



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 09:57 PM EDT

PDB ID : 5X9Z / pdb_00005x9z
Title : Crystal structure of inositol 1,4,5-trisphosphate receptor large cytosolic domain
Authors : Hamada, K.; Miyatake, H.; Terauchi, A.; Mikoshiba, K.
Deposited on : 2017-03-10
Resolution : 7.31 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

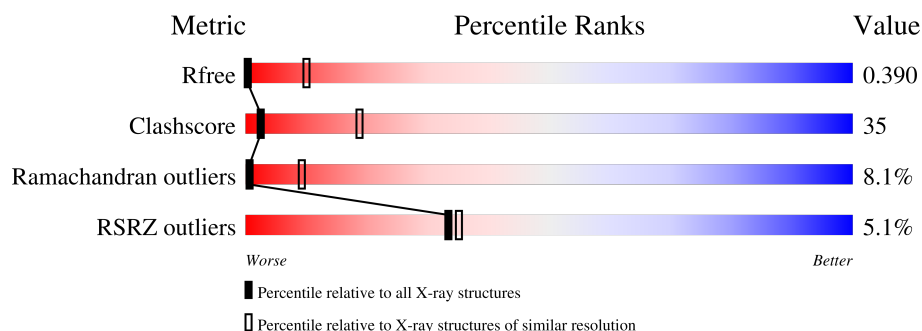
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 7.31 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	1167 (10.00-4.00)
Clashscore	190562	1000 (10.00-4.06)
Ramachandran outliers	187476	1054 (10.00-4.00)
RSRZ outliers	180081	1161 (10.00-4.00)

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	2217	4% 49% 25% • 23%
1	B	2217	4% 50% 23% • 23%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 16948 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.

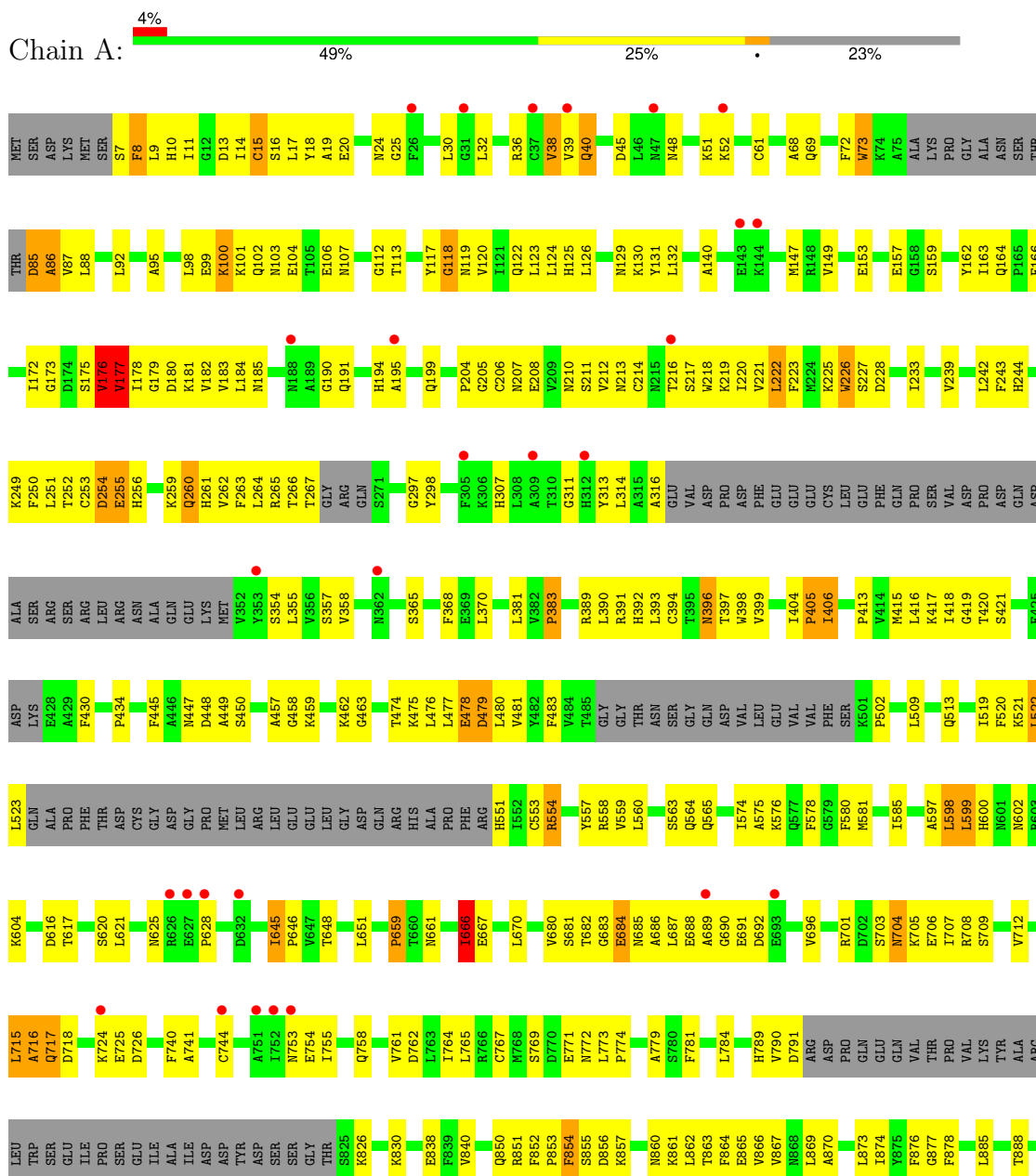
- Molecule 1 is a protein called Inositol 1,4,5-trisphosphate receptor type 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	1710	Total	C	N	O	0	0	0
			8479	5059	1710	1710			
1	B	1708	Total	C	N	O	0	0	0
			8469	5053	1708	1708			

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.

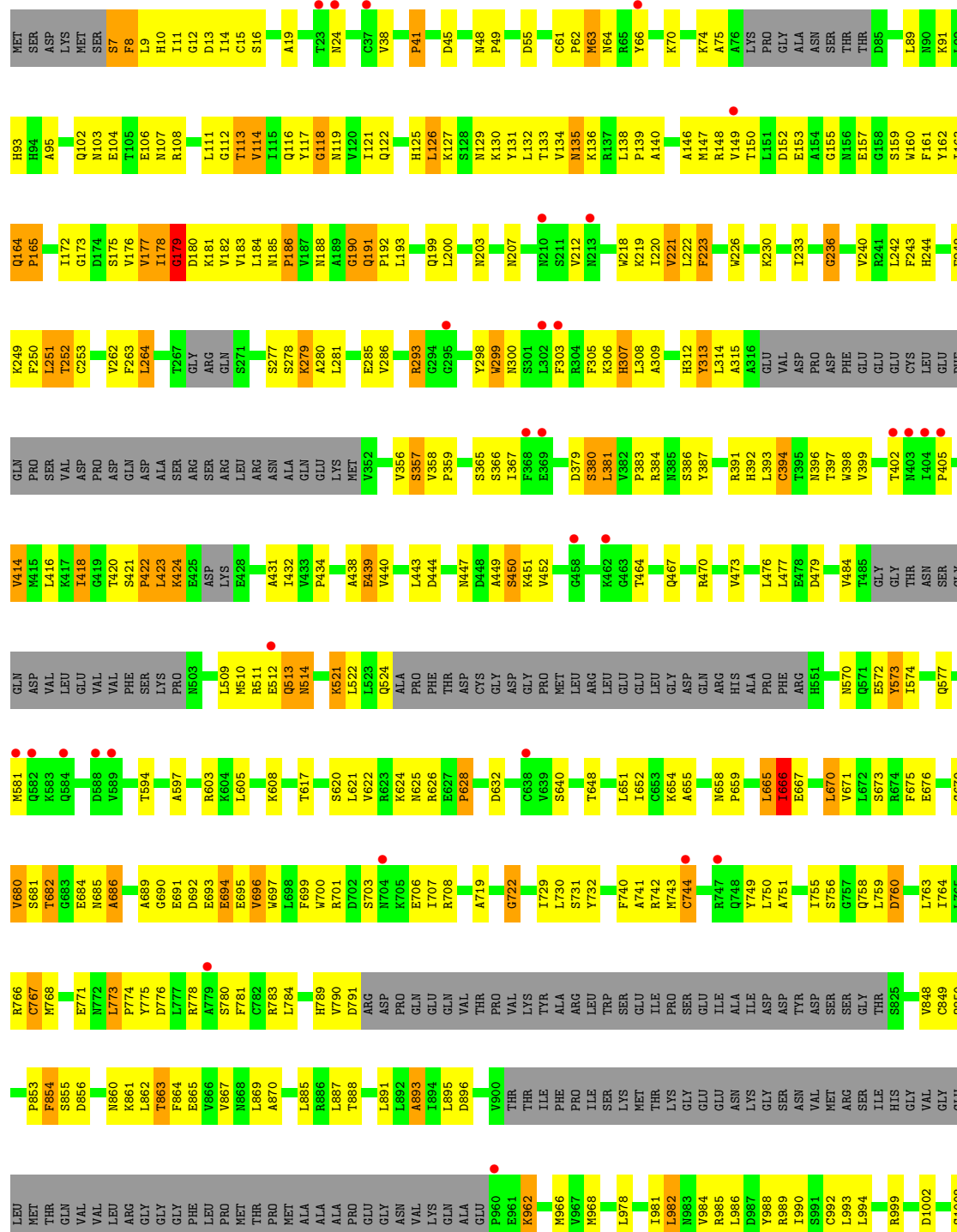
- Molecule 1: Inositol 1,4,5-trisphosphate receptor type 1

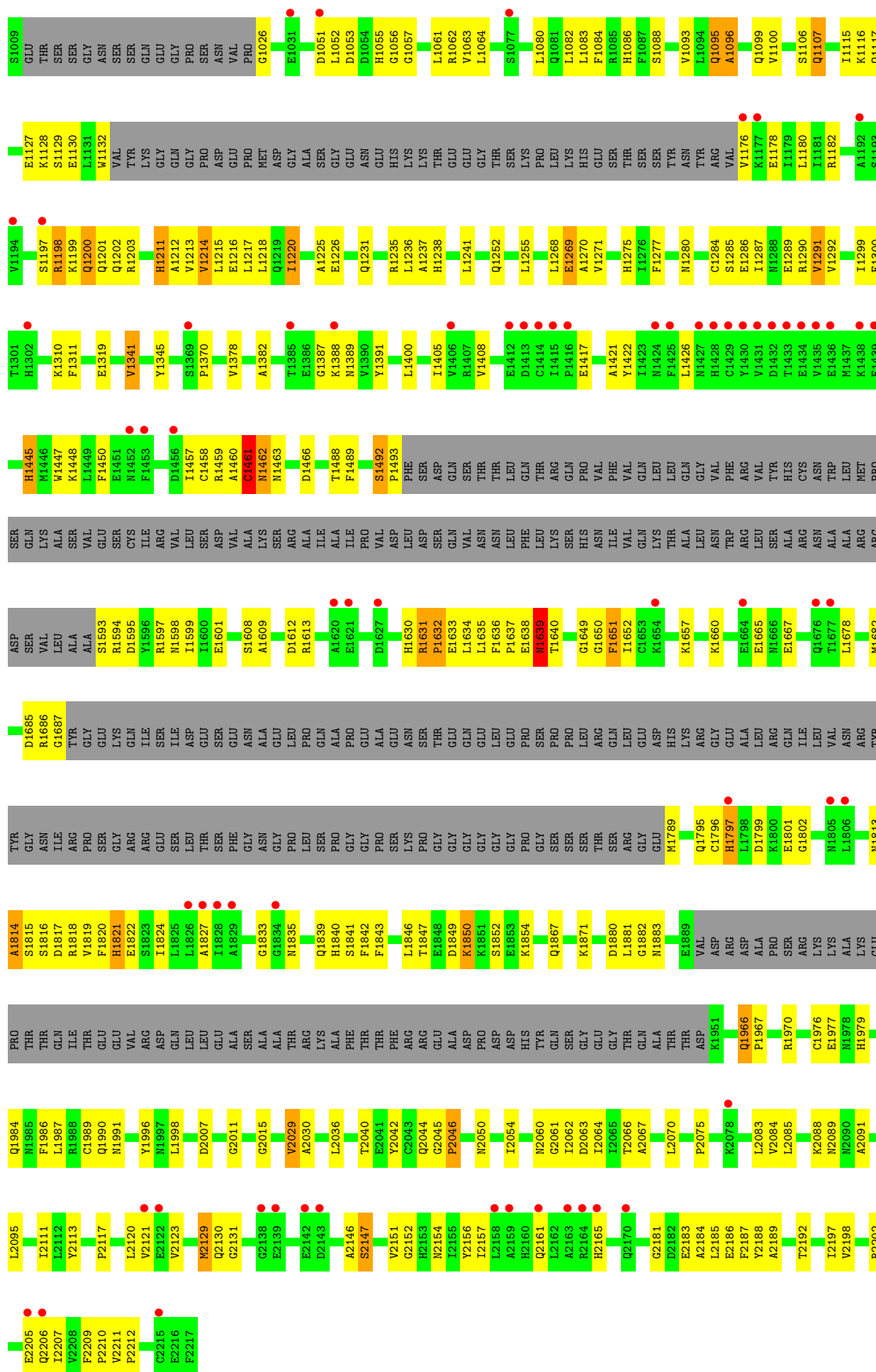






• Molecule 1: Inositol 1,4,5-trisphosphate receptor type 1





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	212.50Å 221.73Å 318.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.15 – 7.31 49.15 – 7.31	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.15-7.31) 88.5 (49.15-7.31)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 7.37Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.317 , 0.394 0.316 , 0.390	Depositor DCC
R_{free} test set	536 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	209.8	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.20 , 406.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.25$, $\langle L^2 \rangle = 0.10$	Xtriage
Estimated twinning fraction	0.219 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.68	EDS
Total number of atoms	16948	wwPDB-VP
Average B, all atoms (Å ²)	170.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% 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	0.65	3/8465 (0.0%)	1.00	25/11786 (0.2%)
1	B	0.69	7/8455 (0.1%)	1.02	22/11772 (0.2%)
All	All	0.67	10/16920 (0.1%)	1.01	47/23558 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	25
1	B	0	22
All	All	0	47

