



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:52 AM UTC

PDB ID : 2B5M / pdb_00002b5m
Title : Crystal Structure of DDB1
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Deposited on : 2005-09-28
Resolution : 2.92 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

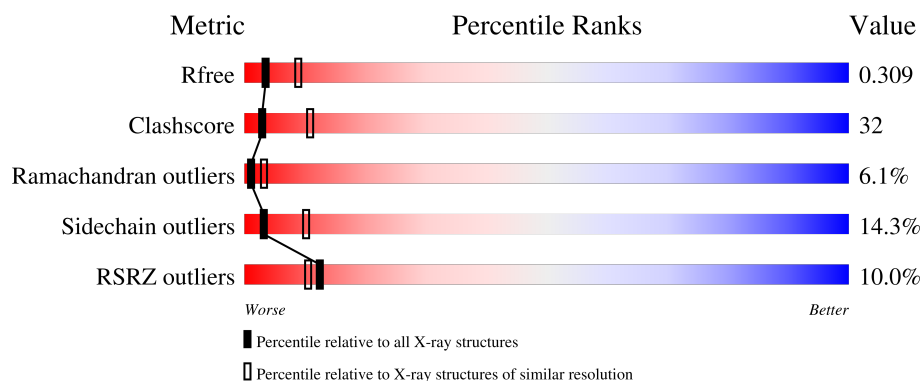
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.92 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	2995 (2.94-2.90)
Clashscore	190562	3213 (2.94-2.90)
Ramachandran outliers	187476	3128 (2.94-2.90)
Sidechain outliers	187428	3130 (2.94-2.90)
RSRZ outliers	180081	2995 (2.94-2.90)

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	A	1140	10% 35% 41% 19% ..

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8768 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.

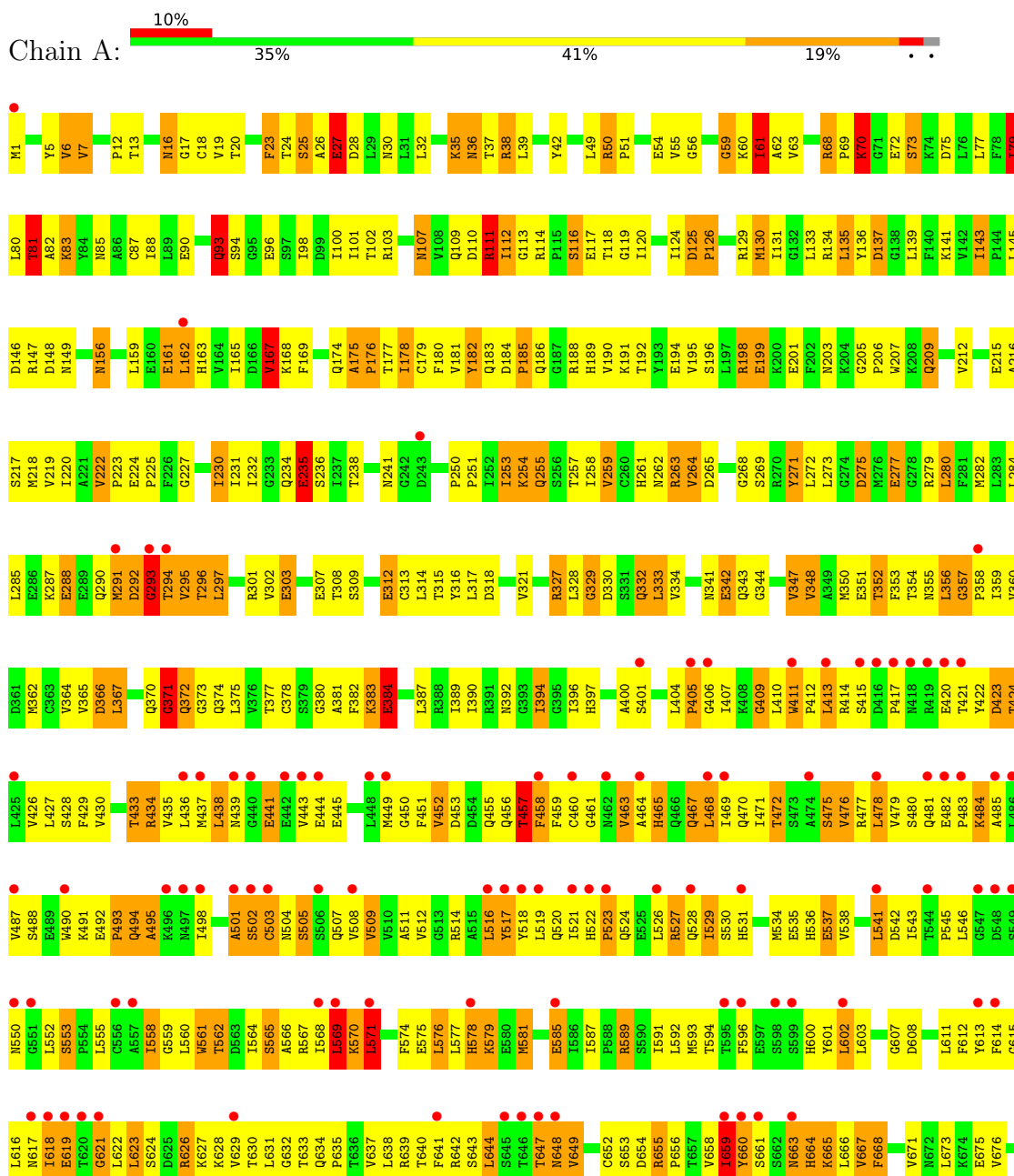
- Molecule 1 is a protein called damage-specific DNA binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1119	8768	5556	1477	1687	48	0	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: damage-specific DNA binding protein 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.38Å 133.83Å 184.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.70 – 2.92 48.70 – 2.92	Depositor EDS
% Data completeness (in resolution range)	(Not available) (48.70-2.92) 92.0 (48.70-2.92)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 2.91Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.232 , 0.277 0.293 , 0.309	Depositor DCC
R_{free} test set	1591 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å ²)	57.4	Xtriage
Anisotropy	0.123	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 13.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	8768	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	2.04	248/8928 (2.8%)	1.68	128/12091 (1.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	2

