



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:32 PM UTC

PDB ID : 4RID / pdb_00004rid
Title : Human FAN1 nuclease
Authors : Pavletich, N.P.; Wang, R.
Deposited on : 2014-10-05
Resolution : 3.30 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

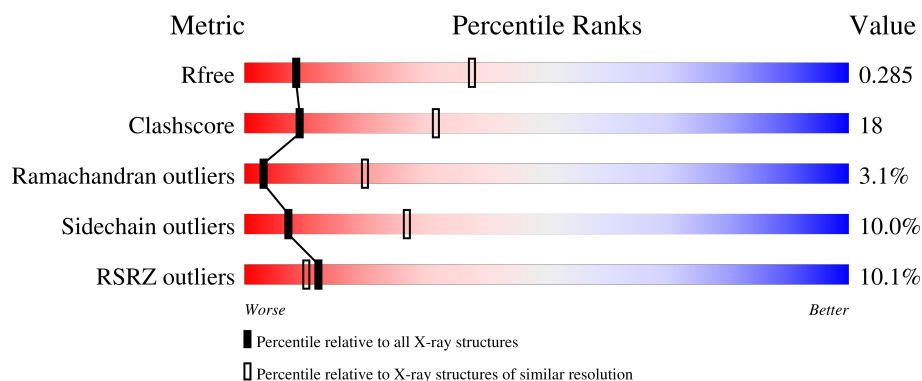
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	640	8% 62% 27% 6% • •
1	B	640	12% 65% 26% 7% • •

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 9981 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.

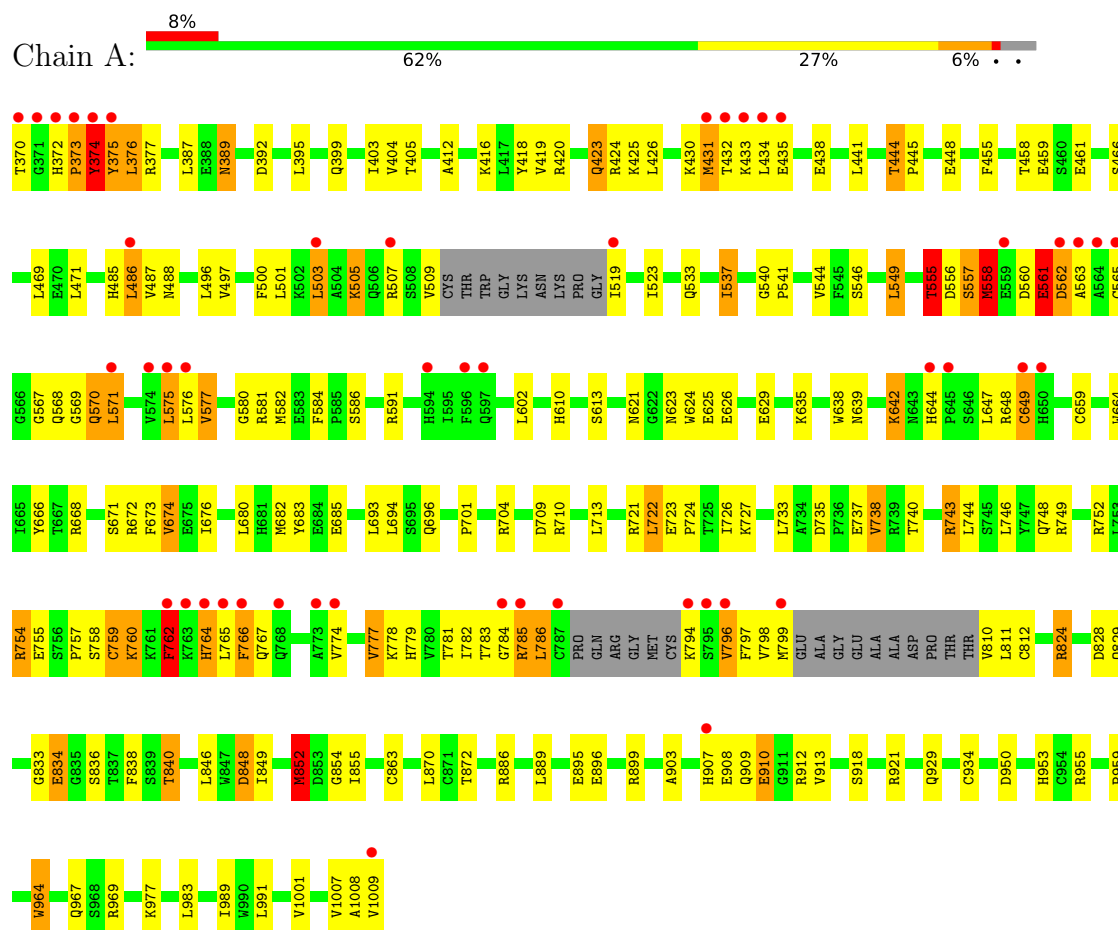
- Molecule 1 is a protein called Fanconi-associated nuclease 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	615	Total	C	N	O	S	0	0	0
			4944	3147	880	890	27			
1	B	628	Total	C	N	O	S	0	0	0
			5037	3201	897	912	27			

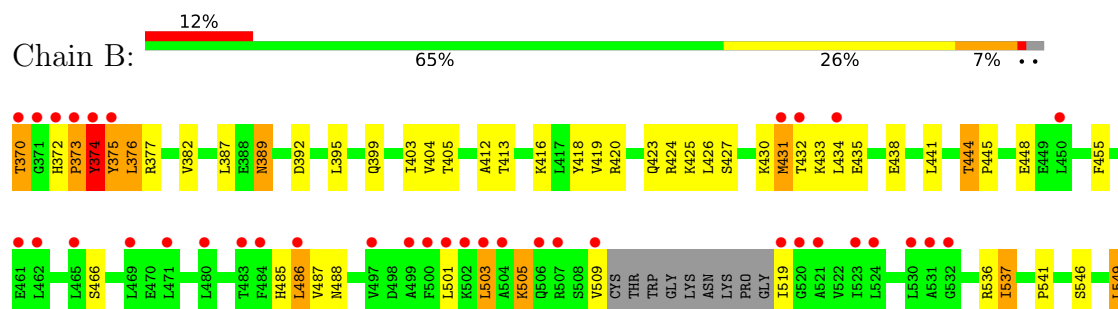
3 Residue-property plots [i](#)

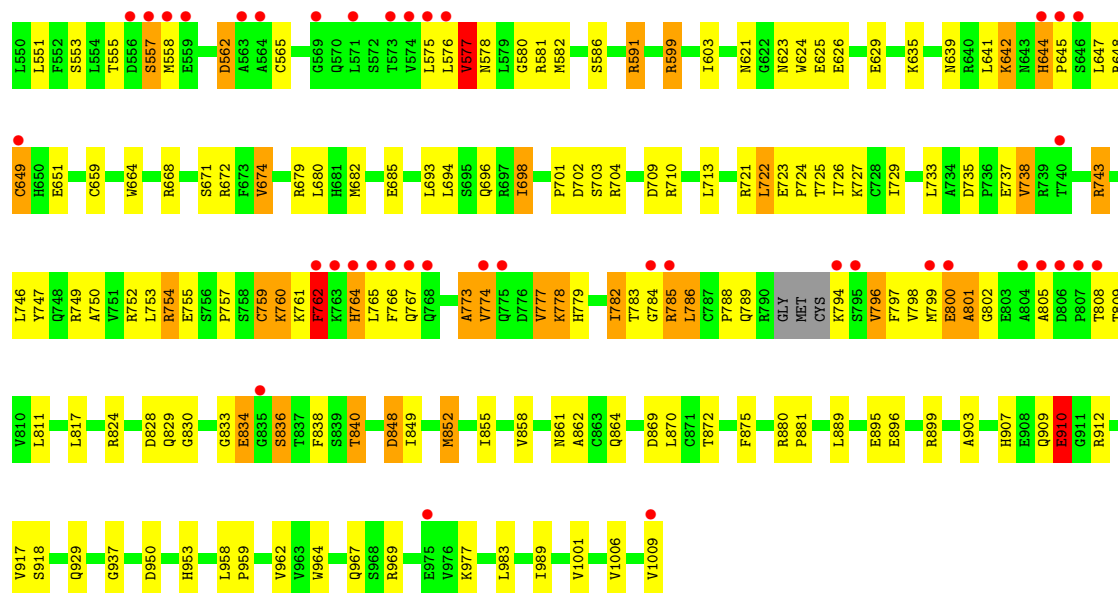
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Fanconi-associated nuclease 1



• Molecule 1: Fanconi-associated nuclease 1





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	146.88Å 156.88Å 205.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.30 30.00 – 3.30	Depositor EDS
% Data completeness (in resolution range)	96.0 (30.00-3.30) 95.9 (30.00-3.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.03 (at 3.07Å)	Xtrriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.246 , 0.288 0.246 , 0.285	Depositor DCC
R_{free} test set	1341 reflections (3.08%)	wwPDB-VP
Wilson B-factor (Å ²)	91.3	Xtrriage
Anisotropy	0.402	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 60.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9981	wwPDB-VP
