



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:54 AM UTC

PDB ID : 6IEH / pdb_00006ieh
Title : Crystal structures of the hMTR4-NRDE2 complex
Authors : Chen, J.Y.; Yun, C.H.
Deposited on : 2018-09-14
Resolution : 2.89 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

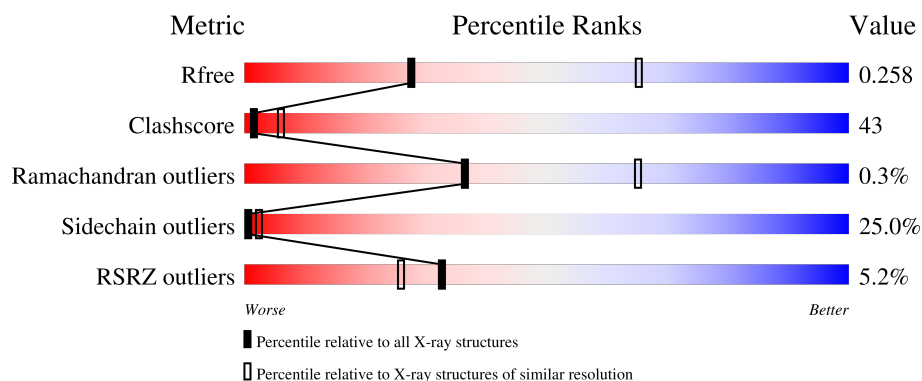
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	B	979	5% 33% 38% 19% 5%
2	A	105	5% 27% 30% 17% 7% 19%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ATP	B	1102	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7647 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 Exosome RNA helicase MTR4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	929	Total	C	N	O	S	0	0	0
			6907	4405	1169	1284	49			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	64	GLY	-	expression tag	UNP P42285
B	65	ALA	-	expression tag	UNP P42285
B	66	MET	-	expression tag	UNP P42285
B	67	ASP	-	expression tag	UNP P42285
B	68	PRO	-	expression tag	UNP P42285
B	69	GLU	-	expression tag	UNP P42285
B	70	PHE	-	expression tag	UNP P42285

- Molecule 2 is a protein called Protein NRDE2 homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	85	Total	C	N	O	S	0	0	0
			676	432	117	124	3			

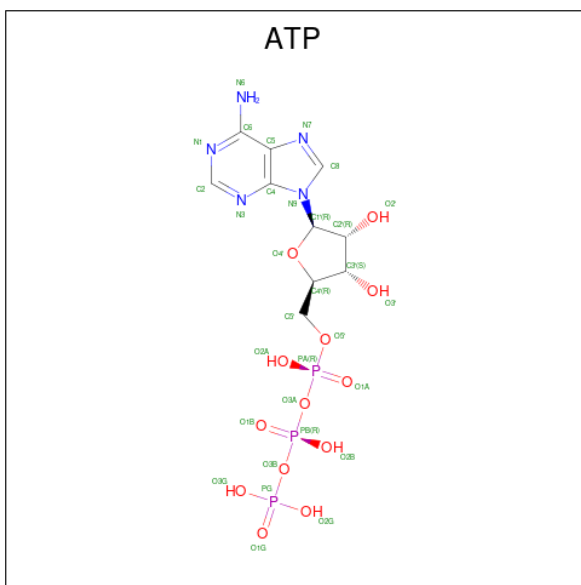
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	162	SER	-	expression tag	UNP Q9H7Z3

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Cl	0	0
			1	1		

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

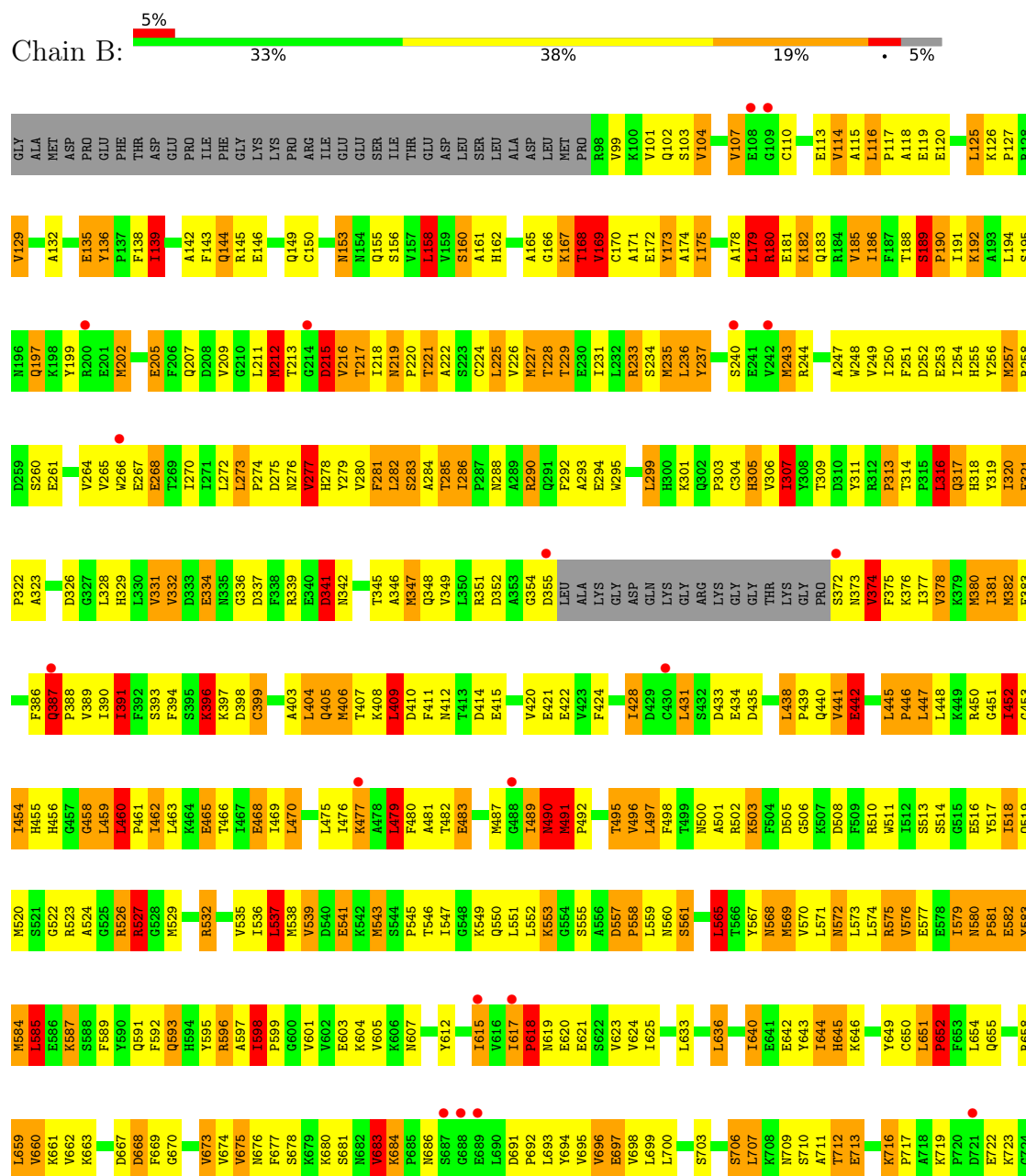
- Molecule 5 is water.

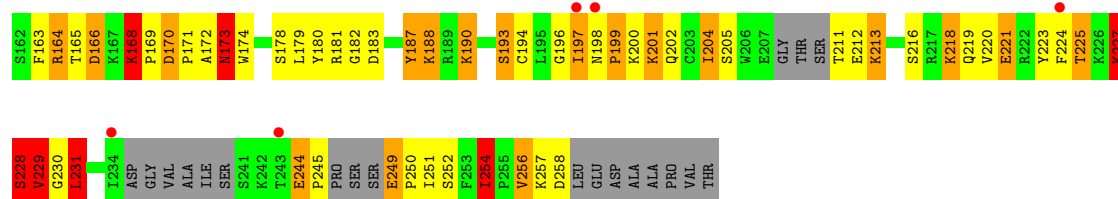
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	27	Total O 27 27	0	0
5	A	5	Total O 5 5	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Exosome RNA helicase MTR4