All (248) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	927	MET	SD-CE	13.40	2.13	1.79
1	A	926	LEU	CA-C	11.39	1.58	1.52
1	A	925	ASP	CA-C	11.19	1.64	1.52
1	A	873	MET	SD-CE	-11.12	1.51	1.79
1	A	808	LEU	C-O	-11.08	1.08	1.23
1	A	581	MET	SD-CE	11.07	2.07	1.79
1	A	308	THR	CA-C	-11.04	1.42	1.53
1	A	667	VAL	CA-CB	11.03	1.69	1.54
1	A	1090	ASP	CA-C	-10.64	1.39	1.52
1	A	1054	MET	SD-CE	10.38	2.05	1.79
1	A	12	PRO	C-O	10.31	1.35	1.23
1	A	370	GLN	C-O	10.18	1.36	1.23
1	A	841	ALA	CA-CB	9.90	1.70	1.53
1	A	360	VAL	C-O	-9.25	1.12	1.24
1	A	1090	ASP	C-O	-9.11	1.13	1.24
1	A	736	LEU	C-O	-9.10	1.13	1.24
1	A	747	GLY	C-O	8.99	1.33	1.23
1	A	222	VAL	CA-CB	-8.94	1.43	1.54
1	A	882	ALA	CA-C	-8.92	1.41	1.52
1	A	354	THR	CA-C	-8.79	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	MET	SD-CE	8.69	2.01	1.79
1	A	182	TYR	CA-C	-8.66	1.42	1.52
1	A	39	LEU	C-O	-8.61	1.13	1.24
1	A	725	CYS	CA-C	-8.44	1.42	1.52
1	A	798	THR	C-O	-8.29	1.13	1.24
1	A	729	VAL	C-O	-8.25	1.14	1.24
1	A	756	ALA	CA-CB	-8.17	1.40	1.53
1	A	1065	VAL	CA-CB	-8.16	1.43	1.54
1	A	925	ASP	N-CA	8.15	1.56	1.46
1	A	954	MET	SD-CE	8.14	2.00	1.79
1	A	79	ILE	CA-C	-8.13	1.42	1.52
1	A	995	VAL	C-O	-8.13	1.15	1.24
1	A	307	GLU	CA-C	-8.08	1.42	1.52
1	A	120	ILE	C-O	-8.03	1.15	1.24
1	A	944	GLU	N-CA	-8.01	1.36	1.46
1	A	885	ASN	C-O	7.91	1.33	1.24
1	A	938	MET	SD-CE	7.90	1.99	1.79
1	A	618	ILE	CA-CB	7.87	1.65	1.54
1	A	831	VAL	CA-CB	-7.79	1.43	1.54
1	A	87	CYS	C-O	-7.74	1.14	1.23
1	A	1013	VAL	CA-C	-7.72	1.42	1.53
1	A	659	ILE	CA-C	7.72	1.60	1.52
1	A	1005	ASN	C-O	-7.70	1.13	1.24
1	A	712	ILE	C-O	-7.69	1.15	1.24
1	A	347	VAL	CA-CB	-7.66	1.44	1.54
1	A	162	LEU	CB-CG	7.63	1.68	1.53
1	A	931	LEU	CA-C	-7.62	1.43	1.52
1	A	357	GLY	CA-C	-7.56	1.41	1.51
1	A	328	LEU	C-O	-7.54	1.13	1.23
1	A	38	ARG	NE-CZ	-7.52	1.24	1.33
1	A	992	LEU	C-O	-7.48	1.15	1.24
1	A	472	THR	CA-CB	7.37	1.65	1.53
1	A	1035	GLY	C-O	-7.34	1.13	1.24
1	A	13	THR	CA-CB	-7.33	1.43	1.54
1	A	720	SER	C-O	-7.31	1.15	1.24
1	A	732	CYS	C-O	-7.30	1.15	1.23
1	A	7	VAL	CA-C	-7.30	1.44	1.52
1	A	857	LYS	CG-CD	7.28	1.74	1.52
1	A	156	ASN	C-O	-7.25	1.15	1.23
1	A	706	GLU	C-N	-7.25	1.23	1.33
1	A	51	PRO	C-O	-7.24	1.15	1.23
1	A	938	MET	CG-SD	7.23	1.98	1.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	35	LYS	C-O	7.17	1.33	1.24
1	A	271	TYR	C-O	7.17	1.32	1.23
1	A	62	ALA	C-O	-7.16	1.15	1.24
1	A	348	VAL	CA-CB	-7.14	1.45	1.54
1	A	61	ILE	C-O	-7.14	1.16	1.24
1	A	755	SER	C-O	-7.08	1.15	1.24
1	A	1126	ALA	C-O	-6.95	1.16	1.24
1	A	1000	LEU	C-O	-6.90	1.16	1.24
1	A	467	GLN	CA-C	6.89	1.61	1.52
1	A	788	VAL	CA-CB	-6.86	1.45	1.54
1	A	50	ARG	CA-C	-6.79	1.44	1.52
1	A	793	ILE	C-O	-6.78	1.16	1.24
1	A	56	GLY	CA-C	6.74	1.57	1.52
1	A	201	GLU	CA-C	-6.73	1.44	1.52
1	A	18	CYS	C-O	-6.73	1.15	1.24
1	A	435	VAL	CA-CB	6.71	1.60	1.54
1	A	844	LYS	CB-CG	6.71	1.72	1.52
1	A	923	VAL	C-O	-6.71	1.16	1.24
1	A	17	GLY	C-O	-6.68	1.14	1.23
1	A	371	GLY	C-O	-6.66	1.15	1.23
1	A	143	ILE	C-O	-6.66	1.16	1.24
1	A	710	LEU	CA-C	6.63	1.60	1.52
1	A	797	HIS	C-O	-6.62	1.16	1.24
1	A	294	THR	CA-CB	6.62	1.64	1.53
1	A	295	VAL	CA-CB	6.61	1.60	1.53
1	A	255	GLN	CA-C	-6.60	1.46	1.53
1	A	1075	SER	C-O	-6.60	1.16	1.23
1	A	498	ILE	CA-CB	6.58	1.61	1.53
1	A	857	LYS	CD-CE	6.58	1.72	1.52
1	A	759	GLN	CG-CD	6.56	1.68	1.52
1	A	910	MET	CG-SD	-6.52	1.64	1.80
1	A	27	GLU	CA-CB	6.50	1.64	1.53
1	A	853	TYR	CA-C	6.50	1.60	1.52
1	A	367	LEU	CA-C	6.48	1.61	1.52
1	A	68	ARG	NE-CZ	6.45	1.40	1.33
1	A	116	SER	C-O	-6.43	1.15	1.23
1	A	852	GLN	CA-C	6.41	1.60	1.52
1	A	984	THR	CA-CB	6.39	1.63	1.53
1	A	80	LEU	CA-C	-6.38	1.44	1.52
1	A	357	GLY	N-CA	6.37	1.53	1.44
1	A	352	THR	C-O	-6.35	1.16	1.24
1	A	93	GLN	CA-C	-6.34	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	627	LYS	CA-C	6.30	1.60	1.52
1	A	930	VAL	CA-CB	-6.29	1.46	1.54
1	A	1033	VAL	CB-CG1	-6.28	1.31	1.52
1	A	280	LEU	CA-C	-6.25	1.45	1.52
1	A	23	PHE	C-O	-6.24	1.16	1.24
1	A	359	ILE	C-O	-6.20	1.17	1.23
1	A	177	THR	CA-C	-6.19	1.45	1.52
1	A	705	ASP	C-O	-6.17	1.17	1.23
1	A	303	GLU	N-CA	-6.16	1.38	1.46
1	A	232	ILE	C-O	-6.16	1.17	1.24
1	A	1002	GLU	C-O	-6.16	1.15	1.23
1	A	989	ARG	NE-CZ	6.15	1.39	1.33
1	A	359	ILE	CA-CB	-6.14	1.46	1.53
1	A	77	LEU	C-O	-6.12	1.16	1.24
1	A	784	GLU	N-CA	6.11	1.54	1.46
1	A	13	THR	C-O	-6.11	1.16	1.24
1	A	951	PRO	C-O	-6.08	1.16	1.24
1	A	111	ARG	NE-CZ	6.07	1.39	1.33
1	A	1080	ARG	NE-CZ	6.06	1.39	1.33
1	A	920	PHE	N-CA	-6.05	1.38	1.46
1	A	118	THR	N-CA	6.04	1.53	1.46
1	A	476	VAL	CA-CB	6.04	1.62	1.54
1	A	875	GLU	C-O	-6.03	1.17	1.24
1	A	996	GLY	C-O	-6.02	1.17	1.24
1	A	362	MET	C-O	-5.99	1.17	1.23
1	A	619	GLU	CA-C	5.99	1.59	1.52
1	A	687	TYR	CA-C	5.99	1.60	1.52
1	A	682	LEU	CA-C	5.98	1.59	1.52
1	A	503	CYS	N-CA	5.96	1.53	1.46
1	A	1094	ILE	C-O	-5.94	1.16	1.24
1	A	976	VAL	C-O	-5.94	1.17	1.24
1	A	93	GLN	CD-NE2	5.94	1.45	1.33
1	A	163	HIS	N-CA	5.91	1.54	1.46
1	A	1000	LEU	CA-C	-5.90	1.45	1.52
1	A	848	ILE	CA-CB	-5.90	1.46	1.53
1	A	1004	VAL	C-O	-5.88	1.17	1.24
1	A	895	THR	CA-CB	-5.87	1.44	1.53
1	A	433	THR	CA-C	5.87	1.59	1.52
1	A	37	THR	N-CA	-5.84	1.39	1.46
1	A	936	LYS	CA-C	5.83	1.60	1.52
1	A	930	VAL	CA-C	-5.83	1.45	1.52
1	A	82	ALA	CA-CB	-5.83	1.43	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	954	MET	C-O	-5.82	1.16	1.23
1	A	932	LEU	N-CA	-5.81	1.39	1.46
1	A	1014	MET	C-O	5.80	1.30	1.23
1	A	923	VAL	CA-C	-5.79	1.45	1.52
1	A	1137	THR	CA-C	-5.76	1.44	1.52
1	A	436	LEU	CA-C	5.76	1.60	1.52
1	A	789	HIS	CA-C	-5.74	1.46	1.52
1	A	1126	ALA	CA-C	-5.73	1.45	1.52
1	A	38	ARG	C-O	-5.72	1.17	1.24
1	A	816	LEU	C-O	-5.71	1.17	1.23
1	A	424	THR	CA-C	-5.69	1.45	1.52
1	A	277	GLU	CD-OE1	5.69	1.36	1.25
1	A	569	LEU	CA-C	5.68	1.59	1.52
1	A	1137	THR	C-O	-5.67	1.16	1.24
1	A	1083	GLU	CA-C	5.67	1.58	1.52
1	A	352	THR	CA-C	5.65	1.59	1.52
1	A	786	VAL	CA-CB	-5.64	1.45	1.55
1	A	736	LEU	CA-C	-5.63	1.45	1.52
1	A	42	TYR	C-O	-5.63	1.16	1.23
1	A	111	ARG	CG-CD	5.63	1.69	1.52
1	A	979	LYS	CA-C	-5.62	1.45	1.52
1	A	578	HIS	CA-C	5.62	1.60	1.52
1	A	501	ALA	CA-C	5.59	1.60	1.53
1	A	137	ASP	C-O	-5.59	1.17	1.24
1	A	329	GLY	C-O	-5.57	1.18	1.23
1	A	282	MET	SD-CE	-5.57	1.65	1.79
1	A	356	LEU	C-O	-5.56	1.16	1.24
1	A	726	TYR	C-O	-5.55	1.17	1.23
1	A	780	THR	N-CA	5.55	1.52	1.45
1	A	1076	PHE	CA-C	-5.54	1.46	1.52
1	A	816	LEU	CA-C	-5.53	1.45	1.52
1	A	660	TYR	CA-C	5.52	1.60	1.52
1	A	112	ILE	CA-CB	5.51	1.61	1.54
1	A	350	MET	CG-SD	5.51	1.94	1.80
1	A	1061	VAL	CA-CB	-5.50	1.47	1.54
1	A	230	ILE	CA-C	-5.50	1.46	1.52
1	A	850	VAL	CA-CB	-5.50	1.47	1.54
1	A	917	LYS	C-O	5.47	1.30	1.24
1	A	516	LEU	CA-C	5.46	1.59	1.52
1	A	394	ILE	C-O	-5.46	1.16	1.24
1	A	725	CYS	C-O	-5.45	1.17	1.23
1	A	713	ARG	N-CA	5.45	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	384	GLU	CA-C	5.44	1.60	1.52
1	A	1014	MET	CG-SD	5.44	1.94	1.80
1	A	124	ILE	CA-CB	-5.43	1.47	1.54
1	A	330	ASP	C-O	-5.43	1.17	1.23
1	A	655	ARG	NE-CZ	5.43	1.39	1.33
1	A	235	GLU	N-CA	5.42	1.53	1.46
1	A	209	GLN	CA-C	-5.42	1.46	1.52
1	A	723	LYS	C-O	-5.42	1.17	1.23
1	A	179	CYS	CA-C	-5.41	1.46	1.52
1	A	1065	VAL	C-O	5.39	1.30	1.24
1	A	212	VAL	CA-C	-5.37	1.47	1.52
1	A	684	SER	N-CA	5.37	1.53	1.46
1	A	1041	THR	CA-C	-5.36	1.46	1.52
1	A	1015	GLN	CG-CD	5.33	1.65	1.52
1	A	259	VAL	CA-CB	-5.31	1.48	1.54
1	A	964	ASN	C-O	5.29	1.30	1.23
1	A	1059	ASN	CA-C	-5.29	1.46	1.53
1	A	716	PRO	CA-C	5.28	1.59	1.52
1	A	70	LYS	CB-CG	5.25	1.68	1.52
1	A	1105	MET	SD-CE	5.23	1.92	1.79
1	A	269	SER	C-O	-5.21	1.17	1.24
1	A	538	VAL	CA-CB	-5.21	1.47	1.54
1	A	284	LEU	CA-C	-5.21	1.46	1.52
1	A	927	MET	CG-SD	5.21	1.93	1.80
1	A	1006	VAL	N-CA	-5.20	1.39	1.46
1	A	390	ILE	CA-CB	-5.20	1.48	1.54
1	A	13	THR	CA-C	-5.20	1.45	1.52
1	A	458	PHE	N-CA	5.17	1.52	1.46
1	A	1011	SER	C-O	-5.17	1.17	1.23
1	A	734	GLY	CA-C	-5.16	1.48	1.52
1	A	93	GLN	C-O	-5.16	1.18	1.23
1	A	966	LEU	C-O	-5.15	1.17	1.23
1	A	491	LYS	CA-C	5.15	1.58	1.52
1	A	1108	VAL	CA-CB	-5.14	1.47	1.54
1	A	716	PRO	CB-CG	-5.13	1.24	1.49
1	A	50	ARG	CG-CD	5.13	1.67	1.52
1	A	772	SER	CA-C	5.13	1.59	1.52
1	A	1003	PHE	C-O	-5.13	1.18	1.24
1	A	859	GLN	CG-CD	5.12	1.64	1.52
1	A	740	ILE	CA-CB	-5.12	1.48	1.54
1	A	719	GLU	C-O	-5.12	1.17	1.23
1	A	139	LEU	CA-C	5.11	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	874	VAL	CA-C	5.10	1.58	1.52
1	A	761	LEU	C-O	-5.10	1.18	1.24
1	A	1015	GLN	CD-OE1	5.10	1.33	1.23
1	A	313	CYS	N-CA	-5.09	1.39	1.46
1	A	259	VAL	CA-C	5.08	1.58	1.53
1	A	1030	PHE	C-O	-5.08	1.17	1.23
1	A	1135	GLU	CD-OE2	5.08	1.34	1.25
1	A	756	ALA	CA-C	-5.07	1.46	1.52
1	A	111	ARG	CZ-NH1	5.06	1.39	1.32
1	A	1024	THR	N-CA	5.06	1.52	1.46
1	A	828	TYR	C-O	-5.04	1.17	1.23
1	A	332	GLN	C-O	-5.04	1.17	1.23
1	A	183	GLN	CA-C	5.04	1.58	1.52
1	A	59	GLY	C-O	-5.03	1.17	1.23
1	A	1078	THR	CA-C	-5.02	1.46	1.52
1	A	16	ASN	CB-CG	5.01	1.64	1.52
1	A	224	GLU	N-CA	5.00	1.53	1.46
1	A	143	ILE	CA-CB	-5.00	1.48	1.53

