SER	N-CA-C	-5.09	101.98	110.17
2	B	259	ASP	CA-CB-CG	-5.08	107.52	112.60
2	D	171	PHE	CA-C-N	-5.08	114.14	122.67
2	D	171	PHE	C-N-CA	-5.08	114.14	122.67
1	A	216	GLY	N-CA-C	5.08	122.72	114.90
2	B	145	HIS	CA-C-N	5.07	126.18	119.84
2	B	145	HIS	C-N-CA	5.07	126.18	119.84
2	D	36	PHE	N-CA-C	-5.07	101.70	109.76
2	B	171	PHE	CA-C-N	-5.07	114.16	122.67
2	B	171	PHE	C-N-CA	-5.07	114.16	122.67
1	A	234	HIS	CA-CB-CG	-5.06	108.74	113.80
2	D	145	HIS	CA-C-N	5.06	126.17	119.84
2	D	145	HIS	C-N-CA	5.06	126.17	119.84
2	D	258	THR	CA-C-O	5.06	125.63	119.05
2	B	225	LYS	O-C-N	5.06	129.87	122.94
1	C	178	SER	CA-C-O	5.06	125.82	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	36	PHE	N-CA-C	-5.05	101.73	109.76
2	D	305	LYS	N-CA-C	5.05	116.79	111.28
1	A	258	THR	N-CA-CB	5.05	119.02	110.49
1	A	347	VAL	N-CA-C	-5.05	107.63	111.62
2	B	305	LYS	N-CA-C	5.04	116.78	111.28
1	C	234	HIS	CA-CB-CG	-5.04	108.76	113.80
2	D	225	LYS	O-C-N	5.03	129.83	122.94
1	C	258	THR	N-CA-CB	5.02	118.98	110.49
2	B	46	PHE	CB-CA-C	-5.01	103.59	111.51
2	D	79	THR	N-CA-CB	5.01	117.48	110.12
2	D	85	ARG	N-CA-C	-5.00	105.71	111.07
2	D	151	TYR	CA-CB-CG	5.00	122.91	113.90
2	D	41	VAL	N-CA-CB	-5.00	104.51	111.41

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	284	ARG	CA
2	B	317	ALA	CA
2	D	284	ARG	CA
2	D	317	ALA	CA

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2679	0	2552	263	2
1	C	2679	0	2552	255	15
2	B	2498	0	2362	168	0
2	D	2498	0	2362	164	11
3	A	5	0	0	2	0
4	A	28	0	0	3	0
4	B	45	0	0	1	2
All	All	10432	0	9828	827	15

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 41.