Average B, all atoms (Å ²)	115.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 19.85 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.8977e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.60	0/5045	0.99	11/6818 (0.2%)
1	B	0.57	0/5141	0.99	11/6952 (0.2%)
All	All	0.59	0/10186	0.99	22/13770 (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	1

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	376	LEU	N-CA-C	9.17	121.04	111.14
1	A	376	LEU	N-CA-C	8.99	120.85	111.14
1	B	557	SER	N-CA-C	6.76	120.40	111.75
1	B	764	HIS	N-CA-C	6.17	120.53	113.19
1	B	698	ILE	N-CA-C	6.09	116.75	110.36
1	A	488	ASN	CA-C-N	6.02	126.18	119.32
1	A	488	ASN	C-N-CA	6.02	126.18	119.32
1	A	764	HIS	N-CA-C	5.61	119.87	113.19
1	B	789	GLN	N-CA-C	5.58	116.55	107.23
1	B	488	ASN	CA-C-N	5.54	125.63	119.32
1	B	488	ASN	C-N-CA	5.54	125.63	119.32
1	B	373	PRO	N-CA-C	5.42	118.81	111.22
1	A	1008	ALA	N-CA-C	5.37	118.68	110.20
1	A	854	GLY	CA-C-N	-5.27	119.01	122.60
1	A	854	GLY	C-N-CA	-5.27	119.01	122.60
1	B	964	TRP	N-CA-C	5.23	117.01	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	373	PRO	N-CA-C	5.22	118.80	111.33
1	A	964	TRP	N-CA-C	5.17	116.93	109.07
1	A	683	TYR	N-CA-C	5.13	116.95	111.36
1	A	562	ASP	N-CA-C	5.12	117.72	110.10
1	B	641	LEU	N-CA-C	5.10	119.58	112.90
1	B	836	SER	N-CA-C	5.02	116.75	111.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	766	PHE	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	4944	0	4981	204	0
1	B	5037	0	5065	192	0
All	All	9981	0	10046	366	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 18.