All (128) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	987	GLU	N-CA-CB	-22.12	77.60	110.12
1	A	986	ASP	CB-CA-C	21.14	152.49	110.42
1	A	987	GLU	N-CA-C	17.58	130.44	111.28
1	A	842	GLU	N-CA-CB	-15.94	82.00	110.37
1	A	309	SER	N-CA-C	-12.62	89.91	109.85
1	A	986	ASP	N-CA-C	-12.10	85.03	110.80
1	A	309	SER	N-CA-CB	-11.57	92.46	111.20
1	A	841	ALA	CB-CA-C	11.29	132.88	110.42
1	A	861	VAL	N-CA-C	11.19	121.87	110.23
1	A	1015	GLN	N-CA-C	-10.67	81.14	111.00
1	A	1014	MET	N-CA-C	10.44	126.67	109.24
1	A	688	PRO	N-CA-C	10.34	133.76	112.47
1	A	649	VAL	N-CA-C	9.35	121.26	108.17
1	A	50	ARG	CB-CA-C	-9.12	101.14	110.17
1	A	1014	MET	CA-C-N	8.64	137.25	121.70
1	A	1014	MET	C-N-CA	8.64	137.25	121.70
1	A	1123	GLU	N-CA-C	-8.51	101.02	111.40
1	A	413	LEU	N-CA-C	8.49	121.94	107.93
1	A	663	ASN	N-CA-C	-8.41	101.50	112.68
1	A	357	GLY	CA-C-O	-8.32	109.62	121.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	308	THR	N-CA-C	-8.32	93.27	108.65
1	A	925	ASP	CB-CA-C	-8.19	99.40	110.79
1	A	49	LEU	N-CA-C	8.03	121.60	108.52
1	A	167	VAL	CB-CA-C	-7.99	96.51	111.30
1	A	1014	MET	CA-C-O	7.98	129.84	120.66
1	A	924	GLY	N-CA-C	-7.33	102.70	112.81
1	A	970	ASN	N-CA-C	-7.11	104.97	112.93
1	A	1015	GLN	N-CA-CB	6.97	122.35	110.50
1	A	1126	ALA	N-CA-C	-6.87	103.40	111.03
1	A	467	GLN	N-CA-C	6.86	120.70	109.24
1	A	884	ILE	N-CA-C	6.85	116.58	106.85
1	A	558	ILE	N-CA-C	6.82	116.78	108.06
1	A	908	ASN	N-CA-C	6.80	119.92	108.23
1	A	1089	ILE	CA-C-N	-6.79	113.55	123.05
1	A	1089	ILE	C-N-CA	-6.79	113.55	123.05
1	A	750	THR	CA-C-O	-6.79	115.41	119.55
1	A	561	TRP	CA-C-N	-6.65	110.95	122.79
1	A	561	TRP	C-N-CA	-6.65	110.95	122.79
1	A	198	ARG	N-CA-C	-6.58	105.26	113.28
1	A	357	GLY	O-C-N	6.53	128.30	121.77
1	A	909	ILE	CA-C-O	-6.52	115.75	121.09
1	A	562	THR	CB-CA-C	6.29	119.09	109.34
1	A	485	ALA	N-CA-C	6.25	115.68	108.49
1	A	161	GLU	CA-C-N	6.23	129.48	120.38
1	A	161	GLU	C-N-CA	6.23	129.48	120.38
1	A	275	ASP	CB-CA-C	-6.20	97.56	110.40
1	A	7	VAL	CB-CA-C	-6.20	99.83	110.30
1	A	439	ASN	N-CA-C	-6.14	104.36	112.72
1	A	259	VAL	N-CA-C	6.11	119.07	112.96
1	A	119	GLY	N-CA-C	6.09	126.26	112.01
1	A	710	LEU	N-CA-C	6.01	118.70	108.90
1	A	73	SER	N-CA-C	-6.00	104.65	111.14
1	A	884	ILE	CB-CA-C	-5.99	103.74	111.53
1	A	917	LYS	O-C-N	5.96	130.39	123.30
1	A	861	VAL	CB-CA-C	-5.96	104.07	111.70
1	A	748	GLY	CA-C-N	-5.96	111.59	120.94
1	A	748	GLY	C-N-CA	-5.96	111.59	120.94
1	A	129	ARG	N-CA-C	-5.93	105.12	112.90
1	A	1090	ASP	N-CA-CB	5.91	119.83	110.55
1	A	687	TYR	CA-C-N	5.90	127.22	119.84
1	A	687	TYR	C-N-CA	5.90	127.22	119.84
1	A	293	GLY	N-CA-C	-5.89	99.22	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	367	LEU	N-CA-C	5.88	118.17	111.11
1	A	798	THR	N-CA-C	5.86	118.62	111.82
1	A	1078	THR	N-CA-C	-5.84	100.27	109.50
1	A	844	LYS	N-CA-C	-5.81	106.35	113.50
1	A	819	CYS	N-CA-C	5.76	117.01	108.60
1	A	553	SER	N-CA-C	5.75	117.78	109.04
1	A	114	ARG	N-CA-C	5.75	116.90	109.72
1	A	295	VAL	CB-CA-C	5.73	119.27	111.88
1	A	315	THR	CB-CA-C	-5.70	103.64	110.94
1	A	1013	VAL	CA-C-O	-5.67	115.66	121.67
1	A	118	THR	N-CA-CB	5.67	120.07	110.49
1	A	908	ASN	CA-C-N	5.67	128.46	122.11
1	A	908	ASN	C-N-CA	5.67	128.46	122.11
1	A	409	GLY	N-CA-C	5.66	119.02	110.18
1	A	6	VAL	CB-CA-C	-5.62	101.84	110.50
1	A	81	THR	N-CA-CB	-5.62	101.25	110.41
1	A	925	ASP	CA-CB-CG	-5.60	107.00	112.60
1	A	648	ASN	N-CA-C	5.59	115.50	108.45
1	A	541	LEU	N-CA-C	5.58	118.56	109.24
1	A	441	GLU	N-CA-C	-5.57	106.49	113.28
1	A	771	PHE	N-CA-C	5.55	118.31	109.81
1	A	457	THR	N-CA-C	-5.54	101.51	110.32
1	A	38	ARG	NE-CZ-NH1	-5.53	115.97	121.50
1	A	712	ILE	N-CA-C	5.49	115.89	107.77
1	A	107	ASN	N-CA-C	5.48	117.66	108.73
1	A	238	THR	N-CA-C	5.47	117.50	109.24
1	A	1071	SER	CA-C-N	5.46	127.87	120.44
1	A	1071	SER	C-N-CA	5.46	127.87	120.44
1	A	1084	PRO	N-CD-CG	-5.45	95.03	103.20
1	A	571	LEU	N-CA-C	5.44	120.15	112.75
1	A	837	TYR	CA-C-N	5.44	126.64	119.84
1	A	837	TYR	C-N-CA	5.44	126.64	119.84
1	A	384	GLU	N-CA-CB	-5.43	101.28	110.41
1	A	321	VAL	CB-CA-C	-5.41	103.80	111.21
1	A	130	MET	N-CA-C	5.41	117.02	108.96
1	A	925	ASP	N-CA-C	5.39	116.99	107.61
1	A	1024	THR	N-CA-C	5.39	122.28	110.80
1	A	88	ILE	CB-CA-C	-5.35	102.85	110.83
1	A	700	THR	N-CA-C	5.35	117.20	109.07
1	A	1004	VAL	N-CA-C	5.33	115.93	108.89
1	A	143	ILE	N-CA-C	5.30	113.27	107.60
1	A	864	LYS	N-CA-C	5.30	122.08	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	626	ARG	N-CA-C	5.29	118.05	109.06
1	A	684	SER	N-CA-C	5.29	122.06	110.80
1	A	434	ARG	CA-C-N	5.25	127.65	120.35
1	A	434	ARG	C-N-CA	5.25	127.65	120.35
1	A	125	ASP	CA-C-N	5.20	124.86	119.56
1	A	125	ASP	C-N-CA	5.20	124.86	119.56
1	A	1041	THR	OG1-CB-CG2	-5.18	98.94	109.30
1	A	328	LEU	CB-CA-C	-5.16	101.47	110.09
1	A	231	ILE	N-CA-C	5.16	115.28	107.75
1	A	61	ILE	CB-CA-C	-5.13	104.49	111.15
1	A	397	HIS	N-CA-C	5.11	117.89	109.76
1	A	36	ASN	N-CA-C	-5.10	99.94	110.80
1	A	808	LEU	CA-C-O	-5.09	115.97	121.87
1	A	844	LYS	CA-CB-CG	5.09	124.28	114.10
1	A	126	PRO	N-CA-C	5.09	120.45	113.84
1	A	411	TRP	O-C-N	5.06	127.25	121.94
1	A	530	SER	N-CA-C	5.06	115.83	108.14
1	A	251	PRO	N-CD-CG	-5.05	95.63	103.20
1	A	920	PHE	N-CA-CB	-5.04	102.01	110.22
1	A	19	VAL	N-CA-CB	-5.03	106.12	112.60
1	A	183	GLN	N-CA-C	5.03	117.59	109.40
1	A	327	ARG	N-CA-CB	-5.01	103.92	110.59
1	A	899	VAL	N-CA-C	-5.01	100.68	107.99
1	A	357	GLY	N-CA-C	-5.00	102.13	112.34

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	841	ALA	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1023	PRO	Peptide
1	A	292	ASP	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	8768	0	8744	563	0
All	All	8768	0	8744	563	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 32.

