



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:01 AM UTC

PDB ID : 1T70 / pdb_00001t70
Title : Crystal structure of a novel phosphatase from *Deinococcus radiodurans*
Authors : Shin, D.H.; Wang, W.; Kim, R.; Yokota, H.; Kim, S.H.; Berkeley Structural Genomics Center (BSGC)
Deposited on : 2004-05-07
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

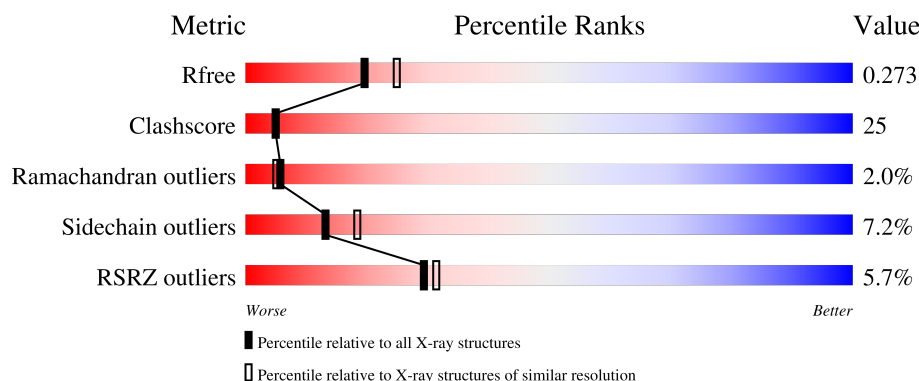
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	255	2% 60% 34% 6%
1	B	255	4% 60% 34% 6%
1	C	255	4% 61% 33% 6%
1	D	255	5% 60% 33% 7%
1	E	255	5% 54% 41% 5%

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Mol	Chain	Length	Quality of chain
1	F	255	5% 58% 36% 5%
1	G	255	18% 48% 45% 7%
1	H	255	2% 60% 35% 5%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 16095 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 Phosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	255	Total	C	N	O	S	0	0	0
			1972	1243	358	363	8			
1	B	255	Total	C	N	O	S	0	0	0
			1972	1243	358	363	8			
1	C	255	Total	C	N	O	S	0	0	0
			1972	1243	358	363	8			
1	D	255	Total	C	N	O	S	0	0	0
			1972	1243	358	363	8			
1	E	255	Total	C	N	O	S	0	0	0
			1972	1243	358	363	8			
1	F	255	Total	C	N	O	S	0	0	0
			1972	1243	358	363	8			
1	G	255	Total	C	N	O	S	0	0	0
			1972	1243	358	363	8			
1	H	255	Total	C	N	O	S	0	0	0
			1972	1243	358	363	8			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	58	Total	O	0	0
			58	58		
2	B	56	Total	O	0	0
			56	56		
2	C	55	Total	O	0	0
			55	55		
2	D	39	Total	O	0	0
			39	39		
2	E	26	Total	O	0	0
			26	26		
2	F	42	Total	O	0	0
			42	42		

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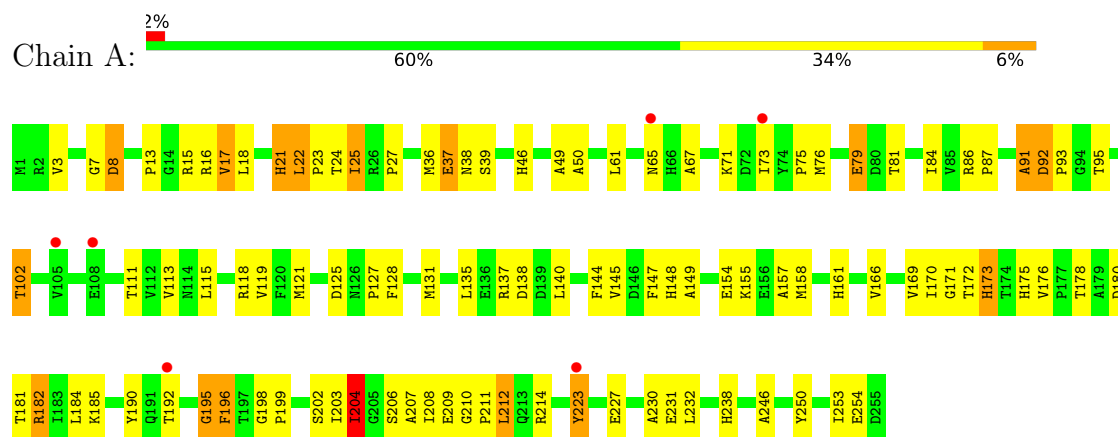
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	16	Total	O	0	0
			16	16		
2	H	27	Total	O	0	0
			27	27		

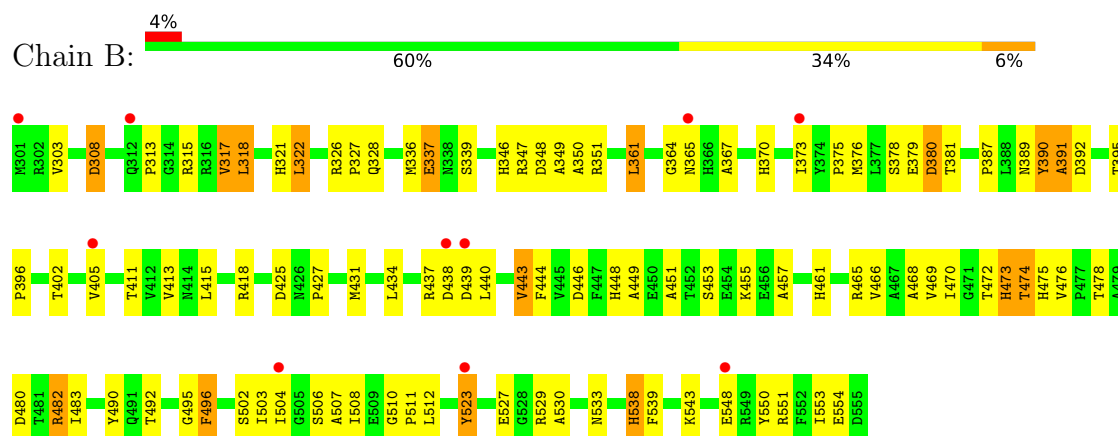
3 Residue-property plots [i](#)

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.

