



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:21 PM UTC

PDB ID : 3T81 / pdb_00003t81
Title : Crystal Structure of diiron adenine deaminase
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Deposited on : 2011-08-01
Resolution : 2.63 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

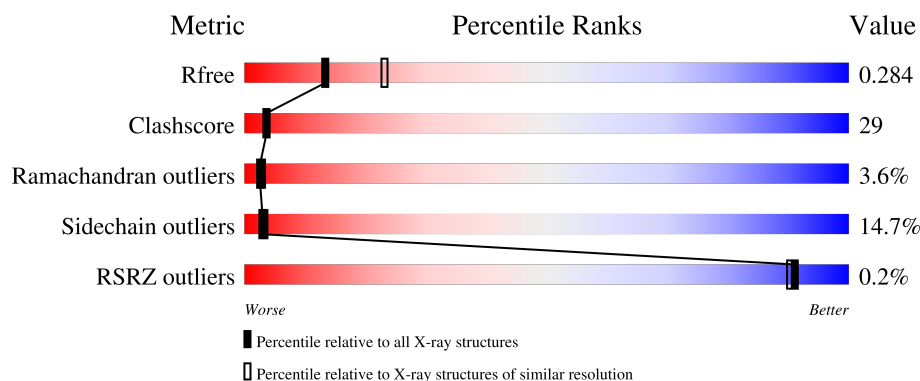
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

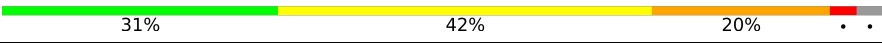
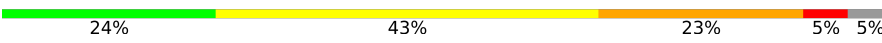
The reported resolution of this entry is 2.63 Å.

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	2053 (2.66-2.62)
Clashscore	190562	2097 (2.66-2.62)
Ramachandran outliers	187476	2066 (2.66-2.62)
Sidechain outliers	187428	2066 (2.66-2.62)
RSRZ outliers	180081	2052 (2.66-2.62)

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	608	
1	B	608	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8674 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 Adenine deaminase 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	587	Total	C	N	O	S	Se	0	0	0
			4337	2723	775	817	6	16			
1	B	579	Total	C	N	O	S	Se	0	0	0
			4277	2685	763	807	6	16			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MSE	-	expression tag	UNP Q7CUX4
A	-1	SER	-	expression tag	UNP Q7CUX4
A	0	LEU	-	expression tag	UNP Q7CUX4
A	598	GLU	-	expression tag	UNP Q7CUX4
A	599	GLY	-	expression tag	UNP Q7CUX4
A	600	HIS	-	expression tag	UNP Q7CUX4
A	601	HIS	-	expression tag	UNP Q7CUX4
A	602	HIS	-	expression tag	UNP Q7CUX4
A	603	HIS	-	expression tag	UNP Q7CUX4
A	604	HIS	-	expression tag	UNP Q7CUX4
A	605	HIS	-	expression tag	UNP Q7CUX4
B	-2	MSE	-	expression tag	UNP Q7CUX4
B	-1	SER	-	expression tag	UNP Q7CUX4
B	0	LEU	-	expression tag	UNP Q7CUX4
B	598	GLU	-	expression tag	UNP Q7CUX4
B	599	GLY	-	expression tag	UNP Q7CUX4
B	600	HIS	-	expression tag	UNP Q7CUX4
B	601	HIS	-	expression tag	UNP Q7CUX4
B	602	HIS	-	expression tag	UNP Q7CUX4
B	603	HIS	-	expression tag	UNP Q7CUX4
B	604	HIS	-	expression tag	UNP Q7CUX4
B	605	HIS	-	expression tag	UNP Q7CUX4

- Molecule 2 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total 3	Fe 3	0	0
2	B	3	Total 3	Fe 3	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	23	Total 23	O 23	0	0
3	B	31	Total 31	O 31	0	0

[illegible]

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	61.66Å 131.84Å 69.63Å 90.00° 97.04° 90.00°	Depositor
Resolution (Å)	48.89 – 2.63 48.89 – 2.63	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.89-2.63) 99.8 (48.89-2.63)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 2.61Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.185 , 0.287 0.186 , 0.284	Depositor DCC
R_{free} test set	1663 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	54.5	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 37.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8674	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% 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

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

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	2.36	183/4402 (4.2%)	2.02	168/5964 (2.8%)
1	B	2.32	201/4340 (4.6%)	2.13	183/5878 (3.1%)
All	All	2.34	384/8742 (4.4%)	2.07	351/11842 (3.0%)

