



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:48 AM UTC

PDB ID : 2ZCI / pdb_00002zci
Title : Structure of a GTP-dependent bacterial PEP-carboxykinase from *Corynebacterium glutamicum*
Authors : Aich, S.; Prasad, L.; Delbaere, L.T.J.
Deposited on : 2007-11-09
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

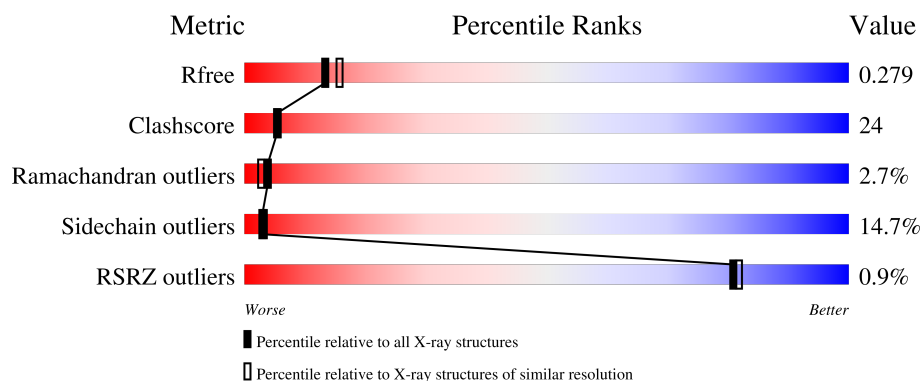
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	610	
1	B	610	
1	C	610	
1	D	610	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18407 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 Phosphoenolpyruvate carboxykinase [GTP].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	586	Total	C	N	O	S	0	0	0
			4539	2871	764	874	30			
1	B	584	Total	C	N	O	S	0	0	0
			4518	2858	761	869	30			
1	C	586	Total	C	N	O	S	0	0	0
			4535	2869	763	873	30			
1	D	578	Total	C	N	O	S	0	0	0
			4489	2840	755	864	30			

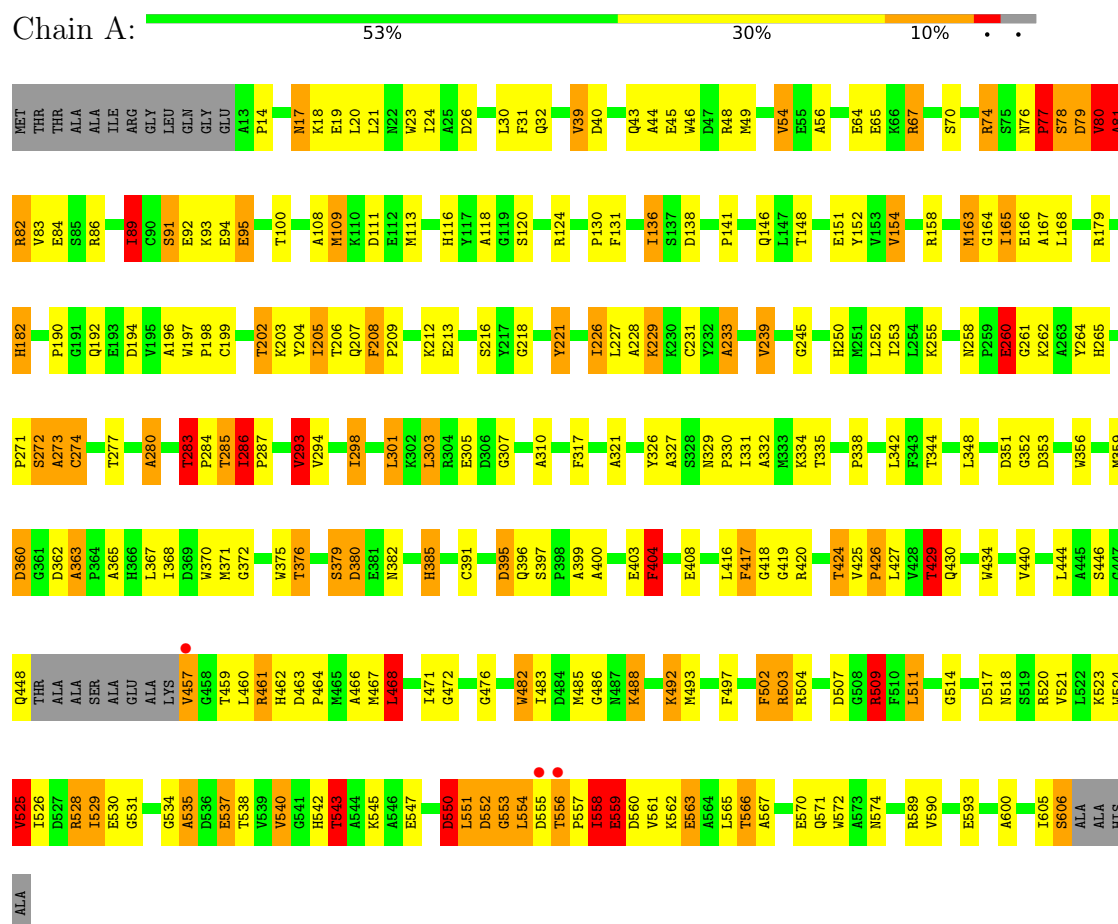
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	109	Total	O	0	0
			109	109		
2	B	69	Total	O	0	0
			69	69		
2	C	89	Total	O	0	0
			89	89		
2	D	59	Total	O	0	0
			59	59		

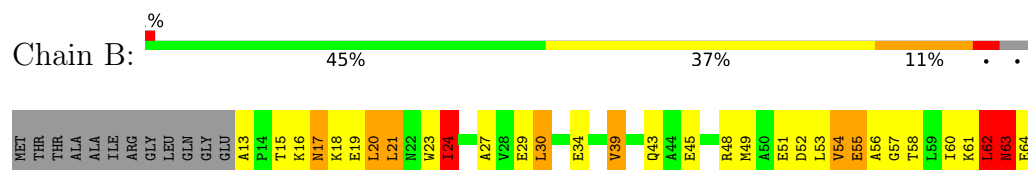
3 Residue-property plots

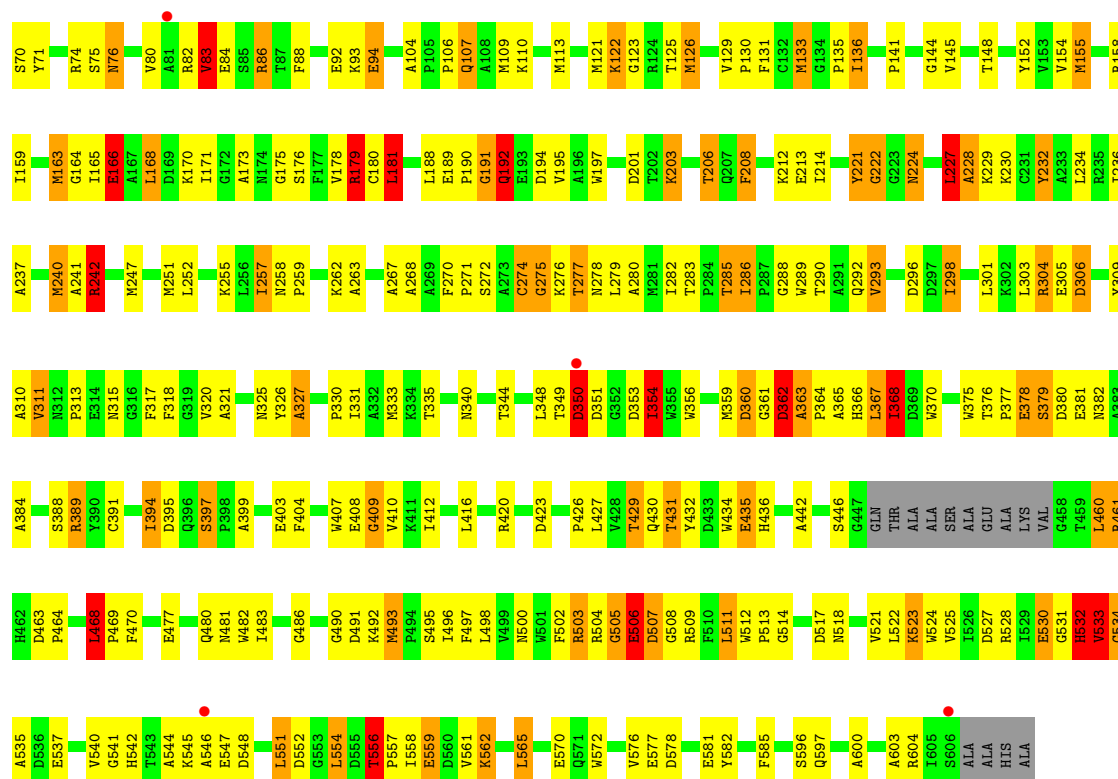
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

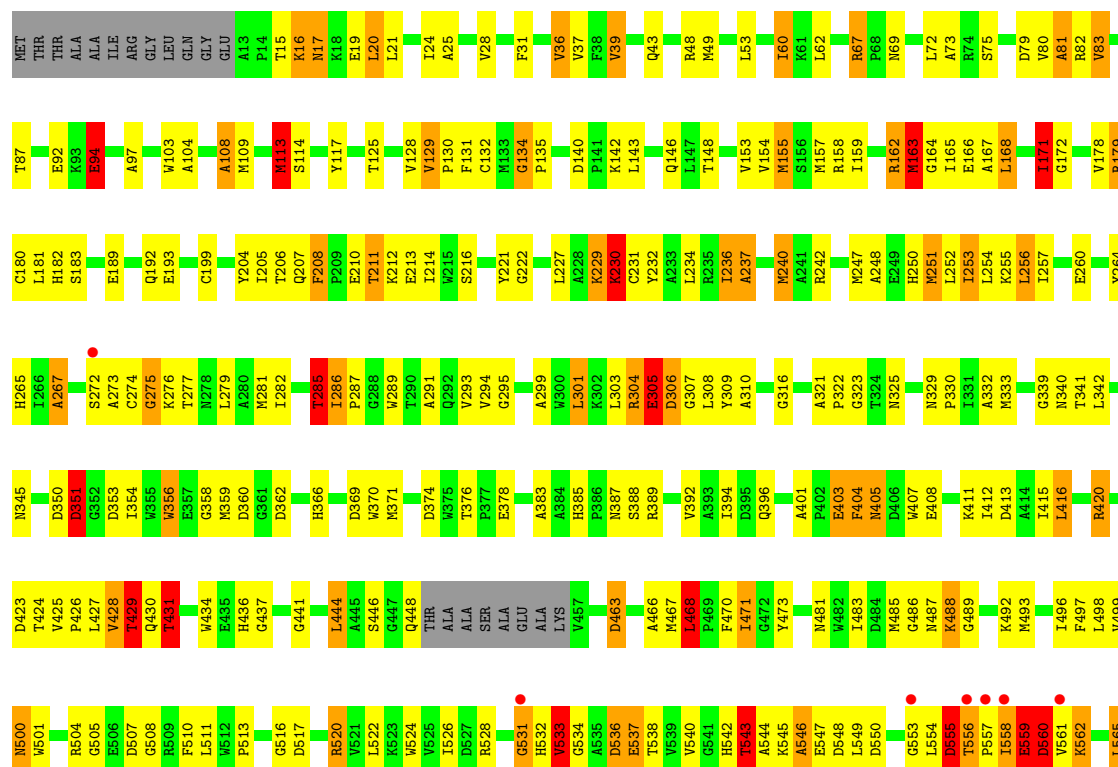


• Molecule 1: Phosphoenolpyruvate carboxykinase [GTP]



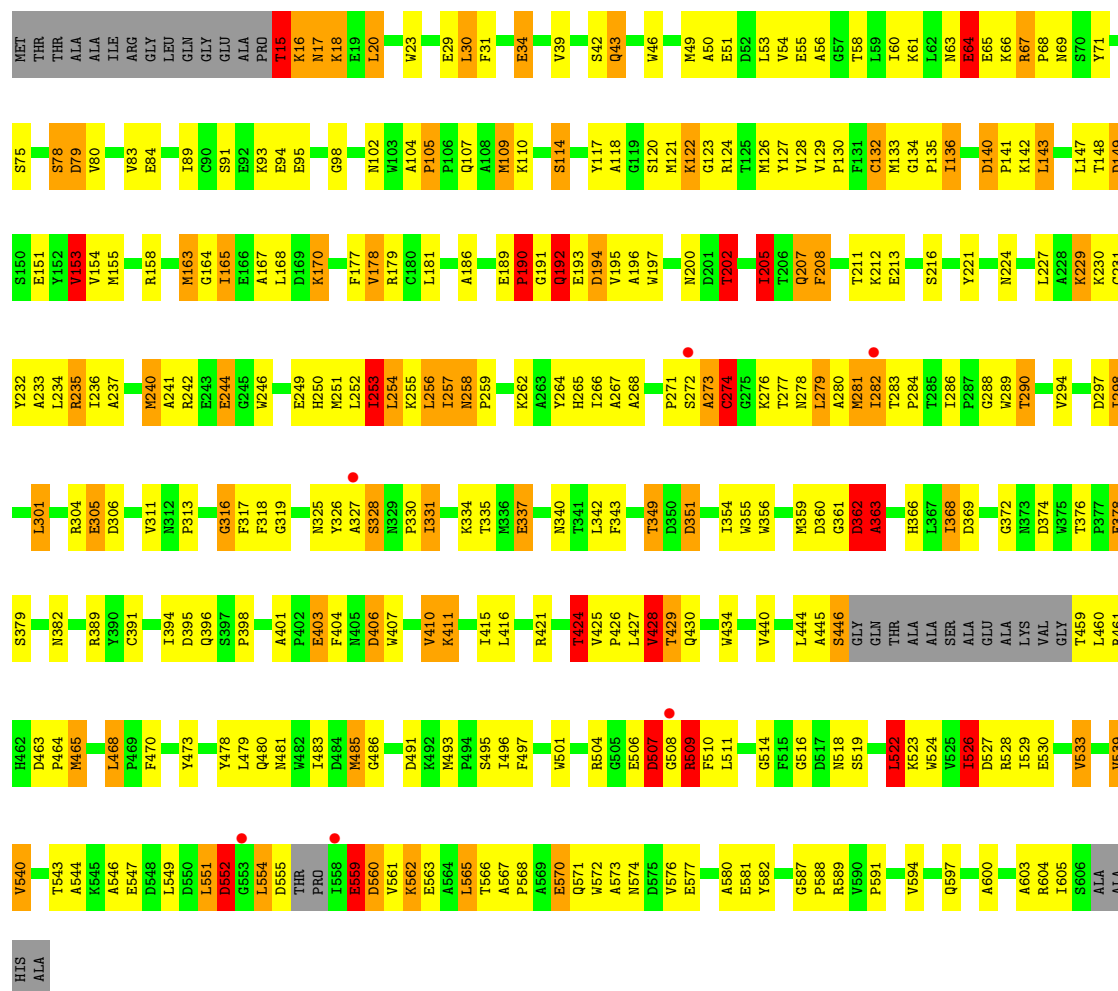
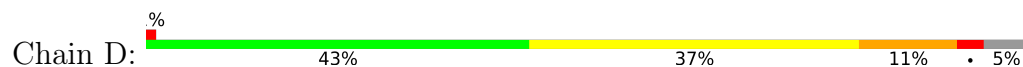


• Molecule 1: Phosphoenolpyruvate carboxykinase [GTP]





• Molecule 1: Phosphoenolpyruvate carboxykinase [GTP]



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.34Å 118.06Å 152.93Å 90.00° 96.44° 90.00°	Depositor
Resolution (Å)	24.83 – 2.30 24.83 – 2.30	Depositor EDS
% Data completeness (in resolution range)	77.0 (24.83-2.30) 76.9 (24.83-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.63 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.188 , 0.279 0.189 , 0.279	Depositor DCC
R_{free} test set	4256 reflections (3.87%)	wwPDB-VP
Wilson B-factor (Å ²)	31.0	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 46.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	18407	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	1.72	58/4658 (1.2%)	1.64	85/6342 (1.3%)
1	B	1.66	48/4637 (1.0%)	1.58	81/6313 (1.3%)
1	C	1.72	55/4654 (1.2%)	1.61	74/6337 (1.2%)
1	D	1.55	28/4605 (0.6%)	1.59	73/6266 (1.2%)
All	All	1.66	189/18554 (1.0%)	1.61	313/25258 (1.2%)

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	3
1	B	0	1
1	C	0	3
1	D	0	2
All	All	0	9