All (366) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:784:GLY:O	1:B:1009:VAL:HG21	1.36	1.26
1:A:784:GLY:O	1:A:1009:VAL:HG21	1.47	1.15
1:B:785:ARG:HB2	1:B:798:VAL:HB	1.28	1.15
1:B:553:SER:HB2	1:B:557:SER:HB2	1.30	1.11
1:A:785:ARG:HB2	1:A:798:VAL:HB	1.27	1.08
1:A:907:HIS:HB3	1:B:374:TYR:H	1.20	1.03
1:B:723:GLU:HB3	1:B:724:PRO:HD3	1.36	1.02
1:A:748:GLN:NE2	1:A:774:VAL:HG21	1.76	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:374:TYR:CE1	1:B:576:LEU:HD23	1.96	1.01
1:B:765:LEU:C	1:B:767:GLN:H	1.69	0.99
1:A:723:GLU:HB3	1:A:724:PRO:HD3	1.47	0.96
1:A:765:LEU:C	1:A:767:GLN:H	1.72	0.95
1:B:786:LEU:HB3	1:B:1009:VAL:HB	1.49	0.93
1:B:785:ARG:HA	1:B:1009:VAL:HG11	1.52	0.92
1:B:836:SER:O	1:B:840:THR:HG23	1.69	0.91
1:A:744:LEU:HD11	1:A:774:VAL:CG2	2.02	0.90
1:B:704:ARG:NH1	1:B:735:ASP:OD2	2.05	0.90
1:A:374:TYR:CE1	1:A:576:LEU:HD23	2.07	0.90
1:A:704:ARG:NH1	1:A:735:ASP:OD2	2.05	0.89
1:A:748:GLN:HE21	1:A:774:VAL:HG21	1.36	0.89
1:A:786:LEU:HB3	1:A:1009:VAL:HB	1.55	0.88
1:A:836:SER:O	1:A:840:THR:HG23	1.74	0.86
1:A:909:GLN:HE22	1:B:370:THR:HA	1.40	0.85
1:A:744:LEU:HD11	1:A:774:VAL:HG22	1.59	0.85
1:A:558:MET:HG3	1:A:563:ALA:H	1.41	0.84
1:B:773:ALA:O	1:B:774:VAL:HG23	1.78	0.84
1:A:389:ASN:HD22	1:A:392:ASP:H	1.24	0.83
1:B:389:ASN:HD22	1:B:392:ASP:H	1.26	0.83
1:A:810:VAL:N	1:B:805:ALA:HA	1.94	0.82
1:B:375:TYR:HB2	1:B:419:VAL:CG1	2.10	0.82
1:A:785:ARG:HA	1:A:1009:VAL:HG11	1.62	0.81
1:A:785:ARG:CB	1:A:798:VAL:HB	2.10	0.81
1:B:377:ARG:HD3	1:B:580:GLY:HA3	1.62	0.81
1:B:784:GLY:O	1:B:1009:VAL:CG2	2.25	0.81
1:A:375:TYR:HB2	1:A:419:VAL:CG1	2.10	0.80
1:B:765:LEU:C	1:B:767:GLN:N	2.38	0.80
1:B:555:THR:HG21	1:B:861:ASN:OD1	1.82	0.80
1:B:784:GLY:C	1:B:1009:VAL:HG21	2.06	0.80
1:B:785:ARG:CB	1:B:798:VAL:HB	2.11	0.79
1:A:426:LEU:HD13	1:A:537:ILE:HG22	1.65	0.79
1:B:786:LEU:CB	1:B:1009:VAL:HB	2.12	0.79
1:A:786:LEU:H	1:A:1009:VAL:CG1	1.95	0.79
1:A:625:GLU:O	1:A:629:GLU:HG2	1.82	0.78
1:A:786:LEU:CB	1:A:1009:VAL:HB	2.13	0.78
1:A:374:TYR:H	1:B:907:HIS:HB3	1.49	0.78
1:A:785:ARG:O	1:A:798:VAL:HG23	1.86	0.76
1:A:556:ASP:HB2	1:A:863:CYS:O	1.87	0.75
1:B:403:ILE:HG21	1:B:541:PRO:HB3	1.67	0.75
1:B:785:ARG:O	1:B:798:VAL:HG23	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:403:ILE:CG2	1:B:541:PRO:HB3	2.17	0.74
1:A:810:VAL:N	1:B:805:ALA:CB	2.51	0.74
1:A:568:GLN:CD	1:A:610:HIS:HB3	2.13	0.73
1:B:786:LEU:H	1:B:1009:VAL:CG1	2.01	0.73
1:B:375:TYR:HB2	1:B:419:VAL:HG12	1.71	0.73
1:A:765:LEU:C	1:A:767:GLN:N	2.40	0.71
1:A:784:GLY:C	1:A:1009:VAL:HG21	2.15	0.71