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	5
1	B	0	9
All	All	0	14

All (384) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	451	MSE	SE-CE	19.80	2.54	1.95
1	A	189	MSE	SE-CE	18.59	2.51	1.95
1	B	396	MSE	SE-CE	14.82	2.39	1.95
1	B	442	MSE	SE-CE	12.35	2.32	1.95
1	B	451	MSE	SE-CE	12.03	2.31	1.95
1	B	496	ALA	CA-CB	-11.67	1.33	1.53
1	B	202	SER	C-O	-11.58	1.10	1.24
1	A	577	MSE	SE-CE	11.21	2.29	1.95
1	A	248	MSE	SE-CE	11.20	2.29	1.95
1	B	435	VAL	CA-CB	10.94	1.65	1.53
1	A	358	ALA	CA-CB	10.93	1.66	1.52
1	B	201	MSE	SE-CE	10.87	2.28	1.95
1	B	300	GLY	N-CA	10.60	1.54	1.44
1	A	396	MSE	SE-CE	10.55	2.27	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	99	MSE	SE-CE	10.51	2.27	1.95
1	B	570	ILE	CA-CB	10.46	1.64	1.54
1	B	584	THR	CA-CB	10.35	1.68	1.53
1	A	399	ASP	CA-C	10.01	1.66	1.52
1	B	25	ALA	CA-CB	-9.89	1.38	1.53
1	B	24	ALA	C-O	9.75	1.35	1.24
1	B	101	THR	CA-CB	9.68	1.69	1.53
1	A	588	MSE	SE-CE	9.53	2.24	1.95
1	B	347	ILE	CA-CB	-9.48	1.38	1.55
1	B	577	MSE	SE-CE	9.41	2.23	1.95
1	A	80	GLY	C-O	9.17	1.35	1.23
1	A	194	VAL	CA-CB	9.06	1.65	1.54
1	B	52	ALA	CA-CB	-8.97	1.39	1.53
1	A	84	VAL	CA-CB	8.86	1.64	1.54
1	A	216	CYS	CA-C	-8.77	1.42	1.52
1	B	256	THR	CA-CB	-8.65	1.39	1.53
1	A	54	ILE	CA-CB	8.63	1.65	1.54
1	A	242	VAL	CA-CB	8.47	1.64	1.54
1	B	78	ASP	C-O	8.42	1.34	1.24
1	A	584	THR	CA-CB	8.29	1.67	1.53
1	B	557	VAL	CA-CB	8.24	1.65	1.54
1	B	448	ARG	CZ-NH1	8.16	1.44	1.32
1	A	472	ALA	C-O	8.16	1.33	1.23
1	B	404	SER	N-CA	8.13	1.56	1.46
1	A	135	TRP	C-O	-8.09	1.14	1.24
1	A	200	ARG	CA-C	8.07	1.63	1.52
1	B	472	ALA	C-O	8.06	1.34	1.23
1	B	534	VAL	N-CA	-8.04	1.36	1.46
1	B	169	ASP	N-CA	8.00	1.55	1.45
1	A	414	ILE	CA-CB	7.97	1.65	1.54
1	A	184	GLY	N-CA	7.93	1.52	1.45
1	B	592	VAL	CA-CB	7.91	1.65	1.54
1	B	72	ASP	CA-C	-7.90	1.42	1.52
1	A	11	ALA	CA-CB	-7.89	1.41	1.53
1	A	195	ILE	CA-CB	-7.87	1.45	1.54
1	B	231	MSE	SE-CE	7.84	2.19	1.95
1	B	403	LYS	N-CA	7.79	1.55	1.46
1	A	517	ILE	C-O	7.78	1.31	1.23
1	A	350	PHE	N-CA	7.75	1.55	1.46
1	A	162	GLU	C-O	-7.70	1.14	1.23
1	B	588	MSE	SE-CE	7.68	2.18	1.95
1	A	66	GLU	N-CA	7.64	1.54	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	127	VAL	CA-C	7.63	1.62	1.52
1	A	442	MSE	SE-CE	7.63	2.18	1.95
1	A	336	LEU	C-O	7.59	1.35	1.24
1	B	61	ILE	C-O	7.57	1.31	1.24
1	B	270	PHE	C-O	7.55	1.32	1.24
1	B	148	ILE	CA-CB	7.52	1.63	1.54
1	B	198	ASP	CA-C	7.52	1.61	1.53
1	A	567	ALA	CA-CB	-7.49	1.40	1.53
1	B	248	MSE	SE-CE	7.47	2.17	1.95
1	B	20	ALA	CA-CB	-7.46	1.41	1.53
1	B	279	HIS	N-CA	-7.45	1.36	1.46
1	B	532	GLU	C-O	7.45	1.32	1.24
1	A	154	CYS	CA-C	-7.42	1.43	1.53
1	B	273	ALA	N-CA	7.42	1.55	1.46
1	B	20	ALA	C-O	7.40	1.32	1.24
1	B	40	THR	CA-CB	-7.39	1.43	1.53
1	B	73	ALA	CA-CB	-7.38	1.41	1.53
1	B	120	ASP	CA-C	7.30	1.62	1.52
1	B	127	VAL	C-O	-7.27	1.15	1.24
1	A	557	VAL	CA-C	7.27	1.61	1.52
1	B	318	TRP	CA-C	-7.26	1.43	1.52
1	B	363	ALA	N-CA	7.26	1.55	1.46
1	B	553	PRO	CA-C	7.26	1.58	1.52
1	B	61	ILE	N-CA	-7.19	1.38	1.46
1	A	514	VAL	CA-CB	7.17	1.63	1.54
1	B	331	LEU	C-O	-7.17	1.14	1.24
1	A	378	ILE	CA-C	7.15	1.58	1.53
1	A	174	ALA	N-CA	7.15	1.55	1.46
1	A	186	ALA	CA-CB	-7.14	1.42	1.53
1	A	201	MSE	CG-SE	7.14	2.16	1.95
1	A	35	LEU	CA-C	-7.12	1.43	1.52
1	A	358	ALA	CA-C	7.07	1.61	1.52
1	B	243	SER	CA-C	7.04	1.61	1.52
1	B	292	PHE	C-O	-7.01	1.15	1.23
1	A	64	VAL	CA-CB	6.97	1.62	1.53
1	B	477	HIS	C-O	6.94	1.32	1.24
1	B	334	SER	C-O	6.93	1.34	1.24
1	A	146	ARG	C-O	-6.91	1.16	1.24
1	B	292	PHE	CA-C	-6.91	1.45	1.53
1	A	557	VAL	CA-CB	-6.89	1.45	1.54
1	A	582	VAL	CA-C	6.89	1.60	1.52
1	A	82	ALA	CA-CB	6.88	1.65	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	306	VAL	CA-C	6.86	1.61	1.52
1	B	135	TRP	CA-C	6.86	1.62	1.52
1	A	472	ALA	CA-CB	-6.84	1.42	1.53
1	A	348	VAL	CA-CB	-6.84	1.46	1.54
1	A	349	VAL	CA-CB	-6.83	1.46	1.54
1	A	103	ALA	CA-CB	6.83	1.64	1.53
1	A	22	ALA	CA-CB	-6.82	1.42	1.53
1	A	519	PRO	C-O	6.81	1.31	1.23
1	B	88	LEU	C-O	6.80	1.33	1.23
1	B	54	ILE	C-O	-6.78	1.16	1.24
1	A	55	GLY	C-O	6.78	1.32	1.23
1	A	540	ASP	C-O	6.78	1.32	1.24
1	A	175	ASP	CA-C	6.76	1.61	1.52
1	B	274	LEU	C-O	-6.72	1.16	1.24
1	A	422	TRP	C-O	6.72	1.32	1.23
1	A	231	MSE	SE-CE	6.71	2.15	1.95
1	A	345	ALA	CA-CB	-6.70	1.43	1.53
1	A	589	GLU	CA-C	6.68	1.61	1.52
1	A	467	TRP	N-CA	6.64	1.55	1.46
1	A	152	PRO	C-O	6.64	1.31	1.23
1	B	288	THR	C-O	6.63	1.32	1.23
1	B	467	TRP	N-CA	6.63	1.54	1.46
1	A	91	THR	CA-C	6.63	1.62	1.52
1	A	16	ASP	N-CA	-6.62	1.38	1.46
1	B	454	PRO	C-O	-6.61	1.15	1.24
1	B	267	LEU	C-O	-6.60	1.18	1.24
1	B	544	ALA	N-CA	-6.59	1.38	1.46
1	B	57	VAL	N-CA	-6.58	1.37	1.46
1	B	357	SER	N-CA	-6.58	1.38	1.46
1	A	257	ILE	C-O	6.56	1.32	1.24
1	B	363	ALA	CA-C	-6.56	1.44	1.52
1	B	586	LYS	CA-C	6.55	1.60	1.52
1	B	35	LEU	N-CA	6.53	1.53	1.46
1	A	513	LYS	CA-C	6.53	1.60	1.52
1	B	34	VAL	CA-C	-6.52	1.44	1.52
1	B	203	GLY	N-CA	6.51	1.53	1.45
1	B	509	ALA	CA-CB	-6.51	1.37	1.54
1	A	108	ALA	C-O	-6.51	1.16	1.24
1	B	72	ASP	C-O	-6.50	1.15	1.24
1	B	51	PRO	N-CA	6.49	1.54	1.47
1	A	94	HIS	N-CA	-6.47	1.38	1.46
1	A	117	ILE	CA-CB	6.46	1.63	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	148	ILE	CA-CB	-6.43	1.46	1.54
1	A	549	VAL	CA-CB	6.43	1.63	1.54
1	A	325	LEU	C-O	6.42	1.31	1.24
1	A	334	SER	CA-C	6.42	1.61	1.52
1	A	581	ASP	CB-CG	6.42	1.68	1.52
1	A	19	ARG	CA-C	-6.42	1.44	1.52
1	B	135	TRP	C-O	6.41	1.31	1.24
1	B	90	ASP	N-CA	6.40	1.53	1.46
1	A	238	ASP	CA-C	6.38	1.60	1.52
1	A	107	ALA	C-O	-6.38	1.16	1.24
1	A	155	VAL	N-CA	-6.36	1.40	1.46
1	B	593	ILE	CA-CB	6.33	1.63	1.54
1	A	476	SER	C-O	-6.33	1.17	1.23
1	A	133	VAL	CA-C	-6.32	1.44	1.52
1	A	119	TRP	CA-C	-6.32	1.45	1.52
1	A	558	PHE	C-O	-6.31	1.16	1.24
1	B	279	HIS	CA-CB	-6.31	1.43	1.53
1	A	275	ASN	N-CA	6.31	1.54	1.46
1	B	306	VAL	C-O	6.30	1.31	1.24
1	A	391	LYS	C-O	6.30	1.31	1.24
1	B	498	ALA	C-O	6.29	1.31	1.24
1	A	107	ALA	CA-C	-6.29	1.44	1.52
1	B	452	ALA	N-CA	-6.29	1.38	1.46
1	A	89	ILE	C-O	-6.28	1.17	1.24
1	A	290	ASP	CA-C	-6.27	1.45	1.52
1	A	341	ALA	CA-CB	6.27	1.64	1.53
1	A	209	LEU	CA-C	-6.27	1.44	1.52
1	B	143	LEU	CA-C	-6.26	1.44	1.53
1	A	318	TRP	CA-C	-6.26	1.44	1.52
1	B	298	GLN	N-CA	6.25	1.53	1.46
1	B	280	LEU	C-O	-6.25	1.16	1.24
1	B	290	ASP	N-CA	6.25	1.53	1.46
1	A	103	ALA	N-CA	6.24	1.53	1.46
1	A	198	ASP	CA-C	-6.24	1.46	1.53
1	A	537	ALA	CA-CB	6.24	1.63	1.53
1	A	110	VAL	C-O	-6.24	1.17	1.24
1	B	311	ARG	CZ-NH1	6.23	1.41	1.32
1	B	86	PRO	CA-C	6.23	1.60	1.52
1	B	360	HIS	C-O	6.21	1.31	1.23
1	A	15	ASP	N-CA	-6.20	1.38	1.46
1	B	266	LEU	C-O	6.20	1.32	1.24
1	B	357	SER	C-O	6.20	1.31	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	335	ASP	C-O	6.19	1.31	1.24
1	A	81	GLY	CA-C	6.18	1.60	1.51
1	B	361	VAL	C-O	-6.16	1.17	1.24
1	A	29	ASP	N-CA	-6.15	1.39	1.46
1	B	434	VAL	CA-CB	6.15	1.62	1.54
1	B	429	VAL	CA-CB	6.15	1.61	1.54
1	A	413	THR	N-CA	6.14	1.53	1.45
1	A	206	GLN	C-O	-6.13	1.16	1.24
1	A	484	VAL	N-CA	6.12	1.53	1.46
1	B	54	ILE	N-CA	-6.12	1.39	1.46
1	B	330	ARG	CA-CB	-6.12	1.43	1.53
1	B	379	PRO	CA-C	6.10	1.60	1.52
1	B	183	GLY	C-O	6.09	1.30	1.23
1	A	421	GLN	CA-C	-6.09	1.44	1.52
1	A	310	VAL	C-O	-6.08	1.16	1.24
1	A	220	ARG	NE-CZ	6.06	1.39	1.33
1	A	126	ASN	N-CA	-6.05	1.39	1.46
1	B	318	TRP	N-CA	-6.05	1.39	1.46
1	A	137	ALA	CA-C	6.04	1.61	1.52
1	A	567	ALA	C-O	-6.04	1.16	1.24
1	B	536	ARG	C-O	6.03	1.31	1.24
1	B	257	ILE	N-CA	6.03	1.53	1.46
1	B	18	LEU	CA-C	6.02	1.60	1.52
1	B	70	ARG	CZ-NH2	6.01	1.41	1.33
1	B	535	ALA	N-CA	6.00	1.53	1.46
1	A	303	ASP	C-O	6.00	1.31	1.24
1	B	216	CYS	CA-CB	-6.00	1.44	1.53
1	B	246	ASP	CA-C	5.99	1.60	1.52
1	A	321	ARG	CA-C	-5.97	1.45	1.52
1	A	384	THR	CA-CB	5.97	1.63	1.53
1	A	594	GLU	N-CA	5.97	1.53	1.45
1	B	79	ALA	CA-CB	-5.97	1.45	1.53
1	B	320	LEU	C-O	5.96	1.31	1.24
1	A	552	GLN	C-O	-5.95	1.17	1.24
1	B	109	VAL	CA-CB	-5.95	1.46	1.54
1	A	117	ILE	N-CA	5.95	1.53	1.46
1	B	174	ALA	N-CA	-5.94	1.38	1.46
1	A	23	VAL	CA-CB	-5.93	1.47	1.54
1	A	397	ALA	CA-CB	5.92	1.63	1.53
1	A	71	ARG	CA-C	-5.91	1.45	1.52
1	B	161	LEU	CA-C	5.90	1.60	1.52
1	B	128	HIS	CA-C	5.90	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	539	GLU	N-CA	5.89	1.53	1.46
1	A	240	GLU	CA-C	-5.88	1.47	1.53
1	A	246	ASP	CB-CG	5.87	1.66	1.52
1	B	236	SER	CA-CB	-5.86	1.44	1.53
1	A	513	LYS	CB-CG	5.86	1.70	1.52
1	B	133	VAL	C-O	-5.86	1.17	1.24
1	B	500	ILE	CA-CB	-5.86	1.46	1.54
1	A	548	VAL	C-O	5.85	1.30	1.24
1	A	413	THR	CA-CB	5.85	1.66	1.54
1	A	37	THR	CA-CB	5.84	1.67	1.53
1	B	159	PRO	CA-C	5.84	1.60	1.52
1	B	41	LEU	C-O	5.83	1.30	1.23
1	A	47	GLY	CA-C	5.83	1.59	1.51
1	A	119	TRP	N-CA	5.83	1.53	1.46
1	B	36	ILE	CA-CB	-5.82	1.47	1.54
1	B	201	MSE	N-CA	5.82	1.53	1.46
1	A	14	ASN	N-CA	5.80	1.53	1.46
1	B	38	GLY	N-CA	5.80	1.54	1.45
1	A	234	GLY	C-O	-5.80	1.16	1.23
1	B	542	ARG	CZ-NH1	5.79	1.40	1.32
1	B	345	ALA	CA-CB	-5.79	1.43	1.53
1	B	42	VAL	CA-C	-5.77	1.46	1.52
1	A	105	TYR	C-O	-5.77	1.16	1.24
1	B	72	ASP	N-CA	5.77	1.53	1.46
1	B	17	THR	CA-CB	5.75	1.62	1.53
1	B	202	SER	CA-C	-5.75	1.45	1.52
1	B	210	ALA	CA-CB	5.75	1.63	1.53
1	A	311	ARG	CD-NE	5.74	1.54	1.46
1	A	452	ALA	CA-C	5.73	1.60	1.52
1	B	586	LYS	N-CA	5.73	1.53	1.45
1	A	489	ALA	CA-C	5.71	1.60	1.52
1	B	248	MSE	CG-SE	5.70	2.12	1.95
1	B	194	VAL	CA-CB	5.70	1.61	1.55
1	A	474	THR	CA-CB	-5.69	1.44	1.53
1	B	368	VAL	CA-CB	-5.69	1.48	1.54
1	A	106	ALA	CA-CB	-5.68	1.44	1.53
1	B	298	GLN	CG-CD	5.68	1.66	1.52
1	B	418	ARG	N-CA	5.68	1.53	1.46
1	A	254	GLY	N-CA	5.68	1.53	1.45
1	A	591	PRO	CA-C	5.67	1.60	1.52
1	B	341	ALA	CA-CB	5.67	1.62	1.53
1	A	79	ALA	CA-CB	5.66	1.63	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	163	ARG	C-O	5.65	1.30	1.23
1	A	201	MSE	SE-CE	5.64	2.12	1.95
1	B	362	LEU	CA-C	5.64	1.59	1.52
1	B	139	ALA	CA-CB	-5.63	1.44	1.53
1	B	288	THR	CA-C	-5.63	1.46	1.52
1	A	348	VAL	C-O	-5.62	1.18	1.24
1	B	526	VAL	CA-CB	5.62	1.62	1.54
1	B	214	LEU	CA-C	-5.62	1.45	1.53
1	A	185	ILE	C-O	5.61	1.31	1.24
1	A	308	ARG	N-CA	-5.59	1.39	1.46
1	A	509	ALA	CA-C	5.59	1.59	1.52
1	B	79	ALA	C-O	5.59	1.31	1.24
1	B	188	ILE	CA-CB	5.59	1.59	1.53
1	B	343	ARG	C-O	5.58	1.31	1.23
1	B	403	LYS	CA-C	5.58	1.60	1.52
1	A	305	VAL	CA-CB	5.58	1.61	1.54
1	A	458	THR	CA-C	-5.58	1.46	1.52
1	B	88	LEU	CA-C	5.56	1.60	1.53
1	A	83	TYR	N-CA	5.56	1.52	1.46
1	B	343	ARG	N-CA	5.56	1.53	1.45
1	A	346	ASP	C-O	5.55	1.30	1.23
1	A	44	VAL	N-CA	5.55	1.54	1.46
1	A	44	VAL	C-O	-5.54	1.16	1.24
1	B	220	ARG	CB-CG	5.54	1.69	1.52
1	A	209	LEU	CA-CB	-5.53	1.44	1.53
1	B	23	VAL	CA-C	5.52	1.59	1.52
1	A	331	LEU	CG-CD2	5.51	1.70	1.52
1	B	88	LEU	C-N	5.51	1.39	1.33
1	B	315	LYS	CG-CD	5.51	1.69	1.52
1	B	248	MSE	CA-C	-5.51	1.45	1.52
1	A	283	THR	CA-CB	-5.48	1.45	1.53
1	A	403	LYS	CG-CD	5.48	1.68	1.52
1	B	290	ASP	C-O	5.48	1.30	1.24
1	A	204	ILE	CB-CG2	5.47	1.70	1.52
1	A	409	VAL	CA-C	-5.47	1.46	1.52
1	B	207	ALA	N-CA	5.45	1.52	1.46
1	B	295	ASP	C-O	-5.45	1.17	1.24
1	A	441	THR	N-CA	-5.44	1.39	1.46
1	A	593	ILE	N-CA	-5.43	1.40	1.46
1	B	316	PRO	N-CA	5.43	1.54	1.47
1	A	486	GLY	N-CA	5.42	1.51	1.45
1	B	18	LEU	N-CA	5.41	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	89	ILE	CA-C	-5.41	1.46	1.52
1	B	348	VAL	C-O	5.40	1.29	1.24
1	B	213	LYS	CA-C	5.40	1.59	1.52
1	A	304	ASP	C-O	5.39	1.30	1.24
1	B	34	VAL	N-CA	5.38	1.53	1.46
1	B	202	SER	N-CA	-5.37	1.40	1.46
1	B	213	LYS	C-O	5.37	1.30	1.23
1	A	122	HIS	CA-C	-5.36	1.45	1.52
1	B	212	GLU	CA-C	5.36	1.59	1.53
1	B	448	ARG	C-O	5.36	1.30	1.23
1	B	508	VAL	CA-CB	5.35	1.61	1.54
1	A	536	ARG	CG-CD	5.35	1.68	1.52
1	A	239	HIS	CA-C	5.34	1.59	1.52
1	B	37	THR	CA-C	-5.34	1.46	1.52
1	B	555	TYR	N-CA	5.34	1.53	1.46
1	A	262	SER	C-O	5.33	1.30	1.24
1	A	177	LEU	N-CA	5.32	1.53	1.46
1	A	89	ILE	CA-C	-5.32	1.46	1.52
1	B	95	ILE	C-O	-5.31	1.18	1.24
1	B	122	HIS	C-O	-5.31	1.17	1.24
1	A	49	LEU	N-CA	5.30	1.52	1.46
1	B	165	GLY	N-CA	5.29	1.51	1.45
1	B	250	LYS	CB-CG	5.29	1.68	1.52
1	B	14	ASN	CG-ND2	5.28	1.44	1.33
1	B	393	PRO	CB-CG	5.27	1.75	1.49
1	B	12	ASP	CA-C	-5.26	1.45	1.52
1	B	242	VAL	N-CA	5.25	1.51	1.46
1	A	233	ALA	CA-C	-5.24	1.45	1.52
1	B	189	MSE	CA-CB	-5.24	1.45	1.53
1	A	444	SER	CA-C	-5.24	1.46	1.52
1	B	133	VAL	CB-CG2	-5.23	1.35	1.52
1	B	185	ILE	N-CA	-5.23	1.40	1.46
1	B	172	ILE	CG1-CD1	5.22	1.72	1.51
1	B	297	LEU	CA-C	-5.22	1.47	1.53
1	A	517	ILE	CA-CB	5.22	1.61	1.54
1	B	374	MSE	CA-C	-5.22	1.46	1.52
1	A	259	LEU	CA-C	-5.21	1.46	1.52
1	B	404	SER	CA-C	5.20	1.58	1.52
1	A	488	ASN	N-CA	5.20	1.52	1.46
1	A	146	ARG	CA-C	5.19	1.59	1.52
1	B	65	HIS	CA-C	-5.18	1.46	1.52
1	A	146	ARG	N-CA	-5.18	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	285	THR	C-O	-5.17	1.16	1.23
1	B	352	ASP	N-CA	5.16	1.53	1.46
1	A	65	HIS	C-O	-5.16	1.17	1.23
1	A	496	ALA	CA-CB	-5.15	1.45	1.53
1	B	570	ILE	CG1-CD1	5.15	1.71	1.51
1	A	326	ASN	N-CA	-5.15	1.40	1.46
1	B	74	ALA	N-CA	5.14	1.52	1.46
1	B	296	LEU	C-O	-5.14	1.18	1.24
1	B	396	MSE	CA-C	-5.14	1.46	1.52
1	B	89	ILE	C-O	-5.14	1.17	1.23
1	B	340	ALA	CA-C	5.13	1.58	1.52
1	A	333	ARG	C-N	-5.13	1.25	1.33
1	A	236	SER	C-O	5.11	1.30	1.24
1	B	9	GLU	C-O	5.10	1.30	1.24
1	A	318	TRP	C-O	-5.09	1.18	1.24
1	A	358	ALA	N-CA	5.09	1.53	1.46
1	A	256	THR	C-O	5.08	1.30	1.23
1	A	220	ARG	CZ-NH2	5.08	1.40	1.33
1	B	422	TRP	N-CA	5.08	1.52	1.45
1	A	56	ILE	CA-CB	5.07	1.62	1.54
1	B	14	ASN	CG-OD1	5.07	1.33	1.23
1	B	145	LEU	CG-CD1	5.07	1.69	1.52
1	B	218	HIS	CA-CB	5.07	1.61	1.53
1	A	309	LEU	C-O	5.05	1.30	1.24
1	B	317	GLU	C-O	-5.05	1.18	1.24
1	B	147	ALA	C-N	-5.05	1.27	1.33
1	B	57	VAL	CA-CB	-5.04	1.47	1.54
1	A	261	GLY	C-O	5.03	1.30	1.23
1	A	406	GLY	N-CA	5.03	1.52	1.45
1	B	387	LYS	N-CA	5.03	1.52	1.45
1	B	344	ARG	C-O	-5.03	1.17	1.24
1	A	302	LEU	N-CA	-5.02	1.40	1.46
1	B	476	SER	CA-C	5.01	1.58	1.52
1	B	173	LEU	N-CA	5.01	1.52	1.46