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	148.31Å 113.73Å 80.72Å 90.00° 96.49° 90.00°	Depositor
Resolution (Å)	40.10 – 2.89 40.10 – 2.89	Depositor EDS
% Data completeness (in resolution range)	98.4 (40.10-2.89) 98.4 (40.10-2.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 2.90Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.235 , 0.252 0.237 , 0.258	Depositor DCC
R_{free} test set	1496 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	52.4	Xtriage
Anisotropy	0.259	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 54.2	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	0.90	EDS
Total number of atoms	7647	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	B	2.46	316/7039 (4.5%)	1.61	120/9575 (1.3%)
2	A	2.00	15/690 (2.2%)	1.84	20/922 (2.2%)
All	All	2.42	331/7729 (4.3%)	1.63	140/10497 (1.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (331) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	219	ASN	C-O	-14.47	1.16	1.23
1	B	398	ASP	C-O	-8.36	1.14	1.24
1	B	290	ARG	C-O	-8.17	1.14	1.24
1	B	535	VAL	C-O	-8.05	1.15	1.24
2	A	198	ASN	C-N	7.97	1.40	1.33
1	B	883	ALA	C-O	-7.97	1.18	1.24
1	B	662	VAL	C-O	-7.93	1.15	1.24
1	B	651	LEU	C-O	-7.92	1.17	1.24
1	B	219	ASN	CA-C	-7.92	1.48	1.53
1	B	197	GLN	C-O	-7.90	1.14	1.24
1	B	674	VAL	C-O	-7.83	1.15	1.24
1	B	103	SER	C-O	-7.83	1.14	1.24
1	B	282	LEU	C-O	-7.82	1.14	1.24
1	B	655	GLN	CA-C	-7.80	1.43	1.52
1	B	660	VAL	C-O	-7.80	1.16	1.23
2	A	170	ASP	C-O	-7.64	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	249	VAL	C-O	-7.62	1.16	1.24
1	B	160	SER	C-O	-7.59	1.15	1.24
1	B	268	GLU	C-O	-7.50	1.15	1.24
2	A	254	ILE	CA-C	-7.46	1.46	1.53
1	B	114	VAL	C-O	-7.45	1.16	1.24
1	B	587	LYS	C-O	-7.42	1.14	1.24
1	B	306	VAL	C-O	-7.41	1.16	1.24
1	B	390	ILE	C-O	-7.39	1.16	1.24
1	B	854	ARG	C-O	-7.38	1.15	1.24
1	B	580	ASN	C-O	-7.38	1.18	1.24
1	B	250	ILE	C-O	-7.33	1.16	1.24
1	B	518	ILE	C-O	-7.31	1.15	1.24
1	B	318	HIS	C-O	-7.29	1.15	1.23
1	B	479	LEU	C-O	-7.22	1.15	1.24
1	B	697	GLU	C-O	-7.20	1.15	1.24
1	B	696	VAL	C-O	-7.19	1.16	1.24
1	B	497	LEU	C-O	-7.14	1.15	1.24
1	B	739	ILE	C-O	-7.08	1.17	1.24
1	B	698	VAL	C-O	-7.03	1.16	1.24
1	B	332	VAL	C-O	-6.96	1.17	1.24
1	B	373	ASN	C-O	-6.94	1.15	1.23
1	B	712	THR	C-O	-6.92	1.16	1.24
1	B	543	MET	C-O	-6.88	1.15	1.24
1	B	251	PHE	C-O	-6.87	1.16	1.24
1	B	226	VAL	C-O	-6.86	1.16	1.24
1	B	455	HIS	CA-C	-6.85	1.44	1.52
1	B	317	GLN	C-O	-6.84	1.16	1.24
1	B	567	TYR	C-O	-6.84	1.16	1.24
1	B	224	CYS	C-O	-6.83	1.16	1.24
1	B	593	GLN	C-O	-6.80	1.16	1.24
1	B	339	ARG	CA-C	-6.78	1.44	1.53
1	B	303	PRO	C-O	-6.75	1.16	1.23
1	B	676	ASN	C-O	-6.73	1.16	1.23
1	B	850	GLU	C-O	-6.72	1.15	1.24
1	B	445	LEU	C-O	-6.69	1.18	1.24
1	B	339	ARG	C-O	-6.67	1.15	1.23
1	B	510	ARG	C-O	-6.67	1.15	1.23
1	B	745	TYR	CA-C	-6.67	1.44	1.52
1	B	281	PHE	C-O	-6.66	1.16	1.24
1	B	513	SER	C-O	-6.65	1.14	1.23
1	B	742	VAL	C-O	-6.64	1.16	1.24
1	B	604	LYS	C-O	-6.63	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	650	CYS	C-O	-6.63	1.15	1.24
1	B	216	VAL	C-O	-6.63	1.17	1.24
1	B	675	VAL	C-O	-6.59	1.16	1.23
1	B	491	MET	CA-C	-6.57	1.47	1.52
1	B	858	LEU	C-O	-6.57	1.16	1.24
1	B	693	LEU	C-O	-6.55	1.16	1.23
1	B	115	ALA	C-O	-6.55	1.16	1.24
1	B	169	VAL	C-O	-6.53	1.15	1.24
1	B	519	GLN	C-O	-6.53	1.16	1.24
1	B	387	GLN	C-N	6.51	1.41	1.33
1	B	376	LYS	C-O	-6.49	1.16	1.24
1	B	234	SER	C-O	-6.48	1.16	1.24
1	B	116	LEU	C-O	-6.47	1.17	1.24
1	B	670	GLY	C-O	-6.46	1.15	1.24
1	B	551	LEU	C-O	-6.44	1.16	1.24
1	B	595	TYR	C-O	-6.41	1.16	1.24
1	B	279	TYR	C-O	-6.41	1.15	1.23
1	B	374	VAL	C-O	-6.40	1.17	1.24
1	B	536	ILE	C-O	-6.40	1.17	1.24
1	B	537	LEU	C-O	-6.39	1.16	1.24
1	B	617	ILE	N-CA	-6.39	1.38	1.46
1	B	170	CYS	CA-C	-6.38	1.44	1.52
1	B	319	TYR	C-O	-6.37	1.15	1.23
1	B	283	SER	CA-C	-6.36	1.44	1.52
1	B	170	CYS	C-O	-6.35	1.16	1.24
1	B	404	LEU	C-O	-6.34	1.16	1.24
1	B	144	GLN	C-O	-6.34	1.16	1.24
1	B	738	ALA	C-O	-6.31	1.16	1.23
1	B	150	CYS	C-O	-6.31	1.16	1.24
1	B	172	GLU	C-O	-6.30	1.16	1.24
1	B	557	ASP	CA-C	-6.30	1.46	1.53
1	B	171	ALA	C-O	-6.30	1.16	1.24
1	B	1004	LEU	C-O	-6.29	1.16	1.24
1	B	314	THR	C-O	-6.28	1.17	1.24
1	B	516	GLU	C-O	-6.27	1.16	1.24
1	B	285	THR	C-O	-6.26	1.16	1.24
1	B	668	ASP	CA-C	-6.25	1.45	1.52
1	B	716	LYS	C-O	-6.25	1.17	1.24
1	B	864	ALA	C-O	-6.22	1.16	1.23
1	B	569	MET	C-O	-6.20	1.17	1.24
1	B	659	LEU	C-O	-6.19	1.16	1.24
1	B	514	SER	C-O	-6.17	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	132	ALA	C-O	-6.15	1.16	1.23
1	B	168	THR	C-O	-6.14	1.16	1.24
1	B	341	ASP	C-O	-6.13	1.17	1.24
1	B	293	ALA	C-O	-6.13	1.16	1.24
1	B	447	LEU	C-O	-6.13	1.17	1.24
1	B	304	CYS	C-O	-6.13	1.17	1.24
1	B	667	ASP	C-O	-6.12	1.17	1.24
1	B	539	VAL	C-O	-6.12	1.17	1.24
1	B	747	PRO	C-O	-6.11	1.16	1.23
1	B	803	ARG	C-O	-6.11	1.17	1.24
2	A	190	LYS	C-O	-6.10	1.16	1.24
1	B	851	LEU	C-O	-6.10	1.17	1.24
1	B	834	SER	C-O	-6.09	1.16	1.24
1	B	547	ILE	C-O	-6.08	1.17	1.24
1	B	643	TYR	C-O	-6.08	1.16	1.24
2	A	182	GLY	C-O	-6.08	1.17	1.24
1	B	649	TYR	C-O	-6.07	1.16	1.24
1	B	377	ILE	C-O	-6.07	1.17	1.24
1	B	145	ARG	C-O	-6.06	1.17	1.24
1	B	763	ILE	C-O	-6.05	1.17	1.24
1	B	839	LEU	C-O	-6.03	1.17	1.24
1	B	729	VAL	C-O	-6.03	1.16	1.24
1	B	316	LEU	C-O	-5.99	1.16	1.24
1	B	405	GLN	C-O	-5.98	1.16	1.24
1	B	212	MET	C-O	-5.98	1.17	1.24
1	B	755	ASN	C-O	-5.97	1.17	1.24
1	B	288	ASN	C-O	-5.96	1.16	1.24
1	B	891	MET	C-O	-5.96	1.17	1.24
1	B	235	MET	C-O	-5.96	1.17	1.24
1	B	422	GLU	C-O	-5.94	1.17	1.24
1	B	381	ILE	C-O	-5.94	1.17	1.24
1	B	592	PHE	C-O	-5.93	1.17	1.24
1	B	320	ILE	C-O	-5.91	1.17	1.24
1	B	517	TYR	C-O	-5.91	1.17	1.24
1	B	677	PHE	C-O	-5.91	1.16	1.23
1	B	222	ALA	CA-C	-5.89	1.45	1.52
1	B	561	SER	CA-C	-5.89	1.45	1.53
1	B	143	PHE	C-O	-5.88	1.17	1.24
1	B	558	PRO	C-O	-5.88	1.17	1.23
1	B	391	ILE	C-O	-5.88	1.17	1.24
1	B	903	GLU	C-O	-5.87	1.17	1.24
1	B	342	ASN	C-O	-5.87	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	378	VAL	C-O	-5.86	1.17	1.24
1	B	173	TYR	C-O	-5.85	1.17	1.24
1	B	202	MET	C-O	-5.85	1.16	1.24
1	B	729	VAL	CA-C	-5.85	1.46	1.52
1	B	620	GLU	C-O	-5.85	1.17	1.24
1	B	495	THR	C-O	-5.85	1.16	1.23
1	B	179	LEU	C-O	-5.84	1.17	1.24
1	B	694	TYR	CA-C	-5.83	1.45	1.52
1	B	796	LYS	C-O	-5.83	1.17	1.24
1	B	673	VAL	C-O	-5.81	1.18	1.24
1	B	501	ALA	C-O	-5.80	1.16	1.24
1	B	420	VAL	C-O	-5.80	1.17	1.24
1	B	299	LEU	C-O	-5.80	1.17	1.24
1	B	571	LEU	C-O	-5.80	1.17	1.24
1	B	581	PRO	C-O	-5.79	1.17	1.24
1	B	318	HIS	CA-C	-5.78	1.45	1.52
1	B	117	PRO	CA-C	-5.76	1.45	1.52
1	B	490	ASN	CA-C	-5.76	1.45	1.52
1	B	571	LEU	CA-C	-5.75	1.45	1.52
1	B	572	ASN	C-O	-5.75	1.17	1.24
1	B	585	LEU	C-O	-5.75	1.17	1.24
1	B	280	VAL	C-O	-5.74	1.18	1.24
1	B	180	ARG	C-O	-5.74	1.17	1.24
1	B	328	LEU	C-O	-5.73	1.16	1.23
1	B	496	VAL	C-O	-5.73	1.18	1.24
2	A	174	TRP	C-O	-5.73	1.17	1.24
1	B	447	LEU	CA-C	-5.72	1.45	1.52
1	B	286	ILE	C-O	-5.71	1.17	1.24
1	B	807	HIS	CA-C	-5.70	1.47	1.53
1	B	199	TYR	CA-C	-5.70	1.45	1.52
1	B	589	PHE	C-O	-5.70	1.17	1.24
1	B	884	ASP	C-O	-5.69	1.15	1.23
1	B	741	SER	C-O	-5.69	1.17	1.24
1	B	225	LEU	CA-C	-5.69	1.45	1.52
1	B	199	TYR	C-O	-5.69	1.17	1.24
1	B	760	LEU	C-O	-5.67	1.17	1.24
1	B	186	ILE	C-O	-5.65	1.18	1.24
1	B	227	MET	CA-C	-5.65	1.45	1.52
1	B	568	ASN	C-O	-5.65	1.17	1.24
1	B	573	LEU	C-O	-5.65	1.17	1.24
1	B	194	LEU	C-O	-5.64	1.17	1.24
1	B	508	ASP	C-O	-5.63	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	565	LEU	C-O	-5.63	1.17	1.23
1	B	652	PRO	C-O	-5.62	1.17	1.24
1	B	135	GLU	C-O	-5.62	1.16	1.23
1	B	468	GLU	C-O	-5.60	1.17	1.24
1	B	321	PHE	C-O	-5.60	1.18	1.24
2	A	173	ASN	CA-C	-5.59	1.45	1.52
1	B	694	TYR	C-O	-5.58	1.17	1.24
1	B	885	GLU	C-O	-5.58	1.17	1.24
1	B	654	LEU	CA-C	-5.57	1.46	1.53
1	B	785	ILE	C-O	-5.57	1.18	1.24
1	B	731	VAL	C-O	-5.57	1.17	1.23
2	A	178	SER	C-O	-5.57	1.17	1.23
1	B	522	GLY	C-O	-5.55	1.16	1.24
2	A	183	ASP	C-O	-5.54	1.17	1.24
1	B	207	GLN	C-O	-5.53	1.17	1.24
1	B	856	ARG	C-O	-5.53	1.17	1.24
1	B	292	PHE	C-O	-5.50	1.17	1.24
1	B	452	ILE	C-O	-5.50	1.18	1.24
1	B	730	PRO	C-O	-5.50	1.18	1.23
1	B	217	THR	C-O	-5.50	1.17	1.23
1	B	211	LEU	C-O	-5.49	1.17	1.24
1	B	998	ARG	C-O	-5.49	1.17	1.24
2	A	256	VAL	CA-CB	-5.48	1.47	1.54
1	B	309	THR	C-O	-5.48	1.17	1.23
1	B	104	VAL	C-O	-5.47	1.18	1.24
1	B	120	GLU	C-O	-5.47	1.17	1.24
1	B	695	VAL	C-O	-5.46	1.18	1.24
1	B	855	LYS	C-O	-5.45	1.17	1.24
1	B	481	ALA	C-O	-5.44	1.17	1.23
1	B	329	HIS	C-O	-5.44	1.17	1.24
1	B	587	LYS	CA-C	-5.44	1.44	1.52
1	B	470	LEU	C-O	-5.43	1.17	1.24
1	B	659	LEU	CA-C	-5.43	1.46	1.52
1	B	827	GLN	C-O	-5.43	1.17	1.24
1	B	853	CYS	C-O	-5.42	1.17	1.24
1	B	640	ILE	C-O	-5.42	1.18	1.24
1	B	146	GLU	C-O	-5.42	1.17	1.24
1	B	441	VAL	C-O	-5.42	1.17	1.24
1	B	603	GLU	C-O	-5.41	1.17	1.24
1	B	226	VAL	CA-C	-5.40	1.46	1.52
1	B	645	HIS	C-O	-5.40	1.17	1.24
1	B	655	GLN	C-O	-5.40	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	462	ILE	C-O	-5.39	1.17	1.24
1	B	727	GLN	C-O	-5.38	1.17	1.23
1	B	103	SER	CA-C	-5.38	1.46	1.52
1	B	142	ALA	C-O	-5.38	1.17	1.24
1	B	191	ILE	C-O	-5.38	1.17	1.24
1	B	295	TRP	C-O	-5.38	1.17	1.24
1	B	465	GLU	C-O	-5.37	1.17	1.24
1	B	854	ARG	CA-C	-5.37	1.45	1.52
1	B	285	THR	CA-C	-5.37	1.45	1.52
1	B	526	ARG	C-O	-5.36	1.17	1.24
1	B	225	LEU	C-O	-5.36	1.17	1.24
1	B	729	VAL	N-CA	-5.36	1.40	1.46
1	B	380	MET	C-O	-5.35	1.17	1.24
1	B	591	GLN	C-O	-5.35	1.17	1.24
1	B	812	ASP	CA-C	-5.35	1.47	1.53
1	B	99	VAL	C-O	-5.35	1.18	1.24
1	B	990	GLU	C-O	-5.34	1.17	1.24
1	B	500	ASN	C-O	-5.34	1.17	1.23
1	B	583	TYR	C-O	-5.33	1.17	1.24
1	B	555	SER	C-O	-5.33	1.16	1.23
1	B	541	GLU	CA-C	-5.33	1.46	1.52
1	B	115	ALA	CA-C	-5.33	1.46	1.52
1	B	607	ASN	C-O	-5.32	1.17	1.24
1	B	165	ALA	C-O	-5.32	1.17	1.24
2	A	204	ILE	C-O	-5.32	1.18	1.24
1	B	636	LEU	C-O	-5.31	1.17	1.24
1	B	168	THR	N-CA	-5.30	1.39	1.46
1	B	228	THR	C-O	-5.30	1.17	1.23
1	B	873	LYS	C-O	-5.30	1.17	1.24
1	B	162	HIS	C-O	-5.29	1.16	1.23
1	B	797	VAL	C-O	-5.29	1.18	1.24
1	B	149	GLN	C-O	-5.28	1.17	1.24
1	B	397	LYS	C-O	-5.28	1.18	1.24
2	A	187	TYR	C-O	-5.28	1.17	1.23
1	B	409	LEU	C-O	-5.28	1.17	1.23
1	B	615	ILE	C-O	-5.28	1.17	1.24
1	B	396	LYS	C-O	-5.27	1.18	1.24
2	A	254	ILE	C-O	-5.27	1.18	1.24
1	B	403	ALA	CA-C	-5.26	1.46	1.52
1	B	502	ARG	C-O	-5.26	1.17	1.23
1	B	857	VAL	C-O	-5.26	1.18	1.24
1	B	624	VAL	C-O	-5.26	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	732	LEU	C-O	-5.26	1.16	1.23
1	B	167	LYS	C-O	-5.25	1.17	1.24
1	B	582	GLU	C-O	-5.25	1.18	1.24
1	B	824	LYS	C-O	-5.25	1.18	1.24
1	B	383	GLU	C-O	-5.24	1.17	1.24
1	B	726	MET	C-O	-5.24	1.17	1.24
1	B	376	LYS	CA-C	-5.23	1.46	1.52
1	B	118	ALA	CA-C	-5.22	1.45	1.52
1	B	741	SER	CA-C	-5.22	1.46	1.52
1	B	248	TRP	C-O	-5.20	1.17	1.23
1	B	277	VAL	C-O	-5.20	1.17	1.24
1	B	479	LEU	CA-C	-5.20	1.46	1.52
1	B	909	LEU	C-O	-5.20	1.17	1.24
1	B	307	ILE	C-O	-5.20	1.18	1.24
2	A	183	ASP	CA-C	-5.20	1.46	1.52
1	B	229	THR	C-O	-5.19	1.18	1.24
1	B	584	MET	C-O	-5.19	1.18	1.24
1	B	175	ILE	C-O	-5.17	1.18	1.24
1	B	190	PRO	C-O	-5.17	1.17	1.24
1	B	264	VAL	C-O	-5.17	1.17	1.24
1	B	326	ASP	C-O	-5.17	1.17	1.24
1	B	535	VAL	CA-C	-5.17	1.46	1.52
1	B	866	SER	C-O	-5.17	1.17	1.24
1	B	491	MET	C-O	-5.16	1.18	1.25
1	B	305	HIS	C-O	-5.15	1.17	1.23
1	B	197	GLN	CA-C	-5.15	1.46	1.52
1	B	102	GLN	C-O	-5.14	1.17	1.24
1	B	139	ILE	C-O	-5.13	1.18	1.24
1	B	178	ALA	C-O	-5.13	1.18	1.24
1	B	146	GLU	CA-C	-5.13	1.46	1.52
1	B	541	GLU	C-O	-5.12	1.17	1.23
1	B	585	LEU	CA-C	-5.12	1.46	1.52
1	B	996	CYS	C-O	-5.12	1.18	1.24
1	B	644	ILE	C-O	-5.12	1.17	1.24
1	B	218	ILE	C-O	-5.11	1.18	1.24
1	B	752	PRO	C-O	-5.11	1.18	1.23
1	B	161	ALA	C-O	-5.11	1.17	1.23
1	B	886	LEU	C-O	-5.11	1.18	1.24
1	B	869	VAL	C-O	-5.10	1.18	1.24
1	B	710	SER	CA-C	-5.10	1.46	1.52
1	B	421	GLU	C-O	-5.09	1.18	1.24
1	B	415	GLU	C-O	-5.09	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	174	ALA	C-O	-5.09	1.18	1.24
2	A	188	LYS	C-O	-5.09	1.18	1.24
1	B	740	SER	CA-C	-5.07	1.46	1.52
1	B	399	CYS	C-O	-5.06	1.18	1.24
1	B	737	SER	C-O	-5.05	1.17	1.24
1	B	834	SER	CA-C	-5.04	1.46	1.52
1	B	944	LYS	C-O	-5.04	1.18	1.24
1	B	850	GLU	CA-C	-5.04	1.46	1.52
1	B	311	TYR	N-CA	-5.03	1.39	1.46
1	B	278	HIS	C-O	-5.03	1.17	1.23
1	B	158	LEU	C-O	-5.03	1.18	1.24
1	B	490	ASN	N-CA	-5.02	1.40	1.46
1	B	982	ILE	C-O	-5.02	1.18	1.24
1	B	570	VAL	C-O	-5.02	1.18	1.24
1	B	270	ILE	C-O	-5.01	1.18	1.24
1	B	728	VAL	C-O	-5.01	1.18	1.24
1	B	1023	PHE	C-O	-5.00	1.18	1.24
1	B	1027	ILE	N-CA	-5.00	1.40	1.46
1	B	195	SER	C-O	-5.00	1.18	1.24
1	B	695	VAL	CA-CB	-5.00	1.48	1.54
1	B	334	GLU	C-O	-5.00	1.17	1.24