1:A:377:ARG:HD3	1:A:580:GLY:HA3	1.70	0.71
1:A:907:HIS:HB3	1:B:374:TYR:N	2.01	0.71
1:A:810:VAL:N	1:B:805:ALA:CA	2.53	0.70
1:B:625:GLU:O	1:B:629:GLU:HG2	1.90	0.70
1:A:375:TYR:HB2	1:A:419:VAL:HG12	1.74	0.70
1:A:912:ARG:HG2	1:B:581:ARG:HH22	1.55	0.70
1:A:759:CYS:HG	1:A:762:PHE:HE1	1.36	0.70
1:B:785:ARG:CA	1:B:1009:VAL:HG11	2.21	0.69
1:A:777:VAL:O	1:A:779:HIS:HD2	1.77	0.68
1:A:784:GLY:O	1:A:1009:VAL:CG2	2.34	0.68
1:B:765:LEU:HA	1:B:767:GLN:HG3	1.76	0.68
1:A:389:ASN:ND2	1:A:392:ASP:H	1.92	0.67
1:A:785:ARG:CA	1:A:1009:VAL:HG11	2.24	0.67
1:A:810:VAL:N	1:B:805:ALA:HB1	2.09	0.67
1:B:849:ILE:O	1:B:852:MET:HB2	1.95	0.67
1:A:375:TYR:HB2	1:A:419:VAL:HG11	1.75	0.66
1:B:849:ILE:HG23	1:B:852:MET:CE	2.25	0.66
1:B:553:SER:HB2	1:B:557:SER:CB	2.18	0.66
1:B:800:GLU:O	1:B:801:ALA:CB	2.42	0.66
1:A:786:LEU:H	1:A:1009:VAL:HG11	1.61	0.66
1:A:765:LEU:HA	1:A:767:GLN:HG3	1.77	0.66
1:B:555:THR:HB	1:B:864:GLN:HG2	1.78	0.66
1:A:565:CYS:O	1:A:613:SER:HB2	1.94	0.66
1:A:797:PHE:O	1:A:811:LEU:HA	1.96	0.66
1:A:375:TYR:HA	1:A:576:LEU:HD21	1.78	0.66
1:A:694:LEU:O	1:A:704:ARG:NH2	2.29	0.65
1:A:833:GLY:O	1:A:834:GLU:HB2	1.96	0.65
1:B:373:PRO:O	1:B:376:LEU:N	2.30	0.65
1:B:762:PHE:CD1	1:B:764:HIS:HB2	2.32	0.64
1:B:800:GLU:O	1:B:801:ALA:HB3	1.98	0.64
1:A:912:ARG:HG2	1:B:581:ARG:NH2	2.13	0.64
1:A:909:GLN:NE2	1:B:370:THR:HA	2.10	0.64
1:A:701:PRO:O	1:A:704:ARG:HG3	1.97	0.64
1:B:777:VAL:O	1:B:779:HIS:HD2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:375:TYR:HB2	1:B:419:VAL:HG11	1.78	0.63
1:B:701:PRO:O	1:B:704:ARG:HG3	1.98	0.63
1:A:777:VAL:HG11	1:A:1001:VAL:HG23	1.81	0.63
1:A:370:THR:HB	1:B:586:SER:OG	1.99	0.62
1:A:908:GLU:HG2	1:B:373:PRO:N	2.14	0.62
1:A:849:ILE:O	1:A:852:MET:HB2	1.99	0.62
1:B:749:ARG:HG3	1:B:752:ARG:HH12	1.63	0.62
1:A:373:PRO:O	1:A:376:LEU:N	2.33	0.62
1:B:659:CYS:HA	1:B:664:TRP:CD2	2.34	0.62
1:B:389:ASN:ND2	1:B:392:ASP:H	1.95	0.61
1:B:797:PHE:O	1:B:811:LEU:HA	2.00	0.61
1:A:430:LYS:HE3	1:A:471:LEU:O	2.00	0.61
1:A:509:VAL:C	1:A:519:ILE:N	2.58	0.61
1:A:762:PHE:CD1	1:A:764:HIS:HB2	2.35	0.61
1:A:423:GLN:HE22	1:A:576:LEU:HD22	1.65	0.61
1:A:431:MET:HA	1:A:434:LEU:HD12	1.82	0.61
1:B:796:VAL:HG12	1:B:811:LEU:HB3	1.82	0.61
1:B:694:LEU:O	1:B:704:ARG:NH2	2.34	0.60
1:B:735:ASP:OD1	1:B:737:GLU:HB2	2.00	0.60
1:A:799:MET:HG3	1:A:799:MET:O	2.01	0.60
1:B:430:LYS:O	1:B:434:LEU:HG	2.02	0.60
1:A:581:ARG:HH22	1:B:912:ARG:HG2	1.65	0.60
1:A:749:ARG:HG3	1:A:752:ARG:HH12	1.67	0.59
1:B:395:LEU:O	1:B:599:ARG:HG3	2.03	0.59
1:A:586:SER:HG	1:B:370:THR:N	2.00	0.59