All (351) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	571	GLY	CA-C-N	17.81	142.10	119.84
1	B	571	GLY	C-N-CA	17.81	142.10	119.84
1	B	436	PRO	CA-C-N	11.27	133.93	119.84
1	B	436	PRO	C-N-CA	11.27	133.93	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	192	ARG	N-CA-C	-10.53	99.88	111.36
1	B	85	SER	CA-C-N	-10.37	109.38	119.85
1	B	85	SER	C-N-CA	-10.37	109.38	119.85
1	A	143	LEU	CA-C-N	-10.33	106.92	119.84
1	A	143	LEU	C-N-CA	-10.33	106.92	119.84
1	A	210	ALA	N-CA-C	-9.98	100.24	111.82
1	A	61	ILE	N-CA-C	-9.94	93.48	107.99
1	B	318	TRP	N-CA-C	-9.69	100.41	110.97
1	A	29	ASP	N-CA-C	-9.67	102.72	112.97
1	B	148	ILE	N-CA-C	-9.61	93.72	107.75
1	B	101	THR	N-CA-C	-9.52	97.15	110.29
1	A	594	GLU	N-CA-C	9.36	123.29	109.07
1	B	586	LYS	N-CA-C	9.35	123.89	110.14
1	B	307	ARG	N-CA-C	-9.30	100.06	111.40
1	B	486	GLY	N-CA-C	9.17	124.57	110.91
1	B	300	GLY	N-CA-C	-9.05	97.03	112.06
1	B	443	ILE	CB-CA-C	-8.95	97.39	110.63
1	B	404	SER	N-CA-C	8.80	122.45	107.93
1	B	93	MSE	N-CA-C	8.78	120.23	108.38
1	B	378	ILE	CA-C-N	-8.56	111.20	119.76
1	B	378	ILE	C-N-CA	-8.56	111.20	119.76
1	B	364	SER	CA-C-N	-8.42	102.41	121.19
1	B	364	SER	C-N-CA	-8.42	102.41	121.19
1	B	532	GLU	CB-CA-C	-8.42	97.53	110.92
1	B	403	LYS	N-CA-C	8.30	121.64	110.35
1	A	133	VAL	N-CA-C	-8.28	102.81	111.58
1	B	494	LEU	N-CA-C	-8.27	102.97	113.23
1	A	231	MSE	N-CA-C	8.24	119.89	111.07
1	B	504	GLY	N-CA-C	-8.20	103.80	112.08
1	B	161	LEU	N-CA-C	8.13	121.06	111.71
1	A	282	GLN	CA-C-N	-8.11	109.19	122.65
1	A	282	GLN	C-N-CA	-8.11	109.19	122.65
1	B	34	VAL	CB-CA-C	-8.09	99.35	111.80
1	A	349	VAL	CB-CA-C	-8.00	99.97	110.84
1	B	98	SER	N-CA-C	7.99	122.12	112.38
1	B	363	ALA	N-CA-C	-7.98	95.91	109.24
1	A	349	VAL	N-CA-C	7.94	119.72	108.36
1	A	50	ARG	NE-CZ-NH2	7.93	126.34	119.20
1	A	317	GLU	N-CA-C	-7.88	102.63	111.14
1	B	18	LEU	N-CA-C	7.81	119.79	111.28
1	B	590	SER	N-CA-C	-7.79	95.61	108.23
1	B	50	ARG	CA-C-N	-7.69	112.07	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	50	ARG	C-N-CA	-7.69	112.07	119.76
1	A	77	ILE	CA-C-N	-7.63	111.43	122.19
1	A	77	ILE	C-N-CA	-7.63	111.43	122.19
1	A	295	ASP	N-CA-C	7.61	120.25	111.11
1	A	155	VAL	N-CA-C	7.59	116.38	107.73
1	B	392	LEU	CA-C-N	7.58	128.17	119.99
1	B	392	LEU	C-N-CA	7.58	128.17	119.99
1	A	33	ASP	N-CA-C	-7.57	104.19	113.50
1	B	353	LEU	N-CA-C	-7.57	102.57	112.41
1	A	45	VAL	N-CA-C	7.55	117.63	110.53
1	B	163	ARG	N-CA-C	7.55	120.86	107.80
1	A	334	SER	N-CA-C	-7.54	103.81	113.16
1	A	364	SER	N-CA-C	-7.53	104.04	113.23
1	B	430	LYS	N-CA-C	-7.47	99.76	110.59
1	A	540	ASP	N-CA-C	7.45	119.41	111.28
1	B	104	ALA	N-CA-C	-7.44	103.25	111.36
1	B	147	ALA	CA-C-N	-7.43	113.21	123.10
1	B	147	ALA	C-N-CA	-7.43	113.21	123.10
1	B	194	VAL	N-CA-C	-7.41	105.19	111.56
1	B	111	ALA	N-CA-C	-7.26	104.57	113.50
1	A	367	ALA	CA-C-N	-7.25	113.22	121.85
1	A	367	ALA	C-N-CA	-7.25	113.22	121.85
1	B	145	LEU	N-CA-C	-7.24	97.88	109.76
1	A	93	MSE	N-CA-C	7.23	118.08	107.88
1	A	195	ILE	N-CA-C	7.23	117.36	110.42
1	A	179	TRP	CA-C-N	7.22	127.06	119.05
1	A	179	TRP	C-N-CA	7.22	127.06	119.05
1	B	270	PHE	CA-C-N	-7.09	111.45	120.60
1	B	270	PHE	C-N-CA	-7.09	111.45	120.60
1	A	305	VAL	N-CA-C	-7.09	103.87	110.53
1	B	338	LEU	CA-C-N	-7.09	114.99	121.65
1	B	338	LEU	C-N-CA	-7.09	114.99	121.65
1	B	260	ARG	N-CA-C	7.07	121.37	110.20
1	B	42	VAL	N-CA-CB	7.05	119.98	111.31
1	B	442	MSE	CG-SE-CE	7.04	114.41	98.92
1	B	248	MSE	N-CA-C	-7.03	103.67	111.82
1	B	294	ASP	N-CA-C	-6.93	103.16	111.69
1	A	498	ALA	CA-C-N	-6.89	114.22	122.35
1	A	498	ALA	C-N-CA	-6.89	114.22	122.35
1	B	272	ALA	CA-C-N	-6.86	110.56	120.29
1	B	272	ALA	C-N-CA	-6.86	110.56	120.29
1	A	229	ALA	N-CA-C	6.84	118.39	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	23	VAL	CB-CA-C	-6.83	103.09	112.04
1	A	86	PRO	N-CA-C	-6.83	100.52	111.38
1	B	31	ARG	N-CA-C	-6.81	101.35	110.55
1	B	326	ASN	N-CA-C	6.81	119.28	111.11
1	B	442	MSE	CB-CG-SE	-6.81	92.27	112.70
1	A	321	ARG	N-CA-C	-6.80	103.87	111.28
1	B	89	ILE	CB-CA-C	-6.76	101.38	111.80
1	A	262	SER	CA-C-N	-6.76	113.45	122.85
1	A	262	SER	C-N-CA	-6.76	113.45	122.85
1	B	173	LEU	CA-CB-CG	-6.75	92.69	116.30
1	A	23	VAL	N-CA-C	6.71	118.27	110.62
1	B	78	ASP	N-CA-C	6.69	120.56	109.46
1	B	196	GLU	N-CA-C	6.58	121.33	113.16
1	A	492	MSE	CG-SE-CE	6.57	113.39	98.92
1	B	416	ARG	CA-C-N	6.57	128.06	119.84
1	B	416	ARG	C-N-CA	6.57	128.06	119.84
1	B	584	THR	N-CA-C	-6.57	105.80	113.88
1	B	117	ILE	CB-CA-C	-6.56	101.81	111.19
1	B	241	LEU	CA-C-N	-6.56	114.86	122.14
1	B	241	LEU	C-N-CA	-6.56	114.86	122.14
1	B	234	GLY	N-CA-C	6.55	125.90	114.76
1	A	571	GLY	CA-C-N	-6.53	113.05	119.78
1	A	571	GLY	C-N-CA	-6.53	113.05	119.78
1	A	50	ARG	NE-CZ-NH1	-6.52	114.98	121.50
1	B	584	THR	CB-CA-C	6.51	119.58	109.03
1	B	537	ALA	N-CA-C	-6.50	104.23	111.71
1	B	235	VAL	N-CA-CB	-6.45	103.69	110.72
1	A	114	VAL	CB-CA-C	-6.45	104.97	111.80
1	A	475	VAL	CB-CA-C	-6.45	102.15	110.98
1	A	292	PHE	CA-C-N	6.44	125.94	119.24
1	A	292	PHE	C-N-CA	6.44	125.94	119.24
1	B	17	THR	CB-CA-C	6.42	120.96	110.88
1	B	335	ASP	N-CA-C	-6.42	105.49	113.38
1	A	26	ALA	N-CA-C	-6.41	103.81	111.69
1	B	128	HIS	N-CA-CB	-6.39	100.88	111.49
1	A	493	ALA	N-CA-C	6.35	118.00	111.14
1	A	24	ALA	N-CA-C	-6.34	103.90	111.69
1	A	241	LEU	CB-CG-CD1	-6.32	91.75	110.70
1	A	242	VAL	CB-CA-C	6.31	117.75	110.88
1	A	553	PRO	N-CA-C	6.30	118.39	110.70
1	B	290	ASP	O-C-N	6.28	130.56	123.27
1	A	186	ALA	N-CA-C	6.26	118.11	110.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	249	ALA	N-CA-C	-6.26	104.46	111.28
1	A	113	GLY	N-CA-C	-6.25	106.42	114.85
1	A	123	GLU	N-CA-C	-6.25	103.78	111.40
1	A	498	ALA	N-CA-C	-6.24	104.76	112.38
1	A	567	ALA	N-CA-C	6.23	119.73	111.75
1	B	402	VAL	CB-CA-C	-6.23	102.45	110.98
1	B	89	ILE	CA-C-O	-6.21	115.12	120.96
1	B	367	ALA	N-CA-C	-6.21	100.47	109.59
1	B	218	HIS	N-CA-C	-6.20	96.98	108.02
1	A	145	LEU	N-CA-C	-6.20	99.09	109.07
1	B	135	TRP	N-CA-C	6.19	121.53	111.37
1	A	541	LEU	N-CA-C	-6.16	104.47	112.23
1	B	548	VAL	CA-C-O	6.15	124.46	119.29
1	B	311	ARG	N-CA-C	-6.14	104.64	111.71
1	A	21	ARG	NE-CZ-NH2	-6.14	113.67	119.20
1	A	314	LEU	O-C-N	-6.14	115.34	122.95
1	B	587	VAL	CB-CA-C	-6.14	103.42	110.41
1	A	501	GLY	CA-C-N	-6.12	112.03	122.56
1	A	501	GLY	C-N-CA	-6.12	112.03	122.56
1	A	403	LYS	CB-CA-C	-6.12	102.28	109.80
1	B	182	ILE	CB-CA-C	-6.11	103.34	110.91
1	B	452	ALA	N-CA-C	-6.10	99.70	108.60
1	A	575	THR	CB-CA-C	-6.08	98.25	110.30
1	B	492	MSE	N-CA-C	6.08	123.76	110.80
1	A	213	LYS	CA-C-N	-6.08	111.30	121.39
1	A	213	LYS	C-N-CA	-6.08	111.30	121.39
1	B	418	ARG	N-CA-C	6.08	123.75	110.80
1	A	228	ASN	N-CA-C	-6.08	104.66	111.28
1	B	128	HIS	N-CA-C	6.05	120.53	112.30
1	B	59	ALA	N-CA-C	-6.04	105.55	113.17
1	B	458	THR	CB-CA-C	-6.04	100.14	110.16
1	A	148	ILE	N-CA-CB	-6.00	104.22	110.95
1	A	334	SER	CA-CB-OG	-6.00	99.10	111.10
1	A	502	THR	CB-CA-C	-6.00	99.70	110.37
1	A	123	GLU	CA-C-N	-5.99	111.65	120.28
1	A	123	GLU	C-N-CA	-5.99	111.65	120.28
1	A	20	ALA	N-CA-C	-5.99	104.66	111.07
1	B	147	ALA	O-C-N	-5.99	115.45	123.23
1	B	435	VAL	CA-C-N	5.97	126.53	120.38
1	B	435	VAL	C-N-CA	5.97	126.53	120.38
1	B	123	GLU	N-CA-C	-5.95	104.42	111.03
1	A	72	ASP	N-CA-C	5.95	118.42	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	365	GLY	N-CA-C	-5.95	107.11	115.32
1	A	174	ALA	N-CA-C	-5.94	104.88	111.36
1	B	463	GLY	N-CA-C	-5.94	102.28	114.16
1	A	372	GLY	N-CA-C	-5.92	106.92	115.27
1	A	168	PHE	N-CA-C	5.91	118.15	108.52
1	B	20	ALA	CA-C-N	-5.91	112.37	120.28
1	B	20	ALA	C-N-CA	-5.91	112.37	120.28
1	B	440	ALA	N-CA-C	5.89	119.08	108.48
1	B	301	GLY	CA-C-O	-5.89	118.39	122.22
1	A	298	GLN	N-CA-CB	5.85	118.91	110.20
1	A	44	VAL	N-CA-C	5.85	120.31	111.89
1	B	580	ALA	N-CA-C	5.84	116.98	107.23
1	A	467	TRP	N-CA-C	5.83	118.24	107.99
1	B	387	LYS	N-CA-C	5.80	119.07	110.48
1	B	364	SER	CA-CB-OG	-5.80	99.50	111.10
1	A	272	ALA	CA-C-O	-5.80	114.73	120.82
1	B	482	LEU	N-CA-C	-5.79	99.76	108.96
1	B	532	GLU	N-CA-C	5.78	118.07	111.02
1	B	236	SER	CA-CB-OG	-5.77	99.55	111.10
1	B	573	HIS	N-CA-C	5.75	119.19	109.76
1	A	300	GLY	N-CA-C	5.75	119.13	110.97
1	A	123	GLU	N-CA-CB	5.74	118.62	110.13
1	B	141	GLU	CA-C-N	-5.74	113.48	122.49
1	B	141	GLU	C-N-CA	-5.74	113.48	122.49
1	A	89	ILE	CB-CA-C	5.72	119.15	110.62
1	A	231	MSE	CA-C-N	5.72	128.22	120.38
1	A	231	MSE	C-N-CA	5.72	128.22	120.38
1	A	203	GLY	N-CA-C	-5.71	99.64	113.18
1	B	372	GLY	N-CA-C	-5.71	107.50	114.92
1	A	470	ALA	N-CA-C	5.70	117.74	109.07
1	A	405	GLN	N-CA-C	5.70	120.61	113.43
1	B	447	HIS	CA-C-O	-5.67	114.91	121.15
1	B	71	ARG	N-CA-C	-5.67	106.24	114.12
1	B	112	ARG	N-CA-C	5.67	120.19	113.16
1	A	378	ILE	N-CA-C	5.67	113.16	107.55
1	B	308	ARG	N-CA-C	5.66	117.45	111.28
1	B	384	THR	N-CA-CB	5.63	118.50	110.16
1	A	581	ASP	N-CA-C	-5.63	99.24	108.41
1	A	141	GLU	CA-C-N	-5.62	113.75	123.25
1	A	141	GLU	C-N-CA	-5.62	113.75	123.25
1	B	117	ILE	CB-CG1-CD1	-5.62	102.00	113.80
1	B	539	GLU	N-CA-CB	5.62	118.49	110.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	73	ALA	N-CA-C	5.62	122.77	110.80
1	B	242	VAL	N-CA-C	-5.61	107.80	113.47
1	B	139	ALA	N-CA-C	5.61	118.59	111.69
1	B	332	GLY	CA-C-N	-5.61	114.84	123.14
1	B	332	GLY	C-N-CA	-5.61	114.84	123.14
1	B	257	ILE	N-CA-C	5.60	116.37	108.36
1	A	435	VAL	CA-C-N	-5.58	114.63	120.38
1	A	435	VAL	C-N-CA	-5.58	114.63	120.38
1	A	126	ASN	CA-C-N	-5.58	113.42	120.56
1	A	126	ASN	C-N-CA	-5.58	113.42	120.56
1	B	422	TRP	N-CA-C	5.57	117.87	109.23
1	B	358	ALA	N-CA-C	5.57	118.72	108.58
1	A	540	ASP	CB-CA-C	5.56	120.02	110.79
1	A	238	ASP	N-CA-C	5.54	117.81	109.23
1	B	202	SER	CA-C-O	-5.53	114.98	120.90
1	B	137	ALA	N-CA-C	5.53	116.99	111.07
1	A	584	THR	N-CA-CB	5.53	118.73	110.22
1	A	344	ARG	N-CA-C	5.53	118.29	110.50
1	B	34	VAL	CA-C-O	-5.52	115.77	120.96
1	A	396	MSE	N-CA-CB	-5.52	101.80	110.69
1	A	509	ALA	N-CA-C	5.52	117.96	109.07
1	A	255	LEU	CB-CA-C	-5.50	100.88	109.84
1	A	508	VAL	CB-CA-C	-5.49	102.65	110.83
1	A	554	PRO	N-CA-C	-5.49	97.83	112.10
1	B	91	THR	CB-CA-C	-5.48	100.61	110.37
1	B	29	ASP	N-CA-C	5.47	119.81	113.18
1	B	61	ILE	CB-CG1-CD1	5.47	125.30	113.80
1	B	305	VAL	CB-CA-C	-5.47	104.81	111.87
1	A	34	VAL	N-CA-C	5.47	116.24	108.42
1	A	118	VAL	N-CA-C	-5.47	98.58	107.28
1	A	140	ILE	CB-CA-C	-5.46	102.20	111.37
1	A	84	VAL	N-CA-C	5.43	115.67	107.80
1	A	86	PRO	CA-C-O	-5.43	115.05	121.67
1	B	484	VAL	CA-C-O	-5.42	114.79	120.27
1	A	218	HIS	N-CA-CB	-5.42	102.26	110.77
1	B	291	VAL	CA-C-N	5.42	128.89	120.60
1	B	291	VAL	C-N-CA	5.42	128.89	120.60
1	A	302	LEU	CA-CB-CG	-5.41	97.35	116.30
1	B	486	GLY	CA-C-N	5.41	126.91	120.14
1	B	486	GLY	C-N-CA	5.41	126.91	120.14
1	B	211	ALA	CA-C-N	-5.40	114.57	122.19
1	B	211	ALA	C-N-CA	-5.40	114.57	122.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	186	ALA	CA-C-N	5.40	131.85	121.54
1	B	186	ALA	C-N-CA	5.40	131.85	121.54
1	B	198	ASP	CA-C-O	5.40	124.83	119.75
1	A	463	GLY	N-CA-C	-5.40	107.59	115.63
1	A	80	GLY	N-CA-C	-5.39	105.19	112.14
1	A	164	GLY	N-CA-C	-5.38	100.42	113.18
1	A	98	SER	CA-CB-OG	-5.38	100.33	111.10
1	B	269	GLU	N-CA-C	5.38	116.95	111.14
1	B	145	LEU	CB-CA-C	5.38	118.52	109.48
1	A	205	VAL	CA-C-N	-5.38	113.02	120.38
1	A	205	VAL	C-N-CA	-5.38	113.02	120.38
1	B	205	VAL	CB-CA-C	-5.38	105.00	111.88
1	A	128	HIS	N-CA-C	5.37	120.70	113.72
1	A	89	ILE	CA-C-N	-5.37	115.49	123.11
1	A	89	ILE	C-N-CA	-5.37	115.49	123.11
1	B	475	VAL	N-CA-C	-5.37	99.43	107.37
1	B	186	ALA	N-CA-C	5.36	117.46	110.43
1	A	83	TYR	N-CA-C	5.36	118.22	109.59
1	B	84	VAL	CB-CA-C	-5.36	102.84	110.83
1	A	220	ARG	NE-CZ-NH2	5.35	124.02	119.20
1	A	83	TYR	CA-C-N	-5.35	116.17	123.12
1	A	83	TYR	C-N-CA	-5.35	116.17	123.12
1	A	135	TRP	N-CA-C	5.35	116.79	111.07
1	A	532	GLU	N-CA-C	-5.34	104.70	111.11
1	A	529	ALA	CA-C-N	-5.33	113.17	119.84
1	A	529	ALA	C-N-CA	-5.33	113.17	119.84
1	A	565	THR	CA-C-N	5.32	129.46	122.06
1	A	565	THR	C-N-CA	5.32	129.46	122.06
1	A	217	GLY	N-CA-C	5.32	121.48	113.02
1	A	520	LEU	CA-C-N	5.32	125.13	119.28
1	A	520	LEU	C-N-CA	5.32	125.13	119.28
1	B	313	GLY	N-CA-C	5.31	125.77	113.18
1	A	49	LEU	CA-CB-CG	-5.31	97.72	116.30
1	A	304	ASP	N-CA-C	5.31	117.06	111.28
1	B	574	GLN	N-CA-C	-5.31	103.52	110.53
1	B	151	ALA	N-CA-C	5.25	121.40	109.81
1	A	178	SER	CA-C-N	-5.24	113.05	120.49
1	A	178	SER	C-N-CA	-5.24	113.05	120.49
1	A	531	LEU	N-CA-C	-5.23	106.05	112.90
1	B	572	PRO	N-CA-C	5.22	123.22	112.47
1	B	71	ARG	CA-C-O	-5.21	113.17	118.90
1	B	544	ALA	N-CA-C	-5.20	105.29	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	484	VAL	CB-CA-C	-5.20	103.40	110.42
1	A	531	LEU	CA-C-N	5.19	127.55	120.54
1	A	531	LEU	C-N-CA	5.19	127.55	120.54
1	B	305	VAL	N-CA-C	-5.19	105.54	110.42
1	A	414	ILE	N-CA-CB	5.19	119.79	111.23
1	A	453	GLU	N-CA-C	5.19	117.13	109.50
1	A	402	VAL	O-C-N	5.19	126.32	121.96
1	B	311	ARG	NE-CZ-NH2	-5.19	114.53	119.20
1	B	325	LEU	CA-C-N	-5.18	113.54	120.54
1	B	325	LEU	C-N-CA	-5.18	113.54	120.54
1	B	413	THR	CB-CA-C	5.18	120.50	109.10
1	B	95	ILE	CB-CA-C	-5.17	105.27	112.04
1	B	575	THR	CB-CA-C	-5.16	101.63	112.82
1	B	90	ASP	N-CA-C	-5.15	98.85	108.02
1	A	372	GLY	CA-C-N	-5.15	115.22	122.94
1	A	372	GLY	C-N-CA	-5.15	115.22	122.94
1	A	226	ASP	N-CA-C	-5.14	105.57	111.07
1	A	231	MSE	CA-CB-CG	-5.14	103.81	114.10
1	B	374	MSE	CB-CA-C	-5.14	100.86	109.65
1	A	403	LYS	CA-CB-CG	5.14	124.37	114.10
1	B	224	ASN	CA-C-N	5.13	127.41	120.38
1	B	224	ASN	C-N-CA	5.13	127.41	120.38
1	A	358	ALA	N-CA-C	5.13	117.05	108.23
1	B	460	PHE	N-CA-C	5.12	121.70	110.80
1	B	548	VAL	CA-C-N	-5.12	116.16	123.17
1	B	548	VAL	C-N-CA	-5.12	116.16	123.17
1	B	126	ASN	CA-C-N	-5.12	112.36	120.55
1	B	126	ASN	C-N-CA	-5.12	112.36	120.55
1	B	169	ASP	N-CA-CB	5.12	118.32	110.70
1	B	450	GLY	N-CA-C	5.09	125.24	113.18
1	A	175	ASP	N-CA-C	5.09	116.51	110.97
1	B	296	LEU	CA-C-N	5.08	128.51	120.89
1	B	296	LEU	C-N-CA	5.08	128.51	120.89
1	A	474	THR	N-CA-C	-5.07	106.34	112.88
1	A	56	ILE	N-CA-C	-5.07	100.91	108.46
1	B	257	ILE	CB-CA-C	-5.07	103.95	110.84
1	B	215	VAL	N-CA-CB	-5.06	102.88	111.23
1	B	84	VAL	N-CA-C	5.06	115.25	108.17
1	B	165	GLY	N-CA-C	-5.05	106.83	115.61
1	A	429	VAL	N-CA-C	5.04	116.42	109.46
1	A	185	ILE	CB-CA-C	-5.04	103.88	110.98
1	A	253	ALA	N-CA-C	-5.04	107.13	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	448	ARG	N-CA-C	5.03	119.51	113.17
1	A	457	LYS	CA-C-N	-5.03	115.89	122.99
1	A	457	LYS	C-N-CA	-5.03	115.89	122.99
1	A	474	THR	CB-CA-C	-5.03	102.22	110.72
1	B	536	ARG	NE-CZ-NH2	-5.03	114.67	119.20
1	B	250	LYS	CG-CD-CE	5.03	122.87	111.30
1	A	484	VAL	N-CA-C	5.02	115.14	108.11
1	B	476	SER	N-CA-C	-5.01	99.67	107.93
1	B	382	ASP	CB-CA-C	5.01	118.00	109.84
1	A	374	MSE	N-CA-C	5.00	117.49	110.23
1	A	351	GLU	N-CA-C	-5.00	105.11	111.11