All (563) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1054:MET:SD	1:A:1054:MET:CE	2.05	1.45
1:A:581:MET:SD	1:A:581:MET:CE	2.07	1.43
1:A:927:MET:SD	1:A:927:MET:CE	2.13	1.37
1:A:781:SER:HB3	1:A:784:GLU:OE1	1.31	1.27
1:A:81:THR:HG21	1:A:85:ASN:HD22	1.07	1.09
1:A:781:SER:HB3	1:A:784:GLU:CD	1.75	1.09
1:A:910:MET:H	1:A:926:LEU:HD13	1.17	1.03
1:A:691:LEU:O	1:A:701:ILE:HA	1.61	1.00
1:A:707:ILE:O	1:A:708:GLN:O	1.81	0.97
1:A:24:THR:HG22	1:A:25:SER:OG	1.64	0.96
1:A:542:ASP:OD1	1:A:593:MET:HG2	1.66	0.95
1:A:413:LEU:HB3	1:A:424:THR:O	1.69	0.93
1:A:910:MET:N	1:A:926:LEU:HD13	1.82	0.92
1:A:218:MET:HE3	1:A:261:HIS:HD2	1.37	0.90
1:A:389:ILE:HD12	1:A:389:ILE:N	1.88	0.89
1:A:81:THR:HG21	1:A:85:ASN:ND2	1.87	0.89
1:A:1051:LEU:HD22	1:A:1094:ILE:HD13	1.54	0.88
1:A:925:ASP:C	1:A:925:ASP:OD1	2.15	0.88
1:A:275:ASP:OD2	1:A:279:ARG:HD2	1.74	0.87
1:A:840:GLU:HB2	1:A:844:LYS:NZ	1.89	0.87
1:A:111:ARG:HA	1:A:111:ARG:HH11	1.38	0.87
1:A:1030:PHE:CZ	1:A:1038:GLY:HA3	2.09	0.87
1:A:664:HIS:ND1	1:A:664:HIS:O	2.09	0.86
1:A:781:SER:CB	1:A:784:GLU:OE1	2.23	0.85
1:A:1112:LEU:HB2	1:A:1122:ARG:HE	1.41	0.85
1:A:848:ILE:O	1:A:863:GLU:O	1.95	0.85
1:A:919:ASP:CG	1:A:920:PHE:H	1.86	0.83
1:A:1101:SER:OG	1:A:1103:PRO:HD2	1.77	0.83
1:A:839:GLU:HG3	1:A:840:GLU:H	1.42	0.82
1:A:61:ILE:HD13	1:A:79:ILE:HD13	1.62	0.81
1:A:478:LEU:HD11	1:A:521:ILE:HG23	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:568:ILE:HD11	1:A:602:LEU:HD21	1.63	0.80
1:A:372:GLN:OE1	1:A:372:GLN:C	2.25	0.79
1:A:413:LEU:HD23	1:A:424:THR:CG2	2.12	0.79
1:A:1109:VAL:O	1:A:1109:VAL:HG12	1.83	0.79
1:A:1112:LEU:HB2	1:A:1122:ARG:HB2	1.66	0.78
1:A:297:LEU:HD12	1:A:297:LEU:O	1.84	0.77
1:A:629:VAL:HG11	1:A:668:PHE:HE2	1.47	0.77
1:A:939:GLU:HB3	1:A:941:ASN:HD22	1.51	0.76
1:A:840:GLU:HB2	1:A:844:LYS:HZ1	1.51	0.75
1:A:568:ILE:O	1:A:577:LEU:HB2	1.87	0.74
1:A:1014:MET:SD	1:A:1015:GLN:N	2.60	0.74
1:A:110:ASP:OD2	1:A:141:LYS:NZ	2.20	0.74
1:A:452:VAL:HG22	1:A:477:ARG:NH2	2.03	0.74
1:A:928:ARG:HD2	1:A:953:TRP:CE3	2.23	0.74
1:A:131:ILE:HG13	1:A:145:LEU:HD11	1.68	0.74
1:A:629:VAL:HG11	1:A:668:PHE:CE2	2.23	0.73
1:A:602:LEU:HD23	1:A:616:LEU:HD22	1.69	0.73
1:A:396:ILE:HD11	1:A:673:LEU:HD11	1.71	0.72
1:A:23:PHE:H	1:A:30:ASN:HD22	1.36	0.72
1:A:24:THR:H	1:A:30:ASN:HD21	1.38	0.71
1:A:69:PRO:O	1:A:72:GLU:HB2	1.90	0.71
1:A:1131:LYS:O	1:A:1135:GLU:HG3	1.90	0.71
1:A:930:VAL:HG22	1:A:954:MET:HE2	1.72	0.71
1:A:275:ASP:HB3	1:A:277:GLU:H	1.56	0.71
1:A:1039:LEU:HD21	1:A:1139:ILE:HG22	1.73	0.70
1:A:616:LEU:HD12	1:A:621:GLY:HA2	1.74	0.70
1:A:411:TRP:HB2	1:A:460:CYS:HB3	1.72	0.70
1:A:511:ALA:HB2	1:A:516:LEU:HD23	1.72	0.70
1:A:742:VAL:O	1:A:749:THR:HA	1.92	0.69
1:A:909:ILE:HG23	1:A:926:LEU:HB2	1.75	0.69
1:A:917:LYS:O	1:A:919:ASP:N	2.26	0.69
1:A:854:SER:O	1:A:855:ASP:C	2.35	0.68
1:A:707:ILE:O	1:A:708:GLN:C	2.36	0.68
1:A:781:SER:CB	1:A:784:GLU:CD	2.61	0.68
1:A:467:GLN:NE2	1:A:524:GLN:HA	2.09	0.68
1:A:503:CYS:HA	1:A:543:ILE:HD11	1.75	0.68
1:A:593:MET:HB3	1:A:602:LEU:HD22	1.74	0.68
1:A:725:CYS:SG	1:A:816:LEU:HD23	2.34	0.68
1:A:81:THR:HB	1:A:85:ASN:HB2	1.76	0.68
1:A:925:ASP:OD1	1:A:925:ASP:O	2.12	0.67
1:A:433:THR:OG1	1:A:455:GLN:O	2.12	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:639:ARG:HG2	1:A:679:MET:O	1.94	0.67
1:A:59:GLY:HA2	1:A:1073:TRP:CZ3	2.29	0.66
1:A:542:ASP:OD1	1:A:593:MET:CG	2.42	0.66
1:A:794:ILE:CD1	1:A:794:ILE:N	2.59	0.66
1:A:568:ILE:CD1	1:A:602:LEU:HD21	2.25	0.66
1:A:292:ASP:C	1:A:293:GLY:O	2.35	0.66
1:A:969:GLU:HG2	1:A:970:ASN:N	2.10	0.66
1:A:90:GLU:HB3	1:A:101:ILE:CG2	2.25	0.66
1:A:950:ASN:OD1	1:A:950:ASN:O	2.13	0.66
1:A:894:THR:HG22	1:A:896:GLU:H	1.61	0.65
1:A:234:GLN:O	1:A:236:SER:N	2.30	0.65
1:A:490:TRP:CD2	1:A:519:LEU:HD11	2.32	0.65
1:A:297:LEU:HD12	1:A:297:LEU:C	2.21	0.65
1:A:571:LEU:HD23	1:A:574:PHE:HE2	1.61	0.65
1:A:1014:MET:SD	1:A:1015:GLN:CA	2.85	0.65
1:A:16:ASN:HD22	1:A:35:LYS:C	2.05	0.65
1:A:979:LYS:NZ	1:A:989:ARG:NH2	2.46	0.64
1:A:504:ASN:HD21	1:A:507:GLN:HG2	1.63	0.64
1:A:569:LEU:HA	1:A:577:LEU:HD13	1.79	0.64
1:A:329:GLY:HA3	1:A:384:GLU:HG2	1.79	0.64
1:A:585:GLU:CD	1:A:585:GLU:N	2.55	0.64
1:A:644:LEU:H	1:A:644:LEU:HD23	1.62	0.64
1:A:6:VAL:HG12	1:A:1040:VAL:HG22	1.79	0.63
1:A:23:PHE:H	1:A:30:ASN:ND2	1.96	0.63
1:A:642:ARG:HA	1:A:647:THR:HG22	1.80	0.63
1:A:654:ASP:HA	1:A:675:GLU:HG3	1.80	0.63
1:A:946:ALA:HA	1:A:990:GLN:OE1	1.98	0.63
1:A:692:ALA:C	1:A:693:LEU:HD12	2.23	0.63
1:A:25:SER:HB2	1:A:28:ASP:HB2	1.79	0.63
1:A:1097:PHE:CZ	1:A:1129:LEU:HD12	2.34	0.63
1:A:5:TYR:OH	1:A:1091:GLY:HA3	1.97	0.63
1:A:218:MET:HE3	1:A:261:HIS:CD2	2.28	0.63
1:A:546:LEU:HD11	1:A:593:MET:HB2	1.81	0.63
1:A:396:ILE:CD1	1:A:673:LEU:HD11	2.29	0.63
1:A:332:GLN:HE21	1:A:352:THR:HG22	1.63	0.63
1:A:511:ALA:HB2	1:A:516:LEU:CD2	2.28	0.63
1:A:747:GLY:O	1:A:748:GLY:C	2.42	0.63
1:A:215:GLU:HG3	1:A:234:GLN:HE21	1.64	0.63
1:A:482:GLU:HB3	1:A:483:PRO:HD3	1.79	0.62
1:A:679:MET:O	1:A:679:MET:SD	2.56	0.62
1:A:38:ARG:NH1	1:A:54:GLU:OE2	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:THR:CG2	1:A:85:ASN:HD22	1.99	0.62
1:A:519:LEU:HD23	1:A:528:GLN:N	2.14	0.62
1:A:558:ILE:CG2	1:A:567:ARG:HB2	2.29	0.62
1:A:660:TYR:CD1	1:A:707:ILE:HG23	2.33	0.62
1:A:938:MET:CE	1:A:939:GLU:OE2	2.47	0.62
1:A:601:TYR:CZ	1:A:666:LEU:HD21	2.33	0.62
1:A:191:LYS:HG2	1:A:192:THR:H	1.63	0.62
1:A:192:THR:HG21	1:A:206:PRO:HD2	1.81	0.62
1:A:1041:THR:HG22	1:A:1042:SER:N	2.14	0.62
1:A:569:LEU:HD22	1:A:576:LEU:HA	1.80	0.62
1:A:893:TRP:CE3	1:A:899:VAL:HG23	2.35	0.62
1:A:743:GLN:HG3	1:A:781:SER:O	2.00	0.62
1:A:131:ILE:HG22	1:A:133:LEU:HD13	1.82	0.61
1:A:494:GLN:O	1:A:495:ALA:HB3	1.99	0.61
1:A:568:ILE:HD11	1:A:602:LEU:CD2	2.29	0.61
1:A:130:MET:HA	1:A:145:LEU:HD13	1.83	0.61
1:A:577:LEU:O	1:A:578:HIS:HB2	2.01	0.60
1:A:660:TYR:CD2	1:A:707:ILE:HG12	2.36	0.60
1:A:371:GLY:C	1:A:1014:MET:HE2	2.26	0.60
1:A:894:THR:HG22	1:A:896:GLU:N	2.15	0.60
1:A:341:ASN:OD1	1:A:342:GLU:O	2.20	0.60
1:A:407:ILE:HD12	1:A:694:ALA:HB1	1.83	0.60
1:A:692:ALA:HA	1:A:700:THR:O	2.01	0.60
1:A:747:GLY:O	1:A:748:GLY:O	2.20	0.60
1:A:464:ALA:O	1:A:467:GLN:OE1	2.20	0.60
1:A:167:VAL:HG13	1:A:180:PHE:HB3	1.84	0.60
1:A:478:LEU:HB3	1:A:487:VAL:CG2	2.31	0.59
1:A:478:LEU:HB3	1:A:487:VAL:HG22	1.83	0.59
1:A:501:ALA:O	1:A:502:SER:HB2	2.01	0.59
1:A:648:ASN:ND2	1:A:660:TYR:HA	2.17	0.59
1:A:839:GLU:HG3	1:A:840:GLU:N	2.16	0.59
1:A:366:ASP:N	1:A:366:ASP:OD1	2.34	0.59
1:A:394:ILE:HD11	1:A:707:ILE:O	2.03	0.59
1:A:643:SER:HB2	1:A:644:LEU:HD23	1.85	0.59
1:A:783:GLY:O	1:A:784:GLU:HG3	2.02	0.59
1:A:928:ARG:HD2	1:A:953:TRP:CD2	2.38	0.59
1:A:939:GLU:O	1:A:941:ASN:ND2	2.36	0.59
1:A:660:TYR:CZ	1:A:707:ILE:HG13	2.38	0.59
1:A:1047:TRP:CZ3	1:A:1132:VAL:HG13	2.38	0.59
1:A:1123:GLU:OE2	1:A:1128:ASP:OD1	2.20	0.58
1:A:130:MET:SD	1:A:195:VAL:HG11	2.44	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1051:LEU:HD22	1:A:1094:ILE:CD1	2.31	0.58
1:A:492:GLU:HG3	1:A:512:VAL:HG11	1.84	0.58
1:A:570:LYS:HG3	1:A:577:LEU:HD11	1.84	0.58
1:A:794:ILE:N	1:A:794:ILE:HD12	2.17	0.58
1:A:392:ASN:HD22	1:A:1012:LEU:HB3	1.68	0.58
1:A:852:GLN:NE2	1:A:859:GLN:OE1	2.37	0.58
1:A:342:GLU:N	1:A:342:GLU:OE1	2.37	0.58
1:A:131:ILE:HB	1:A:143:ILE:HB	1.84	0.58
1:A:507:GLN:CD	1:A:553:SER:H	2.12	0.58
1:A:919:ASP:CG	1:A:920:PHE:N	2.61	0.57
1:A:329:GLY:HA3	1:A:384:GLU:CG	2.34	0.57
1:A:457:THR:HG1	1:A:470:GLN:HE21	1.51	0.57
1:A:516:LEU:O	1:A:531:HIS:HA	2.05	0.57
1:A:223:PRO:C	1:A:225:PRO:HD2	2.29	0.57
1:A:612:PHE:HE2	1:A:628:LYS:HG3	1.69	0.57
1:A:726:TYR:OH	1:A:796:GLN:NE2	2.37	0.57
1:A:191:LYS:HG2	1:A:192:THR:N	2.19	0.57
1:A:839:GLU:HG3	1:A:840:GLU:HG3	1.87	0.57
1:A:1014:MET:SD	1:A:1015:GLN:HA	2.45	0.57
1:A:250:PRO:HG2	1:A:253:ILE:HD12	1.85	0.57
1:A:184:ASP:C	1:A:185:PRO:O	2.46	0.56
1:A:188:ARG:NH1	1:A:216:ALA:O	2.38	0.56
1:A:840:GLU:HB2	1:A:844:LYS:HZ3	1.68	0.56
1:A:753:ARG:HG2	1:A:753:ARG:HH11	1.69	0.56
1:A:1015:GLN:CA	1:A:1015:GLN:OE1	2.52	0.56
1:A:5:TYR:CZ	1:A:1091:GLY:HA3	2.40	0.56
1:A:502:SER:OG	1:A:543:ILE:HG12	2.04	0.56
1:A:493:PRO:O	1:A:494:GLN:HG2	2.04	0.56
1:A:1014:MET:SD	1:A:1014:MET:C	2.89	0.56
1:A:494:GLN:O	1:A:495:ALA:CB	2.53	0.56
1:A:1015:GLN:OE1	1:A:1015:GLN:C	2.49	0.56
1:A:1125:THR:HB	1:A:1128:ASP:CB	2.36	0.56
1:A:111:ARG:HA	1:A:111:ARG:NH1	2.14	0.56