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	178	ILE	C-O	10.83	1.36	1.24
1	A	554	ARG	CA-C	8.30	1.63	1.52
1	B	1445	HIS	CA-C	-8.05	1.42	1.52
1	B	1445	HIS	N-CA	7.73	1.51	1.46
1	B	177	VAL	N-CA	-6.53	1.38	1.46
1	A	176	VAL	C-N	6.37	1.42	1.33
1	B	8	PHE	C-N	6.36	1.42	1.33
1	B	962	LYS	CA-C	5.33	1.59	1.52
1	A	190	GLY	C-N	5.25	1.44	1.33
1	B	178	ILE	C-N	5.02	1.40	1.33

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	177	VAL	N-CA-C	9.47	129.03	109.34
1	A	999	ARG	N-CA-C	-8.87	91.92	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	8	PHE	N-CA-C	8.22	122.44	110.28
1	A	554	ARG	CA-C-O	-8.03	109.02	120.51
1	B	743	MET	CA-C-N	7.86	135.84	121.70
1	B	743	MET	C-N-CA	7.86	135.84	121.70
1	A	2019	LEU	N-CA-C	-7.69	101.91	111.75
1	A	176	VAL	CA-C-N	7.41	135.31	121.97
1	A	176	VAL	C-N-CA	7.41	135.31	121.97
1	B	666	ILE	N-CA-C	7.26	124.45	109.34
1	A	597	ALA	N-CA-C	-7.11	102.73	111.33
1	A	553	CYS	CA-C-N	-6.75	108.65	121.54
1	A	553	CYS	C-N-CA	-6.75	108.65	121.54
1	B	303	PHE	N-CA-C	6.69	118.71	108.07
1	A	998	LYS	CA-C-N	6.64	134.23	121.54
1	A	998	LYS	C-N-CA	6.64	134.23	121.54
1	B	236	GLY	N-CA-C	-6.48	105.20	112.33
1	B	307	HIS	CA-C-N	-6.47	111.83	120.63
1	B	307	HIS	C-N-CA	-6.47	111.83	120.63
1	B	9	LEU	CA-C-N	6.39	133.54	122.81
1	B	9	LEU	C-N-CA	6.39	133.54	122.81
1	A	999	ARG	CA-C-N	-6.25	112.16	122.11
1	A	999	ARG	C-N-CA	-6.25	112.16	122.11
1	A	867	VAL	N-CA-C	-6.12	106.98	112.12
1	B	240	VAL	N-CA-C	6.11	115.16	107.70
1	A	9	LEU	N-CA-C	-5.92	98.19	110.80
1	A	99	GLU	N-CA-C	-5.73	104.73	110.97
1	B	2198	VAL	N-CA-C	5.70	115.50	106.32
1	B	193	LEU	CA-C-N	-5.65	113.13	122.11
1	B	193	LEU	C-N-CA	-5.65	113.13	122.11
1	B	394	CYS	N-CA-C	-5.44	105.04	110.97
1	A	2143	ASP	N-CA-C	-5.26	99.59	110.80
1	A	1461	CYS	N-CA-C	-5.25	99.62	110.80
1	A	666	ILE	N-CA-C	5.24	120.24	109.34
1	A	1349	ALA	N-CA-C	5.17	121.80	110.80
1	A	177	VAL	CB-CA-C	-5.16	102.83	111.29
1	B	1445	HIS	O-C-N	-5.13	118.28	122.03
1	A	2020	LEU	N-CA-C	-5.09	99.96	110.80
1	B	666	ILE	CB-CA-C	-5.06	102.98	111.29
1	A	85	ASP	CA-C-N	5.06	130.81	121.70
1	A	85	ASP	C-N-CA	5.06	130.81	121.70
1	B	414	VAL	N-CA-C	5.05	119.84	109.34
1	B	1284	CYS	CA-C-N	5.04	131.17	121.54
1	B	1284	CYS	C-N-CA	5.04	131.17	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1044	SER	N-CA-C	5.03	117.49	111.71
1	B	1462	ASN	N-CA-C	-5.03	100.09	110.80
1	B	179	GLY	N-CA-C	-5.03	101.27	113.18

There are no chirality outliers.

All (47) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1054	ASP	Peptide
1	A	1055	HIS	Peptide
1	A	118	GLY	Peptide
1	A	1202	GLN	Peptide
1	A	1375	ILE	Peptide
1	A	1380	LEU	Peptide
1	A	1383	VAL	Peptide
1	A	1461	CYS	Peptide
1	A	15	CYS	Peptide
1	A	1639	ASN	Peptide
1	A	176	VAL	Peptide
1	A	1815	SER	Peptide
1	A	2009	ILE	Peptide
1	A	2016	GLY	Peptide
1	A	2071	ASN	Peptide
1	A	2115	MET	Peptide
1	A	2142	GLU	Peptide
1	A	2184	ALA	Peptide
1	A	2192	THR	Peptide
1	A	254	ASP	Peptide
1	A	260	GLN	Peptide
1	A	406	ILE	Peptide
1	A	73	TRP	Peptide
1	A	8	PHE	Peptide
1	A	989	ARG	Peptide
1	B	1269	GLU	Peptide
1	B	1287	ILE	Peptide
1	B	1310	LYS	Peptide
1	B	1461	CYS	Peptide
1	B	1639	ASN	Peptide
1	B	176	VAL	Peptide
1	B	179	GLY	Peptide
1	B	1816	SER	Peptide
1	B	1883	ASN	Peptide

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Mol	Chain	Res	Type	Group
1	B	190	GLY	Peptide
1	B	191	GLN	Peptide
1	B	251	LEU	Peptide
1	B	252	THR	Peptide
1	B	299	TRP	Peptide
1	B	306	LYS	Peptide
1	B	424	LYS	Peptide
1	B	464	THR	Peptide
1	B	670	LEU	Peptide
1	B	7	SER	Peptide
1	B	744	CYS	Peptide
1	B	749	TYR	Peptide
1	B	759	LEU	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	8479	0	3697	432	0
1	B	8469	0	3697	414	0
All	All	16948	0	7394	845	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 35.