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	217	GLY	Peptide
1	A	396	MSE	Peptide
1	A	402	VAL	Peptide
1	A	451	MSE	Peptide
1	A	48	GLU	Peptide
1	B	160	GLY	Peptide
1	B	299	GLY	Peptide
1	B	365	GLY	Peptide
1	B	397	ALA	Peptide
1	B	413	THR	Peptide
1	B	426	GLU	Peptide
1	B	465	GLY	Peptide
1	B	489	ALA	Peptide
1	B	579	ILE	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	4337	0	4344	212	0
1	B	4277	0	4273	303	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	23	0	0	4	0
3	B	31	0	0	4	0
All	All	8674	0	8617	503	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 29.

All (503) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:393:PRO:CG	1:B:393:PRO:CB	1.76	1.45
1:A:231:MSE:SE	1:A:231:MSE:CE	2.15	1.44
1:A:201:MSE:SE	1:A:201:MSE:CG	2.16	1.42
1:B:248:MSE:SE	1:B:248:MSE:CE	2.17	1.42
1:B:588:MSE:SE	1:B:588:MSE:CE	2.18	1.42
1:A:442:MSE:SE	1:A:442:MSE:CE	2.18	1.41
1:B:231:MSE:SE	1:B:231:MSE:CE	2.19	1.40
1:B:577:MSE:CE	1:B:577:MSE:SE	2.23	1.37
1:A:588:MSE:SE	1:A:588:MSE:CE	2.24	1.35
1:A:99:MSE:SE	1:A:99:MSE:CE	2.27	1.33
1:A:396:MSE:SE	1:A:396:MSE:CE	2.27	1.33
1:B:201:MSE:SE	1:B:201:MSE:CE	2.28	1.32
1:A:248:MSE:SE	1:A:248:MSE:CE	2.29	1.31
1:A:577:MSE:SE	1:A:577:MSE:CE	2.29	1.30
1:B:451:MSE:CE	1:B:451:MSE:SE	2.31	1.27
1:B:442:MSE:SE	1:B:442:MSE:CE	2.32	1.26
1:B:396:MSE:SE	1:B:396:MSE:CE	2.39	1.19
1:A:588:MSE:HE2	1:A:590:SER:O	1.45	1.17
1:B:421:GLN:HG3	1:B:422:TRP:H	1.16	1.10
1:B:420:THR:HB	1:B:572:PRO:HD2	1.27	1.10
1:A:189:MSE:SE	1:A:189:MSE:CE	2.51	1.08
1:A:451:MSE:SE	1:A:451:MSE:CE	2.54	1.05
1:B:415:ASP:HB2	1:B:421:GLN:HG2	1.40	1.00
1:B:79:ALA:O	1:B:82:ALA:HB3	1.62	1.00
1:A:588:MSE:CE	1:A:590:SER:O	2.09	1.00
1:B:415:ASP:HB3	1:B:416:ARG:HG2	1.43	1.00
1:B:72:ASP:O	1:B:73:ALA:HB3	1.63	0.98
1:B:179:TRP:HB3	1:B:181:GLU:OE1	1.67	0.94
1:B:311:ARG:HG2	1:B:311:ARG:HH11	1.32	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:421:GLN:HG3	1:B:422:TRP:N	1.84	0.92
1:A:447:HIS:HE1	1:A:451:MSE:H	1.11	0.91
1:A:416:ARG:HG3	1:A:416:ARG:HH11	1.34	0.91
1:B:161:LEU:HD12	1:B:587:VAL:CG2	2.01	0.91
1:B:161:LEU:CD1	1:B:587:VAL:HG23	2.02	0.90
1:B:177:LEU:HD21	1:B:185:ILE:HG12	1.53	0.89
1:B:351:GLU:OE1	1:B:359:ARG:HB2	1.73	0.89
1:B:311:ARG:HD3	3:B:639:HOH:O	1.73	0.87
1:B:397:ALA:HB1	1:B:489:ALA:HB1	1.54	0.86
1:B:192:ARG:HD3	1:B:196:GLU:OE2	1.75	0.86
1:B:161:LEU:HD12	1:B:587:VAL:HG23	1.59	0.84
1:B:556:LEU:HD23	1:B:556:LEU:C	2.02	0.84
1:B:584:THR:HG23	1:B:586:LYS:H	1.43	0.84
1:B:63:SER:OG	1:B:65:HIS:HD2	1.60	0.84
1:B:395:ARG:HD2	1:B:395:ARG:N	1.94	0.82
1:B:71:ARG:O	1:B:72:ASP:O	2.00	0.79
1:A:99:MSE:HE2	1:A:506:MSE:HE1	1.63	0.79
1:A:64:VAL:H	1:B:228:ASN:ND2	1.79	0.79
1:B:415:ASP:CB	1:B:421:GLN:HG2	2.12	0.79
1:A:374:MSE:HE2	1:A:378:ILE:HD11	1.65	0.79
1:A:64:VAL:H	1:B:228:ASN:HD21	1.27	0.79
1:B:189:MSE:HG3	1:B:568:CYS:SG	2.23	0.78
1:A:338:LEU:HD23	1:A:343:ARG:CZ	2.14	0.78
1:B:300:GLY:HA2	3:B:622:HOH:O	1.84	0.78
1:B:397:ALA:HB1	1:B:489:ALA:CB	2.15	0.77
1:B:447:HIS:HD2	1:B:576:ASP:OD1	1.68	0.77
1:B:173:LEU:HD13	1:B:204:ILE:HG12	1.68	0.75
1:B:311:ARG:HG2	1:B:311:ARG:NH1	2.03	0.74
1:B:346:ASP:C	1:B:347:ILE:HG12	2.13	0.73
1:B:18:LEU:HD12	1:B:18:LEU:O	1.88	0.73
1:B:447:HIS:CD2	1:B:576:ASP:OD1	2.41	0.73
1:B:72:ASP:O	1:B:73:ALA:CB	2.24	0.72
1:B:551:TRP:O	1:B:553:PRO:HD3	1.89	0.72
1:A:19:ARG:O	1:A:23:VAL:HG23	1.89	0.72
1:B:173:LEU:CD1	1:B:204:ILE:HG12	2.19	0.72
1:A:53:ASP:C	1:A:54:ILE:HD13	2.15	0.72
1:A:231:MSE:HE1	1:A:253:ALA:O	1.90	0.72
1:A:308:ARG:HG2	1:A:311:ARG:NH2	2.05	0.71
1:B:550:GLU:HA	1:B:550:GLU:OE1	1.88	0.71
1:A:370:GLU:HB3	1:A:375:LEU:HD21	1.72	0.71
1:A:373:ARG:HH11	1:A:373:ARG:HB2	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:ALA:O	1:B:74:ALA:CB	2.36	0.70
1:A:392:LEU:HD21	1:A:500:ILE:HG12	1.72	0.70
1:A:286:LEU:HD12	1:A:323:ALA:HB2	1.74	0.70
1:B:295:ASP:O	1:B:300:GLY:HA3	1.92	0.70
1:B:415:ASP:HB3	1:B:416:ARG:CG	2.20	0.70
1:A:34:VAL:HG12	1:A:35:LEU:N	2.05	0.69
1:A:425:THR:OG1	1:A:426:GLU:O	2.09	0.69
1:A:475:VAL:HG21	1:A:506:MSE:CE	2.23	0.69
1:A:395:ARG:NH2	1:A:454:PRO:O	2.25	0.69
1:A:99:MSE:CE	1:A:506:MSE:HE1	2.23	0.69
1:B:421:GLN:CG	1:B:422:TRP:N	2.54	0.69
1:A:447:HIS:CE1	1:A:451:MSE:H	2.03	0.68
1:B:120:ASP:C	1:B:120:ASP:OD1	2.35	0.68
1:B:402:VAL:HG12	1:B:402:VAL:O	1.93	0.67
1:B:92:HIS:CE1	1:B:239:HIS:CE1	2.82	0.67
1:A:416:ARG:HH11	1:A:416:ARG:CG	2.07	0.67
1:A:496:ALA:O	1:A:499:VAL:HG22	1.94	0.67
1:B:42:VAL:HG22	1:B:42:VAL:O	1.95	0.67
1:B:489:ALA:O	1:B:492:MSE:HB2	1.95	0.67
1:A:592:VAL:HG23	1:A:592:VAL:O	1.95	0.66
1:B:163:ARG:HB2	1:B:447:HIS:CD2	2.30	0.66
1:B:556:LEU:C	1:B:556:LEU:CD2	2.68	0.66
1:B:594:GLU:HA	1:B:594:GLU:OE1	1.94	0.66
1:A:488:ASN:HD21	1:A:491:ASP:CG	2.04	0.66
1:A:429:VAL:HG12	1:A:430:LYS:H	1.60	0.66
1:A:447:HIS:HE1	1:A:451:MSE:N	1.90	0.66
1:B:161:LEU:CD1	1:B:587:VAL:CG2	2.69	0.66
1:B:457:LYS:HB3	1:B:574:GLN:HE21	1.60	0.65
1:B:397:ALA:CB	1:B:489:ALA:HB1	2.26	0.65
1:B:505:GLY:HA2	1:B:520:LEU:HD12	1.77	0.65
1:A:220:ARG:NH2	1:A:418:ARG:HH21	1.95	0.65
1:B:192:ARG:HA	1:B:192:ARG:NE	2.12	0.65
1:A:475:VAL:CG2	1:A:506:MSE:HE2	2.25	0.65
1:B:294:ASP:HA	1:B:535:ALA:HB1	1.78	0.65
1:B:374:MSE:HE2	1:B:378:ILE:HD11	1.77	0.65
1:B:493:ALA:O	1:B:497:ASN:ND2	2.31	0.64
1:B:425:THR:OG1	1:B:426:GLU:N	2.28	0.64
1:A:292:PHE:HB3	1:A:293:PRO:HD2	1.80	0.64
1:A:403:LYS:HA	1:A:432:GLY:O	1.98	0.64
1:B:73:ALA:O	1:B:74:ALA:HB2	1.98	0.64
1:B:259:LEU:HD11	1:B:270:PHE:CD2	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:HIS:CE1	1:B:239:HIS:HE1	2.15	0.63
1:B:161:LEU:HD12	1:B:587:VAL:HG21	1.79	0.63
1:B:446:THR:O	1:B:481:ASN:HB3	1.99	0.63
1:B:551:TRP:O	1:B:553:PRO:CD	2.46	0.63
1:A:228:ASN:HD22	1:B:341:ALA:HB2	1.63	0.63
1:A:85:SER:HB3	1:A:348:VAL:HG13	1.80	0.63
1:B:93:MSE:SE	1:B:117:ILE:HD12	2.49	0.63
1:A:100:ILE:HD12	1:A:104:ALA:CB	2.27	0.63
1:B:584:THR:HG23	1:B:586:LYS:N	2.12	0.63
1:B:418:ARG:O	1:B:418:ARG:HG2	1.98	0.63
1:A:475:VAL:HG21	1:A:506:MSE:HE2	1.80	0.62
1:B:127:VAL:HG12	1:B:128:HIS:CD2	2.34	0.62
1:A:34:VAL:CG1	1:A:35:LEU:N	2.62	0.62
1:B:122:HIS:NE2	1:B:123:GLU:OE2	2.33	0.62
1:B:402:VAL:HB	1:B:434:VAL:HG12	1.82	0.62
1:A:201:MSE:SE	1:A:201:MSE:HA	2.49	0.62
1:A:206:GLN:HE22	1:B:19:ARG:HG3	1.65	0.61
1:B:90:ASP:HA	1:B:302:LEU:HD13	1.81	0.61
1:B:161:LEU:HD11	1:B:587:VAL:HG23	1.81	0.61
1:A:97:SER:OG	1:A:290:ASP:HB3	2.00	0.61
1:A:494:LEU:HD11	1:A:512:GLY:HA2	1.83	0.61
1:B:89:ILE:HA	1:B:116:THR:O	2.00	0.61
1:B:197:ARG:HH22	1:B:206:GLN:NE2	1.99	0.61
1:B:173:LEU:HD13	1:B:204:ILE:HG23	1.83	0.61
1:B:549:VAL:HG22	1:B:550:GLU:H	1.66	0.61
1:B:474:THR:CG2	1:B:505:GLY:H	2.13	0.60
1:A:520:LEU:HD13	1:A:525:LEU:O	2.02	0.60
1:B:155:VAL:HG13	1:B:168:PHE:HB2	1.83	0.60
1:A:100:ILE:HD12	1:A:104:ALA:HB1	1.84	0.60
1:B:270:PHE:O	1:B:271:VAL:C	2.41	0.60
1:A:75:GLN:HG2	1:A:76:VAL:N	2.17	0.60
1:B:238:ASP:OD1	1:B:239:HIS:N	2.35	0.59
1:B:306:VAL:O	1:B:310:VAL:HG23	2.02	0.59
1:A:263:HIS:HB3	1:A:265:HIS:CE1	2.37	0.59
1:B:190:ASN:HB3	1:B:201:MSE:SE	2.51	0.59
1:B:53:ASP:OD2	1:B:68:ALA:N	2.34	0.59
1:B:134:ARG:CZ	1:B:179:TRP:CZ2	2.85	0.59
1:B:468:ASN:C	1:B:548:VAL:HG13	2.28	0.59
1:A:488:ASN:ND2	1:A:491:ASP:H	2.01	0.58
1:A:187:GLU:HA	1:A:216:CYS:O	2.03	0.58
1:A:575:THR:C	1:A:577:MSE:H	2.11	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:468:ASN:O	1:B:548:VAL:HG13	2.03	0.58
1:B:31:ARG:HA	1:B:72:ASP:HB3	1.86	0.58
1:B:479:SER:O	1:B:480:HIS:C	2.45	0.58
1:B:538:PHE:HE2	1:B:542:ARG:NH2	2.01	0.58
1:A:302:LEU:O	1:A:302:LEU:HG	2.00	0.58
1:A:266:LEU:O	1:A:269:GLU:HB2	2.03	0.58