All (827) 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:A:266:GLN:HG3	1:A:268:LYS:HB3	1.50	0.94
1:C:266:GLN:HG3	1:C:268:LYS:HB3	1.50	0.94
2:D:181:GLU:HG3	2:D:182:TRP:H	1.33	0.94
1:A:106:CYS:HB2	1:A:173:VAL:HG22	1.51	0.92
1:C:106:CYS:HB2	1:C:173:VAL:HG22	1.51	0.91
2:D:114:MET:HE3	2:D:119:ARG:HB3	1.53	0.91
2:D:43:GLU:HB2	2:D:55:PRO:HG3	1.52	0.91
2:B:181:GLU:HG3	2:B:182:TRP:H	1.33	0.90
1:A:47:THR:HG22	1:A:49:PHE:H	1.36	0.90
1:C:157:GLN:NE2	1:C:159:ASN:HD21	1.68	0.90
2:D:82:HIS:HD2	2:D:84:VAL:H	1.18	0.90
2:B:114:MET:HE3	2:B:119:ARG:HB3	1.53	0.90
1:A:157:GLN:NE2	1:A:159:ASN:HD21	1.68	0.90
1:C:47:THR:HG22	1:C:49:PHE:H	1.36	0.89
2:B:82:HIS:HD2	2:B:84:VAL:H	1.18	0.89
1:A:156:ILE:HD13	2:B:46:PHE:CE1	2.07	0.89
1:A:157:GLN:HE21	1:A:159:ASN:HD21	1.18	0.89
1:C:157:GLN:HE21	1:C:159:ASN:HD21	1.18	0.89
2:B:43:GLU:HB2	2:B:55:PRO:HG3	1.52	0.88
1:C:156:ILE:HD13	2:D:46:PHE:CE1	2.07	0.88
1:C:129:ASP:HA	1:C:182:TRP:CZ2	2.09	0.88
1:A:129:ASP:HA	1:A:182:TRP:CZ2	2.09	0.87
2:B:146:PRO:HG3	2:B:153:PHE:CZ	2.10	0.87
1:C:73:THR:HB	1:C:76:ILE:HD12	1.56	0.87
1:A:106:CYS:HB2	1:A:173:VAL:CG2	2.04	0.87
1:A:226:LEU:HB2	1:A:323:ILE:HG22	1.55	0.87
1:C:106:CYS:HB2	1:C:173:VAL:CG2	2.04	0.87
2:D:146:PRO:HG3	2:D:153:PHE:CZ	2.09	0.87
1:C:354:LYS:HE2	1:C:355:GLN:HB3	1.57	0.87
1:A:73:THR:HB	1:A:76:ILE:HD12	1.56	0.87
1:A:354:LYS:HE2	1:A:355:GLN:HB3	1.57	0.86
1:A:205:LEU:HD13	1:A:318:THR:HG22	1.57	0.86
1:C:226:LEU:HB2	1:C:323:ILE:HG22	1.55	0.86
1:C:205:LEU:HD13	1:C:318:THR:HG22	1.57	0.85
1:A:226:LEU:HD12	1:A:323:ILE:CG2	2.07	0.85
1:A:3:PHE:CD2	1:A:348:MET:HE2	2.12	0.84
1:A:36:PHE:CE2	1:A:340:MET:HE3	2.13	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3:PHE:CD2	1:C:348:MET:HE2	2.12	0.84
1:C:36:PHE:CE2	1:C:340:MET:HE3	2.13	0.84
1:C:226:LEU:HD12	1:C:323:ILE:CG2	2.07	0.84
2:D:146:PRO:HG3	2:D:153:PHE:CE1	2.14	0.82
2:B:184:ALA:HB2	2:B:208:TYR:CD1	2.15	0.82
2:B:146:PRO:HG3	2:B:153:PHE:CE1	2.14	0.81
2:D:184:ALA:HB2	2:D:208:TYR:CD1	2.15	0.81
1:A:226:LEU:HD12	1:A:323:ILE:HG22	1.63	0.81
2:B:106:SER:HB2	2:B:173:ASN:HB3	1.64	0.80
1:C:251:TYR:O	1:C:255:VAL:HG23	1.82	0.80
1:C:180:THR:HG23	1:C:190:MET:HE1	1.64	0.80
2:D:106:SER:HB2	2:D:173:ASN:HB3	1.64	0.80
1:C:153:PHE:HB2	2:D:116:PHE:CE2	2.17	0.79
1:A:153:PHE:HB2	2:B:116:PHE:CE2	2.17	0.79
1:A:251:TYR:O	1:A:255:VAL:HG23	1.82	0.79
1:C:92:LEU:HD13	1:C:160:PRO:HD3	1.65	0.79
2:B:85:ARG:O	2:B:89:GLU:HG3	1.83	0.78
1:A:180:THR:HG23	1:A:190:MET:HE1	1.64	0.78
1:C:226:LEU:HD12	1:C:323:ILE:HG22	1.63	0.78
2:D:85:ARG:O	2:D:89:GLU:HG3	1.83	0.78
2:D:181:GLU:HG3	2:D:182:TRP:N	1.98	0.78
1:A:92:LEU:HD13	1:A:160:PRO:HD3	1.65	0.78
1:C:156:ILE:HD13	2:D:46:PHE:HE1	1.49	0.77
2:D:139:PHE:CE2	2:D:168:PRO:HD2	2.19	0.77
2:B:139:PHE:CE2	2:B:168:PRO:HD2	2.19	0.77
2:B:181:GLU:HG3	2:B:182:TRP:N	1.98	0.77
1:A:156:ILE:HD13	2:B:46:PHE:HE1	1.49	0.76
1:C:108:GLY:C	1:C:109:LEU:HD23	2.11	0.76
2:D:17:SER:O	2:D:21:ILE:HD12	1.86	0.76
1:C:208:TYR:CE2	1:C:224:HIS:HE1	2.04	0.75
2:D:217:VAL:HG23	2:D:219:VAL:HG13	1.66	0.75
1:A:73:THR:CB	1:A:76:ILE:HD12	2.17	0.75
1:A:208:TYR:CE2	1:A:224:HIS:HE1	2.04	0.75
1:C:134:LEU:HA	1:C:137:GLU:OE1	1.87	0.75
1:C:191:ILE:HG23	1:C:225:CYS:HB3	1.69	0.75
1:A:134:LEU:HA	1:A:137:GLU:OE1	1.87	0.75
1:A:108:GLY:C	1:A:109:LEU:HD23	2.11	0.75
2:B:217:VAL:HG23	2:B:219:VAL:HG13	1.66	0.74
1:C:123:ASN:HB2	1:C:127:LEU:CD1	2.17	0.74
1:A:191:ILE:HG23	1:A:225:CYS:HB3	1.69	0.74
2:B:123:SER:HA	2:B:126:GLN:NE2	2.03	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:ASN:HB2	1:A:127:LEU:CD1	2.17	0.74
1:C:73:THR:CB	1:C:76:ILE:HD12	2.17	0.74
1:A:121:MET:HE1	1:A:267:THR:HG21	1.70	0.74
2:B:207:LEU:HD12	2:B:207:LEU:O	1.88	0.74
1:A:157:GLN:HE21	1:A:159:ASN:ND2	1.87	0.73
2:D:207:LEU:HD12	2:D:207:LEU:O	1.88	0.73
2:B:17:SER:O	2:B:21:ILE:HD12	1.86	0.73
1:C:129:ASP:HA	1:C:182:TRP:HZ2	1.51	0.73
1:C:121:MET:HE1	1:C:267:THR:HG21	1.70	0.73
2:D:123:SER:HA	2:D:126:GLN:NE2	2.03	0.73
1:C:27:LEU:N	1:C:27:LEU:HD23	2.03	0.72
2:D:119:ARG:HG2	2:D:127:LEU:HD21	1.71	0.72
1:A:184:ALA:HB2	1:A:208:TYR:CD1	2.25	0.72
1:C:157:GLN:HE21	1:C:159:ASN:ND2	1.87	0.72
1:A:89:ASP:O	1:A:93:LEU:HB2	1.89	0.72
1:C:336:ILE:O	1:C:340:MET:HG2	1.89	0.71
2:B:184:ALA:HA	2:B:208:TYR:CE1	2.25	0.71
1:C:89:ASP:O	1:C:93:LEU:HB2	1.89	0.71
2:B:119:ARG:HG2	2:B:127:LEU:HD21	1.71	0.71
1:C:184:ALA:HB2	1:C:208:TYR:CD1	2.25	0.71
1:A:1:MET:HB2	1:A:321:ASP:O	1.90	0.71
1:A:336:ILE:O	1:A:340:MET:HG2	1.89	0.71
2:D:82:HIS:CD2	2:D:84:VAL:HG23	2.26	0.71
1:A:27:LEU:N	1:A:27:LEU:HD23	2.03	0.71
1:A:205:LEU:CD1	1:A:318:THR:HG22	2.21	0.71
2:D:184:ALA:HA	2:D:208:TYR:CE1	2.25	0.71
1:C:1:MET:HB2	1:C:321:ASP:O	1.90	0.71
1:A:129:ASP:HA	1:A:182:TRP:HZ2	1.51	0.70
1:A:129:ASP:HB2	1:A:182:TRP:NE1	2.07	0.70
1:C:45:HIS:HB3	1:C:46:PHE:CE1	2.27	0.70
1:C:184:ALA:HA	1:C:208:TYR:CE1	2.26	0.70
1:A:23:ARG:O	1:A:27:LEU:HG	1.92	0.70
1:A:45:HIS:HB3	1:A:46:PHE:CE1	2.27	0.70
1:C:259:LYS:HG3	1:C:260:ILE:N	2.07	0.70
1:A:259:LYS:HG3	1:A:260:ILE:N	2.07	0.70
1:C:129:ASP:HB2	1:C:182:TRP:NE1	2.07	0.70
1:C:205:LEU:CD1	1:C:318:THR:HG22	2.21	0.70
1:A:184:ALA:HA	1:A:208:TYR:CE1	2.26	0.69
2:B:82:HIS:CD2	2:B:84:VAL:HG23	2.26	0.69
2:D:241:ALA:O	2:D:245:VAL:HG23	1.92	0.69
2:D:225:LYS:CG	2:D:294:ASP:HB2	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:276:TYR:O	2:D:280:THR:HG22	1.92	0.69
2:B:225:LYS:CG	2:B:294:ASP:HB2	2.22	0.69
2:B:241:ALA:O	2:B:245:VAL:HG23	1.92	0.69
2:B:276:TYR:O	2:B:280:THR:HG22	1.92	0.69
1:C:184:ALA:HB1	1:C:211:VAL:HB	1.75	0.68
1:C:95:GLN:NE2	1:C:161:SER:O	2.27	0.68
1:A:354:LYS:HG2	1:A:355:GLN:N	2.09	0.68
1:A:184:ALA:HB1	1:A:211:VAL:HB	1.75	0.68
1:C:23:ARG:O	1:C:27:LEU:HG	1.92	0.68
1:C:354:LYS:HG2	1:C:355:GLN:H	1.59	0.68
1:A:123:ASN:HB2	1:A:127:LEU:HD11	1.76	0.68
1:C:123:ASN:HB2	1:C:127:LEU:HD11	1.76	0.68
1:C:354:LYS:HG2	1:C:355:GLN:N	2.09	0.68
1:C:82:HIS:HD2	1:C:84:VAL:H	1.42	0.68
1:C:133:ASP:O	1:C:136:LYS:HB3	1.94	0.67
1:A:82:HIS:HD2	1:A:84:VAL:H	1.42	0.67
1:A:133:ASP:O	1:A:136:LYS:HB3	1.94	0.67
1:C:193:SER:OG	1:C:195:ILE:HB	1.95	0.67
1:A:354:LYS:HG2	1:A:355:GLN:H	1.59	0.67
2:B:82:HIS:CD2	2:B:84:VAL:H	2.09	0.67
1:C:295:SER:O	1:C:299:ASN:ND2	2.28	0.66
1:A:295:SER:O	1:A:299:ASN:ND2	2.28	0.66
1:A:95:GLN:NE2	1:A:161:SER:O	2.27	0.66
1:A:193:SER:OG	1:A:195:ILE:HB	1.95	0.66
1:C:12:PRO:HG2	1:C:15:LEU:HG	1.77	0.66
1:C:69:LEU:HG	1:C:70:ASN:N	2.10	0.66
1:C:42:LEU:HG	1:C:43:GLU:N	2.11	0.66
1:C:323:ILE:HD13	1:C:323:ILE:N	2.11	0.66
1:C:136:LYS:O	1:C:139:PHE:HB2	1.96	0.66
2:D:12:ASN:OD1	2:D:15:ARG:N	2.28	0.65
1:C:129:ASP:HB2	1:C:182:TRP:HE1	1.61	0.65
1:A:1:MET:HE1	1:A:351:LEU:HB3	1.79	0.65
1:A:12:PRO:HG2	1:A:15:LEU:HG	1.77	0.65
2:D:112:ALA:O	2:D:115:ARG:N	2.29	0.65
2:B:112:ALA:O	2:B:115:ARG:N	2.29	0.65
1:A:266:GLN:HG3	1:A:268:LYS:CB	2.26	0.65
2:B:12:ASN:OD1	2:B:15:ARG:N	2.28	0.65
1:A:69:LEU:HG	1:A:70:ASN:N	2.10	0.65
1:A:42:LEU:HG	1:A:43:GLU:N	2.11	0.64
1:A:136:LYS:O	1:A:139:PHE:HB2	1.96	0.64
1:C:82:HIS:O	1:C:86:GLN:HG3	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:17:GLN:O	1:C:21:MET:HG2	1.96	0.64
1:A:17:GLN:O	1:A:21:MET:HG2	1.96	0.64
2:B:146:PRO:HB2	2:B:151:TYR:O	1.98	0.64
1:A:323:ILE:HD13	1:A:323:ILE:N	2.11	0.64
1:A:129:ASP:HB2	1:A:182:TRP:HE1	1.61	0.64
1:A:82:HIS:O	1:A:86:GLN:HG3	1.98	0.64
2:B:107:ASP:OD1	2:B:108:CYS:N	2.29	0.64
1:C:300:PRO:HG3	1:C:311:ILE:CD1	2.28	0.64
2:B:75:ASN:OD1	2:B:75:ASN:N	2.30	0.63
1:C:226:LEU:CB	1:C:323:ILE:HG22	2.27	0.63
2:D:146:PRO:HB2	2:D:151:TYR:O	1.98	0.63
2:D:15:ARG:NH2	2:D:300:GLU:O	2.29	0.63
1:A:300:PRO:HG3	1:A:311:ILE:CD1	2.28	0.63
2:D:27:THR:O	2:D:31:VAL:HG23	1.99	0.63
2:D:193:ARG:NH2	2:D:196:ASP:OD1	2.29	0.63
1:C:1:MET:HE1	1:C:351:LEU:HB3	1.78	0.63
1:C:47:THR:CG2	1:C:49:PHE:H	2.11	0.63
2:B:15:ARG:NH2	2:B:300:GLU:O	2.29	0.63
2:B:27:THR:O	2:B:31:VAL:HG23	1.99	0.63
2:D:75:ASN:OD1	2:D:75:ASN:N	2.30	0.63
2:D:10:PHE:CD1	2:D:49:ASN:HA	2.34	0.63
1:A:300:PRO:HG3	1:A:311:ILE:HD11	1.81	0.63
1:C:156:ILE:HB	2:D:46:PHE:CD1	2.34	0.63
1:A:81:ALA:HB3	1:A:86:GLN:NE2	2.14	0.62
1:C:81:ALA:HB3	1:C:86:GLN:NE2	2.14	0.62
2:D:82:HIS:CD2	2:D:84:VAL:H	2.09	0.62
1:A:226:LEU:CB	1:A:323:ILE:HG22	2.27	0.62
2:B:233:ASN:HD22	2:B:234:VAL:N	1.98	0.62
1:C:300:PRO:HG3	1:C:311:ILE:HD11	1.81	0.62
1:C:323:ILE:O	1:C:323:ILE:HG12	1.99	0.62
2:D:107:ASP:OD1	2:D:108:CYS:N	2.29	0.62
1:C:346:ASP:OD1	1:C:346:ASP:N	2.31	0.62
1:A:52:LEU:HD11	1:A:58:ALA:HB2	1.82	0.62
1:A:156:ILE:HB	2:B:46:PHE:CD1	2.34	0.62
2:B:207:LEU:HD12	2:B:207:LEU:C	2.25	0.62
1:A:83:PRO:HD3	1:A:131:TRP:CE2	2.35	0.62
2:B:10:PHE:CD1	2:B:49:ASN:HA	2.34	0.62
2:B:193:ARG:NH2	2:B:196:ASP:OD1	2.29	0.62
1:C:83:PRO:HD3	1:C:131:TRP:CE2	2.35	0.62
1:A:323:ILE:HG12	1:A:323:ILE:O	1.99	0.61
2:D:233:ASN:HD22	2:D:234:VAL:N	1.98	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:266:GLN:HG3	1:C:268:LYS:CB	2.26	0.61
2:B:147:ASN:HA	2:B:152:SER:OG	2.01	0.61
1:A:86:GLN:O	1:A:90:VAL:HG23	2.00	0.61