All (189) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	171	ILE	CA-CB	10.01	1.66	1.54
1	B	468	LEU	N-CA	9.92	1.55	1.46
1	B	483	ILE	CA-CB	9.63	1.65	1.54
1	B	236	ILE	CA-CB	9.25	1.64	1.54
1	A	483	ILE	CA-CB	8.89	1.64	1.54
1	D	483	ILE	CA-CB	8.70	1.64	1.54
1	C	108	ALA	CA-CB	8.60	1.67	1.53
1	C	163	MET	CA-C	8.48	1.63	1.52
1	D	153	VAL	CA-CB	8.41	1.65	1.54
1	D	129	VAL	CA-CB	8.14	1.64	1.54
1	A	48	ARG	CA-C	8.10	1.63	1.52
1	C	446	SER	N-CA	7.96	1.56	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	423	ASP	CA-C	7.92	1.62	1.52
1	A	376	THR	CA-CB	7.90	1.64	1.54
1	C	597	GLN	CA-C	-7.73	1.42	1.52
1	D	202	THR	CA-CB	7.66	1.64	1.53
1	C	248	ALA	CA-CB	-7.43	1.43	1.53
1	B	500	ASN	CA-C	7.41	1.60	1.52
1	C	599	ASP	N-CA	7.38	1.55	1.46
1	A	365	ALA	CA-CB	7.27	1.64	1.53
1	B	498	LEU	N-CA	-7.21	1.37	1.46
1	B	24	ILE	CA-CB	7.18	1.64	1.54
1	B	155	MET	CA-C	7.15	1.62	1.52
1	D	236	ILE	CA-CB	7.14	1.63	1.54
1	C	128	VAL	CA-CB	7.14	1.62	1.53
1	A	152	TYR	C-O	-7.12	1.15	1.24
1	B	468	LEU	C-O	7.08	1.31	1.24
1	A	39	VAL	CA-CB	7.03	1.62	1.54
1	D	109	MET	CA-C	7.03	1.61	1.52
1	C	500	ASN	N-CA	-7.00	1.37	1.46
1	B	321	ALA	CA-C	6.98	1.60	1.52
1	C	83	VAL	N-CA	6.92	1.54	1.46
1	B	327	ALA	CA-C	6.91	1.61	1.52
1	C	164	GLY	C-O	-6.87	1.14	1.23
1	B	533	VAL	CA-C	6.82	1.61	1.52
1	B	496	ILE	CA-CB	6.78	1.62	1.54
1	D	58	THR	C-O	-6.68	1.16	1.24
1	D	286	ILE	CA-CB	6.66	1.60	1.53
1	C	533	VAL	CA-CB	6.65	1.63	1.54
1	D	140	ASP	N-CA	6.63	1.53	1.46
1	B	446	SER	N-CA	6.58	1.53	1.45
1	A	198	PRO	C-O	6.52	1.31	1.23
1	D	485	MET	N-CA	-6.48	1.38	1.46
1	C	72	LEU	CA-C	6.45	1.60	1.52
1	D	240	MET	N-CA	6.42	1.54	1.46
1	C	267	ALA	CA-C	6.37	1.61	1.52
1	A	154	VAL	N-CA	6.37	1.53	1.46
1	B	164	GLY	C-O	-6.36	1.20	1.24
1	D	559	GLU	CA-C	6.34	1.61	1.52
1	B	277	THR	CA-CB	6.31	1.63	1.53
1	A	130	PRO	C-O	6.28	1.30	1.23
1	A	556	THR	CA-CB	6.25	1.63	1.53
1	A	605	ILE	CA-CB	6.25	1.62	1.54
1	A	226	ILE	CA-CB	6.20	1.62	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	32	GLN	N-CA	6.18	1.50	1.46
1	D	127	TYR	CA-C	-6.18	1.45	1.52
1	B	395	ASP	N-CA	6.18	1.54	1.46
1	A	70	SER	N-CA	6.15	1.53	1.45
1	C	237	ALA	CA-CB	-6.12	1.43	1.53
1	A	280	ALA	N-CA	6.12	1.53	1.46
1	C	60	ILE	CA-CB	6.11	1.61	1.54
1	C	321	ALA	N-CA	-6.10	1.42	1.46
1	C	425	VAL	N-CA	6.10	1.50	1.46
1	C	579	ASN	C-O	-6.08	1.17	1.24
1	C	72	LEU	N-CA	-6.06	1.38	1.46
1	A	89	ILE	N-CA	-6.05	1.38	1.46
1	A	382	ASN	C-O	-6.04	1.16	1.23
1	A	521	VAL	CA-CB	6.01	1.61	1.54
1	A	165	ILE	CA-CB	6.00	1.61	1.54
1	C	113	MET	CA-C	5.99	1.60	1.52
1	B	130	PRO	C-O	5.99	1.30	1.23
1	C	425	VAL	CA-CB	5.99	1.60	1.53
1	D	143	LEU	N-CA	-5.95	1.38	1.45
1	A	334	LYS	CA-C	5.93	1.60	1.52
1	C	578	ASP	C-O	5.93	1.30	1.24
1	C	333	MET	N-CA	5.92	1.53	1.46
1	C	583	LEU	N-CA	5.92	1.53	1.46
1	C	97	ALA	CA-CB	-5.90	1.43	1.53
1	A	467	MET	C-O	-5.89	1.16	1.24
1	B	83	VAL	CA-CB	5.88	1.62	1.54
1	C	140	ASP	CA-C	5.88	1.60	1.52
1	A	205	ILE	CA-CB	5.87	1.62	1.54
1	B	556	THR	CA-CB	5.87	1.61	1.52
1	D	104	ALA	CA-CB	-5.87	1.45	1.54
1	A	301	LEU	N-CA	5.86	1.53	1.45
1	A	283	THR	CA-CB	5.85	1.61	1.53
1	A	120	SER	N-CA	5.85	1.54	1.46
1	C	131	PHE	CA-C	-5.82	1.45	1.52
1	A	344	THR	CA-C	5.81	1.59	1.52
1	A	502	PHE	N-CA	5.81	1.52	1.46
1	B	350	ASP	N-CA	5.78	1.53	1.46
1	B	350	ASP	CA-C	5.77	1.60	1.52
1	A	56	ALA	C-O	5.75	1.31	1.24
1	C	207	GLN	N-CA	-5.75	1.39	1.46
1	B	331	ILE	CA-C	5.75	1.59	1.52
1	C	182	HIS	CA-C	-5.74	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	310	ALA	C-O	-5.74	1.16	1.24
1	B	240	MET	N-CA	5.72	1.53	1.46
1	C	332	ALA	C-O	-5.69	1.17	1.24
1	A	228	ALA	N-CA	5.69	1.53	1.46
1	C	405	ASN	N-CA	5.67	1.53	1.46
1	B	252	LEU	CA-C	5.66	1.60	1.53
1	A	164	GLY	C-O	-5.66	1.16	1.23
1	B	293	VAL	CA-CB	5.63	1.61	1.54
1	B	442	ALA	CA-CB	-5.63	1.44	1.53
1	B	62	LEU	N-CA	-5.62	1.38	1.46
1	B	121	MET	N-CA	5.60	1.52	1.46
1	B	537	GLU	C-O	-5.60	1.17	1.24
1	D	120	SER	N-CA	5.58	1.53	1.46
1	A	239	VAL	C-O	-5.56	1.18	1.24
1	A	202	THR	CA-CB	5.54	1.60	1.53
1	A	429	THR	CA-CB	5.53	1.63	1.53
1	C	415	ILE	CA-CB	-5.53	1.47	1.54
1	A	146	GLN	C-O	-5.53	1.17	1.24
1	B	359	MET	N-CA	5.53	1.52	1.46
1	D	343	PHE	N-CA	5.53	1.53	1.46
1	C	542	HIS	N-CA	5.53	1.53	1.46
1	B	145	VAL	CA-CB	5.52	1.62	1.54
1	C	37	VAL	CA-CB	5.52	1.61	1.54
1	A	81	ALA	CA-CB	5.51	1.62	1.53
1	A	425	VAL	CA-CB	5.51	1.59	1.53
1	B	282	ILE	CA-CB	5.49	1.60	1.54
1	A	351	ASP	CA-C	5.47	1.60	1.52
1	C	73	ALA	CA-CB	-5.47	1.45	1.53
1	A	509	ARG	CA-C	5.46	1.59	1.52
1	C	412	ILE	CA-CB	5.46	1.61	1.54
1	D	382	ASN	CA-C	5.44	1.59	1.52
1	B	166	GLU	CG-CD	5.42	1.65	1.52
1	C	403	GLU	C-O	5.42	1.31	1.24
1	C	73	ALA	N-CA	-5.41	1.39	1.46
1	D	368	ILE	CA-CB	5.41	1.60	1.54
1	B	354	ILE	CA-CB	5.39	1.62	1.54
1	C	556	THR	CA-CB	5.39	1.64	1.54
1	B	603	ALA	C-O	-5.39	1.17	1.24
1	C	129	VAL	CA-CB	5.38	1.61	1.54
1	D	425	VAL	CA-CB	5.37	1.59	1.53
1	D	311	VAL	CA-C	5.37	1.59	1.52
1	C	356	TRP	N-CA	-5.37	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	363	ALA	CA-CB	5.36	1.61	1.53
1	D	178	VAL	CA-CB	-5.36	1.45	1.53
1	A	424	THR	CA-CB	5.34	1.62	1.53
1	C	383	ALA	N-CA	5.32	1.52	1.46
1	B	181	LEU	N-CA	-5.30	1.39	1.45
1	B	232	TYR	CA-C	-5.30	1.47	1.52
1	D	594	VAL	CA-CB	5.29	1.61	1.54
1	A	24	ILE	CA-CB	5.27	1.60	1.54
1	D	224	ASN	N-CA	5.26	1.53	1.46
1	A	233	ALA	CA-CB	-5.26	1.44	1.53
1	C	498	LEU	N-CA	-5.25	1.40	1.46
1	A	79	ASP	CA-C	-5.24	1.46	1.53
1	B	283	THR	CA-CB	5.24	1.61	1.53
1	A	303	LEU	N-CA	-5.24	1.39	1.46
1	B	130	PRO	N-CA	-5.24	1.40	1.46
1	C	20	LEU	CA-C	-5.24	1.46	1.52
1	A	54	VAL	CA-C	5.23	1.59	1.52
1	A	182	HIS	C-O	-5.23	1.17	1.23
1	C	81	ALA	CA-CB	5.22	1.60	1.53
1	A	566	THR	CA-CB	5.21	1.62	1.53
1	A	426	PRO	N-CA	5.19	1.53	1.47
1	A	167	ALA	C-O	-5.19	1.18	1.24
1	B	213	GLU	CA-C	-5.19	1.46	1.52
1	A	419	GLY	N-CA	5.18	1.50	1.44
1	B	596	SER	C-O	5.18	1.30	1.24
1	D	102	ASN	CA-C	-5.18	1.46	1.52
1	A	600	ALA	CA-C	5.18	1.59	1.52
1	C	148	THR	CA-C	5.17	1.58	1.52
1	B	80	VAL	N-CA	5.16	1.51	1.46
1	C	94	GLU	N-CA	5.15	1.52	1.46
1	B	93	LYS	CA-C	5.14	1.59	1.52
1	A	556	THR	C-N	5.13	1.39	1.33
1	B	534	GLY	C-O	5.13	1.30	1.23
1	A	471	ILE	CA-CB	5.13	1.59	1.54
1	B	495	SER	CA-C	5.13	1.60	1.53
1	D	236	ILE	N-CA	5.12	1.52	1.46
1	A	593	GLU	N-CA	-5.12	1.40	1.46
1	A	14	PRO	CA-C	-5.11	1.47	1.52
1	A	550	ASP	CA-C	-5.11	1.48	1.53
1	C	351	ASP	CB-CG	5.10	1.64	1.52
1	C	428	VAL	CA-CB	5.10	1.61	1.54
1	A	14	PRO	N-CA	-5.08	1.41	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	351	ASP	N-CA	5.08	1.52	1.46
1	C	558	ILE	CA-CB	5.08	1.61	1.54
1	B	228	ALA	C-O	-5.05	1.17	1.24
1	A	404	PHE	CA-C	5.03	1.59	1.52
1	C	183	SER	CA-C	5.02	1.58	1.52
1	B	331	ILE	CG1-CD1	5.02	1.71	1.51
1	D	337	GLU	C-N	5.02	1.39	1.34
1	D	164	GLY	N-CA	5.00	1.52	1.45
1	C	573	ALA	C-O	-5.00	1.18	1.24