All (845) 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:1208:MET:O	1:A:1212:ALA:HB3	1.49	1.10
1:A:162:TYR:O	1:A:184:LEU:C	1.97	1.07
1:A:405:PRO:HA	1:A:416:LEU:HA	1.39	1.04
1:B:1682:MET:O	1:B:1686:ARG:N	1.93	1.01
1:A:1472:SER:O	1:A:1476:LYS:CB	2.10	1.00
1:A:866:VAL:O	1:A:870:ALA:HB2	1.62	1.00
1:A:1371:LEU:O	1:A:1375:ILE:N	1.94	1.00
1:A:1605:ASP:O	1:A:1609:ALA:HB2	1.62	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:PHE:HA	1:B:177:VAL:HA	1.42	0.99
1:A:1208:MET:O	1:A:1212:ALA:CB	2.10	0.98
1:A:2020:LEU:O	1:A:2024:ILE:N	1.96	0.98
1:A:162:TYR:O	1:A:184:LEU:CA	2.11	0.98
1:A:314:LEU:HA	1:A:357:SER:HA	1.47	0.95
1:A:1125:ILE:O	1:A:1129:SER:CB	2.14	0.94
1:A:581:MET:O	1:A:585:ILE:N	2.00	0.94
1:A:1798:LEU:HA	1:A:1802:GLY:HA3	1.50	0.94
1:B:242:LEU:O	1:B:251:LEU:N	2.00	0.94
1:A:243:PHE:HA	1:A:250:PHE:HA	1.50	0.94
1:A:521:LYS:O	1:A:523:LEU:N	2.01	0.93
1:A:1118:ASP:O	1:A:1122:LEU:N	2.01	0.93
1:B:2040:THR:O	1:B:2044:GLN:CB	2.17	0.93
1:A:1231:GLN:O	1:A:1235:ARG:CB	2.17	0.92
1:A:1379:GLU:HA	1:A:1382:ALA:HB3	1.47	0.92
1:B:117:TYR:C	1:B:173:GLY:H	1.77	0.92
1:B:1417:GLU:O	1:B:1421:ALA:N	2.02	0.91
1:A:708:ARG:O	1:A:712:VAL:N	2.03	0.91
1:A:1210:ALA:O	1:A:1214:VAL:CB	2.19	0.91
1:B:314:LEU:HA	1:B:357:SER:HA	1.52	0.91
1:A:117:TYR:O	1:A:173:GLY:N	2.02	0.91
1:A:458:GLY:O	1:A:462:LYS:CB	2.18	0.91
1:A:981:ILE:O	1:A:985:ARG:CB	2.19	0.90
1:A:2125:LYS:O	1:A:2129:MET:CB	2.20	0.90
1:B:1095:GLN:O	1:B:1099:GLN:N	2.05	0.90
1:B:467:GLN:O	1:B:470:ARG:N	2.04	0.90
1:A:8:PHE:H	1:A:177:VAL:C	1.80	0.89
1:B:7:SER:O	1:B:178:ILE:N	2.04	0.89
1:B:1214:VAL:O	1:B:1218:LEU:N	2.06	0.89
1:A:1378:VAL:O	1:A:1382:ALA:HB2	1.73	0.88
1:B:315:ALA:HA	1:B:366:SER:HA	1.55	0.88
1:A:2083:LEU:O	1:A:2087:LEU:CB	2.22	0.88
1:A:856:ASP:O	1:A:860:ASN:CB	2.22	0.88
1:A:1864:LYS:O	1:A:1868:GLN:N	2.07	0.87
1:A:2189:ALA:O	1:A:2193:ALA:N	2.06	0.87
1:A:1380:LEU:O	1:A:1384:CYS:CB	2.23	0.86
1:B:981:ILE:O	1:B:985:ARG:CB	2.23	0.86
1:A:2124:ILE:O	1:A:2128:TYR:CB	2.24	0.86
1:A:19:ALA:N	1:A:25:GLY:O	2.09	0.85
1:B:696:VAL:O	1:B:700:TRP:N	2.10	0.85
1:B:2183:GLU:O	1:B:2187:PHE:CB	2.24	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:686:ALA:O	1:B:689:ALA:HB3	1.77	0.84
1:B:19:ALA:HA	1:B:218:TRP:HA	1.58	0.84
1:A:2036:LEU:O	1:A:2040:THR:CB	2.25	0.84
1:A:162:TYR:O	1:A:184:LEU:HA	1.74	0.84
1:B:244:HIS:O	1:B:248:GLU:N	2.10	0.83
1:B:140:ALA:N	1:B:146:ALA:O	2.11	0.83
1:B:130:LYS:HA	1:B:153:GLU:HA	1.58	0.83
1:B:1212:ALA:O	1:B:1216:GLU:CB	2.26	0.83
1:A:1421:ALA:O	1:A:1425:PHE:CB	2.26	0.83
1:B:1594:ARG:O	1:B:1598:ASN:CB	2.27	0.83
1:B:391:ARG:HA	1:B:398:TRP:HA	1.59	0.83
1:A:125:HIS:O	1:A:129:ASN:N	2.11	0.83
1:A:1861:ASP:O	1:A:1865:VAL:CB	2.26	0.83
1:B:103:ASN:O	1:B:107:ASN:CB	2.26	0.83
1:B:865:GLU:O	1:B:869:LEU:CB	2.27	0.82
1:A:1605:ASP:O	1:A:1609:ALA:CB	2.27	0.82
1:A:354:SER:HA	1:A:419:GLY:HA3	1.61	0.82
1:B:1096:ALA:O	1:B:1100:VAL:N	2.13	0.82
1:A:2189:ALA:O	1:A:2192:THR:N	2.13	0.82
1:A:621:LEU:O	1:A:625:ASN:N	2.10	0.81
1:A:1849:ASP:O	1:A:1853:GLU:N	2.12	0.81
1:A:298:TYR:HA	1:A:381:LEU:HA	1.61	0.81
1:A:480:LEU:O	1:A:483:PHE:N	2.14	0.81
1:B:392:HIS:N	1:B:397:THR:O	2.12	0.81
1:A:975:ILE:O	1:A:979:GLN:CB	2.28	0.81
1:A:1417:GLU:O	1:A:1421:ALA:N	2.10	0.81
1:A:162:TYR:CB	1:A:185:ASN:O	2.29	0.81
1:A:2188:TYR:O	1:A:2192:THR:CB	2.29	0.81
1:B:392:HIS:O	1:B:396:ASN:N	2.13	0.81
1:B:764:ILE:O	1:B:768:MET:CB	2.29	0.81
1:A:1224:LYS:HA	1:A:1270:ALA:HB3	1.63	0.80
1:B:162:TYR:O	1:B:184:LEU:C	2.24	0.80
1:B:666:ILE:CB	1:B:670:LEU:H	1.93	0.80
1:B:697:TRP:O	1:B:701:ARG:N	2.10	0.80
1:A:866:VAL:O	1:A:870:ALA:CB	2.30	0.80
1:B:767:CYS:O	1:B:771:GLU:CB	2.30	0.80
1:A:251:LEU:HA	1:A:264:LEU:HA	1.64	0.80
1:A:8:PHE:N	1:A:177:VAL:O	2.14	0.79
1:B:670:LEU:HA	1:B:673:SER:H	1.47	0.79
1:B:605:LEU:O	1:B:608:LYS:N	2.16	0.79
1:B:163:ILE:HA	1:B:184:LEU:HA	1.63	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:398:TRP:H	1:B:422:PRO:HA	1.47	0.78
1:A:118:GLY:N	1:A:163:ILE:O	2.13	0.78
1:A:1381:LEU:O	1:A:1385:THR:CB	2.32	0.78
1:A:761:VAL:O	1:A:764:ILE:N	2.17	0.78
1:A:1992:ASN:O	1:A:1994:THR:N	2.15	0.78
1:A:1252:GLN:O	1:A:1256:HIS:CB	2.31	0.78
1:B:61:CYS:CB	1:B:122:GLN:O	2.32	0.78
1:B:162:TYR:CB	1:B:185:ASN:O	2.31	0.78
1:A:252:THR:O	1:A:263:PHE:O	2.01	0.77
1:A:1862:ARG:O	1:A:1866:ALA:CB	2.33	0.77
1:B:1813:ASN:O	1:B:1815:SER:N	2.17	0.77
1:A:1792:ALA:O	1:A:1796:CYS:CB	2.31	0.77
1:B:1632:PRO:O	1:B:1635:LEU:N	2.17	0.77
1:A:853:PRO:O	1:A:855:SER:N	2.17	0.77
1:A:1862:ARG:O	1:A:1866:ALA:HB3	1.85	0.77
1:A:1126:VAL:O	1:A:1130:GLU:CB	2.33	0.76
1:B:15:CYS:HA	1:B:222:LEU:HA	1.67	0.76
1:B:313:TYR:CB	1:B:358:VAL:O	2.34	0.76
1:A:666:ILE:CB	1:A:670:LEU:H	1.98	0.76
1:A:16:SER:O	1:A:221:VAL:N	2.19	0.76
1:A:2035:THR:O	1:A:2039:LEU:CB	2.34	0.76
1:A:194:HIS:H	1:A:211:SER:HA	1.51	0.76
1:A:253:CYS:C	1:A:261:HIS:O	2.29	0.75
1:A:2116:ARG:O	1:A:2120:LEU:N	2.18	0.75
1:A:392:HIS:O	1:A:396:ASN:N	2.20	0.75
1:A:1377:LEU:O	1:A:1381:LEU:CB	2.34	0.75
1:B:1795:GLN:O	1:B:1799:ASP:N	2.20	0.75
1:A:1795:GLN:O	1:A:1799:ASP:N	2.19	0.74
1:B:161:PHE:HA	1:B:186:PRO:HA	1.68	0.74
1:B:891:LEU:O	1:B:895:LEU:CB	2.35	0.74
1:A:767:CYS:O	1:A:771:GLU:CB	2.35	0.74
1:A:2189:ALA:C	1:A:2193:ALA:H	1.96	0.74
1:A:32:LEU:H	1:A:448:ASP:CB	2.01	0.74
1:B:252:THR:O	1:B:262:VAL:HA	1.88	0.74
1:A:254:ASP:O	1:A:261:HIS:CB	2.36	0.74
1:B:185:ASN:HA	1:B:192:PRO:HA	1.68	0.74
1:B:15:CYS:HA	1:B:223:PHE:H	1.53	0.73
1:B:252:THR:O	1:B:262:VAL:CA	2.36	0.73
1:A:1848:GLU:O	1:A:1850:LYS:N	2.18	0.73
1:B:305:PHE:O	1:B:314:LEU:N	2.20	0.73
1:A:2088:LYS:O	1:A:2092:SER:N	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:SER:HA	1:A:394:CYS:CB	2.19	0.72
1:A:2147:SER:O	1:A:2151:VAL:CB	2.38	0.72
1:B:162:TYR:O	1:B:184:LEU:HA	1.89	0.72
1:A:212:VAL:O	1:A:214:CYS:N	2.21	0.72
1:A:255:GLU:HA	1:A:260:GLN:HA	1.72	0.72
1:B:509:LEU:O	1:B:513:GLN:N	2.19	0.72
1:B:982:LEU:O	1:B:986:LEU:N	2.23	0.72
1:B:102:GLN:O	1:B:106:GLU:CB	2.37	0.72
1:B:1818:ARG:O	1:B:1821:HIS:N	2.22	0.72
1:B:11:ILE:H	1:B:113:THR:C	1.98	0.71
1:B:199:GLN:HA	1:B:207:ASN:HA	1.71	0.71
1:B:252:THR:HA	1:B:280:ALA:HA	1.72	0.71
1:B:1052:LEU:O	1:B:1057:GLY:N	2.23	0.71
1:B:315:ALA:HB3	1:B:356:VAL:O	1.89	0.71
1:B:1422:TYR:O	1:B:1426:LEU:CB	2.38	0.71
1:A:474:THR:O	1:A:477:LEU:N	2.24	0.71
1:A:15:CYS:HA	1:A:222:LEU:HA	1.72	0.71
1:B:773:LEU:O	1:B:775:TYR:N	2.20	0.71
1:A:741:ALA:HB2	1:A:876:PHE:HA	1.73	0.71
1:A:973:LYS:O	1:A:977:ILE:CB	2.39	0.71
1:A:2021:GLY:O	1:A:2025:ASN:N	2.24	0.71
1:A:181:LYS:HA	1:A:218:TRP:O	1.90	0.70
1:B:2152:GLY:O	1:B:2156:TYR:CB	2.39	0.70
1:A:20:GLU:N	1:A:217:SER:O	2.22	0.70
1:A:1371:LEU:O	1:A:1374:HIS:N	2.24	0.70
1:A:118:GLY:H	1:A:163:ILE:C	2.00	0.70
1:A:1297:HIS:HA	1:A:1301:THR:HA	1.73	0.70
1:A:102:GLN:O	1:A:106:GLU:CB	2.40	0.70
1:A:1040:ILE:O	1:A:1043:GLY:N	2.25	0.70
1:A:8:PHE:N	1:A:176:VAL:O	2.26	0.69
1:B:104:GLU:O	1:B:108:ARG:CB	2.40	0.69
1:B:1636:PHE:O	1:B:1638:GLU:N	2.23	0.69
1:A:253:CYS:O	1:A:261:HIS:O	2.10	0.69
1:A:1178:GLU:O	1:A:1182:ARG:CB	2.41	0.69
1:A:1378:VAL:O	1:A:1382:ALA:CB	2.40	0.69
1:A:1118:ASP:O	1:A:1121:GLN:N	2.25	0.69
1:A:2115:MET:O	1:A:2119:GLU:N	2.22	0.69