1:A:509:VAL:HG12	1:A:541:LEU:HD13	1.87	0.56
1:A:522:HIS:HB2	1:A:527:ARG:NH1	2.20	0.56
1:A:1122:ARG:O	1:A:1122:ARG:HG3	2.05	0.56
1:A:1129:LEU:HD13	1:A:1129:LEU:O	2.06	0.56
1:A:16:ASN:ND2	1:A:35:LYS:O	2.33	0.55
1:A:116:SER:HB3	1:A:137:ASP:OD1	2.06	0.55
1:A:570:LYS:NZ	1:A:570:LYS:HB3	2.21	0.55
1:A:35:LYS:HB2	1:A:38:ARG:HB2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1026:GLY:O	1:A:1041:THR:HG23	2.06	0.55
1:A:125:ASP:OD1	1:A:126:PRO:HD2	2.06	0.55
1:A:342:GLU:C	1:A:344:GLY:H	2.15	0.55
1:A:567:ARG:HG2	1:A:579:LYS:HB2	1.88	0.55
1:A:458:PHE:HB3	1:A:501:ALA:CB	2.37	0.55
1:A:24:THR:H	1:A:30:ASN:ND2	2.05	0.55
1:A:615:GLY:HA3	1:A:624:SER:HB2	1.89	0.55
1:A:518:TYR:CD1	1:A:571:LEU:HD22	2.42	0.55
1:A:546:LEU:HD11	1:A:593:MET:SD	2.47	0.55
1:A:907:ASN:OD1	1:A:909:ILE:HD12	2.06	0.55
1:A:695:ASN:ND2	1:A:697:SER:H	2.04	0.55
1:A:649:VAL:HG23	1:A:659:ILE:HB	1.88	0.54
1:A:930:VAL:HG12	1:A:931:LEU:N	2.22	0.54
1:A:262:ASN:ND2	1:A:316:TYR:H	2.06	0.54
1:A:372:GLN:OE1	1:A:373:GLY:N	2.40	0.54
1:A:389:ILE:HD12	1:A:389:ILE:H	1.66	0.54
1:A:452:VAL:HG22	1:A:477:ARG:CZ	2.36	0.54
1:A:979:LYS:HZ2	1:A:989:ARG:NH2	2.05	0.54
1:A:509:VAL:CG2	1:A:571:LEU:HD11	2.37	0.54
1:A:404:LEU:O	1:A:405:PRO:O	2.26	0.54
1:A:455:GLN:HB3	1:A:472:THR:OG1	2.06	0.54
1:A:264:VAL:HG12	1:A:265:ASP:N	2.22	0.54
1:A:503:CYS:CA	1:A:543:ILE:HD11	2.37	0.54
1:A:467:GLN:HE22	1:A:524:GLN:HA	1.73	0.54
1:A:509:VAL:HG22	1:A:571:LEU:HD21	1.89	0.54
1:A:546:LEU:CD1	1:A:593:MET:HB2	2.38	0.54
1:A:907:ASN:OD1	1:A:909:ILE:CD1	2.56	0.54
1:A:659:ILE:HD13	1:A:668:PHE:HE1	1.73	0.54
1:A:296:THR:OG1	1:A:297:LEU:N	2.39	0.53
1:A:429:PHE:O	1:A:456:GLN:HG3	2.08	0.53
1:A:687:TYR:CD1	1:A:701:ILE:HG13	2.43	0.53
1:A:667:VAL:HG21	1:A:707:ILE:CG2	2.39	0.53
1:A:1134:GLU:O	1:A:1137:THR:OG1	2.26	0.53
1:A:634:GLN:HB3	1:A:635:PRO:HD2	1.89	0.53
1:A:1102:ARG:N	1:A:1103:PRO:CD	2.71	0.53
1:A:268:GLY:O	1:A:285:LEU:HD22	2.08	0.53
1:A:912:LEU:HD12	1:A:928:ARG:HH22	1.72	0.53
1:A:546:LEU:HD21	1:A:593:MET:HG3	1.90	0.53
1:A:770:LEU:HD13	1:A:865:GLU:HB2	1.91	0.53
1:A:234:GLN:O	1:A:235:GLU:C	2.51	0.53
1:A:596:PHE:CE2	1:A:648:ASN:HA	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:690:SER:O	1:A:691:LEU:HD23	2.09	0.53
1:A:585:GLU:N	1:A:585:GLU:OE2	2.41	0.53
1:A:576:LEU:HD13	1:A:577:LEU:C	2.35	0.53
1:A:614:PHE:CE1	1:A:626:ARG:HG3	2.44	0.53
1:A:413:LEU:HD23	1:A:424:THR:HG22	1.89	0.52
1:A:559:GLY:HA2	1:A:565:SER:O	2.10	0.52
1:A:615:GLY:CA	1:A:624:SER:HB2	2.38	0.52
1:A:643:SER:CB	1:A:644:LEU:HD23	2.39	0.52
1:A:1090:ASP:OD2	1:A:1090:ASP:N	2.41	0.52
1:A:24:THR:HG22	1:A:25:SER:HG	1.72	0.52
1:A:602:LEU:O	1:A:614:PHE:HB2	2.09	0.52
1:A:1014:MET:HA	1:A:1015:GLN:O	2.10	0.52
1:A:555:LEU:HD13	1:A:568:ILE:HG21	1.92	0.52
1:A:600:HIS:CD2	1:A:618:ILE:HG12	2.45	0.52
1:A:945:ILE:O	1:A:946:ALA:HB2	2.10	0.52
1:A:110:ASP:HB2	1:A:136:TYR:HE1	1.76	0.51
1:A:264:VAL:HG12	1:A:265:ASP:OD1	2.11	0.51
1:A:421:THR:C	1:A:422:TYR:CD1	2.88	0.51
1:A:730:SER:HB2	1:A:732:CYS:SG	2.50	0.51
1:A:1094:ILE:CG2	1:A:1094:ILE:O	2.57	0.51
1:A:555:LEU:HD13	1:A:568:ILE:CG2	2.41	0.51
1:A:1055:GLN:HE22	1:A:1089:ILE:HA	1.75	0.51
1:A:206:PRO:O	1:A:207:TRP:HB3	2.10	0.51
1:A:463:VAL:HA	1:A:505:SER:O	2.10	0.51
1:A:564:ILE:N	1:A:564:ILE:HD12	2.25	0.51
1:A:1108:VAL:O	1:A:1109:VAL:HB	2.09	0.51
1:A:1123:GLU:O	1:A:1124:ALA:HB3	2.09	0.51
1:A:413:LEU:HD23	1:A:424:THR:CB	2.40	0.51
1:A:5:TYR:HB2	1:A:1043:LEU:HD11	1.92	0.51
1:A:881:LEU:HD12	1:A:889:ARG:O	2.11	0.51
1:A:102:THR:O	1:A:102:THR:HG22	2.09	0.51
1:A:290:GLN:O	1:A:291:MET:C	2.53	0.51
1:A:910:MET:O	1:A:910:MET:HG2	2.10	0.51
1:A:90:GLU:O	1:A:101:ILE:HG22	2.11	0.50
1:A:522:HIS:HB3	1:A:523:PRO:HD2	1.93	0.50
1:A:441:GLU:HA	1:A:687:TYR:CE2	2.47	0.50
1:A:1091:GLY:HA2	1:A:1094:ILE:HB	1.93	0.50
1:A:1125:THR:HB	1:A:1128:ASP:HB2	1.93	0.50
1:A:36:ASN:OD1	1:A:60:LYS:HG2	2.12	0.50
1:A:909:ILE:HA	1:A:926:LEU:HD22	1.94	0.50
1:A:1055:GLN:O	1:A:1059:ASN:ND2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:576:LEU:HD13	1:A:577:LEU:N	2.26	0.50
1:A:275:ASP:HB2	1:A:279:ARG:H	1.76	0.50
1:A:317:LEU:O	1:A:318:ASP:HB2	2.10	0.50
1:A:358:PRO:HA	1:A:1033:VAL:O	2.12	0.50
1:A:558:ILE:HG22	1:A:567:ARG:HB2	1.92	0.50
1:A:917:LYS:C	1:A:919:ASP:N	2.70	0.50
1:A:938:MET:HE3	1:A:939:GLU:OE2	2.12	0.50
1:A:351:GLU:OE2	1:A:353:PHE:HE2	1.95	0.50
1:A:480:SER:O	1:A:484:LYS:HA	2.12	0.49
1:A:589:ARG:HG3	1:A:635:PRO:HB2	1.93	0.49
1:A:928:ARG:HD3	1:A:953:TRP:HA	1.93	0.49
1:A:1041:THR:HG22	1:A:1042:SER:H	1.77	0.49
1:A:909:ILE:HA	1:A:926:LEU:CD2	2.42	0.49
1:A:81:THR:CG2	1:A:83:LYS:H	2.26	0.49
1:A:184:ASP:O	1:A:185:PRO:C	2.55	0.49
1:A:59:GLY:HA2	1:A:1073:TRP:CE3	2.46	0.49
1:A:110:ASP:HB2	1:A:136:TYR:CE1	2.48	0.49
1:A:261:HIS:HA	1:A:272:LEU:O	2.12	0.49
1:A:923:VAL:HG21	1:A:959:ILE:HG13	1.93	0.49
1:A:1125:THR:HB	1:A:1128:ASP:H	1.78	0.49
1:A:459:PHE:CD2	1:A:460:CYS:N	2.80	0.49
1:A:864:LYS:HD2	1:A:899:VAL:O	2.13	0.49
1:A:90:GLU:HB3	1:A:101:ILE:HG23	1.93	0.49
1:A:564:ILE:HD11	1:A:585:GLU:HA	1.95	0.49
1:A:660:TYR:CE1	1:A:707:ILE:HG13	2.47	0.49
1:A:1000:LEU:HD13	1:A:1002:GLU:HB2	1.95	0.49
1:A:134:ARG:C	1:A:135:LEU:HD23	2.38	0.49
1:A:614:PHE:HE1	1:A:626:ARG:HG3	1.77	0.49
1:A:641:PHE:HA	1:A:681:PRO:CG	2.43	0.49
1:A:1051:LEU:O	1:A:1054:MET:HB2	2.13	0.49
1:A:467:GLN:HE22	1:A:524:GLN:H	1.60	0.49
1:A:679:MET:SD	1:A:679:MET:C	2.95	0.49
1:A:175:ALA:O	1:A:176:PRO:C	2.56	0.49
1:A:927:MET:CE	1:A:927:MET:CG	2.90	0.49
1:A:1051:LEU:CD2	1:A:1094:ILE:HD13	2.35	0.49
1:A:182:TYR:HE2	1:A:191:LYS:HB2	1.78	0.48
1:A:617:ASN:ND2	1:A:622:LEU:HD13	2.28	0.48
1:A:667:VAL:HG21	1:A:707:ILE:HG21	1.96	0.48
1:A:392:ASN:HD22	1:A:1012:LEU:CB	2.26	0.48
1:A:185:PRO:O	1:A:186:GLN:HB2	2.12	0.48
1:A:656:PRO:HB2	1:A:671:VAL:HB	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:ILE:HG21	1:A:217:SER:HA	1.95	0.48
1:A:355:ASN:ND2	1:A:357:GLY:HA2	2.28	0.48
1:A:458:PHE:HB3	1:A:501:ALA:HB3	1.95	0.48
1:A:923:VAL:HG21	1:A:959:ILE:CG1	2.43	0.48
1:A:954:MET:HE3	1:A:957:VAL:HG23	1.96	0.48
1:A:979:LYS:HZ3	1:A:989:ARG:NH2	2.10	0.48
1:A:637:VAL:HB	1:A:652:CYS:HB2	1.96	0.48
1:A:864:LYS:HD2	1:A:899:VAL:HG12	1.94	0.48
1:A:903:CYS:C	1:A:905:HIS:H	2.22	0.48
1:A:933:LEU:HG	1:A:944:GLU:HA	1.96	0.48
1:A:695:ASN:O	1:A:696:ASN:C	2.56	0.48
1:A:507:GLN:NE2	1:A:553:SER:HB3	2.29	0.48
1:A:294:THR:CG2	1:A:295:VAL:H	2.27	0.48
1:A:743:GLN:HA	1:A:747:GLY:O	2.13	0.47
1:A:70:LYS:H	1:A:70:LYS:CD	2.27	0.47
1:A:38:ARG:HD2	1:A:54:GLU:OE1	2.14	0.47
1:A:413:LEU:HD23	1:A:424:THR:HB	1.95	0.47
1:A:659:ILE:HG22	1:A:666:LEU:HB3	1.96	0.47
1:A:789:HIS:ND1	1:A:812:TYR:HA	2.29	0.47
1:A:854:SER:O	1:A:856:GLY:N	2.47	0.47
1:A:948:ASP:HB2	1:A:992:LEU:CD1	2.44	0.47
1:A:826:ASN:ND2	1:A:852:GLN:OE1	2.48	0.47
1:A:222:VAL:HA	1:A:223:PRO:HD3	1.73	0.47
1:A:543:ILE:O	1:A:543:ILE:HG13	2.15	0.47
1:A:652:CYS:HB3	1:A:676:VAL:O	2.15	0.47
1:A:661:SER:HA	1:A:665:LYS:O	2.15	0.47
1:A:886:SER:C	1:A:909:ILE:O	2.58	0.47
1:A:607:GLY:HA2	1:A:635:PRO:HB3	1.96	0.47
1:A:25:SER:O	1:A:26:ALA:C	2.56	0.47
1:A:381:ALA:O	1:A:382:PHE:C	2.57	0.47
1:A:400:ALA:HB3	1:A:701:ILE:HD11	1.97	0.47
1:A:396:ILE:HD11	1:A:673:LEU:HD21	1.96	0.46
1:A:665:LYS:HB2	1:A:665:LYS:NZ	2.30	0.46
1:A:394:ILE:HD11	1:A:707:ILE:HA	1.97	0.46
1:A:765:VAL:HG12	1:A:806:GLN:HB3	1.98	0.46
1:A:174:GLN:O	1:A:175:ALA:HB2	2.15	0.46
1:A:168:LYS:HE2	1:A:219:VAL:O	2.15	0.46
1:A:478:LEU:HD21	1:A:521:ILE:CG2	2.46	0.46
1:A:558:ILE:O	1:A:566:ALA:HA	2.15	0.46
1:A:459:PHE:HE2	1:A:461:GLY:HA3	1.80	0.46
1:A:509:VAL:HG21	1:A:571:LEU:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:642:ARG:HH22	1:A:683:ASN:CG	2.24	0.46
1:A:107:ASN:OD1	1:A:109:GLN:HB2	2.16	0.46
1:A:367:LEU:HB2	1:A:374:GLN:OE1	2.15	0.46
1:A:377:THR:O	1:A:387:LEU:HA	2.16	0.46
1:A:932:LEU:C	1:A:933:LEU:HD12	2.40	0.46
1:A:1051:LEU:HA	1:A:1054:MET:HB2	1.98	0.46
1:A:110:ASP:O	1:A:111:ARG:C	2.59	0.46
1:A:182:TYR:OH	1:A:209:GLN:NE2	2.49	0.46
1:A:184:ASP:O	1:A:185:PRO:O	2.33	0.46
1:A:343:GLN:HE21	1:A:343:GLN:HA	1.81	0.46
1:A:706:GLU:HA	1:A:707:ILE:HD12	1.98	0.46
1:A:979:LYS:HZ3	1:A:989:ARG:HH21	1.62	0.46
1:A:1047:TRP:HZ3	1:A:1132:VAL:HG13	1.79	0.46
1:A:768:SER:C	1:A:769:LYS:HD3	2.41	0.45
1:A:881:LEU:HD11	1:A:888:VAL:CG1	2.45	0.45
1:A:347:VAL:C	1:A:348:VAL:HG23	2.41	0.45