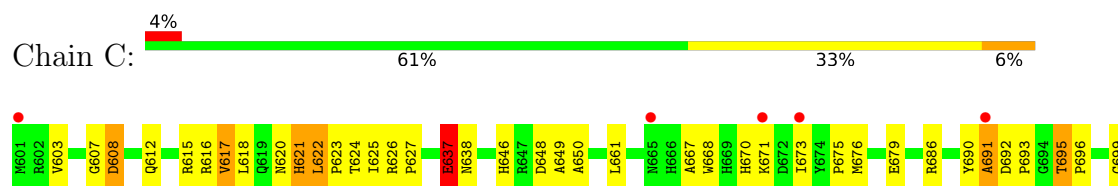
• Molecule 1: Phosphatase

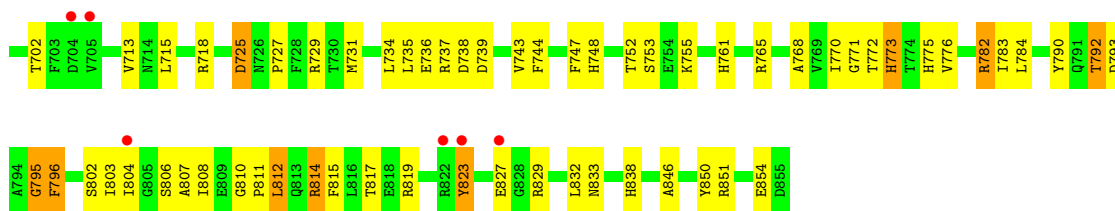


• Molecule 1: Phosphatase

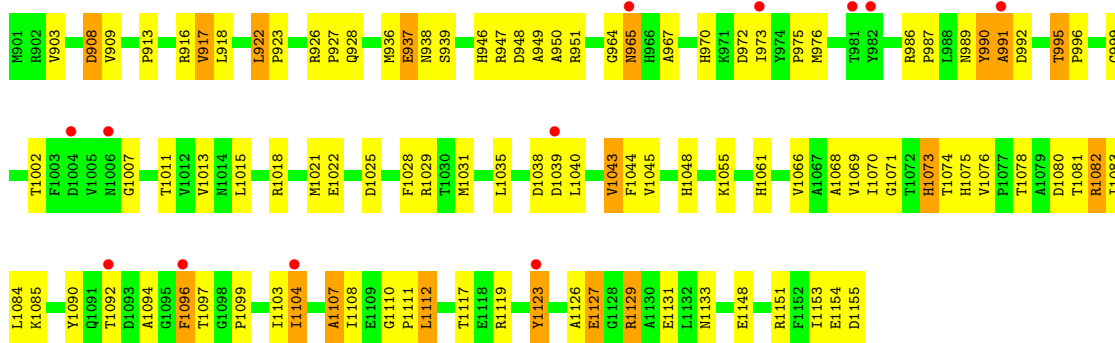


• Molecule 1: Phosphatase

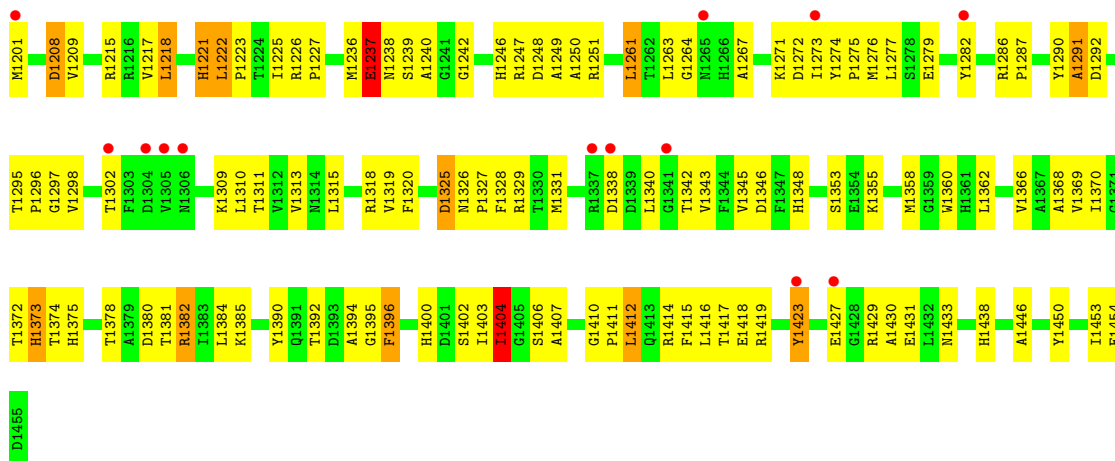




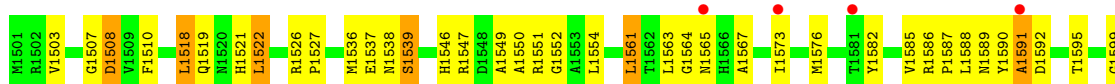
• Molecule 1: Phosphatase

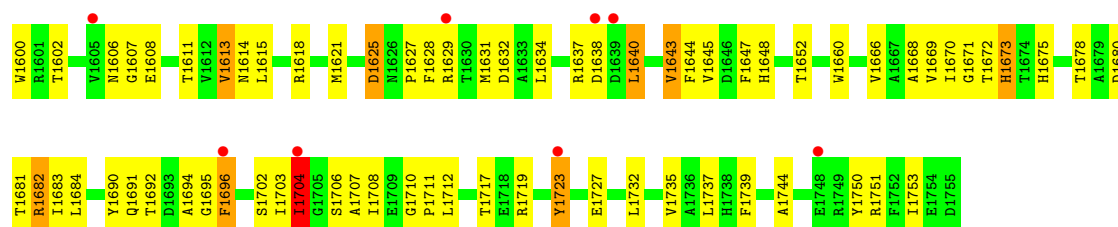


• Molecule 1: Phosphatase

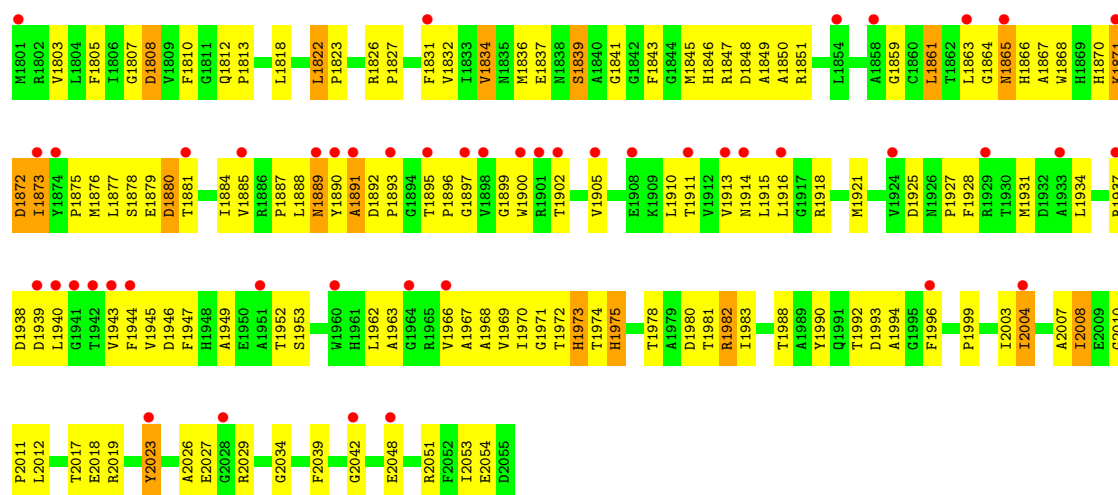


• Molecule 1: Phosphatase

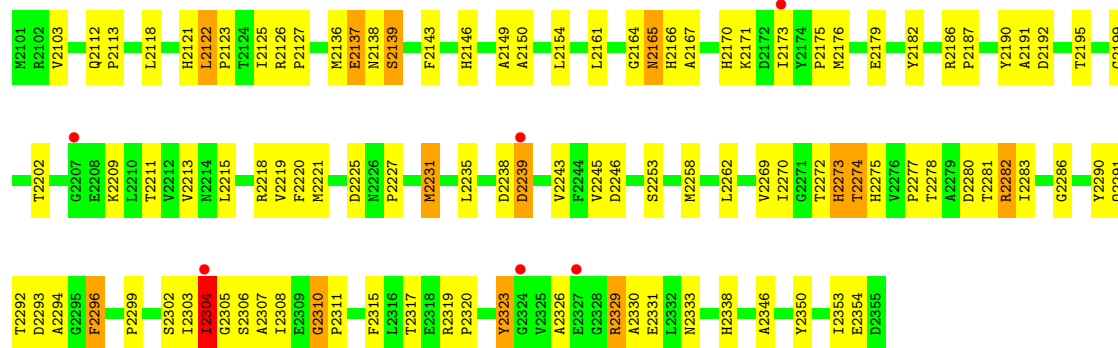




● Molecule 1: Phosphatase



● Molecule 1: Phosphatase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	242.79Å 116.61Å 89.28Å 90.00° 109.40° 90.00°	Depositor
Resolution (Å)	19.95 – 2.30 19.95 – 2.30	Depositor EDS
% Data completeness (in resolution range)	78.5 (19.95-2.30) 90.3 (19.95-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.22 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.207 , 0.260 0.222 , 0.273	Depositor DCC
R_{free} test set	10028 reflections (10.02%)	wwPDB-VP
Wilson B-factor (Å ²)	36.0	Xtriage
Anisotropy	0.504	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.016 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16095	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.00% 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	0.49	0/2022	1.00	9/2743 (0.3%)
1	B	0.48	0/2022	0.99	8/2743 (0.3%)
1	C	0.47	0/2022	1.00	9/2743 (0.3%)
1	D	0.46	0/2022	0.99	11/2743 (0.4%)
1	E	0.43	0/2022	0.94	7/2743 (0.3%)
1	F	0.44	0/2022	1.00	8/2743 (0.3%)
1	G	0.42	1/2022 (0.0%)	0.96	8/2743 (0.3%)
1	H	0.48	1/2022 (0.0%)	0.94	4/2743 (0.1%)
All	All	0.46	2/16176 (0.0%)	0.98	64/21944 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	2231	MET	SD-CE	-6.55	1.63	1.79
1	G	1974	THR	N-CA	5.49	1.53	1.46

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	440	LEU	N-CA-C	10.54	122.35	111.07
1	G	1974	THR	N-CA-C	-9.49	101.70	113.38
1	C	808	ILE	N-CA-C	8.18	118.96	110.62
1	A	208	ILE	N-CA-C	7.50	118.27	110.62
1	F	1640	LEU	N-CA-C	7.32	119.04	111.14
1	F	1708	ILE	N-CA-C	7.29	118.09	110.72
1	H	2274	THR	N-CA-C	-7.15	104.56	113.28
1	D	1040	LEU	N-CA-C	7.05	120.36	111.69
1	C	795	GLY	N-CA-C	-7.03	102.41	112.81
1	B	391	ALA	N-CA-C	7.00	119.76	111.71
1	A	195	GLY	N-CA-C	-6.98	103.88	112.33
1	B	508	ILE	N-CA-C	6.94	117.70	110.62
1	A	21	HIS	N-CA-C	6.77	120.01	111.69
1	C	691	ALA	N-CA-C	6.70	119.41	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1108	ILE	N-CA-C	6.61	117.39	110.72
1	E	1209	VAL	N-CA-C	-6.55	100.19	109.63
1	B	474	THR	N-CA-C	-6.54	105.46	113.50
1	B	495	GLY	N-CA-C	-6.39	103.36	112.81
1	D	995	THR	CA-C-N	6.29	126.26	119.78
1	D	995	THR	C-N-CA	6.29	126.26	119.78
1	C	621	HIS	N-CA-C	6.18	119.30	111.69
1	H	2243	VAL	N-CA-C	6.10	117.09	108.36
1	F	1591	ALA	N-CA-C	6.04	118.36	111.11
1	F	1643	VAL	N-CA-C	6.04	116.80	107.99
1	D	991	ALA	N-CA-C	6.03	117.94	111.36
1	F	1707	ALA	N-CA-C	-5.97	102.23	110.35
1	B	451	ALA	N-CA-C	5.96	118.85	109.96
1	A	91	ALA	N-CA-C	5.94	119.62	112.38
1	D	1007	GLY	N-CA-C	-5.93	107.47	115.36
1	G	1891	ALA	N-CA-C	5.93	119.98	112.87
1	E	1221	HIS	N-CA-C	5.86	120.45	113.12
1	D	1043	VAL	N-CA-C	5.73	116.19	108.17
1	E	1343	VAL	N-CA-C	5.73	116.55	108.36
1	G	2008	ILE	N-CA-C	5.63	115.82	110.53
1	F	1539	SER	N-CA-C	5.61	117.85	111.11
1	E	1291	ALA	N-CA-C	5.61	118.33	111.82
1	A	198	GLY	CA-C-N	5.57	126.81	119.84
1	A	198	GLY	C-N-CA	5.57	126.81	119.84
1	C	695	THR	CA-C-N	5.55	125.86	119.92
1	C	695	THR	C-N-CA	5.55	125.86	119.92
1	B	390	TYR	N-CA-C	-5.52	98.28	107.99
1	A	209	GLU	N-CA-C	5.48	116.93	111.07
1	C	743	VAL	N-CA-C	5.44	115.78	108.17
1	H	2308	ILE	N-CA-C	5.38	116.16	110.72
1	B	443	VAL	N-CA-C	5.34	115.99	108.36
1	E	1407	ALA	N-CA-C	-5.33	103.44	110.43
1	A	92	ASP	CA-C-N	5.32	124.93	119.56
1	A	92	ASP	C-N-CA	5.32	124.93	119.56
1	G	1807	GLY	N-CA-C	5.28	119.29	112.54
1	D	1096	PHE	N-CA-C	5.27	118.32	110.52
1	D	1107	ALA	N-CA-C	-5.26	103.54	110.43
1	F	1696	PHE	N-CA-C	5.25	117.46	110.53
1	H	2286	GLY	N-CA-C	-5.24	107.83	115.63
1	D	990	TYR	N-CA-C	-5.22	100.01	108.41
1	C	637	GLU	N-CA-C	5.20	119.11	112.87
1	G	1975	HIS	CA-C-N	-5.19	118.33	122.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	1975	HIS	C-N-CA	-5.19	118.33	122.85
1	D	909	VAL	N-CA-C	-5.15	102.86	109.30
1	G	1839	SER	N-CA-C	5.15	117.31	111.02
1	C	807	ALA	N-CA-C	-5.10	102.84	110.23
1	G	1834	VAL	N-CA-C	5.08	115.35	107.78
1	F	1607	GLY	N-CA-C	-5.04	108.87	115.47
1	E	1237	GLU	N-CA-C	5.01	117.47	111.71
1	E	1395	GLY	N-CA-C	-5.01	103.57	112.58

There are no chirality outliers.

There are no planarity outliers.

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	1972	0	1904	84	0
1	B	1972	0	1901	93	0
1	C	1972	0	1901	109	0
1	D	1972	0	1901	119	0
1	E	1972	0	1901	119	0
1	F	1972	0	1901	102	0
1	G	1972	0	1901	140	0
1	H	1972	0	1901	87	0
2	A	58	0	0	1	0
2	B	56	0	0	2	0
2	C	55	0	0	2	0
2	D	39	0	0	5	0
2	E	26	0	0	2	0
2	F	42	0	0	1	0
2	G	16	0	0	0	0
2	H	27	0	0	0	0
All	All	16095	0	15211	778	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 25.