1:A:762:PHE:C	1:A:762:PHE:CD2	2.80	0.59
1:B:786:LEU:H	1:B:1009:VAL:HG11	1.67	0.59
1:A:373:PRO:HD3	1:A:416:LYS:HE2	1.84	0.58
1:B:431:MET:HA	1:B:434:LEU:HD12	1.85	0.58
1:A:849:ILE:HG23	1:A:852:MET:CE	2.33	0.58
1:B:659:CYS:HA	1:B:664:TRP:CG	2.38	0.58
1:B:762:PHE:C	1:B:762:PHE:CD2	2.80	0.58
1:B:671:SER:O	1:B:674:VAL:HG13	2.04	0.58
1:B:833:GLY:O	1:B:834:GLU:HB2	2.04	0.58
1:A:444:THR:N	1:A:445:PRO:HD2	2.18	0.58
1:A:723:GLU:HB3	1:A:724:PRO:CD	2.29	0.58
1:B:418:TYR:CE1	1:B:455:PHE:HB3	2.39	0.57
1:B:903:ALA:HB2	1:B:929:GLN:NE2	2.19	0.57
1:A:430:LYS:O	1:A:434:LEU:HG	2.03	0.57
1:A:895:GLU:O	1:A:899:ARG:HG3	2.04	0.57
1:B:635:LYS:HE3	1:B:639:ASN:HD21	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:GLN:HE22	1:A:403:ILE:HD11	1.69	0.56
1:B:785:ARG:O	1:B:798:VAL:N	2.38	0.56
1:A:635:LYS:HE3	1:A:639:ASN:HD21	1.71	0.56
1:B:723:GLU:HB3	1:B:724:PRO:CD	2.20	0.56
1:A:840:THR:CG2	1:A:918:SER:H	2.17	0.56
1:B:373:PRO:HD3	1:B:416:LYS:HE2	1.87	0.56
1:A:671:SER:O	1:A:674:VAL:HG13	2.05	0.56
1:A:903:ALA:HB2	1:A:929:GLN:NE2	2.21	0.56
1:A:757:PRO:C	1:A:759:CYS:H	2.14	0.55
1:B:374:TYR:CE1	1:B:576:LEU:CD2	2.82	0.55
1:B:759:CYS:HG	1:B:762:PHE:HE1	1.53	0.55
1:A:403:ILE:CG2	1:A:541:PRO:HB3	2.36	0.55
1:A:738:VAL:O	1:A:743:ARG:NH1	2.39	0.55
1:A:458:THR:HG22	1:A:459:GLU:H	1.72	0.55
1:B:773:ALA:O	1:B:774:VAL:CG2	2.53	0.55
1:A:759:CYS:SG	1:A:762:PHE:CE1	2.99	0.55
1:A:387:LEU:HD11	1:A:404:VAL:HG11	1.88	0.55
1:A:693:LEU:O	1:A:696:GLN:HG3	2.07	0.55
1:A:659:CYS:HA	1:A:664:TRP:CD2	2.41	0.55
1:A:430:LYS:HB2	1:A:433:LYS:CG	2.37	0.55
1:A:659:CYS:HA	1:A:664:TRP:CG	2.42	0.55
1:A:639:ASN:HA	1:A:642:LYS:HE2	1.88	0.55
1:B:765:LEU:O	1:B:767:GLN:N	2.35	0.55
1:B:444:THR:N	1:B:445:PRO:HD2	2.22	0.54
1:A:735:ASP:OD1	1:A:737:GLU:HB2	2.07	0.54
1:A:748:GLN:HE21	1:A:774:VAL:CG2	2.15	0.54
1:B:639:ASN:HA	1:B:642:LYS:HE2	1.90	0.54
1:A:624:TRP:HB2	1:A:680:LEU:HD21	1.89	0.54
1:B:799:MET:O	1:B:799:MET:HG3	2.08	0.54
1:B:796:VAL:CG1	1:B:811:LEU:HB3	2.38	0.54
1:A:765:LEU:CA	1:A:767:GLN:HG3	2.38	0.54
1:B:840:THR:CG2	1:B:918:SER:H	2.21	0.54
1:B:765:LEU:CA	1:B:767:GLN:HG3	2.37	0.53
1:B:430:LYS:HB2	1:B:433:LYS:CG	2.38	0.53
1:B:777:VAL:HG11	1:B:1001:VAL:HG23	1.89	0.53
1:A:786:LEU:N	1:A:1009:VAL:HG11	2.24	0.53
1:B:773:ALA:C	1:B:774:VAL:HG23	2.33	0.53
1:B:509:VAL:C	1:B:519:ILE:N	2.67	0.53
1:A:668:ARG:O	1:A:672:ARG:HG2	2.08	0.53
1:B:581:ARG:HD2	1:B:581:ARG:N	2.22	0.52
1:A:777:VAL:O	1:A:779:HIS:CD2	2.61	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:668:ARG:O	1:B:672:ARG:HG2	2.09	0.52