1:B:461:LEU:HB3	1:B:464:TRP:CD1	2.38	0.58
1:B:154:CYS:HB2	1:B:189:MSE:HE3	1.86	0.57
1:A:57:VAL:O	1:A:57:VAL:HG12	2.01	0.57
1:A:93:MSE:HE3	1:A:105:TYR:CZ	2.39	0.57
1:A:110:VAL:O	1:A:112:ARG:N	2.38	0.57
1:B:466:ARG:O	1:B:549:VAL:HG23	2.04	0.57
1:B:149:LEU:HB3	1:B:182:ILE:HD13	1.86	0.57
1:B:417:PRO:O	1:B:419:PHE:N	2.37	0.57
1:A:308:ARG:HG2	1:A:311:ARG:HH21	1.68	0.57
1:B:476:SER:H	1:B:480:HIS:HD2	1.51	0.57
1:A:413:THR:N	1:A:423:GLY:O	2.36	0.57
1:A:448:ARG:H	1:A:481:ASN:ND2	2.01	0.57
1:B:35:LEU:HD12	1:B:73:ALA:HB2	1.87	0.57
1:B:476:SER:O	1:B:480:HIS:CD2	2.57	0.57
1:A:27:ARG:HH11	1:B:196:GLU:HA	1.69	0.56
1:A:99:MSE:HE2	1:A:506:MSE:CE	2.35	0.56
1:B:129:GLY:O	1:B:130:VAL:C	2.45	0.56
1:B:129:GLY:O	1:B:132:GLY:N	2.38	0.56
1:B:154:CYS:SG	1:B:189:MSE:HE3	2.46	0.56
1:B:420:THR:CB	1:B:572:PRO:HD2	2.19	0.56
1:A:119:TRP:CZ3	1:A:136:ALA:HB1	2.40	0.56
1:A:340:ALA:HA	3:A:631:HOH:O	2.04	0.56
1:B:420:THR:HB	1:B:572:PRO:CD	2.19	0.56
1:B:590:SER:OG	1:B:592:VAL:HG13	2.06	0.56
1:B:236:SER:C	1:B:255:LEU:HD23	2.31	0.56
1:B:155:VAL:HG13	1:B:168:PHE:CG	2.41	0.56
1:A:184:GLY:HA2	1:A:213:LYS:HB3	1.88	0.55
1:A:592:VAL:O	1:A:592:VAL:CG2	2.54	0.55
1:B:344:ARG:HG3	1:B:344:ARG:NH1	2.20	0.55
1:A:341:ALA:HB2	1:B:228:ASN:HD22	1.71	0.55
1:B:95:ILE:O	1:B:98:SER:HB2	2.06	0.55
1:B:363:ALA:O	1:B:366:ARG:N	2.29	0.55
1:A:374:MSE:HE2	1:A:378:ILE:CD1	2.34	0.55
1:A:120:ASP:OD1	1:A:122:HIS:HB3	2.07	0.55
1:B:192:ARG:HA	1:B:192:ARG:HE	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:MSE:O	1:B:252:ARG:HG3	2.07	0.54
1:A:522:LEU:HB2	1:A:526:VAL:HG23	1.90	0.54
1:A:426:GLU:O	1:A:427:ALA:HB2	2.08	0.54
1:B:545:VAL:HG11	1:B:558:PHE:CD1	2.43	0.54
1:A:88:LEU:HB3	1:A:302:LEU:HD23	1.90	0.54
1:B:187:GLU:HG3	1:B:218:HIS:HB2	1.90	0.54
1:B:270:PHE:CD1	1:B:270:PHE:N	2.73	0.53
1:B:241:LEU:HA	1:B:246:ASP:OD2	2.07	0.53
1:A:432:GLY:O	1:A:433:PHE:CD1	2.61	0.53
1:B:110:VAL:O	1:B:110:VAL:HG12	2.09	0.53
1:B:173:LEU:HD13	1:B:204:ILE:CG1	2.36	0.53
1:B:457:LYS:HB3	1:B:574:GLN:NE2	2.23	0.53
1:A:97:SER:OG	1:A:290:ASP:CB	2.56	0.53
1:A:498:ALA:HB1	1:A:517:ILE:HD13	1.90	0.53
1:B:394:LEU:C	1:B:395:ARG:HD2	2.33	0.53
1:B:46:THR:OG1	1:B:48:GLU:HG3	2.09	0.53
1:A:416:ARG:HB3	1:A:419:PHE:O	2.08	0.53
1:B:95:ILE:HG13	1:B:119:TRP:CE2	2.43	0.53
1:A:411:LEU:O	1:A:424:GLU:HB2	2.09	0.53
1:B:140:ILE:HD12	1:B:147:ALA:HB3	1.90	0.53
1:B:369:ALA:HA	1:B:375:LEU:HG	1.89	0.53
1:A:373:ARG:HB2	1:A:373:ARG:NH1	2.24	0.53
1:B:146:ARG:NH2	1:B:344:ARG:HD3	2.23	0.53
1:A:329:GLN:O	1:A:330:ARG:C	2.52	0.52
1:B:153:SER:CB	1:B:188:ILE:HG12	2.39	0.52
1:A:449:HIS:CD2	1:A:481:ASN:HD21	2.27	0.52
1:A:474:THR:O	1:A:480:HIS:HB3	2.09	0.52
1:B:476:SER:H	1:B:480:HIS:CD2	2.26	0.52
1:A:543:GLU:O	1:A:544:ALA:C	2.52	0.52
1:A:228:ASN:ND2	1:B:64:VAL:H	2.08	0.52
1:A:197:ARG:HH22	1:A:206:GLN:HE21	1.56	0.52
1:A:201:MSE:SE	1:A:201:MSE:CB	3.02	0.52
1:A:314:LEU:O	1:A:315:LYS:C	2.48	0.52
1:A:488:ASN:O	1:A:492:MSE:HG3	2.09	0.52
1:B:351:GLU:HB2	1:B:357:SER:HB3	1.91	0.52
1:B:18:LEU:HD12	1:B:18:LEU:C	2.32	0.52
1:B:474:THR:HG23	1:B:524:GLY:O	2.09	0.52
1:A:425:THR:OG1	1:A:426:GLU:N	2.42	0.52
1:B:154:CYS:CB	1:B:189:MSE:HE3	2.39	0.52
1:A:414:ILE:HG23	1:A:572:PRO:HG2	1.92	0.51
1:B:346:ASP:C	1:B:347:ILE:CG1	2.80	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:390:MSE:HE3	1:B:392:LEU:CD2	2.41	0.51
1:A:10:PRO:O	1:A:11:ALA:C	2.54	0.51
1:A:248:MSE:O	1:A:252:ARG:HG3	2.11	0.51
1:B:453:GLU:OE2	1:B:453:GLU:HA	2.11	0.51
1:A:95:ILE:HD11	1:A:117:ILE:HD11	1.92	0.51
1:B:122:HIS:HA	1:B:152:PRO:HG3	1.93	0.51
1:B:146:ARG:HH22	1:B:344:ARG:HD3	1.75	0.51
1:B:221:GLY:O	1:B:222:LEU:C	2.52	0.51
1:A:449:HIS:CD2	1:A:481:ASN:ND2	2.79	0.51
1:A:480:HIS:CG	1:A:525:LEU:HD21	2.46	0.51
1:B:581:ASP:HB3	1:B:584:THR:HG22	1.93	0.51
1:A:9:GLU:N	3:A:622:HOH:O	2.42	0.50
1:A:428:ASP:O	1:A:435:VAL:HG23	2.10	0.50
1:A:448:ARG:HG3	1:A:481:ASN:HA	1.93	0.50
1:B:541:LEU:HD23	1:B:558:PHE:HZ	1.75	0.50
1:B:28:GLY:HA2	1:B:70:ARG:NH1	2.27	0.50
1:A:134:ARG:O	1:A:137:ALA:HB3	2.11	0.50
1:A:448:ARG:HG3	1:A:481:ASN:HD22	1.76	0.50
1:B:150:LEU:HD13	1:B:186:ALA:HA	1.92	0.50
1:B:488:ASN:O	1:B:489:ALA:C	2.55	0.50
1:B:573:HIS:ND1	1:B:573:HIS:N	2.60	0.50
1:A:588:MSE:HE1	1:A:590:SER:O	2.04	0.50
1:B:485:PHE:CD2	1:B:485:PHE:N	2.79	0.50
1:B:108:ALA:O	1:B:112:ARG:HD2	2.12	0.49
1:B:126:ASN:ND2	1:B:155:VAL:HB	2.27	0.49
1:B:163:ARG:N	1:B:576:ASP:OD2	2.35	0.49
1:A:280:LEU:HD13	1:A:318:TRP:HB3	1.94	0.49
1:A:466:ARG:HB2	1:A:466:ARG:HH11	1.77	0.49
1:B:42:VAL:O	1:B:42:VAL:CG2	2.54	0.49
1:B:471:PHE:HE1	1:B:541:LEU:HD21	1.76	0.49
1:A:482:LEU:HD12	1:A:483:THR:N	2.27	0.49
1:A:136:ALA:O	1:A:137:ALA:C	2.54	0.49
1:B:223:LYS:O	1:B:224:ASN:C	2.53	0.49
1:B:474:THR:HG22	1:B:505:GLY:H	1.77	0.49
1:B:474:THR:HG21	1:B:505:GLY:H	1.77	0.49
1:B:527:SER:OG	1:B:528:ASP:N	2.45	0.49
1:A:321:ARG:HD2	3:A:624:HOH:O	2.12	0.49
1:A:197:ARG:HH22	1:A:206:GLN:NE2	2.09	0.49
1:B:93:MSE:HE3	1:B:105:TYR:CZ	2.47	0.49
1:B:317:GLU:HB3	3:B:628:HOH:O	2.12	0.48
1:B:443:ILE:HD11	1:B:461:LEU:HG	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:475:VAL:HB	1:B:506:MSE:HE2	1.93	0.48
1:A:75:GLN:CG	1:A:76:VAL:N	2.76	0.48
1:A:493:ALA:O	1:A:494:LEU:C	2.54	0.48
1:B:272:ALA:O	1:B:276:THR:OG1	2.28	0.48
1:A:29:ASP:O	1:A:30:GLN:HG3	2.14	0.48
1:B:67:PRO:O	1:B:68:ALA:HB3	2.14	0.48
1:B:187:GLU:O	1:B:189:MSE:HE2	2.14	0.48
1:B:477:HIS:O	1:B:566:LEU:N	2.46	0.48
1:A:551:TRP:CZ2	1:A:558:PHE:HB2	2.49	0.48
1:B:28:GLY:HA2	1:B:70:ARG:HH12	1.78	0.48
1:B:191:MSE:O	1:B:195:ILE:HD12	2.13	0.48
1:A:351:GLU:OE1	1:A:359:ARG:NE	2.38	0.48
1:B:294:ASP:CA	1:B:535:ALA:HB1	2.44	0.48
1:A:308:ARG:CG	1:A:311:ARG:HH21	2.27	0.48
1:A:448:ARG:H	1:A:481:ASN:HD22	1.59	0.48
1:A:100:ILE:HD11	1:A:105:TYR:HA	1.96	0.47
1:B:173:LEU:HD13	1:B:204:ILE:CG2	2.44	0.47
1:B:71:ARG:C	1:B:72:ASP:O	2.51	0.47
1:B:264:ASP:OD2	1:B:308:ARG:NH1	2.44	0.47
1:B:173:LEU:HD12	1:B:204:ILE:HG12	1.95	0.47
1:A:93:MSE:HE3	1:A:105:TYR:OH	2.14	0.47
1:B:505:GLY:HA2	1:B:520:LEU:HB2	1.97	0.47
1:B:10:PRO:O	1:B:11:ALA:C	2.55	0.47
1:A:28:GLY:C	1:A:30:GLN:H	2.21	0.47
1:A:46:THR:O	1:B:277:LEU:HD11	2.14	0.47
1:A:430:LYS:HG3	1:A:431:ASP:OD1	2.15	0.47
1:B:118:VAL:HG21	1:B:331:LEU:HD21	1.97	0.47
1:B:181:GLU:CD	1:B:181:GLU:H	2.23	0.47
1:B:344:ARG:HG3	1:B:344:ARG:HH11	1.79	0.47
1:B:550:GLU:O	1:B:552:GLN:N	2.48	0.47
1:A:161:LEU:HD23	1:A:161:LEU:N	2.29	0.47
1:A:201:MSE:SE	1:A:201:MSE:CA	3.13	0.46
1:A:248:MSE:CE	1:A:248:MSE:HB3	2.45	0.46
1:B:94:HIS:O	1:B:95:ILE:C	2.55	0.46
1:B:507:ALA:HB2	1:B:517:ILE:HD12	1.96	0.46
1:B:593:ILE:O	1:B:593:ILE:HG22	2.14	0.46
1:A:31:ARG:O	1:A:31:ARG:HG3	2.16	0.46
1:A:93:MSE:SE	1:A:117:ILE:HD12	2.64	0.46
1:A:239:HIS:HB3	1:A:258:GLU:HB2	1.96	0.46
1:A:304:ASP:OD1	1:A:307:ARG:HD2	2.14	0.46
1:B:251:LEU:HA	1:B:251:LEU:HD23	1.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:ARG:HH11	1:B:21:ARG:HD2	1.51	0.46
1:B:123:GLU:C	1:B:125:GLY:N	2.72	0.46
1:B:187:GLU:CG	1:B:218:HIS:HB2	2.45	0.46
1:A:447:HIS:CE1	1:A:452:ALA:HB3	2.51	0.46
1:B:256:THR:HG22	1:B:257:ILE:N	2.25	0.46
1:A:424:GLU:CG	1:A:425:THR:N	2.78	0.46
1:B:209:LEU:O	1:B:210:ALA:C	2.58	0.46
1:B:285:THR:O	1:B:286:LEU:HD23	2.15	0.46
1:B:352:ASP:OD1	1:B:352:ASP:C	2.58	0.46
1:B:505:GLY:N	1:B:520:LEU:HB2	2.30	0.46
1:B:584:THR:CG2	1:B:586:LYS:H	2.22	0.46
1:B:295:ASP:O	1:B:300:GLY:CA	2.62	0.46
1:B:464:TRP:O	1:B:465:GLY:O	2.34	0.46
1:B:15:ASP:OD2	1:B:17:THR:CG2	2.63	0.46
1:A:217:GLY:HA3	1:A:237:SER:O	2.16	0.46
1:B:536:ARG:O	1:B:537:ALA:C	2.58	0.46