All (313) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	468	LEU	CA-C-N	-15.29	103.97	119.87
1	D	468	LEU	C-N-CA	-15.29	103.97	119.87
1	A	468	LEU	CA-C-N	-13.93	106.63	120.83
1	A	468	LEU	C-N-CA	-13.93	106.63	120.83
1	C	532	HIS	N-CA-C	-13.85	96.93	112.72
1	A	606	SER	CA-C-O	9.58	137.09	120.80
1	D	43	GLN	N-CA-C	-9.49	100.27	112.23
1	C	208	PHE	CA-C-N	9.48	130.12	119.32
1	C	208	PHE	C-N-CA	9.48	130.12	119.32
1	D	540	VAL	N-CA-C	9.40	120.21	110.62
1	A	321	ALA	CA-C-N	-8.91	110.58	119.76
1	A	321	ALA	C-N-CA	-8.91	110.58	119.76
1	D	395	ASP	CB-CA-C	-8.75	95.81	110.68
1	A	558	ILE	CB-CA-C	-8.74	100.03	111.13
1	A	526	ILE	N-CA-C	8.60	118.61	110.53
1	C	165	ILE	N-CA-C	8.60	119.39	110.36
1	B	435	GLU	N-CA-C	-8.57	101.44	112.23
1	D	208	PHE	CA-C-N	8.46	127.77	118.97
1	D	208	PHE	C-N-CA	8.46	127.77	118.97
1	A	76	ASN	CA-C-N	8.43	130.37	119.84
1	A	76	ASN	C-N-CA	8.43	130.37	119.84
1	A	197	TRP	CA-C-N	-8.43	112.05	120.31
1	A	197	TRP	C-N-CA	-8.43	112.05	120.31
1	C	436	HIS	CA-C-N	8.39	129.30	119.98
1	C	436	HIS	C-N-CA	8.39	129.30	119.98
1	A	286	ILE	CA-C-N	8.29	129.60	119.98
1	A	286	ILE	C-N-CA	8.29	129.60	119.98
1	A	89	ILE	CB-CA-C	8.24	122.65	111.19
1	A	385	HIS	N-CA-C	-8.18	98.79	110.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	194	ASP	N-CA-C	8.10	120.23	110.19
1	A	424	THR	CA-C-N	-8.07	116.78	122.59
1	A	424	THR	C-N-CA	-8.07	116.78	122.59
1	B	360	ASP	N-CA-C	8.04	122.17	109.39
1	B	165	ILE	N-CA-C	8.01	121.11	111.09
1	D	153	VAL	N-CA-C	7.97	118.75	110.62
1	B	191	GLY	N-CA-C	-7.96	97.15	111.15
1	C	468	LEU	CA-C-N	-7.91	111.33	120.12
1	C	468	LEU	C-N-CA	-7.91	111.33	120.12
1	A	503	ARG	CG-CD-NE	-7.90	94.61	112.00
1	D	605	ILE	N-CA-C	7.86	117.97	110.42
1	C	113	MET	N-CA-C	7.82	120.79	111.33
1	B	27	ALA	N-CA-C	7.82	119.58	111.14
1	B	197	TRP	CA-C-N	7.79	128.07	119.90
1	B	197	TRP	C-N-CA	7.79	128.07	119.90
1	D	540	VAL	CB-CA-C	-7.74	101.69	112.14
1	B	242	ARG	N-CA-C	-7.68	102.55	112.23
1	A	79	ASP	N-CA-C	7.68	119.36	108.54
1	B	397	SER	CA-C-N	-7.61	111.67	120.12
1	B	397	SER	C-N-CA	-7.61	111.67	120.12
1	A	40	ASP	N-CA-C	7.60	122.31	112.89
1	C	275	GLY	N-CA-C	-7.59	103.69	112.50
1	B	597	GLN	N-CA-C	-7.55	103.05	111.28
1	C	587	GLY	CA-C-N	7.45	127.16	119.56
1	C	587	GLY	C-N-CA	7.45	127.16	119.56
1	A	192	GLN	N-CA-C	7.44	126.65	110.80
1	A	205	ILE	N-CA-C	-7.42	96.72	107.78
1	D	573	ALA	CA-C-N	7.42	131.22	120.38
1	D	573	ALA	C-N-CA	7.42	131.22	120.38
1	D	105	PRO	CA-C-N	7.41	126.94	119.24
1	D	105	PRO	C-N-CA	7.41	126.94	119.24
1	B	379	SER	N-CA-C	7.31	121.44	112.23
1	A	327	ALA	N-CA-C	7.26	119.27	111.36
1	A	293	VAL	CB-CA-C	7.19	119.82	110.91
1	B	367	LEU	CA-C-N	-7.17	112.66	122.91
1	B	367	LEU	C-N-CA	-7.17	112.66	122.91
1	C	304	ARG	CA-C-N	-7.17	111.41	122.16
1	C	304	ARG	C-N-CA	-7.17	111.41	122.16
1	D	286	ILE	CB-CA-C	7.12	118.33	110.71
1	B	480	GLN	N-CA-C	-7.08	103.30	112.23
1	B	221	TYR	N-CA-C	7.06	121.17	109.46
1	C	543	THR	N-CA-C	7.02	121.11	109.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	30	LEU	CA-CB-CG	7.00	140.81	116.30
1	A	21	LEU	N-CA-C	7.00	118.91	111.28
1	A	165	ILE	N-CA-C	6.99	117.70	110.36
1	C	104	ALA	N-CA-C	-6.96	101.96	108.22
1	D	167	ALA	N-CA-C	-6.94	103.16	111.69
1	C	590	VAL	N-CA-CB	6.93	117.86	110.17
1	A	78	SER	CA-C-N	-6.87	113.72	123.20
1	A	78	SER	C-N-CA	-6.87	113.72	123.20
1	D	127	TYR	N-CA-C	-6.86	98.54	109.59
1	B	274	CYS	N-CA-C	-6.86	100.13	110.28
1	D	273	ALA	N-CA-C	-6.85	100.15	110.28
1	B	556	THR	CA-C-N	6.85	127.92	119.98
1	B	556	THR	C-N-CA	6.85	127.92	119.98
1	C	429	THR	N-CA-C	6.84	120.69	109.06
1	A	111	ASP	N-CA-C	6.80	118.49	111.14
1	C	483	ILE	N-CA-C	-6.79	104.15	110.53
1	B	286	ILE	CA-C-N	6.74	126.70	119.76
1	B	286	ILE	C-N-CA	6.74	126.70	119.76
1	A	553	GLY	N-CA-C	-6.67	105.96	114.37
1	B	286	ILE	CB-CA-C	-6.63	99.29	111.36
1	A	525	VAL	N-CA-C	-6.63	103.86	110.62
1	B	505	GLY	N-CA-C	-6.61	102.49	112.41
1	B	208	PHE	CA-C-N	6.59	127.11	119.47
1	B	208	PHE	C-N-CA	6.59	127.11	119.47
1	B	523	LYS	N-CA-C	-6.57	104.04	111.14
1	D	597	GLN	N-CA-C	6.57	118.10	111.07
1	C	431	THR	N-CA-CB	-6.57	101.38	110.38
1	B	533	VAL	CB-CA-C	6.56	122.05	111.29
1	A	363	ALA	CA-C-N	-6.55	113.03	119.78
1	A	363	ALA	C-N-CA	-6.55	113.03	119.78
1	A	283	THR	CB-CA-C	6.54	117.42	110.17
1	D	509	ARG	N-CA-C	6.53	119.99	109.02
1	B	493	MET	N-CA-C	-6.50	101.32	110.29
1	A	462	HIS	CA-C-N	6.49	128.00	122.28
1	A	462	HIS	C-N-CA	6.49	128.00	122.28
1	C	36	VAL	N-CA-C	6.47	117.92	108.53
1	C	562	LYS	N-CA-C	-6.47	105.42	113.38
1	A	395	ASP	CB-CA-C	-6.47	97.55	110.42
1	D	587	GLY	CA-C-N	6.45	126.21	119.05
1	D	587	GLY	C-N-CA	6.45	126.21	119.05
1	A	352	GLY	N-CA-C	6.44	124.86	115.32
1	C	360	ASP	N-CA-C	6.43	120.23	112.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	285	THR	N-CA-C	-6.40	103.91	112.94
1	A	26	ASP	N-CA-C	6.38	118.77	111.11
1	A	221	TYR	N-CA-C	6.35	119.59	109.24
1	A	590	VAL	CA-C-N	-6.33	113.26	119.78
1	A	590	VAL	C-N-CA	-6.33	113.26	119.78
1	B	55	GLU	N-CA-C	-6.33	103.68	111.40
1	C	240	MET	N-CA-C	-6.31	104.32	111.07
1	B	596	SER	CB-CA-C	-6.31	100.98	110.88
1	C	329	ASN	CA-C-N	-6.29	112.53	119.19
1	C	329	ASN	C-N-CA	-6.29	112.53	119.19
1	B	270	PHE	CA-C-N	6.24	127.64	119.84
1	B	270	PHE	C-N-CA	6.24	127.64	119.84
1	A	360	ASP	N-CA-C	-6.24	104.59	111.82
1	A	540	VAL	N-CA-C	6.22	117.01	110.72
1	B	30	LEU	N-CA-C	6.22	117.85	111.14
1	B	576	VAL	N-CA-C	6.19	116.94	110.62
1	B	39	VAL	CB-CA-C	6.17	120.19	110.81
1	C	501	TRP	CB-CA-C	-6.16	99.77	110.17
1	A	131	PHE	N-CA-C	6.15	118.42	109.07
1	C	516	GLY	N-CA-C	-6.14	107.05	114.66
1	B	460	LEU	N-CA-C	6.12	123.83	110.80
1	B	168	LEU	N-CA-C	6.11	118.72	111.33
1	D	594	VAL	N-CA-C	-6.06	104.60	110.72
1	C	556	THR	CA-C-N	6.06	127.42	119.84
1	C	556	THR	C-N-CA	6.06	127.42	119.84
1	D	192	GLN	N-CA-C	6.03	123.65	110.80
1	D	235	ARG	NE-CZ-NH2	6.02	124.61	119.20
1	B	356	TRP	N-CA-C	5.98	118.17	109.07
1	A	556	THR	CA-C-N	-5.97	112.88	120.23
1	A	556	THR	C-N-CA	-5.97	112.88	120.23
1	A	550	ASP	CB-CA-C	-5.96	109.69	116.54
1	C	286	ILE	CA-C-N	5.96	126.27	119.83
1	C	286	ILE	C-N-CA	5.96	126.27	119.83
1	C	567	ALA	CA-C-N	5.95	126.88	119.98
1	C	567	ALA	C-N-CA	5.95	126.88	119.98
1	C	82	ARG	N-CA-C	5.94	123.46	110.80
1	A	376	THR	CA-C-N	-5.94	112.42	119.84
1	A	376	THR	C-N-CA	-5.94	112.42	119.84
1	D	30	LEU	CA-CB-CG	5.92	137.04	116.30
1	C	159	ILE	N-CA-C	5.92	117.45	111.00
1	A	559	GLU	CA-C-N	5.91	128.68	120.29
1	A	559	GLU	C-N-CA	5.91	128.68	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	605	ILE	N-CA-C	5.91	116.65	110.62
1	A	338	PRO	N-CA-C	5.89	121.28	114.03
1	D	55	GLU	N-CA-C	5.87	117.67	111.28
1	A	91	SER	N-CA-C	-5.86	101.80	110.48
1	C	134	GLY	N-CA-C	-5.85	100.41	112.34
1	D	526	ILE	N-CA-C	5.85	116.03	110.42
1	C	155	MET	N-CA-C	5.82	117.42	111.14
1	C	251	MET	N-CA-C	5.82	118.95	109.59
1	D	493	MET	CA-C-N	5.81	125.77	119.78
1	D	493	MET	C-N-CA	5.81	125.77	119.78
1	B	293	VAL	CB-CA-C	-5.80	103.60	111.15
1	C	171	ILE	CB-CA-C	5.79	119.38	111.97
1	B	84	GLU	N-CA-C	5.78	118.36	111.71
1	B	368	ILE	CB-CA-C	5.78	119.13	110.98
1	C	425	VAL	CA-C-N	-5.78	114.02	119.85
1	C	425	VAL	C-N-CA	-5.78	114.02	119.85
1	D	424	THR	N-CA-C	5.78	123.11	110.80
1	D	80	VAL	N-CA-C	5.77	117.72	112.29
1	C	387	ASN	N-CA-C	5.76	120.01	113.15
1	D	560	ASP	N-CA-C	-5.76	106.23	113.20
1	C	171	ILE	N-CA-C	-5.75	104.90	110.42
1	D	445	ALA	N-CA-C	5.74	117.69	109.14
1	A	196	ALA	N-CA-C	5.71	118.28	111.71
1	D	279	LEU	N-CA-C	5.68	117.56	111.36
1	A	233	ALA	N-CA-C	5.65	118.99	111.75
1	C	537	GLU	N-CA-C	5.65	118.21	110.24
1	C	401	ALA	CA-C-N	-5.65	113.07	119.28
1	C	401	ALA	C-N-CA	-5.65	113.07	119.28
1	A	543	THR	CB-CA-C	5.64	119.16	109.51
1	A	208	PHE	CA-C-N	5.63	125.48	119.28
1	A	208	PHE	C-N-CA	5.63	125.48	119.28
1	A	154	VAL	CB-CA-C	-5.62	104.68	111.88
1	C	362	ASP	N-CA-C	-5.61	101.39	110.32
1	B	232	TYR	N-CA-C	-5.61	105.47	112.93
1	C	146	GLN	N-CA-C	5.60	118.09	109.07
1	A	368	ILE	N-CA-C	-5.59	100.53	108.58
1	D	253	ILE	CB-CA-C	5.58	118.70	110.77
1	D	580	ALA	N-CA-C	5.58	117.36	111.28
1	D	522	LEU	CA-C-N	5.57	128.01	120.38
1	D	522	LEU	C-N-CA	5.57	128.01	120.38
1	C	285	THR	N-CA-CB	-5.57	102.25	110.49
1	B	423	ASP	N-CA-C	5.57	115.90	108.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	539	VAL	CA-C-N	5.55	128.06	120.46
1	D	539	VAL	C-N-CA	5.55	128.06	120.46
1	A	44	ALA	N-CA-C	-5.55	105.31	111.36
1	A	476	GLY	N-CA-C	-5.54	105.54	113.86
1	D	186	ALA	N-CA-C	5.54	118.66	109.79
1	B	306	ASP	N-CA-C	5.54	121.92	113.61
1	A	65	GLU	N-CA-C	-5.53	106.49	113.18
1	C	231	CYS	N-CA-C	-5.52	105.34	111.36
1	B	236	ILE	N-CA-CB	5.51	116.63	110.51
1	C	307	GLY	N-CA-C	5.51	119.04	110.88
1	D	306	ASP	N-CA-C	5.51	119.99	112.88
1	A	310	ALA	N-CA-C	5.51	117.88	108.90
1	A	67	ARG	CA-C-N	5.50	125.78	119.83
1	A	67	ARG	C-N-CA	5.50	125.78	119.83
1	D	56	ALA	N-CA-C	-5.50	106.52	113.18
1	B	121	MET	N-CA-C	5.50	118.99	112.72
1	B	30	LEU	N-CA-CB	5.49	118.03	110.07
1	B	559	GLU	N-CA-C	-5.49	106.17	112.92
1	C	546	ALA	CA-C-N	5.47	128.59	120.17
1	C	546	ALA	C-N-CA	5.47	128.59	120.17
1	B	502	PHE	CA-C-N	-5.47	111.22	120.95
1	B	502	PHE	C-N-CA	-5.47	111.22	120.95
1	C	230	LYS	N-CA-C	-5.47	107.16	113.88
1	D	382	ASN	N-CA-C	5.45	117.93	110.24
1	D	582	TYR	CA-CB-CG	-5.45	104.09	113.90
1	B	376	THR	CA-C-N	-5.44	114.08	120.12
1	B	376	THR	C-N-CA	-5.44	114.08	120.12
1	B	224	ASN	N-CA-C	5.43	117.96	111.71
1	B	320	VAL	CA-C-N	-5.43	113.80	119.83
1	B	320	VAL	C-N-CA	-5.43	113.80	119.83
1	D	508	GLY	N-CA-C	-5.42	108.22	115.32
1	B	227	LEU	N-CA-C	5.40	117.92	111.71
1	D	363	ALA	CA-C-N	5.40	125.32	119.76
1	D	363	ALA	C-N-CA	5.40	125.32	119.76
1	A	80	VAL	N-CA-C	5.37	118.15	112.83
1	C	499	VAL	N-CA-C	5.37	116.58	108.96
1	D	258	ASN	CA-C-N	-5.36	113.38	119.28
1	D	258	ASN	C-N-CA	-5.36	113.38	119.28
1	C	536	ASP	CA-C-N	5.36	128.46	120.90
1	C	536	ASP	C-N-CA	5.36	128.46	120.90
1	C	236	ILE	N-CA-CB	5.34	116.68	110.65
1	C	463	ASP	CA-C-N	5.34	126.51	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	463	ASP	C-N-CA	5.34	126.51	119.84
1	D	398	PRO	N-CA-C	-5.33	106.26	113.40
1	C	323	GLY	CA-C-N	5.32	128.40	120.95
1	C	323	GLY	C-N-CA	5.32	128.40	120.95
1	D	237	ALA	N-CA-C	5.32	117.08	111.28
1	A	380	ASP	O-C-N	5.31	128.67	122.24
1	A	19	GLU	N-CA-C	-5.31	105.39	111.07
1	B	267	ALA	CA-C-N	-5.31	112.60	121.94
1	B	267	ALA	C-N-CA	-5.31	112.60	121.94
1	B	468	LEU	CB-CA-C	-5.30	102.90	112.76
1	D	316	GLY	N-CA-C	5.29	118.83	111.10
1	B	13	ALA	CA-C-N	-5.29	115.43	120.83
1	B	13	ALA	C-N-CA	-5.29	115.43	120.83
1	C	83	VAL	CA-C-N	5.29	127.68	120.54
1	C	83	VAL	C-N-CA	5.29	127.68	120.54
1	A	528	ARG	CB-CG-CD	5.28	123.45	111.30
1	A	92	GLU	N-CA-C	5.27	117.70	111.33
1	D	91	SER	N-CA-C	-5.27	103.73	110.53
1	B	482	TRP	CA-C-N	5.27	127.19	120.56
1	B	482	TRP	C-N-CA	5.27	127.19	120.56
1	A	303	LEU	CB-CG-CD2	-5.26	94.92	110.70
1	A	529	ILE	CA-C-N	5.26	130.34	121.14
1	A	529	ILE	C-N-CA	5.26	130.34	121.14
1	A	482	TRP	CA-C-N	5.25	127.13	120.72
1	A	482	TRP	C-N-CA	5.25	127.13	120.72
1	B	179	ARG	N-CA-C	5.25	117.28	109.25
1	D	298	ILE	N-CA-C	5.23	116.26	108.46
1	B	482	TRP	N-CA-C	5.22	117.38	111.11
1	B	159	ILE	CB-CA-C	-5.22	105.01	112.22
1	C	471	ILE	N-CA-CB	5.21	116.21	110.53
1	D	440	VAL	CA-C-N	5.21	125.87	119.99
1	D	440	VAL	C-N-CA	5.21	125.87	119.99
1	A	31	PHE	N-CA-C	5.20	117.85	111.82
1	C	295	GLY	N-CA-C	-5.19	103.17	110.91
1	B	409	GLY	CA-C-O	-5.19	117.19	122.59
1	D	406	ASP	CA-C-N	5.19	127.24	120.28
1	D	406	ASP	C-N-CA	5.19	127.24	120.28
1	B	532	HIS	CA-C-N	-5.17	112.66	121.97
1	B	532	HIS	C-N-CA	-5.17	112.66	121.97
1	B	86	ARG	N-CA-C	5.17	118.90	112.59
1	C	199	CYS	N-CA-C	5.17	116.06	107.73
1	D	411	LYS	N-CA-CB	5.17	118.30	109.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	192	GLN	CA-C-N	5.17	128.21	120.87
1	C	192	GLN	C-N-CA	5.17	128.21	120.87
1	A	372	GLY	N-CA-C	-5.16	107.99	115.27
1	C	148	THR	N-CA-C	5.16	117.23	109.23
1	D	554	LEU	N-CA-C	5.15	117.01	108.20
1	A	151	GLU	N-CA-C	-5.14	106.96	113.18
1	A	417	PHE	N-CA-C	-5.13	101.04	109.40
1	D	445	ALA	CA-C-N	5.13	130.93	121.70
1	D	445	ALA	C-N-CA	5.13	130.93	121.70
1	A	486	GLY	CA-C-N	5.13	127.15	120.28
1	A	486	GLY	C-N-CA	5.13	127.15	120.28
1	B	80	VAL	CB-CA-C	-5.12	105.09	110.62
1	D	98	GLY	CA-C-N	5.11	124.72	119.56
1	D	98	GLY	C-N-CA	5.11	124.72	119.56
1	B	389	ARG	NE-CZ-NH1	-5.10	116.40	121.50
1	D	147	LEU	N-CA-C	-5.10	100.86	109.07
1	D	428	VAL	CB-CA-C	-5.08	101.70	110.65
1	D	205	ILE	CB-CA-C	5.08	119.62	111.29
1	C	48	ARG	N-CA-C	-5.08	105.74	111.28
1	D	249	GLU	N-CA-C	5.08	117.84	109.72
1	B	241	ALA	N-CA-C	5.06	116.80	111.28
1	A	504	ARG	N-CA-C	5.05	117.67	109.24
1	B	68	PRO	CA-C-O	-5.03	115.61	121.34
1	C	520	ARG	N-CA-C	-5.03	105.51	111.69
1	D	221	TYR	N-CA-C	5.02	117.16	109.07
1	B	229	LYS	N-CA-C	-5.02	100.55	108.73
1	B	54	VAL	CA-C-N	5.02	129.09	120.71
1	B	54	VAL	C-N-CA	5.02	129.09	120.71
1	D	42	SER	N-CA-C	5.02	117.00	110.53
1	B	275	GLY	N-CA-C	-5.01	101.30	113.18
1	C	83	VAL	N-CA-CB	5.01	119.50	111.23
1	B	133	MET	N-CA-C	5.01	118.47	110.70

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	261	GLY	Peptide
1	A	559	GLU	Peptide
1	A	81	ALA	Peptide
1	B	350	ASP	Peptide
1	C	305	GLU	Peptide

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Mol	Chain	Res	Type	Group
1	C	560	ASP	Peptide
1	C	81	ALA	Peptide
1	D	15	THR	Peptide
1	D	361	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	4539	0	4342	162	0
1	B	4518	0	4320	237	0
1	C	4535	0	4336	221	0
1	D	4489	0	4292	242	0
2	A	109	0	0	9	0
2	B	69	0	0	6	0
2	C	89	0	0	8	0
2	D	59	0	0	9	0
All	All	18407	0	17290	849	0

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 24.