1:A:403:ILE:HG21	1:A:541:PRO:HB3	1.90	0.52
1:A:431:MET:HE2	1:A:533:GLN:OE1	2.09	0.52
1:A:740:THR:HG21	1:A:953:HIS:O	2.10	0.52
1:B:693:LEU:O	1:B:696:GLN:HG3	2.10	0.52
1:B:764:HIS:O	1:B:765:LEU:HG	2.10	0.52
1:A:372:HIS:O	1:A:377:ARG:HG2	2.11	0.51
1:A:785:ARG:O	1:A:798:VAL:N	2.44	0.51
1:A:848:ASP:N	1:A:848:ASP:OD1	2.44	0.51
1:A:642:LYS:HA	1:A:647:LEU:HD12	1.92	0.51
1:B:374:TYR:HE1	1:B:576:LEU:HD23	1.66	0.51
1:A:581:ARG:HD2	1:A:581:ARG:N	2.25	0.51
1:B:725:THR:O	1:B:729:ILE:HG13	2.10	0.51
1:A:431:MET:HA	1:A:434:LEU:HB2	1.92	0.51
1:A:562:ASP:HB3	1:A:668:ARG:NH1	2.26	0.51
1:A:726:ILE:O	1:A:727:LYS:C	2.52	0.51
1:B:624:TRP:HB2	1:B:680:LEU:HD21	1.91	0.51
1:B:855:ILE:HD12	1:B:855:ILE:N	2.26	0.51
1:B:828:ASP:OD2	1:B:829:GLN:HG2	2.11	0.50
1:A:370:THR:N	1:B:909:GLN:HE22	2.09	0.50
1:A:412:ALA:O	1:A:416:LYS:HG3	2.12	0.50
1:B:762:PHE:C	1:B:762:PHE:HD2	2.20	0.50
1:A:765:LEU:O	1:A:767:GLN:N	2.37	0.50
1:A:561:GLU:HB2	1:A:955:ARG:HH22	1.77	0.50
1:A:762:PHE:C	1:A:762:PHE:HD2	2.19	0.50
1:B:576:LEU:O	1:B:577:VAL:C	2.55	0.50
1:B:423:GLN:HE22	1:B:576:LEU:HD22	1.77	0.50
1:B:426:LEU:HD13	1:B:537:ILE:HG22	1.94	0.50
1:A:556:ASP:O	1:A:557:SER:C	2.55	0.49
1:B:387:LEU:HD11	1:B:404:VAL:HG11	1.94	0.49
1:A:486:LEU:HD13	1:A:503:LEU:HD21	1.94	0.49
1:A:722:LEU:O	1:A:723:GLU:C	2.56	0.49
1:A:581:ARG:HE	1:B:910:GLU:C	2.16	0.49
1:B:651:GLU:HG2	1:B:698:ILE:HG21	1.94	0.49
1:B:412:ALA:O	1:B:416:LYS:HG3	2.13	0.49
1:A:505:LYS:C	1:A:505:LYS:HE2	2.38	0.49
1:A:373:PRO:O	1:A:374:TYR:C	2.56	0.49
1:A:950:ASP:OD1	1:A:953:HIS:HD2	1.96	0.48
1:B:621:ASN:HB2	1:B:623:ASN:ND2	2.28	0.48
1:B:757:PRO:C	1:B:759:CYS:H	2.20	0.48
1:A:912:ARG:NH2	1:B:377:ARG:HH22	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:486:LEU:HD13	1:B:503:LEU:HD21	1.96	0.48
1:A:833:GLY:HA2	1:A:921:ARG:NH1	2.28	0.48
1:A:485:HIS:H	1:A:485:HIS:CD2	2.31	0.48
1:A:838:PHE:HE2	1:A:959:PRO:HG2	1.79	0.48
1:A:733:LEU:O	1:A:743:ARG:NH2	2.47	0.48
1:A:430:LYS:HD2	1:A:433:LYS:HG3	1.96	0.48
1:A:581:ARG:NE	1:B:910:GLU:O	2.33	0.48
1:A:896:GLU:CD	1:A:896:GLU:H	2.21	0.48
1:B:578:ASN:O	1:B:582:MET:HG3	2.14	0.48
1:B:777:VAL:O	1:B:779:HIS:CD2	2.63	0.48
1:A:459:GLU:C	1:A:461:GLU:H	2.22	0.47
1:A:744:LEU:HD11	1:A:774:VAL:HG23	1.90	0.47
1:B:466:SER:HB3	1:B:501:LEU:HD21	1.95	0.47
1:A:828:ASP:OD2	1:A:829:GLN:HG2	2.14	0.47
1:B:785:ARG:HA	1:B:1009:VAL:CG1	2.36	0.47
1:B:373:PRO:HD2	1:B:376:LEU:HB3	1.97	0.47
1:B:726:ILE:O	1:B:727:LYS:C	2.57	0.47
1:B:738:VAL:O	1:B:743:ARG:NH1	2.48	0.47
1:A:757:PRO:C	1:A:759:CYS:N	2.73	0.47