1:A:307:HIS:O	1:A:311:GLY:N	2.26	0.69
1:B:14:ILE:O	1:B:223:PHE:N	2.26	0.68
1:B:55:ASP:HA	1:B:127:LYS:CB	2.23	0.68
1:A:1294:HIS:O	1:A:1298:CYS:N	2.21	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:TYR:O	1:B:184:LEU:CA	2.41	0.68
1:B:853:PRO:O	1:B:855:SER:N	2.25	0.68
1:A:874:ILE:O	1:A:878:PHE:N	2.26	0.68
1:A:243:PHE:HA	1:A:250:PHE:CA	2.23	0.68
1:B:1593:SER:O	1:B:1597:ARG:N	2.18	0.68
1:A:2117:PRO:O	1:A:2121:VAL:CB	2.41	0.68
1:B:315:ALA:HB2	1:B:358:VAL:CB	2.23	0.68
1:B:1489:PHE:HA	1:B:1493:PRO:C	2.18	0.68
1:A:162:TYR:O	1:A:184:LEU:O	2.10	0.67
1:B:1991:ASN:CB	1:B:1998:LEU:HA	2.25	0.67
1:B:628:PRO:O	1:B:632:ASP:N	2.22	0.67
1:B:2050:ASN:O	1:B:2054:ILE:CB	2.42	0.67
1:A:390:LEU:O	1:A:398:TRP:HA	1.93	0.67
1:B:398:TRP:O	1:B:421:SER:O	2.13	0.67
1:B:476:LEU:O	1:B:479:ASP:N	2.28	0.67
1:A:14:ILE:O	1:A:223:PHE:N	2.23	0.67
1:B:8:PHE:HA	1:B:177:VAL:CA	2.22	0.67
1:A:244:HIS:N	1:A:249:LYS:O	2.28	0.67
1:A:255:GLU:HA	1:A:259:LYS:O	1.95	0.67
1:A:769:SER:HA	1:A:779:ALA:HA	1.77	0.67
1:A:1476:LYS:HA	1:A:1884:LYS:HA	1.75	0.66
1:A:391:ARG:HA	1:A:398:TRP:HA	1.77	0.66
1:A:998:LYS:O	1:A:1007:GLN:HA	1.95	0.66
1:B:421:SER:O	1:B:423:LEU:N	2.28	0.66
1:B:1820:PHE:C	1:B:1822:GLU:H	2.04	0.66
1:B:135:ASN:CB	1:B:148:ARG:O	2.42	0.66
1:B:279:LYS:HA	1:B:309:ALA:H	1.60	0.66
1:A:255:GLU:CA	1:A:259:LYS:O	2.42	0.66
1:B:1986:PHE:O	1:B:1990:GLN:N	2.29	0.66
1:A:7:SER:C	1:A:176:VAL:O	2.39	0.66
1:B:152:ASP:O	1:B:155:GLY:N	2.28	0.66
1:B:223:PHE:HA	1:B:293:ARG:HA	1.76	0.66
1:B:398:TRP:N	1:B:422:PRO:HA	2.10	0.66
1:B:680:VAL:O	1:B:682:THR:N	2.28	0.66
1:A:1062:ARG:O	1:A:1066:HIS:N	2.23	0.66
1:A:7:SER:HA	1:A:177:VAL:N	2.11	0.65
1:A:19:ALA:O	1:A:25:GLY:N	2.29	0.65
1:B:1597:ARG:O	1:B:1601:GLU:CB	2.44	0.65
1:A:1108:ASP:O	1:A:1112:TYR:N	2.26	0.65
1:A:1848:GLU:C	1:A:1850:LYS:H	2.03	0.65
1:B:1225:ALA:H	1:B:1270:ALA:HB3	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:THR:CB	1:B:280:ALA:HA	2.27	0.65
1:B:1459:ARG:C	1:B:1461:CYS:H	2.04	0.65
1:A:478:GLU:O	1:A:480:LEU:N	2.29	0.65
1:B:118:GLY:H	1:B:163:ILE:C	2.04	0.65
1:A:179:GLY:HA2	1:A:220:ILE:O	1.96	0.65
1:A:355:LEU:H	1:A:419:GLY:HA2	1.61	0.64
1:B:621:LEU:O	1:B:625:ASN:N	2.30	0.64
1:B:1850:LYS:O	1:B:1854:LYS:N	2.30	0.64
1:A:2076:LEU:HA	1:A:2080:ARG:CB	2.27	0.64
1:A:61:CYS:CB	1:A:122:GLN:O	2.45	0.64
1:A:32:LEU:CB	1:A:445:PHE:HA	2.28	0.64
1:B:70:LYS:O	1:B:74:LYS:CB	2.46	0.64
1:A:2123:VAL:O	1:A:2127:ALA:HB3	1.98	0.63
1:B:313:TYR:O	1:B:357:SER:C	2.41	0.63
1:A:100:LYS:O	1:A:103:ASN:N	2.31	0.63
1:B:252:THR:CA	1:B:280:ALA:HA	2.27	0.63
1:B:2091:ALA:O	1:B:2095:LEU:CB	2.46	0.63
1:A:16:SER:N	1:A:221:VAL:O	2.31	0.63
1:A:313:TYR:O	1:A:358:VAL:CB	2.46	0.63
1:A:2020:LEU:O	1:A:2021:GLY:C	2.42	0.63
1:A:124:LEU:HA	1:A:131:TYR:HA	1.80	0.63
1:A:253:CYS:CB	1:A:262:VAL:HA	2.28	0.62
1:B:134:VAL:O	1:B:136:LYS:N	2.32	0.62
1:B:125:HIS:N	1:B:130:LYS:O	2.25	0.62
1:B:1986:PHE:O	1:B:1989:CYS:N	2.32	0.62
1:B:252:THR:O	1:B:262:VAL:C	2.42	0.62
1:B:132:LEU:HA	1:B:150:THR:O	1.99	0.62
1:B:1966:GLN:O	1:B:1970:ARG:CB	2.48	0.62
1:B:138:LEU:O	1:B:148:ARG:N	2.22	0.62
1:A:2168:GLU:O	1:A:2172:MET:CB	2.48	0.62
1:A:404:ILE:O	1:A:417:LYS:N	2.33	0.61
1:A:1033:ILE:HA	1:A:1036:GLN:CB	2.30	0.61
1:B:789:HIS:O	1:B:791:ASP:N	2.33	0.61
1:B:1269:GLU:HA	1:B:1319:GLU:CB	2.30	0.61
1:B:1457:ILE:O	1:B:1459:ARG:N	2.33	0.61
1:A:39:VAL:N	1:A:207:ASN:O	2.32	0.61
1:A:888:THR:O	1:A:891:LEU:N	2.33	0.61
1:B:666:ILE:H	1:B:667:GLU:HA	1.66	0.61
1:B:11:ILE:C	1:B:13:ASP:H	2.09	0.61
1:B:1849:ASP:O	1:B:1850:LYS:C	2.43	0.61
1:B:1849:ASP:O	1:B:1852:SER:N	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:279:LYS:N	1:B:309:ALA:HB2	2.15	0.61
1:A:69:GLN:O	1:A:73:TRP:CB	2.49	0.61
1:B:125:HIS:O	1:B:129:ASN:N	2.33	0.61
1:A:666:ILE:N	1:A:667:GLU:HA	2.16	0.60
1:A:683:GLY:O	1:A:685:ASN:N	2.34	0.60
1:B:449:ALA:O	1:B:452:VAL:N	2.34	0.60
1:B:1051:ASP:O	1:B:1055:HIS:N	2.32	0.60
1:B:2120:LEU:O	1:B:2123:VAL:N	2.34	0.60
1:A:252:THR:C	1:A:263:PHE:O	2.44	0.60
1:A:885:LEU:O	1:A:888:THR:N	2.34	0.60
1:A:998:LYS:C	1:A:1007:GLN:HA	2.26	0.60
1:A:1030:PHE:O	1:A:1034:GLU:CB	2.50	0.60
1:B:1609:ALA:O	1:B:1613:ARG:CB	2.50	0.60
1:B:2061:GLY:O	1:B:2064:ILE:N	2.31	0.60
1:A:1480:GLU:CB	1:A:1882:GLY:H	2.15	0.60
1:B:1128:LYS:O	1:B:1132:TRP:CB	2.50	0.60
1:B:7:SER:O	1:B:178:ILE:C	2.44	0.60
1:B:692:ASP:O	1:B:696:VAL:N	2.35	0.60
1:B:2188:TYR:O	1:B:2192:THR:CB	2.49	0.60
1:A:130:LYS:HA	1:A:153:GLU:HA	1.83	0.59
1:A:704:ASN:C	1:A:706:GLU:H	2.10	0.59
1:B:117:TYR:O	1:B:173:GLY:N	2.35	0.59
1:A:103:ASN:O	1:A:107:ASN:CB	2.50	0.59
1:A:1371:LEU:O	1:A:1372:MET:C	2.42	0.59
1:A:11:ILE:H	1:A:113:THR:C	2.09	0.59
1:A:1291:VAL:O	1:A:1295:PHE:N	2.35	0.59
1:B:398:TRP:H	1:B:422:PRO:CA	2.13	0.59
1:A:893:ALA:O	1:A:897:CYS:CB	2.51	0.59
1:B:117:TYR:C	1:B:119:ASN:H	2.11	0.59
1:B:127:LYS:C	1:B:129:ASN:N	2.57	0.59
1:B:680:VAL:C	1:B:682:THR:H	2.11	0.59
1:B:1231:GLN:HA	1:B:1275:HIS:CB	2.33	0.59
1:B:1231:GLN:O	1:B:1235:ARG:CB	2.51	0.59
1:B:2157:ILE:O	1:B:2161:GLN:CB	2.51	0.59
1:A:755:ILE:O	1:A:758:GLN:N	2.35	0.59
1:B:691:GLU:O	1:B:695:GLU:N	2.35	0.59
1:B:1445:HIS:C	1:B:1447:TRP:H	2.11	0.58
1:B:117:TYR:O	1:B:119:ASN:N	2.37	0.58
1:B:962:LYS:O	1:B:966:MET:CB	2.51	0.58
1:A:680:VAL:O	1:A:682:THR:N	2.34	0.58
1:A:1251:ASN:O	1:A:1255:LEU:CB	2.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1417:GLU:O	1:A:1420:ILE:N	2.36	0.58
1:A:1682:MET:C	1:A:1685:ASP:H	2.12	0.58
1:A:1453:PHE:O	1:A:1457:ILE:CB	2.52	0.58
1:B:299:TRP:H	1:B:380:SER:C	2.10	0.58
1:B:978:LEU:O	1:B:982:LEU:CB	2.52	0.58
1:A:1208:MET:O	1:A:1212:ALA:HB2	2.02	0.58
1:A:8:PHE:N	1:A:177:VAL:C	2.59	0.57
1:A:164:GLN:CB	1:A:183:VAL:O	2.52	0.57
1:A:242:LEU:O	1:A:250:PHE:HA	2.04	0.57
1:B:1489:PHE:HA	1:B:1493:PRO:HA	1.86	0.57
1:B:1839:GLN:O	1:B:1842:PHE:CB	2.52	0.57
1:A:85:ASP:HA	1:A:86:ALA:C	2.30	0.57
1:A:256:HIS:H	1:A:261:HIS:H	1.51	0.57
1:B:45:ASP:O	1:B:49:PRO:HA	2.05	0.57
1:A:978:LEU:O	1:A:982:LEU:CB	2.53	0.56
1:B:242:LEU:C	1:B:251:LEU:H	2.06	0.56
1:A:125:HIS:N	1:A:130:LYS:O	2.38	0.56
1:B:233:ILE:HA	1:B:384:ARG:N	2.19	0.56
1:B:399:VAL:HA	1:B:420:THR:HA	1.87	0.56
1:A:30:LEU:CB	1:A:36:ARG:H	2.18	0.56
1:A:1798:LEU:CA	1:A:1802:GLY:HA3	2.30	0.56
1:B:277:SER:O	1:B:280:ALA:HB3	2.06	0.56
1:B:313:TYR:O	1:B:357:SER:CA	2.53	0.56
1:B:253:CYS:HA	1:B:262:VAL:HA	1.88	0.56
1:B:386:SER:O	1:B:432:ILE:N	2.29	0.56
1:B:1976:CYS:O	1:B:1979:HIS:N	2.39	0.56
1:B:1200:GLN:O	1:B:1203:ARG:N	2.39	0.56
1:B:1595:ASP:O	1:B:1599:ILE:CB	2.54	0.56
1:B:773:LEU:C	1:B:775:TYR:H	2.13	0.56
1:B:856:ASP:O	1:B:860:ASN:CB	2.53	0.56
1:A:896:ASP:C	1:A:898:VAL:H	2.13	0.56
1:A:563:SER:O	1:A:565:GLN:N	2.39	0.56
1:A:233:ILE:HA	1:A:383:PRO:HA	1.86	0.56
1:A:254:ASP:O	1:A:256:HIS:N	2.39	0.56
1:A:256:HIS:H	1:A:261:HIS:N	2.03	0.56
1:A:1048:THR:O	1:A:1050:LEU:N	2.36	0.56
1:A:1476:LYS:CA	1:A:1884:LYS:HA	2.36	0.56
1:B:2181:GLY:HA2	1:B:2184:ALA:HB3	1.88	0.56
1:A:40:GLN:HA	1:A:206:CYS:HA	1.87	0.55
1:A:551:HIS:O	1:A:554:ARG:N	2.37	0.55
1:A:1682:MET:O	1:A:1686:ARG:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:676:GLU:O	1:B:680:VAL:N	2.35	0.55
1:A:617:THR:O	1:A:621:LEU:CB	2.55	0.55