All (849) 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:D:355:TRP:HA	1:D:359:MET:CE	1.70	1.22
1:B:129:VAL:HG13	1:B:163:MET:CE	1.70	1.19
1:C:534:GLY:HA3	1:C:548:ASP:OD2	1.38	1.18
1:D:132:CYS:HB2	1:D:143:LEU:HD23	1.18	1.16
1:A:558:ILE:H	1:A:558:ILE:HD12	1.00	1.16
1:B:129:VAL:CG1	1:B:163:MET:CE	2.29	1.10
1:B:74:ARG:NH1	1:B:368:ILE:CD1	2.17	1.08
1:C:113:MET:HE1	1:C:206:THR:HB	1.35	1.06
1:D:132:CYS:HB2	1:D:143:LEU:CD2	1.88	1.04
1:B:129:VAL:HG13	1:B:163:MET:HE2	1.08	1.04
1:B:109:MET:HE2	1:D:105:PRO:HD3	1.38	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:ARG:NH1	1:B:368:ILE:HD11	1.72	1.02
1:C:366:HIS:HE1	1:C:374:ASP:OD1	1.43	1.01
1:A:558:ILE:H	1:A:558:ILE:CD1	1.70	1.00
1:B:74:ARG:HH12	1:B:368:ILE:CD1	1.73	1.00
1:C:247:MET:HE1	1:C:308:LEU:HD21	1.44	0.99
1:D:355:TRP:HA	1:D:359:MET:HE2	1.41	0.99
1:D:511:LEU:HD13	1:D:563:GLU:HG3	1.43	0.98
1:A:429:THR:HG22	2:A:627:HOH:O	1.62	0.98
1:A:550:ASP:O	1:A:551:LEU:HD13	1.63	0.97
1:B:180:CYS:HB3	1:B:227:LEU:HD23	1.47	0.97
1:B:304:ARG:O	1:B:306:ASP:N	1.96	0.96
1:B:577:GLU:O	1:B:581:GLU:HG3	1.65	0.96
1:D:71:TYR:CE2	2:D:643:HOH:O	2.17	0.96
1:A:550:ASP:O	1:A:551:LEU:CD1	2.14	0.95
1:B:69:ASN:HD22	1:B:340:ASN:HD22	1.03	0.95
1:D:78:SER:O	1:D:79:ASP:HB2	1.63	0.95
1:A:558:ILE:HD12	1:A:558:ILE:N	1.82	0.94
1:D:63:ASN:HD22	1:D:66:LYS:HB2	1.34	0.93
1:D:17:ASN:HD22	1:D:18:LYS:H	1.12	0.93
1:B:129:VAL:CG1	1:B:163:MET:HE2	1.94	0.92
1:C:16:LYS:HD3	1:C:16:LYS:N	1.84	0.92
1:C:273:ALA:O	1:C:274:CYS:SG	2.27	0.92
1:B:506:GLU:O	1:B:508:GLY:N	2.03	0.92
1:A:429:THR:CG2	2:A:627:HOH:O	2.16	0.91
1:D:49:MET:HG2	1:D:151:GLU:OE1	1.71	0.90
1:C:16:LYS:HD3	1:C:16:LYS:H	1.38	0.88
1:A:77:PRO:HG3	1:A:371:MET:HE3	1.56	0.88
1:C:17:ASN:O	1:C:21:LEU:HD12	1.73	0.88
1:C:16:LYS:H	1:C:16:LYS:CD	1.87	0.88
1:C:341:THR:HG22	1:C:392:VAL:HB	1.53	0.88
1:D:376:THR:OG1	1:D:378:GLU:HG2	1.75	0.86
1:D:278:ASN:O	1:D:282:ILE:HG23	1.76	0.85
1:A:507:ASP:OD1	1:A:509:ARG:HD2	1.77	0.85
1:B:43:GLN:HE22	1:B:158:ARG:HH12	1.22	0.85
1:B:129:VAL:CG1	1:B:163:MET:HE3	2.04	0.85
1:C:179:ARG:HG2	1:C:179:ARG:HH11	1.40	0.85
1:D:278:ASN:O	1:D:282:ILE:CG2	2.25	0.85
1:C:285:THR:HG21	1:C:517:ASP:OD1	1.75	0.84
1:D:318:PHE:CE2	1:D:389:ARG:HD2	2.11	0.84
1:C:154:VAL:O	1:C:163:MET:HE1	1.77	0.84
1:A:503:ARG:HH22	1:A:566:THR:CG2	1.91	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:VAL:HB	1:A:459:THR:HG23	1.60	0.83
1:C:69:ASN:HD22	1:C:340:ASN:HD22	1.24	0.83
1:D:273:ALA:O	1:D:274:CYS:HB2	1.77	0.82
1:C:366:HIS:CE1	1:C:374:ASP:OD1	2.32	0.82
1:D:511:LEU:CD1	1:D:563:GLU:HG3	2.08	0.82
1:A:326:TYR:O	1:A:330:PRO:HG3	1.79	0.82
1:D:355:TRP:HA	1:D:359:MET:HE1	1.62	0.82
1:A:429:THR:HB	1:A:543:THR:HB	1.60	0.82
1:C:413:ASP:OD1	2:C:667:HOH:O	1.98	0.81
1:A:430:GLN:OE1	1:A:528:ARG:HD2	1.81	0.81
1:C:211:THR:OG1	1:C:213:GLU:HG3	1.81	0.80
1:D:325:ASN:OD1	1:D:328:SER:HB3	1.80	0.80
1:A:503:ARG:HH22	1:A:566:THR:HG23	1.46	0.80
1:C:113:MET:CE	1:C:206:THR:HB	2.11	0.80
1:A:558:ILE:O	1:A:560:ASP:N	2.15	0.79
1:B:544:ALA:O	1:B:565:LEU:HG	1.83	0.79
1:B:129:VAL:HG11	1:B:163:MET:CE	2.13	0.79
1:A:555:ASP:O	1:A:557:PRO:HD3	1.83	0.79
1:D:229:LYS:NZ	1:D:297:ASP:OD2	2.16	0.78
1:D:424:THR:HG22	1:D:571:GLN:HB3	1.64	0.78
1:B:237:ALA:HA	1:B:240:MET:HE2	1.64	0.78
1:B:561:VAL:O	1:B:565:LEU:HD22	1.84	0.78
1:B:255:LYS:HD3	1:B:292:GLN:HE21	1.49	0.77
1:A:86:ARG:HE	1:C:94:GLU:HG3	1.49	0.77
1:B:74:ARG:CZ	1:B:368:ILE:HD11	2.14	0.77
1:C:113:MET:HE1	1:C:206:THR:CB	2.15	0.77
1:A:331:ILE:HD12	1:A:399:ALA:HB2	1.66	0.77
1:B:189:GLU:N	1:B:192:GLN:OE1	2.17	0.77
1:D:242:ARG:HH21	1:D:481:ASN:HD22	1.33	0.76
1:B:506:GLU:C	1:B:508:GLY:H	1.93	0.76
1:D:53:LEU:HD12	1:D:155:MET:HE3	1.67	0.76
1:B:109:MET:CE	1:D:105:PRO:HD3	2.14	0.76
1:C:210:GLU:HG2	2:C:620:HOH:O	1.84	0.76
1:C:69:ASN:HD22	1:C:340:ASN:ND2	1.83	0.76
1:A:563:GLU:O	1:A:566:THR:HG22	1.86	0.76
1:B:74:ARG:NH1	1:B:368:ILE:HD13	2.01	0.76
1:D:17:ASN:ND2	1:D:18:LYS:H	1.84	0.75
1:C:242:ARG:HH11	1:C:481:ASN:HD22	1.34	0.75
1:A:79:ASP:HB2	2:A:694:HOH:O	1.86	0.75
1:C:179:ARG:NH1	2:C:670:HOH:O	2.17	0.75
1:C:407:TRP:H	1:C:407:TRP:HE3	1.34	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:509:ARG:HA	1:D:509:ARG:NE	2.02	0.75
1:D:274:CYS:SG	2:D:646:HOH:O	2.44	0.74
1:B:109:MET:HE2	1:D:105:PRO:CD	2.17	0.74
1:B:378:GLU:O	1:B:378:GLU:HG3	1.85	0.74
1:D:540:VAL:HG22	1:D:572:TRP:CZ2	2.23	0.74
1:A:136:ILE:HG22	2:A:651:HOH:O	1.88	0.74
1:B:364:PRO:HG2	1:B:367:LEU:HG	1.70	0.74
1:C:430:GLN:NE2	1:C:528:ARG:HE	1.86	0.73
1:C:179:ARG:HH11	1:C:179:ARG:CG	1.99	0.73
1:C:53:LEU:HD12	1:C:155:MET:HE1	1.70	0.73
1:D:600:ALA:O	1:D:604:ARG:HD3	1.89	0.73
1:C:129:VAL:CG1	1:C:163:MET:HE2	2.19	0.73
1:B:62:LEU:HD21	1:B:354:ILE:HD13	1.71	0.73
1:D:240:MET:O	1:D:244:GLU:HB2	1.88	0.73
1:D:253:ILE:HD11	1:D:410:VAL:HG21	1.71	0.73
1:B:505:GLY:O	1:B:506:GLU:O	2.06	0.73
1:C:426:PRO:HG2	1:C:429:THR:CG2	2.19	0.73
1:B:429:THR:HG23	2:B:619:HOH:O	1.88	0.72
1:D:16:LYS:C	1:D:16:LYS:HD2	2.14	0.72
1:C:16:LYS:N	1:C:16:LYS:CD	2.51	0.72
1:D:327:ALA:O	1:D:328:SER:CB	2.37	0.72
1:C:20:LEU:CD2	1:C:24:ILE:HD11	2.19	0.72
1:C:237:ALA:HA	1:C:240:MET:HE2	1.71	0.72
1:B:503:ARG:HG2	1:B:503:ARG:HH11	1.54	0.71
1:B:275:GLY:H	1:B:278:ASN:HD22	1.38	0.71
1:C:286:ILE:HD11	1:C:520:ARG:CZ	2.20	0.71
1:D:255:LYS:NZ	1:D:257:ILE:HD11	2.05	0.71
1:C:129:VAL:HG11	1:C:163:MET:HE2	1.73	0.71
1:B:271:PRO:HB3	1:B:463:ASP:OD2	1.91	0.71
1:B:17:ASN:HA	1:B:173:ALA:O	1.91	0.71
1:C:256:LEU:HD12	1:C:289:TRP:CZ3	2.25	0.71
1:B:351:ASP:N	2:B:646:HOH:O	2.22	0.70
1:B:62:LEU:HB2	1:B:70:SER:O	1.91	0.70
1:B:69:ASN:HD22	1:B:340:ASN:ND2	1.86	0.70
1:C:53:LEU:HD12	1:C:155:MET:CE	2.21	0.70
1:B:427:LEU:HB3	1:B:565:LEU:HD13	1.73	0.70
1:B:34:GLU:HG2	1:B:123:GLY:H	1.57	0.70
1:A:430:GLN:HB2	1:A:497:PHE:CE2	2.27	0.70
1:B:201:ASP:OD2	1:D:588:PRO:HG3	1.92	0.70
1:B:69:ASN:ND2	1:B:340:ASN:HD22	1.86	0.70
1:A:82:ARG:HH12	1:A:84:GLU:HB2	1.55	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:THR:HG21	1:A:208:PHE:CZ	2.27	0.70
1:D:49:MET:HB3	1:D:155:MET:HE2	1.73	0.70
1:B:277:THR:HG22	1:B:296:ASP:OD2	1.91	0.69
1:C:113:MET:CE	1:C:206:THR:CB	2.70	0.69
1:C:511:LEU:HD22	1:C:561:VAL:HG11	1.74	0.69
1:A:260:GLU:OE2	1:A:260:GLU:HA	1.90	0.69
1:B:43:GLN:HE22	1:B:158:ARG:NH1	1.91	0.69
1:C:20:LEU:O	1:C:24:ILE:HG13	1.93	0.69
1:C:206:THR:HG21	1:C:208:PHE:CZ	2.28	0.69
1:C:429:THR:HB	1:C:543:THR:HB	1.74	0.69
1:C:431:THR:HB	1:C:496:ILE:O	1.92	0.69
1:D:50:ALA:HB1	1:D:71:TYR:CZ	2.27	0.69
1:D:189:GLU:HB2	1:D:192:GLN:HG3	1.75	0.68
1:A:514:GLY:HA2	1:A:518:ASN:OD1	1.94	0.68
1:C:256:LEU:CD1	1:C:289:TRP:CE3	2.76	0.68
1:C:487:ASN:C	1:C:489:GLY:N	2.51	0.68
1:D:205:ILE:HD11	1:D:231:CYS:SG	2.33	0.68
1:D:376:THR:OG1	1:D:378:GLU:CG	2.41	0.68
1:D:426:PRO:HG3	1:D:567:ALA:HB2	1.74	0.68
1:B:506:GLU:N	1:B:506:GLU:OE2	2.26	0.68
1:D:132:CYS:CB	1:D:143:LEU:HD23	2.11	0.68
1:B:63:ASN:HD21	1:B:65:GLU:HB3	1.59	0.68
1:B:67:ARG:HD2	1:B:353:ASP:OD1	1.93	0.68
1:D:255:LYS:HZ3	1:D:257:ILE:HD11	1.57	0.68
1:D:349:THR:HG21	1:D:351:ASP:OD1	1.94	0.68
1:D:355:TRP:CA	1:D:359:MET:HE2	2.22	0.68
1:B:24:ILE:C	1:B:24:ILE:HD13	2.19	0.67
1:B:179:ARG:HD3	2:B:623:HOH:O	1.93	0.67
1:C:286:ILE:HD11	1:C:520:ARG:NH1	2.09	0.67
1:D:465:MET:HE2	1:D:479:LEU:HD23	1.75	0.67
1:B:61:LYS:HG3	1:B:71:TYR:CE2	2.28	0.67
1:B:74:ARG:HH12	1:B:368:ILE:HD13	1.55	0.67
1:C:17:ASN:HD21	1:C:19:GLU:HB2	1.59	0.67
1:A:503:ARG:NH2	1:A:566:THR:CG2	2.57	0.67
1:D:509:ARG:HA	1:D:509:ARG:CZ	2.24	0.67
1:B:242:ARG:HH21	1:B:481:ASN:HD22	1.40	0.67
1:C:424:THR:HA	1:C:571:GLN:HE21	1.59	0.67
1:B:333:MET:HE3	1:B:333:MET:HA	1.75	0.67
1:D:255:LYS:HZ3	1:D:257:ILE:CD1	2.08	0.67
1:D:17:ASN:HD22	1:D:18:LYS:N	1.90	0.67
1:A:380:ASP:OD2	2:A:697:HOH:O	2.13	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:582:TYR:O	1:C:585:PHE:HB3	1.94	0.67
1:A:255:LYS:HE3	1:A:403:GLU:OE2	1.95	0.67
1:C:179:ARG:NH1	1:C:179:ARG:CG	2.55	0.66
1:C:157:MET:CB	1:C:163:MET:HE3	2.25	0.66
1:B:135:PRO:HG2	1:B:407:TRP:HA	1.78	0.66
1:A:77:PRO:CG	1:A:371:MET:HE3	2.26	0.66
1:B:230:LYS:N	2:B:638:HOH:O	2.13	0.66
1:C:157:MET:HB3	1:C:163:MET:HE3	1.77	0.66
1:C:553:GLY:O	1:C:554:LEU:HG	1.96	0.66
1:B:503:ARG:HG2	1:B:503:ARG:NH1	2.10	0.66
1:C:69:ASN:ND2	1:C:340:ASN:HD22	1.94	0.66
1:D:464:PRO:HD2	1:D:468:LEU:HD13	1.76	0.66
1:B:49:MET:HE1	1:B:154:VAL:HG11	1.77	0.65
1:C:16:LYS:H	1:C:16:LYS:CE	2.08	0.65
1:A:17:ASN:ND2	1:A:20:LEU:H	1.95	0.65
1:B:524:TRP:NE1	1:B:533:VAL:CG1	2.59	0.65
1:D:305:GLU:OE2	1:D:305:GLU:N	2.26	0.65
1:B:362:ASP:O	1:B:363:ALA:CB	2.45	0.65
1:B:17:ASN:O	1:B:21:LEU:HD12	1.96	0.65
1:D:67:ARG:HH22	1:D:354:ILE:HD11	1.62	0.65
1:B:394:ILE:HD13	1:B:404:PHE:CD1	2.32	0.65
1:D:511:LEU:HD22	1:D:560:ASP:HB3	1.77	0.65
1:C:304:ARG:HG3	1:C:309:TYR:CD1	2.33	0.64
1:A:427:LEU:HB3	1:A:565:LEU:HD23	1.78	0.64
1:D:16:LYS:HD2	1:D:17:ASN:N	2.11	0.64
1:A:89:ILE:HD13	1:A:472:GLY:O	1.97	0.64
1:B:107:GLN:H	1:B:107:GLN:NE2	1.97	0.63
1:B:171:ILE:O	1:B:175:GLY:HA3	1.98	0.63
1:B:311:VAL:HG12	1:B:409:GLY:CA	2.28	0.63
1:D:53:LEU:HD12	1:D:155:MET:CE	2.28	0.63
1:B:554:LEU:HD13	1:B:556:THR:HG22	1.81	0.63
1:D:507:ASP:HA	1:D:509:ARG:NH1	2.13	0.63
1:B:133:MET:HE3	1:B:313:PRO:HB2	1.80	0.63
1:D:43:GLN:HE22	1:D:158:ARG:HH12	1.47	0.63
1:C:511:LEU:HB3	1:C:561:VAL:HG11	1.80	0.63
1:B:86:ARG:HE	1:D:94:GLU:HG2	1.64	0.62
1:D:429:THR:HG23	2:D:634:HOH:O	1.98	0.62
1:B:63:ASN:C	1:B:63:ASN:HD22	2.06	0.62
1:D:17:ASN:HB3	1:D:20:LEU:HB2	1.80	0.62
1:D:30:LEU:HD22	1:D:117:TYR:HB3	1.80	0.62
1:D:267:ALA:O	1:D:415:ILE:HA	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:427:LEU:HB3	1:D:565:LEU:HD13	1.81	0.62
1:A:216:SER:HB2	1:A:227:LEU:HD21	1.82	0.62
1:A:553:GLY:O	1:A:555:ASP:N	2.32	0.62
1:B:430:GLN:NE2	1:B:528:ARG:HE	1.97	0.62
1:B:304:ARG:HE	1:B:304:ARG:HA	1.64	0.62
1:C:272:SER:HB2	1:C:275:GLY:HA3	1.82	0.62
1:C:426:PRO:HG2	1:C:429:THR:HG21	1.80	0.62
1:B:430:GLN:HG2	1:B:431:THR:O	2.00	0.62
1:D:507:ASP:OD1	1:D:509:ARG:NH1	2.32	0.62
1:C:559:GLU:O	1:C:560:ASP:HB2	2.00	0.62
1:D:265:HIS:HE1	1:D:403:GLU:OE2	1.83	0.62
1:A:136:ILE:HG13	1:A:136:ILE:O	2.00	0.62
1:B:528:ARG:HH12	1:B:534:GLY:HA2	1.64	0.62
1:B:434:TRP:CD1	1:B:486:GLY:HA3	2.35	0.61
1:B:15:THR:HG21	1:B:20:LEU:HD13	1.82	0.61
1:C:540:VAL:HG22	1:C:572:TRP:CZ2	2.35	0.61
1:D:523:LYS:HG3	2:D:620:HOH:O	2.00	0.61
1:B:34:GLU:CG	1:B:123:GLY:H	2.13	0.61
1:D:53:LEU:CD1	1:D:155:MET:HE3	2.30	0.61
1:D:277:THR:O	1:D:281:MET:HG3	2.01	0.61
1:B:74:ARG:HD2	1:B:370:TRP:O	2.00	0.61
1:C:430:GLN:HE22	1:C:528:ARG:HE	1.46	0.61
1:A:17:ASN:HD22	1:A:20:LEU:H	1.46	0.61
1:B:524:TRP:NE1	1:B:533:VAL:HG11	2.16	0.61
1:D:208:PHE:HB2	1:D:213:GLU:HB2	1.82	0.61
1:D:234:LEU:HD11	1:D:250:HIS:CD2	2.36	0.61
1:A:264:TYR:OH	1:A:530:GLU:OE2	2.13	0.60
1:A:503:ARG:NH2	1:A:566:THR:HG22	2.16	0.60
1:C:429:THR:HG23	2:C:635:HOH:O	2.02	0.60
1:C:109:MET:O	1:C:113:MET:HG3	2.01	0.60
1:A:67:ARG:HD2	1:A:353:ASP:OD2	2.02	0.60
1:C:256:LEU:HD13	1:C:289:TRP:HE3	1.65	0.60
1:A:550:ASP:O	1:A:551:LEU:HD12	2.00	0.60
1:B:129:VAL:HG11	1:B:163:MET:HE3	1.79	0.60
1:B:530:GLU:HB3	1:B:532:HIS:CE1	2.36	0.60
1:A:511:LEU:HD23	1:A:563:GLU:HB3	1.83	0.60
1:B:379:SER:O	1:B:380:ASP:HB2	2.02	0.60
1:C:256:LEU:HD12	1:C:289:TRP:CE3	2.37	0.60
1:A:113:MET:HE3	1:A:204:TYR:HB2	1.84	0.60
1:B:514:GLY:HA2	1:B:518:ASN:OD1	2.01	0.60
1:D:559:GLU:OE2	1:D:559:GLU:O	2.20	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:ARG:HD3	1:B:477:GLU:OE1	2.02	0.59
1:D:136:ILE:O	1:D:170:LYS:NZ	2.33	0.59
1:D:507:ASP:HA	1:D:509:ARG:HH12	1.67	0.59
1:A:520:ARG:NE	1:A:554:LEU:HD23	2.18	0.59
1:A:551:LEU:O	1:A:552:ASP:HB2	2.02	0.59
1:B:432:TYR:CE2	1:B:541:GLY:HA2	2.37	0.59
1:A:86:ARG:HE	1:C:94:GLU:CG	2.15	0.59
1:C:17:ASN:C	1:C:17:ASN:HD22	2.11	0.59
1:C:487:ASN:O	1:C:488:LYS:C	2.46	0.59
1:D:195:VAL:HG12	1:D:196:ALA:H	1.66	0.59
1:B:349:THR:O	1:B:350:ASP:HB2	2.03	0.59
1:D:507:ASP:CG	1:D:509:ARG:HH12	2.11	0.59
1:C:463:ASP:OD1	1:C:468:LEU:HB2	2.03	0.59
1:D:30:LEU:CD2	1:D:117:TYR:HB3	2.33	0.59
1:B:535:ALA:CB	1:B:542:HIS:HB3	2.31	0.59
1:C:265:HIS:HE1	1:C:403:GLU:OE2	1.86	0.59
1:D:50:ALA:O	1:D:54:VAL:HG23	2.02	0.59
1:D:69:ASN:HB3	1:D:340:ASN:OD1	2.01	0.59
1:D:354:ILE:HD13	1:D:356:TRP:CZ3	2.38	0.59
1:A:448:GLN:C	1:A:461:ARG:HH12	2.11	0.58
1:B:24:ILE:HD13	1:B:24:ILE:O	2.03	0.58
1:C:232:TYR:HA	1:C:236:ILE:CG1	2.34	0.58
1:D:255:LYS:NZ	1:D:257:ILE:CD1	2.67	0.58