All (778) 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:C:729:ARG:NH2	1:E:1291:ALA:HB3	1.67	1.09
1:D:991:ALA:HB3	1:F:1629:ARG:HH22	1.08	1.08
1:C:729:ARG:HH22	1:E:1291:ALA:HB3	0.97	1.08
1:D:1029:ARG:HH22	1:F:1591:ALA:HB3	0.98	1.07
1:E:1315:LEU:HG	1:E:1331:MET:HE2	1.37	1.06
1:D:1013:VAL:HG21	1:D:1031:MET:HE1	1.42	1.00
1:C:667:ALA:O	1:C:673:ILE:HD13	1.63	0.98
1:D:992:ASP:HB3	1:D:995:THR:HG23	1.47	0.97
1:A:67:ALA:O	1:A:73:ILE:HD13	1.64	0.96
1:D:1029:ARG:NH2	1:F:1591:ALA:HB3	1.80	0.95
1:A:25:ILE:HG23	1:D:1148:GLU:OE1	1.66	0.94
1:B:548:GLU:OE1	1:C:625:ILE:HG23	1.66	0.94
1:D:991:ALA:HB3	1:F:1629:ARG:NH2	1.83	0.94
1:F:1567:ALA:O	1:F:1573:ILE:HD13	1.68	0.93
1:D:967:ALA:O	1:D:973:ILE:HD13	1.67	0.93
1:F:1613:VAL:HG21	1:F:1631:MET:HE1	1.51	0.93
1:E:1382:ARG:HH11	1:E:1382:ARG:HB3	1.32	0.91
1:E:1267:ALA:O	1:E:1273:ILE:HD13	1.72	0.89
1:H:2170:HIS:O	1:H:2173:ILE:HD12	1.76	0.86
1:B:415:LEU:HG	1:B:431:MET:HE2	1.57	0.85
1:F:1615:LEU:HG	1:F:1631:MET:HE3	1.57	0.84
1:G:1945:VAL:HG21	1:G:1962:LEU:HD23	1.58	0.84
1:C:650:ALA:CB	1:C:676:MET:HE1	2.08	0.84
1:B:367:ALA:O	1:B:373:ILE:HD13	1.78	0.83
1:F:1547:ARG:HG3	1:F:1576:MET:HE3	1.60	0.83
1:H:2213:VAL:HG21	1:H:2231:MET:HE1	1.60	0.83
1:B:418:ARG:HD2	1:B:427:PRO:HD3	1.59	0.82
1:D:1080:ASP:OD1	1:D:1092:THR:HG23	1.80	0.82
1:C:713:VAL:HG21	1:C:731:MET:HE1	1.62	0.82
1:E:1380:ASP:OD1	1:E:1392:THR:HG23	1.80	0.82
1:B:391:ALA:HB2	1:B:425:ASP:CG	2.05	0.81
1:F:1602:THR:HG22	1:F:1611:THR:OG1	1.80	0.81
1:G:1868:TRP:HA	1:G:1873:ILE:HD13	1.62	0.81
1:H:2192:ASP:HB3	1:H:2195:THR:HG23	1.63	0.81
1:A:92:ASP:HB3	1:A:95:THR:HG23	1.64	0.80
1:B:548:GLU:HG2	1:C:624:THR:HB	1.64	0.80
1:A:91:ALA:HB2	1:A:125:ASP:CG	2.07	0.80
1:C:621:HIS:HE1	1:C:850:TYR:OH	1.63	0.80
1:C:691:ALA:HB2	1:C:725:ASP:OD1	1.82	0.79
1:F:1591:ALA:HB2	1:F:1625:ASP:OD1	1.82	0.79
1:G:1845:MET:HE2	1:G:1863:LEU:HD21	1.63	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:964:GLY:HA2	1:D:987:PRO:CG	2.14	0.78
1:B:490:TYR:OH	1:B:492:THR:HG22	1.81	0.78
1:E:1326:ASN:HB2	1:E:1329:ARG:HH21	1.49	0.77
1:G:1913:VAL:HG21	1:G:1931:MET:HE1	1.66	0.77
1:A:46:HIS:HD2	1:A:49:ALA:H	1.29	0.77
1:C:718:ARG:HD2	1:C:727:PRO:HD3	1.66	0.77
1:C:650:ALA:HB3	1:C:676:MET:HE1	1.66	0.76
1:G:2051:ARG:HE	1:G:2053:ILE:HD11	1.49	0.76
1:E:1315:LEU:HD11	1:E:1331:MET:HG2	1.65	0.76
1:E:1375:HIS:HD2	1:E:1404:ILE:O	1.69	0.76
1:F:1550:ALA:HB3	1:F:1576:MET:HE1	1.67	0.76
1:E:1292:ASP:HB3	1:E:1295:THR:HG23	1.68	0.76
1:F:1592:ASP:HB3	1:F:1595:THR:HG23	1.67	0.76
1:D:991:ALA:CB	1:F:1629:ARG:HH22	1.95	0.75
1:G:1850:ALA:HB3	1:G:1876:MET:HE1	1.66	0.75
1:C:729:ARG:HH22	1:E:1291:ALA:CB	1.90	0.75
1:H:2121:HIS:HE1	1:H:2350:TYR:OH	1.68	0.75
1:F:1690:TYR:OH	1:F:1692:THR:HG22	1.86	0.75
1:H:2167:ALA:O	1:H:2173:ILE:HD13	1.86	0.75
1:E:1382:ARG:HH11	1:E:1382:ARG:CB	1.99	0.75
1:C:692:ASP:N	1:E:1329:ARG:NH1	2.36	0.74
1:B:434:LEU:HD12	1:B:437:ARG:HE	1.53	0.74
1:A:190:TYR:OH	1:A:192:THR:HG22	1.89	0.73
1:H:2215:LEU:HG	1:H:2231:MET:HE3	1.70	0.73
1:E:1302:THR:HG22	1:E:1311:THR:OG1	1.88	0.73
1:G:1822:LEU:HD11	1:G:1832:VAL:HG11	1.71	0.73
1:G:1867:ALA:O	1:G:1873:ILE:HD13	1.88	0.73
1:D:964:GLY:HA2	1:D:987:PRO:HG3	1.71	0.72
1:A:46:HIS:CD2	1:A:49:ALA:H	2.07	0.72
1:H:2282:ARG:HH11	1:H:2282:ARG:HB3	1.53	0.72
1:C:646:HIS:CD2	1:C:649:ALA:H	2.08	0.72
1:E:1390:TYR:OH	1:E:1392:THR:HG22	1.90	0.72
1:E:1315:LEU:CG	1:E:1331:MET:HE2	2.16	0.72
1:D:1090:TYR:OH	1:D:1092:THR:HG22	1.90	0.72
1:G:1846:HIS:HD2	1:G:1849:ALA:H	1.37	0.72
1:G:1861:LEU:N	1:G:1861:LEU:HD22	2.05	0.72
1:B:375:PRO:O	1:B:379:GLU:HG2	1.90	0.71
1:C:782:ARG:HH11	1:C:782:ARG:HB3	1.54	0.71
1:A:25:ILE:HG23	1:D:1148:GLU:CD	2.14	0.71
1:E:1416:LEU:HD23	1:F:1629:ARG:HG3	1.72	0.71
1:C:646:HIS:HD2	1:C:649:ALA:H	1.38	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1889:ASN:HB2	1:G:1925:ASP:O	1.91	0.70
1:G:1846:HIS:CD2	1:G:1849:ALA:H	2.09	0.70
1:A:24:THR:HB	1:D:1148:GLU:HG2	1.71	0.70
1:H:2213:VAL:CG2	1:H:2231:MET:HE1	2.21	0.70
1:C:692:ASP:HB3	1:C:695:THR:HG23	1.74	0.70
1:G:1803:VAL:HG21	1:G:2039:PHE:CE2	2.27	0.70
1:C:691:ALA:HB3	1:E:1329:ARG:NH1	2.06	0.69
1:C:718:ARG:HD2	1:C:727:PRO:CD	2.22	0.69
1:H:2191:ALA:HB2	1:H:2225:ASP:OD1	1.91	0.69
1:A:161:HIS:HB2	1:B:512:LEU:HD21	1.73	0.69
1:B:350:ALA:HB3	1:B:376:MET:HE1	1.72	0.69
1:C:675:PRO:O	1:C:679:GLU:HG2	1.93	0.68
1:B:379:GLU:O	1:B:381:THR:HG23	1.92	0.68
1:G:1836:MET:HB3	1:G:1839:SER:OG	1.94	0.68
1:G:2011:PRO:HG3	1:G:2023:TYR:HD1	1.59	0.68
1:A:178:THR:HG21	1:A:192:THR:OG1	1.93	0.68
1:F:1680:ASP:OD1	1:F:1692:THR:HG23	1.93	0.68
1:G:1864:GLY:HA2	1:G:1887:PRO:HG3	1.75	0.68
1:B:503:ILE:O	1:B:504:ILE:HG22	1.93	0.68
1:G:1847:ARG:HA	1:G:1876:MET:CE	2.23	0.67
1:C:691:ALA:HB3	1:E:1329:ARG:HH12	1.58	0.67
1:D:1015:LEU:HD11	1:D:1031:MET:HG2	1.75	0.67
1:E:1438:HIS:HB2	1:E:1446:ALA:HB3	1.77	0.67
1:F:1546:HIS:HD2	1:F:1549:ALA:H	1.41	0.67
1:D:1029:ARG:HH12	1:F:1591:ALA:HB1	1.60	0.67
1:E:1403:ILE:O	1:E:1404:ILE:HG22	1.94	0.67
1:H:2290:TYR:OH	1:H:2292:THR:HG22	1.95	0.67
1:H:2191:ALA:HB2	1:H:2225:ASP:CG	2.20	0.67
1:A:8:ASP:HB3	1:A:38:ASN:HD22	1.58	0.66
1:A:75:PRO:O	1:A:79:GLU:HG2	1.94	0.66
1:A:202:SER:HB2	1:A:206:SER:O	1.94	0.66
1:F:1546:HIS:CD2	1:F:1549:ALA:H	2.13	0.66
1:H:2280:ASP:OD1	1:H:2292:THR:HG23	1.94	0.66
1:F:1613:VAL:CG2	1:F:1631:MET:HE1	2.24	0.66
1:A:21:HIS:HE1	1:A:250:TYR:OH	1.79	0.66
1:A:204:ILE:HD12	1:B:453:SER:HB3	1.77	0.66
1:G:1990:TYR:OH	1:G:1992:THR:HG22	1.95	0.66
1:D:1103:ILE:O	1:D:1104:ILE:HG22	1.94	0.66
1:G:1871:LYS:HG2	1:G:1872:ASP:N	2.10	0.66
1:A:79:GLU:O	1:A:81:THR:HG23	1.96	0.65
1:G:2004:ILE:HD12	1:H:2253:SER:HB3	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:2215:LEU:HD11	1:H:2231:MET:HG2	1.77	0.65
1:D:991:ALA:HB1	1:F:1629:ARG:HH12	1.60	0.65
1:F:1618:ARG:HD2	1:F:1627:PRO:HD3	1.79	0.65
1:D:1015:LEU:HD11	1:D:1031:MET:CG	2.26	0.65
1:B:418:ARG:HD2	1:B:427:PRO:CD	2.26	0.65
1:G:1879:GLU:O	1:G:1881:THR:HG23	1.96	0.65
1:H:2275:HIS:HD2	1:H:2304:ILE:O	1.79	0.65
1:B:415:LEU:CG	1:B:431:MET:HE2	2.26	0.64
1:D:936:MET:HB3	1:D:939:SER:OG	1.98	0.64
1:E:1222:LEU:N	1:E:1223:PRO:HD2	2.10	0.64
1:G:1915:LEU:HG	1:G:1931:MET:HE2	1.80	0.64
1:G:1967:ALA:HB1	1:G:2039:PHE:CE1	2.32	0.64
1:G:1902:THR:HG22	1:G:1911:THR:OG1	1.98	0.64
1:F:1703:ILE:O	1:F:1704:ILE:HG22	1.97	0.64
1:E:1291:ALA:HB2	1:E:1325:ASP:OD1	1.97	0.64
1:D:1066:VAL:HG12	1:D:1068:ALA:H	1.63	0.64
1:E:1237:GLU:HG2	1:E:1238:ASN:ND2	2.13	0.64
1:F:1710:GLY:HA3	1:F:1723:TYR:HB3	1.80	0.64
1:E:1378:THR:HG21	1:E:1392:THR:OG1	1.97	0.63
1:E:1326:ASN:CB	1:E:1329:ARG:HH21	2.10	0.63
1:H:2202:THR:HG22	1:H:2211:THR:OG1	1.99	0.63
1:A:176:VAL:HG21	1:B:492:THR:HG21	1.81	0.63
1:A:210:GLY:HA3	1:A:223:TYR:HB3	1.80	0.63
1:B:482:ARG:HB3	1:B:482:ARG:HH11	1.64	0.63
1:F:1643:VAL:O	1:F:1666:VAL:HG13	1.99	0.63
1:A:113:VAL:HG21	1:A:131:MET:HE1	1.79	0.62
1:F:1735:VAL:HG12	1:F:1737:LEU:HD21	1.81	0.62
1:E:1247:ARG:HA	1:E:1276:MET:CE	2.30	0.62
1:E:1372:THR:O	1:E:1373:HIS:HB3	1.99	0.62
1:G:1843:PHE:HD1	1:G:1866:HIS:CD2	2.17	0.62
1:F:1675:HIS:HD2	1:F:1704:ILE:O	1.83	0.62
1:G:1872:ASP:O	1:G:1876:MET:HG3	1.99	0.62
1:G:1921:MET:HE3	1:G:1973:HIS:CE1	2.35	0.62
1:G:1953:SER:HB3	1:H:2304:ILE:HD12	1.81	0.62
1:B:321:HIS:HE1	1:B:550:TYR:OH	1.82	0.62
1:B:351:ARG:HD2	2:B:583:HOH:O	1.99	0.62
1:G:1947:PHE:O	1:G:1971:GLY:HA2	2.00	0.62
1:H:2338:HIS:HB2	1:H:2346:ALA:HB3	1.80	0.62
1:A:172:THR:O	1:A:173:HIS:HB3	1.98	0.62
1:D:1029:ARG:HH12	1:F:1591:ALA:CB	2.12	0.62
1:D:1110:GLY:HA3	1:D:1123:TYR:HB3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1250:ALA:HB3	1:E:1276:MET:HE1	1.81	0.61
1:E:1275:PRO:O	1:E:1279:GLU:HG2	2.00	0.61
1:G:1864:GLY:HA2	1:G:1887:PRO:CG	2.30	0.61
1:H:2150:ALA:HB3	1:H:2176:MET:HE1	1.83	0.61
1:C:612:GLN:HG3	1:C:615:ARG:NH2	2.15	0.61
1:D:1015:LEU:CG	1:D:1031:MET:HE3	2.30	0.61
1:G:1803:VAL:HG21	1:G:2039:PHE:HE2	1.65	0.61
1:H:2215:LEU:HG	1:H:2231:MET:CE	2.30	0.61
1:D:946:HIS:HD2	1:D:949:ALA:H	1.49	0.61
1:A:180:ASP:OD1	1:A:192:THR:HG23	2.00	0.61
1:H:2121:HIS:CE1	1:H:2350:TYR:OH	2.54	0.60
1:B:478:THR:HG21	1:B:492:THR:OG1	2.01	0.60
1:H:2215:LEU:HD13	1:H:2258:MET:HE3	1.84	0.60
1:G:1913:VAL:CG2	1:G:1931:MET:HE1	2.31	0.60
1:E:1414:ARG:HD2	2:E:185:HOH:O	2.01	0.60
1:A:212:LEU:HD21	1:B:461:HIS:HB2	1.84	0.60
1:B:391:ALA:HB2	1:B:425:ASP:OD1	2.00	0.60
1:D:1015:LEU:HG	1:D:1031:MET:HE3	1.84	0.60
1:G:1891:ALA:HB2	1:G:1925:ASP:OD1	2.02	0.60
1:G:1975:HIS:O	1:G:1996:PHE:HB2	2.01	0.60
1:B:548:GLU:CD	1:C:625:ILE:HG23	2.26	0.60
1:A:131:MET:HE2	1:A:131:MET:HA	1.82	0.59
1:E:1246:HIS:CD2	1:E:1249:ALA:H	2.20	0.59
1:E:1366:VAL:HG12	1:E:1368:ALA:H	1.67	0.59
1:H:2215:LEU:HD11	1:H:2231:MET:CG	2.32	0.59
1:B:480:ASP:OD1	1:B:492:THR:HG23	2.02	0.59
1:C:621:HIS:CE1	1:C:850:TYR:OH	2.52	0.59
1:B:415:LEU:HD11	1:B:431:MET:HG2	1.84	0.59
1:H:2219:VAL:HG12	1:H:2220:PHE:CD2	2.36	0.59
1:C:692:ASP:N	1:E:1329:ARG:HH12	1.99	0.59