1:A:682:THR:O	1:A:686:ALA:HB3	2.07	0.55
1:A:1848:GLU:C	1:A:1850:LYS:N	2.64	0.55
1:B:11:ILE:C	1:B:13:ASP:N	2.63	0.55
1:B:127:LYS:C	1:B:129:ASN:H	2.11	0.55
1:B:1638:GLU:O	1:B:1640:THR:N	2.39	0.55
1:A:263:PHE:CB	1:A:416:LEU:H	2.19	0.55
1:A:457:ALA:HA	1:A:522:LEU:HA	1.88	0.55
1:B:885:LEU:C	1:B:888:THR:H	2.14	0.55
1:B:1378:VAL:O	1:B:1382:ALA:HB2	2.05	0.55
1:A:297:GLY:O	1:A:381:LEU:HA	2.06	0.55
1:A:100:LYS:O	1:A:101:LYS:C	2.48	0.55
1:A:1952:ALA:O	1:A:1954:ASP:N	2.40	0.55
1:B:421:SER:O	1:B:422:PRO:C	2.49	0.55
1:B:1286:GLU:O	1:B:1289:GLU:O	2.25	0.55
1:B:1682:MET:CB	1:B:1687:GLY:H	2.19	0.55
1:B:1797:HIS:O	1:B:1802:GLY:N	2.29	0.55
1:A:1864:LYS:O	1:A:1867:GLN:N	2.39	0.55
1:A:7:SER:CB	1:A:179:GLY:N	2.69	0.55
1:B:848:VAL:O	1:B:850:GLN:N	2.40	0.55
1:B:2062:ILE:O	1:B:2066:THR:CB	2.55	0.55
1:B:1095:GLN:O	1:B:1096:ALA:C	2.50	0.55
1:A:195:ALA:HB3	1:A:216:THR:CB	2.37	0.55
1:A:2018:GLY:C	1:A:2020:LEU:N	2.62	0.55
1:A:40:GLN:CA	1:A:206:CYS:HA	2.37	0.54
1:A:1317:LYS:HA	1:A:1323:ILE:CB	2.37	0.54
1:A:1476:LYS:CB	1:A:1883:ASN:HA	2.38	0.54
1:B:139:PRO:HA	1:B:147:MET:HA	1.89	0.54
1:B:1636:PHE:C	1:B:1638:GLU:H	2.13	0.54
1:A:1862:ARG:O	1:A:1866:ALA:HB2	2.07	0.54
1:A:2114:ASN:C	1:A:2116:ARG:N	2.66	0.54
1:B:1129:SER:CB	1:B:1180:LEU:HA	2.38	0.54
1:B:91:LYS:O	1:B:95:ALA:HB2	2.07	0.54
1:B:1115:ILE:C	1:B:1117:GLN:H	2.16	0.54
1:A:255:GLU:C	1:A:259:LYS:O	2.51	0.54
1:B:863:THR:O	1:B:867:VAL:CB	2.55	0.54
1:B:1093:VAL:HA	1:B:1176:VAL:N	2.22	0.54
1:A:253:CYS:HA	1:A:263:PHE:H	1.73	0.54
1:A:475:LYS:O	1:A:479:ASP:CB	2.56	0.54
1:B:2185:LEU:HA	1:B:2188:TYR:CB	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1405:ILE:O	1:B:1408:VAL:N	2.41	0.54
1:A:11:ILE:H	1:A:113:THR:N	2.06	0.54
1:B:780:SER:O	1:B:783:ARG:N	2.40	0.54
1:B:1235:ARG:O	1:B:1238:HIS:N	2.41	0.54
1:B:1289:GLU:C	1:B:1291:VAL:N	2.64	0.54
1:A:199:GLN:HA	1:A:207:ASN:HA	1.89	0.54
1:B:1682:MET:O	1:B:1685:ASP:N	2.41	0.54
1:B:1682:MET:C	1:B:1686:ARG:H	2.16	0.54
1:A:45:ASP:N	1:A:48:ASN:O	2.36	0.53
1:A:2020:LEU:O	1:A:2023:TYR:N	2.40	0.53
1:B:1052:LEU:HA	1:B:1056:GLY:H	1.72	0.53
1:A:123:LEU:O	1:A:132:LEU:N	2.36	0.53
1:B:570:ASN:O	1:B:573:TYR:N	2.42	0.53
1:B:860:ASN:O	1:B:861:LYS:C	2.51	0.53
1:A:1798:LEU:HA	1:A:1802:GLY:CA	2.30	0.53
1:A:39:VAL:C	1:A:207:ASN:H	2.16	0.53
1:A:1682:MET:HA	1:A:1685:ASP:CB	2.39	0.53
1:B:729:ILE:O	1:B:732:TYR:N	2.41	0.53
1:B:986:LEU:C	1:B:988:TYR:H	2.16	0.53
1:B:1026:GLY:HA2	1:B:1594:ARG:CB	2.38	0.53
1:B:1796:CYS:HA	1:B:1799:ASP:CB	2.39	0.53
1:B:2044:GLN:C	1:B:2046:PRO:N	2.65	0.53
1:A:2043:CYS:C	1:A:2097:ALA:HB1	2.34	0.53
1:A:38:VAL:HA	1:A:208:GLU:HA	1.91	0.53
1:B:62:PRO:O	1:B:64:ASN:N	2.42	0.53
1:A:865:GLU:O	1:A:869:LEU:CB	2.57	0.53
1:B:180:ASP:C	1:B:219:LYS:HA	2.34	0.53
1:A:1209:GLY:O	1:A:1213:VAL:CB	2.57	0.52
1:A:2010:CYS:O	1:A:2012:SER:N	2.43	0.52
1:B:1199:LYS:C	1:B:1201:GLN:N	2.67	0.52
1:B:1211:HIS:O	1:B:1214:VAL:N	2.42	0.52
1:B:1341:VAL:O	1:B:1345:TYR:N	2.42	0.52
1:B:200:LEU:O	1:B:203:ASN:N	2.41	0.52
1:B:1277:PHE:O	1:B:1280:ASN:N	2.43	0.52
1:A:17:LEU:HA	1:A:219:LYS:O	2.10	0.52
1:B:10:HIS:H	1:B:13:ASP:CB	2.22	0.52
1:B:163:ILE:O	1:B:164:GLN:O	2.27	0.52
1:B:305:PHE:C	1:B:314:LEU:H	2.15	0.52
1:B:236:GLY:HA3	1:B:286:VAL:H	1.74	0.52
1:B:111:LEU:C	1:B:113:THR:H	2.18	0.52
1:B:315:ALA:HA	1:B:366:SER:CA	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:315:ALA:H	1:B:357:SER:HA	1.75	0.52
1:B:577:GLN:O	1:B:581:MET:N	2.32	0.52
1:A:204:PRO:O	1:A:205:GLY:C	2.51	0.52
1:A:1111:ASN:O	1:A:1115:ILE:N	2.43	0.52
1:A:1297:HIS:O	1:A:1301:THR:N	2.43	0.52
1:B:1608:SER:O	1:B:1612:ASP:CB	2.57	0.52
1:B:2186:GLU:O	1:B:2189:ALA:N	2.41	0.52
1:A:19:ALA:HA	1:A:217:SER:O	2.09	0.52
1:A:684:GLU:O	1:A:687:LEU:CB	2.58	0.52
1:A:977:ILE:O	1:A:981:ILE:CB	2.58	0.52
1:A:2184:ALA:HA	1:A:2187:PHE:CB	2.40	0.52
1:A:1986:PHE:O	1:A:1990:GLN:N	2.43	0.52
1:A:2114:ASN:O	1:A:2116:ARG:N	2.43	0.52
1:A:7:SER:HA	1:A:177:VAL:CA	2.40	0.51
1:A:265:ARG:O	1:A:267:THR:N	2.44	0.51
1:A:459:LYS:O	1:A:463:GLY:N	2.31	0.51
1:B:136:LYS:HA	1:B:147:MET:CB	2.40	0.51
1:A:854:PHE:O	1:A:857:LYS:N	2.41	0.51
1:B:696:VAL:O	1:B:697:TRP:C	2.53	0.51
1:B:117:TYR:HA	1:B:163:ILE:O	2.10	0.51
1:B:654:LYS:O	1:B:658:ASN:N	2.39	0.51
1:B:984:VAL:O	1:B:989:ARG:N	2.43	0.51
1:A:316:ALA:HA	1:A:354:SER:O	2.10	0.51
1:A:1341:VAL:O	1:A:1344:PHE:N	2.43	0.51
1:B:242:LEU:O	1:B:250:PHE:HA	2.10	0.51
1:B:1488:THR:O	1:B:1492:SER:N	2.42	0.51
1:B:1850:LYS:O	1:B:1854:LYS:CB	2.59	0.51
1:A:1179:ILE:O	1:A:1183:LEU:CB	2.58	0.51
1:B:7:SER:N	1:B:177:VAL:CB	2.73	0.51
1:B:867:VAL:O	1:B:870:ALA:N	2.43	0.51
1:B:1880:ASP:C	1:B:1882:GLY:H	2.18	0.51
1:B:2063:ASP:HA	1:B:2113:TYR:CB	2.41	0.51
1:A:19:ALA:O	1:A:24:ASN:HA	2.11	0.51
1:A:399:VAL:HA	1:A:421:SER:H	1.76	0.51
1:B:2129:MET:O	1:B:2131:GLY:N	2.43	0.51
1:A:13:ASP:HA	1:A:225:LYS:C	2.36	0.51
1:A:692:ASP:O	1:A:696:VAL:N	2.43	0.51
1:A:1636:PHE:O	1:A:1638:GLU:N	2.44	0.51
1:B:165:PRO:HA	1:B:182:VAL:HA	1.92	0.51
1:B:1387:GLY:O	1:B:1389:ASN:N	2.44	0.51
1:A:1085:ARG:O	1:A:1087:PHE:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:476:LEU:O	1:B:477:LEU:C	2.53	0.50
1:B:680:VAL:C	1:B:682:THR:N	2.67	0.50
1:B:397:THR:HA	1:B:422:PRO:HA	1.93	0.50
1:B:652:ILE:O	1:B:655:ALA:HB3	2.12	0.50
1:A:393:LEU:C	1:A:396:ASN:H	2.20	0.50
1:A:558:ARG:C	1:A:560:LEU:N	2.67	0.50
1:A:2003:LEU:O	1:A:2007:ASP:CB	2.60	0.50
1:B:665:LEU:O	1:B:671:VAL:N	2.45	0.50
1:B:1214:VAL:O	1:B:1215:LEU:C	2.55	0.50
1:B:1489:PHE:HA	1:B:1493:PRO:CA	2.42	0.50
1:B:1867:GLN:O	1:B:1871:LYS:N	2.27	0.50
1:A:221:VAL:O	1:A:222:LEU:O	2.29	0.50
1:B:1986:PHE:O	1:B:1987:LEU:C	2.54	0.50
1:A:140:ALA:HB2	1:A:147:MET:C	2.37	0.50
1:A:476:LEU:O	1:A:479:ASP:N	2.44	0.50
1:A:1116:LYS:O	1:A:1117:GLN:C	2.55	0.50
1:A:1238:HIS:O	1:A:1240:PHE:N	2.45	0.49
1:B:1820:PHE:O	1:B:1822:GLU:N	2.45	0.49
1:A:554:ARG:HA	1:A:557:TYR:CB	2.42	0.49
1:B:243:PHE:HA	1:B:249:LYS:O	2.11	0.49
1:B:281:LEU:O	1:B:308:LEU:CB	2.60	0.49
1:B:387:TYR:HA	1:B:431:ALA:HA	1.94	0.49
1:B:2036:LEU:O	1:B:2040:THR:CB	2.60	0.49
1:A:391:ARG:HA	1:A:398:TRP:N	2.27	0.49
1:A:2173:LEU:O	1:A:2177:GLY:N	2.45	0.49
1:B:118:GLY:N	1:B:163:ILE:C	2.69	0.49
1:B:1225:ALA:HB1	1:B:1226:GLU:HA	1.94	0.49
1:A:15:CYS:HA	1:A:223:PHE:N	2.27	0.49
1:A:480:LEU:C	1:A:483:PHE:H	2.20	0.49
1:A:1863:MET:O	1:A:1867:GLN:N	2.38	0.49
1:A:2119:GLU:O	1:A:2123:VAL:CB	2.60	0.49
1:B:666:ILE:H	1:B:667:GLU:CA	2.26	0.49
1:B:1682:MET:O	1:B:1685:ASP:C	2.54	0.49
1:B:2007:ASP:O	1:B:2011:GLY:N	2.46	0.49
1:B:279:LYS:H	1:B:309:ALA:HB2	1.76	0.49
1:B:112:GLY:HA2	1:B:226:TRP:CB	2.43	0.49
1:A:391:ARG:HA	1:A:398:TRP:CA	2.42	0.49
1:B:1218:LEU:C	1:B:1220:ILE:H	2.20	0.49
1:A:1251:ASN:CB	1:A:1283:LEU:HA	2.43	0.49
1:A:558:ARG:C	1:A:560:LEU:H	2.21	0.49
1:A:2019:LEU:O	1:A:2021:GLY:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:763:LEU:O	1:B:767:CYS:CB	2.60	0.49
1:B:1127:GLU:O	1:B:1130:GLU:N	2.41	0.49
1:B:1682:MET:C	1:B:1685:ASP:H	2.21	0.49
1:A:2189:ALA:O	1:A:2191:HIS:N	2.45	0.48
1:B:113:THR:O	1:B:114:VAL:C	2.56	0.48
1:A:13:ASP:HA	1:A:226:TRP:N	2.28	0.48
1:A:690:GLY:O	1:A:691:GLU:C	2.56	0.48
1:A:826:LYS:O	1:A:830:LYS:CB	2.61	0.48