1:A:558:ILE:CD1	1:A:558:ILE:N	2.46	0.58
1:B:325:ASN:ND2	1:B:327:ALA:HB3	2.18	0.58
1:B:503:ARG:HH11	1:B:503:ARG:CG	2.17	0.58
1:B:528:ARG:NH1	1:B:534:GLY:HA2	2.18	0.58
1:C:306:ASP:O	1:C:411:LYS:NZ	2.31	0.58
1:B:344:THR:O	1:B:388:SER:HB2	2.03	0.58
1:D:416:LEU:HD11	1:D:522:LEU:HD11	1.85	0.58
1:D:514:GLY:HA2	1:D:518:ASN:OD1	2.04	0.58
1:A:464:PRO:HD2	1:A:468:LEU:HG	1.86	0.58
1:B:43:GLN:NE2	1:B:158:ARG:HH12	1.95	0.58
1:B:63:ASN:HD22	1:B:65:GLU:H	1.50	0.58
1:D:235:ARG:NH2	1:D:470:PHE:HD2	2.01	0.58
1:D:254:LEU:HD11	1:D:256:LEU:HD22	1.86	0.58
1:A:550:ASP:C	1:A:551:LEU:HD12	2.28	0.57
1:C:507:ASP:C	1:C:507:ASP:OD1	2.46	0.57
1:D:78:SER:O	1:D:79:ASP:CB	2.45	0.57
1:D:577:GLU:O	1:D:581:GLU:HG3	2.03	0.57
1:B:521:VAL:O	1:B:525:VAL:HG23	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:GLN:OE1	1:A:158:ARG:NH1	2.37	0.57
1:A:109:MET:HE1	1:C:103:TRP:HZ3	1.69	0.57
1:A:221:TYR:C	1:A:221:TYR:CD2	2.82	0.57
1:A:80:VAL:CG1	1:A:80:VAL:O	2.53	0.57
1:C:113:MET:HE2	1:C:206:THR:OG1	2.04	0.57
1:C:487:ASN:C	1:C:489:GLY:H	2.11	0.57
1:D:34:GLU:CD	1:D:123:GLY:H	2.13	0.57
1:D:114:SER:HA	1:D:117:TYR:HB2	1.85	0.57
1:A:80:VAL:HG11	1:A:385:HIS:NE2	2.20	0.57
1:C:350:ASP:OD2	1:C:366:HIS:HD2	1.88	0.57
1:C:330:PRO:HD2	2:C:627:HOH:O	2.04	0.56
1:C:166:GLU:HA	1:D:406:ASP:OD1	2.05	0.56
1:C:255:LYS:HD2	1:C:265:HIS:CE1	2.41	0.56
1:B:94:GLU:OE1	1:D:202:THR:HB	2.06	0.56
1:D:46:TRP:CD1	1:D:46:TRP:C	2.83	0.56
1:B:53:LEU:HD22	1:B:58:THR:OG1	2.05	0.56
1:B:82:ARG:HB2	1:B:82:ARG:CZ	2.36	0.56
1:B:388:SER:C	1:B:389:ARG:HG2	2.31	0.56
1:B:325:ASN:HD21	1:B:327:ALA:HB3	1.71	0.56
1:C:467:MET:O	1:C:468:LEU:C	2.47	0.56
1:D:67:ARG:NH2	1:D:67:ARG:HG3	2.21	0.56
1:D:465:MET:CE	1:D:479:LEU:HD23	2.35	0.56
1:B:122:LYS:HD2	1:B:188:LEU:O	2.05	0.56
1:C:214:ILE:HD11	1:C:236:ILE:HG12	1.88	0.56
1:C:487:ASN:O	1:C:489:GLY:N	2.38	0.56
1:D:189:GLU:H	1:D:192:GLN:NE2	2.03	0.56
1:A:204:TYR:C	1:A:205:ILE:HD12	2.31	0.55
1:C:536:ASP:OD1	1:C:536:ASP:O	2.24	0.55
1:D:465:MET:HG3	1:D:478:TYR:HE2	1.70	0.55
1:B:503:ARG:C	1:B:504:ARG:HG3	2.31	0.55
1:B:122:LYS:HD3	1:B:122:LYS:C	2.31	0.55
1:B:325:ASN:HB2	1:B:360:ASP:OD2	2.06	0.55
1:B:427:LEU:HB3	1:B:565:LEU:CD1	2.36	0.55
1:A:258:ASN:C	1:A:258:ASN:OD1	2.49	0.55
1:B:524:TRP:NE1	1:B:533:VAL:HG13	2.21	0.55
1:D:279:LEU:HD11	1:D:522:LEU:HD21	1.89	0.55
1:D:349:THR:CG2	1:D:351:ASP:OD1	2.53	0.55
1:D:17:ASN:HB3	1:D:20:LEU:CB	2.36	0.55
1:B:48:ARG:HH21	1:B:52:ASP:N	2.05	0.55
1:D:259:PRO:HA	1:D:288:GLY:O	2.07	0.55
1:D:244:GLU:HB3	1:D:246:TRP:CD1	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:THR:O	1:A:396:GLN:NE2	2.36	0.54
1:A:511:LEU:CD2	1:A:563:GLU:HB3	2.37	0.54
1:B:214:ILE:HG21	1:B:227:LEU:HG	1.89	0.54
1:B:532:HIS:ND1	1:B:532:HIS:N	2.54	0.54
1:C:598:PHE:CE1	1:C:602:LYS:HD2	2.42	0.54
1:A:77:PRO:HG3	1:A:371:MET:CE	2.34	0.54
1:B:51:GLU:O	1:B:54:VAL:HG12	2.07	0.54
1:B:63:ASN:ND2	1:B:65:GLU:H	2.06	0.54
1:B:82:ARG:HG3	1:B:82:ARG:HH11	1.72	0.54
1:B:255:LYS:CD	1:B:292:GLN:HE21	2.18	0.54
1:C:264:TYR:CG	1:C:526:ILE:HD12	2.42	0.54
1:A:531:GLY:HA2	2:A:671:HOH:O	2.07	0.54
1:B:259:PRO:HG3	1:B:288:GLY:HA3	1.90	0.54
1:D:253:ILE:HG13	1:D:294:VAL:HB	1.90	0.54
1:B:141:PRO:HG3	1:B:170:LYS:HG2	1.89	0.54
1:B:349:THR:HA	1:B:367:LEU:HD23	1.89	0.54
1:C:424:THR:HA	1:C:571:GLN:NE2	2.20	0.54
1:D:421:ARG:HD2	1:D:446:SER:HB2	1.90	0.54
1:D:278:ASN:O	1:D:282:ILE:HG21	2.04	0.54
1:D:317:PHE:O	1:D:391:CYS:HA	2.07	0.54
1:D:571:GLN:O	1:D:574:ASN:HB3	2.08	0.54
1:B:17:ASN:O	1:B:21:LEU:CD1	2.56	0.53
1:B:524:TRP:CE2	1:B:533:VAL:HG11	2.43	0.53
1:C:369:ASP:C	1:C:371:MET:H	2.16	0.53
1:D:465:MET:HG3	1:D:478:TYR:CE2	2.43	0.53
1:C:545:LYS:O	1:C:546:ALA:HB3	2.07	0.53
1:B:311:VAL:HG12	1:B:409:GLY:HA2	1.90	0.53
1:B:325:ASN:HD22	1:B:327:ALA:H	1.57	0.53
1:B:528:ARG:NH1	1:B:534:GLY:CA	2.71	0.53
1:D:327:ALA:O	1:D:328:SER:HB3	2.06	0.53
1:C:555:ASP:HB2	1:C:559:GLU:OE2	2.08	0.53
1:D:368:ILE:HG23	1:D:372:GLY:O	2.08	0.53
1:D:524:TRP:CZ2	1:D:544:ALA:HA	2.44	0.53
1:A:540:VAL:HG22	1:A:572:TRP:CZ2	2.42	0.53
1:A:558:ILE:C	1:A:560:ASP:H	2.14	0.53
1:C:254:LEU:HD11	1:C:291:ALA:HB1	1.90	0.53
1:C:256:LEU:CD1	1:C:289:TRP:HE3	2.20	0.53
1:D:501:TRP:HE3	1:D:501:TRP:HA	1.73	0.53
1:D:335:THR:O	1:D:396:GLN:HG2	2.09	0.53
1:D:403:GLU:O	1:D:404:PHE:C	2.52	0.53
1:D:507:ASP:CG	1:D:509:ARG:NH1	2.67	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:543:THR:O	1:C:544:ALA:C	2.50	0.53
1:D:67:ARG:CG	1:D:67:ARG:HH21	2.22	0.53
1:A:555:ASP:O	2:A:706:HOH:O	2.18	0.53
1:D:368:ILE:HD12	2:D:619:HOH:O	2.08	0.53
1:A:461:ARG:O	1:A:461:ARG:HG2	2.09	0.52
1:C:129:VAL:CG1	1:C:163:MET:HG3	2.39	0.52
1:D:15:THR:O	1:D:15:THR:OG1	2.28	0.52
1:D:121:MET:HG2	1:D:149:ASP:HB3	1.92	0.52
1:C:83:VAL:HG23	1:C:205:ILE:HD13	1.92	0.52
1:D:68:PRO:O	1:D:69:ASN:C	2.52	0.52
1:A:80:VAL:O	1:A:80:VAL:HG13	2.10	0.52
1:B:255:LYS:HZ2	1:B:263:ALA:HB1	1.74	0.52
1:D:165:ILE:N	1:D:165:ILE:HD12	2.24	0.52
1:D:480:GLN:HA	1:D:591:PRO:HG3	1.91	0.52
1:B:426:PRO:HB2	1:B:429:THR:HG22	1.91	0.52
1:D:283:THR:OG1	1:D:331:ILE:CD1	2.58	0.52
1:B:62:LEU:HD21	1:B:354:ILE:CD1	2.38	0.52
1:B:71:TYR:N	1:B:71:TYR:CD1	2.77	0.52
1:B:464:PRO:HD2	1:B:468:LEU:HG	1.92	0.52
1:B:258:ASN:O	1:B:259:PRO:C	2.50	0.52
1:B:289:TRP:CZ2	1:B:523:LYS:HG3	2.45	0.52
1:B:228:ALA:HA	1:B:232:TYR:HB3	1.91	0.52
1:C:252:LEU:O	1:C:267:ALA:HA	2.10	0.52
1:C:511:LEU:HD22	1:C:561:VAL:CG1	2.38	0.52
1:C:538:THR:OG1	1:C:543:THR:CG2	2.58	0.52
1:D:501:TRP:HA	1:D:501:TRP:CE3	2.45	0.52
1:C:17:ASN:ND2	1:C:20:LEU:H	2.07	0.52
1:C:75:SER:OG	1:C:80:VAL:HG12	2.10	0.52
1:B:18:LYS:HA	1:B:21:LEU:HD12	1.92	0.51
1:B:191:GLY:O	1:B:192:GLN:HB3	2.10	0.51
1:D:235:ARG:NH2	1:D:470:PHE:CD2	2.78	0.51
1:D:251:MET:HE2	1:D:415:ILE:HG23	1.90	0.51
1:D:268:ALA:HA	1:D:416:LEU:O	2.11	0.51
1:D:273:ALA:HA	1:D:276:LYS:HE3	1.91	0.51
1:A:550:ASP:C	1:A:551:LEU:CD1	2.82	0.51
1:B:503:ARG:O	1:B:504:ARG:HG3	2.11	0.51
1:C:277:THR:HG23	1:C:281:MET:HE3	1.93	0.51
1:C:429:THR:CG2	1:C:543:THR:HB	2.41	0.51
1:D:121:MET:SD	1:D:126:MET:HB2	2.50	0.51
1:D:318:PHE:CD2	1:D:389:ARG:HD2	2.44	0.51
1:A:113:MET:HE3	1:A:204:TYR:CB	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:157:MET:HB2	1:C:163:MET:CE	2.41	0.51
1:C:230:LYS:HE2	1:C:470:PHE:CZ	2.46	0.51
1:A:554:LEU:HD22	1:A:554:LEU:O	2.11	0.51
1:B:104:ALA:CB	1:B:109:MET:HE3	2.41	0.51
1:B:533:VAL:O	1:B:548:ASP:OD2	2.29	0.51
1:A:537:GLU:OE2	1:A:542:HIS:ND1	2.42	0.51
1:C:25:ALA:O	1:C:28:VAL:HG12	2.10	0.51
1:A:95:GLU:OE2	1:A:589:ARG:NH2	2.39	0.51
1:D:229:LYS:O	1:D:233:ALA:HB3	2.11	0.51
1:D:254:LEU:O	1:D:265:HIS:HA	2.11	0.51
1:B:315:ASN:O	1:B:394:ILE:HG22	2.10	0.51
1:B:530:GLU:OE1	1:B:530:GLU:HA	2.11	0.51
1:A:23:TRP:CZ2	1:A:179:ARG:HB3	2.46	0.50
1:A:108:ALA:HB2	1:C:108:ALA:CB	2.41	0.50
1:D:49:MET:HE3	1:D:155:MET:HG2	1.92	0.50
1:D:266:ILE:HD13	1:D:522:LEU:HD12	1.92	0.50
1:A:525:VAL:O	1:A:529:ILE:HG12	2.10	0.50
1:C:211:THR:OG1	1:C:211:THR:O	2.29	0.50
1:D:134:GLY:O	1:D:135:PRO:C	2.53	0.50
1:D:604:ARG:HD2	2:D:658:HOH:O	2.11	0.50
1:A:100:THR:HB	1:A:468:LEU:CD2	2.42	0.50
1:B:106:PRO:O	1:B:110:LYS:HG3	2.12	0.50
1:D:570:GLU:O	1:D:574:ASN:HB2	2.11	0.50
1:A:221:TYR:HB3	2:A:694:HOH:O	2.11	0.50
1:A:272:SER:OG	1:A:420:ARG:NH2	2.43	0.50
1:A:285:THR:HG21	1:A:517:ASP:OD1	2.12	0.50
1:A:429:THR:HB	1:A:543:THR:CB	2.35	0.50
1:B:468:LEU:N	1:B:469:PRO:CD	2.74	0.50
1:C:142:LYS:HG2	1:C:240:MET:HE1	1.94	0.50
1:A:274:CYS:HA	1:A:277:THR:HB	1.92	0.50
1:D:246:TRP:HB2	1:D:301:LEU:O	2.12	0.50
1:B:275:GLY:H	1:B:278:ASN:ND2	2.07	0.50
1:C:129:VAL:HG13	1:C:163:MET:HE2	1.90	0.50
1:C:404:PHE:CD1	1:C:404:PHE:C	2.89	0.50
1:A:280:ALA:HB1	1:A:293:VAL:HG23	1.93	0.49
1:A:523:LYS:HE3	1:A:551:LEU:HD11	1.94	0.49
1:B:64:GLU:O	1:B:64:GLU:HG3	2.12	0.49
1:B:382:ASN:HB3	1:B:384:ALA:O	2.12	0.49
1:B:507:ASP:OD2	1:B:509:ARG:HB3	2.11	0.49
1:D:67:ARG:HH22	1:D:354:ILE:CD1	2.24	0.49
1:B:136:ILE:HG21	1:B:166:GLU:HG3	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:167:ALA:O	1:C:171:ILE:HG23	2.11	0.49
1:A:563:GLU:O	1:A:566:THR:CG2	2.58	0.49
1:C:247:MET:HE3	1:C:301:LEU:HB2	1.94	0.49
1:C:407:TRP:CE3	1:C:407:TRP:N	2.70	0.49
1:D:278:ASN:ND2	1:D:328:SER:O	2.45	0.49
1:D:430:GLN:HG3	1:D:497:PHE:CZ	2.46	0.49
1:B:82:ARG:HH11	1:B:82:ARG:CG	2.26	0.49
1:C:305:GLU:HB2	2:C:640:HOH:O	2.11	0.49
1:D:17:ASN:ND2	1:D:18:LYS:N	2.56	0.49
1:D:189:GLU:H	1:D:192:GLN:HE21	1.61	0.49
1:A:427:LEU:HB3	1:A:565:LEU:CD2	2.42	0.49
1:C:211:THR:OG1	1:C:213:GLU:CG	2.58	0.49
1:A:404:PHE:CD1	1:A:404:PHE:C	2.91	0.49
1:B:285:THR:O	1:B:285:THR:HG23	2.13	0.49
1:C:369:ASP:C	1:C:371:MET:N	2.70	0.49
1:D:559:GLU:C	1:D:561:VAL:H	2.20	0.49
1:B:366:HIS:O	1:B:367:LEU:HG	2.12	0.49
1:C:316:GLY:HA2	1:C:394:ILE:HG13	1.95	0.49
1:C:424:THR:H	1:C:571:GLN:HE22	1.60	0.49
1:A:253:ILE:CG2	1:A:294:VAL:HB	2.43	0.49
1:A:307:GLY:HA2	1:A:492:LYS:HB2	1.94	0.49
1:A:538:THR:OG1	1:A:543:THR:CG2	2.61	0.49
1:A:271:PRO:HB3	1:A:463:ASP:OD2	2.12	0.48
1:B:432:TYR:CZ	1:B:541:GLY:HA2	2.48	0.48
1:D:205:ILE:CD1	1:D:231:CYS:SG	3.01	0.48
1:A:550:ASP:HB3	1:A:552:ASP:H	1.78	0.48
1:C:142:LYS:HG2	1:C:240:MET:CE	2.43	0.48
1:C:473:TYR:HB2	2:C:616:HOH:O	2.12	0.48
1:D:428:VAL:O	1:D:543:THR:HG23	2.12	0.48
1:A:252:LEU:HB2	1:A:280:ALA:HB2	1.95	0.48
1:C:555:ASP:OD2	1:C:559:GLU:HG2	2.12	0.48
1:D:148:THR:HG21	1:D:153:VAL:HG22	1.96	0.48
1:A:80:VAL:CG1	1:A:385:HIS:CE1	2.96	0.48
1:C:429:THR:HB	1:C:543:THR:CB	2.43	0.48
1:D:603:ALA:O	1:D:604:ARG:C	2.56	0.48
1:C:162:ARG:H	1:C:162:ARG:HD2	1.77	0.48
1:C:206:THR:CG2	1:C:208:PHE:CZ	2.96	0.48
1:C:232:TYR:CG	1:C:236:ILE:HD11	2.48	0.48
1:C:92:GLU:HG2	1:C:210:GLU:HG3	1.96	0.48
1:C:546:ALA:HB2	1:C:565:LEU:HD23	1.95	0.48
1:D:109:MET:O	1:D:110:LYS:C	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:434:TRP:CD1	1:D:486:GLY:HA3	2.49	0.48
1:B:43:GLN:NE2	1:B:158:ARG:NH1	2.57	0.48
1:B:506:GLU:CD	1:B:506:GLU:H	2.21	0.48
1:B:524:TRP:CE2	1:B:533:VAL:CG1	2.96	0.48
1:C:129:VAL:HG13	1:C:163:MET:HG3	1.94	0.48
1:C:339:GLY:O	1:C:396:GLN:NE2	2.34	0.48
1:D:362:ASP:O	1:D:363:ALA:HB3	2.13	0.48
1:D:572:TRP:O	1:D:576:VAL:HG23	2.14	0.48
1:A:233:ALA:HB1	1:A:298:ILE:HG21	1.95	0.48
1:A:253:ILE:HG22	1:A:294:VAL:HB	1.95	0.48
1:D:241:ALA:HB1	1:D:246:TRP:O	2.14	0.48
1:C:531:GLY:C	1:C:533:VAL:H	2.10	0.48
1:C:568:PRO:O	1:C:571:GLN:HB2	2.14	0.48
1:D:23:TRP:CZ2	1:D:179:ARG:HB3	2.49	0.48
1:D:544:ALA:HB3	1:D:565:LEU:HD11	1.96	0.48
1:D:133:MET:HE3	1:D:313:PRO:O	2.14	0.48
1:A:342:LEU:HD12	1:A:342:LEU:HA	1.65	0.47
1:B:362:ASP:O	1:B:363:ALA:HB3	2.14	0.47
1:C:232:TYR:CD2	1:C:236:ILE:HD11	2.48	0.47
1:A:79:ASP:HB3	1:A:203:LYS:HE3	1.95	0.47
1:B:107:GLN:H	1:B:107:GLN:CD	2.21	0.47
1:B:577:GLU:O	1:B:581:GLU:CG	2.51	0.47
1:B:600:ALA:O	1:B:604:ARG:HG3	2.14	0.47
1:C:434:TRP:CD1	1:C:486:GLY:HA3	2.49	0.47
1:D:195:VAL:HG12	1:D:196:ALA:N	2.28	0.47
1:D:568:PRO:O	1:D:571:GLN:HB2	2.15	0.47
1:A:199:CYS:HB2	1:A:218:GLY:O	2.15	0.47
1:A:286:ILE:HA	1:A:287:PRO:HD3	1.67	0.47
1:B:505:GLY:H	1:B:511:LEU:HD13	1.78	0.47
1:B:506:GLU:C	1:B:508:GLY:N	2.57	0.47
1:C:157:MET:CB	1:C:163:MET:CE	2.92	0.47
1:D:178:VAL:HG21	1:D:232:TYR:CZ	2.49	0.47
1:A:46:TRP:CD1	1:A:46:TRP:C	2.93	0.47
1:A:317:PHE:O	1:A:391:CYS:HA	2.14	0.47
1:C:132:CYS:HB2	1:C:143:LEU:HD23	1.97	0.47
1:D:128:VAL:O	1:D:130:PRO:HD3	2.14	0.47
1:A:138:ASP:O	1:A:141:PRO:HG3	2.15	0.47
1:D:135:PRO:HG2	1:D:407:TRP:HA	1.97	0.47
1:A:262:LYS:NZ	2:A:709:HOH:O	2.48	0.47
1:A:271:PRO:HD2	1:A:418:GLY:O	2.15	0.47
1:A:426:PRO:HG3	1:A:567:ALA:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:317:PHE:O	1:B:391:CYS:HA	2.15	0.47
1:B:365:ALA:HA	1:B:377:PRO:HD3	1.96	0.47
1:B:436:HIS:HE1	1:B:540:VAL:O	1.98	0.47
1:B:514:GLY:O	1:B:517:ASP:HB2	2.14	0.47
1:C:247:MET:CE	1:C:301:LEU:HB2	2.45	0.47
1:C:416:LEU:HD12	1:C:497:PHE:HB2	1.97	0.47
1:C:427:LEU:HA	1:C:500:ASN:O	2.14	0.47
1:D:67:ARG:NH2	1:D:67:ARG:CG	2.75	0.47
1:D:465:MET:HE2	1:D:479:LEU:CD2	2.44	0.47
1:B:179:ARG:CD	2:B:623:HOH:O	2.57	0.47
1:C:20:LEU:CD2	1:C:24:ILE:CD1	2.92	0.47
1:C:423:ASP:OD2	1:C:448:GLN:C	2.57	0.47
1:C:485:MET:C	1:C:493:MET:HE2	2.39	0.47
1:A:148:THR:HA	1:A:182:HIS:O	2.14	0.47
1:B:34:GLU:HG2	1:B:123:GLY:N	2.26	0.47
1:B:62:LEU:HD11	1:B:354:ILE:HD13	1.96	0.47
1:B:562:LYS:HD2	1:B:562:LYS:HA	1.47	0.47
1:C:471:ILE:HG22	1:C:473:TYR:H	1.80	0.47
1:D:194:ASP:OD2	1:D:195:VAL:N	2.42	0.47
1:B:16:LYS:HB2	1:B:16:LYS:HE2	1.40	0.47
1:B:251:MET:HA	1:B:268:ALA:O	2.15	0.47