1:C:23:ARG:NH2	1:C:331:GLY:O	2.27	0.61
1:C:52:LEU:HD11	1:C:58:ALA:HB2	1.82	0.61
2:D:63:LEU:HD12	2:D:93:LEU:HD22	1.82	0.61
1:A:233:ASP:O	1:A:303:THR:HA	2.00	0.61
1:C:86:GLN:O	1:C:90:VAL:HG23	2.00	0.61
1:C:233:ASP:O	1:C:303:THR:HA	2.00	0.61
2:D:119:ARG:HG2	2:D:127:LEU:CD2	2.30	0.61
1:A:47:THR:CG2	1:A:49:PHE:H	2.11	0.61
2:B:84:VAL:O	2:B:88:GLU:HG3	2.00	0.61
1:C:355:GLN:HG2	1:C:355:GLN:OXT	2.01	0.61
2:D:204:TYR:O	2:D:207:LEU:HB3	2.01	0.61
1:A:123:ASN:C	1:A:127:LEU:HD12	2.26	0.60
2:B:114:MET:HE2	2:B:124:GLN:HG3	1.83	0.60
1:C:13:PRO:HD2	1:C:14:GLU:OE1	2.01	0.60
2:B:204:TYR:O	2:B:207:LEU:HB3	2.01	0.60
2:B:2:LYS:HB2	2:B:294:ASP:OD1	2.02	0.60
2:D:63:LEU:HD12	2:D:93:LEU:CD2	2.32	0.60
2:D:84:VAL:O	2:D:88:GLU:HG3	2.00	0.60
2:B:63:LEU:HD12	2:B:93:LEU:HD22	1.82	0.60
2:D:2:LYS:HB2	2:D:294:ASP:OD1	2.02	0.60
1:A:346:ASP:OD1	1:A:346:ASP:N	2.31	0.60
2:B:172:VAL:HG22	2:B:173:ASN:N	2.16	0.60
1:C:123:ASN:C	1:C:127:LEU:HD12	2.26	0.60
2:D:114:MET:HE2	2:D:124:GLN:HG3	1.83	0.60
2:B:119:ARG:HG2	2:B:127:LEU:CD2	2.30	0.60
1:C:197:ASN:OD1	1:C:200:GLU:HG3	2.02	0.60
1:A:79:PRO:HB3	1:A:127:LEU:HD22	1.84	0.60
1:A:205:LEU:O	1:A:208:TYR:N	2.34	0.60
1:C:205:LEU:O	1:C:208:TYR:N	2.34	0.60
2:D:147:ASN:HA	2:D:152:SER:OG	2.01	0.60
1:C:170:VAL:O	1:C:189:PRO:HD2	2.02	0.60
2:D:247:LEU:N	2:D:247:LEU:HD22	2.17	0.60
1:C:231:SER:HB3	1:C:301:VAL:HG13	1.84	0.60
2:B:225:LYS:HG3	2:B:294:ASP:HB2	1.84	0.60
1:A:13:PRO:HD2	1:A:14:GLU:OE1	2.01	0.59
1:A:170:VAL:O	1:A:189:PRO:HD2	2.02	0.59
1:A:197:ASN:OD1	1:A:200:GLU:HG3	2.02	0.59
1:C:79:PRO:HB3	1:C:127:LEU:HD22	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:130:GLU:O	2:B:133:LYS:N	2.36	0.59
2:B:63:LEU:HD12	2:B:93:LEU:CD2	2.32	0.59
1:C:256:ASN:C	1:C:258:THR:H	2.08	0.59
2:D:207:LEU:HD12	2:D:207:LEU:C	2.25	0.59
1:A:256:ASN:C	1:A:258:THR:H	2.08	0.59
1:A:345:SER:HB2	1:A:346:ASP:OD1	2.02	0.59
1:C:310:ILE:O	1:C:310:ILE:HD13	2.03	0.59
2:D:172:VAL:HG22	2:D:173:ASN:N	2.16	0.59
1:A:231:SER:HB3	1:A:301:VAL:HG13	1.84	0.59
1:A:226:LEU:HD12	1:A:323:ILE:HG21	1.85	0.59
1:C:170:VAL:HG12	1:C:171:TYR:N	2.18	0.59
1:A:310:ILE:HD13	1:A:310:ILE:O	2.03	0.59
1:A:355:GLN:OXT	1:A:355:GLN:HG2	2.01	0.59
1:C:345:SER:HB2	1:C:346:ASP:OD1	2.02	0.59
1:A:123:ASN:HB2	1:A:127:LEU:HD12	1.84	0.58
1:C:123:ASN:HB2	1:C:127:LEU:HD12	1.84	0.58
2:D:225:LYS:HG3	2:D:294:ASP:HB2	1.84	0.58
1:A:115:ARG:HD2	1:A:267:THR:HB	1.86	0.58
1:A:176:SER:N	3:A:356:PO4:O2	2.33	0.58
2:B:247:LEU:HD22	2:B:247:LEU:N	2.17	0.58
1:C:36:PHE:HE2	1:C:340:MET:HE3	1.66	0.58
2:B:44:ASN:HB3	2:B:50:GLY:HA3	1.85	0.58
1:C:115:ARG:HD2	1:C:267:THR:HB	1.86	0.58
1:C:92:LEU:HD13	1:C:160:PRO:CD	2.33	0.58
1:A:240:LYS:O	1:A:244:ARG:HG3	2.04	0.58
2:B:193:ARG:HH21	2:B:196:ASP:CG	2.11	0.58
2:B:6:PHE:HE1	2:B:8:LEU:HD21	1.69	0.58
2:D:193:ARG:HH21	2:D:196:ASP:CG	2.11	0.58
1:A:13:PRO:HD2	1:A:14:GLU:CD	2.29	0.58
1:C:140:ASN:N	1:C:140:ASN:OD1	2.37	0.58
2:D:6:PHE:HE1	2:D:8:LEU:HD21	1.69	0.58
2:D:130:GLU:O	2:D:133:LYS:N	2.36	0.58
1:A:92:LEU:HD13	1:A:160:PRO:CD	2.33	0.58
1:A:134:LEU:HD22	1:A:145:ALA:O	2.04	0.58
2:D:65:MET:O	2:D:65:MET:HG2	2.03	0.58
2:D:231:ASN:C	2:D:231:ASN:HD22	2.12	0.58
2:B:217:VAL:CG2	2:B:219:VAL:HG13	2.34	0.57
1:C:134:LEU:HD22	1:C:145:ALA:O	2.04	0.57
1:C:207:LEU:O	1:C:211:VAL:HG23	2.05	0.57
1:C:226:LEU:HD12	1:C:323:ILE:HG21	1.85	0.57
2:B:134:ILE:HG22	2:B:135:ILE:N	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:PRO:HD2	1:C:14:GLU:CD	2.29	0.57
1:A:140:ASN:N	1:A:140:ASN:OD1	2.37	0.57
1:A:207:LEU:O	1:A:211:VAL:HG23	2.05	0.57
1:C:110:TYR:CB	1:C:112:LYS:HE3	2.35	0.57
2:D:217:VAL:CG2	2:D:219:VAL:HG13	2.34	0.57
1:A:170:VAL:HG12	1:A:171:TYR:N	2.18	0.57
1:C:54:ASN:HD21	2:D:88:GLU:HB3	1.70	0.57
1:C:240:LYS:O	1:C:244:ARG:HG3	2.04	0.57
2:B:8:LEU:O	2:B:50:GLY:HA2	2.04	0.57
2:D:44:ASN:HB3	2:D:50:GLY:HA3	1.85	0.57
1:A:54:ASN:HD21	2:B:88:GLU:HB3	1.70	0.57
2:B:65:MET:O	2:B:65:MET:HG2	2.03	0.57
1:C:266:GLN:O	1:C:266:GLN:HG2	1.96	0.57
1:A:23:ARG:NH2	1:A:331:GLY:O	2.27	0.57
1:C:28:GLY:HA3	1:C:62:LEU:HD22	1.87	0.57
1:A:184:ALA:HB2	1:A:208:TYR:HD1	1.69	0.56
1:C:61:HIS:CE1	2:D:64:GLY:HA2	2.40	0.56
1:C:159:ASN:HB3	2:D:51:VAL:HG22	1.87	0.56
1:A:110:TYR:CB	1:A:112:LYS:HE3	2.35	0.56
2:D:8:LEU:O	2:D:50:GLY:HA2	2.04	0.56
2:D:134:ILE:HG22	2:D:135:ILE:N	2.19	0.56
1:A:194:TRP:HB2	1:A:299:ASN:OD1	2.05	0.56
2:B:189:PRO:HB3	2:B:223:ARG:O	2.06	0.56
2:B:231:ASN:C	2:B:231:ASN:HD22	2.12	0.56
1:C:318:THR:HB	1:C:320:ILE:HD12	1.88	0.56
1:C:115:ARG:CD	1:C:267:THR:HB	2.36	0.56
1:A:28:GLY:HA3	1:A:62:LEU:HD22	1.87	0.56
1:A:61:HIS:CE1	2:B:64:GLY:HA2	2.40	0.56
1:C:312:GLN:HA	1:C:312:GLN:NE2	2.20	0.56
1:C:184:ALA:HA	1:C:208:TYR:HE1	1.71	0.56
1:A:87:ALA:CA	1:A:135:MET:HE3	2.36	0.55
1:A:303:THR:OG1	1:A:306:GLU:HG3	2.06	0.55
1:A:159:ASN:HB3	2:B:51:VAL:HG22	1.87	0.55
1:C:194:TRP:HB2	1:C:299:ASN:OD1	2.05	0.55
1:A:312:GLN:HA	1:A:312:GLN:NE2	2.20	0.55
2:B:25:LEU:HD22	2:B:65:MET:HE1	1.87	0.55
1:C:26:ASN:HD22	1:C:26:ASN:N	2.02	0.55
2:D:25:LEU:HD22	2:D:65:MET:HE1	1.87	0.55
1:A:226:LEU:CD1	1:A:323:ILE:HG22	2.35	0.55
1:C:226:LEU:CD1	1:C:323:ILE:HG22	2.35	0.55
2:D:243:ALA:O	2:D:247:LEU:HD23	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:ARG:CD	1:A:267:THR:HB	2.36	0.55
2:B:72:ALA:HB2	2:B:102:ALA:HB3	1.89	0.55
2:B:200:GLN:CA	2:B:200:GLN:HE21	2.19	0.55
1:C:186:ARG:HG3	1:C:186:ARG:HH11	1.72	0.55
1:A:110:TYR:CD1	1:A:110:TYR:N	2.75	0.55
2:B:221:GLN:O	2:B:223:ARG:HG2	2.06	0.55
1:C:303:THR:OG1	1:C:306:GLU:HG3	2.06	0.55
2:B:185:LYS:O	2:B:217:VAL:HG11	2.07	0.55
2:D:189:PRO:HB3	2:D:223:ARG:O	2.06	0.55
2:B:243:ALA:O	2:B:247:LEU:HD23	2.07	0.55
1:C:115:ARG:HH11	1:C:267:THR:CG2	2.20	0.55
2:D:40:ALA:HA	2:D:72:ALA:O	2.06	0.55
1:A:105:ILE:HG13	1:A:128:MET:HE1	1.89	0.55
1:C:17:GLN:OE1	2:D:160:PRO:HA	2.07	0.55
1:A:186:ARG:HG3	1:A:186:ARG:HH11	1.72	0.54
2:B:218:ASP:C	2:B:220:SER:H	2.15	0.54
2:D:221:GLN:O	2:D:223:ARG:HG2	2.06	0.54
1:A:171:TYR:N	1:A:171:TYR:CD1	2.75	0.54
1:C:184:ALA:HB2	1:C:208:TYR:HD1	1.69	0.54
2:D:218:ASP:C	2:D:220:SER:H	2.15	0.54
1:C:105:ILE:HG13	1:C:128:MET:HE1	1.89	0.54
1:C:134:LEU:O	1:C:144:ILE:HD13	2.08	0.54
2:D:82:HIS:NE2	2:D:84:VAL:HG23	2.22	0.54
1:A:17:GLN:OE1	2:B:160:PRO:HA	2.07	0.54
1:A:332:SER:HB3	1:A:335:GLU:OE2	2.07	0.54
2:B:40:ALA:HA	2:B:72:ALA:O	2.06	0.54
2:B:82:HIS:NE2	2:B:84:VAL:HG23	2.22	0.54
1:C:87:ALA:CA	1:C:135:MET:HE3	2.36	0.54
1:A:115:ARG:HH11	1:A:267:THR:CG2	2.20	0.54
1:A:318:THR:HB	1:A:320:ILE:HD12	1.88	0.54
1:C:171:TYR:N	1:C:171:TYR:CD1	2.75	0.54
2:D:72:ALA:HB2	2:D:102:ALA:HB3	1.89	0.54
1:A:184:ALA:HA	1:A:208:TYR:HE1	1.70	0.54
1:C:1:MET:CE	1:C:351:LEU:HB3	2.38	0.54
2:D:185:LYS:O	2:D:217:VAL:HG11	2.07	0.54
1:A:1:MET:CE	1:A:351:LEU:HB3	2.38	0.54
1:A:266:GLN:O	1:A:266:GLN:HG2	1.97	0.54
1:A:333:GLU:O	1:A:337:ILE:HG12	2.08	0.54
1:C:110:TYR:CD1	1:C:110:TYR:N	2.75	0.54
1:A:85:ARG:HG2	4:A:2007:HOH:O	2.08	0.53
1:C:208:TYR:CE2	1:C:224:HIS:CE1	2.92	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:TYR:CE2	1:A:224:HIS:CE1	2.92	0.53
2:B:126:GLN:HA	2:B:129:SER:OG	2.08	0.53
1:C:218:ASP:C	1:C:220:THR:H	2.17	0.53
1:C:333:GLU:O	1:C:337:ILE:HG12	2.08	0.53
1:A:134:LEU:O	1:A:144:ILE:HD13	2.08	0.53
1:C:332:SER:HB3	1:C:335:GLU:OE2	2.07	0.53
2:D:200:GLN:HE21	2:D:200:GLN:CA	2.19	0.53
2:D:105:PHE:N	2:D:105:PHE:CD1	2.77	0.53
1:A:36:PHE:HE2	1:A:340:MET:HE3	1.66	0.53
1:A:350:TYR:CD1	1:A:350:TYR:N	2.77	0.53
1:C:88:GLU:O	1:C:92:LEU:HD22	2.09	0.53
1:C:123:ASN:CB	1:C:127:LEU:HD12	2.39	0.53
2:D:126:GLN:HA	2:D:129:SER:OG	2.08	0.53
1:C:87:ALA:HA	1:C:135:MET:HE3	1.91	0.52
1:C:224:HIS:CD2	1:C:224:HIS:N	2.77	0.52
1:A:181:GLU:O	1:A:185:GLU:HG3	2.09	0.52
2:B:105:PHE:CD1	2:B:105:PHE:N	2.77	0.52
1:C:109:LEU:HD23	1:C:109:LEU:N	2.24	0.52
1:C:115:ARG:HH11	1:C:267:THR:HG22	1.74	0.52
1:C:181:GLU:O	1:C:185:GLU:HG3	2.09	0.52
2:B:95:GLN:HE21	2:B:95:GLN:CA	2.23	0.52
1:A:26:ASN:N	1:A:26:ASN:HD22	2.02	0.52
1:A:88:GLU:O	1:A:92:LEU:HD22	2.09	0.52
1:C:230:THR:OG1	1:C:325:CYS:HB3	2.10	0.52
1:A:224:HIS:N	1:A:224:HIS:CD2	2.77	0.52
1:A:287:ASP:O	1:A:288:THR:HG23	2.10	0.52
1:A:109:LEU:HD23	1:A:109:LEU:N	2.24	0.52
1:A:115:ARG:HH11	1:A:267:THR:HG22	1.74	0.52
1:A:143:TYR:HB2	4:A:2014:HOH:O	2.10	0.52
2:B:184:ALA:CA	2:B:208:TYR:CE1	2.93	0.52
1:C:350:TYR:N	1:C:350:TYR:CD1	2.77	0.52
2:D:136:ASN:O	2:D:140:THR:OG1	2.28	0.52
1:A:291:ARG:HE	1:A:293:ASP:CG	2.18	0.52
2:B:259:ASP:HB3	2:B:262:GLN:HB3	1.92	0.52
1:C:73:THR:HG23	1:C:101:PHE:CE1	2.45	0.52
2:D:95:GLN:HE21	2:D:95:GLN:CA	2.23	0.52
1:A:123:ASN:CB	1:A:127:LEU:HD12	2.39	0.52
1:C:299:ASN:O	1:C:301:VAL:N	2.41	0.52
2:D:146:PRO:CG	2:D:153:PHE:CE1	2.90	0.52
2:D:184:ALA:HB2	2:D:208:TYR:CE1	2.45	0.52
1:A:73:THR:HG23	1:A:101:PHE:CE1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:THR:OG1	1:A:325:CYS:HB3	2.10	0.51
2:B:136:ASN:O	2:B:140:THR:OG1	2.28	0.51
1:C:177:ALA:O	1:C:181:GLU:HG3	2.10	0.51
1:C:287:ASP:O	1:C:288:THR:HG23	2.10	0.51