1:H:2282:ARG:HH11	1:H:2282:ARG:CB	2.16	0.59
1:B:523:TYR:N	1:B:523:TYR:CD2	2.69	0.59
1:E:1311:THR:HG21	1:E:1340:LEU:HD22	1.85	0.59
1:F:1669:VAL:C	1:F:1670:ILE:HD12	2.28	0.59
1:H:2319:ARG:HB3	1:H:2320:PRO:HD2	1.85	0.59
1:D:1078:THR:HG21	1:D:1092:THR:OG1	2.02	0.59
1:E:1375:HIS:CD2	1:E:1404:ILE:HG12	2.38	0.59
1:A:27:PRO:HA	1:D:928:GLN:HE22	1.67	0.58
1:G:1847:ARG:HG3	1:G:1876:MET:HE3	1.85	0.58
1:H:2272:THR:O	1:H:2273:HIS:HB3	2.03	0.58
1:D:950:ALA:HB3	1:D:976:MET:HE1	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1075:HIS:O	1:D:1096:PHE:HB2	2.03	0.58
1:A:182:ARG:HH11	1:A:182:ARG:HB3	1.69	0.58
1:C:772:THR:O	1:C:773:HIS:HB3	2.03	0.58
1:G:1826:ARG:O	1:G:1826:ARG:HD3	2.03	0.58
1:C:715:LEU:HD11	1:C:731:MET:HG2	1.84	0.58
1:E:1353:SER:HB3	1:F:1704:ILE:HD12	1.84	0.58
1:G:1847:ARG:HG2	1:G:1851:ARG:NH2	2.18	0.58
1:F:1682:ARG:HG2	1:F:1683:ILE:H	1.66	0.58
1:G:1847:ARG:HA	1:G:1876:MET:HE3	1.85	0.58
1:G:1945:VAL:HG21	1:G:1962:LEU:CD2	2.33	0.58
1:C:670:HIS:O	1:C:673:ILE:HD12	2.04	0.58
1:B:469:VAL:C	1:B:470:ILE:HD12	2.28	0.58
1:G:1971:GLY:O	1:G:1993:ASP:HA	2.02	0.58
1:D:916:ARG:NH1	1:D:1154:GLU:OE1	2.37	0.58
1:D:1099:PRO:CB	1:D:1126:ALA:HB3	2.33	0.58
1:E:1246:HIS:HD2	1:E:1249:ALA:H	1.49	0.58
1:G:1839:SER:HB2	1:G:1845:MET:HA	1.86	0.58
1:A:25:ILE:HA	1:D:1148:GLU:OE2	2.03	0.57
1:D:972:ASP:O	1:D:976:MET:HG3	2.04	0.57
1:D:913:PRO:O	1:D:917:VAL:HG22	2.03	0.57
1:G:1848:ASP:HA	1:G:1851:ARG:NH1	2.19	0.57
1:C:782:ARG:HG2	1:C:783:ILE:H	1.68	0.57
1:H:2190:TYR:HB3	1:H:2195:THR:HG21	1.86	0.57
1:C:753:SER:HB3	1:D:1104:ILE:HD12	1.86	0.57
1:D:948:ASP:HA	1:D:951:ARG:HH12	1.70	0.57
1:A:91:ALA:HB2	1:A:125:ASP:OD1	2.05	0.57
1:E:1236:MET:HG3	1:E:1261:LEU:HG	1.86	0.57
1:F:1672:THR:O	1:F:1673:HIS:HB3	2.03	0.57
1:H:2218:ARG:HD2	1:H:2227:PRO:HD2	1.87	0.57
1:H:2329:ARG:HD2	1:H:2354:GLU:O	2.05	0.57
1:C:718:ARG:HD3	2:C:163:HOH:O	2.04	0.57
1:A:115:LEU:HD11	1:A:131:MET:HG2	1.87	0.57
1:D:1075:HIS:HD2	1:D:1104:ILE:HG12	1.70	0.57
1:G:1949:ALA:O	1:G:1973:HIS:HB3	2.05	0.57
1:A:203:ILE:O	1:A:204:ILE:HG22	2.05	0.56
1:E:1375:HIS:CD2	1:E:1404:ILE:O	2.55	0.56
1:G:2011:PRO:HG3	1:G:2023:TYR:CD1	2.39	0.56
1:A:182:ARG:HH11	1:A:182:ARG:CB	2.19	0.56
1:D:1111:PRO:HG3	1:D:1123:TYR:CD1	2.40	0.56
1:F:1588:LEU:HD22	1:F:1634:LEU:HD22	1.86	0.56
1:G:2003:ILE:O	1:G:2004:ILE:HG22	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:833:ASN:OD1	1:C:851:ARG:HG3	2.06	0.56
1:F:1675:HIS:O	1:F:1696:PHE:HB2	2.04	0.56
1:B:548:GLU:OE2	1:C:625:ILE:HA	2.04	0.56
1:F:1670:ILE:HD12	1:F:1670:ILE:N	2.21	0.56
1:D:948:ASP:HA	1:D:951:ARG:NH1	2.21	0.56
1:F:1589:ASN:O	1:F:1625:ASP:HB2	2.04	0.56
1:H:2310:GLY:HA3	1:H:2323:TYR:HB3	1.87	0.56
1:D:1082:ARG:HH11	1:D:1082:ARG:HB3	1.70	0.56
1:H:2303:ILE:O	1:H:2304:ILE:HG22	2.06	0.56
1:B:402:THR:HG22	1:B:411:THR:OG1	2.06	0.56
1:B:472:THR:O	1:B:473:HIS:HB3	2.06	0.56
1:D:1013:VAL:CG1	1:D:1045:VAL:HG22	2.36	0.56
1:E:1272:ASP:O	1:E:1275:PRO:HG2	2.06	0.56
1:G:1915:LEU:HD11	1:G:1931:MET:HG2	1.88	0.56
1:F:1563:LEU:C	1:F:1614:ASN:HD21	2.14	0.55
1:G:1803:VAL:HG12	1:G:1831:PHE:HB3	1.87	0.55
1:G:1818:LEU:HD13	1:G:1818:LEU:C	2.30	0.55
1:D:1082:ARG:HG2	2:D:52:HOH:O	2.06	0.55
1:G:1982:ARG:HG2	1:G:1983:ILE:H	1.70	0.55
1:B:326:ARG:O	1:B:326:ARG:HD3	2.06	0.55
1:G:1812:GLN:HB2	1:G:1813:PRO:HD3	1.87	0.55
1:H:2112:GLN:HB2	1:H:2113:PRO:HD3	1.89	0.55
1:A:118:ARG:HD2	1:A:127:PRO:CD	2.36	0.55
1:F:1735:VAL:CG1	1:F:1737:LEU:HD21	2.37	0.55
1:E:1217:VAL:HG12	1:E:1454:GLU:OE2	2.07	0.55
1:G:1969:VAL:C	1:G:1970:ILE:HD12	2.31	0.55
1:D:946:HIS:CD2	1:D:949:ALA:H	2.24	0.55
1:D:1129:ARG:HD2	1:D:1155:ASP:OXT	2.06	0.55
1:E:1271:LYS:O	1:E:1275:PRO:HD2	2.05	0.55
1:F:1621:MET:HE3	1:F:1673:HIS:CE1	2.42	0.55
1:E:1277:LEU:HD22	1:E:1297:GLY:HA3	1.88	0.55
1:H:2175:PRO:O	1:H:2179:GLU:HG2	2.06	0.55
1:E:1423:TYR:HD2	1:E:1423:TYR:O	1.89	0.55
1:D:1043:VAL:O	1:D:1066:VAL:HG13	2.06	0.54
1:E:1247:ARG:HA	1:E:1276:MET:HE3	1.89	0.54
1:F:1735:VAL:HG12	1:F:1737:LEU:CD2	2.37	0.54
1:G:1826:ARG:HG2	1:G:1832:VAL:HG21	1.88	0.54
1:G:1999:PRO:HG3	1:G:2026:ALA:HB3	1.88	0.54
1:C:832:LEU:C	1:C:832:LEU:HD23	2.32	0.54
1:E:1431:GLU:HB2	1:E:1453:ILE:HD13	1.89	0.54
1:H:2146:HIS:CD2	1:H:2149:ALA:H	2.26	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:VAL:HG12	1:A:144:PHE:O	2.08	0.54
1:B:482:ARG:HH11	1:B:482:ARG:CB	2.20	0.54
1:D:1129:ARG:HD2	1:D:1155:ASP:C	2.33	0.54
1:G:1970:ILE:HD12	1:G:1970:ILE:N	2.22	0.54
1:G:2023:TYR:CD2	1:G:2023:TYR:N	2.74	0.54
1:G:1888:LEU:CD1	1:G:1899:GLY:HA3	2.38	0.53
1:A:91:ALA:HB2	1:A:125:ASP:OD2	2.08	0.53
1:C:752:THR:HG21	1:D:1074:THR:HB	1.89	0.53
1:D:1002:THR:HG22	1:D:1011:THR:OG1	2.09	0.53
1:C:729:ARG:NH2	1:E:1291:ALA:CB	2.57	0.53
1:G:2007:ALA:O	1:G:2011:PRO:HD2	2.09	0.53
1:C:838:HIS:HB2	1:C:846:ALA:HB3	1.90	0.53
1:A:7:GLY:HA3	1:A:195:GLY:O	2.08	0.53
1:C:782:ARG:HG2	1:C:783:ILE:N	2.23	0.53
1:A:137:ARG:HD2	1:A:140:LEU:HD21	1.90	0.53
1:B:548:GLU:CG	1:C:624:THR:HB	2.35	0.53
1:H:2191:ALA:O	1:H:2192:ASP:C	2.51	0.53
1:A:76:MET:HE2	1:A:84:ILE:HD11	1.90	0.53
1:D:1069:VAL:C	1:D:1070:ILE:HD12	2.34	0.53
1:C:782:ARG:HH11	1:C:782:ARG:CB	2.22	0.53
1:H:2113:PRO:HB2	1:H:2299:PRO:HD3	1.90	0.53
1:B:347:ARG:HG3	1:B:376:MET:HE3	1.91	0.52
1:G:1943:VAL:O	1:G:1966:VAL:HG13	2.09	0.52
1:G:1945:VAL:HG23	1:G:1966:VAL:HG11	1.90	0.52
1:A:172:THR:O	1:A:173:HIS:CB	2.58	0.52
1:E:1287:PRO:HB2	1:E:1290:TYR:CE2	2.43	0.52
1:C:810:GLY:HA3	1:C:823:TYR:HB3	1.92	0.52
1:D:1148:GLU:HB3	2:D:69:HOH:O	2.08	0.52
1:G:1818:LEU:HD13	1:G:1818:LEU:O	2.09	0.52
1:G:1978:THR:HA	1:H:2278:THR:HA	1.91	0.52
1:B:496:PHE:CD1	1:B:496:PHE:C	2.86	0.52
1:E:1374:THR:HB	1:F:1652:THR:HG21	1.91	0.52
1:A:232:LEU:HD23	1:A:232:LEU:C	2.35	0.52
1:F:1618:ARG:HD2	1:F:1627:PRO:CD	2.40	0.52
1:G:2023:TYR:H	1:G:2023:TYR:HD2	1.54	0.52
1:A:16:ARG:NH1	1:A:254:GLU:OE1	2.41	0.52
1:E:1402:SER:HB2	1:E:1406:SER:O	2.10	0.52
1:G:1891:ALA:HB2	1:G:1925:ASP:HB2	1.91	0.52
1:C:802:SER:HB2	1:C:806:SER:O	2.10	0.52
1:E:1372:THR:O	1:E:1373:HIS:CB	2.57	0.52
1:B:523:TYR:H	1:B:523:TYR:HD2	1.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:616:ARG:NH1	1:C:854:GLU:OE1	2.42	0.52
1:C:691:ALA:CB	1:E:1329:ARG:HH12	2.23	0.52
1:E:1355:LYS:HD3	1:E:1392:THR:O	2.10	0.52
1:F:1678:THR:HG21	1:F:1692:THR:OG1	2.09	0.52
1:B:472:THR:O	1:B:473:HIS:CB	2.57	0.52
1:B:523:TYR:N	1:B:523:TYR:HD2	2.07	0.52
1:D:990:TYR:HB3	1:D:995:THR:HG21	1.91	0.52
1:D:995:THR:HG22	1:E:1419:ARG:HH11	1.74	0.52
1:B:315:ARG:HD2	2:B:606:HOH:O	2.08	0.52
1:E:1411:PRO:HG3	1:E:1423:TYR:CD1	2.45	0.52
1:H:2302:SER:HB2	1:H:2306:SER:O	2.09	0.52
1:H:2330:ALA:O	1:H:2354:GLU:HG2	2.10	0.51
1:H:2272:THR:O	1:H:2273:HIS:CB	2.58	0.51
1:C:608:ASP:OD1	1:C:772:THR:HB	2.11	0.51
1:A:8:ASP:HB3	1:A:38:ASN:ND2	2.24	0.51
1:B:392:ASP:O	1:B:395:THR:HG23	2.11	0.51
1:C:737:ARG:HG2	1:C:737:ARG:HH11	1.76	0.51
1:D:991:ALA:HB2	1:D:1025:ASP:CG	2.35	0.51
1:A:13:PRO:O	1:A:17:VAL:HG22	2.11	0.51
1:D:1131:GLU:OE2	1:D:1133:ASN:ND2	2.43	0.51
1:C:607:GLY:HA3	1:C:795:GLY:O	2.10	0.51
1:A:118:ARG:HD2	1:A:127:PRO:HD2	1.91	0.51
1:B:313:PRO:O	1:B:317:VAL:HG23	2.10	0.51
1:B:474:THR:O	1:B:475:HIS:HB2	2.10	0.51
1:F:1521:HIS:HE1	1:F:1750:TYR:OH	1.94	0.51
1:F:1547:ARG:HA	1:F:1576:MET:CE	2.41	0.51
1:H:2280:ASP:O	1:H:2281:THR:C	2.53	0.51
1:B:328:GLN:HE22	1:C:627:PRO:HA	1.75	0.51
1:G:1990:TYR:CD1	1:G:1990:TYR:C	2.89	0.51
1:F:1554:LEU:CD1	1:F:1582:TYR:HD2	2.24	0.51
1:A:65:ASN:ND2	1:A:121:MET:HE3	2.26	0.50
1:C:686:ARG:O	1:C:699:GLY:HA2	2.12	0.50
1:C:782:ARG:HD3	1:C:783:ILE:C	2.36	0.50
1:A:238:HIS:HB2	1:A:246:ALA:HB3	1.92	0.50
1:E:1248:ASP:HA	1:E:1251:ARG:HH12	1.75	0.50
1:E:1380:ASP:O	1:E:1381:THR:C	2.54	0.50
1:D:1055:LYS:HD3	1:D:1092:THR:O	2.10	0.50
1:G:1972:THR:O	1:G:1973:HIS:CB	2.60	0.50
1:H:2202:THR:HA	1:H:2211:THR:HA	1.94	0.50
1:B:439:ASP:OD2	1:B:439:ASP:N	2.40	0.50
1:D:965:ASN:HD22	1:D:1021:MET:HE3	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1221:HIS:HE1	1:E:1450:TYR:OH	1.95	0.50
1:G:1810:PHE:HB2	1:G:1996:PHE:CE2	2.46	0.50
1:G:1885:VAL:HG12	1:G:1914:ASN:HB2	1.93	0.50
1:G:2017:THR:HB	1:G:2019:ARG:NH1	2.26	0.50
1:C:691:ALA:HB3	1:E:1329:ARG:CZ	2.41	0.50
1:B:347:ARG:HA	1:B:376:MET:CE	2.42	0.50
1:B:548:GLU:OE2	1:C:624:THR:O	2.30	0.50
1:C:782:ARG:HD2	1:C:784:LEU:HD23	1.92	0.50
1:D:1071:GLY:HA3	1:D:1092:THR:O	2.11	0.50
1:F:1691:GLN:NE2	1:F:1694:ALA:HA	2.27	0.50
1:C:646:HIS:CD2	1:C:649:ALA:N	2.80	0.50
1:A:231:GLU:HB2	1:A:253:ILE:HD13	1.94	0.50
1:B:308:ASP:HB2	1:B:496:PHE:HB2	1.92	0.50
1:G:1875:PRO:O	1:G:1879:GLU:HG2	2.11	0.50
1:G:1888:LEU:HD22	1:G:1934:LEU:HD22	1.94	0.50
1:A:230:ALA:H	1:A:254:GLU:HG2	1.77	0.50
1:G:1888:LEU:HD13	1:G:1899:GLY:HA3	1.93	0.50
1:H:2291:GLN:HE21	1:H:2294:ALA:HA	1.76	0.49
1:E:1396:PHE:CD1	1:E:1396:PHE:C	2.88	0.49
1:A:22:LEU:N	1:A:23:PRO:HD2	2.26	0.49
1:D:1127:GLU:O	1:D:1127:GLU:CD	2.55	0.49
1:E:1431:GLU:OE2	1:E:1433:ASN:ND2	2.46	0.49
1:F:1526:ARG:O	1:F:1526:ARG:HD3	2.12	0.49