1:B:559:LYS:HB2	3:B:623:HOH:O	2.15	0.46
1:A:395:ARG:N	1:A:497:ASN:OD1	2.42	0.46
1:A:410:ARG:HD3	1:A:594:GLU:CG	2.46	0.46
1:A:433:PHE:O	1:A:434:VAL:C	2.58	0.46
1:A:449:HIS:HD2	1:A:481:ASN:HD21	1.63	0.46
1:B:224:ASN:O	1:B:227:LEU:HB3	2.16	0.46
1:A:445:VAL:HG12	1:A:446:THR:N	2.31	0.45
1:A:575:THR:C	1:A:577:MSE:N	2.71	0.45
1:B:318:TRP:O	1:B:319:ALA:C	2.60	0.45
1:A:477:HIS:HA	1:A:478:ASP:HA	1.75	0.45
1:B:153:SER:HB2	1:B:188:ILE:HG12	1.98	0.45
1:A:129:GLY:O	1:A:130:VAL:C	2.59	0.45
1:A:497:ASN:O	1:A:498:ALA:C	2.59	0.45
1:B:549:VAL:HG22	1:B:550:GLU:N	2.29	0.45
1:B:112:ARG:HG2	1:B:112:ARG:HH11	1.80	0.45
1:B:443:ILE:CD1	1:B:461:LEU:HG	2.46	0.45
1:B:112:ARG:HG2	1:B:112:ARG:NH1	2.30	0.45
1:B:436:PRO:HG2	1:B:442:MSE:CE	2.47	0.45
1:B:129:GLY:O	1:B:131:ASP:N	2.50	0.45
1:B:336:LEU:CD2	1:B:344:ARG:HD2	2.47	0.45
1:A:43:ASP:OD2	1:A:50:ARG:NE	2.47	0.45
1:A:92:HIS:O	1:A:287:CYS:HB2	2.16	0.45
1:A:280:LEU:HD23	3:A:624:HOH:O	2.17	0.45
1:B:93:MSE:HE1	1:B:95:ILE:HG12	1.99	0.45
1:A:185:ILE:HG22	1:A:186:ALA:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:390:MSE:HE3	1:B:392:LEU:HD21	1.99	0.45
1:B:542:ARG:O	1:B:543:GLU:C	2.60	0.45
1:A:443:ILE:HG23	1:A:443:ILE:O	2.17	0.44
1:B:536:ARG:C	1:B:538:PHE:N	2.71	0.44
1:B:538:PHE:O	1:B:539:GLU:C	2.56	0.44
1:B:156:PRO:HD2	1:B:156:PRO:O	2.16	0.44
1:B:245:GLU:OE1	1:B:245:GLU:HA	2.17	0.44
1:B:436:PRO:HA	1:B:437:PRO:HD2	1.39	0.44
1:B:469:GLY:HA3	1:B:509:ALA:O	2.17	0.44
1:B:477:HIS:HA	1:B:478:ASP:HA	1.57	0.44
1:A:49:LEU:N	1:A:49:LEU:HD23	2.29	0.44
1:A:59:ALA:HA	1:A:364:SER:O	2.18	0.44
1:B:446:THR:OG1	1:B:456:THR:HG23	2.17	0.44
1:B:506:MSE:HE3	1:B:520:LEU:CD1	2.47	0.44
1:A:189:MSE:H	1:A:189:MSE:HG2	1.53	0.44
1:B:63:SER:OG	1:B:65:HIS:CD2	2.52	0.44
1:A:27:ARG:NH1	1:B:196:GLU:HA	2.33	0.44
1:A:117:ILE:HD13	1:A:117:ILE:HG21	1.78	0.44
1:B:436:PRO:HG2	1:B:442:MSE:HE2	1.98	0.44
1:A:18:LEU:HD12	1:A:57:VAL:HG12	1.99	0.44
1:B:557:VAL:O	1:B:558:PHE:C	2.61	0.44
1:B:53:ASP:OD2	1:B:67:PRO:HA	2.18	0.44
1:A:38:GLY:O	1:A:80:GLY:HA2	2.17	0.43
1:B:231:MSE:HE2	1:B:231:MSE:HB3	1.99	0.43
1:A:217:GLY:CA	1:A:237:SER:O	2.67	0.43
1:A:252:ARG:HG2	1:B:46:THR:HG21	2.00	0.43
1:A:339:ILE:N	1:A:339:ILE:HD13	2.30	0.43
1:B:155:VAL:HA	1:B:156:PRO:HA	1.66	0.43
1:B:156:PRO:O	1:B:156:PRO:CD	2.63	0.43
1:A:18:LEU:CD1	1:A:57:VAL:HG12	2.48	0.43
1:A:160:GLY:C	1:A:161:LEU:HD23	2.43	0.43
1:B:150:LEU:HB3	1:B:186:ALA:HB2	2.00	0.43
1:B:294:ASP:HA	1:B:535:ALA:CB	2.47	0.43
1:B:294:ASP:HB3	1:B:535:ALA:HB1	2.00	0.43
1:B:533:GLU:O	1:B:534:VAL:C	2.56	0.43
1:A:89:ILE:O	1:A:302:LEU:HD22	2.18	0.43
1:A:123:GLU:O	1:A:124:PHE:C	2.56	0.43
1:A:293:PRO:HB3	1:A:534:VAL:HG12	2.00	0.43
1:B:161:LEU:HD12	1:B:161:LEU:HA	1.60	0.43
1:A:231:MSE:SE	1:A:255:LEU:HG	2.68	0.43
1:A:295:ASP:O	1:A:299:GLY:N	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:HIS:CG	1:A:452:ALA:HB3	2.54	0.43
1:B:217:GLY:N	1:B:237:SER:O	2.50	0.43
1:B:385:VAL:O	1:B:385:VAL:HG12	2.18	0.43
1:A:198:ASP:HA	1:A:199:PRO:HD3	1.75	0.43
1:A:482:LEU:HD12	1:A:482:LEU:C	2.43	0.43
1:A:335:ASP:OD1	1:A:335:ASP:N	2.51	0.43
1:B:366:ARG:O	1:B:368:VAL:HG13	2.19	0.43
1:B:459:GLY:C	1:B:460:PHE:CG	2.97	0.43
1:A:105:TYR:CE2	1:A:109:VAL:HG11	2.53	0.43
1:A:416:ARG:HG3	1:A:416:ARG:NH1	2.13	0.43
1:B:477:HIS:HB3	1:B:478:ASP:OD1	2.19	0.43
1:A:271:VAL:O	1:A:272:ALA:C	2.60	0.42
1:B:66:GLU:HA	1:B:67:PRO:HD3	1.66	0.42
1:B:122:HIS:CB	1:B:152:PRO:HB3	2.49	0.42
1:B:155:VAL:HG13	1:B:168:PHE:CB	2.47	0.42
1:B:415:ASP:OD2	1:B:421:GLN:NE2	2.49	0.42
1:B:590:SER:OG	1:B:592:VAL:CG1	2.67	0.42
1:A:575:THR:O	1:A:577:MSE:N	2.52	0.42
1:B:123:GLU:C	1:B:125:GLY:H	2.27	0.42
1:B:426:GLU:O	1:B:427:ALA:HB2	2.19	0.42
1:A:18:LEU:O	1:A:22:ALA:N	2.52	0.42
1:A:55:GLY:O	1:A:62:ALA:N	2.48	0.42
1:A:472:ALA:CB	1:A:484:VAL:HG22	2.49	0.42
1:A:556:LEU:O	1:A:556:LEU:HG	2.19	0.42
1:B:90:ASP:OD1	1:B:288:THR:N	2.52	0.42
1:B:276:THR:O	1:B:277:LEU:C	2.61	0.42
1:B:308:ARG:O	1:B:309:LEU:C	2.61	0.42
1:B:474:THR:HG22	1:B:505:GLY:O	2.18	0.42
1:A:205:VAL:O	1:A:206:GLN:C	2.57	0.42
1:B:117:ILE:HG21	1:B:117:ILE:HD13	1.75	0.42
1:A:288:THR:O	1:A:289:ASP:C	2.60	0.42
1:A:527:SER:OG	1:A:528:ASP:N	2.50	0.42
1:B:93:MSE:HB3	1:B:289:ASP:H	1.85	0.42
1:B:109:VAL:HG23	1:B:110:VAL:N	2.33	0.42
1:B:302:LEU:O	1:B:302:LEU:HG	2.16	0.42
1:B:385:VAL:O	1:B:385:VAL:CG1	2.67	0.42
1:A:11:ALA:O	1:A:12:ASP:C	2.61	0.42
1:A:137:ALA:O	1:A:140:ILE:HG12	2.19	0.42
1:A:429:VAL:HG12	1:A:430:LYS:N	2.32	0.42
1:B:117:ILE:HG23	1:B:145:LEU:HD11	2.02	0.42
1:A:49:LEU:HD23	1:A:49:LEU:HA	1.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:ILE:O	1:A:216:CYS:HB2	2.19	0.42
1:A:467:TRP:O	1:A:469:GLY:N	2.53	0.42
1:B:24:ALA:HB1	1:B:30:GLN:HG3	2.02	0.42
1:B:123:GLU:OE1	1:B:480:HIS:CE1	2.73	0.42
1:B:140:ILE:O	1:B:141:GLU:C	2.63	0.42
1:B:472:ALA:HA	1:B:483:THR:O	2.20	0.42
1:A:404:SER:OG	1:A:405:GLN:N	2.49	0.41
1:B:155:VAL:O	1:B:168:PHE:N	2.51	0.41
1:B:218:HIS:CE1	1:B:240:GLU:OE2	2.73	0.41
1:B:239:HIS:HD2	1:B:240:GLU:HG2	1.85	0.41
1:B:404:SER:O	1:B:405:GLN:C	2.63	0.41
1:B:416:ARG:HA	1:B:417:PRO:HD3	1.91	0.41
1:B:76:VAL:HG12	1:B:76:VAL:O	2.20	0.41
1:B:393:PRO:O	1:B:395:ARG:NH1	2.31	0.41
1:A:63:SER:OG	1:A:65:HIS:HD2	2.03	0.41
1:B:227:LEU:C	1:B:227:LEU:HD12	2.43	0.41
1:B:549:VAL:CG2	1:B:550:GLU:H	2.32	0.41
1:B:583:LEU:HD23	1:B:583:LEU:HA	1.71	0.41
1:A:378:ILE:O	1:A:379:PRO:C	2.62	0.41
1:B:258:GLU:O	1:B:287:CYS:SG	2.77	0.41
1:A:28:GLY:HA2	1:A:70:ARG:NH2	2.36	0.41
1:A:51:PRO:O	1:A:52:ALA:HB2	2.20	0.41
1:A:447:HIS:ND1	1:A:452:ALA:HB3	2.35	0.41
1:A:467:TRP:HB3	1:A:469:GLY:O	2.21	0.41
1:A:155:VAL:HA	1:A:156:PRO:HA	1.86	0.41
1:A:384:THR:O	1:A:387:LYS:HG3	2.20	0.41
1:B:19:ARG:HA	1:B:19:ARG:HD3	1.74	0.41
1:B:137:ALA:O	1:B:138:LYS:C	2.63	0.41
1:A:50:ARG:O	1:A:50:ARG:CG	2.69	0.41
1:B:550:GLU:OE1	1:B:550:GLU:CA	2.65	0.41
1:B:551:TRP:CE2	1:B:558:PHE:HB2	2.55	0.41
1:A:305:VAL:O	1:A:306:VAL:C	2.64	0.41
1:A:554:PRO:O	1:A:555:TYR:HB2	2.21	0.41
1:B:190:ASN:HD22	1:B:201:MSE:SE	2.54	0.41
1:A:248:MSE:O	1:A:249:ALA:C	2.62	0.41
1:A:554:PRO:O	1:A:555:TYR:CB	2.67	0.41
1:B:127:VAL:HG12	1:B:128:HIS:NE2	2.36	0.41
1:B:505:GLY:HA2	1:B:520:LEU:CD1	2.46	0.41
1:A:110:VAL:C	1:A:112:ARG:H	2.29	0.41
1:A:196:GLU:OE1	1:B:27:ARG:HD2	2.20	0.41
1:A:416:ARG:CG	1:A:416:ARG:NH1	2.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:305:VAL:O	1:B:306:VAL:C	2.63	0.41
1:B:413:THR:HG23	1:B:423:GLY:O	2.21	0.41
1:A:331:LEU:O	1:A:332:GLY:C	2.61	0.40
1:B:499:VAL:O	1:B:500:ILE:C	2.63	0.40
1:B:505:GLY:CA	1:B:520:LEU:HB2	2.51	0.40
1:A:23:VAL:HG23	1:A:23:VAL:H	1.56	0.40
1:A:393:PRO:O	1:A:394:LEU:C	2.63	0.40
1:B:122:HIS:HA	1:B:152:PRO:CG	2.52	0.40
1:B:296:LEU:HA	1:B:300:GLY:HA3	2.02	0.40
1:B:392:LEU:HA	1:B:393:PRO:HD3	1.64	0.40
1:A:228:ASN:ND2	1:B:341:ALA:HB2	2.33	0.40
1:B:99:MSE:HE2	1:B:506:MSE:HE1	2.03	0.40
1:B:117:ILE:O	1:B:117:ILE:HG13	2.20	0.40
1:B:153:SER:HB3	1:B:186:ALA:O	2.20	0.40
1:A:95:ILE:H	1:A:119:TRP:CD1	2.40	0.40
1:A:436:PRO:HA	1:A:437:PRO:HD2	1.78	0.40
1:A:453:GLU:O	1:A:455:THR:N	2.48	0.40
1:B:218:HIS:CE1	1:B:240:GLU:CD	3.00	0.40
1:B:370:GLU:O	1:B:371:GLY:C	2.64	0.40
1:B:505:GLY:HA2	1:B:520:LEU:CG	2.51	0.40
1:B:531:LEU:HD12	1:B:531:LEU:O	2.21	0.40
1:A:552:GLN:O	1:A:553:PRO:C	2.61	0.40
1:B:24:ALA:O	1:B:25:ALA:C	2.65	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	585/608 (96%)	516 (88%)	54 (9%)	15 (3%)	4 5
1	B	573/608 (94%)	474 (83%)	72 (13%)	27 (5%)	2 1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1158/1216 (95%)	990 (86%)	126 (11%)	42 (4%)	2 3