1:A:151:ILE:HD12	1:A:153:PHE:CE2	2.45	0.51
1:A:177:ALA:O	1:A:181:GLU:HG3	2.10	0.51
1:C:205:LEU:O	1:C:208:TYR:HB3	2.10	0.51
1:A:299:ASN:O	1:A:301:VAL:N	2.41	0.51
2:B:31:VAL:HG13	2:B:36:PHE:CD2	2.46	0.51
2:B:146:PRO:CG	2:B:153:PHE:CE1	2.90	0.51
1:A:332:SER:O	1:A:336:ILE:HG13	2.10	0.51
2:D:184:ALA:CA	2:D:208:TYR:CE1	2.93	0.51
1:A:205:LEU:O	1:A:208:TYR:HB3	2.10	0.51
1:C:151:ILE:HD12	1:C:153:PHE:CE2	2.45	0.51
1:C:291:ARG:HE	1:C:293:ASP:CG	2.18	0.51
1:C:230:THR:HG23	1:C:300:PRO:HB2	1.93	0.51
1:A:87:ALA:HA	1:A:135:MET:HE3	1.91	0.50
1:A:121:MET:HE1	1:A:267:THR:CG2	2.40	0.50
1:A:218:ASP:C	1:A:220:THR:H	2.16	0.50
2:D:259:ASP:HB3	2:D:262:GLN:HB3	1.92	0.50
2:D:31:VAL:HG13	2:D:36:PHE:CD2	2.46	0.50
2:B:133:LYS:O	2:B:137:ASP:N	2.45	0.50
2:B:184:ALA:HB2	2:B:208:TYR:CE1	2.45	0.50
2:B:193:ARG:O	2:B:196:ASP:HB2	2.11	0.50
1:C:138:GLY:HA2	1:C:143:TYR:O	2.11	0.50
1:C:332:SER:O	1:C:336:ILE:HG13	2.11	0.50
2:D:177:LYS:H	2:D:177:LYS:CD	2.25	0.50
1:C:259:LYS:O	1:C:261:PHE:N	2.45	0.50
1:C:354:LYS:CE	1:C:355:GLN:HB3	2.37	0.50
2:D:193:ARG:O	2:D:196:ASP:HB2	2.11	0.50
2:B:200:GLN:HA	2:B:200:GLN:NE2	2.26	0.50
1:A:138:GLY:HA2	1:A:143:TYR:O	2.11	0.50
1:A:307:CYS:O	1:A:311:ILE:HG12	2.11	0.50
2:B:63:LEU:CD1	2:B:93:LEU:HD22	2.41	0.50
2:B:200:GLN:CA	2:B:200:GLN:NE2	2.75	0.50
2:D:187:GLY:HA3	2:D:217:VAL:HG21	1.93	0.50
2:B:159:ASN:HA	2:B:160:PRO:C	2.36	0.50
1:C:46:PHE:CD1	1:C:46:PHE:N	2.80	0.50
1:C:204:GLN:O	1:C:207:LEU:HB3	2.12	0.50
2:D:63:LEU:CD1	2:D:93:LEU:HD22	2.41	0.50
1:A:354:LYS:CE	1:A:355:GLN:HB3	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:LEU:HD13	1:A:228:TYR:OH	2.12	0.49
1:A:184:ALA:CB	1:A:211:VAL:HB	2.42	0.49
1:A:230:THR:HG23	1:A:300:PRO:HB2	1.93	0.49
2:B:187:GLY:HA3	2:B:217:VAL:HG21	1.93	0.49
1:C:307:CYS:O	1:C:311:ILE:HG12	2.11	0.49
1:A:184:ALA:CA	1:A:208:TYR:CE1	2.95	0.49
1:A:209:ASN:O	1:A:213:THR:OG1	2.28	0.49
1:A:259:LYS:O	1:A:261:PHE:N	2.45	0.49
1:C:123:ASN:O	1:C:127:LEU:HD12	2.12	0.49
1:A:3:PHE:CG	1:A:348:MET:HE2	2.47	0.49
1:A:294:TYR:O	1:A:297:GLU:HB2	2.13	0.49
1:C:226:LEU:HD13	1:C:228:TYR:OH	2.12	0.49
2:D:200:GLN:NE2	2:D:200:GLN:HA	2.26	0.49
1:A:143:TYR:CD2	1:A:155:LYS:HE2	2.47	0.49
1:A:144:ILE:HG22	1:A:145:ALA:N	2.27	0.49
2:B:134:ILE:O	2:B:137:ASP:N	2.46	0.49
2:B:177:LYS:CD	2:B:177:LYS:H	2.25	0.49
1:C:3:PHE:CG	1:C:348:MET:HE2	2.47	0.49
1:C:73:THR:HG21	1:C:76:ILE:CD1	2.43	0.49
1:C:294:TYR:O	1:C:297:GLU:HB2	2.13	0.49
2:D:133:LYS:O	2:D:137:ASP:N	2.45	0.49
2:B:147:ASN:HA	2:B:152:SER:CB	2.43	0.49
2:D:159:ASN:HA	2:D:160:PRO:C	2.36	0.49
2:D:200:GLN:CA	2:D:200:GLN:NE2	2.75	0.49
2:D:123:SER:O	2:D:126:GLN:HG3	2.13	0.49
1:A:123:ASN:O	1:A:127:LEU:HD12	2.12	0.49
1:A:182:TRP:O	1:A:186:ARG:NH1	2.46	0.49
2:B:197:SER:HA	2:B:270:GLU:OE1	2.13	0.49
1:C:250:TRP:CD1	1:C:250:TRP:C	2.90	0.49
2:B:177:LYS:H	2:B:177:LYS:HD2	1.77	0.49
1:C:184:ALA:CA	1:C:208:TYR:CE1	2.95	0.49
1:A:314:ASP:O	1:A:318:THR:OG1	2.29	0.49
2:B:311:VAL:O	2:B:314:VAL:HB	2.13	0.49
2:D:134:ILE:O	2:D:137:ASP:N	2.46	0.49
2:D:172:VAL:HG22	2:D:173:ASN:H	1.77	0.49
1:C:121:MET:HE1	1:C:267:THR:CG2	2.40	0.48
1:A:204:GLN:O	1:A:207:LEU:HB3	2.12	0.48
2:B:89:GLU:O	2:B:92:LEU:HB3	2.13	0.48
2:D:89:GLU:O	2:D:92:LEU:HB3	2.13	0.48
2:D:177:LYS:H	2:D:177:LYS:HD2	1.77	0.48
2:D:225:LYS:HB3	2:D:294:ASP:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:PHE:CD1	1:A:46:PHE:N	2.80	0.48
1:A:73:THR:HG21	1:A:76:ILE:CD1	2.43	0.48
2:B:123:SER:O	2:B:126:GLN:HG3	2.13	0.48
1:C:143:TYR:CD2	1:C:155:LYS:HE2	2.47	0.48
2:D:305:LYS:O	2:D:309:ARG:HB3	2.13	0.48
1:A:320:ILE:HG22	1:A:320:ILE:O	2.12	0.48
1:C:144:ILE:HG22	1:C:145:ALA:N	2.27	0.48
1:A:85:ARG:NH2	4:A:2123:HOH:O	2.46	0.48
2:D:197:SER:HA	2:D:270:GLU:OE1	2.13	0.48
1:A:250:TRP:CD1	1:A:250:TRP:C	2.90	0.48
2:B:95:GLN:CA	2:B:95:GLN:NE2	2.76	0.48
2:B:172:VAL:HG22	2:B:173:ASN:H	1.77	0.48
1:C:314:ASP:O	1:C:318:THR:OG1	2.29	0.48
2:D:147:ASN:HA	2:D:152:SER:CB	2.43	0.48
2:B:130:GLU:OE1	2:B:148:ASN:ND2	2.47	0.48
2:B:305:LYS:O	2:B:309:ARG:HB3	2.13	0.48
1:C:194:TRP:HB3	1:C:228:TYR:HA	1.96	0.48
2:B:225:LYS:HB3	2:B:294:ASP:O	2.13	0.48
2:B:231:ASN:C	2:B:231:ASN:ND2	2.72	0.47
1:C:119:THR:HG22	1:C:120:ASP:N	2.29	0.47
1:C:182:TRP:O	1:C:186:ARG:NH1	2.46	0.47
2:D:231:ASN:C	2:D:231:ASN:ND2	2.72	0.47
2:D:311:VAL:O	2:D:314:VAL:HB	2.13	0.47
1:A:123:ASN:N	1:A:123:ASN:ND2	2.62	0.47
1:C:102:ARG:NH1	1:C:169:PRO:HG2	2.30	0.47
1:C:184:ALA:CB	1:C:211:VAL:HB	2.42	0.47
1:C:186:ARG:HH11	1:C:186:ARG:CG	2.27	0.47
2:D:314:VAL:HG12	2:D:315:VAL:N	2.29	0.47
1:A:119:THR:HG22	1:A:120:ASP:N	2.29	0.47
2:B:314:VAL:HG12	2:B:315:VAL:N	2.29	0.47
2:D:213:GLN:O	2:D:215:HIS:N	2.47	0.47
2:B:213:GLN:O	2:B:215:HIS:N	2.47	0.47
1:C:121:MET:HE3	1:C:121:MET:HB2	1.77	0.47
2:D:221:GLN:OE1	2:D:221:GLN:HA	2.13	0.47
1:A:69:LEU:CG	1:A:70:ASN:N	2.78	0.47
2:B:221:GLN:HA	2:B:221:GLN:OE1	2.13	0.47
1:C:190:MET:O	1:C:225:CYS:N	2.40	0.47
1:C:323:ILE:N	1:C:323:ILE:CD1	2.76	0.47
2:D:95:GLN:HG3	2:D:160:PRO:HB2	1.97	0.47
2:B:8:LEU:N	2:B:300:GLU:OE2	2.32	0.47
1:C:123:ASN:N	1:C:123:ASN:HD22	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:ASN:N	1:A:123:ASN:HD22	2.13	0.47
2:B:30:TYR:CZ	2:B:309:ARG:HD2	2.50	0.47
2:B:170:GLN:HG3	4:B:2091:HOH:O	2.15	0.47
2:D:130:GLU:OE1	2:D:148:ASN:ND2	2.47	0.47
1:A:173:VAL:HG23	1:A:173:VAL:O	2.16	0.47
1:C:45:HIS:HB3	1:C:46:PHE:CD1	2.49	0.47
1:C:208:TYR:CD2	1:C:224:HIS:HE1	2.33	0.47
1:C:225:CYS:SG	1:C:322:ASN:ND2	2.88	0.47
1:C:312:GLN:NE2	1:C:316:ASP:OD1	2.47	0.47
2:D:299:PHE:CD1	2:D:299:PHE:N	2.83	0.47
2:D:308:GLN:HE21	2:D:308:GLN:HB2	1.47	0.47
1:A:47:THR:HG22	1:A:49:PHE:N	2.17	0.46
1:A:186:ARG:NH1	1:A:186:ARG:CG	2.78	0.46
1:A:194:TRP:HB3	1:A:228:TYR:HA	1.96	0.46
1:C:49:PHE:CZ	1:C:250:TRP:CH2	3.03	0.46
1:C:123:ASN:N	1:C:123:ASN:ND2	2.62	0.46
1:C:151:ILE:HD12	1:C:153:PHE:HE2	1.80	0.46
2:B:218:ASP:O	2:B:220:SER:N	2.47	0.46
1:C:170:VAL:CG1	1:C:171:TYR:N	2.78	0.46
1:A:45:HIS:HB3	1:A:46:PHE:CD1	2.49	0.46
1:A:197:ASN:O	1:A:200:GLU:HB2	2.16	0.46
1:A:312:GLN:NE2	1:A:316:ASP:OD1	2.48	0.46
2:D:30:TYR:CZ	2:D:309:ARG:HD2	2.50	0.46
1:A:186:ARG:HH11	1:A:186:ARG:CG	2.27	0.46
1:A:202:LYS:O	1:A:205:LEU:HB2	2.16	0.46
1:A:225:CYS:SG	1:A:322:ASN:ND2	2.88	0.46
2:B:70:LYS:HA	2:B:100:ARG:HG2	1.98	0.46
1:C:72:GLY:HA3	1:C:102:ARG:HB2	1.97	0.46
1:C:173:VAL:HG23	1:C:173:VAL:O	2.15	0.46
2:D:70:LYS:HA	2:D:100:ARG:HG2	1.98	0.46
1:A:49:PHE:CZ	1:A:250:TRP:CH2	3.03	0.46
1:A:102:ARG:NH1	1:A:169:PRO:HG2	2.30	0.46
1:A:176:SER:HB2	3:A:356:PO4:O4	2.15	0.46
2:B:19:GLN:NE2	2:B:23:GLU:OE2	2.49	0.46
1:C:186:ARG:NH1	1:C:186:ARG:CG	2.78	0.46
1:C:202:LYS:O	1:C:205:LEU:HB2	2.16	0.46
1:C:320:ILE:O	1:C:320:ILE:HG22	2.12	0.46
1:A:54:ASN:HD21	2:B:88:GLU:CB	2.28	0.46
1:A:170:VAL:CG1	1:A:171:TYR:N	2.78	0.46
1:A:190:MET:O	1:A:225:CYS:N	2.40	0.46
2:B:299:PHE:N	2:B:299:PHE:CD1	2.83	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:TYR:O	1:C:144:ILE:HG12	2.16	0.46
1:C:312:GLN:NE2	1:C:312:GLN:CA	2.79	0.46
2:D:8:LEU:HA	2:D:42:TYR:HB3	1.98	0.46
2:D:30:TYR:CE2	2:D:309:ARG:CD	2.99	0.46
1:A:73:THR:CB	1:A:76:ILE:CD1	2.93	0.46
1:A:105:ILE:HD12	1:A:128:MET:CE	2.46	0.46
2:B:246:TYR:HD2	2:B:247:LEU:HD22	1.81	0.46
1:C:111:ASP:O	1:C:114:PHE:N	2.46	0.46
1:C:250:TRP:CD1	1:C:251:TYR:N	2.84	0.46
1:C:354:LYS:CG	1:C:355:GLN:N	2.79	0.46
2:D:38:THR:CG2	2:D:39:LEU:N	2.76	0.46
2:D:82:HIS:HD2	2:D:84:VAL:N	2.00	0.46
2:D:95:GLN:CA	2:D:95:GLN:NE2	2.76	0.46
2:D:218:ASP:O	2:D:220:SER:N	2.47	0.46
1:A:242:ILE:HG22	1:A:243:CYS:N	2.29	0.46
1:C:304:PRO:O	1:C:308:ILE:HG13	2.16	0.46
1:A:24:LEU:O	1:A:24:LEU:HD12	2.16	0.45
1:A:47:THR:CG2	1:A:48:GLU:N	2.79	0.45
1:A:250:TRP:CD1	1:A:251:TYR:N	2.84	0.45
2:B:30:TYR:CE2	2:B:309:ARG:CD	2.99	0.45
2:B:123:SER:HB3	2:B:150:PHE:HZ	1.81	0.45
1:C:52:LEU:O	1:C:52:LEU:HG	2.14	0.45
1:A:11:GLN:HB2	1:A:51:LEU:HD11	1.98	0.45
1:A:52:LEU:CD1	1:A:58:ALA:HB2	2.46	0.45
1:A:159:ASN:HB3	1:A:160:PRO:HA	1.98	0.45
1:A:226:LEU:HG	1:A:320:ILE:HG21	1.98	0.45
1:A:304:PRO:O	1:A:308:ILE:HG13	2.16	0.45
2:B:51:VAL:HG13	2:B:51:VAL:O	2.16	0.45
2:B:95:GLN:HG3	2:B:160:PRO:HB2	1.97	0.45
1:C:54:ASN:HD21	2:D:88:GLU:CB	2.28	0.45
1:C:110:TYR:CG	1:C:112:LYS:HE3	2.51	0.45
1:C:323:ILE:HD13	1:C:323:ILE:H	1.79	0.45
2:D:19:GLN:NE2	2:D:23:GLU:OE2	2.49	0.45
1:C:105:ILE:HD12	1:C:128:MET:CE	2.46	0.45
1:C:143:TYR:CD2	1:C:155:LYS:CE	3.00	0.45
1:C:197:ASN:H	1:C:200:GLU:HB2	1.82	0.45
2:D:30:TYR:CE2	2:D:309:ARG:HD3	2.52	0.45
2:D:76:HIS:HD1	2:D:76:HIS:HA	1.62	0.45
1:A:110:TYR:CG	1:A:112:LYS:HE3	2.51	0.45
2:B:184:ALA:CB	2:B:208:TYR:CE1	2.99	0.45
1:C:188:LEU:HA	1:C:188:LEU:HD23	1.67	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:24:LEU:HD12	1:C:24:LEU:O	2.16	0.45
1:C:226:LEU:HG	1:C:320:ILE:HG21	1.98	0.45
1:A:143:TYR:O	1:A:144:ILE:HG12	2.16	0.45
1:A:354:LYS:CG	1:A:355:GLN:N	2.79	0.45
1:C:69:LEU:CG	1:C:70:ASN:N	2.78	0.45
1:C:197:ASN:O	1:C:200:GLU:HB2	2.16	0.45
2:D:184:ALA:CB	2:D:208:TYR:CE1	2.99	0.45