All (140) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	807	HIS	CA-C-N	18.21	139.26	119.05
1	B	807	HIS	C-N-CA	18.21	139.26	119.05
1	B	1037	ALA	N-CA-C	16.89	129.69	111.28
2	A	231	LEU	N-CA-C	14.45	126.75	111.14
1	B	812	ASP	CA-C-N	13.98	133.97	119.85
1	B	812	ASP	C-N-CA	13.98	133.97	119.85
1	B	577	GLU	N-CA-C	13.74	126.26	111.28
2	A	170	ASP	CA-C-N	12.66	132.35	119.56
2	A	170	ASP	C-N-CA	12.66	132.35	119.56
1	B	651	LEU	CA-C-N	11.85	132.31	119.28
1	B	651	LEU	C-N-CA	11.85	132.31	119.28
1	B	774	ILE	CA-C-N	11.43	131.53	119.76
1	B	774	ILE	C-N-CA	11.43	131.53	119.76
1	B	963	LYS	CA-C-N	11.29	133.81	120.94
1	B	963	LYS	C-N-CA	11.29	133.81	120.94
1	B	286	ILE	CA-C-N	11.25	131.66	119.28
1	B	286	ILE	C-N-CA	11.25	131.66	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	930	GLY	CA-C-N	10.98	130.82	119.19
1	B	930	GLY	C-N-CA	10.98	130.82	119.19
1	B	529	MET	N-CA-C	10.81	126.47	113.28
1	B	260	SER	N-CA-C	10.23	122.02	111.07
1	B	1040	LEU	N-CA-C	-10.12	94.88	109.96
1	B	189	SER	CA-C-N	9.54	129.63	119.05
1	B	189	SER	C-N-CA	9.54	129.63	119.05
2	A	168	LYS	CA-C-N	9.52	129.28	119.76
2	A	168	LYS	C-N-CA	9.52	129.28	119.76
1	B	460	LEU	CA-C-N	9.24	129.31	119.05
1	B	460	LEU	C-N-CA	9.24	129.31	119.05
1	B	244	ARG	N-CA-C	9.14	121.24	111.28
1	B	722	GLU	N-CA-C	8.98	123.76	110.48
1	B	175	ILE	CB-CA-C	-8.80	100.07	112.22
2	A	163	PHE	N-CA-C	8.77	122.87	110.50
1	B	691	ASP	CA-C-N	8.21	131.34	120.25
1	B	691	ASP	C-N-CA	8.21	131.34	120.25
1	B	913	VAL	N-CA-C	8.21	119.97	112.17
1	B	240	SER	N-CA-C	8.21	121.18	110.43
1	B	1038	ALA	N-CA-C	7.95	122.28	112.58
2	A	252	SER	N-CA-C	7.91	120.81	111.71
1	B	527	ARG	N-CA-C	7.88	119.50	111.07
2	A	225	THR	N-CA-C	-7.88	102.68	111.82
1	B	107	VAL	N-CA-C	7.82	125.61	109.34
1	B	1033	ASP	N-CA-C	7.78	121.23	108.08
2	A	201	LYS	N-CA-C	-7.72	103.76	113.02
1	B	618	PRO	N-CA-C	-7.57	99.30	111.19
1	B	733	VAL	N-CA-C	7.57	118.34	110.62
1	B	387	GLN	CA-C-N	-7.47	112.06	119.90
1	B	387	GLN	C-N-CA	-7.47	112.06	119.90
1	B	667	ASP	CB-CA-C	7.47	122.56	110.16
1	B	458	GLY	N-CA-C	7.38	122.91	113.24
1	B	505	ASP	CB-CA-C	-7.11	97.02	110.67
1	B	1034	ILE	CB-CA-C	-7.11	100.75	112.26
1	B	683	VAL	N-CA-CB	-7.10	99.52	111.23
2	A	229	VAL	CB-CA-C	-7.05	100.54	111.26
1	B	207	GLN	N-CA-C	6.96	118.94	111.36
1	B	136	TYR	CA-C-N	6.95	126.76	119.05
1	B	136	TYR	C-N-CA	6.95	126.76	119.05
1	B	306	VAL	CB-CA-C	-6.94	100.83	110.96
1	B	215	ASP	N-CA-C	6.93	118.92	111.36
1	B	1030	ILE	N-CA-C	6.88	117.67	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	261	GLU	N-CA-C	6.87	118.56	111.14
1	B	757	GLN	CA-C-N	6.76	129.33	120.28
1	B	757	GLN	C-N-CA	6.76	129.33	120.28
1	B	985	MET	N-CA-C	6.74	118.63	111.28
1	B	954	ASP	CB-CA-C	6.70	122.61	109.35
2	A	198	ASN	CA-C-N	-6.66	112.83	120.89
2	A	198	ASN	C-N-CA	-6.66	112.83	120.89
1	B	331	VAL	N-CA-C	6.63	119.38	111.09
2	A	227	LYS	N-CA-C	6.45	119.04	110.53
1	B	619	ASN	N-CA-C	6.42	118.28	111.28
1	B	539	VAL	N-CA-C	6.41	117.26	107.77
1	B	921	MET	CA-C-N	6.33	127.76	119.84
1	B	921	MET	C-N-CA	6.33	127.76	119.84
1	B	667	ASP	N-CA-CB	6.33	120.52	110.65
1	B	226	VAL	CB-CA-C	-6.32	102.32	110.98
1	B	924	LEU	N-CA-C	6.30	119.68	109.40
1	B	899	ASP	N-CA-C	6.19	120.97	113.17
1	B	913	VAL	CB-CA-C	-6.11	104.09	111.85
1	B	617	ILE	CA-C-N	-6.10	113.66	119.76
1	B	617	ILE	C-N-CA	-6.10	113.66	119.76
1	B	506	GLY	N-CA-C	-6.08	106.71	114.37
1	B	477	LYS	N-CA-C	5.94	117.84	111.36
1	B	118	ALA	N-CA-C	5.92	119.60	112.38
1	B	483	GLU	N-CA-C	5.92	119.60	112.38
1	B	1031	LYS	N-CA-C	5.90	119.08	107.98
1	B	104	VAL	N-CA-C	5.88	116.40	108.17
1	B	438	LEU	CA-C-N	5.88	125.74	119.28
1	B	438	LEU	C-N-CA	5.88	125.74	119.28
1	B	442	GLU	N-CA-C	5.88	117.68	111.28
1	B	993	ILE	CB-CA-C	-5.87	104.45	111.97
1	B	942	ILE	CB-CA-C	-5.84	104.25	112.14
1	B	256	TYR	CA-C-N	5.82	128.66	120.28
1	B	256	TYR	C-N-CA	5.82	128.66	120.28
1	B	273	LEU	CA-C-N	5.71	125.91	120.31
1	B	273	LEU	C-N-CA	5.71	125.91	120.31
2	A	229	VAL	N-CA-C	5.68	116.90	109.58
1	B	621	GLU	N-CA-C	5.63	119.62	112.87
1	B	713	GLU	N-CA-C	5.60	118.32	111.82
1	B	557	ASP	CA-C-N	5.58	125.34	119.76
1	B	557	ASP	C-N-CA	5.58	125.34	119.76
1	B	649	TYR	N-CA-C	5.58	117.45	111.36
1	B	476	ILE	N-CA-C	5.55	115.58	107.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1006	GLN	N-CA-C	-5.48	105.31	111.28
1	B	646	LYS	N-CA-C	-5.46	102.89	109.83
1	B	279	TYR	N-CA-C	5.43	118.08	109.50
1	B	846	LEU	N-CA-C	5.42	117.19	111.28
1	B	947	ALA	CA-C-N	5.38	127.50	120.28
1	B	947	ALA	C-N-CA	5.38	127.50	120.28
1	B	205	GLU	N-CA-C	5.35	117.19	111.36
1	B	598	ILE	CA-C-N	5.33	124.96	119.05
1	B	598	ILE	C-N-CA	5.33	124.96	119.05
1	B	1025	GLU	CA-C-N	5.24	125.77	120.00
1	B	1025	GLU	C-N-CA	5.24	125.77	120.00
2	A	205	SER	N-CA-C	5.23	116.94	108.41
1	B	1039	SER	CA-C-N	-5.22	113.30	121.02
1	B	1039	SER	C-N-CA	-5.22	113.30	121.02
1	B	237	TYR	N-CA-C	5.21	117.04	111.36
1	B	650	CYS	N-CA-C	5.21	119.35	112.89
1	B	168	THR	N-CA-C	5.18	117.66	111.71
2	A	228	SER	N-CA-C	5.18	117.25	109.23
2	A	254	ILE	N-CA-C	-5.16	101.84	107.73
1	B	597	ALA	CA-C-N	5.16	123.49	120.24
1	B	597	ALA	C-N-CA	5.16	123.49	120.24
1	B	640	ILE	CB-CA-C	-5.16	105.27	112.02
1	B	1032	ARG	N-CA-C	5.16	116.91	109.07
1	B	753	VAL	CB-CA-C	-5.12	105.23	112.14
1	B	925	THR	N-CA-C	-5.12	103.39	110.35
1	B	684	LYS	N-CA-C	5.11	120.41	113.16
1	B	275	ASP	CA-C-N	5.10	127.62	120.28
1	B	275	ASP	C-N-CA	5.10	127.62	120.28
2	A	179	LEU	CA-C-N	5.09	131.37	122.81
2	A	179	LEU	C-N-CA	5.09	131.37	122.81
1	B	624	VAL	CB-CA-C	-5.07	105.30	112.14
1	B	920	GLU	N-CA-C	5.06	116.53	108.79
1	B	774	ILE	N-CA-C	-5.05	104.32	109.02
1	B	751	ARG	CA-C-N	5.04	124.94	119.85
1	B	751	ARG	C-N-CA	5.04	124.94	119.85
1	B	1036	PHE	N-CA-C	5.04	118.98	111.87
2	A	199	PRO	CA-N-CD	-5.02	104.97	112.00
1	B	579	ILE	CG1-CB-CG2	-5.01	95.66	110.70
1	B	813	PRO	N-CA-C	-5.01	103.41	111.38

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	684	LYS	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	B	6907	0	6547	586	0
2	A	676	0	661	95	0
3	B	1	0	0	0	0
4	B	31	0	12	10	0
5	A	5	0	0	1	0
5	B	27	0	0	8	0
All	All	7647	0	7220	631	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 43.