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	111	ALA
1	A	397	ALA
1	A	430	LYS
1	A	431	ASP
1	A	588	MSE
1	B	72	ASP
1	B	73	ALA
1	B	74	ALA
1	B	371	GLY
1	B	398	ASN
1	B	417	PRO
1	B	418	ARG
1	B	437	PRO
1	B	465	GLY
1	B	556	LEU
1	B	558	PHE
1	B	566	LEU
1	A	69	SER
1	A	406	GLY
1	A	516	ALA
1	A	553	PRO
1	B	129	GLY
1	B	303	ASP
1	B	364	SER
1	B	551	TRP
1	B	552	GLN
1	A	68	ALA
1	B	177	LEU
1	B	187	GLU
1	B	262	SER
1	A	74	ALA
1	A	224	ASN
1	A	416	ARG
1	A	489	ALA
1	B	224	ASN
1	B	492	MSE
1	B	568	CYS

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Mol	Chain	Res	Type
1	A	454	PRO
1	B	546	GLY
1	B	385	VAL
1	B	427	ALA
1	B	572	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	445/444 (100%)	385 (86%)	60 (14%)	4	4
1	B	439/444 (99%)	369 (84%)	70 (16%)	2	2
All	All	884/888 (100%)	754 (85%)	130 (15%)	3	3