2:D:247:LEU:N	2:D:247:LEU:CD2	2.79	0.45
1:A:81:ALA:HB3	1:A:86:GLN:CD	2.42	0.45
1:A:143:TYR:CD2	1:A:155:LYS:CE	3.00	0.45
1:A:151:ILE:HD12	1:A:153:PHE:HE2	1.81	0.45
1:A:208:TYR:CD2	1:A:224:HIS:HE1	2.33	0.45
2:B:10:PHE:CE1	2:B:49:ASN:C	2.95	0.45
2:B:100:ARG:HH11	2:B:100:ARG:HD3	1.61	0.45
2:B:257:ASN:C	2:B:259:ASP:H	2.23	0.45
1:A:72:GLY:HA3	1:A:102:ARG:HB2	1.98	0.45
1:A:289:ASN:HB3	1:A:290:ARG:H	1.39	0.45
2:B:172:VAL:CG2	2:B:173:ASN:N	2.80	0.45
1:C:81:ALA:HB3	1:C:86:GLN:CD	2.42	0.45
1:C:159:ASN:HB3	1:C:160:PRO:HA	1.98	0.45
2:D:10:PHE:CE1	2:D:49:ASN:C	2.95	0.45
2:D:51:VAL:O	2:D:51:VAL:HG13	2.16	0.45
1:A:323:ILE:HD13	1:A:323:ILE:H	1.79	0.45
2:D:172:VAL:O	2:D:190:LEU:HA	2.17	0.45
1:A:163:TYR:CD2	1:A:163:TYR:C	2.95	0.44
1:A:327:PHE:CD1	1:A:327:PHE:N	2.85	0.44
2:B:8:LEU:HA	2:B:42:TYR:HB3	1.98	0.44
2:B:227:THR:HA	2:B:296:LEU:O	2.18	0.44
1:C:52:LEU:CD1	1:C:58:ALA:HB2	2.46	0.44
2:D:246:TYR:HD2	2:D:247:LEU:HD22	1.81	0.44
1:A:241:ASP:O	1:A:244:ARG:N	2.50	0.44
1:C:125:ARG:O	1:C:129:ASP:HB3	2.18	0.44
2:D:123:SER:HB3	2:D:150:PHE:HZ	1.81	0.44
1:A:52:LEU:O	1:A:52:LEU:HG	2.14	0.44
1:A:189:PRO:HB3	1:A:223:ASP:O	2.17	0.44
1:A:207:LEU:O	1:A:207:LEU:HD12	2.18	0.44
2:B:30:TYR:CE2	2:B:309:ARG:HD3	2.52	0.44
2:B:172:VAL:O	2:B:190:LEU:HA	2.17	0.44
1:C:189:PRO:HB3	1:C:223:ASP:O	2.17	0.44
2:B:247:LEU:N	2:B:247:LEU:CD2	2.79	0.44
1:C:218:ASP:C	1:C:220:THR:N	2.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:ASN:H	1:A:200:GLU:HB2	1.82	0.44
1:A:218:ASP:C	1:A:220:THR:N	2.76	0.44
2:D:227:THR:HA	2:D:296:LEU:O	2.18	0.44
2:D:257:ASN:C	2:D:259:ASP:H	2.23	0.44
1:A:6:PHE:CD1	1:A:6:PHE:C	2.95	0.44
1:A:72:GLY:CA	1:A:102:ARG:HB2	2.48	0.44
2:B:6:PHE:CE1	2:B:8:LEU:HD21	2.52	0.44
2:B:31:VAL:HG23	2:B:31:VAL:H	1.55	0.44
1:C:236:SER:HB2	1:C:240:LYS:HE3	2.00	0.44
1:A:111:ASP:O	1:A:114:PHE:N	2.46	0.44
1:C:11:GLN:HB2	1:C:51:LEU:HD11	1.98	0.44
1:C:241:ASP:O	1:C:244:ARG:N	2.50	0.44
1:A:112:LYS:NZ	1:A:113:ASP:OD1	2.44	0.44
2:B:82:HIS:HD2	2:B:84:VAL:N	2.00	0.44
2:B:106:SER:OG	2:B:107:ASP:O	2.36	0.44
1:C:207:LEU:O	1:C:207:LEU:HD12	2.18	0.44
2:D:126:GLN:HG3	2:D:126:GLN:H	1.39	0.44
2:D:195:ASP:O	2:D:263:LYS:NZ	2.47	0.44
1:A:183:ALA:O	1:A:187:GLY:N	2.51	0.43
1:A:194:TRP:HB3	1:A:227:SER:O	2.18	0.43
1:C:72:GLY:CA	1:C:102:ARG:HB2	2.48	0.43
1:C:94:ASP:OD1	1:C:164:THR:OG1	2.36	0.43
1:C:242:ILE:HG22	1:C:243:CYS:N	2.29	0.43
1:C:327:PHE:CD1	1:C:327:PHE:N	2.85	0.43
2:D:131:CYS:O	2:D:135:ILE:HG13	2.18	0.43
2:D:213:GLN:HB3	2:D:214:ALA:H	1.53	0.43
2:D:268:LEU:HA	2:D:268:LEU:HD12	1.44	0.43
1:C:194:TRP:HB3	1:C:227:SER:O	2.18	0.43
1:A:236:SER:HB2	1:A:240:LYS:HE3	2.00	0.43
1:C:47:THR:CG2	1:C:48:GLU:N	2.79	0.43
1:C:209:ASN:O	1:C:213:THR:OG1	2.28	0.43
1:C:349:PRO:HB2	1:C:350:TYR:CD1	2.53	0.43
1:A:312:GLN:NE2	1:A:312:GLN:CA	2.79	0.43
1:C:300:PRO:HG3	1:C:311:ILE:HD13	1.99	0.43
2:D:100:ARG:HH11	2:D:100:ARG:HD3	1.61	0.43
2:D:190:LEU:HD12	2:D:224:HIS:ND1	2.32	0.43
1:A:125:ARG:O	1:A:129:ASP:HB3	2.18	0.43
1:C:154:PRO:HD2	2:D:116:PHE:CD2	2.54	0.43
1:C:343:PHE:CD1	1:C:343:PHE:C	2.96	0.43
2:D:106:SER:OG	2:D:107:ASP:O	2.36	0.43
1:A:3:PHE:CE2	1:A:348:MET:HG2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:190:LEU:HD12	2:B:224:HIS:ND1	2.32	0.43
2:B:209:HIS:CD2	2:B:209:HIS:C	2.96	0.43
1:C:163:TYR:CD2	1:C:163:TYR:C	2.95	0.43
2:D:164:THR:HG22	2:D:167:GLY:O	2.19	0.43
1:A:188:LEU:HD23	1:A:188:LEU:HA	1.67	0.43
1:A:343:PHE:CD1	1:A:343:PHE:C	2.96	0.43
2:B:164:THR:HG22	2:B:167:GLY:O	2.19	0.43
2:B:195:ASP:O	2:B:263:LYS:NZ	2.47	0.43
1:A:349:PRO:HB2	1:A:350:TYR:CD1	2.53	0.42
2:B:213:GLN:HB3	2:B:214:ALA:H	1.53	0.42
1:C:192:LEU:HD12	1:C:225:CYS:O	2.19	0.42
2:D:209:HIS:C	2:D:209:HIS:CD2	2.96	0.42
1:A:94:ASP:OD1	1:A:164:THR:OG1	2.36	0.42
1:A:110:TYR:HB2	1:A:112:LYS:HE3	2.01	0.42
1:A:191:ILE:HG23	1:A:225:CYS:CB	2.45	0.42
1:A:192:LEU:HD12	1:A:225:CYS:O	2.19	0.42
2:B:38:THR:CG2	2:B:39:LEU:N	2.76	0.42
2:B:131:CYS:O	2:B:135:ILE:HG13	2.18	0.42
1:A:3:PHE:CE1	1:A:323:ILE:HD11	2.54	0.42
2:B:144:CYS:O	2:B:155:LYS:HA	2.19	0.42
2:B:232:GLN:HG2	2:B:279:SER:CB	2.50	0.42
1:C:6:PHE:CD1	1:C:6:PHE:C	2.95	0.42
1:C:48:GLU:H	1:C:48:GLU:HG3	1.56	0.42
1:C:184:ALA:CA	1:C:208:TYR:HE1	2.32	0.42
1:C:207:LEU:HD12	1:C:207:LEU:C	2.44	0.42
1:C:259:LYS:CG	1:C:260:ILE:N	2.78	0.42
2:D:12:ASN:HD21	2:D:15:ARG:HD3	1.84	0.42
2:D:231:ASN:HB3	2:D:273:ILE:HG23	2.01	0.42
1:A:300:PRO:HG3	1:A:311:ILE:HD13	1.99	0.42
1:C:3:PHE:CE2	1:C:348:MET:HG2	2.54	0.42
1:C:293:ASP:OD1	1:C:293:ASP:N	2.52	0.42
2:D:25:LEU:HA	2:D:25:LEU:HD23	1.70	0.42
2:D:144:CYS:O	2:D:155:LYS:HA	2.19	0.42
1:A:154:PRO:HD2	2:B:116:PHE:CD2	2.54	0.42
1:C:106:CYS:CB	1:C:173:VAL:HG22	2.36	0.42
1:C:183:ALA:O	1:C:187:GLY:N	2.51	0.42
2:B:62:LEU:HA	2:B:65:MET:HE3	2.00	0.42
1:C:26:ASN:N	1:C:26:ASN:ND2	2.67	0.42
1:C:129:ASP:O	1:C:132:TYR:HB3	2.20	0.42
1:C:338:ALA:O	1:C:342:LEU:HB2	2.20	0.42
2:D:62:LEU:HA	2:D:65:MET:HE3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:ASP:OD1	1:A:220:THR:OG1	2.28	0.42
1:A:256:ASN:O	1:A:258:THR:N	2.53	0.42
2:B:246:TYR:HD2	2:B:247:LEU:CD2	2.32	0.42
1:C:43:GLU:HB2	1:C:55:PRO:HG3	2.02	0.42
1:C:102:ARG:HH11	1:C:102:ARG:HD3	1.74	0.42
2:D:246:TYR:HD2	2:D:247:LEU:CD2	2.32	0.42
1:A:144:ILE:HG22	1:A:153:PHE:CE1	2.55	0.42
2:D:8:LEU:N	2:D:300:GLU:OE2	2.32	0.42
2:D:232:GLN:HG2	2:D:279:SER:CB	2.50	0.42
2:B:56:LEU:HD23	2:B:56:LEU:HA	1.94	0.42
1:A:1:MET:HB2	1:A:2:LYS:H	1.56	0.41
1:A:129:ASP:O	1:A:132:TYR:HB3	2.20	0.41
2:B:2:LYS:O	2:B:294:ASP:HA	2.20	0.41
2:B:10:PHE:CD1	2:B:49:ASN:CA	3.02	0.41
2:B:12:ASN:HD21	2:B:15:ARG:HD3	1.84	0.41
2:B:200:GLN:HE21	2:B:200:GLN:C	2.28	0.41
1:C:3:PHE:CE1	1:C:323:ILE:HD11	2.54	0.41
1:C:144:ILE:HG22	1:C:153:PHE:CE1	2.55	0.41
1:C:308:ILE:O	1:C:308:ILE:HG22	2.20	0.41
2:D:178:GLU:O	2:D:181:GLU:HG2	2.20	0.41
1:A:121:MET:HE3	1:A:121:MET:HB2	1.77	0.41
1:A:338:ALA:O	1:A:342:LEU:HB2	2.20	0.41
2:B:65:MET:HE3	2:B:65:MET:HB3	1.78	0.41
1:A:160:PRO:HB2	2:B:17:SER:HB2	2.02	0.41
1:A:293:ASP:OD1	1:A:293:ASP:N	2.52	0.41
2:B:6:PHE:HA	2:B:40:ALA:O	2.20	0.41
2:B:194:TRP:HB3	2:B:227:THR:O	2.20	0.41
2:D:6:PHE:HA	2:D:40:ALA:O	2.20	0.41
2:B:259:ASP:HB3	2:B:262:GLN:HG2	2.03	0.41
2:D:10:PHE:CD1	2:D:49:ASN:CA	3.02	0.41
1:A:49:PHE:HZ	1:A:250:TRP:CH2	2.39	0.41
1:A:332:SER:OG	1:A:333:GLU:N	2.49	0.41
1:A:226:LEU:CG	1:A:323:ILE:HG22	2.51	0.41
2:B:19:GLN:O	2:B:23:GLU:HG3	2.21	0.41
1:C:49:PHE:HZ	1:C:250:TRP:CH2	2.39	0.41
2:D:259:ASP:HB3	2:D:262:GLN:HG2	2.03	0.41
2:B:143:TYR:CD2	2:B:155:LYS:HE3	2.56	0.41
1:C:110:TYR:HB2	1:C:112:LYS:HE3	2.01	0.41
1:A:6:PHE:HD1	1:A:7:LEU:N	2.19	0.41
2:B:178:GLU:O	2:B:181:GLU:HG2	2.20	0.41
2:B:231:ASN:HB3	2:B:273:ILE:HG23	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:6:PHE:HD1	1:C:7:LEU:N	2.19	0.41
1:C:160:PRO:HB2	2:D:17:SER:HB2	2.02	0.41
1:C:226:LEU:CG	1:C:323:ILE:HG22	2.51	0.41
1:A:81:ALA:O	1:A:131:TRP:NE1	2.48	0.41
1:A:93:LEU:HD12	1:A:93:LEU:HA	1.92	0.41
1:A:94:ASP:CG	1:A:163:TYR:HB3	2.45	0.41
1:A:308:ILE:O	1:A:308:ILE:HG22	2.20	0.41
2:B:62:LEU:HD12	2:B:65:MET:CE	2.51	0.41
2:B:119:ARG:HA	2:B:120:PRO:HD3	1.94	0.41
2:B:244:ARG:HB2	2:B:264:MET:SD	2.61	0.41
2:B:246:TYR:CD2	2:B:247:LEU:HD22	2.56	0.41
1:C:1:MET:HB3	1:C:321:ASP:HB2	2.03	0.41
1:C:37:ASP:O	1:C:70:ASN:HB2	2.21	0.41
1:C:94:ASP:CG	1:C:163:TYR:HB3	2.45	0.41
1:C:332:SER:OG	1:C:333:GLU:N	2.49	0.41
2:D:19:GLN:O	2:D:23:GLU:HG3	2.21	0.41
2:D:56:LEU:HD23	2:D:56:LEU:HA	1.94	0.41
2:D:61:PHE:C	2:D:61:PHE:CD1	2.99	0.41
2:D:62:LEU:HD12	2:D:65:MET:CE	2.51	0.41
2:D:194:TRP:HB3	2:D:227:THR:O	2.20	0.41
2:D:200:GLN:HE21	2:D:200:GLN:C	2.28	0.41
1:A:37:ASP:O	1:A:70:ASN:HB2	2.21	0.41
1:A:64:GLY:HA2	2:B:61:PHE:CZ	2.56	0.41
2:B:111:SER:O	2:B:114:MET:HB3	2.21	0.41
1:C:256:ASN:O	1:C:258:THR:N	2.53	0.41
1:A:63:LEU:HD23	1:A:63:LEU:HA	1.78	0.40
1:A:156:ILE:H	1:A:156:ILE:HG13	1.59	0.40
1:A:182:TRP:CD1	1:A:186:ARG:HH12	2.40	0.40
1:C:73:THR:CB	1:C:76:ILE:CD1	2.93	0.40
1:C:172:VAL:O	1:C:190:MET:HB2	2.21	0.40
1:C:310:ILE:HG23	1:C:310:ILE:HD12	1.79	0.40
2:D:2:LYS:O	2:D:294:ASP:HA	2.20	0.40
2:D:15:ARG:HB3	2:D:19:GLN:OE1	2.21	0.40
1:A:43:GLU:HB2	1:A:55:PRO:HG3	2.02	0.40
1:A:172:VAL:O	1:A:190:MET:HB2	2.21	0.40
1:A:310:ILE:HG23	1:A:310:ILE:HD12	1.79	0.40
2:B:31:VAL:HG12	2:B:36:PHE:HB2	2.03	0.40
2:B:61:PHE:CD1	2:B:61:PHE:C	2.99	0.40
2:B:155:LYS:CG	2:B:156:ILE:N	2.84	0.40
2:B:305:LYS:O	2:B:309:ARG:N	2.48	0.40
1:C:26:ASN:C	1:C:27:LEU:HD23	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:182:TRP:CD1	1:C:186:ARG:HH12	2.40	0.40
2:D:31:VAL:HG12	2:D:36:PHE:HB2	2.03	0.40
1:A:26:ASN:C	1:A:27:LEU:HD23	2.46	0.40
2:B:12:ASN:HB2	2:B:13:SER:H	1.59	0.40
1:C:323:ILE:HD13	1:C:323:ILE:HG23	1.77	0.40
1:A:170:VAL:C	1:A:171:TYR:CD1	3.00	0.40
2:D:244:ARG:HB2	2:D:264:MET:SD	2.61	0.40
1:A:1:MET:HB3	1:A:321:ASP:HB2	2.03	0.40
2:D:30:TYR:CE2	2:D:309:ARG:HD2	2.57	0.40
2:D:66:THR:OG1	2:D:100:ARG:NH2	2.54	0.40
2:D:246:TYR:CD2	2:D:247:LEU:HD22	2.56	0.40