All (631) 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:686:ASN:CB	1:B:960:SER:CB	1.75	1.56
1:B:313:PRO:CB	1:B:527:ARG:NH1	1.72	1.53
1:B:686:ASN:CB	1:B:960:SER:HB3	1.07	1.49
1:B:313:PRO:CG	1:B:527:ARG:NH1	1.77	1.45
1:B:465:GLU:OE2	1:B:1040:LEU:CB	1.65	1.42
1:B:396:LYS:HG2	1:B:456:HIS:CE1	1.53	1.42
1:B:396:LYS:CG	1:B:456:HIS:ND1	1.83	1.40
1:B:615:ILE:HD11	1:B:825:LYS:CG	1.53	1.38
1:B:884:ASP:O	1:B:888:LEU:CD2	1.76	1.32
1:B:896:LEU:O	1:B:900:LEU:CD2	1.76	1.32
1:B:713:GLU:OE2	2:A:200:LYS:HE3	1.18	1.32
1:B:968:ASP:HB3	5:B:1221:HOH:O	1.19	1.28
1:B:168:THR:CG2	4:B:1102:ATP:O2A	1.80	1.27
1:B:615:ILE:CD1	1:B:825:LYS:CG	2.16	1.22
1:B:897:PHE:CA	1:B:900:LEU:HD23	1.69	1.22
1:B:396:LYS:HG2	1:B:456:HIS:ND1	0.88	1.20
1:B:888:LEU:HD22	1:B:912:PHE:CE2	1.75	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:170:ASP:HB2	2:A:181:ARG:NH1	1.57	1.20
1:B:884:ASP:O	1:B:888:LEU:HD23	1.27	1.19
1:B:468:GLU:O	1:B:491:MET:CE	1.90	1.19
1:B:880:ILE:HD13	1:B:888:LEU:HD12	1.21	1.16
1:B:168:THR:HB	4:B:1102:ATP:O2A	1.46	1.15
1:B:375:PHE:HZ	1:B:409:LEU:HD21	1.05	1.15
1:B:880:ILE:HG21	1:B:888:LEU:HD11	1.28	1.15
1:B:615:ILE:CD1	1:B:825:LYS:HG2	1.75	1.14
1:B:168:THR:CB	4:B:1102:ATP:O2A	1.97	1.12
1:B:431:LEU:HD11	1:B:1034:ILE:CG2	1.80	1.11
1:B:375:PHE:CZ	1:B:409:LEU:HD21	1.85	1.11
1:B:896:LEU:C	1:B:900:LEU:HD21	1.75	1.10
2:A:244:GLU:HG2	2:A:245:PRO:HD2	1.31	1.10
2:A:249:GLU:HB3	2:A:250:PRO:HD2	1.22	1.10
1:B:233:ARG:NH2	1:B:568:ASN:OD1	1.83	1.09
1:B:897:PHE:HA	1:B:900:LEU:CD2	1.80	1.09
1:B:431:LEU:CD1	1:B:1034:ILE:HG22	1.82	1.09
1:B:468:GLU:O	1:B:491:MET:HE1	1.45	1.09
1:B:896:LEU:O	1:B:900:LEU:HD21	0.92	1.09
1:B:313:PRO:HG2	1:B:527:ARG:NH1	1.62	1.07
1:B:192:LYS:HE3	1:B:213:THR:HG21	1.33	1.07
1:B:615:ILE:CD1	1:B:825:LYS:HG3	1.80	1.05
1:B:884:ASP:C	1:B:888:LEU:HD21	1.80	1.05
1:B:612:TYR:CE1	1:B:825:LYS:HD3	1.89	1.05
1:B:313:PRO:HB3	1:B:527:ARG:NH1	1.44	1.05
1:B:880:ILE:HG21	1:B:888:LEU:CD1	1.87	1.04
1:B:396:LYS:CG	1:B:456:HIS:CE1	2.31	1.04
1:B:468:GLU:C	1:B:491:MET:HE1	1.82	1.04
1:B:168:THR:HG22	4:B:1102:ATP:O2A	1.51	1.04
2:A:244:GLU:HG2	2:A:245:PRO:CD	1.89	1.02
1:B:236:LEU:HB3	1:B:272:LEU:HD13	1.39	1.02
1:B:713:GLU:OE2	2:A:200:LYS:CE	2.08	1.02
1:B:968:ASP:CB	5:B:1221:HOH:O	1.85	1.02
1:B:897:PHE:HA	1:B:900:LEU:HD23	1.02	1.01
1:B:482:THR:HG21	5:B:1202:HOH:O	1.61	1.01
1:B:468:GLU:CA	1:B:491:MET:HE1	1.92	0.99
1:B:139:ILE:HD12	1:B:139:ILE:H	1.24	0.99
1:B:347:MET:HE2	1:B:543:MET:H	1.27	0.99
1:B:897:PHE:C	1:B:900:LEU:HD23	1.88	0.98
1:B:387:GLN:HB3	1:B:388:PRO:CD	1.94	0.97
1:B:884:ASP:O	1:B:888:LEU:HD21	1.60	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:997:MET:HE1	1:B:1030:ILE:HG23	1.44	0.97
1:B:406:MET:HB3	1:B:452:ILE:CD1	1.95	0.97
1:B:686:ASN:CB	1:B:960:SER:HB2	1.91	0.96
1:B:460:LEU:HD22	1:B:460:LEU:H	1.28	0.96
1:B:749:ASP:OD1	1:B:751:ARG:HG3	1.63	0.96
1:B:977:ALA:O	1:B:1032:ARG:NH1	2.00	0.94
2:A:249:GLU:CB	2:A:250:PRO:HD2	1.94	0.94
1:B:431:LEU:HD11	1:B:1034:ILE:HG22	0.95	0.93
1:B:258:ARG:NH1	1:B:557:ASP:O	2.02	0.93
1:B:450:ARG:NH1	1:B:450:ARG:HB2	1.84	0.93
1:B:686:ASN:CB	1:B:960:SER:CA	2.48	0.92
1:B:770:PHE:CD2	1:B:775:PRO:HD3	2.04	0.92
1:B:498:PHE:O	1:B:538:MET:HG3	1.70	0.92
1:B:598:ILE:CD1	1:B:842:ALA:HB1	2.00	0.90
1:B:897:PHE:CA	1:B:900:LEU:CD2	2.44	0.89
1:B:598:ILE:HD13	1:B:842:ALA:HB1	1.53	0.89
2:A:170:ASP:HB2	2:A:181:ARG:HH12	1.27	0.89
1:B:511:TRP:CZ3	1:B:543:MET:HE3	2.08	0.88
1:B:841:LYS:O	1:B:844:THR:HG23	1.71	0.88
1:B:888:LEU:CD2	1:B:912:PHE:CE2	2.57	0.88
1:B:633:LEU:CD1	1:B:804:MET:HE1	2.04	0.88
1:B:490:ASN:ND2	1:B:490:ASN:O	2.07	0.87
1:B:254:ILE:HG22	1:B:283:SER:HB2	1.57	0.87
1:B:253:GLU:OE1	5:B:1201:HOH:O	1.91	0.87
1:B:751:ARG:HG3	1:B:751:ARG:HH11	1.39	0.87
2:A:231:LEU:HD23	2:A:231:LEU:H	1.39	0.86
2:A:213:LYS:HE3	2:A:213:LYS:HA	1.58	0.86
1:B:894:ASN:O	1:B:894:ASN:ND2	2.07	0.86
1:B:884:ASP:C	1:B:888:LEU:CD2	2.45	0.85
1:B:997:MET:CE	1:B:1030:ILE:HG23	2.07	0.85
1:B:465:GLU:OE2	1:B:1040:LEU:CA	2.25	0.85
2:A:164:ARG:HD2	5:A:302:HOH:O	1.75	0.85
1:B:700:LEU:HD12	1:B:729:VAL:CG1	2.07	0.84
1:B:347:MET:HE2	1:B:543:MET:N	1.92	0.84
1:B:442:GLU:OE1	2:A:221:GLU:OE1	1.94	0.84
1:B:254:ILE:CG2	1:B:283:SER:HB2	2.06	0.84
1:B:380:MET:HE1	2:A:254:ILE:HG21	1.60	0.84
1:B:192:LYS:CE	1:B:213:THR:HG21	2.08	0.83
1:B:880:ILE:CG2	1:B:888:LEU:HD11	2.08	0.83
2:A:172:ALA:HB1	2:A:180:TYR:CD2	2.13	0.83
1:B:888:LEU:HD22	1:B:912:PHE:HE2	1.44	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:388:PRO:HG3	1:B:526:ARG:HH12	1.44	0.82
1:B:615:ILE:HD11	1:B:825:LYS:HG2	0.84	0.82
1:B:743:ARG:HG3	2:A:166:ASP:HB3	1.61	0.82
1:B:313:PRO:HG3	1:B:527:ARG:NH1	1.95	0.82
1:B:633:LEU:CD1	1:B:804:MET:CE	2.58	0.82
1:B:321:PHE:HE2	1:B:372:SER:HB2	1.45	0.82
1:B:388:PRO:HG3	1:B:526:ARG:NH1	1.94	0.81
1:B:468:GLU:O	1:B:491:MET:HE2	1.78	0.81
1:B:727:GLN:HE22	2:A:190:LYS:HD3	1.46	0.81
1:B:336:GLY:O	1:B:553:LYS:HD3	1.79	0.81
1:B:458:GLY:O	1:B:991:GLY:N	2.13	0.81
1:B:404:LEU:CD2	2:A:224:PHE:CZ	2.63	0.81
1:B:703:SER:HB2	1:B:706:SER:HB2	1.61	0.81
1:B:735:LEU:HD11	2:A:196:GLY:HA2	1.62	0.81
1:B:460:LEU:H	1:B:460:LEU:CD2	1.94	0.80
1:B:897:PHE:C	1:B:900:LEU:CD2	2.54	0.80
1:B:511:TRP:CZ3	1:B:543:MET:CE	2.63	0.80
1:B:815:LEU:HD22	1:B:815:LEU:O	1.81	0.80
1:B:237:TYR:OH	1:B:268:GLU:OE1	2.00	0.79
1:B:380:MET:HE1	2:A:254:ILE:CG2	2.12	0.79
1:B:125:LEU:HG	1:B:153:ASN:OD1	1.82	0.79
1:B:431:LEU:CD1	1:B:1034:ILE:CG2	2.52	0.79
1:B:347:MET:CE	1:B:543:MET:H	1.95	0.78
1:B:735:LEU:HD11	2:A:196:GLY:CA	2.14	0.78
1:B:779:PRO:HA	1:B:783:MET:HG3	1.66	0.77
1:B:101:VAL:HG11	1:B:290:ARG:HD2	1.65	0.77
1:B:267:GLU:OE1	1:B:561:SER:HB2	1.84	0.77
1:B:406:MET:HB3	1:B:452:ILE:HD11	1.63	0.77
1:B:598:ILE:HD11	1:B:842:ALA:CB	2.15	0.77
2:A:231:LEU:HD23	2:A:231:LEU:N	2.00	0.76
1:B:351:ARG:O	1:B:352:ASP:HB2	1.85	0.76
1:B:404:LEU:CD2	2:A:224:PHE:HZ	1.98	0.76
1:B:953:ILE:HD12	1:B:953:ILE:N	2.02	0.75
1:B:598:ILE:HD11	1:B:842:ALA:HA	1.69	0.75
1:B:751:ARG:HG3	1:B:751:ARG:NH1	2.00	0.75
1:B:848:MET:HE2	1:B:851:LEU:HD23	1.68	0.75
1:B:880:ILE:HD13	1:B:888:LEU:CD1	2.11	0.75
1:B:711:ALA:O	2:A:190:LYS:HE3	1.86	0.75
1:B:644:ILE:HD11	1:B:779:PRO:HG3	1.67	0.74
1:B:456:HIS:HB2	1:B:482:THR:HB	1.68	0.74
1:B:598:ILE:HD11	1:B:842:ALA:CA	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:749:ASP:CG	1:B:751:ARG:NH1	2.44	0.74
1:B:700:LEU:HD12	1:B:729:VAL:HG11	1.69	0.74
1:B:633:LEU:HD11	1:B:804:MET:CE	2.18	0.74
1:B:673:VAL:HG12	1:B:699:LEU:HB3	1.70	0.74
1:B:888:LEU:HB2	1:B:1007:MET:HE1	1.69	0.74
1:B:651:LEU:N	1:B:652:PRO:HD2	2.02	0.74
1:B:659:LEU:HD12	1:B:742:VAL:HB	1.68	0.74
1:B:891:MET:HE3	1:B:935:MET:HB2	1.70	0.73
1:B:585:LEU:HD23	1:B:848:MET:HE3	1.69	0.73
1:B:482:THR:CB	5:B:1202:HOH:O	2.35	0.73
1:B:953:ILE:HD12	1:B:953:ILE:H	1.53	0.73
2:A:249:GLU:HB3	2:A:250:PRO:CD	2.11	0.73
1:B:870:ILE:HG23	1:B:875:ARG:NH1	2.04	0.73
1:B:465:GLU:CD	1:B:1040:LEU:N	2.47	0.72
1:B:381:ILE:HG23	1:B:386:PHE:HB2	1.71	0.72
1:B:972:THR:HG21	1:B:985:MET:HE1	1.71	0.72
1:B:598:ILE:CD1	1:B:842:ALA:CB	2.68	0.72
1:B:888:LEU:HD22	1:B:912:PHE:CD2	2.21	0.72
1:B:482:THR:CG2	5:B:1202:HOH:O	2.29	0.72
1:B:236:LEU:CB	1:B:272:LEU:HD13	2.19	0.71
1:B:572:ASN:O	1:B:576:VAL:HG13	1.90	0.71
1:B:596:ARG:HH11	1:B:596:ARG:CG	2.04	0.71
1:B:406:MET:HB3	1:B:452:ILE:HD13	1.73	0.71
1:B:460:LEU:HD22	1:B:460:LEU:N	2.05	0.71
1:B:774:ILE:C	1:B:774:ILE:HD12	2.15	0.71
1:B:144:GLN:NE2	1:B:169:VAL:HG13	2.05	0.71
1:B:972:THR:HG21	1:B:985:MET:CE	2.20	0.71
1:B:294:GLU:OE2	1:B:596:ARG:NH2	2.24	0.70
1:B:565:LEU:HD22	1:B:847:GLN:HE21	1.56	0.70
1:B:882:SER:OG	1:B:1006:GLN:HG3	1.90	0.70
1:B:848:MET:HE2	1:B:851:LEU:CD2	2.21	0.70
1:B:465:GLU:OE2	1:B:1040:LEU:N	2.24	0.70
1:B:974:ALA:O	1:B:1029:LYS:HB3	1.92	0.69
1:B:334:GLU:OE2	1:B:532:ARG:HG2	1.92	0.69
1:B:997:MET:HE1	1:B:1030:ILE:CG2	2.22	0.69
2:A:173:ASN:OD1	2:A:173:ASN:N	2.22	0.69
1:B:881:SER:H	1:B:1006:GLN:HE21	1.39	0.69
1:B:243:MET:HG3	1:B:243:MET:O	1.90	0.69
1:B:456:HIS:CB	1:B:482:THR:HB	2.22	0.69
1:B:888:LEU:CD2	1:B:912:PHE:HE2	1.99	0.69
1:B:900:LEU:HD22	1:B:900:LEU:H	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:815:LEU:HD22	1:B:815:LEU:C	2.16	0.69
2:A:170:ASP:CB	2:A:181:ARG:NH1	2.48	0.69
1:B:404:LEU:HD21	2:A:224:PHE:HZ	1.58	0.69
1:B:411:PHE:HB3	1:B:477:LYS:HD2	1.74	0.69
1:B:456:HIS:HB2	5:B:1202:HOH:O	1.93	0.68
1:B:144:GLN:HE22	1:B:169:VAL:CG1	2.05	0.68
1:B:751:ARG:HH11	1:B:751:ARG:CG	2.06	0.68
1:B:387:GLN:HB3	1:B:388:PRO:HD3	1.76	0.68
1:B:144:GLN:NE2	1:B:166:GLY:O	2.27	0.68
1:B:615:ILE:C	1:B:615:ILE:HD12	2.18	0.68
1:B:770:PHE:HD2	1:B:775:PRO:HD3	1.59	0.68
1:B:202:MET:HA	1:B:202:MET:HE2	1.75	0.68
1:B:1024:ALA:O	1:B:1027:ILE:HD11	1.94	0.68
1:B:859:ARG:HE	1:B:866:SER:HA	1.60	0.67
1:B:225:LEU:HD23	1:B:227:MET:HE2	1.77	0.67
1:B:233:ARG:HH11	1:B:268:GLU:CD	2.03	0.67
1:B:888:LEU:HB3	1:B:912:PHE:HE2	1.58	0.67
1:B:749:ASP:OD1	1:B:751:ARG:CG	2.42	0.67
2:A:213:LYS:HA	2:A:213:LYS:CE	2.25	0.67
1:B:334:GLU:OE2	1:B:532:ARG:CG	2.43	0.67
1:B:636:LEU:HD22	1:B:793:VAL:HG13	1.77	0.67
1:B:465:GLU:CD	1:B:1040:LEU:CB	2.63	0.67
1:B:215:ASP:OD1	1:B:215:ASP:N	2.23	0.66
1:B:445:LEU:HD12	1:B:445:LEU:O	1.95	0.66
1:B:582:GLU:HG3	1:B:851:LEU:CD2	2.26	0.66
1:B:243:MET:HE2	1:B:243:MET:HA	1.77	0.66
1:B:252:ASP:OD1	1:B:282:LEU:HD12	1.95	0.66
1:B:1014:ILE:C	1:B:1014:ILE:HD12	2.20	0.66
1:B:749:ASP:OD1	1:B:751:ARG:NH1	2.29	0.66