1:F:1634:LEU:HD12	1:F:1637:ARG:HE	1.76	0.49
1:F:1672:THR:O	1:F:1673:HIS:CB	2.59	0.49
1:G:1871:LYS:O	1:G:1875:PRO:HD2	2.12	0.49
1:A:21:HIS:CE1	1:A:250:TYR:OH	2.63	0.49
1:D:1075:HIS:CD2	1:D:1104:ILE:HG12	2.48	0.49
1:G:1836:MET:HB3	1:G:1839:SER:HG	1.76	0.49
1:G:1928:PHE:CE2	1:H:2315:PHE:HB3	2.47	0.49
1:D:964:GLY:O	1:D:967:ALA:N	2.43	0.49
1:D:1048:HIS:CE1	1:D:1073:HIS:CD2	3.01	0.49
1:D:1111:PRO:HG3	1:D:1123:TYR:HD1	1.77	0.49
1:B:548:GLU:CD	1:C:624:THR:C	2.80	0.49
1:F:1732:LEU:C	1:F:1732:LEU:HD23	2.38	0.49
1:H:2215:LEU:CG	1:H:2231:MET:HE3	2.40	0.49
1:B:504:ILE:HG23	1:B:504:ILE:O	2.12	0.49
1:D:937:GLU:HG3	1:D:938:ASN:N	2.28	0.49
1:E:1218:LEU:C	1:E:1218:LEU:HD13	2.38	0.49
1:G:1845:MET:SD	1:G:1850:ALA:HB2	2.52	0.49
1:E:1369:VAL:C	1:E:1370:ILE:HD12	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1900:TRP:CZ2	1:G:1937:ARG:NE	2.80	0.49
1:G:1963:ALA:HA	1:G:1988:THR:OG1	2.12	0.49
1:C:772:THR:O	1:C:773:HIS:CB	2.60	0.49
1:C:812:LEU:HD21	1:D:1061:HIS:HB2	1.94	0.49
1:G:1822:LEU:N	1:G:1823:PRO:HD2	2.27	0.49
1:G:1996:PHE:CZ	1:G:1999:PRO:HD2	2.47	0.49
1:D:991:ALA:CB	1:F:1629:ARG:NH2	2.66	0.49
1:D:1104:ILE:HG23	1:D:1104:ILE:O	2.13	0.49
1:E:1328:PHE:HA	1:E:1358:MET:HE1	1.95	0.49
1:G:1878:SER:C	1:G:1880:ASP:H	2.21	0.49
1:G:2010:GLY:HA3	1:G:2023:TYR:HB3	1.94	0.49
1:A:13:PRO:HB2	1:A:199:PRO:HD3	1.95	0.48
1:C:691:ALA:CB	1:E:1329:ARG:NH1	2.75	0.48
1:C:761:HIS:HB2	1:D:1112:LEU:HD21	1.95	0.48
1:D:970:HIS:HA	2:D:317:HOH:O	2.13	0.48
1:E:1277:LEU:HD22	1:E:1297:GLY:CA	2.43	0.48
1:H:2186:ARG:O	1:H:2199:GLY:HA2	2.13	0.48
1:B:548:GLU:OE2	1:C:625:ILE:HG22	2.14	0.48
1:C:608:ASP:HB3	1:C:638:ASN:HD22	1.78	0.48
1:G:1826:ARG:N	1:G:1827:PRO:CD	2.76	0.48
1:H:2136:MET:HB3	1:H:2139:SER:OG	2.12	0.48
1:C:817:THR:HB	1:C:819:ARG:NH1	2.27	0.48
1:D:1013:VAL:CG2	1:D:1031:MET:HE1	2.29	0.48
1:D:1097:THR:HA	1:D:1131:GLU:O	2.14	0.48
1:E:1276:MET:HE2	1:E:1282:TYR:CE1	2.47	0.48
1:F:1554:LEU:HD11	1:F:1582:TYR:HD2	1.78	0.48
1:H:2307:ALA:O	1:H:2311:PRO:HD2	2.14	0.48
1:F:1644:PHE:CD1	1:F:1644:PHE:C	2.92	0.48
1:G:1946:ASP:C	1:G:1946:ASP:OD2	2.55	0.48
1:H:2122:LEU:N	1:H:2123:PRO:HD2	2.28	0.48
1:E:1412:LEU:HD22	1:E:1416:LEU:HD12	1.95	0.48
1:G:1864:GLY:O	1:G:1865:ASN:C	2.57	0.48
1:B:415:LEU:CD1	1:B:431:MET:HE2	2.44	0.48
1:D:1082:ARG:HH11	1:D:1082:ARG:CB	2.26	0.48
1:F:1702:SER:HB2	1:F:1706:SER:O	2.13	0.48
1:C:691:ALA:HB3	1:E:1329:ARG:NH2	2.29	0.48
1:E:1221:HIS:C	1:E:1223:PRO:HD2	2.39	0.48
1:F:1565:ASN:HB2	1:F:1648:HIS:CE1	2.49	0.48
1:B:466:VAL:HG12	1:B:468:ALA:H	1.78	0.47
1:B:548:GLU:OE2	1:C:625:ILE:CG2	2.62	0.47
1:F:1723:TYR:N	1:F:1723:TYR:CD2	2.82	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1915:LEU:CG	1:G:1931:MET:HE2	2.42	0.47
1:G:2004:ILE:HG23	1:G:2004:ILE:O	2.14	0.47
1:C:811:PRO:HG3	1:C:823:TYR:CD1	2.50	0.47
1:D:1070:ILE:CG2	1:D:1094:ALA:HB2	2.44	0.47
1:F:1508:ASP:HB3	1:F:1538:ASN:HD22	1.79	0.47
1:C:748:HIS:CE1	1:C:773:HIS:CD2	3.02	0.47
1:C:775:HIS:CD2	1:C:804:ILE:HG12	2.50	0.47
1:E:1318:ARG:HD2	1:E:1327:PRO:CD	2.45	0.47
1:F:1536:MET:HE3	1:F:1539:SER:OG	2.14	0.47
1:F:1588:LEU:HD13	1:F:1600:TRP:HD1	1.79	0.47
1:A:155:LYS:HD3	1:A:192:THR:O	2.14	0.47
1:A:230:ALA:H	1:A:254:GLU:CG	2.27	0.47
1:B:538:HIS:HD2	1:C:620:ASN:O	1.97	0.47
1:C:626:ARG:N	1:C:627:PRO:CD	2.78	0.47
1:C:782:ARG:CD	1:C:784:LEU:HD23	2.44	0.47
1:E:1313:VAL:HG13	1:E:1345:VAL:HG13	1.96	0.47
1:G:1810:PHE:HB2	1:G:1996:PHE:HE2	1.78	0.47
1:A:27:PRO:CA	1:D:928:GLN:HE22	2.26	0.47
1:C:622:LEU:N	1:C:623:PRO:HD2	2.30	0.47
1:D:947:ARG:HG3	1:D:976:MET:HE3	1.96	0.47
1:E:1226:ARG:N	1:E:1227:PRO:CD	2.78	0.47
1:D:1029:ARG:HD3	1:F:1592:ASP:OD1	2.15	0.47
1:E:1217:VAL:HG11	1:E:1430:ALA:HB3	1.97	0.47
1:G:1871:LYS:HG2	1:G:1872:ASP:H	1.80	0.47
1:G:1911:THR:HG21	1:G:1940:LEU:HD22	1.97	0.47
1:H:2239:ASP:OD2	1:H:2239:ASP:N	2.46	0.47
1:C:615:ARG:HD2	2:C:167:HOH:O	2.13	0.47
1:C:755:LYS:HD3	1:C:792:THR:O	2.15	0.47
1:G:1868:TRP:HA	1:G:1873:ILE:CD1	2.39	0.47
1:A:196:PHE:CD1	1:A:196:PHE:C	2.92	0.47
1:D:950:ALA:CB	1:D:976:MET:HE1	2.45	0.47
1:E:1263:LEU:HD12	1:E:1286:ARG:HB3	1.95	0.47
1:G:1967:ALA:HB2	1:G:2042:GLY:O	2.15	0.47
1:D:995:THR:HG22	1:E:1419:ARG:NH1	2.29	0.47
1:G:1863:LEU:C	1:G:1914:ASN:HD21	2.22	0.47
1:H:2218:ARG:HD2	1:H:2227:PRO:CD	2.44	0.47
1:A:192:THR:HG21	1:B:476:VAL:HG21	1.97	0.46
1:E:1236:MET:HE3	1:E:1239:SER:OG	2.15	0.46
1:G:1803:VAL:CG2	1:G:2039:PHE:CE2	2.98	0.46
1:C:667:ALA:O	1:C:673:ILE:HG21	2.15	0.46
1:C:776:VAL:HG21	1:D:1092:THR:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:790:TYR:OH	1:C:792:THR:HG22	2.15	0.46
1:E:1248:ASP:HA	1:E:1251:ARG:NH1	2.30	0.46
1:E:1348:HIS:CE1	1:E:1373:HIS:CD2	3.03	0.46
1:E:1348:HIS:HE1	1:E:1373:HIS:HD2	1.63	0.46
1:F:1670:ILE:CG2	1:F:1694:ALA:HB2	2.45	0.46
1:F:1682:ARG:HG2	1:F:1683:ILE:N	2.31	0.46
1:B:336:MET:HB3	1:B:339:SER:OG	2.14	0.46
1:B:346:HIS:CD2	1:B:348:ASP:HB2	2.50	0.46
1:D:1015:LEU:HD21	1:D:1031:MET:HE3	1.97	0.46
1:E:1263:LEU:HD13	1:E:1267:ALA:HB1	1.96	0.46
1:E:1394:ALA:O	1:E:1433:ASN:HB3	2.15	0.46
1:F:1668:ALA:HB1	1:F:1670:ILE:CD1	2.45	0.46
1:F:1704:ILE:O	1:F:1704:ILE:HG23	2.15	0.46
1:G:1999:PRO:CG	1:G:2026:ALA:HB3	2.44	0.46
1:A:71:LYS:O	1:A:75:PRO:HD2	2.16	0.46
1:B:507:ALA:O	1:B:511:PRO:HD2	2.16	0.46
1:F:1551:ARG:HH11	1:F:1551:ARG:HB3	1.79	0.46
1:F:1618:ARG:HD3	2:F:210:HOH:O	2.15	0.46
1:A:180:ASP:O	1:A:181:THR:C	2.59	0.46
1:D:1031:MET:O	1:D:1035:LEU:HG	2.14	0.46
1:H:2246:ASP:OD2	1:H:2246:ASP:C	2.58	0.46
1:D:965:ASN:ND2	1:D:1021:MET:HE3	2.31	0.46
1:A:175:HIS:CD2	1:A:204:ILE:HG12	2.50	0.46
1:A:175:HIS:HD2	1:A:204:ILE:O	1.98	0.46
1:C:690:TYR:HB3	1:C:695:THR:HG21	1.98	0.46
1:D:918:LEU:HD13	1:D:918:LEU:C	2.41	0.46
1:F:1634:LEU:O	1:F:1640:LEU:HD11	2.16	0.46
1:B:318:LEU:O	1:B:322:LEU:HB2	2.15	0.46
1:D:1022:GLU:OE1	1:E:1414:ARG:NH2	2.49	0.46
1:D:1123:TYR:N	1:D:1123:TYR:CD2	2.83	0.46
1:G:1848:ASP:HA	1:G:1851:ARG:HH12	1.80	0.46
1:B:390:TYR:HB3	1:B:395:THR:HG21	1.97	0.46
1:C:770:ILE:HD12	1:C:770:ILE:N	2.31	0.46
1:D:964:GLY:O	1:D:965:ASN:C	2.59	0.46
1:E:1237:GLU:CG	1:E:1238:ASN:ND2	2.78	0.46
1:F:1518:LEU:O	1:F:1522:LEU:HB2	2.15	0.46
1:F:1536:MET:HG3	1:F:1561:LEU:HG	1.98	0.46
1:H:2269:VAL:C	1:H:2270:ILE:HD12	2.41	0.46
1:F:1680:ASP:O	1:F:1681:THR:C	2.59	0.45
1:G:1831:PHE:CD1	1:G:1910:LEU:HD23	2.51	0.45
1:G:2011:PRO:HD3	1:G:2023:TYR:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:637:GLU:OE2	1:C:638:ASN:ND2	2.48	0.45
1:C:771:GLY:O	1:C:793:ASP:HA	2.16	0.45
1:F:1519:GLN:OE1	1:F:1552:GLY:HA3	2.16	0.45
1:A:50:ALA:CB	1:A:76:MET:HE1	2.47	0.45
1:B:326:ARG:N	1:B:327:PRO:CD	2.80	0.45
1:E:1267:ALA:O	1:E:1273:ILE:HG21	2.16	0.45
1:E:1430:ALA:O	1:E:1454:GLU:HG2	2.15	0.45
1:F:1510:PHE:HB2	1:F:1696:PHE:CE2	2.52	0.45
1:F:1550:ALA:CB	1:F:1576:MET:HE1	2.39	0.45
1:B:395:THR:HA	1:B:396:PRO:HD3	1.86	0.45
1:B:530:ALA:H	1:B:554:GLU:HG2	1.80	0.45
1:F:1565:ASN:HD22	1:F:1621:MET:CE	2.30	0.45
1:H:2215:LEU:CD1	1:H:2231:MET:HE3	2.46	0.45
1:A:204:ILE:O	1:A:204:ILE:HG23	2.16	0.45
1:C:811:PRO:HD3	1:C:823:TYR:HB3	1.99	0.45
1:E:1400:HIS:CE1	1:E:1453:ILE:HD12	2.51	0.45
1:F:1587:PRO:HB2	1:F:1590:TYR:CD2	2.52	0.45
1:H:2150:ALA:CB	1:H:2176:MET:HE1	2.45	0.45
1:A:25:ILE:CG2	1:D:1148:GLU:OE2	2.65	0.45
1:B:548:GLU:CD	1:C:625:ILE:CG2	2.89	0.45
1:E:1218:LEU:O	1:E:1218:LEU:HD22	2.17	0.45
1:G:2048:GLU:HG3	1:G:2048:GLU:O	2.17	0.45
1:H:2182:TYR:HD1	1:H:2182:TYR:H	1.64	0.45
1:B:470:ILE:HD12	1:B:470:ILE:N	2.31	0.45
1:C:668:TRP:CD2	1:F:1719:ARG:HD2	2.51	0.45
1:C:792:THR:OG1	1:D:1076:VAL:HG11	2.16	0.45
1:D:986:ARG:O	1:D:999:GLY:HA2	2.17	0.45
1:G:1837:GLU:OE1	1:G:1865:ASN:HB3	2.16	0.45
1:G:1864:GLY:O	1:G:1867:ALA:N	2.47	0.45
1:G:2003:ILE:HD11	1:G:2008:ILE:HG23	1.99	0.45
1:A:24:THR:C	1:D:1148:GLU:CD	2.85	0.45
1:C:734:LEU:C	1:C:736:GLU:H	2.25	0.45
1:F:1711:PRO:HG3	1:F:1723:TYR:CD1	2.52	0.45
1:G:1918:ARG:HD2	1:G:1927:PRO:CD	2.46	0.45
1:H:2136:MET:O	1:H:2139:SER:OG	2.35	0.45
1:A:102:THR:HG22	1:A:111:THR:OG1	2.17	0.45
1:A:203:ILE:HD13	1:B:457:ALA:HB2	1.99	0.45
1:C:792:THR:HG21	1:D:1076:VAL:HG21	1.98	0.45
1:E:1274:TYR:N	1:E:1275:PRO:HD2	2.32	0.45
1:G:1826:ARG:HD3	1:G:1826:ARG:C	2.42	0.45
1:H:2118:LEU:C	1:H:2118:LEU:HD13	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:2245:VAL:HG21	1:H:2262:LEU:HD23	1.97	0.45
1:A:119:VAL:HG23	1:A:154:GLU:OE1	2.16	0.45
1:B:482:ARG:HG2	1:B:483:ILE:H	1.82	0.45
1:D:926:ARG:C	1:D:926:ARG:HD2	2.42	0.45
1:G:1889:ASN:OD1	1:G:1889:ASN:N	2.49	0.45
1:G:1892:ASP:HB3	1:G:1895:THR:HG23	1.98	0.45
1:G:1970:ILE:N	1:G:1970:ILE:CD1	2.80	0.44
1:H:2282:ARG:CG	1:H:2283:ILE:H	2.30	0.44
1:A:169:VAL:C	1:A:170:ILE:HD12	2.42	0.44
1:A:182:ARG:HD2	1:A:184:LEU:HD23	1.99	0.44
1:B:449:ALA:O	1:B:455:LYS:HE3	2.18	0.44
1:C:815:PHE:HB3	1:D:1028:PHE:CD2	2.53	0.44
1:H:2164:GLY:HA2	1:H:2187:PRO:HG3	1.99	0.44
1:H:2304:ILE:O	1:H:2304:ILE:HG23	2.17	0.44
1:A:207:ALA:O	1:A:211:PRO:HD2	2.18	0.44
1:B:337:GLU:OE2	1:B:448:HIS:CE1	2.70	0.44