All (15) 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:C:345:SER:O	2:D:237:GLU:CD[4_467]	0.67	1.53
1:C:345:SER:O	2:D:237:GLU:OE2[4_467]	0.78	1.42
1:C:141:GLU:OE2	2:D:26:ASP:OD2[4_567]	1.08	1.12
1:A:237:ASN:ND2	1:C:291:ARG:CB[2_464]	1.10	1.10
1:C:345:SER:C	2:D:237:GLU:OE2[4_467]	1.38	0.82
1:A:237:ASN:ND2	1:C:291:ARG:CG[2_464]	1.46	0.74
1:C:141:GLU:CD	2:D:26:ASP:OD2[4_567]	1.46	0.74
1:C:345:SER:C	2:D:237:GLU:CD[4_467]	1.57	0.63
1:C:345:SER:O	2:D:237:GLU:CG[4_467]	1.63	0.57
1:C:268:LYS:CB	4:B:2119:HOH:O[4_566]	1.75	0.45
1:C:141:GLU:OE1	2:D:26:ASP:OD2[4_567]	1.84	0.36
1:C:345:SER:O	2:D:237:GLU:OE1[4_467]	1.94	0.26
1:C:268:LYS:N	4:B:2119:HOH:O[4_566]	2.01	0.19
1:C:346:ASP:CG	2:D:237:GLU:OE1[4_467]	2.09	0.11
1:C:346:ASP:N	2:D:237:GLU:OE2[4_467]	2.10	0.10