1:B:912:PHE:HE1	1:B:935:MET:HE1	1.61	0.66
1:B:399:CYS:SG	1:B:480:PHE:O	2.53	0.66
1:B:797:VAL:O	1:B:801:GLU:HG3	1.96	0.66
1:B:888:LEU:CB	1:B:1007:MET:HE1	2.25	0.66
2:A:172:ALA:HB1	2:A:180:TYR:HD2	1.60	0.66
2:A:244:GLU:CG	2:A:245:PRO:CD	2.71	0.66
1:B:188:THR:HA	1:B:227:MET:O	1.96	0.65
1:B:615:ILE:HD13	1:B:825:LYS:HG3	1.76	0.65
1:B:749:ASP:OD2	1:B:751:ARG:NH1	2.29	0.65
1:B:971:TYR:O	1:B:975:THR:HG23	1.95	0.65
1:B:973:TRP:O	1:B:1032:ARG:NH2	2.29	0.65
1:B:468:GLU:HA	1:B:491:MET:HE1	1.76	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:617:ILE:H	1:B:618:PRO:HD3	1.62	0.65
1:B:440:GLN:NE2	2:A:216:SER:OG	2.30	0.65
1:B:212:MET:HE2	1:B:235:MET:HE3	1.78	0.65
1:B:532:ARG:NH2	2:A:249:GLU:HA	2.12	0.65
1:B:144:GLN:NE2	1:B:169:VAL:CG1	2.61	0.64
1:B:382:MET:HE3	1:B:382:MET:HA	1.77	0.64
1:B:968:ASP:OD1	1:B:968:ASP:N	2.29	0.64
1:B:139:ILE:H	1:B:139:ILE:CD1	2.00	0.64
1:B:448:LEU:HD23	1:B:470:LEU:CD1	2.28	0.64
1:B:404:LEU:CD2	2:A:224:PHE:CE1	2.81	0.64
1:B:138:PHE:CD1	4:B:1102:ATP:C6	2.86	0.64
1:B:615:ILE:HD13	1:B:825:LYS:CG	2.22	0.64
1:B:237:TYR:O	1:B:575:ARG:NH2	2.25	0.63
1:B:932:LEU:HD22	1:B:932:LEU:O	1.97	0.63
1:B:406:MET:CB	1:B:452:ILE:CD1	2.75	0.63
1:B:465:GLU:CD	1:B:1040:LEU:CA	2.71	0.63
1:B:450:ARG:HB2	1:B:450:ARG:CZ	2.27	0.63
1:B:686:ASN:CB	1:B:960:SER:HA	2.26	0.63
1:B:809:LEU:HD22	1:B:809:LEU:O	1.99	0.63
1:B:1025:GLU:OE2	1:B:1025:GLU:HA	1.97	0.63
1:B:744:LEU:HD12	1:B:762:SER:HB3	1.81	0.63
1:B:450:ARG:HB2	1:B:450:ARG:HH11	1.59	0.63
1:B:633:LEU:HD11	1:B:804:MET:HE3	1.80	0.63
1:B:617:ILE:N	1:B:618:PRO:HD3	2.14	0.62
1:B:732:LEU:HD23	1:B:734:HIS:HE1	1.65	0.62
1:B:274:PRO:HD2	1:B:277:VAL:HG21	1.82	0.62
1:B:387:GLN:HA	1:B:387:GLN:NE2	2.15	0.62
1:B:313:PRO:HB2	1:B:527:ARG:NH1	2.03	0.61
1:B:891:MET:CE	1:B:935:MET:HB2	2.29	0.61
1:B:888:LEU:HB3	1:B:912:PHE:CE2	2.35	0.61
2:A:170:ASP:HB2	2:A:181:ARG:HH11	1.63	0.61
1:B:460:LEU:CD1	1:B:990:GLU:HB2	2.30	0.61
1:B:375:PHE:HE2	1:B:405:GLN:O	1.84	0.61
1:B:460:LEU:HD13	1:B:990:GLU:HB2	1.81	0.61
1:B:675:VAL:HG11	2:A:187:TYR:CD2	2.36	0.61
1:B:404:LEU:HD21	2:A:224:PHE:CZ	2.32	0.61
1:B:645:HIS:CE1	1:B:734:HIS:O	2.53	0.61
1:B:532:ARG:NH2	2:A:249:GLU:N	2.48	0.61
1:B:404:LEU:HD22	2:A:224:PHE:CE1	2.35	0.61
1:B:727:GLN:HE22	2:A:190:LYS:HB2	1.66	0.61
1:B:1003:LEU:HD12	1:B:1003:LEU:O	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:347:MET:HE2	1:B:543:MET:CB	2.31	0.60
1:B:930:GLY:N	1:B:931:PRO:CD	2.64	0.60
1:B:1009:GLN:HE21	1:B:1009:GLN:CA	2.14	0.60
1:B:233:ARG:NH1	1:B:268:GLU:OE2	2.32	0.60
1:B:468:GLU:CB	1:B:491:MET:HE1	2.31	0.60
1:B:396:LYS:CD	1:B:456:HIS:CE1	2.84	0.60
1:B:744:LEU:N	1:B:744:LEU:HD23	2.16	0.60
1:B:633:LEU:HD12	1:B:804:MET:HE1	1.84	0.60
1:B:372:SER:O	1:B:372:SER:OG	2.14	0.60
1:B:374:VAL:O	1:B:378:VAL:HG23	2.01	0.60
1:B:446:PRO:O	1:B:450:ARG:NH1	2.34	0.60
2:A:256:VAL:O	2:A:256:VAL:HG13	2.00	0.60
1:B:1009:GLN:HA	1:B:1009:GLN:NE2	2.16	0.60
1:B:633:LEU:HD12	1:B:804:MET:CE	2.30	0.60
1:B:144:GLN:HE22	1:B:169:VAL:HG13	1.65	0.59
2:A:219:GLN:O	2:A:223:TYR:CE2	2.55	0.59
1:B:532:ARG:HH22	2:A:249:GLU:N	2.00	0.59
1:B:651:LEU:N	1:B:652:PRO:CD	2.66	0.59
1:B:812:ASP:CB	1:B:813:PRO:HD2	2.32	0.59
1:B:880:ILE:HG21	1:B:888:LEU:HD12	1.80	0.59
1:B:465:GLU:CD	1:B:1040:LEU:H	2.11	0.59
1:B:601:VAL:O	1:B:605:VAL:HG23	2.03	0.59
1:B:617:ILE:N	1:B:618:PRO:CD	2.66	0.59
1:B:511:TRP:CE3	1:B:543:MET:HE2	2.38	0.59
1:B:582:GLU:HG3	1:B:851:LEU:HD21	1.84	0.59
1:B:888:LEU:CB	1:B:912:PHE:HE2	2.15	0.59
1:B:661:LYS:HB2	1:B:738:ALA:HB3	1.85	0.58
1:B:900:LEU:HD22	1:B:900:LEU:N	2.17	0.58
1:B:964:PRO:HA	1:B:967:MET:HG3	1.83	0.58
2:A:219:GLN:O	2:A:223:TYR:CD2	2.56	0.58
1:B:450:ARG:HE	2:A:227:LYS:HZ2	1.50	0.58
1:B:470:LEU:CD2	1:B:475:LEU:HD12	2.34	0.58
1:B:483:GLU:O	1:B:483:GLU:HG2	2.03	0.57
2:A:199:PRO:HB2	2:A:201:LYS:HE3	1.86	0.57
1:B:243:MET:HA	1:B:243:MET:CE	2.34	0.57
1:B:972:THR:CB	1:B:985:MET:HE1	2.35	0.57
1:B:492:PRO:HB2	1:B:526:ARG:HG2	1.87	0.57
2:A:213:LYS:HG3	2:A:213:LYS:O	2.05	0.57
1:B:888:LEU:CG	1:B:912:PHE:HE2	2.18	0.57
1:B:1000:LEU:O	1:B:1000:LEU:HD23	2.05	0.57
1:B:139:ILE:HD12	1:B:139:ILE:N	2.07	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:396:LYS:CB	1:B:456:HIS:CE1	2.89	0.56
1:B:233:ARG:NH1	1:B:268:GLU:CD	2.63	0.56
1:B:407:THR:O	1:B:407:THR:HG22	2.05	0.56
1:B:877:ALA:HB2	1:B:889:THR:HG21	1.87	0.56
1:B:1039:SER:O	1:B:1040:LEU:C	2.42	0.56
1:B:381:ILE:HG23	1:B:386:PHE:CB	2.35	0.56
1:B:257:MET:HB3	1:B:559:LEU:HD11	1.87	0.56
1:B:410:ASP:O	2:A:230:GLY:HA2	2.06	0.56
1:B:511:TRP:CZ3	1:B:543:MET:HE2	2.41	0.56
1:B:539:VAL:O	1:B:539:VAL:HG12	2.06	0.56
1:B:972:THR:CG2	1:B:985:MET:HE1	2.36	0.56
2:A:244:GLU:HG2	2:A:245:PRO:HD3	1.82	0.56
2:A:187:TYR:CD1	2:A:187:TYR:C	2.84	0.55
2:A:244:GLU:CG	2:A:245:PRO:HD2	2.20	0.55
1:B:615:ILE:HD12	1:B:615:ILE:O	2.07	0.55
1:B:908:LEU:HD22	1:B:931:PRO:HB3	1.88	0.55
1:B:1031:LYS:O	1:B:1031:LYS:HG2	2.06	0.55
1:B:190:PRO:HG3	1:B:266:TRP:CZ2	2.41	0.55
1:B:770:PHE:CE2	1:B:775:PRO:HD3	2.40	0.55
1:B:404:LEU:HD22	2:A:224:PHE:HE1	1.70	0.55
2:A:213:LYS:CE	2:A:213:LYS:CA	2.85	0.55
1:B:323:ALA:HA	1:B:372:SER:CB	2.36	0.55
1:B:387:GLN:HB3	1:B:388:PRO:HD2	1.87	0.55
1:B:408:LYS:O	2:A:228:SER:CB	2.55	0.55
1:B:341:ASP:OD1	1:B:341:ASP:N	2.27	0.54
1:B:219:ASN:N	1:B:220:PRO:HD3	2.22	0.54
1:B:409:LEU:N	1:B:409:LEU:HD23	2.22	0.54
1:B:565:LEU:HD22	1:B:847:GLN:NE2	2.20	0.54
1:B:879:GLU:O	1:B:1006:GLN:NE2	2.40	0.54
2:A:231:LEU:H	2:A:231:LEU:CD2	2.07	0.54
1:B:582:GLU:CG	1:B:848:MET:HE1	2.37	0.54
1:B:612:TYR:CD1	1:B:825:LYS:HD3	2.39	0.54
1:B:389:VAL:HG23	1:B:495:THR:HB	1.89	0.54
1:B:911:CYS:SG	1:B:964:PRO:HA	2.48	0.53
1:B:560:ASN:HA	1:B:593:GLN:HE22	1.72	0.53
1:B:727:GLN:NE2	2:A:190:LYS:HB2	2.24	0.53
1:B:912:PHE:HE1	1:B:935:MET:CE	2.21	0.53
1:B:997:MET:HE1	1:B:1030:ILE:HG12	1.90	0.53
1:B:202:MET:HE2	1:B:202:MET:CA	2.37	0.53
1:B:113:GLU:OE1	1:B:290:ARG:HD3	2.09	0.53
1:B:190:PRO:HG3	1:B:266:TRP:CH2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:532:ARG:NH2	2:A:249:GLU:CA	2.72	0.52
1:B:703:SER:HB2	1:B:706:SER:H	1.73	0.52
1:B:751:ARG:N	1:B:752:PRO:CD	2.72	0.52
1:B:1039:SER:O	1:B:1041:TYR:N	2.43	0.52
1:B:799:ALA:O	1:B:802:HIS:HB3	2.09	0.52
1:B:888:LEU:HD23	1:B:888:LEU:H	1.73	0.52
1:B:252:ASP:HA	1:B:282:LEU:HB2	1.91	0.52
1:B:596:ARG:HH11	1:B:596:ARG:HG2	1.73	0.52
1:B:387:GLN:NE2	1:B:387:GLN:CA	2.73	0.52
1:B:965:HIS:N	1:B:965:HIS:CD2	2.75	0.52
2:A:199:PRO:CB	2:A:201:LYS:HE3	2.40	0.52
2:A:224:PHE:CD1	2:A:224:PHE:N	2.73	0.52
1:B:158:LEU:HA	1:B:281:PHE:HB2	1.92	0.52
1:B:615:ILE:HD12	1:B:825:LYS:HG3	1.85	0.52
1:B:700:LEU:HD12	1:B:729:VAL:HG13	1.90	0.52
2:A:249:GLU:CB	2:A:250:PRO:CD	2.63	0.52
1:B:167:LYS:HD3	1:B:283:SER:O	2.09	0.52
1:B:217:THR:HG22	1:B:220:PRO:HG3	1.92	0.52
1:B:450:ARG:HD3	2:A:228:SER:OG	2.10	0.52
1:B:880:ILE:CD1	1:B:888:LEU:HD12	2.15	0.52
1:B:180:ARG:NH1	1:B:180:ARG:HG2	2.24	0.51
1:B:374:VAL:O	1:B:374:VAL:HG23	2.10	0.51
1:B:394:PHE:CD1	1:B:503:LYS:HD2	2.46	0.51
1:B:136:TYR:OH	1:B:173:TYR:HB2	2.11	0.51
1:B:994:ILE:HG23	1:B:1035:VAL:HG13	1.92	0.51
1:B:732:LEU:HD23	1:B:734:HIS:CE1	2.46	0.51
1:B:841:LYS:C	1:B:844:THR:HG23	2.33	0.51
1:B:922:PRO:CG	1:B:968:ASP:CG	2.83	0.51
2:A:172:ALA:CB	2:A:180:TYR:CD2	2.89	0.51
1:B:408:LYS:HB2	1:B:409:LEU:HD23	1.93	0.51
1:B:468:GLU:HB3	1:B:491:MET:HE1	1.93	0.51
1:B:1009:GLN:HE21	1:B:1009:GLN:HA	1.72	0.51
1:B:683:VAL:HG12	1:B:683:VAL:O	2.11	0.51
1:B:236:LEU:HG	1:B:272:LEU:HB3	1.93	0.51
1:B:347:MET:CE	1:B:543:MET:N	2.65	0.51
1:B:412:ASN:ND2	1:B:451:GLY:CA	2.73	0.51
1:B:841:LYS:HA	1:B:844:THR:CG2	2.41	0.51
1:B:354:GLY:O	1:B:355:ASP:O	2.29	0.51
1:B:380:MET:CE	2:A:254:ILE:CG2	2.86	0.50
1:B:442:GLU:OE1	2:A:221:GLU:CD	2.53	0.50
2:A:221:GLU:O	2:A:221:GLU:HG3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:SER:OG	1:B:284:ALA:O	2.29	0.50
1:B:180:ARG:HG2	1:B:180:ARG:HH11	1.75	0.50
1:B:596:ARG:HH11	1:B:596:ARG:HG3	1.76	0.50
1:B:347:MET:HE2	1:B:543:MET:HB3	1.93	0.50
1:B:922:PRO:HG3	1:B:968:ASP:OD1	2.11	0.50
1:B:168:THR:HG21	4:B:1102:ATP:O2A	1.99	0.50
1:B:321:PHE:CE2	1:B:372:SER:HB2	2.36	0.50
1:B:814:ASN:HD22	1:B:814:ASN:C	2.19	0.50
1:B:891:MET:HE1	1:B:935:MET:HE2	1.92	0.50
1:B:732:LEU:HD13	2:A:194:CYS:SG	2.52	0.50
1:B:841:LYS:O	1:B:844:THR:CG2	2.54	0.49
1:B:891:MET:CE	1:B:935:MET:HE2	2.42	0.49
1:B:316:LEU:HD11	1:B:524:ALA:O	2.11	0.49
1:B:180:ARG:HH11	1:B:180:ARG:CG	2.24	0.49
1:B:897:PHE:O	1:B:900:LEU:HD23	2.10	0.49
1:B:1021:ASN:O	1:B:1025:GLU:HG2	2.10	0.49
1:B:221:THR:O	1:B:221:THR:OG1	2.13	0.49
1:B:406:MET:CB	1:B:452:ILE:HD13	2.38	0.49
1:B:809:LEU:HD13	1:B:815:LEU:HD23	1.94	0.49
1:B:968:ASP:HB2	5:B:1221:HOH:O	1.81	0.49
1:B:160:SER:OG	1:B:285:THR:HA	2.12	0.49
1:B:598:ILE:N	1:B:599:PRO:CD	2.75	0.49
1:B:465:GLU:OE1	1:B:1040:LEU:N	2.45	0.49
1:B:932:LEU:HD22	1:B:932:LEU:C	2.38	0.49
1:B:814:ASN:C	1:B:814:ASN:ND2	2.71	0.48
1:B:119:GLU:H	1:B:119:GLU:CD	2.22	0.48
1:B:582:GLU:HG3	1:B:848:MET:CE	2.42	0.48
1:B:706:SER:O	2:A:190:LYS:NZ	2.45	0.48
1:B:125:LEU:CG	1:B:153:ASN:OD1	2.59	0.48
1:B:446:PRO:HB2	2:A:224:PHE:CD2	2.48	0.48
1:B:456:HIS:HD2	1:B:459:LEU:HD22	1.78	0.48
1:B:1014:ILE:C	1:B:1014:ILE:CD1	2.85	0.48
1:B:804:MET:O	1:B:804:MET:HG2	2.14	0.48
1:B:458:GLY:O	1:B:991:GLY:CA	2.62	0.48
1:B:790:LEU:O	1:B:790:LEU:HG	2.09	0.48
1:B:431:LEU:CG	1:B:1034:ILE:CG2	2.91	0.48
1:B:814:ASN:ND2	1:B:814:ASN:O	2.46	0.48