1:B:468:LEU:CB	1:B:469:PRO:HD3	2.45	0.47
1:B:524:TRP:HE1	1:B:533:VAL:HG13	1.80	0.47
1:C:253:ILE:HB	1:C:294:VAL:HB	1.97	0.46
1:B:505:GLY:N	1:B:511:LEU:HD13	2.30	0.46
1:C:31:PHE:HE2	1:C:117:TYR:CD2	2.32	0.46
1:C:513:PRO:HG3	1:C:554:LEU:HD22	1.97	0.46
1:D:34:GLU:HG2	1:D:124:ARG:N	2.31	0.46
1:A:154:VAL:O	1:A:163:MET:HE1	2.14	0.46
1:A:509:ARG:HD3	1:A:509:ARG:C	2.41	0.46
1:B:110:LYS:HG2	1:B:208:PHE:CZ	2.51	0.46
1:B:122:LYS:HD3	1:B:123:GLY:N	2.30	0.46
1:C:113:MET:HE2	1:C:206:THR:CB	2.45	0.46
1:C:251:MET:HB2	1:C:299:ALA:HB3	1.97	0.46
1:A:94:GLU:HG2	1:C:204:TYR:OH	2.16	0.46
1:B:113:MET:SD	1:B:206:THR:HG23	2.55	0.46
1:B:122:LYS:CD	1:B:188:LEU:O	2.63	0.46
1:B:292:GLN:HA	1:B:399:ALA:O	2.15	0.46
1:B:335:THR:HG23	1:B:397:SER:HA	1.97	0.46
1:D:122:LYS:HE2	1:D:122:LYS:HB2	1.70	0.46
1:A:420:ARG:HG2	1:A:502:PHE:CD1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:VAL:HG21	1:B:203:LYS:HD3	1.97	0.46
1:B:461:ARG:HD2	1:B:461:ARG:HA	1.85	0.46
1:C:279:LEU:HD11	1:C:522:LEU:HD11	1.98	0.46
1:C:180:CYS:HB3	1:C:227:LEU:HD12	1.97	0.46
1:D:284:PRO:HB3	1:D:519:SER:CB	2.46	0.46
1:A:116:HIS:CE1	1:A:202:THR:HG21	2.50	0.46
1:B:104:ALA:HB1	1:B:109:MET:HE3	1.98	0.46
1:C:162:ARG:HD2	1:C:162:ARG:N	2.29	0.46
1:C:210:GLU:CG	2:C:620:HOH:O	2.52	0.46
1:D:43:GLN:NE2	1:D:158:ARG:HH12	2.11	0.46
1:A:136:ILE:CD1	1:A:166:GLU:HB3	2.46	0.46
1:B:551:LEU:O	1:B:552:ASP:C	2.59	0.46
1:C:25:ALA:O	1:C:28:VAL:CG1	2.64	0.46
1:D:349:THR:CG2	1:D:351:ASP:CG	2.89	0.46
1:B:232:TYR:C	1:B:232:TYR:CD2	2.93	0.46
1:C:53:LEU:CD1	1:C:155:MET:CE	2.93	0.46
1:C:132:CYS:HB2	1:C:143:LEU:CD2	2.46	0.46
1:C:430:GLN:NE2	1:C:528:ARG:NE	2.61	0.46
1:A:553:GLY:C	1:A:555:ASP:H	2.24	0.46
1:C:83:VAL:CG2	1:C:205:ILE:CD1	2.94	0.46
1:C:255:LYS:HD2	1:C:265:HIS:HE1	1.80	0.46
1:C:429:THR:CB	1:C:543:THR:HB	2.44	0.46
1:D:71:TYR:HE2	2:D:643:HOH:O	1.72	0.46
1:D:89:ILE:O	1:D:89:ILE:HG22	2.15	0.46
1:D:304:ARG:O	1:D:305:GLU:C	2.59	0.46
1:A:272:SER:HB3	1:A:273:ALA:H	1.60	0.45
1:A:448:GLN:C	1:A:461:ARG:NH1	2.73	0.45
1:A:206:THR:CG2	1:A:208:PHE:CZ	2.99	0.45
1:B:86:ARG:HE	1:D:94:GLU:CG	2.28	0.45
1:B:416:LEU:HD22	1:B:497:PHE:HB2	1.99	0.45
1:C:15:THR:HG21	1:C:20:LEU:HD13	1.97	0.45
1:C:274:CYS:HA	1:C:277:THR:HB	1.97	0.45
1:C:341:THR:HG22	1:C:392:VAL:CB	2.38	0.45
1:D:230:LYS:HA	1:D:230:LYS:HD3	1.73	0.45
1:D:326:TYR:O	1:D:330:PRO:HD3	2.15	0.45
1:A:417:PHE:HZ	1:A:482:TRP:CH2	2.34	0.45
1:C:322:PRO:HD3	1:C:388:SER:OG	2.17	0.45
1:D:63:ASN:O	1:D:65:GLU:N	2.49	0.45
1:C:130:PRO:HG2	1:C:168:LEU:HG	1.99	0.45
1:C:134:GLY:O	1:C:135:PRO:C	2.60	0.45
1:C:255:LYS:HB2	1:C:265:HIS:CE1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:362:ASP:O	1:D:363:ALA:CB	2.64	0.45
1:D:416:LEU:HD11	1:D:522:LEU:CD1	2.46	0.45
1:B:257:ILE:HB	1:B:290:THR:HG22	1.99	0.45
1:B:375:TRP:CE3	1:B:375:TRP:C	2.95	0.45
1:D:327:ALA:O	1:D:328:SER:HB2	2.16	0.45
1:A:124:ARG:NH2	1:A:194:ASP:OD2	2.49	0.45
1:A:540:VAL:CG2	1:A:572:TRP:CZ2	3.00	0.45
1:B:88:PHE:HB2	1:B:206:THR:HB	1.98	0.45
1:B:286:ILE:CG2	1:B:289:TRP:HD1	2.29	0.45
1:C:369:ASP:O	1:C:371:MET:N	2.50	0.45
1:D:516:GLY:C	1:D:518:ASN:H	2.24	0.45
1:D:528:ARG:HD2	1:D:533:VAL:HG23	1.98	0.45
1:A:424:THR:H	1:A:571:GLN:NE2	2.14	0.45
1:B:188:LEU:HD11	1:B:194:ASP:OD1	2.17	0.45
1:C:212:LYS:HE2	1:C:240:MET:HG2	1.98	0.45
1:C:232:TYR:HA	1:C:236:ILE:HG13	1.99	0.45
1:D:31:PHE:HE1	1:D:181:LEU:HD12	1.80	0.45
1:D:194:ASP:CG	1:D:195:VAL:H	2.25	0.45
1:A:255:LYS:HD2	1:A:403:GLU:OE2	2.16	0.45
1:C:273:ALA:C	1:C:274:CYS:SG	2.97	0.45
1:A:520:ARG:HE	1:A:554:LEU:HD23	1.81	0.45
1:B:257:ILE:HB	1:B:290:THR:CG2	2.47	0.45
1:B:513:PRO:HG2	1:B:554:LEU:HD21	1.97	0.45
1:C:39:VAL:HG22	1:C:129:VAL:HA	1.99	0.45
1:C:67:ARG:HD3	1:C:353:ASP:OD2	2.17	0.45
1:C:216:SER:HB2	1:C:227:LEU:HD21	1.99	0.45
1:D:298:ILE:O	2:D:637:HOH:O	2.21	0.45
1:A:509:ARG:HD3	1:A:509:ARG:O	2.17	0.44
1:A:554:LEU:HD13	1:A:557:PRO:HG2	1.99	0.44
1:B:431:THR:HB	1:B:436:HIS:ND1	2.32	0.44
1:D:211:THR:OG1	1:D:213:GLU:OE2	2.30	0.44
1:A:255:LYS:CE	1:A:403:GLU:OE2	2.63	0.44
1:B:34:GLU:HG3	1:B:123:GLY:CA	2.46	0.44
1:B:286:ILE:HG21	1:B:289:TRP:CD1	2.52	0.44
1:B:505:GLY:C	1:B:506:GLU:O	2.60	0.44
1:D:207:GLN:HE21	1:D:207:GLN:HB3	1.29	0.44
1:D:271:PRO:HB3	1:D:463:ASP:OD2	2.17	0.44
1:D:524:TRP:CZ3	1:D:528:ARG:HG3	2.53	0.44
1:D:93:LYS:HE2	1:D:93:LYS:HB2	1.81	0.44
1:C:504:ARG:NH2	1:C:510:PHE:CZ	2.85	0.44
1:A:524:TRP:O	1:A:525:VAL:C	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:555:ASP:OD2	1:C:559:GLU:CG	2.66	0.44
1:B:304:ARG:C	1:B:306:ASP:N	2.73	0.44
1:C:424:THR:H	1:C:571:GLN:NE2	2.15	0.44
1:D:234:LEU:HD11	1:D:250:HIS:HD2	1.81	0.44
1:D:509:ARG:HG3	1:D:510:PHE:H	1.81	0.44
1:A:424:THR:H	1:A:571:GLN:HE22	1.65	0.44
1:C:49:MET:HE1	1:C:154:VAL:HG11	1.99	0.44
1:C:168:LEU:HA	1:C:168:LEU:HD23	1.77	0.44
1:B:192:GLN:O	1:B:192:GLN:CG	2.65	0.44
1:B:222:GLY:HA2	1:B:318:PHE:CZ	2.52	0.44
1:B:546:ALA:H	1:B:562:LYS:HD3	1.83	0.44
1:C:264:TYR:CE1	1:C:526:ILE:HG21	2.53	0.44
1:D:522:LEU:O	1:D:526:ILE:HG23	2.17	0.43
1:A:124:ARG:NH1	1:A:194:ASP:OD1	2.50	0.43
1:A:424:THR:HA	1:A:571:GLN:HE21	1.83	0.43
1:B:286:ILE:CG2	1:B:289:TRP:CD1	3.02	0.43
1:B:430:GLN:HE22	1:B:528:ARG:HE	1.63	0.43
1:C:242:ARG:NH1	1:C:481:ASN:HA	2.32	0.43
1:D:334:LYS:O	1:D:337:GLU:HB2	2.18	0.43
1:A:207:GLN:NE2	1:A:231:CYS:SG	2.91	0.43
1:A:209:PRO:HB3	1:A:239:VAL:HG21	2.00	0.43
1:A:245:GLY:O	1:A:485:MET:HE1	2.18	0.43
1:D:200:ASN:OD1	1:D:202:THR:N	2.43	0.43
1:D:257:ILE:HB	1:D:290:THR:HG22	1.99	0.43
1:B:104:ALA:HB3	1:B:109:MET:HG3	2.00	0.43
1:C:135:PRO:HB3	1:C:405:ASN:O	2.18	0.43
1:D:63:ASN:C	1:D:65:GLU:H	2.25	0.43
1:D:252:LEU:HB2	1:D:280:ALA:HB2	2.00	0.43
1:B:286:ILE:HG21	1:B:286:ILE:HD13	1.72	0.43
1:C:389:ARG:HH11	1:C:389:ARG:HD2	1.65	0.43
1:D:501:TRP:CE3	1:D:501:TRP:CA	3.01	0.43
1:A:250:HIS:ND1	1:A:466:ALA:O	2.46	0.43
1:B:136:ILE:H	1:B:136:ILE:HG13	1.66	0.43
1:B:578:ASP:OD1	1:B:578:ASP:C	2.61	0.43
1:C:420:ARG:H	1:C:420:ARG:HG2	1.51	0.43
1:D:426:PRO:HG2	1:D:429:THR:HG21	2.00	0.43
1:C:31:PHE:CE2	1:C:117:TYR:CD2	3.06	0.43
1:C:250:HIS:HD2	1:C:466:ALA:O	2.01	0.43
1:C:301:LEU:HA	1:C:309:TYR:O	2.19	0.43
1:A:80:VAL:HG11	1:A:385:HIS:CD2	2.54	0.43
1:B:76:ASN:HD22	1:B:76:ASN:HA	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:SER:OG	1:B:274:CYS:O	2.25	0.43
1:B:403:GLU:HG3	1:B:410:VAL:CG1	2.49	0.43
1:D:141:PRO:O	1:D:142:LYS:HB2	2.18	0.43
1:D:416:LEU:HD23	1:D:497:PHE:HB2	2.00	0.43
1:A:74:ARG:HD2	1:A:370:TRP:O	2.18	0.43
1:B:280:ALA:O	1:B:293:VAL:HG22	2.19	0.43
1:C:505:GLY:O	1:C:508:GLY:N	2.49	0.43
1:C:513:PRO:HG3	1:C:554:LEU:CD2	2.49	0.43
1:D:69:ASN:HA	2:D:643:HOH:O	2.18	0.43
1:D:524:TRP:CH2	1:D:528:ARG:HG3	2.54	0.43
1:A:528:ARG:HH21	1:A:534:GLY:C	2.26	0.43
1:B:326:TYR:O	1:B:330:PRO:HG3	2.19	0.43
1:C:17:ASN:HB2	1:C:172:GLY:O	2.19	0.43
1:D:429:THR:HG22	1:D:543:THR:HG23	2.00	0.43
1:D:464:PRO:CD	1:D:468:LEU:HD13	2.47	0.43
1:D:528:ARG:HG2	1:D:533:VAL:HG23	2.00	0.43
1:A:280:ALA:O	1:A:293:VAL:HB	2.18	0.42
1:A:356:TRP:CD1	1:A:359:MET:HG3	2.54	0.42
1:C:316:GLY:CA	1:C:394:ILE:HG13	2.49	0.42
1:C:431:THR:HG21	1:C:437:GLY:CA	2.49	0.42
1:D:17:ASN:CB	1:D:20:LEU:HB2	2.46	0.42
1:A:554:LEU:HD23	1:A:554:LEU:HA	1.83	0.42
1:B:75:SER:O	1:B:76:ASN:C	2.62	0.42
1:C:424:THR:N	1:C:571:GLN:NE2	2.67	0.42
1:A:229:LYS:HB2	1:A:229:LYS:HE2	1.45	0.42
1:B:232:TYR:C	1:B:232:TYR:HD2	2.26	0.42
1:B:234:LEU:HG	1:B:298:ILE:HD12	2.01	0.42
1:A:557:PRO:HA	1:A:558:ILE:HD12	2.00	0.42
1:B:512:TRP:HA	1:B:513:PRO:HD3	1.88	0.42
1:C:75:SER:N	1:C:345:ASN:OD1	2.44	0.42
1:D:177:PHE:CE1	1:D:179:ARG:HG2	2.54	0.42
1:D:316:GLY:HA2	1:D:394:ILE:HG13	2.02	0.42
1:D:551:LEU:O	1:D:552:ASP:C	2.62	0.42
1:B:82:ARG:CG	1:B:82:ARG:NH1	2.80	0.42
1:B:230:LYS:HD2	1:B:470:PHE:CE2	2.54	0.42
1:C:87:THR:HA	1:C:205:ILE:O	2.20	0.42
1:C:178:VAL:HG21	1:C:236:ILE:CD1	2.50	0.42
1:D:234:LEU:HD13	1:D:470:PHE:HB2	2.00	0.42
1:B:45:GLU:O	1:B:49:MET:HG3	2.20	0.42
1:C:178:VAL:HG11	1:C:236:ILE:HD13	2.02	0.42
1:A:397:SER:HB3	1:A:400:ALA:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:VAL:HG22	1:B:212:LYS:HB3	2.02	0.42
1:D:49:MET:HE3	1:D:155:MET:CG	2.50	0.42
1:D:421:ARG:NH2	1:D:424:THR:OG1	2.53	0.42
1:D:459:THR:HG23	1:D:460:LEU:H	1.83	0.42
1:A:535:ALA:H	1:A:545:LYS:HE2	1.84	0.42
1:B:279:LEU:HD11	1:B:522:LEU:HD11	2.02	0.42
1:B:554:LEU:HD22	1:B:556:THR:HB	2.02	0.42
1:B:582:TYR:O	1:B:585:PHE:HB3	2.19	0.42
1:A:202:THR:CG2	1:A:204:TYR:CE2	3.03	0.42
1:C:221:TYR:O	1:C:222:GLY:C	2.62	0.42
1:D:67:ARG:HA	1:D:67:ARG:HD2	1.60	0.42
1:D:75:SER:HA	1:D:197:TRP:CD2	2.54	0.42
1:D:473:TYR:OH	1:D:478:TYR:HA	2.19	0.42
1:A:375:TRP:CD1	1:A:379:SER:HG	2.38	0.42
1:B:301:LEU:HA	1:B:309:TYR:O	2.20	0.42
1:D:189:GLU:O	1:D:191:GLY:N	2.53	0.42
1:D:401:ALA:O	1:D:404:PHE:HD1	2.03	0.42
1:A:45:GLU:O	1:A:49:MET:HG3	2.20	0.41
1:B:125:THR:HG22	1:B:126:MET:N	2.34	0.41
1:B:310:ALA:HB3	1:B:412:ILE:HD11	2.02	0.41
1:B:335:THR:HG23	1:B:397:SER:CA	2.50	0.41
1:C:113:MET:CE	1:C:206:THR:OG1	2.67	0.41
1:D:256:LEU:HD12	1:D:289:TRP:HE3	1.85	0.41
1:D:485:MET:HB3	1:D:485:MET:HE3	1.48	0.41
1:C:114:SER:HA	1:C:117:TYR:HB2	2.01	0.41
1:C:234:LEU:HB3	1:C:470:PHE:HB3	2.01	0.41
1:C:247:MET:HE2	1:C:308:LEU:HD11	2.02	0.41
1:C:255:LYS:HD2	1:C:403:GLU:OE2	2.19	0.41
1:C:428:VAL:HG13	1:C:544:ALA:HB2	2.00	0.41
1:D:61:LYS:HE3	1:D:64:GLU:OE2	2.20	0.41
1:D:93:LYS:HB3	1:D:95:GLU:OE1	2.20	0.41
1:D:276:LYS:HE2	1:D:297:ASP:OD1	2.19	0.41
1:A:77:PRO:CG	1:A:371:MET:CE	2.96	0.41
1:A:305:GLU:CD	1:A:305:GLU:H	2.28	0.41
1:C:277:THR:HG23	1:C:281:MET:CE	2.50	0.41
1:B:63:ASN:C	1:B:63:ASN:ND2	2.77	0.41
1:B:82:ARG:CZ	1:B:82:ARG:CB	2.99	0.41
1:C:43:GLN:OE1	1:C:158:ARG:NH2	2.54	0.41
1:C:441:GLY:O	1:C:444:LEU:HB2	2.20	0.41
1:C:492:LYS:HD2	1:C:492:LYS:HA	1.83	0.41
1:B:62:LEU:HD11	1:B:354:ILE:CD1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:MET:HB2	1:B:301:LEU:HB2	2.03	0.41
1:D:528:ARG:HD2	1:D:533:VAL:O	2.19	0.41
1:A:82:ARG:HB3	1:A:83:VAL:H	1.44	0.41
1:A:255:LYS:HG3	1:A:265:HIS:CE1	2.55	0.41
1:A:367:LEU:HA	1:A:367:LEU:HD23	1.84	0.41
1:A:553:GLY:C	1:A:555:ASP:N	2.73	0.41
1:C:524:TRP:CZ2	1:C:544:ALA:HA	2.54	0.41
1:D:554:LEU:HA	1:D:554:LEU:HD23	1.74	0.41
1:A:329:ASN:O	1:A:332:ALA:HB3	2.21	0.41
1:C:256:LEU:HD22	1:C:291:ALA:HB2	2.03	0.41
1:D:526:ILE:HG13	1:D:527:ASP:N	2.35	0.41
1:D:194:ASP:CG	1:D:195:VAL:N	2.78	0.41
1:B:23:TRP:CZ2	1:B:181:LEU:CD1	3.04	0.41
1:B:131:PHE:CZ	1:B:144:GLY:HA3	2.55	0.41
1:B:557:PRO:O	1:B:559:GLU:N	2.54	0.41
1:C:286:ILE:HA	1:C:287:PRO:HD3	1.95	0.41
1:C:528:ARG:HD2	1:C:533:VAL:HG12	2.03	0.41
1:C:531:GLY:C	1:C:533:VAL:N	2.72	0.41
1:D:93:LYS:O	1:D:94:GLU:C	2.64	0.41
1:D:154:VAL:HG12	1:D:163:MET:HE1	2.02	0.41
1:D:319:GLY:O	1:D:389:ARG:HA	2.21	0.41
1:D:366:HIS:NE2	1:D:374:ASP:OD1	2.52	0.41
1:D:369:ASP:OD1	1:D:369:ASP:C	2.64	0.41
1:D:378:GLU:HG2	1:D:378:GLU:H	1.57	0.41
1:D:549:LEU:HB3	1:D:551:LEU:HD21	2.02	0.41
1:C:577:GLU:OE1	1:C:581:GLU:OE2	2.39	0.41
1:A:89:ILE:O	1:A:89:ILE:HG13	2.21	0.40
1:C:370:TRP:CZ2	1:C:385:HIS:HD2	2.39	0.40
1:A:165:ILE:HD12	1:A:168:LEU:HD23	2.03	0.40
1:A:485:MET:HE2	1:A:488:LYS:HE3	2.02	0.40
1:B:155:MET:HE2	1:B:155:MET:HB3	1.94	0.40
1:B:429:THR:CG2	2:B:619:HOH:O	2.60	0.40
1:C:325:ASN:ND2	1:C:358:GLY:O	2.53	0.40
1:C:354:ILE:HD13	1:C:356:TRP:CZ3	2.56	0.40
1:D:264:TYR:CE1	1:D:526:ILE:HD13	2.56	0.40
1:D:334:LYS:O	1:D:335:THR:C	2.63	0.40
1:A:283:THR:HA	1:A:284:PRO:HD3	1.92	0.40
1:A:305:GLU:O	1:A:492:LYS:HE3	2.22	0.40
1:A:503:ARG:HH22	1:A:566:THR:HG22	1.69	0.40
1:B:166:GLU:OE2	1:B:166:GLU:HA	2.21	0.40
1:B:304:ARG:HA	1:B:304:ARG:NE	2.31	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:430:GLN:HB2	1:C:497:PHE:CE2	2.57	0.40
1:D:251:MET:HE1	1:D:415:ILE:HD13	2.03	0.40
1:D:258:ASN:OD1	1:D:258:ASN:C	2.65	0.40
1:D:562:LYS:O	1:D:566:THR:HG23	2.20	0.40
1:B:66:LYS:HB3	1:B:66:LYS:HE2	1.82	0.40
1:B:221:TYR:O	1:B:224:ASN:HB2	2.21	0.40
1:B:275:GLY:N	1:B:278:ASN:HD22	2.11	0.40
1:B:540:VAL:HG22	1:B:572:TRP:CZ2	2.57	0.40
1:C:94:GLU:O	1:C:94:GLU:HG2	2.21	0.40
1:C:221:TYR:CD2	1:C:221:TYR:C	2.99	0.40
1:C:232:TYR:HA	1:C:236:ILE:HG12	2.02	0.40
1:A:424:THR:HA	1:A:571:GLN:NE2	2.36	0.40
1:A:434:TRP:NE1	1:A:482:TRP:O	2.43	0.40
1:A:434:TRP:CH2	1:A:493:MET:HE3	2.57	0.40
1:B:527:ASP:HB3	1:B:533:VAL:CG2	2.51	0.40
1:D:34:GLU:HG2	1:D:124:ARG:H	1.86	0.40
1:D:189:GLU:O	1:D:190:PRO:C	2.65	0.40
1:D:242:ARG:NH2	1:D:481:ASN:HD22	2.10	0.40