1:B:786:LEU:H	1:B:1009:VAL:HB	1.80	0.47
1:A:562:ASP:HB3	1:A:668:ARG:CZ	2.44	0.47
1:A:912:ARG:NE	1:B:377:ARG:HH22	2.13	0.47
1:B:485:HIS:CD2	1:B:485:HIS:H	2.33	0.47
1:B:848:ASP:OD1	1:B:848:ASP:N	2.47	0.47
1:A:623:ASN:HB3	1:A:626:GLU:HB3	1.97	0.47
1:A:723:GLU:CB	1:A:724:PRO:HD3	2.32	0.47
1:B:642:LYS:HA	1:B:647:LEU:HD12	1.96	0.47
1:A:764:HIS:O	1:A:765:LEU:HG	2.15	0.47
1:B:431:MET:HA	1:B:434:LEU:HB2	1.97	0.46
1:B:505:LYS:C	1:B:505:LYS:HE2	2.41	0.46
1:B:648:ARG:O	1:B:649:CYS:C	2.57	0.46
1:B:722:LEU:O	1:B:723:GLU:C	2.59	0.46
1:A:466:SER:HB3	1:A:501:LEU:HD21	1.96	0.46
1:B:840:THR:HB	1:B:917:VAL:HA	1.98	0.46
1:A:423:GLN:OE1	1:A:576:LEU:HD13	2.16	0.46
1:A:418:TYR:CE1	1:A:455:PHE:HB3	2.51	0.46
1:A:638:TRP:HB2	1:A:666:TYR:CD1	2.51	0.46
1:B:581:ARG:HA	1:B:581:ARG:NH1	2.32	0.45
1:A:586:SER:H	1:B:370:THR:N	2.14	0.45
1:A:799:MET:O	1:A:799:MET:CG	2.64	0.45
1:A:555:THR:O	1:A:556:ASP:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:796:VAL:HG12	1:A:811:LEU:HB3	1.98	0.45
1:A:855:ILE:N	1:A:855:ILE:HD12	2.30	0.45
1:B:399:GLN:HE22	1:B:403:ILE:HD11	1.81	0.45
1:B:777:VAL:O	1:B:778:LYS:C	2.60	0.45
1:B:373:PRO:O	1:B:374:TYR:C	2.60	0.45
1:B:855:ILE:O	1:B:858:VAL:HG22	2.16	0.45
1:A:648:ARG:O	1:A:649:CYS:C	2.60	0.45
1:A:760:LYS:HA	1:A:762:PHE:CE2	2.52	0.45
1:A:418:TYR:O	1:A:419:VAL:C	2.59	0.45
1:B:830:GLY:HA2	1:B:962:VAL:O	2.16	0.45
1:A:824:ARG:HE	1:A:824:ARG:HB3	1.44	0.45
1:B:733:LEU:O	1:B:743:ARG:NH2	2.49	0.45
1:A:907:HIS:CD2	1:B:374:TYR:HB2	2.53	0.44
1:B:701:PRO:C	1:B:703:SER:H	2.26	0.44
1:A:567:GLY:HA3	1:A:570:GLN:HE22	1.83	0.44
1:A:395:LEU:HD13	1:A:602:LEU:HD22	2.00	0.44
1:A:576:LEU:O	1:A:577:VAL:C	2.61	0.44
1:B:419:VAL:O	1:B:423:GLN:HG3	2.17	0.44
1:B:786:LEU:N	1:B:1009:VAL:HG11	2.30	0.44
1:A:430:LYS:HD2	1:A:433:LYS:CG	2.47	0.44
1:A:403:ILE:HD12	1:A:544:VAL:HG21	1.99	0.44
1:A:909:GLN:HE22	1:B:370:THR:CA	2.22	0.44
1:A:895:GLU:OE1	1:A:899:ARG:HD2	2.18	0.44
1:B:682:MET:HE2	1:B:685:GLU:HG3	2.00	0.44
1:B:760:LYS:HA	1:B:762:PHE:CE2	2.53	0.44
1:A:374:TYR:N	1:B:907:HIS:HB3	2.27	0.43
1:B:895:GLU:OE1	1:B:899:ARG:HD2	2.17	0.43
1:B:896:GLU:H	1:B:896:GLU:CD	2.26	0.43
1:B:562:ASP:HA	1:B:668:ARG:HH22	1.83	0.43
1:B:786:LEU:H	1:B:1009:VAL:CB	2.30	0.43
1:B:802:GLY:HA2	1:B:805:ALA:HB3	2.01	0.43
1:A:682:MET:HE2	1:A:685:GLU:HG3	1.99	0.43
1:B:389:ASN:HA	1:B:591:ARG:NH2	2.33	0.43
1:A:375:TYR:CE2	1:A:420:ARG:HG2	2.52	0.43
1:A:934:CYS:HG	1:A:964:TRP:CD1	2.37	0.43
1:A:549:LEU:HD21	1:A:571:LEU:HD12	2.00	0.43
1:B:599:ARG:O	1:B:603:ILE:HG13	2.19	0.43