1:B:233:ARG:NH1	1:B:268:GLU:OE1	2.47	0.48
1:B:126:LYS:HA	1:B:127:PRO:HD3	1.77	0.48
1:B:167:LYS:HB2	4:B:1102:ATP:O1B	2.14	0.47
1:B:243:MET:CE	1:B:243:MET:CA	2.91	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:410:ASP:HA	1:B:450:ARG:HG2	1.96	0.47
1:B:445:LEU:HB3	1:B:446:PRO:HD3	1.96	0.47
1:B:582:GLU:CB	1:B:848:MET:HE1	2.45	0.47
1:B:699:LEU:CD2	1:B:726:MET:HE3	2.44	0.47
1:B:841:LYS:HA	1:B:844:THR:HG21	1.96	0.47
1:B:900:LEU:CD2	1:B:900:LEU:H	2.24	0.47
1:B:168:THR:CG2	4:B:1102:ATP:PA	2.95	0.47
1:B:922:PRO:HG3	1:B:968:ASP:CG	2.38	0.47
1:B:697:GLU:OE2	2:A:187:TYR:OH	2.32	0.47
1:B:412:ASN:HD22	1:B:451:GLY:N	2.12	0.47
1:B:699:LEU:HD23	1:B:726:MET:HE3	1.97	0.47
1:B:841:LYS:C	1:B:844:THR:CG2	2.87	0.47
1:B:144:GLN:HE22	1:B:169:VAL:HG11	1.77	0.47
1:B:189:SER:O	1:B:228:THR:HA	2.13	0.47
1:B:254:ILE:HG22	1:B:282:LEU:O	2.14	0.47
1:B:257:MET:HG3	1:B:266:TRP:CB	2.45	0.47
1:B:809:LEU:HD22	1:B:809:LEU:C	2.39	0.47
1:B:322:PRO:HG3	1:B:346:ALA:HB1	1.97	0.47
1:B:404:LEU:CD1	2:A:220:VAL:HG22	2.44	0.47
1:B:460:LEU:HA	1:B:461:PRO:HD3	1.71	0.47
1:B:496:VAL:HG23	1:B:524:ALA:HB2	1.95	0.47
1:B:412:ASN:HD21	1:B:451:GLY:HA2	1.80	0.47
1:B:642:GLU:HA	1:B:645:HIS:NE2	2.30	0.47
1:B:1027:ILE:H	1:B:1027:ILE:HG13	1.50	0.47
1:B:267:GLU:OE1	1:B:561:SER:CB	2.60	0.47
1:B:583:TYR:CE1	1:B:587:LYS:HE3	2.50	0.47
1:B:197:GLN:CB	1:B:489:ILE:HG12	2.45	0.46
1:B:1024:ALA:O	1:B:1027:ILE:CD1	2.62	0.46
1:B:183:GLN:OE1	1:B:247:ALA:CB	2.62	0.46
1:B:404:LEU:HD23	2:A:224:PHE:CZ	2.50	0.46
1:B:804:MET:HG2	1:B:810:HIS:HD2	1.79	0.46
1:B:1003:LEU:HD12	1:B:1003:LEU:C	2.40	0.46
1:B:255:HIS:HB2	1:B:258:ARG:NH2	2.31	0.46
1:B:323:ALA:HA	1:B:372:SER:HB2	1.95	0.46
1:B:410:ASP:N	2:A:229:VAL:O	2.38	0.46
1:B:538:MET:HE2	1:B:538:MET:HB3	1.80	0.46
1:B:182:LYS:HD2	1:B:182:LYS:HA	1.43	0.46
1:B:320:ILE:HG13	1:B:331:VAL:HG21	1.97	0.46
1:B:511:TRP:CE3	1:B:543:MET:CE	2.97	0.46
1:B:559:LEU:O	1:B:559:LEU:HG	2.16	0.46
1:B:381:ILE:HD13	1:B:389:VAL:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:490:ASN:HD22	1:B:490:ASN:C	2.21	0.46
1:B:579:ILE:HD12	1:B:579:ILE:HG23	1.53	0.46
1:B:783:MET:HB3	1:B:783:MET:HE3	1.72	0.46
1:B:435:ASP:OD2	1:B:1033:ASP:HB3	2.16	0.46
1:B:732:LEU:HB2	2:A:196:GLY:HA3	1.98	0.46
1:B:912:PHE:CE1	1:B:935:MET:HE1	2.48	0.46
1:B:585:LEU:CD2	1:B:848:MET:HE3	2.44	0.46
1:B:424:PHE:CE1	1:B:445:LEU:HD22	2.51	0.46
1:B:479:LEU:HD23	1:B:479:LEU:HA	1.69	0.46
1:B:896:LEU:C	1:B:900:LEU:CD2	2.57	0.46
1:B:901:SER:HB2	1:B:904:GLN:H	1.81	0.46
1:B:911:CYS:HA	1:B:963:LYS:O	2.16	0.46
2:A:199:PRO:HG2	2:A:201:LYS:HD2	1.98	0.46
2:A:170:ASP:OD2	2:A:181:ARG:HB2	2.16	0.45
1:B:181:GLU:OE2	1:B:181:GLU:HA	2.14	0.45
1:B:582:GLU:CG	1:B:848:MET:CE	2.94	0.45
1:B:615:ILE:CD1	1:B:615:ILE:C	2.84	0.45
1:B:880:ILE:CG2	1:B:888:LEU:CD1	2.75	0.45
1:B:490:ASN:ND2	1:B:490:ASN:C	2.72	0.45
1:B:584:MET:HE3	1:B:584:MET:HB2	1.81	0.45
1:B:156:SER:O	1:B:305:HIS:HD2	1.99	0.45
1:B:231:ILE:HD12	1:B:231:ILE:HG23	1.64	0.45
1:B:454:ILE:HA	1:B:480:PHE:O	2.17	0.45
1:B:565:LEU:CD2	1:B:847:GLN:HE21	2.28	0.45
1:B:977:ALA:O	1:B:1032:ARG:CZ	2.64	0.45
1:B:114:VAL:HB	1:B:305:HIS:HD1	1.81	0.45
1:B:489:ILE:HD12	1:B:490:ASN:H	1.81	0.45
1:B:583:TYR:HE1	1:B:587:LYS:HE3	1.82	0.45
1:B:645:HIS:HB3	1:B:736:LEU:HD12	1.98	0.45
1:B:880:ILE:HA	1:B:1006:GLN:HB3	1.98	0.45
1:B:257:MET:HG3	1:B:266:TRP:HB2	1.98	0.45
1:B:450:ARG:HH11	1:B:450:ARG:CB	2.29	0.45
1:B:774:ILE:HB	1:B:775:PRO:HD2	1.99	0.45
2:A:168:LYS:HA	2:A:169:PRO:HD2	1.68	0.45
1:B:456:HIS:HB2	1:B:482:THR:CB	2.43	0.44
1:B:870:ILE:CG2	1:B:875:ARG:NH1	2.77	0.44
2:A:187:TYR:CD1	2:A:187:TYR:O	2.70	0.44
1:B:658:ARG:NH2	2:A:166:ASP:OD2	2.50	0.44
2:A:170:ASP:HA	2:A:171:PRO:HD2	1.76	0.44
1:B:167:LYS:HE3	4:B:1102:ATP:O1B	2.17	0.44
1:B:448:LEU:HD23	1:B:470:LEU:HD11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:SER:HA	1:B:190:PRO:HD3	1.64	0.44
1:B:881:SER:O	1:B:881:SER:OG	2.35	0.44
1:B:922:PRO:CG	1:B:968:ASP:OD1	2.65	0.44
1:B:446:PRO:HB2	2:A:224:PHE:HD2	1.82	0.44
1:B:460:LEU:CD2	1:B:990:GLU:HG3	2.46	0.44
1:B:900:LEU:N	1:B:900:LEU:HD13	2.31	0.44
1:B:153:ASN:HD22	1:B:153:ASN:HA	1.53	0.44
1:B:410:ASP:CG	1:B:450:ARG:HG3	2.42	0.44
1:B:863:PHE:HE1	1:B:889:THR:OG1	2.01	0.44
1:B:712:THR:HG21	2:A:193:SER:C	2.43	0.44
2:A:227:LYS:HA	2:A:227:LYS:HD2	1.51	0.44
1:B:307:ILE:O	1:B:307:ILE:HG22	2.18	0.44
1:B:334:GLU:OE2	1:B:532:ARG:HG3	2.17	0.44
1:B:740:SER:HA	1:B:776:LEU:HA	1.99	0.44
1:B:999:ARG:O	1:B:1002:GLU:HB3	2.17	0.44
1:B:815:LEU:C	1:B:815:LEU:CD2	2.84	0.43
1:B:828:ILE:H	1:B:828:ILE:HG12	1.46	0.43
1:B:997:MET:CE	1:B:1030:ILE:CG2	2.87	0.43
1:B:399:CYS:SG	1:B:480:PHE:C	3.00	0.43
1:B:612:TYR:HE1	1:B:825:LYS:HD3	1.69	0.43
1:B:740:SER:CB	1:B:774:ILE:HD11	2.48	0.43
1:B:751:ARG:HB2	1:B:752:PRO:HD3	2.00	0.43
2:A:196:GLY:O	2:A:197:ILE:C	2.59	0.43
1:B:669:PHE:N	1:B:669:PHE:CD1	2.86	0.43
1:B:431:LEU:HG	1:B:1034:ILE:HG23	2.01	0.43
1:B:299:LEU:CD1	1:B:587:LYS:HD2	2.48	0.43
1:B:179:LEU:HD12	1:B:179:LEU:HA	1.66	0.43
1:B:323:ALA:HA	1:B:372:SER:HB3	2.00	0.43
1:B:404:LEU:HD11	2:A:220:VAL:HG22	2.00	0.43
1:B:428:ILE:HD11	1:B:441:VAL:HG11	2.00	0.43
1:B:713:GLU:CD	2:A:200:LYS:HE3	2.23	0.43
1:B:749:ASP:CG	1:B:751:ARG:HH12	2.16	0.43
1:B:863:PHE:HE1	1:B:889:THR:HG1	1.65	0.43
1:B:192:LYS:CG	1:B:213:THR:CG2	2.96	0.43
1:B:470:LEU:HD23	1:B:475:LEU:HD12	1.99	0.43
1:B:596:ARG:CG	1:B:596:ARG:NH1	2.71	0.43
1:B:192:LYS:CG	1:B:213:THR:HG23	2.49	0.43
1:B:212:MET:HE2	1:B:235:MET:CE	2.44	0.43
1:B:888:LEU:HB2	1:B:1007:MET:CE	2.43	0.43
2:A:218:LYS:HA	2:A:218:LYS:CE	2.48	0.43
1:B:274:PRO:HD2	1:B:277:VAL:CG2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:404:LEU:HD11	2:A:220:VAL:CG2	2.49	0.43
1:B:744:LEU:HD23	1:B:744:LEU:H	1.82	0.43
1:B:557:ASP:HA	1:B:558:PRO:HD3	1.81	0.43
1:B:483:GLU:HG3	1:B:520:MET:HE2	2.00	0.42
1:B:537:LEU:HA	1:B:537:LEU:HD23	1.75	0.42
1:B:735:LEU:N	1:B:735:LEU:HD23	2.33	0.42
2:A:224:PHE:N	2:A:224:PHE:HD1	2.17	0.42
1:B:336:GLY:O	1:B:553:LYS:CD	2.61	0.42
1:B:347:MET:HE2	1:B:543:MET:CA	2.49	0.42
1:B:168:THR:HG22	4:B:1102:ATP:PA	2.51	0.42
1:B:683:VAL:O	1:B:683:VAL:CG1	2.67	0.42
1:B:764:GLN:HE21	1:B:764:GLN:HB3	1.60	0.42
1:B:770:PHE:CE2	1:B:775:PRO:HG3	2.55	0.42
1:B:942:ILE:HD12	1:B:942:ILE:HA	1.80	0.42
1:B:408:LYS:N	1:B:408:LYS:CD	2.81	0.42
1:B:460:LEU:HD23	1:B:463:LEU:HD12	2.00	0.42
1:B:848:MET:O	1:B:848:MET:HG3	2.18	0.42
1:B:580:ASN:HB2	1:B:581:PRO:CD	2.49	0.42
1:B:585:LEU:HA	1:B:585:LEU:HD12	1.84	0.42
1:B:727:GLN:HE21	1:B:727:GLN:HB3	1.55	0.42
1:B:809:LEU:HD23	1:B:809:LEU:HA	1.75	0.42
1:B:942:ILE:HD13	1:B:942:ILE:N	2.35	0.42
1:B:989:PHE:N	1:B:989:PHE:CD1	2.87	0.42
1:B:582:GLU:HG3	1:B:848:MET:HE2	2.02	0.42
1:B:678:SER:OG	1:B:680:LYS:HE2	2.20	0.42
1:B:408:LYS:O	2:A:228:SER:HB2	2.18	0.42
1:B:821:LEU:HD23	1:B:821:LEU:HA	1.73	0.42
1:B:802:HIS:ND1	1:B:802:HIS:C	2.78	0.42
1:B:125:LEU:HD12	1:B:125:LEU:HA	1.67	0.42
1:B:669:PHE:HA	1:B:717:PRO:HB3	2.01	0.42
1:B:707:LEU:HD21	1:B:725:GLU:HG2	2.01	0.42
1:B:458:GLY:O	1:B:991:GLY:HA3	2.20	0.41
1:B:598:ILE:N	1:B:599:PRO:HD2	2.35	0.41
1:B:459:LEU:HA	1:B:459:LEU:HD12	1.78	0.41
1:B:550:GLN:HE21	1:B:550:GLN:HB2	1.58	0.41
1:B:897:PHE:N	1:B:900:LEU:CD2	2.83	0.41
1:B:202:MET:HE2	1:B:202:MET:N	2.35	0.41
1:B:273:LEU:HA	1:B:274:PRO:HD3	1.85	0.41
1:B:468:GLU:HB3	1:B:491:MET:CE	2.50	0.41
1:B:663:LYS:HA	1:B:668:ASP:HA	2.02	0.41
1:B:807:HIS:HA	1:B:808:PRO:HD3	1.22	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:244:GLU:CB	2:A:245:PRO:CD	2.97	0.41
1:B:382:MET:HG3	1:B:411:PHE:CE1	2.56	0.41
1:B:404:LEU:HD23	1:B:404:LEU:HA	1.75	0.41
1:B:523:ARG:HA	1:B:523:ARG:HD2	1.95	0.41
1:B:727:GLN:NE2	2:A:190:LYS:HD3	2.24	0.41
1:B:1031:LYS:HA	1:B:1036:PHE:CE2	2.55	0.41
1:B:692:PRO:HG2	1:B:692:PRO:O	2.21	0.41
1:B:1019:LEU:HA	1:B:1019:LEU:HD23	1.69	0.41
1:B:574:LEU:HD23	1:B:574:LEU:HA	1.79	0.41
1:B:744:LEU:CD1	1:B:762:SER:HB3	2.48	0.41
2:A:197:ILE:HG12	2:A:202:GLN:HB2	2.03	0.41
1:B:408:LYS:C	2:A:228:SER:CB	2.94	0.41
1:B:659:LEU:HD12	1:B:742:VAL:CB	2.45	0.41
1:B:809:LEU:C	1:B:809:LEU:CD2	2.91	0.41
1:B:1008:CYS:SG	1:B:1024:ALA:HB2	2.61	0.41
1:B:732:LEU:CD1	2:A:194:CYS:SG	3.09	0.41
1:B:175:ILE:HG23	1:B:185:VAL:HG11	2.03	0.41
1:B:332:VAL:HA	1:B:337:ASP:O	2.20	0.41
1:B:431:LEU:HG	1:B:1034:ILE:CG2	2.50	0.41
1:B:453:GLY:C	1:B:479:LEU:HD23	2.46	0.41
1:B:470:LEU:HD22	1:B:475:LEU:HD12	2.01	0.41
1:B:569:MET:HE2	1:B:569:MET:HB3	1.84	0.41
1:B:764:GLN:HA	1:B:767:GLN:HB2	2.03	0.41
1:B:433:ASP:OD1	1:B:433:ASP:N	2.54	0.41
1:B:434:GLU:CD	1:B:434:GLU:C	2.88	0.41
1:B:885:GLU:HA	1:B:888:LEU:HG	2.02	0.41
1:B:391:ILE:HG23	1:B:497:LEU:HD23	2.02	0.40
1:B:456:HIS:HB3	1:B:482:THR:HB	2.01	0.40
1:B:953:ILE:O	1:B:953:ILE:CD1	2.69	0.40
1:B:129:VAL:O	1:B:129:VAL:CG2	2.68	0.40
1:B:243:MET:HE3	1:B:243:MET:HB2	1.83	0.40
1:B:645:HIS:HB3	1:B:736:LEU:CD1	2.52	0.40
1:B:847:GLN:HE21	1:B:847:GLN:HB3	1.65	0.40
2:A:227:LYS:HD2	2:A:228:SER:H	1.86	0.40
1:B:438:LEU:HA	1:B:439:PRO:HD3	1.79	0.40
1:B:644:ILE:O	1:B:644:ILE:CG2	2.69	0.40
1:B:760:LEU:HA	1:B:760:LEU:HD23	1.64	0.40
1:B:450:ARG:HE	2:A:227:LYS:NZ	2.16	0.40
1:B:459:LEU:N	1:B:459:LEU:HD13	2.35	0.40
1:B:922:PRO:HG2	1:B:968:ASP:CG	2.47	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	B	925/979 (94%)	905 (98%)	18 (2%)	2 (0%)	43	72
2	A	77/105 (73%)	72 (94%)	4 (5%)	1 (1%)	9	32
All	All	1002/1084 (92%)	977 (98%)	22 (2%)	3 (0%)	36	65