1:A:1872:ALA:O	1:A:1876:VAL:CB	2.61	0.48
1:B:16:SER:N	1:B:221:VAL:O	2.30	0.48
1:B:117:TYR:C	1:B:119:ASN:N	2.70	0.48
1:B:1843:PHE:O	1:B:1846:LEU:N	2.45	0.48
1:B:2029:VAL:O	1:B:2030:ALA:C	2.55	0.48
1:B:2186:GLU:C	1:B:2189:ALA:H	2.19	0.48
1:A:724:LYS:O	1:A:726:ASP:N	2.47	0.48
1:A:2043:CYS:O	1:A:2097:ALA:HB1	2.14	0.48
1:B:298:TYR:HA	1:B:381:LEU:CA	2.43	0.48
1:B:298:TYR:HA	1:B:381:LEU:HA	1.95	0.48
1:A:7:SER:HA	1:A:177:VAL:C	2.38	0.48
1:A:355:LEU:H	1:A:419:GLY:CA	2.27	0.48
1:A:551:HIS:C	1:A:554:ARG:H	2.22	0.48
1:A:715:LEU:O	1:A:716:ALA:C	2.57	0.48
1:A:2150:ASN:O	1:A:2153:HIS:N	2.46	0.48
1:A:1631:ARG:CB	1:A:1648:SER:H	2.26	0.48
1:B:719:ALA:C	1:B:722:GLY:H	2.22	0.48
1:B:1634:LEU:O	1:B:1638:GLU:O	2.31	0.48
1:A:659:PRO:C	1:A:661:ASN:H	2.21	0.48
1:A:781:PHE:O	1:A:784:LEU:N	2.46	0.48
1:A:1270:ALA:HB2	1:A:1319:GLU:CB	2.44	0.48
1:B:118:GLY:C	1:B:163:ILE:H	2.21	0.48
1:B:233:ILE:CB	1:B:383:PRO:HA	2.44	0.48
1:A:117:TYR:C	1:A:172:ILE:HA	2.39	0.47
1:A:862:LEU:O	1:A:863:THR:C	2.55	0.47
1:A:1049:PRO:O	1:A:1053:ASP:N	2.43	0.47
1:A:225:LYS:H	1:A:228:ASP:CB	2.25	0.47
1:A:1332:ALA:O	1:A:1335:VAL:N	2.42	0.47
1:A:1417:GLU:O	1:A:1418:VAL:C	2.57	0.47
1:B:2015:GLY:O	1:B:2067:ALA:HB1	2.14	0.47
1:A:15:CYS:HA	1:A:222:LEU:CA	2.42	0.47
1:A:239:VAL:O	1:A:434:PRO:HA	2.14	0.47
1:A:480:LEU:O	1:A:481:VAL:C	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1061:LEU:O	1:B:1064:LEU:CB	2.63	0.47
1:B:2061:GLY:C	1:B:2064:ILE:H	2.19	0.47
1:A:391:ARG:HA	1:A:397:THR:C	2.39	0.47
1:A:1789:MET:N	1:B:1789:MET:N	2.62	0.47
1:A:2068:LEU:O	1:A:2072:ASP:HA	2.14	0.47
1:B:1457:ILE:C	1:B:1459:ARG:N	2.72	0.47
1:B:1649:GLY:O	1:B:1650:GLY:C	2.55	0.47
1:B:278:SER:O	1:B:279:LYS:C	2.58	0.47
1:A:598:LEU:O	1:A:599:LEU:C	2.57	0.47
1:A:1341:VAL:O	1:A:1345:TYR:N	2.44	0.47
1:A:2189:ALA:O	1:A:2190:LYS:C	2.58	0.47
1:B:365:SER:HA	1:B:394:CYS:CB	2.44	0.47
1:B:773:LEU:C	1:B:775:TYR:N	2.72	0.47
1:B:1459:ARG:C	1:B:1461:CYS:N	2.72	0.47
1:A:680:VAL:C	1:A:682:THR:H	2.21	0.47
1:A:1369:SER:C	1:A:1371:LEU:N	2.73	0.47
1:B:617:THR:O	1:B:621:LEU:CB	2.63	0.47
1:A:10:HIS:CB	1:A:112:GLY:HA2	2.45	0.47
1:B:315:ALA:CB	1:B:358:VAL:H	2.27	0.47
1:B:1813:ASN:O	1:B:1814:ALA:C	2.58	0.47
1:A:1980:ASN:HA	1:A:2038:SER:HA	1.97	0.47
1:B:15:CYS:CA	1:B:223:PHE:H	2.25	0.47
1:B:2184:ALA:O	1:B:2188:TYR:CB	2.62	0.47
1:A:149:VAL:CB	1:A:210:ASN:HA	2.45	0.46
1:A:576:LYS:O	1:A:578:PHE:N	2.48	0.46
1:A:761:VAL:O	1:A:762:ASP:C	2.56	0.46
1:B:125:HIS:O	1:B:127:LYS:N	2.48	0.46
1:B:1818:ARG:C	1:B:1820:PHE:N	2.72	0.46
1:B:1820:PHE:C	1:B:1822:GLU:N	2.69	0.46
1:B:690:GLY:O	1:B:691:GLU:C	2.58	0.46
1:A:869:LEU:O	1:A:873:LEU:CB	2.64	0.46
1:B:305:PHE:O	1:B:313:TYR:HA	2.16	0.46
1:A:16:SER:C	1:A:221:VAL:H	2.22	0.46
1:A:98:LEU:O	1:A:101:LYS:N	2.48	0.46
1:A:1680:GLU:C	1:A:1682:MET:N	2.71	0.46
1:B:299:TRP:H	1:B:380:SER:CB	2.28	0.46
1:B:620:SER:O	1:B:624:LYS:N	2.43	0.46
1:B:1053:ASP:O	1:B:1057:GLY:HA3	2.16	0.46
1:B:62:PRO:O	1:B:63:MET:C	2.58	0.46
1:B:1199:LYS:O	1:B:1200:GLN:C	2.58	0.46
1:B:1632:PRO:O	1:B:1634:LEU:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:ASP:O	1:A:219:LYS:HA	2.15	0.46
1:A:1973:GLN:O	1:A:1976:CYS:N	2.48	0.46
1:B:1236:LEU:O	1:B:1237:ALA:C	2.58	0.46
1:B:1632:PRO:O	1:B:1636:PHE:N	2.41	0.46
1:B:1840:HIS:O	1:B:1841:SER:C	2.58	0.46
1:B:2197:ILE:HA	1:B:2212:PRO:CA	2.46	0.46
1:A:68:ALA:O	1:A:72:PHE:CB	2.63	0.46
1:A:724:LYS:C	1:A:726:ASP:H	2.22	0.46
1:A:772:ASN:O	1:A:773:LEU:C	2.57	0.46
1:B:862:LEU:O	1:B:863:THR:C	2.59	0.46
1:B:1062:ARG:O	1:B:1063:VAL:C	2.59	0.46
1:B:1199:LYS:O	1:B:1202:GLN:N	2.47	0.46
1:A:2020:LEU:C	1:A:2024:ILE:H	2.16	0.46
1:A:979:GLN:O	1:A:982:LEU:N	2.49	0.46
1:A:1001:PHE:O	1:A:1003:GLU:N	2.44	0.46
1:A:1271:VAL:O	1:A:1275:HIS:N	2.46	0.46
1:B:117:TYR:CB	1:B:172:ILE:HA	2.46	0.46
1:A:708:ARG:O	1:A:709:SER:C	2.59	0.45
1:A:1245:CYS:CB	1:A:1285:SER:O	2.64	0.45
1:B:131:TYR:O	1:B:152:ASP:O	2.34	0.45
1:A:659:PRO:O	1:A:661:ASN:N	2.48	0.45
1:B:862:LEU:O	1:B:864:PHE:N	2.49	0.45
1:B:2147:SER:O	1:B:2151:VAL:CB	2.65	0.45
1:A:1966:GLN:O	1:A:1970:ARG:CB	2.63	0.45
1:B:594:THR:O	1:B:597:ALA:HB3	2.15	0.45
1:B:1843:PHE:O	1:B:1847:THR:N	2.45	0.45
1:A:1118:ASP:C	1:A:1122:LEU:H	2.11	0.45
1:A:1953:LYS:O	1:A:1954:ASP:C	2.59	0.45
1:B:444:ASP:O	1:B:447:ASN:N	2.49	0.45
1:B:1966:GLN:C	1:B:1970:ARG:H	2.25	0.45
1:A:616:ASP:O	1:A:620:SER:CB	2.65	0.45
1:B:11:ILE:O	1:B:13:ASP:N	2.50	0.45
1:B:356:VAL:O	1:B:358:VAL:N	2.50	0.45
1:A:580:PHE:O	1:A:581:MET:C	2.59	0.45
1:A:1207:ASN:C	1:A:1209:GLY:N	2.73	0.45
1:A:1954:ASP:O	1:A:1955:ASP:C	2.60	0.45
1:B:15:CYS:HA	1:B:223:PHE:N	2.25	0.45
1:B:183:VAL:O	1:B:185:ASN:N	2.44	0.45
1:B:1847:THR:O	1:B:1850:LYS:N	2.50	0.45
1:A:870:ALA:HA	1:A:873:LEU:CB	2.47	0.45
1:A:1118:ASP:O	1:A:1119:LEU:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1680:GLU:C	1:A:1682:MET:H	2.24	0.45
1:B:2211:VAL:O	1:B:2212:PRO:C	2.59	0.45
1:A:7:SER:CB	1:A:180:ASP:N	2.80	0.45
1:A:253:CYS:HA	1:A:263:PHE:N	2.31	0.45
1:A:716:ALA:O	1:A:718:ASP:N	2.50	0.45
1:B:313:TYR:O	1:B:357:SER:HA	2.17	0.45
1:B:986:LEU:C	1:B:988:TYR:N	2.75	0.45
1:A:16:SER:O	1:A:221:VAL:C	2.60	0.45
1:A:445:PHE:O	1:A:449:ALA:HB2	2.17	0.45
1:B:188:ASN:C	1:B:190:GLY:N	2.74	0.45
1:B:1976:CYS:O	1:B:1977:GLU:C	2.59	0.45
1:B:2151:VAL:C	1:B:2154:ASN:H	2.25	0.45
1:A:1295:PHE:C	1:A:1297:HIS:N	2.72	0.45
1:A:753:ASN:O	1:A:754:GLU:C	2.60	0.44
1:A:1197:SER:O	1:A:1200:GLN:N	2.50	0.44
1:B:279:LYS:CA	1:B:309:ALA:HB2	2.47	0.44
1:B:397:THR:CA	1:B:422:PRO:HA	2.47	0.44
1:B:648:THR:O	1:B:651:LEU:N	2.49	0.44
1:B:2202:ARG:CB	1:B:2206:GLN:HA	2.47	0.44
1:A:40:GLN:N	1:A:206:CYS:HA	2.31	0.44
1:A:1410:THR:C	1:A:1412:GLU:H	2.26	0.44
1:A:1952:ALA:C	1:A:1954:ASP:H	2.25	0.44
1:B:121:ILE:O	1:B:160:TRP:HA	2.17	0.44
1:A:1802:GLY:C	1:A:1804:SER:H	2.24	0.44
1:B:116:GLN:HA	1:B:175:SER:HA	1.99	0.44
1:A:370:LEU:HA	1:A:389:ARG:O	2.17	0.44
1:A:399:VAL:HA	1:A:420:THR:HA	2.00	0.44
1:A:838:GLU:O	1:A:840:VAL:N	2.50	0.44
1:A:2044:GLN:HA	1:A:2097:ALA:HB1	1.99	0.44
1:B:89:LEU:O	1:B:93:HIS:CB	2.65	0.44
1:B:185:ASN:O	1:B:186:PRO:C	2.60	0.44
1:B:421:SER:C	1:B:423:LEU:H	2.26	0.44
1:B:1211:HIS:O	1:B:1213:VAL:N	2.50	0.44
1:A:1682:MET:CA	1:A:1686:ARG:H	2.31	0.44
1:B:521:LYS:O	1:B:524:GLN:N	2.51	0.44
1:A:399:VAL:HA	1:A:421:SER:N	2.31	0.44
1:A:1094:LEU:O	1:A:1095:GLN:C	2.60	0.44
1:A:1476:LYS:HA	1:A:1884:LYS:CA	2.47	0.44
1:B:179:GLY:HA2	1:B:220:ILE:O	2.18	0.44
1:B:730:LEU:O	1:B:731:SER:C	2.59	0.44
1:A:1835:ASN:C	1:A:1837:THR:N	2.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:TRP:O	1:A:421:SER:CB	2.66	0.44
1:A:979:GLN:O	1:A:983:ASN:N	2.41	0.44
1:A:2060:ASN:O	1:A:2061:GLY:C	2.61	0.44
1:A:2126:LYS:O	1:A:2130:GLN:CB	2.66	0.44
1:B:692:ASP:O	1:B:693:GLU:C	2.60	0.44
1:B:1178:GLU:O	1:B:1182:ARG:CB	2.66	0.44
1:B:2120:LEU:O	1:B:2121:VAL:C	2.61	0.44
1:B:2186:GLU:O	1:B:2189:ALA:HB3	2.17	0.44
1:A:406:ILE:H	1:A:415:MET:C	2.26	0.44
1:A:701:ARG:C	1:A:703:SER:N	2.75	0.44
1:A:896:ASP:C	1:A:898:VAL:N	2.74	0.44
1:A:1795:GLN:HA	1:A:1798:LEU:CB	2.48	0.44
1:A:1849:ASP:O	1:A:1850:LYS:C	2.61	0.44
1:B:125:HIS:O	1:B:126:LEU:C	2.61	0.44
1:B:312:HIS:O	1:B:313:TYR:C	2.61	0.44