All (130) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	THR
1	A	31	ARG
1	A	36	ILE
1	A	54	ILE
1	A	57	VAL
1	A	61	ILE
1	A	66	GLU
1	A	71	ARG
1	A	84	VAL
1	A	98	SER
1	A	155	VAL
1	A	172	ILE
1	A	188	ILE
1	A	189	MSE
1	A	200	ARG
1	A	214	LEU
1	A	262	SER
1	A	280	LEU

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Mol	Chain	Res	Type
1	A	290	ASP
1	A	298	GLN
1	A	336	LEU
1	A	338	LEU
1	A	348	VAL
1	A	364	SER
1	A	370	GLU
1	A	373	ARG
1	A	375	LEU
1	A	378	ILE
1	A	380	THR
1	A	387	LYS
1	A	395	ARG
1	A	401	LEU
1	A	408	LYS
1	A	409	VAL
1	A	416	ARG
1	A	420	THR
1	A	424	GLU
1	A	425	THR
1	A	428	ASP
1	A	429	VAL
1	A	430	LYS
1	A	442	MSE
1	A	455	THR
1	A	462	THR
1	A	466	ARG
1	A	482	LEU
1	A	513	LYS
1	A	517	ILE
1	A	518	LEU
1	A	527	SER
1	A	528	ASP
1	A	531	LEU
1	A	536	ARG
1	A	547	LYS
1	A	548	VAL
1	A	553	PRO
1	A	584	THR
1	A	588	MSE
1	A	589	GLU
1	A	595	VAL

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Mol	Chain	Res	Type
1	B	42	VAL
1	B	75	GLN
1	B	76	VAL
1	B	77	ILE
1	B	85	SER
1	B	95	ILE
1	B	96	GLU
1	B	97	SER
1	B	100	ILE
1	B	101	THR
1	B	102	PRO
1	B	140	ILE
1	B	154	CYS
1	B	155	VAL
1	B	161	LEU
1	B	173	LEU
1	B	175	ASP
1	B	177	LEU
1	B	178	SER
1	B	181	GLU
1	B	185	ILE
1	B	189	MSE
1	B	192	ARG
1	B	198	ASP
1	B	200	ARG
1	B	227	LEU
1	B	239	HIS
1	B	241	LEU
1	B	255	LEU
1	B	257	ILE
1	B	268	PRO
1	B	288	THR
1	B	290	ASP
1	B	298	GLN
1	B	311	ARG
1	B	321	ARG
1	B	334	SER
1	B	347	ILE
1	B	373	ARG
1	B	380	THR
1	B	384	THR
1	B	387	LYS

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Mol	Chain	Res	Type
1	B	405	GLN
1	B	413	THR
1	B	415	ASP
1	B	420	THR
1	B	425	THR
1	B	430	LYS
1	B	431	ASP
1	B	435	VAL
1	B	438	GLU
1	B	441	THR
1	B	442	MSE
1	B	443	ILE
1	B	462	THR
1	B	478	ASP
1	B	485	PHE
1	B	517	ILE
1	B	523	SER
1	B	532	GLU
1	B	550	GLU
1	B	555	TYR
1	B	570	ILE
1	B	573	HIS
1	B	575	THR
1	B	577	MSE
1	B	586	LYS
1	B	588	MSE
1	B	592	VAL
1	B	594	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	HIS
1	A	206	GLN
1	A	228	ASN
1	A	279	HIS
1	A	282	GLN
1	A	447	HIS
1	A	481	ASN
1	A	488	ASN
1	B	65	HIS
1	B	126	ASN

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Mol	Chain	Res	Type
1	B	190	ASN
1	B	206	GLN
1	B	228	ASN
1	B	279	HIS
1	B	329	GLN
1	B	447	HIS
1	B	480	HIS
1	B	481	ASN
1	B	488	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	571/608 (93%)	-0.55	1 (0%) 91 90	28, 46, 68, 80	0
1	B	563/608 (92%)	-0.36	1 (0%) 91 90	31, 50, 89, 100	0
All	All	1134/1216 (93%)	-0.46	2 (0%) 91 90	28, 48, 83, 100	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	425	THR	2.1
1	A	595	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FE	A	607	1/1	0.97	0.04	45,45,45,45	0
2	FE	A	608	1/1	0.98	0.03	50,50,50,50	0
2	FE	A	606	1/1	0.99	0.02	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FE	B	606	1/1	0.99	0.03	52,52,52,52	0
2	FE	B	607	1/1	0.99	0.02	64,64,64,64	0
2	FE	B	608	1/1	0.99	0.04	59,59,59,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.