1:C:692:ASP:HA	1:C:693:PRO:HD3	1.86	0.44
1:C:782:ARG:CG	1:C:783:ILE:N	2.80	0.44
1:C:823:TYR:HD2	1:C:823:TYR:O	2.01	0.44
1:E:1348:HIS:CE1	1:E:1373:HIS:HB2	2.53	0.44
1:G:1861:LEU:N	1:G:1861:LEU:CD2	2.76	0.44
1:B:482:ARG:HD3	1:B:483:ILE:O	2.17	0.44
1:D:1080:ASP:O	1:D:1081:THR:C	2.61	0.44
1:D:1148:GLU:O	1:D:1148:GLU:HG3	2.18	0.44
1:H:2291:GLN:NE2	1:H:2294:ALA:HA	2.32	0.44
1:B:321:HIS:O	1:B:322:LEU:C	2.60	0.44
1:C:715:LEU:HG	1:C:731:MET:HE3	1.99	0.44
1:D:926:ARG:HB3	1:D:927:PRO:HD3	2.00	0.44
1:D:1055:LYS:HD2	2:D:146:HOH:O	2.17	0.44
1:E:1217:VAL:CG1	1:E:1430:ALA:HB3	2.47	0.44
1:E:1309:LYS:HE3	1:E:1309:LYS:HB2	1.85	0.44
1:E:1382:ARG:CB	1:E:1382:ARG:NH1	2.76	0.44
1:E:1415:PHE:HB3	1:F:1628:PHE:CE2	2.52	0.44
1:H:2331:GLU:HB2	1:H:2353:ILE:HD13	1.99	0.44
1:A:79:GLU:HG2	1:A:79:GLU:H	1.62	0.44
1:B:443:VAL:O	1:B:466:VAL:HG13	2.17	0.44
1:C:803:ILE:O	1:C:804:ILE:HG22	2.18	0.44
1:G:1877:LEU:HD22	1:G:1897:GLY:HA3	2.00	0.44
1:G:1892:ASP:HA	1:G:1893:PRO:HD3	1.82	0.44
1:H:2182:TYR:N	1:H:2182:TYR:CD1	2.86	0.44
1:B:387:PRO:HB2	1:B:390:TYR:CE2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:908:ASP:HB3	1:D:938:ASN:HD22	1.83	0.44
1:E:1370:ILE:HD12	1:E:1370:ILE:N	2.33	0.44
1:B:510:GLY:HA3	1:B:523:TYR:HB3	2.00	0.44
1:G:1870:HIS:H	1:G:1873:ILE:HD12	1.83	0.44
1:F:1585:VAL:HG12	1:F:1614:ASN:HB2	2.00	0.43
1:B:387:PRO:HB2	1:B:390:TYR:CD2	2.53	0.43
1:F:1526:ARG:N	1:F:1527:PRO:CD	2.81	0.43
1:F:1606:ASN:C	1:F:1608:GLU:H	2.26	0.43
1:A:8:ASP:OD1	1:A:172:THR:HB	2.17	0.43
1:A:92:ASP:HA	1:A:93:PRO:HD3	1.84	0.43
1:B:392:ASP:HB3	1:B:395:THR:HG23	1.99	0.43
1:C:617:VAL:HG13	1:C:854:GLU:OE2	2.18	0.43
1:C:718:ARG:HD2	1:C:727:PRO:HD2	2.00	0.43
1:E:1221:HIS:CE1	1:E:1450:TYR:OH	2.72	0.43
1:H:2191:ALA:HB2	1:H:2225:ASP:OD2	2.17	0.43
1:D:1084:LEU:O	1:D:1085:LYS:C	2.61	0.43
1:F:1660:TRP:CH2	1:F:1684:LEU:HD22	2.54	0.43
1:G:1982:ARG:HG2	1:G:1983:ILE:N	2.33	0.43
1:H:2282:ARG:HG2	1:H:2283:ILE:H	1.82	0.43
1:E:1310:LEU:HD12	1:E:1342:THR:O	2.18	0.43
1:G:2017:THR:O	1:G:2018:GLU:HB2	2.19	0.43
1:B:378:SER:C	1:B:380:ASP:H	2.25	0.43
1:D:972:ASP:O	1:D:975:PRO:HG2	2.18	0.43
1:D:1029:ARG:NH1	1:F:1592:ASP:N	2.66	0.43
1:D:1111:PRO:CD	1:D:1123:TYR:HD1	2.32	0.43
1:F:1588:LEU:HD23	1:F:1631:MET:HE2	1.99	0.43
1:H:2192:ASP:HB3	1:H:2195:THR:CG2	2.42	0.43
1:A:147:PHE:O	1:A:171:GLY:HA2	2.19	0.43
1:E:1240:ALA:C	1:E:1242:GLY:H	2.27	0.43
1:E:1319:VAL:HG12	1:E:1320:PHE:CD2	2.54	0.43
1:B:336:MET:HG3	1:B:361:LEU:HG	2.01	0.43
1:C:811:PRO:O	1:C:814:ARG:HB2	2.19	0.43
1:E:1264:GLY:HA2	1:E:1287:PRO:HG3	2.00	0.43
1:G:1884:ILE:HG22	1:G:1885:VAL:N	2.34	0.43
1:D:1015:LEU:CD2	1:D:1031:MET:HE3	2.48	0.43
1:D:1082:ARG:HD3	1:D:1083:ILE:O	2.18	0.43
1:B:370:HIS:O	1:B:373:ILE:HD12	2.18	0.43
1:C:695:THR:HA	1:C:696:PRO:HD3	1.88	0.43
1:E:1417:THR:O	1:E:1418:GLU:HB2	2.18	0.43
1:F:1503:VAL:HG21	1:F:1739:PHE:CE2	2.54	0.43
1:G:1980:ASP:O	1:G:1981:THR:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1999:PRO:CB	1:G:2026:ALA:HB3	2.48	0.43
1:C:715:LEU:HB3	1:C:747:PHE:HD1	1.84	0.42
1:D:1117:THR:HB	1:D:1119:ARG:NH1	2.34	0.42
1:E:1348:HIS:CE1	1:E:1373:HIS:HD2	2.37	0.42
1:G:1902:THR:HG22	1:G:1911:THR:CG2	2.49	0.42
1:A:37:GLU:OE2	1:A:148:HIS:CE1	2.72	0.42
1:E:1247:ARG:HH22	1:E:1279:GLU:CD	2.26	0.42
1:G:1808:ASP:OD1	1:G:1972:THR:HB	2.19	0.42
1:A:118:ARG:HD2	1:A:127:PRO:HD3	2.00	0.42
1:C:796:PHE:C	1:C:796:PHE:CD1	2.96	0.42
1:E:1378:THR:HA	1:F:1678:THR:HA	2.01	0.42
1:G:1822:LEU:HD21	1:G:1832:VAL:HG11	2.01	0.42
1:G:1865:ASN:N	1:G:1916:LEU:HD21	2.34	0.42
1:G:1895:THR:HA	1:G:1896:PRO:HD3	1.90	0.42
1:H:2122:LEU:O	1:H:2122:LEU:HD22	2.19	0.42
1:H:2219:VAL:O	1:H:2221:MET:HG3	2.19	0.42
1:D:1013:VAL:HG11	1:D:1045:VAL:HG22	2.01	0.42
1:F:1551:ARG:HH11	1:F:1551:ARG:CB	2.32	0.42
1:H:2275:HIS:HA	1:H:2296:PHE:HB3	2.01	0.42
1:H:2317:THR:HB	1:H:2319:ARG:CZ	2.49	0.42
1:C:744:PHE:CD1	1:C:744:PHE:C	2.96	0.42
1:D:1048:HIS:CE1	1:D:1073:HIS:HD2	2.37	0.42
1:B:389:ASN:O	1:B:425:ASP:HB2	2.20	0.42
1:B:533:ASN:OD1	1:B:551:ARG:HG3	2.20	0.42
1:D:1044:PHE:CD1	1:D:1044:PHE:C	2.97	0.42
1:F:1739:PHE:HD1	1:F:1744:ALA:HA	1.84	0.42
1:G:1968:ALA:HB1	1:G:1970:ILE:HD13	2.02	0.42
1:G:1970:ILE:HG21	1:G:1994:ALA:HB2	2.02	0.42
1:B:364:GLY:HA2	1:B:387:PRO:HG3	2.01	0.42
1:C:608:ASP:O	1:C:796:PHE:HB2	2.19	0.42
1:C:691:ALA:C	1:E:1329:ARG:NH1	2.77	0.42
1:G:2053:ILE:O	1:G:2054:GLU:C	2.63	0.42
1:A:149:ALA:O	1:A:155:LYS:HE3	2.19	0.42
1:A:157:ALA:HB2	1:B:503:ILE:HD13	2.02	0.42
1:B:539:PHE:HA	1:B:543:LYS:O	2.19	0.42
1:C:811:PRO:HD3	1:C:823:TYR:CB	2.49	0.42
1:D:922:LEU:N	1:D:923:PRO:HD2	2.33	0.42
1:F:1682:ARG:CG	1:F:1683:ILE:N	2.83	0.42
1:G:1887:PRO:HB3	1:G:1916:LEU:HG	2.01	0.42
1:G:1918:ARG:HD2	1:G:1927:PRO:HD3	2.02	0.42
1:A:86:ARG:HB2	1:A:87:PRO:CD	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1215:ARG:NH2	2:E:9:HOH:O	2.51	0.42
1:F:1675:HIS:CD2	1:F:1704:ILE:HG12	2.54	0.42
1:F:1751:ARG:NH1	1:F:1753:ILE:HD11	2.34	0.42
1:A:128:PHE:HA	1:A:158:MET:HE1	2.01	0.42
1:D:1039:ASP:OD2	1:D:1039:ASP:N	2.48	0.42
1:G:1805:PHE:O	1:G:2034:GLY:HA3	2.20	0.42
1:G:1812:GLN:O	1:G:1813:PRO:C	2.63	0.42
1:G:1952:THR:HG21	1:H:2274:THR:HB	2.02	0.42
1:H:2126:ARG:N	1:H:2127:PRO:CD	2.83	0.41
1:C:692:ASP:N	1:E:1329:ARG:HH11	2.15	0.41
1:C:768:ALA:HB1	1:C:770:ILE:CD1	2.50	0.41
1:E:1208:ASP:HB2	1:E:1396:PHE:HB2	2.01	0.41
1:F:1613:VAL:HG13	1:F:1645:VAL:HG22	2.02	0.41
1:F:1615:LEU:HB3	1:F:1647:PHE:HD1	1.85	0.41
1:A:15:ARG:NH2	2:A:256:HOH:O	2.51	0.41
1:A:113:VAL:CG1	1:A:145:VAL:HG22	2.49	0.41
1:E:1226:ARG:O	1:E:1226:ARG:HD3	2.20	0.41
1:G:1982:ARG:HD3	1:G:1983:ILE:C	2.46	0.41
1:H:2137:GLU:HG3	1:H:2138:ASN:CG	2.45	0.41
1:D:926:ARG:C	1:D:926:ARG:CD	2.93	0.41
1:D:1151:ARG:NE	1:D:1153:ILE:HD11	2.35	0.41
1:G:1836:MET:O	1:G:1839:SER:OG	2.32	0.41
1:H:2209:LYS:HE3	1:H:2209:LYS:HB2	1.95	0.41
1:C:691:ALA:HB2	1:C:725:ASP:CG	2.44	0.41
1:D:964:GLY:O	1:D:967:ALA:HB2	2.21	0.41
1:F:1586:ARG:O	1:F:1599:GLY:HA2	2.20	0.41
1:A:36:MET:HB3	1:A:39:SER:OG	2.21	0.41
1:B:346:HIS:CD2	1:B:349:ALA:H	2.38	0.41
1:E:1346:ASP:OD2	1:E:1346:ASP:C	2.62	0.41
1:F:1631:MET:O	1:F:1632:ASP:C	2.63	0.41
1:G:1890:TYR:HB3	1:G:1895:THR:HG21	2.02	0.41
1:H:2143:PHE:HD1	1:H:2166:HIS:CD2	2.38	0.41
1:F:1564:GLY:HA2	1:F:1587:PRO:HG3	2.01	0.41
1:G:1810:PHE:CB	1:G:1996:PHE:CE2	3.03	0.41
1:G:1837:GLU:HG3	1:G:1866:HIS:HB2	2.02	0.41
1:H:2294:ALA:O	1:H:2333:ASN:HB3	2.21	0.41
1:D:995:THR:HA	1:D:996:PRO:HD3	1.78	0.41
1:E:1315:LEU:CD1	1:E:1331:MET:HE2	2.51	0.41
1:E:1384:LEU:O	1:E:1385:LYS:C	2.64	0.41
1:F:1671:GLY:HA3	1:F:1692:THR:O	2.21	0.41
1:H:2299:PRO:HG2	1:H:2305:GLY:HA2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:502:SER:HB2	1:B:506:SER:O	2.21	0.41
1:C:804:ILE:HG12	1:C:804:ILE:O	2.21	0.41
1:D:1099:PRO:HB2	1:D:1126:ALA:HB3	2.02	0.41
1:D:1127:GLU:HG3	2:D:230:HOH:O	2.21	0.41
1:E:1292:ASP:HB3	1:E:1295:THR:CG2	2.43	0.41
1:E:1313:VAL:CG1	1:E:1345:VAL:HG22	2.50	0.41
1:G:1944:PHE:CD2	1:G:1968:ALA:HB3	2.56	0.41
1:B:415:LEU:HD11	1:B:431:MET:CG	2.48	0.41
1:B:444:PHE:CD1	1:B:444:PHE:C	2.98	0.41
1:C:739:ASP:OD2	1:C:739:ASP:N	2.54	0.41
1:F:1536:MET:HB3	1:F:1539:SER:OG	2.20	0.41
1:H:2154:LEU:HD11	1:H:2182:TYR:CD2	2.55	0.41
1:H:2164:GLY:O	1:H:2165:ASN:C	2.63	0.41
1:A:24:THR:O	1:D:1148:GLU:CD	2.64	0.40
1:A:184:LEU:O	1:A:185:LYS:C	2.62	0.40
1:C:715:LEU:HB3	1:C:747:PHE:CD1	2.56	0.40
1:G:1891:ALA:HB2	1:G:1925:ASP:CG	2.46	0.40
1:H:2277:PRO:HA	1:H:2293:ASP:O	2.21	0.40
1:B:446:ASP:OD2	1:B:446:ASP:C	2.65	0.40
1:B:511:PRO:HG3	1:B:523:TYR:HD1	1.86	0.40
1:E:1247:ARG:HG3	1:E:1276:MET:HE3	2.03	0.40
1:E:1360:TRP:CH2	1:E:1384:LEU:HD22	2.55	0.40
1:F:1591:ALA:O	1:F:1592:ASP:C	2.62	0.40
1:G:1902:THR:HG22	1:G:1911:THR:HG23	2.02	0.40
1:B:365:ASN:HB2	1:B:448:HIS:CE1	2.56	0.40
1:B:490:TYR:CD1	1:B:490:TYR:C	2.99	0.40
1:C:782:ARG:HD3	1:C:783:ILE:O	2.21	0.40
1:F:1507:GLY:HA3	1:F:1695:GLY:O	2.22	0.40
1:G:1834:VAL:O	1:G:1861:LEU:HA	2.21	0.40
1:H:2303:ILE:CD1	1:H:2311:PRO:HB2	2.51	0.40
1:E:1225:ILE:C	1:E:1227:PRO:HD2	2.46	0.40
1:E:1295:THR:HA	1:E:1296:PRO:HD3	1.90	0.40
1:H:2219:VAL:HG12	1:H:2220:PHE:CG	2.56	0.40
1:H:2302:SER:HB3	1:H:2326:ALA:CB	2.52	0.40
1:H:2323:TYR:HD2	1:H:2323:TYR:O	2.04	0.40
1:D:1107:ALA:O	1:D:1111:PRO:HD2	2.21	0.40
1:F:1717:THR:HB	1:F:1719:ARG:NH1	2.36	0.40
1:G:1803:VAL:HG23	1:G:1803:VAL:O	2.21	0.40
1:G:1831:PHE:CE2	1:G:1859:GLY:HA3	2.56	0.40
1:G:1967:ALA:HB1	1:G:2039:PHE:CD1	2.56	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	253/255 (99%)	236 (93%)	13 (5%)	4 (2%)	7	7
1	B	253/255 (99%)	234 (92%)	15 (6%)	4 (2%)	7	7
1	C	253/255 (99%)	238 (94%)	12 (5%)	3 (1%)	10	12
1	D	253/255 (99%)	235 (93%)	13 (5%)	5 (2%)	6	5
1	E	253/255 (99%)	228 (90%)	21 (8%)	4 (2%)	7	7
1	F	253/255 (99%)	236 (93%)	14 (6%)	3 (1%)	10	12
1	G	253/255 (99%)	206 (81%)	36 (14%)	11 (4%)	2	1
1	H	253/255 (99%)	229 (90%)	17 (7%)	7 (3%)	4	2
All	All	2024/2040 (99%)	1842 (91%)	141 (7%)	41 (2%)	6	5