1:A:690:SER:HB3	1:A:701:ILE:HB	1.98	0.45
1:A:909:ILE:HG12	1:A:926:LEU:HD22	1.98	0.45
1:A:148:ASP:O	1:A:149:ASN:HB3	2.16	0.45
1:A:367:LEU:HA	1:A:367:LEU:HD23	1.76	0.45
1:A:706:GLU:O	1:A:707:ILE:HG13	2.16	0.45
1:A:63:VAL:O	1:A:79:ILE:HA	2.16	0.45
1:A:294:THR:HG22	1:A:295:VAL:N	2.32	0.45
1:A:297:LEU:C	1:A:297:LEU:CD1	2.88	0.45
1:A:333:LEU:HD12	1:A:333:LEU:HA	1.73	0.45
1:A:347:VAL:HG12	1:A:348:VAL:N	2.27	0.45
1:A:687:TYR:N	1:A:688:PRO:HD3	2.32	0.45
1:A:294:THR:CG2	1:A:295:VAL:N	2.80	0.45
1:A:342:GLU:C	1:A:344:GLY:N	2.74	0.45
1:A:421:THR:C	1:A:422:TYR:CG	2.94	0.45
1:A:695:ASN:OD1	1:A:698:THR:HB	2.16	0.45
1:A:161:GLU:CD	1:A:191:LYS:HE3	2.42	0.45
1:A:536:HIS:ND1	1:A:562:THR:HB	2.33	0.45
1:A:926:LEU:HD12	1:A:927:MET:SD	2.57	0.45
1:A:1058:LEU:HD11	1:A:1097:PHE:HB2	1.99	0.45
1:A:254:LYS:O	1:A:254:LYS:HD3	2.18	0.44
1:A:378:CYS:HB3	1:A:721:PRO:HB2	1.98	0.44
1:A:828:TYR:CE2	1:A:861:VAL:HG21	2.52	0.44
1:A:966:LEU:HD13	1:A:1007:PHE:CE2	2.53	0.44
1:A:60:LYS:HE2	1:A:972:PHE:CE1	2.52	0.44
1:A:396:ILE:CG1	1:A:396:ILE:O	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:GLY:HA3	1:A:428:SER:OG	2.17	0.44
1:A:706:GLU:C	1:A:707:ILE:HD12	2.42	0.44
1:A:468:LEU:HD11	1:A:481:GLN:OE1	2.17	0.44
1:A:518:TYR:CD1	1:A:571:LEU:CD2	3.00	0.44
1:A:1051:LEU:HB3	1:A:1094:ILE:CD1	2.48	0.44
1:A:133:LEU:HB3	1:A:135:LEU:HD21	2.00	0.44
1:A:452:VAL:HG11	1:A:455:GLN:HG3	2.00	0.44
1:A:504:ASN:ND2	1:A:507:GLN:HG2	2.31	0.44
1:A:529:ILE:HG22	1:A:529:ILE:O	2.17	0.44
1:A:433:THR:HB	1:A:452:VAL:O	2.18	0.44
1:A:511:ALA:CB	1:A:516:LEU:HD23	2.43	0.44
1:A:578:HIS:CD2	1:A:623:LEU:HG	2.52	0.44
1:A:612:PHE:HE2	1:A:628:LYS:CG	2.29	0.44
1:A:928:ARG:NE	1:A:928:ARG:H	2.16	0.44
1:A:263:ARG:HA	1:A:271:TYR:CD2	2.52	0.44
1:A:451:PHE:CE1	1:A:479:VAL:HG21	2.52	0.44
1:A:455:GLN:O	1:A:456:GLN:C	2.60	0.44
1:A:472:THR:HG22	1:A:475:SER:O	2.18	0.44
1:A:507:GLN:HE21	1:A:571:LEU:HD13	1.83	0.44
1:A:667:VAL:O	1:A:668:PHE:HD1	2.01	0.44
1:A:753:ARG:HG2	1:A:753:ARG:NH1	2.31	0.44
1:A:1065:VAL:HG12	1:A:1066:GLY:N	2.32	0.44
1:A:932:LEU:HD13	1:A:965:PHE:CZ	2.53	0.43
1:A:220:ILE:HB	1:A:230:ILE:HB	1.99	0.43
1:A:223:PRO:O	1:A:225:PRO:HD2	2.19	0.43
1:A:653:SER:C	1:A:655:ARG:H	2.25	0.43
1:A:116:SER:HB3	1:A:137:ASP:CG	2.44	0.43
1:A:356:LEU:HD21	1:A:712:ILE:HD13	2.01	0.43
1:A:763:SER:C	1:A:803:HIS:HE1	2.25	0.43
1:A:949:PHE:O	1:A:950:ASN:CG	2.62	0.43
1:A:185:PRO:O	1:A:186:GLN:CB	2.64	0.43
1:A:414:ARG:HA	1:A:422:TYR:HA	1.99	0.43
1:A:433:THR:O	1:A:453:ASP:HA	2.19	0.43
1:A:458:PHE:CB	1:A:501:ALA:HB2	2.49	0.43
1:A:508:VAL:HG12	1:A:509:VAL:N	2.33	0.43
1:A:93:GLN:HB2	1:A:98:ILE:HG23	1.99	0.43
1:A:658:VAL:CG1	1:A:659:ILE:N	2.82	0.43
1:A:894:THR:CG2	1:A:896:GLU:HB2	2.48	0.43
1:A:984:THR:C	1:A:986:ASP:H	2.27	0.43
1:A:840:GLU:OE1	1:A:844:LYS:HE3	2.19	0.43
1:A:25:SER:O	1:A:27:GLU:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:GLN:OE1	1:A:279:ARG:NH2	2.52	0.43
1:A:639:ARG:HG3	1:A:640:THR:N	2.34	0.43
1:A:660:TYR:OH	1:A:704:ILE:CG2	2.67	0.43
1:A:793:ILE:C	1:A:794:ILE:HD12	2.43	0.43
1:A:905:HIS:O	1:A:906:TYR:HB3	2.19	0.43
1:A:253:ILE:O	1:A:255:GLN:N	2.51	0.43
1:A:600:HIS:NE2	1:A:618:ILE:HD13	2.33	0.43
1:A:196:SER:OG	1:A:199:GLU:HG2	2.19	0.42
1:A:839:GLU:CG	1:A:840:GLU:OE2	2.67	0.42
1:A:893:TRP:CZ3	1:A:899:VAL:HG23	2.54	0.42
1:A:949:PHE:HD1	1:A:949:PHE:H	1.65	0.42
1:A:520:GLN:HB2	1:A:527:ARG:HB3	2.01	0.42
1:A:534:MET:CE	1:A:560:LEU:HD11	2.49	0.42
1:A:592:LEU:O	1:A:603:LEU:N	2.38	0.42
1:A:706:GLU:CA	1:A:707:ILE:HD12	2.49	0.42
1:A:1041:THR:CG2	1:A:1042:SER:N	2.82	0.42
1:A:55:VAL:HG11	1:A:100:ILE:HG13	2.01	0.42
1:A:275:ASP:OD2	1:A:279:ARG:HB2	2.19	0.42
1:A:478:LEU:HD21	1:A:521:ILE:HG23	2.01	0.42
1:A:517:TYR:N	1:A:517:TYR:CD1	2.87	0.42
1:A:643:SER:OG	1:A:644:LEU:HD23	2.19	0.42
1:A:931:LEU:HB2	1:A:933:LEU:HD11	2.01	0.42
1:A:608:ASP:O	1:A:633:THR:O	2.37	0.42
1:A:949:PHE:CD1	1:A:949:PHE:N	2.87	0.42
1:A:159:LEU:CD2	1:A:161:GLU:HB2	2.48	0.42
1:A:358:PRO:HD2	1:A:380:GLY:HA2	2.02	0.42
1:A:492:GLU:O	1:A:494:GLN:N	2.51	0.42
1:A:816:LEU:HD12	1:A:831:VAL:HG22	2.01	0.42
1:A:909:ILE:HA	1:A:926:LEU:HD13	2.01	0.42
1:A:1064:SER:O	1:A:1065:VAL:C	2.62	0.42
1:A:1097:PHE:HA	1:A:1100:ILE:HD12	2.02	0.42
1:A:1139:ILE:HD13	1:A:1139:ILE:HG21	1.60	0.42
1:A:312:GLU:HG3	1:A:327:ARG:HE	1.84	0.42
1:A:413:LEU:HD23	1:A:424:THR:HG21	1.98	0.42
1:A:130:MET:HE1	1:A:195:VAL:HG12	2.02	0.42
1:A:135:LEU:HD23	1:A:135:LEU:N	2.35	0.42
1:A:156:ASN:HD22	1:A:156:ASN:HA	1.51	0.42
1:A:537:GLU:HB3	1:A:561:TRP:CG	2.55	0.42
1:A:1102:ARG:HB2	1:A:1103:PRO:HD3	2.01	0.42
1:A:1108:VAL:H	1:A:1108:VAL:HG23	1.64	0.42
1:A:490:TRP:HB2	1:A:526:LEU:HD13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:731:GLN:HA	1:A:796:GLN:HE21	1.85	0.42
1:A:763:SER:O	1:A:803:HIS:HE1	2.03	0.42
1:A:23:PHE:N	1:A:30:ASN:ND2	2.66	0.42
1:A:301:ARG:NH1	1:A:303:GLU:OE2	2.53	0.42
1:A:642:ARG:HH22	1:A:683:ASN:CB	2.32	0.42
1:A:706:GLU:OE2	1:A:707:ILE:HD12	2.20	0.42
1:A:798:THR:HB	1:A:800:GLU:HG3	2.02	0.42
1:A:1125:THR:O	1:A:1129:LEU:HB2	2.20	0.42
1:A:275:ASP:HB3	1:A:277:GLU:N	2.31	0.41
1:A:507:GLN:NE2	1:A:553:SER:H	2.18	0.41
1:A:522:HIS:CB	1:A:527:ARG:NH1	2.83	0.41
1:A:617:ASN:C	1:A:619:GLU:H	2.28	0.41
1:A:909:ILE:HA	1:A:926:LEU:CD1	2.49	0.41
1:A:194:GLU:HB2	1:A:203:ASN:HB2	2.01	0.41
1:A:815:SER:HB3	1:A:872:SER:HA	2.01	0.41
1:A:192:THR:HB	1:A:205:GLY:HA3	2.03	0.41
1:A:643:SER:H	1:A:647:THR:HG22	1.85	0.41
1:A:939:GLU:HB3	1:A:941:ASN:ND2	2.28	0.41
1:A:413:LEU:CB	1:A:424:THR:O	2.55	0.41
1:A:534:MET:O	1:A:535:GLU:C	2.63	0.41
1:A:629:VAL:CG1	1:A:668:PHE:HE2	2.25	0.41
1:A:165:ILE:HB	1:A:181:VAL:O	2.20	0.41
1:A:364:VAL:C	1:A:365:VAL:HG23	2.45	0.41
1:A:410:LEU:HB3	1:A:680:CYS:SG	2.61	0.41
1:A:459:PHE:CZ	1:A:503:CYS:O	2.73	0.41
1:A:347:VAL:CG1	1:A:348:VAL:N	2.81	0.41
1:A:375:LEU:HD12	1:A:1037:ILE:HD13	2.03	0.41
1:A:415:SER:HB2	1:A:423:ASP:OD2	2.21	0.41
1:A:507:GLN:OE1	1:A:552:LEU:HA	2.20	0.41
1:A:920:PHE:N	1:A:920:PHE:CD2	2.85	0.41
1:A:1104:LYS:O	1:A:1108:VAL:HG23	2.19	0.41
1:A:222:VAL:O	1:A:227:GLY:HA2	2.21	0.41
1:A:145:LEU:N	1:A:145:LEU:CD1	2.84	0.41
1:A:467:GLN:HE22	1:A:524:GLN:CA	2.34	0.41
1:A:706:GLU:OE2	1:A:707:ILE:CD1	2.69	0.41
1:A:169:PHE:CE2	1:A:178:ILE:HD12	2.55	0.41
1:A:190:VAL:HG13	1:A:190:VAL:O	2.21	0.41
1:A:215:GLU:CB	1:A:234:GLN:HG3	2.50	0.41
1:A:458:PHE:HB3	1:A:501:ALA:HB2	2.01	0.41
1:A:464:ALA:O	1:A:465:HIS:HB2	2.20	0.41
1:A:569:LEU:HA	1:A:577:LEU:HD22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:805:HIS:CD2	1:A:851:PHE:CZ	3.09	0.41
1:A:984:THR:O	1:A:984:THR:OG1	2.18	0.41
1:A:1030:PHE:CE1	1:A:1038:GLY:HA3	2.52	0.41
1:A:207:TRP:CZ3	1:A:241:ASN:ND2	2.88	0.41
1:A:375:LEU:O	1:A:389:ILE:HA	2.21	0.41
1:A:471:ILE:HD11	1:A:503:CYS:HB2	2.03	0.41
1:A:534:MET:HE2	1:A:560:LEU:HD11	2.03	0.41
1:A:207:TRP:CD1	1:A:207:TRP:C	2.99	0.40
1:A:280:LEU:CD1	1:A:314:LEU:HD21	2.51	0.40
1:A:383:LYS:HE2	1:A:384:GLU:OE2	2.21	0.40
1:A:537:GLU:OE2	1:A:561:TRP:CE2	2.75	0.40
1:A:830:ILE:HG22	1:A:873:MET:HE1	2.02	0.40
1:A:926:LEU:O	1:A:928:ARG:NH2	2.54	0.40
1:A:1030:PHE:CE2	1:A:1038:GLY:HA3	2.53	0.40
1:A:218:MET:CE	1:A:261:HIS:HD2	2.19	0.40
1:A:569:LEU:HB3	1:A:575:GLU:O	2.21	0.40
1:A:617:ASN:C	1:A:619:GLU:N	2.79	0.40
1:A:854:SER:C	1:A:856:GLY:N	2.78	0.40
1:A:909:ILE:HG22	1:A:910:MET:N	2.37	0.40
1:A:107:ASN:OD1	1:A:109:GLN:CB	2.69	0.40
1:A:285:LEU:N	1:A:285:LEU:HD12	2.36	0.40
1:A:375:LEU:HD23	1:A:375:LEU:HA	1.84	0.40
1:A:631:LEU:HD23	1:A:631:LEU:HA	1.86	0.40
1:A:763:SER:C	1:A:803:HIS:CE1	3.00	0.40
1:A:839:GLU:HG3	1:A:840:GLU:CG	2.52	0.40
1:A:893:TRP:C	1:A:894:THR:O	2.63	0.40
1:A:917:LYS:O	1:A:919:ASP:C	2.65	0.40
1:A:258:ILE:HD13	1:A:273:LEU:HD13	2.02	0.40
1:A:389:ILE:N	1:A:389:ILE:CD1	2.64	0.40
1:A:437:MET:C	1:A:438:LEU:HG	2.46	0.40
1:A:612:PHE:CE2	1:A:628:LYS:HA	2.56	0.40
1:A:931:LEU:HD23	1:A:947:ARG:HB2	2.02	0.40
1:A:1112:LEU:HB3	1:A:1122:ARG:HH21	1.87	0.40
1:A:413:LEU:HD22	1:A:426:VAL:HG23	2.03	0.40
1:A:469:ILE:HG21	1:A:503:CYS:SG	2.62	0.40
1:A:478:LEU:HD12	1:A:526:LEU:CD2	2.52	0.40
1:A:504:ASN:HB3	1:A:543:ILE:O	2.21	0.40
1:A:611:LEU:C	1:A:611:LEU:HD23	2.46	0.40
1:A:786:VAL:HG12	1:A:787:GLU:N	2.36	0.40
1:A:902:GLU:O	1:A:905:HIS:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1111/1140 (98%)	888 (80%)	155 (14%)	68 (6%)	1 3