1:B:440:VAL:O	1:B:443:LEU:N	2.51	0.44
1:B:512:GLU:C	1:B:514:ASN:H	2.25	0.44
1:B:893:ALA:O	1:B:896:ASP:N	2.51	0.44
1:B:1252:GLN:O	1:B:1255:LEU:N	2.51	0.44
1:A:645:ILE:O	1:A:648:THR:N	2.51	0.43
1:B:358:VAL:O	1:B:359:PRO:C	2.59	0.43
1:B:1086:HIS:C	1:B:1088:SER:H	2.26	0.43
1:A:1420:ILE:O	1:A:1424:ASN:CB	2.67	0.43
1:B:450:SER:O	1:B:451:LYS:C	2.60	0.43
1:B:755:ILE:O	1:B:758:GLN:N	2.50	0.43
1:B:1880:ASP:C	1:B:1882:GLY:N	2.76	0.43
1:A:978:LEU:HA	1:A:981:ILE:CB	2.49	0.43
1:B:1289:GLU:O	1:B:1291:VAL:N	2.51	0.43
1:A:20:GLU:HA	1:A:24:ASN:HA	2.00	0.43
1:A:688:GLU:O	1:A:689:ALA:C	2.61	0.43
1:B:750:LEU:O	1:B:751:ALA:C	2.60	0.43
1:B:1682:MET:CA	1:B:1686:ARG:H	2.32	0.43
1:B:510:MET:O	1:B:511:ARG:C	2.62	0.43
1:B:572:GLU:O	1:B:574:ILE:N	2.52	0.43
1:B:1682:MET:CB	1:B:1687:GLY:N	2.82	0.43
1:A:7:SER:CB	1:A:179:GLY:H	2.31	0.43
1:A:1376:HIS:O	1:A:1380:LEU:CB	2.66	0.43
1:A:1410:THR:C	1:A:1412:GLU:N	2.75	0.43
1:A:1883:ASN:HA	1:A:1884:LYS:HA	1.75	0.43
1:B:402:THR:CB	1:B:418:ILE:HA	2.48	0.43
1:A:13:ASP:HA	1:A:226:TRP:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:850:GLN:O	1:A:851:ARG:C	2.61	0.43
1:A:1297:HIS:O	1:A:1298:CYS:C	2.60	0.43
1:A:1864:LYS:O	1:A:1865:VAL:C	2.62	0.43
1:B:308:LEU:O	1:B:309:ALA:C	2.62	0.43
1:B:670:LEU:HA	1:B:673:SER:CB	2.48	0.43
1:A:8:PHE:H	1:A:177:VAL:CA	2.31	0.43
1:B:860:ASN:O	1:B:863:THR:N	2.51	0.43
1:B:1849:ASP:O	1:B:1850:LYS:O	2.36	0.43
1:A:1477:TYR:HA	1:A:1881:LEU:O	2.19	0.43
1:A:85:ASP:HA	1:A:86:ALA:O	2.18	0.43
1:A:2150:ASN:C	1:A:2153:HIS:H	2.27	0.43
1:A:715:LEU:O	1:A:717:GLN:N	2.51	0.42
1:B:118:GLY:H	1:B:164:GLN:N	2.17	0.42
1:B:181:LYS:HA	1:B:218:TRP:O	2.19	0.42
1:B:572:GLU:C	1:B:574:ILE:H	2.27	0.42
1:B:992:CYS:C	1:B:994:LEU:N	2.76	0.42
1:A:11:ILE:O	1:A:112:GLY:N	2.52	0.42
1:A:101:LYS:O	1:A:104:GLU:N	2.49	0.42
1:A:1375:ILE:HA	1:A:1378:VAL:CB	2.49	0.42
1:A:2019:LEU:O	1:A:2020:LEU:C	2.62	0.42
1:B:45:ASP:O	1:B:48:ASN:C	2.63	0.42
1:B:133:THR:O	1:B:149:VAL:HA	2.19	0.42
1:B:854:PHE:O	1:B:855:SER:C	2.63	0.42
1:B:134:VAL:HA	1:B:149:VAL:CB	2.49	0.42
1:B:315:ALA:CA	1:B:366:SER:HA	2.39	0.42
1:B:393:LEU:C	1:B:396:ASN:H	2.26	0.42
1:B:1080:LEU:O	1:B:1084:PHE:N	2.35	0.42
1:B:2042:TYR:C	1:B:2044:GLN:H	2.27	0.42
1:A:354:SER:CA	1:A:419:GLY:HA3	2.40	0.42
1:A:519:ILE:O	1:A:520:PHE:C	2.61	0.42
1:A:683:GLY:O	1:A:684:GLU:C	2.60	0.42
1:A:982:LEU:O	1:A:986:LEU:N	2.36	0.42
1:B:622:VAL:O	1:B:626:ARG:HA	2.20	0.42
1:B:781:PHE:O	1:B:784:LEU:N	2.51	0.42
1:A:117:TYR:C	1:A:119:ASN:H	2.28	0.42
1:B:421:SER:C	1:B:423:LEU:N	2.78	0.42
1:B:1880:ASP:O	1:B:1882:GLY:N	2.44	0.42
1:A:19:ALA:HA	1:A:218:TRP:HA	2.02	0.42
1:A:92:LEU:O	1:A:95:ALA:HB3	2.19	0.42
1:A:252:THR:N	1:A:263:PHE:O	2.52	0.42
1:A:355:LEU:N	1:A:418:ILE:O	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:772:ASN:C	1:A:774:PRO:N	2.76	0.42
1:A:789:HIS:O	1:A:791:ASP:N	2.52	0.42
1:A:1270:ALA:O	1:A:1272:THR:N	2.48	0.42
1:A:2183:GLU:HA	1:A:2186:GLU:CB	2.50	0.42
1:B:685:ASN:O	1:B:686:ALA:C	2.62	0.42
1:A:125:HIS:O	1:A:126:LEU:C	2.63	0.42
1:A:854:PHE:C	1:A:856:ASP:N	2.76	0.42
1:A:157:GLU:C	1:A:159:SER:N	2.75	0.42
1:A:666:ILE:N	1:A:667:GLU:CA	2.80	0.42
1:A:1637:PRO:C	1:A:1639:ASN:H	2.27	0.42
1:B:694:GLU:O	1:B:695:GLU:C	2.62	0.42
1:A:648:THR:O	1:A:651:LEU:N	2.53	0.41
1:A:1377:LEU:C	1:A:1381:LEU:H	2.27	0.41
1:A:1793:GLU:HA	1:A:1796:CYS:CB	2.50	0.41
1:A:2116:ARG:O	1:A:2117:PRO:C	2.62	0.41
1:B:250:PHE:O	1:B:264:LEU:HA	2.20	0.41
1:B:1638:GLU:O	1:B:1639:ASN:C	2.63	0.41
1:A:191:GLN:CB	1:A:212:VAL:HA	2.50	0.41
1:A:1095:GLN:O	1:A:1096:ALA:C	2.63	0.41
1:A:1973:GLN:O	1:A:1974:LEU:C	2.64	0.41
1:B:263:PHE:CB	1:B:416:LEU:O	2.68	0.41
1:A:18:TYR:O	1:A:218:TRP:HA	2.21	0.41
1:A:1381:LEU:HA	1:A:1384:CYS:CB	2.50	0.41
1:A:2123:VAL:O	1:A:2127:ALA:CB	2.64	0.41
1:B:1093:VAL:O	1:B:1096:ALA:HB3	2.20	0.41
1:B:2111:ILE:C	1:B:2113:TYR:N	2.78	0.41
1:A:997:PHE:O	1:A:998:LYS:C	2.61	0.41
1:B:91:LYS:O	1:B:95:ALA:CB	2.66	0.41
1:B:1633:GLU:HA	1:B:1636:PHE:CB	2.50	0.41
1:B:2083:LEU:O	1:B:2084:VAL:C	2.62	0.41
1:A:645:ILE:O	1:A:646:PRO:C	2.64	0.41
1:B:756:SER:O	1:B:760:ASP:HA	2.20	0.41
1:B:1080:LEU:O	1:B:1083:LEU:CB	2.68	0.41
1:B:1197:SER:O	1:B:1198:ARG:C	2.63	0.41
1:B:1651:PHE:O	1:B:1652:ILE:C	2.64	0.41
1:A:166:PHE:N	1:A:182:VAL:HA	2.35	0.41
1:A:478:GLU:O	1:A:479:ASP:C	2.64	0.41
1:A:478:GLU:C	1:A:480:LEU:N	2.76	0.41
1:A:1274:GLN:O	1:A:1275:HIS:C	2.64	0.41
1:A:1836:THR:HA	1:A:1839:GLN:CB	2.50	0.41
1:A:2010:CYS:O	1:A:2011:GLY:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:GLN:C	1:B:117:TYR:O	2.64	0.41
1:B:253:CYS:O	1:B:279:LYS:CB	2.68	0.41
1:B:766:ARG:C	1:B:768:MET:N	2.79	0.41
1:A:724:LYS:C	1:A:726:ASP:N	2.79	0.41
1:A:1375:ILE:C	1:A:1378:VAL:H	2.28	0.41
1:B:251:LEU:HA	1:B:264:LEU:HA	2.03	0.41
1:B:2197:ILE:HA	1:B:2212:PRO:CB	2.51	0.41
1:A:86:ALA:O	1:A:88:LEU:N	2.54	0.41
1:A:861:LYS:O	1:A:864:PHE:N	2.54	0.41
1:A:1061:LEU:HA	1:A:1101:GLN:CB	2.50	0.41
1:A:1211:HIS:O	1:A:1215:LEU:CB	2.68	0.41
1:B:1106:SER:O	1:B:1107:GLN:CB	2.69	0.41
1:A:125:HIS:H	1:A:130:LYS:C	2.29	0.41
1:A:509:LEU:O	1:A:513:GLN:N	2.54	0.41
1:A:1986:PHE:O	1:A:1987:LEU:C	2.63	0.41
1:B:449:ALA:O	1:B:450:SER:C	2.63	0.41
1:B:675:PHE:O	1:B:679:GLY:HA3	2.21	0.41
1:B:853:PRO:O	1:B:854:PHE:C	2.64	0.41
1:B:992:CYS:C	1:B:994:LEU:H	2.29	0.41
1:B:1387:GLY:C	1:B:1389:ASN:H	2.28	0.41
1:B:1630:HIS:O	1:B:1631:ARG:C	2.63	0.41
1:A:574:ILE:O	1:A:575:ALA:C	2.62	0.41
1:A:1245:CYS:CB	1:A:1341:VAL:H	2.34	0.41
1:B:157:GLU:C	1:B:159:SER:N	2.75	0.41
1:B:438:ALA:O	1:B:439:GLU:C	2.61	0.41
1:B:620:SER:O	1:B:621:LEU:C	2.63	0.41
1:B:706:GLU:O	1:B:708:ARG:N	2.44	0.41
1:B:1488:THR:O	1:B:1489:PHE:C	2.63	0.41
1:B:1833:GLY:C	1:B:1835:ASN:H	2.29	0.41
1:A:368:PHE:HA	1:A:392:HIS:HA	2.04	0.40
1:B:1657:LYS:O	1:B:1660:LYS:N	2.44	0.40
1:B:1678:LEU:HA	1:B:1827:ALA:HA	2.02	0.40
1:B:2088:LYS:O	1:B:2089:ASN:C	2.64	0.40
1:A:243:PHE:O	1:A:430:PHE:CB	2.69	0.40
1:A:680:VAL:C	1:A:682:THR:N	2.79	0.40
1:B:24:ASN:O	1:B:41:PRO:HA	2.22	0.40
1:B:689:ALA:O	1:B:690:GLY:C	2.63	0.40
1:B:740:PHE:O	1:B:742:ARG:N	2.55	0.40
1:B:1214:VAL:O	1:B:1217:LEU:N	2.55	0.40
1:B:1665:GLU:C	1:B:1667:GLU:N	2.74	0.40
1:B:1824:ILE:O	1:B:1827:ALA:HB3	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:LEU:CA	1:A:264:LEU:HA	2.42	0.40
1:A:255:GLU:HA	1:A:261:HIS:H	1.86	0.40
1:A:406:ILE:N	1:A:415:MET:O	2.55	0.40
1:B:888:THR:C	1:B:891:LEU:H	2.29	0.40
1:B:1682:MET:CB	1:B:1686:ARG:H	2.34	0.40
1:B:1813:ASN:C	1:B:1818:ARG:CB	2.95	0.40
1:A:100:LYS:O	1:A:103:ASN:CB	2.70	0.40
1:A:764:ILE:O	1:A:765:LEU:C	2.64	0.40
1:A:1134:TYR:O	1:A:1230:MET:N	2.52	0.40
1:B:1082:LEU:O	1:B:1083:LEU:C	2.64	0.40
1:B:1448:LYS:C	1:B:1450:PHE:N	2.78	0.40
1:A:17:LEU:CB	1:A:220:ILE:HA	2.52	0.40
1:A:874:ILE:O	1:A:877:GLY:C	2.64	0.40
1:A:1998:LEU:C	1:A:2000:CYS:N	2.79	0.40
1:B:161:PHE:O	1:B:162:TYR:C	2.63	0.40
1:B:1115:ILE:C	1:B:1117:GLN:N	2.78	0.40
1:B:1818:ARG:O	1:B:1819:VAL:C	2.65	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	1682/2217 (76%)	1265 (75%)	296 (18%)	121 (7%)	1	11
1	B	1680/2217 (76%)	1193 (71%)	337 (20%)	150 (9%)	0	8
All	All	3362/4434 (76%)	2458 (73%)	633 (19%)	271 (8%)	1	9