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	380	ASP
1	D	965	ASN
1	G	1880	ASP
1	B	473	HIS
1	C	608	ASP
1	E	1208	ASP
1	F	1508	ASP
1	F	1704	ILE
1	G	1808	ASP
1	G	1872	ASP
1	G	1973	HIS
1	H	2171	LYS
1	B	308	ASP
1	C	735	LEU
1	C	773	HIS
1	D	908	ASP
1	E	1373	HIS

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Mol	Chain	Res	Type
1	F	1673	HIS
1	G	1865	ASN
1	H	2239	ASP
1	H	2273	HIS
1	H	2304	ILE
1	A	8	ASP
1	A	135	LEU
1	A	173	HIS
1	A	204	ILE
1	D	989	ASN
1	D	1073	HIS
1	E	1404	ILE
1	G	1889	ASN
1	G	1939	ASP
1	H	2235	LEU
1	B	405	VAL
1	D	1104	ILE
1	G	2004	ILE
1	H	2165	ASN
1	H	2310	GLY
1	E	1410	GLY
1	G	1841	GLY
1	G	1873	ILE
1	G	1905	VAL

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	199/199 (100%)	181 (91%)	18 (9%)	9	12
1	B	199/199 (100%)	183 (92%)	16 (8%)	11	15
1	C	199/199 (100%)	179 (90%)	20 (10%)	7	9
1	D	199/199 (100%)	188 (94%)	11 (6%)	19	28
1	E	199/199 (100%)	183 (92%)	16 (8%)	11	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	199/199 (100%)	187 (94%)	12 (6%)	17	25
1	G	199/199 (100%)	190 (96%)	9 (4%)	24	37
1	H	199/199 (100%)	187 (94%)	12 (6%)	17	25
All	All	1592/1592 (100%)	1478 (93%)	114 (7%)	13	18