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	336/355 (95%)	288 (86%)	36 (11%)	12 (4%)	2	2
1	C	336/355 (95%)	288 (86%)	36 (11%)	12 (4%)	2	2
2	B	317/324 (98%)	265 (84%)	42 (13%)	10 (3%)	3	3
2	D	317/324 (98%)	265 (84%)	42 (13%)	10 (3%)	3	3
All	All	1306/1358 (96%)	1106 (85%)	156 (12%)	44 (3%)	3	2

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	147	ASP
1	A	257	ALA
1	A	260	ILE
1	A	263	ASP
1	A	270	TYR
1	A	288	THR
2	B	162	ALA
2	B	214	ALA
2	B	219	VAL
2	B	256	SER
2	B	259	ASP
1	C	147	ASP
1	C	257	ALA
1	C	260	ILE
1	C	263	ASP
1	C	270	TYR
1	C	288	THR
2	D	162	ALA
2	D	214	ALA
2	D	219	VAL
2	D	256	SER
2	D	259	ASP
1	A	124	SER
1	A	331	GLY
1	A	353	GLU
2	B	213	GLN
1	C	124	SER
1	C	331	GLY
1	C	353	GLU
2	D	213	GLN

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Mol	Chain	Res	Type
2	D	317	ALA
1	A	150	HIS
2	B	124	GLN
2	B	146	PRO
2	B	317	ALA
1	C	150	HIS
2	D	124	GLN
2	D	146	PRO
2	B	257	ASN
2	D	257	ASN
1	A	316	ASP
1	C	316	ASP
1	A	300	PRO
1	C	300	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	286/303 (94%)	201 (70%)	85 (30%)	0	0
1	C	286/303 (94%)	201 (70%)	85 (30%)	0	0
2	B	265/274 (97%)	195 (74%)	70 (26%)	0	0
2	D	265/274 (97%)	195 (74%)	70 (26%)	0	0
All	All	1102/1154 (96%)	792 (72%)	310 (28%)	0	0