All (271) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	86	ALA

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Mol	Chain	Res	Type
1	A	87	VAL
1	A	213	ASN
1	A	222	LEU
1	A	226	TRP
1	A	255	GLU
1	A	266	THR
1	A	478	GLU
1	A	479	ASP
1	A	502	PRO
1	A	522	LEU
1	A	598	LEU
1	A	628	PRO
1	A	659	PRO
1	A	666	ILE
1	A	681	SER
1	A	744	CYS
1	A	899	HIS
1	A	990	ILE
1	A	1239	GLU
1	A	1264	ASN
1	A	1370	PRO
1	A	1400	LEU
1	A	1637	PRO
1	A	1849	ASP
1	A	1864	LYS
1	A	1885	LYS
1	A	1966	GLN
1	A	1993	LYS
1	A	2013	THR
1	A	2046	PRO
1	A	2071	ASN
1	A	2104	ASP
1	A	2143	ASP
1	A	2178	GLN
1	A	2210	PRO
1	B	38	VAL
1	B	113	THR
1	B	164	GLN
1	B	165	PRO
1	B	223	PHE
1	B	293	ARG
1	B	300	ASN

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Mol	Chain	Res	Type
1	B	357	SER
1	B	405	PRO
1	B	513	GLN
1	B	628	PRO
1	B	659	PRO
1	B	666	ILE
1	B	681	SER
1	B	696	VAL
1	B	741	ALA
1	B	744	CYS
1	B	760	ASP
1	B	773	LEU
1	B	774	PRO
1	B	854	PHE
1	B	990	ILE
1	B	999	ARG
1	B	1008	SER
1	B	1095	GLN
1	B	1096	ALA
1	B	1107	GLN
1	B	1214	VAL
1	B	1220	ILE
1	B	1285	SER
1	B	1292	VAL
1	B	1300	GLU
1	B	1311	PHE
1	B	1400	LEU
1	B	1458	CYS
1	B	1462	ASN
1	B	1463	ASN
1	B	1492	SER
1	B	1637	PRO
1	B	1814	ALA
1	B	1966	GLN
1	B	1967	PRO
1	B	1984	GLN
1	B	2046	PRO
1	B	2075	PRO
1	B	2117	PRO
1	B	2129	MET
1	B	2210	PRO
1	A	52	LYS

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Mol	Chain	Res	Type
1	A	175	SER
1	A	177	VAL
1	A	564	GLN
1	A	600	HIS
1	A	684	GLU
1	A	716	ALA
1	A	717	GLN
1	A	725	GLU
1	A	740	PHE
1	A	854	PHE
1	A	1027	ALA
1	A	1095	GLN
1	A	1267	ILE
1	A	1288	ASN
1	A	1346	ASN
1	A	1347	ASP
1	A	1349	ALA
1	A	1372	MET
1	A	1435	VAL
1	A	1458	CYS
1	A	1461	CYS
1	A	1464	THR
1	A	1865	VAL
1	A	1881	LEU
1	A	1984	GLN
1	A	2011	GLY
1	A	2021	GLY
1	A	2115	MET
1	A	2146	ALA
1	A	2148	PRO
1	B	12	GLY
1	B	63	MET
1	B	75	ALA
1	B	118	GLY
1	B	135	ASN
1	B	221	VAL
1	B	307	HIS
1	B	313	TYR
1	B	380	SER
1	B	381	LEU
1	B	414	VAL
1	B	422	PRO

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Mol	Chain	Res	Type
1	B	423	LEU
1	B	450	SER
1	B	484	VAL
1	B	573	TYR
1	B	603	ARG
1	B	640	SER
1	B	665	LEU
1	B	767	CYS
1	B	790	VAL
1	B	849	CYS
1	B	893	ALA
1	B	1460	ALA
1	B	1461	CYS
1	B	1639	ASN
1	B	1797	HIS
1	B	1801	GLU
1	B	1817	ASP
1	B	1850	LYS
1	B	2146	ALA
1	A	100	LYS
1	A	227	SER
1	A	396	ASN
1	A	405	PRO
1	A	413	PRO
1	A	450	SER
1	A	604	LYS
1	A	1061	LEU
1	A	1086	HIS
1	A	1462	ASN
1	A	1630	HIS
1	A	1820	PHE
1	A	1953	LYS
1	A	2060	ASN
1	A	2165	HIS
1	B	66	TYR
1	B	114	VAL
1	B	126	LEU
1	B	264	LEU
1	B	379	ASP
1	B	434	PRO
1	B	514	ASN
1	B	521	LYS

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Mol	Chain	Res	Type
1	B	682	THR
1	B	686	ALA
1	B	707	ILE
1	B	722	GLY
1	B	776	ASP
1	B	993	LEU
1	B	1002	ASP
1	B	1116	LYS
1	B	1200	GLN
1	B	1241	LEU
1	B	1268	LEU
1	B	1388	LYS
1	B	1391	TYR
1	B	1821	HIS
1	B	2060	ASN
1	B	2085	LEU
1	B	2130	GLN
1	B	2165	HIS
1	B	2205	GLU
1	A	40	GLN
1	A	51	LYS
1	A	447	ASN
1	A	599	LEU
1	A	704	ASN
1	A	1096	ALA
1	A	1221	PRO
1	A	1299	ILE
1	A	1887	ASP
1	A	2202	ARG
1	B	41	PRO
1	B	279	LYS
1	B	684	GLU
1	B	694	GLU
1	B	699	PHE
1	B	778	ARG
1	B	887	LEU
1	B	968	MET
1	B	982	LEU
1	B	1198	ARG
1	B	1211	HIS
1	B	1290	ARG
1	B	1632	PRO

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Mol	Chain	Res	Type
1	B	1881	LEU
1	B	2070	LEU
1	A	602	ASN
1	A	645	ILE
1	A	790	VAL
1	A	852	PHE
1	A	895	LEU
1	A	897	CYS
1	A	1275	HIS
1	A	1463	ASN
1	A	2020	LEU
1	A	2190	LYS
1	A	2215	CYS
1	B	230	LYS
1	B	285	GLU
1	B	424	LYS
1	B	439	GLU
1	B	473	VAL
1	B	522	LEU
1	B	703	SER
1	B	863	THR
1	B	1271	VAL
1	B	1996	TYR
1	B	2029	VAL
1	B	2147	SER
1	B	2207	ILE
1	B	2209	PHE
1	A	120	VAL
1	A	705	LYS
1	A	715	LEU
1	A	1369	SER
1	A	1466	ASP
1	A	1991	ASN
1	A	2147	SER
1	B	418	ILE
1	B	680	VAL
1	B	1466	ASP
1	B	1651	PHE
1	A	38	VAL
1	A	178	ILE
1	A	383	PRO
1	B	191	GLN

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Mol	Chain	Res	Type
1	B	367	ILE
1	B	1299	ILE
1	A	559	VAL
1	A	707	ILE
1	A	1874	VAL
1	A	2062	ILE
1	B	1291	VAL
1	B	1341	VAL
1	B	1370	PRO
1	A	1418	VAL
1	B	179	GLY
1	B	1631	ARG
1	A	894	ILE
1	A	1838	ILE
1	A	1967	PRO
1	B	212	VAL
1	B	2045	GLY
1	B	186	PRO

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	1710/2217 (77%)	-0.13	78 (4%) 37 37	0, 157, 428, 888	0
1	B	1708/2217 (77%)	-0.08	97 (5%) 29 33	0, 136, 432, 776	0
All	All	3418/4434 (77%)	-0.11	175 (5%) 33 35	0, 147, 430, 888	0

All (175) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1429	CYS	11.3
1	B	1432	ASP	9.8
1	B	1428	HIS	7.8
1	B	2164	ARG	6.6
1	A	1888	ASP	6.2
1	B	1430	TYR	6.2
1	B	1414	CYS	6.0
1	B	1177	LYS	5.8
1	B	2163	ALA	5.2
1	A	1889	GLU	5.2
1	A	1489	PHE	4.7
1	B	66	TYR	4.6
1	A	1427	ASN	4.6
1	B	2206	GLN	4.4
1	B	2165	HIS	4.3
1	A	627	GLU	4.3
1	B	960	PRO	4.3
1	B	23	THR	4.3
1	B	1676	GLN	4.2
1	A	1384	CYS	4.2
1	B	589	VAL	4.2
1	A	2051	GLN	4.1
1	B	24	ASN	4.1
1	B	1051	ASP	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	1398	SER	4.0
1	A	1132	TRP	4.0
1	A	144	LYS	4.0
1	B	404	ILE	4.0
1	B	1413	ASP	4.0
1	B	302	LEU	3.9
1	A	2203	THR	3.9
1	A	693	GLU	3.9
1	B	1424	ASN	3.9
1	A	2050	ASN	3.8
1	A	752	ILE	3.8
1	B	1415	ILE	3.8
1	B	1416	PRO	3.8
1	B	1427	ASN	3.7
1	A	1466	ASP	3.7
1	B	2205	GLU	3.7
1	B	1621	GLU	3.7
1	B	1435	VAL	3.6
1	B	462	LYS	3.6
1	B	2215	CYS	3.6
1	A	724	LYS	3.6
1	B	403	ASN	3.5
1	B	1434	GLU	3.5
1	B	1197	SER	3.5
1	B	582	GLN	3.5
1	B	1654	LYS	3.4
1	B	1433	THR	3.3
1	B	303	PHE	3.3
1	A	1387	GLY	3.3
1	B	1425	PHE	3.3
1	B	588	ASP	3.3
1	A	1987	LEU	3.2
1	A	1386	GLU	3.2
1	A	626	ARG	3.2
1	A	2147	SER	3.2
1	B	1031	GLU	3.2
1	B	402	THR	3.2
1	A	1471	ASP	3.1
1	B	1431	VAL	3.1
1	A	47	ASN	3.1
1	B	149	VAL	3.0
1	B	1077	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	2158	LEU	3.0
1	A	2047	CYS	3.0
1	A	1637	PRO	3.0
1	A	1434	GLU	3.0
1	B	1677	THR	3.0
1	B	638	CYS	3.0
1	A	353	TYR	2.9
1	A	2104	ASP	2.9
1	B	2078	LYS	2.9
1	B	1439	GLU	2.9
1	A	2158	LEU	2.9
1	B	1192	ALA	2.9
1	A	1982	ASP	2.9
1	B	1627	ASP	2.8
1	B	368	PHE	2.8
1	B	405	PRO	2.8
1	B	1388	LYS	2.8
1	A	2157	ILE	2.8
1	A	1133	VAL	2.8
1	B	213	ASN	2.7
1	B	581	MET	2.7
1	A	143	GLU	2.7
1	B	369	GLU	2.7
1	B	584	GLN	2.7
1	B	2161	GLN	2.7
1	B	1369	SER	2.7
1	A	216	THR	2.7
1	A	188	ASN	2.7
1	B	1834	GLY	2.7
1	B	2159	ALA	2.7
1	A	1814	ALA	2.6
1	A	2106	GLU	2.6
1	B	747	ARG	2.6
1	B	37	CYS	2.6
1	B	1456	ASP	2.6
1	A	39	VAL	2.6
1	A	753	ASN	2.6
1	A	1264	ASN	2.6
1	A	2196	GLU	2.5
1	B	744	CYS	2.5
1	B	1385	THR	2.5
1	A	751	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	2103	HIS	2.5
1	A	2142	GLU	2.4
1	B	2121	VAL	2.4
1	A	1676	GLN	2.4
1	B	512	GLU	2.4
1	A	2105	SER	2.4
1	A	1279	ASN	2.4
1	B	1797	HIS	2.4
1	A	309	ALA	2.4
1	B	1829	ALA	2.4
1	B	1176	VAL	2.4
1	A	1376	HIS	2.4
1	A	305	PHE	2.3
1	B	295	GLY	2.3
1	B	1826	LEU	2.3
1	B	1828	ILE	2.3
1	A	1435	VAL	2.3
1	A	26	PHE	2.3
1	A	2098	ILE	2.3
1	A	37	CYS	2.2
1	A	1396	CYS	2.2
1	A	1441	TYR	2.2
1	B	2142	GLU	2.2
1	A	2053	CYS	2.2
1	A	1381	LEU	2.2
1	A	628	PRO	2.2
1	B	1438	LYS	2.2
1	A	1332	ALA	2.2
1	B	458	GLY	2.2
1	B	1436	GLU	2.2
1	B	2139	GLU	2.2
1	B	779	ALA	2.2
1	B	704	ASN	2.2
1	B	1805	ASN	2.2
1	A	1333	GLU	2.2
1	B	210	ASN	2.2
1	B	1453	PHE	2.2
1	B	2122	GLU	2.2
1	B	1452	ASN	2.1
1	A	1385	THR	2.1
1	B	1302	HIS	2.1
1	B	1827	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	52	LYS	2.1
1	A	362	ASN	2.1
1	A	31	GLY	2.1
1	A	689	ALA	2.1
1	B	1194	VAL	2.1
1	B	1406	VAL	2.1
1	A	1089	GLN	2.1
1	B	2143	ASP	2.1
1	A	744	CYS	2.1
1	A	1989	CYS	2.1
1	A	1983	LEU	2.1
1	B	1620	ALA	2.1
1	B	2170	GLN	2.1
1	A	632	ASP	2.0
1	B	2138	GLY	2.0
1	B	1412	GLU	2.0
1	B	1664	GLU	2.0
1	A	1636	PHE	2.0
1	A	1834	GLY	2.0
1	A	2108	ALA	2.0
1	A	312	HIS	2.0
1	A	195	ALA	2.0
1	A	1336	ASN	2.0
1	A	2154	ASN	2.0
1	B	1806	LEU	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.