There are no symmetry-related clashes.

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	582/610 (95%)	528 (91%)	39 (7%)	15 (3%)	4	3
1	B	580/610 (95%)	523 (90%)	38 (7%)	19 (3%)	3	2
1	C	582/610 (95%)	527 (90%)	42 (7%)	13 (2%)	5	4
1	D	572/610 (94%)	519 (91%)	37 (6%)	16 (3%)	4	2
All	All	2316/2440 (95%)	2097 (90%)	156 (7%)	63 (3%)	4	3

All (63) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	260	GLU
1	A	273	ALA
1	A	362	ASP
1	A	551	LEU
1	A	556	THR
1	A	559	GLU
1	B	56	ALA
1	B	94	GLU
1	B	305	GLU
1	B	363	ALA
1	B	460	LEU
1	B	506	GLU
1	B	507	ASP
1	C	79	ASP
1	C	488	LYS
1	C	533	VAL
1	C	559	GLU
1	D	17	ASN
1	D	79	ASP
1	D	190	PRO
1	D	192	GLN
1	D	193	GLU
1	D	274	CYS
1	D	328	SER
1	D	362	ASP
1	D	424	THR
1	D	507	ASP
1	A	82	ARG
1	A	395	ASP
1	B	192	GLN
1	B	361	GLY
1	B	362	ASP
1	C	229	LYS
1	C	558	ILE
1	D	552	ASP
1	A	81	ALA
1	A	535	ALA
1	B	17	ASN
1	C	555	ASP
1	C	557	PRO
1	C	560	ASP
1	D	118	ALA
1	D	363	ALA