All (68) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	235	GLU
1	A	291	MET
1	A	405	PRO
1	A	417	PRO
1	A	430	VAL
1	A	494	GLN
1	A	495	ALA
1	A	502	SER
1	A	505	SER
1	A	523	PRO
1	A	684	SER
1	A	696	ASN
1	A	706	GLU
1	A	707	ILE
1	A	708	GLN
1	A	839	GLU
1	A	951	PRO
1	A	952	ASN
1	A	1024	THR
1	A	1065	VAL
1	A	287	LYS
1	A	371	GLY
1	A	406	GLY
1	A	463	VAL
1	A	623	LEU
1	A	632	GLY
1	A	748	GLY
1	A	751	ALA

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Mol	Chain	Res	Type
1	A	772	SER
1	A	841	ALA
1	A	864	LYS
1	A	894	THR
1	A	906	TYR
1	A	918	GLY
1	A	938	MET
1	A	950	ASN
1	A	985	THR
1	A	146	ASP
1	A	254	LYS
1	A	450	GLY
1	A	475	SER
1	A	493	PRO
1	A	826	ASN
1	A	876	PHE
1	A	897	LYS
1	A	919	ASP
1	A	983	ALA
1	A	1025	GLN
1	A	175	ALA
1	A	199	GLU
1	A	288	GLU
1	A	412	PRO
1	A	664	HIS
1	A	856	GLY
1	A	885	ASN
1	A	465	HIS
1	A	621	GLY
1	A	840	GLU
1	A	855	ASP
1	A	998	PHE
1	A	113	GLY
1	A	484	LYS
1	A	509	VAL
1	A	264	VAL
1	A	185	PRO
1	A	545	PRO
1	A	112	ILE
1	A	293	GLY