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	17	VAL
1	A	18	LEU
1	A	22	LEU
1	A	25	ILE
1	A	37	GLU
1	A	61	LEU
1	A	79	GLU
1	A	102	THR
1	A	138	ASP
1	A	166	VAL
1	A	182	ARG
1	A	196	PHE
1	A	204	ILE
1	A	212	LEU
1	A	214	ARG
1	A	223	TYR
1	A	227	GLU
1	B	303	VAL
1	B	317	VAL
1	B	318	LEU
1	B	322	LEU
1	B	337	GLU
1	B	361	LEU
1	B	413	VAL
1	B	438	ASP
1	B	465	ARG
1	B	482	ARG
1	B	496	PHE
1	B	523	TYR
1	B	527	GLU
1	B	529	ARG
1	B	538	HIS

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Mol	Chain	Res	Type
1	B	553	ILE
1	C	603	VAL
1	C	617	VAL
1	C	618	LEU
1	C	622	LEU
1	C	637	GLU
1	C	648	ASP
1	C	661	LEU
1	C	671	LYS
1	C	702	THR
1	C	725	ASP
1	C	738	ASP
1	C	765	ARG
1	C	782	ARG
1	C	792	THR
1	C	796	PHE
1	C	812	LEU
1	C	814	ARG
1	C	823	TYR
1	C	827	GLU
1	C	829	ARG
1	D	903	VAL
1	D	917	VAL
1	D	922	LEU
1	D	937	GLU
1	D	1018	ARG
1	D	1038	ASP
1	D	1082	ARG
1	D	1112	LEU
1	D	1123	TYR
1	D	1127	GLU
1	D	1129	ARG
1	E	1201	MET
1	E	1218	LEU
1	E	1222	LEU
1	E	1237	GLU
1	E	1261	LEU
1	E	1298	VAL
1	E	1325	ASP
1	E	1338	ASP
1	E	1362	LEU
1	E	1382	ARG

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Mol	Chain	Res	Type
1	E	1396	PHE
1	E	1404	ILE
1	E	1412	LEU
1	E	1423	TYR
1	E	1427	GLU
1	E	1429	ARG
1	F	1518	LEU
1	F	1522	LEU
1	F	1537	GLU
1	F	1561	LEU
1	F	1613	VAL
1	F	1625	ASP
1	F	1638	ASP
1	F	1682	ARG
1	F	1704	ILE
1	F	1712	LEU
1	F	1723	TYR
1	F	1727	GLU
1	G	1822	LEU
1	G	1861	LEU
1	G	1871	LYS
1	G	1938	ASP
1	G	1982	ARG
1	G	2012	LEU
1	G	2023	TYR
1	G	2027	GLU
1	G	2029	ARG
1	H	2103	VAL
1	H	2122	LEU
1	H	2125	ILE
1	H	2137	GLU
1	H	2139	SER
1	H	2161	LEU
1	H	2238	ASP
1	H	2282	ARG
1	H	2296	PHE
1	H	2304	ILE
1	H	2323	TYR
1	H	2329	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (73) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	HIS
1	A	28	GLN
1	A	38	ASN
1	A	46	HIS
1	A	148	HIS
1	A	161	HIS
1	A	173	HIS
1	A	175	HIS
1	B	319	GLN
1	B	321	HIS
1	B	328	GLN
1	B	366	HIS
1	B	414	ASN
1	B	448	HIS
1	B	473	HIS
1	B	475	HIS
1	B	538	HIS
1	C	619	GLN
1	C	621	HIS
1	C	628	GLN
1	C	638	ASN
1	C	646	HIS
1	C	666	HIS
1	C	669	HIS
1	C	748	HIS
1	C	761	HIS
1	C	773	HIS
1	C	775	HIS
1	D	921	HIS
1	D	928	GLN
1	D	938	ASN
1	D	946	HIS
1	D	965	ASN
1	D	966	HIS
1	D	969	HIS
1	D	1014	ASN
1	D	1048	HIS
1	D	1061	HIS
1	D	1073	HIS
1	D	1075	HIS
1	E	1221	HIS
1	E	1228	GLN
1	E	1238	ASN

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Mol	Chain	Res	Type
1	E	1246	HIS
1	E	1348	HIS
1	E	1373	HIS
1	E	1375	HIS
1	E	1413	GLN
1	E	1438	HIS
1	F	1519	GLN
1	F	1521	HIS
1	F	1538	ASN
1	F	1546	HIS
1	F	1565	ASN
1	F	1566	HIS
1	F	1569	HIS
1	F	1648	HIS
1	F	1661	HIS
1	F	1673	HIS
1	F	1675	HIS
1	G	1821	HIS
1	G	1828	GLN
1	G	1846	HIS
1	G	1869	HIS
1	G	1973	HIS
1	H	2121	HIS
1	H	2128	GLN
1	H	2138	ASN
1	H	2169	HIS
1	H	2248	HIS
1	H	2275	HIS
1	H	2321	HIS
1	H	2338	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	255/255 (100%)	-0.05	6 (2%) 59 62	21, 31, 55, 92	0
1	B	255/255 (100%)	0.12	10 (3%) 43 45	22, 35, 69, 102	0
1	C	255/255 (100%)	0.09	11 (4%) 40 41	22, 33, 62, 93	0
1	D	255/255 (100%)	0.23	12 (4%) 36 38	22, 39, 72, 90	0
1	E	255/255 (100%)	0.51	13 (5%) 33 35	26, 44, 73, 102	0
1	F	255/255 (100%)	0.25	12 (4%) 36 38	24, 37, 68, 113	0
1	G	255/255 (100%)	1.25	47 (18%) 3 4	33, 55, 88, 109	0
1	H	255/255 (100%)	0.40	6 (2%) 59 62	25, 40, 70, 104	0
All	All	2040/2040 (100%)	0.35	117 (5%) 29 31	21, 39, 73, 113	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	1905	VAL	4.5
1	G	2023	TYR	4.2
1	C	673	ILE	4.2
1	E	1273	ILE	4.1
1	G	1873	ILE	4.1
1	G	1996	PHE	3.9
1	E	1305	VAL	3.9
1	F	1573	ILE	3.7
1	C	691	ALA	3.6
1	A	73	ILE	3.6
1	G	1900	TRP	3.6
1	D	991	ALA	3.6
1	H	2327	GLU	3.5
1	E	1265	ASN	3.5
1	G	1891	ALA	3.5
1	D	973	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	373	ILE	3.4
1	F	1565	ASN	3.4
1	C	827	GLU	3.3
1	E	1427	GLU	3.3
1	F	1605	VAL	3.3
1	B	405	VAL	3.3
1	G	1944	PHE	3.2
1	E	1423	TYR	3.2
1	G	1881	THR	3.2
1	E	1201	MET	3.2
1	B	523	TYR	3.2
1	B	548	GLU	3.1
1	C	704	ASP	3.1
1	G	2028	GLY	3.1
1	F	1639	ASP	3.1
1	B	365	ASN	3.0
1	G	2048	GLU	3.0
1	A	223	TYR	3.0
1	F	1704	ILE	3.0
1	E	1304	ASP	3.0
1	G	2004	ILE	3.0
1	G	1801	MET	3.0
1	G	1939	ASP	2.9
1	D	1123	TYR	2.9
1	F	1748	GLU	2.9
1	E	1282	TYR	2.9
1	F	1723	TYR	2.9
1	C	705	VAL	2.9
1	D	1096	PHE	2.8
1	C	804	ILE	2.8
1	G	1951	ALA	2.8
1	G	1966	VAL	2.8
1	D	1039	ASP	2.8
1	G	1914	ASN	2.8
1	H	2304	ILE	2.7
1	H	2173	ILE	2.7
1	H	2239	ASP	2.7
1	G	1960	TRP	2.7
1	G	1929	ARG	2.7
1	C	665	ASN	2.7
1	D	1092	THR	2.7
1	G	1897	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	1629	ARG	2.7
1	G	1933	ALA	2.7
1	G	1831	PHE	2.7
1	G	1924	VAL	2.6
1	C	823	TYR	2.6
1	G	1901	ARG	2.6
1	F	1696	PHE	2.6
1	G	1941	GLY	2.6
1	G	1890	TYR	2.5
1	G	1940	LEU	2.5
1	B	439	ASP	2.5
1	G	1895	THR	2.5
1	D	1104	ILE	2.5
1	G	1874	TYR	2.5
1	G	1913	VAL	2.4
1	E	1337	ARG	2.4
1	G	1964	GLY	2.4
1	H	2207	GLY	2.4
1	G	1902	THR	2.4
1	F	1638	ASP	2.4
1	G	1908	GLU	2.4
1	E	1341	GLY	2.4
1	F	1581	THR	2.4
1	E	1306	ASN	2.4
1	B	312	GLN	2.4
1	G	1889	ASN	2.3
1	B	301	MET	2.3
1	B	504	ILE	2.3
1	E	1302	THR	2.3
1	A	105	VAL	2.3
1	A	65	ASN	2.3
1	G	1893	PRO	2.3
1	C	601	MET	2.3
1	F	1591	ALA	2.3
1	G	1885	VAL	2.3
1	G	1943	VAL	2.3
1	G	1863	LEU	2.3
1	G	1898	VAL	2.3
1	C	671	LYS	2.2
1	H	2324	GLY	2.2
1	G	1871	LYS	2.2
1	G	1942	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	965	ASN	2.2
1	G	2042	GLY	2.2
1	G	1854	LEU	2.2
1	D	1006	ASN	2.1
1	G	1911	THR	2.1
1	G	1937	ARG	2.1
1	G	1916	LEU	2.1
1	B	438	ASP	2.1
1	A	192	THR	2.0
1	G	1858	ALA	2.0
1	G	1865	ASN	2.0
1	D	982	TYR	2.0
1	A	108	GLU	2.0
1	D	981	THR	2.0
1	D	1004	ASP	2.0
1	E	1338	ASP	2.0
1	C	822	ARG	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.