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Mol	Chain	Res	Type
1	A	363	ALA
1	B	57	GLY
1	B	63	ASN
1	B	190	PRO
1	B	350	ASP
1	B	490	GLY
1	B	531	GLY
1	C	351	ASP
1	D	64	GLU
1	D	546	ALA
1	A	118	ALA
1	A	552	ASP
1	B	558	ILE
1	C	162	ARG
1	C	531	GLY
1	C	550	ASP
1	D	18	LYS
1	A	561	VAL
1	B	222	GLY
1	A	77	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	474/487 (97%)	410 (86%)	64 (14%)	4	4
1	B	471/487 (97%)	399 (85%)	72 (15%)	3	3
1	C	473/487 (97%)	416 (88%)	57 (12%)	5	5
1	D	469/487 (96%)	384 (82%)	85 (18%)	2	2
All	All	1887/1948 (97%)	1609 (85%)	278 (15%)	3	3

All (278) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ASN

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Mol	Chain	Res	Type
1	A	18	LYS
1	A	30	LEU
1	A	39	VAL
1	A	54	VAL
1	A	64	GLU
1	A	74	ARG
1	A	77	PRO
1	A	78	SER
1	A	80	VAL
1	A	89	ILE
1	A	91	SER
1	A	93	LYS
1	A	95	GLU
1	A	109	MET
1	A	136	ILE
1	A	163	MET
1	A	190	PRO
1	A	212	LYS
1	A	213	GLU
1	A	226	ILE
1	A	229	LYS
1	A	260	GLU
1	A	272	SER
1	A	274	CYS
1	A	283	THR
1	A	285	THR
1	A	286	ILE
1	A	293	VAL
1	A	298	ILE
1	A	301	LEU
1	A	303	LEU
1	A	348	LEU
1	A	360	ASP
1	A	376	THR
1	A	379	SER
1	A	404	PHE
1	A	408	GLU
1	A	416	LEU
1	A	429	THR
1	A	440	VAL
1	A	444	LEU
1	A	446	SER

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Mol	Chain	Res	Type
1	A	457	VAL
1	A	460	LEU
1	A	461	ARG
1	A	468	LEU
1	A	488	LYS
1	A	492	LYS
1	A	509	ARG
1	A	511	LEU
1	A	525	VAL
1	A	537	GLU
1	A	543	THR
1	A	547	GLU
1	A	550	ASP
1	A	554	LEU
1	A	558	ILE
1	A	559	GLU
1	A	562	LYS
1	A	563	GLU
1	A	570	GLU
1	A	574	ASN
1	A	606	SER
1	B	19	GLU
1	B	20	LEU
1	B	21	LEU
1	B	24	ILE
1	B	29	GLU
1	B	30	LEU
1	B	39	VAL
1	B	55	GLU
1	B	60	ILE
1	B	62	LEU
1	B	63	ASN
1	B	65	GLU
1	B	67	ARG
1	B	76	ASN
1	B	83	VAL
1	B	92	GLU
1	B	107	GLN
1	B	122	LYS
1	B	126	MET
1	B	136	ILE
1	B	148	THR

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Mol	Chain	Res	Type
1	B	152	TYR
1	B	163	MET
1	B	166	GLU
1	B	168	LEU
1	B	176	SER
1	B	179	ARG
1	B	181	LEU
1	B	192	GLN
1	B	195	VAL
1	B	203	LYS
1	B	206	THR
1	B	227	LEU
1	B	242	ARG
1	B	257	ILE
1	B	262	LYS
1	B	276	LYS
1	B	298	ILE
1	B	303	LEU
1	B	304	ARG
1	B	311	VAL
1	B	348	LEU
1	B	354	ILE
1	B	362	ASP
1	B	368	ILE
1	B	378	GLU
1	B	381	GLU
1	B	394	ILE
1	B	408	GLU
1	B	420	ARG
1	B	429	THR
1	B	431	THR
1	B	435	GLU
1	B	461	ARG
1	B	468	LEU
1	B	491	ASP
1	B	492	LYS
1	B	493	MET
1	B	503	ARG
1	B	506	GLU
1	B	511	LEU
1	B	530	GLU
1	B	532	HIS

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Mol	Chain	Res	Type
1	B	533	VAL
1	B	545	LYS
1	B	547	GLU
1	B	551	LEU
1	B	554	LEU
1	B	556	THR
1	B	562	LYS
1	B	565	LEU
1	B	570	GLU
1	C	16	LYS
1	C	17	ASN
1	C	36	VAL
1	C	39	VAL
1	C	60	ILE
1	C	62	LEU
1	C	67	ARG
1	C	94	GLU
1	C	113	MET
1	C	125	THR
1	C	153	VAL
1	C	163	MET
1	C	168	LEU
1	C	171	ILE
1	C	179	ARG
1	C	181	LEU
1	C	189	GLU
1	C	193	GLU
1	C	211	THR
1	C	229	LYS
1	C	230	LYS
1	C	253	ILE
1	C	256	LEU
1	C	257	ILE
1	C	260	GLU
1	C	276	LYS
1	C	282	ILE
1	C	285	THR
1	C	293	VAL
1	C	301	LEU
1	C	303	LEU
1	C	305	GLU
1	C	306	ASP

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Mol	Chain	Res	Type
1	C	342	LEU
1	C	351	ASP
1	C	359	MET
1	C	376	THR
1	C	378	GLU
1	C	404	PHE
1	C	408	GLU
1	C	416	LEU
1	C	420	ARG
1	C	429	THR
1	C	431	THR
1	C	444	LEU
1	C	468	LEU
1	C	537	GLU
1	C	543	THR
1	C	547	GLU
1	C	549	LEU
1	C	555	ASP
1	C	556	THR
1	C	559	GLU
1	C	562	LYS
1	C	565	LEU
1	C	589	ARG
1	C	606	SER
1	D	15	THR
1	D	16	LYS
1	D	20	LEU
1	D	29	GLU
1	D	34	GLU
1	D	39	VAL
1	D	51	GLU
1	D	60	ILE
1	D	64	GLU
1	D	67	ARG
1	D	78	SER
1	D	83	VAL
1	D	84	GLU
1	D	107	GLN
1	D	114	SER
1	D	122	LYS
1	D	132	CYS
1	D	136	ILE

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Mol	Chain	Res	Type
1	D	140	ASP
1	D	149	ASP
1	D	153	VAL
1	D	163	MET
1	D	165	ILE
1	D	168	LEU
1	D	170	LYS
1	D	190	PRO
1	D	202	THR
1	D	205	ILE
1	D	207	GLN
1	D	212	LYS
1	D	216	SER
1	D	227	LEU
1	D	229	LYS
1	D	244	GLU
1	D	253	ILE
1	D	254	LEU
1	D	256	LEU
1	D	257	ILE
1	D	262	LYS
1	D	272	SER
1	D	274	CYS
1	D	281	MET
1	D	282	ILE
1	D	290	THR
1	D	301	LEU
1	D	305	GLU
1	D	331	ILE
1	D	342	LEU
1	D	349	THR
1	D	351	ASP
1	D	360	ASP
1	D	362	ASP
1	D	378	GLU
1	D	379	SER
1	D	403	GLU
1	D	410	VAL
1	D	411	LYS
1	D	428	VAL
1	D	429	THR
1	D	444	LEU

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Mol	Chain	Res	Type
1	D	446	SER
1	D	461	ARG
1	D	465	MET
1	D	491	ASP
1	D	495	SER
1	D	496	ILE
1	D	504	ARG
1	D	506	GLU
1	D	507	ASP
1	D	509	ARG
1	D	522	LEU
1	D	526	ILE
1	D	529	ILE
1	D	530	GLU
1	D	533	VAL
1	D	539	VAL
1	D	547	GLU
1	D	551	LEU
1	D	552	ASP
1	D	555	ASP
1	D	559	GLU
1	D	562	LYS
1	D	565	LEU
1	D	570	GLU
1	D	589	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	32	GLN
1	A	101	ASN
1	A	102	ASN
1	A	107	GLN
1	A	207	GLN
1	A	265	HIS
1	A	571	GLN
1	B	43	GLN
1	B	63	ASN
1	B	76	ASN
1	B	107	GLN
1	B	146	GLN

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Mol	Chain	Res	Type
1	B	278	ASN
1	B	292	GLN
1	B	325	ASN
1	B	340	ASN
1	B	430	GLN
1	B	474	ASN
1	B	481	ASN
1	B	571	GLN
1	C	17	ASN
1	C	76	ASN
1	C	101	ASN
1	C	207	GLN
1	C	265	HIS
1	C	340	ASN
1	C	366	HIS
1	C	430	GLN
1	C	480	GLN
1	C	481	ASN
1	C	487	ASN
1	C	571	GLN
1	C	574	ASN
1	D	17	ASN
1	D	43	GLN
1	D	63	ASN
1	D	76	ASN
1	D	101	ASN
1	D	107	GLN
1	D	192	GLN
1	D	207	GLN
1	D	250	HIS
1	D	265	HIS
1	D	278	ASN
1	D	480	GLN
1	D	481	ASN
1	D	574	ASN
1	D	597	GLN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	586/610 (96%)	-0.39	3 (0%) 87 87	14, 25, 44, 62	0
1	B	584/610 (95%)	-0.11	4 (0%) 84 85	15, 32, 51, 62	0
1	C	586/610 (96%)	-0.22	7 (1%) 76 77	17, 28, 46, 72	0
1	D	578/610 (94%)	0.04	6 (1%) 79 80	23, 35, 54, 74	0
All	All	2334/2440 (95%)	-0.17	20 (0%) 81 82	14, 30, 50, 74	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	556	THR	4.7
1	D	327	ALA	4.2
1	C	561	VAL	3.8
1	D	508	GLY	3.6
1	C	557	PRO	3.1
1	D	282	ILE	3.1
1	D	558	ILE	3.0
1	A	556	THR	2.9
1	D	553	GLY	2.8
1	C	558	ILE	2.8
1	A	555	ASP	2.6
1	C	553	GLY	2.5
1	B	606	SER	2.5
1	A	457	VAL	2.5
1	B	546	ALA	2.3
1	D	272	SER	2.3
1	C	272	SER	2.3
1	B	81	ALA	2.2
1	B	350	ASP	2.1
1	C	531	GLY	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.