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	387	GLN
2	A	244	GLU
1	B	922	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	B	689/860 (80%)	523 (76%)	166 (24%)	1	2
2	A	72/94 (77%)	48 (67%)	24 (33%)	0	0
All	All	761/954 (80%)	571 (75%)	190 (25%)	0	2

All (190) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	104	VAL
1	B	107	VAL
1	B	110	CYS

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Mol	Chain	Res	Type
1	B	116	LEU
1	B	125	LEU
1	B	129	VAL
1	B	135	GLU
1	B	139	ILE
1	B	153	ASN
1	B	155	GLN
1	B	158	LEU
1	B	168	THR
1	B	169	VAL
1	B	179	LEU
1	B	180	ARG
1	B	182	LYS
1	B	185	VAL
1	B	186	ILE
1	B	189	SER
1	B	192	LYS
1	B	205	GLU
1	B	209	VAL
1	B	212	MET
1	B	215	ASP
1	B	216	VAL
1	B	221	THR
1	B	229	THR
1	B	233	ARG
1	B	236	LEU
1	B	243	MET
1	B	257	MET
1	B	265	VAL
1	B	276	ASN
1	B	277	VAL
1	B	286	ILE
1	B	301	LYS
1	B	307	ILE
1	B	313	PRO
1	B	316	LEU
1	B	317	GLN
1	B	341	ASP
1	B	345	THR
1	B	347	MET
1	B	348	GLN
1	B	349	VAL

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Mol	Chain	Res	Type
1	B	374	VAL
1	B	382	MET
1	B	387	GLN
1	B	391	ILE
1	B	393	SER
1	B	396	LYS
1	B	406	MET
1	B	409	LEU
1	B	414	ASP
1	B	428	ILE
1	B	431	LEU
1	B	442	GLU
1	B	446	PRO
1	B	447	LEU
1	B	452	ILE
1	B	454	ILE
1	B	459	LEU
1	B	460	LEU
1	B	462	ILE
1	B	466	THR
1	B	469	ILE
1	B	479	LEU
1	B	487	MET
1	B	489	ILE
1	B	490	ASN
1	B	491	MET
1	B	503	LYS
1	B	518	ILE
1	B	527	ARG
1	B	532	ARG
1	B	537	LEU
1	B	541	GLU
1	B	545	PRO
1	B	546	THR
1	B	549	LYS
1	B	552	LEU
1	B	553	LYS
1	B	565	LEU
1	B	575	ARG
1	B	576	VAL
1	B	585	LEU
1	B	596	ARG

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Mol	Chain	Res	Type
1	B	598	ILE
1	B	618	PRO
1	B	623	VAL
1	B	625	ILE
1	B	640	ILE
1	B	652	PRO
1	B	660	VAL
1	B	681	SER
1	B	683	VAL
1	B	696	VAL
1	B	706	SER
1	B	707	LEU
1	B	709	ASN
1	B	716	LYS
1	B	719	LYS
1	B	723	LYS
1	B	727	GLN
1	B	728	VAL
1	B	729	VAL
1	B	732	LEU
1	B	733	VAL
1	B	736	LEU
1	B	737	SER
1	B	750	LEU
1	B	751	ARG
1	B	757	GLN
1	B	759	VAL
1	B	760	LEU
1	B	764	GLN
1	B	766	VAL
1	B	774	ILE
1	B	778	ASP
1	B	780	ILE
1	B	783	MET
1	B	787	ASP
1	B	794	ILE
1	B	802	HIS
1	B	807	HIS
1	B	809	LEU
1	B	814	ASN
1	B	815	LEU
1	B	825	LYS