All (310) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	8	LEU
1	A	9	THR
1	A	15	LEU
1	A	22	LYS
1	A	23	ARG
1	A	24	LEU

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Mol	Chain	Res	Type
1	A	27	LEU
1	A	32	GLU
1	A	42	LEU
1	A	46	PHE
1	A	47	THR
1	A	48	GLU
1	A	52	LEU
1	A	62	LEU
1	A	76	ILE
1	A	84	VAL
1	A	85	ARG
1	A	92	LEU
1	A	93	LEU
1	A	95	GLN
1	A	106	CYS
1	A	107	ARG
1	A	109	LEU
1	A	112	LYS
1	A	115	ARG
1	A	121	MET
1	A	123	ASN
1	A	124	SER
1	A	125	ARG
1	A	127	LEU
1	A	128	MET
1	A	129	ASP
1	A	131	TRP
1	A	137	GLU
1	A	140	ASN
1	A	144	ILE
1	A	148	ASN
1	A	151	ILE
1	A	152	LYS
1	A	155	LYS
1	A	156	ILE
1	A	164	THR
1	A	176	SER
1	A	178	SER
1	A	186	ARG
1	A	191	ILE
1	A	199	HIS
1	A	205	LEU

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Mol	Chain	Res	Type
1	A	207	LEU
1	A	213	THR
1	A	219	VAL
1	A	224	HIS
1	A	225	CYS
1	A	227	SER
1	A	232	VAL
1	A	238	ARG
1	A	242	ILE
1	A	250	TRP
1	A	258	THR
1	A	259	LYS
1	A	260	ILE
1	A	263	ASP
1	A	265	ASP
1	A	266	GLN
1	A	289	ASN
1	A	290	ARG
1	A	298	ILE
1	A	308	ILE
1	A	310	ILE
1	A	311	ILE
1	A	312	GLN
1	A	318	THR
1	A	323	ILE
1	A	324	CYS
1	A	332	SER
1	A	337	ILE
1	A	339	SER
1	A	340	MET
1	A	342	LEU
1	A	345	SER
1	A	348	MET
1	A	350	TYR
1	A	351	LEU
1	A	355	GLN
2	B	1	MET
2	B	2	LYS
2	B	6	PHE
2	B	12	ASN
2	B	15	ARG
2	B	17	SER

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Mol	Chain	Res	Type
2	B	18	ASP
2	B	19	GLN
2	B	20	VAL
2	B	37	ASP
2	B	38	THR
2	B	51	VAL
2	B	62	LEU
2	B	65	MET
2	B	70	LYS
2	B	81	HIS
2	B	84	VAL
2	B	95	GLN
2	B	100	ARG
2	B	106	SER
2	B	115	ARG
2	B	119	ARG
2	B	122	ASP
2	B	123	SER
2	B	124	GLN
2	B	126	GLN
2	B	129	SER
2	B	130	GLU
2	B	140	THR
2	B	149	ASP
2	B	157	SER
2	B	175	THR
2	B	176	SER
2	B	177	LYS
2	B	179	VAL
2	B	180	VAL
2	B	181	GLU
2	B	188	LEU
2	B	190	LEU
2	B	200	GLN
2	B	207	LEU
2	B	210	GLU
2	B	213	GLN
2	B	217	VAL
2	B	223	ARG
2	B	224	HIS
2	B	225	LYS
2	B	226	LEU

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Mol	Chain	Res	Type
2	B	228	LEU
2	B	231	ASN
2	B	233	ASN
2	B	253	GLU
2	B	256	SER
2	B	259	ASP
2	B	261	GLU
2	B	262	GLN
2	B	269	SER
2	B	273	ILE
2	B	275	THR
2	B	277	GLU
2	B	281	GLN
2	B	284	ARG
2	B	289	CYS
2	B	295	LEU
2	B	301	SER
2	B	303	GLU
2	B	307	GLN
2	B	309	ARG
2	B	318	ASN
2	B	319	ILE
1	C	1	MET
1	C	8	LEU
1	C	9	THR
1	C	15	LEU
1	C	22	LYS
1	C	23	ARG
1	C	24	LEU
1	C	27	LEU
1	C	32	GLU
1	C	42	LEU
1	C	46	PHE
1	C	47	THR
1	C	48	GLU
1	C	52	LEU
1	C	62	LEU
1	C	76	ILE
1	C	84	VAL
1	C	85	ARG
1	C	92	LEU
1	C	93	LEU

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Mol	Chain	Res	Type
1	C	95	GLN
1	C	106	CYS
1	C	107	ARG
1	C	109	LEU
1	C	112	LYS
1	C	115	ARG
1	C	121	MET
1	C	123	ASN
1	C	124	SER
1	C	125	ARG
1	C	127	LEU
1	C	128	MET
1	C	129	ASP
1	C	131	TRP
1	C	137	GLU
1	C	140	ASN
1	C	144	ILE
1	C	148	ASN
1	C	151	ILE
1	C	152	LYS
1	C	155	LYS
1	C	156	ILE
1	C	164	THR
1	C	176	SER
1	C	178	SER
1	C	186	ARG
1	C	191	ILE
1	C	199	HIS
1	C	205	LEU
1	C	207	LEU
1	C	213	THR
1	C	219	VAL
1	C	224	HIS
1	C	225	CYS
1	C	227	SER
1	C	232	VAL
1	C	238	ARG
1	C	242	ILE
1	C	250	TRP
1	C	258	THR
1	C	259	LYS
1	C	260	ILE

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Mol	Chain	Res	Type
1	C	263	ASP
1	C	265	ASP
1	C	266	GLN
1	C	289	ASN
1	C	290	ARG
1	C	298	ILE
1	C	308	ILE
1	C	310	ILE
1	C	311	ILE
1	C	312	GLN
1	C	318	THR
1	C	323	ILE
1	C	324	CYS
1	C	332	SER
1	C	337	ILE
1	C	339	SER
1	C	340	MET
1	C	342	LEU
1	C	345	SER
1	C	348	MET
1	C	350	TYR
1	C	351	LEU
1	C	355	GLN
2	D	1	MET
2	D	2	LYS
2	D	6	PHE
2	D	12	ASN
2	D	15	ARG
2	D	17	SER
2	D	18	ASP
2	D	19	GLN
2	D	20	VAL
2	D	37	ASP
2	D	38	THR
2	D	51	VAL
2	D	62	LEU
2	D	65	MET
2	D	70	LYS
2	D	81	HIS
2	D	84	VAL
2	D	95	GLN
2	D	100	ARG

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Mol	Chain	Res	Type
2	D	106	SER
2	D	115	ARG
2	D	119	ARG
2	D	122	ASP
2	D	123	SER
2	D	124	GLN
2	D	126	GLN
2	D	129	SER
2	D	130	GLU
2	D	140	THR
2	D	149	ASP
2	D	157	SER
2	D	175	THR
2	D	176	SER
2	D	177	LYS
2	D	179	VAL
2	D	180	VAL
2	D	181	GLU
2	D	188	LEU
2	D	190	LEU
2	D	200	GLN
2	D	207	LEU
2	D	210	GLU
2	D	213	GLN
2	D	217	VAL
2	D	223	ARG
2	D	224	HIS
2	D	225	LYS
2	D	226	LEU
2	D	228	LEU
2	D	231	ASN
2	D	233	ASN
2	D	253	GLU
2	D	256	SER
2	D	259	ASP
2	D	261	GLU
2	D	262	GLN
2	D	269	SER
2	D	273	ILE
2	D	275	THR
2	D	277	GLU
2	D	281	GLN

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Mol	Chain	Res	Type
2	D	284	ARG
2	D	289	CYS
2	D	295	LEU
2	D	301	SER
2	D	303	GLU
2	D	307	GLN
2	D	309	ARG
2	D	318	ASN
2	D	319	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	44	HIS
1	A	54	ASN
1	A	61	HIS
1	A	82	HIS
1	A	95	GLN
1	A	157	GLN
1	A	165	GLN
1	A	204	GLN
1	A	224	HIS
1	A	237	ASN
1	A	256	ASN
1	A	322	ASN
1	A	344	GLN
2	B	9	ASN
2	B	68	ASN
2	B	81	HIS
2	B	82	HIS
2	B	95	GLN
2	B	118	ASN
2	B	145	HIS
2	B	173	ASN
2	B	200	GLN
2	B	209	HIS
2	B	215	HIS
2	B	231	ASN
2	B	232	GLN
2	B	233	ASN
2	B	308	GLN

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Mol	Chain	Res	Type
2	B	318	ASN
1	C	26	ASN
1	C	54	ASN
1	C	82	HIS
1	C	95	GLN
1	C	157	GLN
1	C	165	GLN
1	C	204	GLN
1	C	224	HIS
1	C	237	ASN
1	C	256	ASN
1	C	266	GLN
1	C	322	ASN
1	C	344	GLN
2	D	9	ASN
2	D	68	ASN
2	D	81	HIS
2	D	82	HIS
2	D	95	GLN
2	D	118	ASN
2	D	145	HIS
2	D	173	ASN
2	D	200	GLN
2	D	209	HIS
2	D	215	HIS
2	D	231	ASN
2	D	232	GLN
2	D	233	ASN
2	D	308	GLN
2	D	318	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	PO4	A	356	-	4,4,4	2.79	4 (100%)	6,6,6	0.64	0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	356	PO4	P-O2	-3.11	1.45	1.54
3	A	356	PO4	P-O4	-3.10	1.45	1.54
3	A	356	PO4	P-O3	-2.75	1.46	1.54
3	A	356	PO4	P-O1	-2.09	1.45	1.50

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	356	PO4	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.