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	982/999 (98%)	842 (86%)	140 (14%)	3 10

All (140) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	20	THR
1	A	25	SER
1	A	27	GLU
1	A	32	LEU
1	A	50	ARG
1	A	61	ILE
1	A	68	ARG
1	A	70	LYS
1	A	73	SER
1	A	75	ASP
1	A	79	ILE
1	A	81	THR
1	A	83	LYS
1	A	93	GLN
1	A	94	SER
1	A	96	GLU
1	A	103	ARG
1	A	111	ARG
1	A	117	GLU
1	A	135	LEU
1	A	147	ARG
1	A	162	LEU
1	A	167	VAL
1	A	176	PRO
1	A	178	ILE
1	A	189	HIS
1	A	198	ARG
1	A	253	ILE
1	A	257	THR

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Mol	Chain	Res	Type
1	A	259	VAL
1	A	263	ARG
1	A	288	GLU
1	A	296	THR
1	A	297	LEU
1	A	302	VAL
1	A	312	GLU
1	A	333	LEU
1	A	334	VAL
1	A	342	GLU
1	A	366	ASP
1	A	372	GLN
1	A	383	LYS
1	A	384	GLU
1	A	401	SER
1	A	420	GLU
1	A	423	ASP
1	A	427	LEU
1	A	434	ARG
1	A	438	LEU
1	A	443	VAL
1	A	444	GLU
1	A	445	GLU
1	A	449	MET
1	A	452	VAL
1	A	457	THR
1	A	468	LEU
1	A	476	VAL
1	A	478	LEU
1	A	488	SER
1	A	514	ARG
1	A	517	TYR
1	A	527	ARG
1	A	529	ILE
1	A	537	GLU
1	A	550	ASN
1	A	565	SER
1	A	569	LEU
1	A	570	LYS
1	A	571	LEU
1	A	576	LEU
1	A	579	LYS

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Mol	Chain	Res	Type
1	A	585	GLU
1	A	587	ILE
1	A	589	ARG
1	A	591	ILE
1	A	594	THR
1	A	602	LEU
1	A	613	TYR
1	A	630	THR
1	A	638	LEU
1	A	644	LEU
1	A	647	THR
1	A	659	ILE
1	A	663	ASN
1	A	665	LYS
1	A	668	PHE
1	A	679	MET
1	A	685	ASP
1	A	688	PRO
1	A	700	THR
1	A	701	ILE
1	A	704	ILE
1	A	708	GLN
1	A	766	SER
1	A	780	THR
1	A	782	PHE
1	A	794	ILE
1	A	840	GLU
1	A	842	GLU
1	A	843	PRO
1	A	844	LYS
1	A	857	LYS
1	A	864	LYS
1	A	866	VAL
1	A	899	VAL
1	A	900	ARG
1	A	922	LEU
1	A	923	VAL
1	A	925	ASP
1	A	927	MET
1	A	949	PHE
1	A	957	VAL
1	A	966	LEU

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Mol	Chain	Res	Type
1	A	969	GLU
1	A	980	ASP
1	A	985	THR
1	A	992	LEU
1	A	993	GLN
1	A	1000	LEU
1	A	1014	MET
1	A	1015	GLN
1	A	1050	LEU
1	A	1052	LEU
1	A	1054	MET
1	A	1058	LEU
1	A	1069	GLU
1	A	1086	THR
1	A	1092	ASP
1	A	1093	LEU
1	A	1094	ILE
1	A	1106	GLN
1	A	1108	VAL
1	A	1111	ASN
1	A	1112	LEU
1	A	1122	ARG
1	A	1125	THR
1	A	1129	LEU
1	A	1131	LYS
1	A	1132	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	30	ASN
1	A	85	ASN
1	A	156	ASN
1	A	163	HIS
1	A	189	HIS
1	A	209	GLN
1	A	234	GLN
1	A	241	ASN
1	A	261	HIS
1	A	262	ASN
1	A	332	GLN

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Mol	Chain	Res	Type
1	A	343	GLN
1	A	370	GLN
1	A	392	ASN
1	A	399	HIS
1	A	455	GLN
1	A	456	GLN
1	A	462	ASN
1	A	467	GLN
1	A	648	ASN
1	A	663	ASN
1	A	670	ASN
1	A	683	ASN
1	A	695	ASN
1	A	708	GLN
1	A	711	HIS
1	A	727	GLN
1	A	796	GLN
1	A	797	HIS
1	A	885	ASN
1	A	941	ASN
1	A	1055	GLN
1	A	1056	ASN
1	A	1059	ASN
1	A	1070	HIS

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 ⓘ

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	1119/1140 (98%)	0.68	112 (10%)	12 10	8, 20, 28, 40	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	439	ASN	6.2
1	A	508	VAL	6.1
1	A	660	TYR	6.0
1	A	571	LEU	5.3
1	A	547	GLY	4.7
1	A	449	MET	4.4
1	A	517	TYR	4.3
1	A	444	GLU	4.1
1	A	924	GLY	4.1
1	A	519	LEU	4.0
1	A	474	ALA	4.0
1	A	684	SER	4.0
1	A	551	GLY	3.9
1	A	613	TYR	3.9
1	A	405	PRO	3.9
1	A	569	LEU	3.8
1	A	549	SER	3.8
1	A	528	GLN	3.7
1	A	501	ALA	3.6
1	A	460	CYS	3.6
1	A	413	LEU	3.6
1	A	425	LEU	3.6
1	A	401	SER	3.6
1	A	641	PHE	3.6
1	A	294	THR	3.6
1	A	483	PRO	3.5
1	A	496	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	436	LEU	3.4
1	A	599	SER	3.4
1	A	970	ASN	3.3
1	A	462	ASN	3.3
1	A	620	THR	3.3
1	A	416	ASP	3.3
1	A	685	ASP	3.2
1	A	618	ILE	3.1
1	A	293	GLY	3.1
1	A	585	GLU	3.1
1	A	661	SER	3.1
1	A	518	TYR	3.1
1	A	502	SER	3.1
1	A	682	LEU	3.1
1	A	595	THR	3.0
1	A	596	PHE	3.0
1	A	598	SER	3.0
1	A	925	ASP	3.0
1	A	440	GLY	3.0
1	A	556	CYS	3.0
1	A	578	HIS	3.0
1	A	419	ARG	2.9
1	A	541	LEU	2.9
1	A	482	GLU	2.9
1	A	648	ASN	2.9
1	A	647	THR	2.9
1	A	531	HIS	2.8
1	A	420	GLU	2.8
1	A	614	PHE	2.8
1	A	406	GLY	2.8
1	A	448	LEU	2.8
1	A	291	MET	2.8
1	A	417	PRO	2.8
1	A	621	GLY	2.8
1	A	498	ILE	2.7
1	A	443	VAL	2.7
1	A	663	ASN	2.7
1	A	506	SER	2.7
1	A	485	ALA	2.7
1	A	437	MET	2.7
1	A	645	SER	2.7
1	A	523	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	646	THR	2.6
1	A	619	GLU	2.6
1	A	415	SER	2.6
1	A	550	ASN	2.6
1	A	481	GLN	2.6
1	A	841	ALA	2.5
1	A	521	ILE	2.5
1	A	497	ASN	2.5
1	A	544	THR	2.5
1	A	458	PHE	2.5
1	A	468	LEU	2.4
1	A	469	ILE	2.4
1	A	557	ALA	2.4
1	A	1	MET	2.4
1	A	487	VAL	2.4
1	A	983	ALA	2.4
1	A	659	ILE	2.3
1	A	243	ASP	2.3
1	A	442	GLU	2.3
1	A	690	SER	2.3
1	A	773	SER	2.3
1	A	918	GLY	2.3
1	A	418	ASN	2.2
1	A	568	ILE	2.2
1	A	162	LEU	2.2
1	A	486	LEU	2.2
1	A	982	ALA	2.2
1	A	629	VAL	2.2
1	A	503	CYS	2.2
1	A	411	TRP	2.2
1	A	358	PRO	2.1
1	A	1109	VAL	2.1
1	A	478	LEU	2.1
1	A	464	ALA	2.1
1	A	516	LEU	2.1
1	A	548	ASP	2.1
1	A	602	LEU	2.1
1	A	522	HIS	2.1
1	A	526	LEU	2.1
1	A	736	LEU	2.1
1	A	617	ASN	2.0
1	A	421	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	490	TRP	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.