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Mol	Chain	Res	Type
1	B	828	ILE
1	B	836	LYS
1	B	844	THR
1	B	847	GLN
1	B	848	MET
1	B	861	LEU
1	B	865	THR
1	B	871	GLU
1	B	872	MET
1	B	882	SER
1	B	885	GLU
1	B	887	LEU
1	B	888	LEU
1	B	889	THR
1	B	894	ASN
1	B	901	SER
1	B	910	SER
1	B	916	GLU
1	B	932	LEU
1	B	935	MET
1	B	942	ILE
1	B	953	ILE
1	B	968	ASP
1	B	982	ILE
1	B	988	VAL
1	B	994	ILE
1	B	997	MET
1	B	1000	LEU
1	B	1004	LEU
1	B	1007	MET
1	B	1008	CYS
1	B	1009	GLN
1	B	1027	ILE
1	B	1028	THR
1	B	1030	ILE
1	B	1032	ARG
1	B	1042	LEU
2	A	164	ARG
2	A	165	THR
2	A	166	ASP
2	A	168	LYS
2	A	173	ASN

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Mol	Chain	Res	Type
2	A	188	LYS
2	A	193	SER
2	A	197	ILE
2	A	204	ILE
2	A	211	THR
2	A	212	GLU
2	A	213	LYS
2	A	218	LYS
2	A	221	GLU
2	A	225	THR
2	A	227	LYS
2	A	228	SER
2	A	229	VAL
2	A	231	LEU
2	A	249	GLU
2	A	251	ILE
2	A	254	ILE
2	A	257	LYS
2	A	258	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	112	HIS
1	B	144	GLN
1	B	155	GLN
1	B	255	HIS
1	B	278	HIS
1	B	317	GLN
1	B	344	ASN
1	B	387	GLN
1	B	405	GLN
1	B	412	ASN
1	B	440	GLN
1	B	550	GLN
1	B	593	GLN
1	B	727	GLN
1	B	734	HIS
1	B	764	GLN
1	B	810	HIS
1	B	814	ASN
1	B	827	GLN

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Mol	Chain	Res	Type
1	B	847	GLN
1	B	894	ASN
1	B	965	HIS
1	B	1006	GLN
1	B	1009	GLN
2	A	202	GLN
2	A	233	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	ATP	B	1102	-	32,33,33	2.47	14 (43%)	48,52,52	1.83	11 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ATP	B	1102	-	-	1/22/38/38	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1102	ATP	PA-O3A	-6.64	1.52	1.59
4	B	1102	ATP	C5-N7	-5.05	1.29	1.39
4	B	1102	ATP	C4-N9	-4.21	1.28	1.37
4	B	1102	ATP	C8-N9	-3.59	1.31	1.37
4	B	1102	ATP	PB-O3A	-3.47	1.55	1.59
4	B	1102	ATP	O4'-C4'	-3.21	1.37	1.45
4	B	1102	ATP	PB-O2B	-2.65	1.43	1.55
4	B	1102	ATP	PG-O3G	-2.65	1.45	1.54
4	B	1102	ATP	PA-O1A	-2.50	1.42	1.50
4	B	1102	ATP	C4-N3	-2.34	1.30	1.34
4	B	1102	ATP	PA-O2A	-2.32	1.44	1.55
4	B	1102	ATP	PG-O2G	-2.32	1.46	1.54
4	B	1102	ATP	C2-N3	-2.29	1.29	1.33
4	B	1102	ATP	PB-O1B	-2.26	1.43	1.50

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1102	ATP	C5-C4-N3	-5.46	119.20	126.72
4	B	1102	ATP	O2A-PA-O3A	4.62	119.76	107.27
4	B	1102	ATP	C2-N3-C4	3.68	120.83	111.83
4	B	1102	ATP	C4-C5-N7	-3.59	106.47	110.58
4	B	1102	ATP	N3-C4-N9	3.48	133.08	127.17
4	B	1102	ATP	N3-C2-N1	-3.26	123.65	128.58
4	B	1102	ATP	O4'-C1'-N9	-2.77	102.78	108.09
4	B	1102	ATP	O3A-PA-O1A	-2.69	102.61	110.70
4	B	1102	ATP	C5-N7-C8	2.30	107.06	103.45
4	B	1102	ATP	C6-C5-N7	2.04	136.01	132.09
4	B	1102	ATP	O3G-PG-O1G	2.01	118.66	110.83

There are no chirality outliers.

All (1) torsion outliers are listed below:

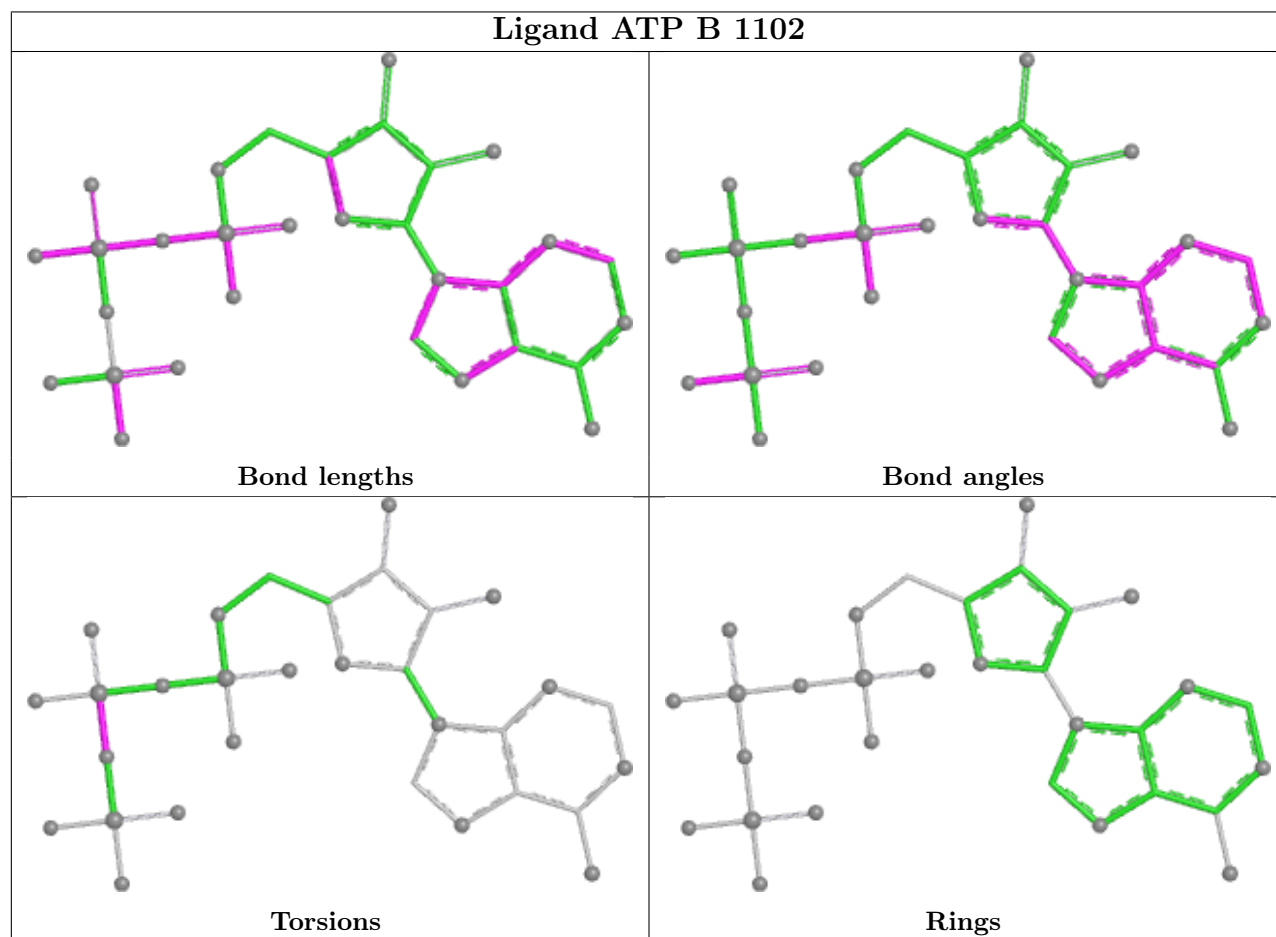
Mol	Chain	Res	Type	Atoms
4	B	1102	ATP	PG-O3B-PB-O1B

There are no ring outliers.

1 monomer is involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1102	ATP	10	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	B	929/979 (94%)	0.47	48 (5%) 33 26	25, 48, 71, 99	0
2	A	85/105 (80%)	0.81	5 (5%) 28 22	35, 55, 84, 102	0
All	All	1014/1084 (93%)	0.50	53 (5%) 33 26	25, 48, 74, 102	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	976	GLY	5.5
2	A	198	ASN	5.0
1	B	355	ASP	4.9
1	B	430	CYS	4.3
1	B	897	PHE	3.9
1	B	1006	GLN	3.9
1	B	902	ALA	3.9
1	B	242	VAL	3.6
1	B	888	LEU	3.6
1	B	926	GLU	3.3
1	B	974	ALA	3.2
1	B	387	GLN	3.2
1	B	477	LYS	3.2
1	B	906	THR	3.2
1	B	109	GLY	3.2
1	B	921	MET	3.1
1	B	721	ASP	3.0
1	B	688	GLY	2.8
1	B	919	SER	2.8
1	B	108	GLU	2.8
1	B	200	ARG	2.8
1	B	785	ILE	2.8
1	B	981	HIS	2.7
2	A	224	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
2	A	234	ILE	2.7
1	B	689	GLU	2.7
1	B	881	SER	2.6
1	B	687	SER	2.5
1	B	615	ILE	2.5
1	B	889	THR	2.5
1	B	903	GLU	2.5
1	B	1020	GLU	2.4
1	B	1040	LEU	2.4
1	B	928	LEU	2.3
1	B	266	TRP	2.3
1	B	978	THR	2.3
1	B	488	GLY	2.3
1	B	1016	ASN	2.3
1	B	372	SER	2.3
2	A	243	THR	2.3
1	B	939	ALA	2.2
1	B	983	CYS	2.2
1	B	811	ASN	2.2
1	B	214	GLY	2.2
1	B	1034	ILE	2.1
1	B	959	LEU	2.1
1	B	806	SER	2.1
1	B	1019	LEU	2.1
2	A	197	ILE	2.1
1	B	895	GLY	2.1
1	B	240	SER	2.0
1	B	1039	SER	2.0
1	B	617	ILE	2.0

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

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

6.3 Carbohydrates ⓘ

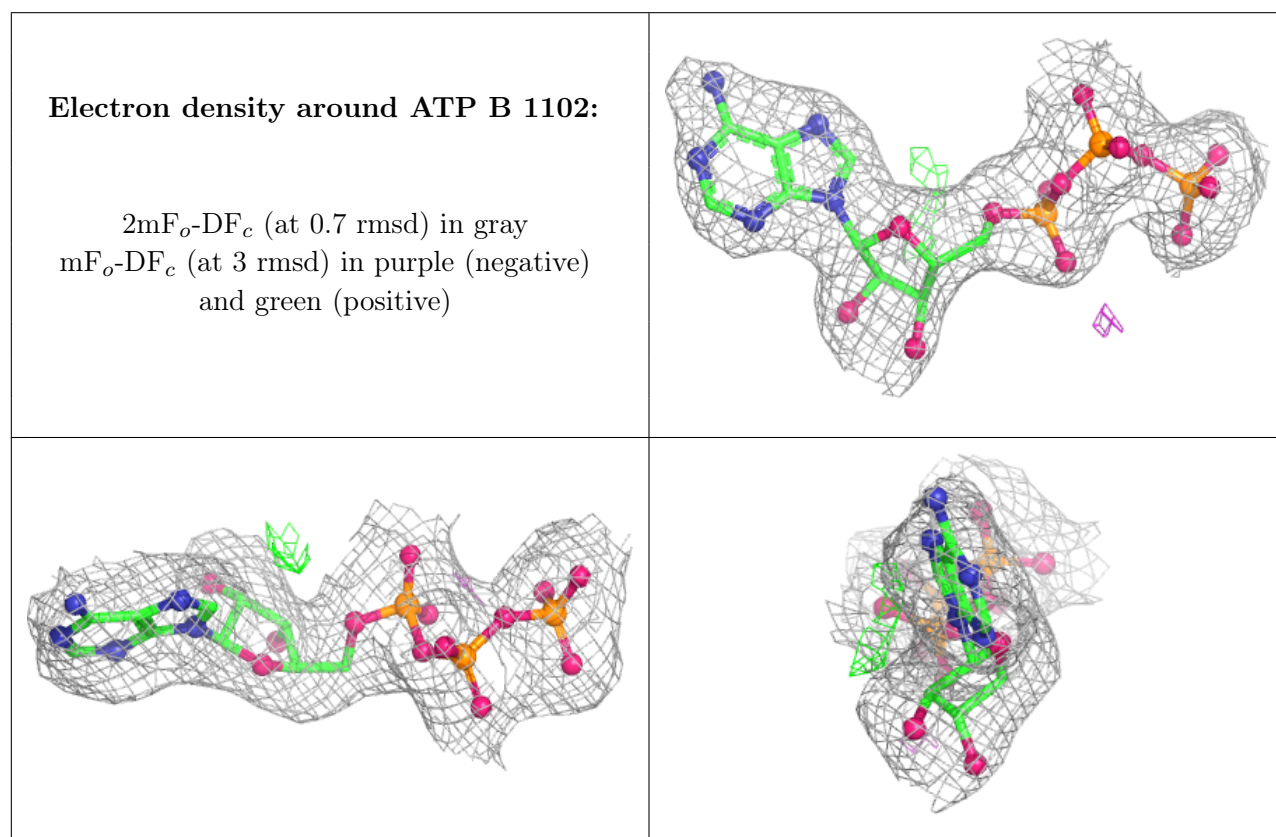
There are no oligosaccharides in this entry.

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($\text{\AA}^2$)	Q<0.9
3	CL	B	1101	1/1	0.90	0.10	52,52,52,52	0
4	ATP	B	1102	31/31	0.95	0.09	33,43,53,62	0

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



6.5 Other polymers [i](#)

There are no such residues in this entry.