1:B:624:TRP:CE2	1:B:679:ARG:HG2	2.54	0.43
1:A:584:PHE:O	1:A:912:ARG:HD2	2.19	0.43
1:B:861:ASN:HB2	1:B:862:ALA:H	1.70	0.43
1:B:392:ASP:CG	1:B:551:LEU:HD13	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:503:LEU:HD23	1:A:523:ILE:HD11	2.00	0.43
1:B:427:SER:C	1:B:536:ARG:HD3	2.43	0.43
1:B:754:ARG:HG3	1:B:755:GLU:N	2.33	0.43
1:B:817:LEU:HD23	1:B:1006:VAL:HG13	2.01	0.43
1:A:571:LEU:HD13	1:A:576:LEU:HD12	2.00	0.42
1:B:757:PRO:C	1:B:759:CYS:N	2.76	0.42
1:A:582:MET:HG2	1:A:913:VAL:HG21	2.01	0.42
1:A:785:ARG:O	1:A:798:VAL:CG2	2.62	0.42
1:A:496:LEU:O	1:A:500:PHE:HD2	2.03	0.42
1:A:912:ARG:HH21	1:B:377:ARG:HH22	1.68	0.42
1:B:382:VAL:HG11	1:B:549:LEU:HG	2.01	0.42
1:B:765:LEU:N	1:B:767:GLN:HG3	2.35	0.42
1:A:419:VAL:O	1:A:423:GLN:HG3	2.19	0.42
1:A:709:ASP:HA	1:A:746:LEU:HD21	2.00	0.42
1:B:762:PHE:HB2	1:B:764:HIS:HD2	1.84	0.42
1:A:507:ARG:HH22	1:A:519:ILE:HD12	1.85	0.42
1:B:759:CYS:SG	1:B:762:PHE:CE1	3.11	0.42
1:B:869:ASP:O	1:B:875:PHE:HB2	2.20	0.42
1:B:950:ASP:OD1	1:B:953:HIS:HD2	2.03	0.42
1:A:754:ARG:HG3	1:A:755:GLU:N	2.34	0.42
1:B:430:LYS:HD2	1:B:433:LYS:HG3	2.02	0.42
1:B:895:GLU:O	1:B:899:ARG:HG3	2.20	0.42
1:B:375:TYR:HA	1:B:576:LEU:HD21	2.01	0.42
1:B:444:THR:O	1:B:448:GLU:HB2	2.19	0.42
1:A:621:ASN:HB2	1:A:623:ASN:ND2	2.35	0.41
1:A:977:LYS:HD3	1:A:977:LYS:HA	1.69	0.41
1:B:753:LEU:HG	1:B:759:CYS:SG	2.60	0.41
1:B:782:ILE:HG13	1:B:1006:VAL:HG22	2.02	0.41
1:B:838:PHE:HE2	1:B:959:PRO:HG2	1.84	0.41
1:A:907:HIS:CG	1:B:374:TYR:HB2	2.55	0.41
1:A:370:THR:OG1	1:B:909:GLN:OE1	2.38	0.41
1:A:556:ASP:OD1	1:A:575:LEU:HD22	2.20	0.41
1:A:762:PHE:HB2	1:A:764:HIS:HD2	1.85	0.41
1:A:765:LEU:N	1:A:767:GLN:HG3	2.35	0.41
1:B:710:ARG:NH1	1:B:713:LEU:HD13	2.35	0.41
1:A:469:LEU:HB3	1:A:497:VAL:HG22	2.03	0.41
1:A:561:GLU:CB	1:A:955:ARG:HH22	2.33	0.41
1:B:372:HIS:O	1:B:377:ARG:HG2	2.21	0.41
1:B:709:ASP:HA	1:B:746:LEU:HD21	2.02	0.41
1:B:759:CYS:O	1:B:761:LYS:N	2.53	0.41
1:A:710:ARG:NH1	1:A:713:LEU:HD13	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:912:ARG:CZ	1:B:377:ARG:HH22	2.34	0.41
1:B:644:HIS:CG	1:B:645:PRO:HD2	2.55	0.41
1:B:838:PHE:CD2	1:B:958:LEU:HD22	2.55	0.41
1:A:799:MET:SD	1:A:812:CYS:SG	3.13	0.41
1:B:747:TYR:O	1:B:750:ALA:HB3	2.20	0.41
1:A:912:ARG:HE	1:B:377:ARG:HH22	1.69	0.41
1:A:989:ILE:HD13	1:A:989:ILE:HA	1.88	0.41
1:B:623:ASN:HB3	1:B:626:GLU:HB3	2.02	0.41
1:A:374:TYR:CD1	1:A:576:LEU:HD23	2.54	0.41
1:A:581:ARG:NH2	1:B:912:ARG:HG2	2.34	0.41
1:A:781:THR:HG23	1:A:1007:VAL:HG23	2.03	0.41
1:B:849:ILE:HG23	1:B:852:MET:HE2	2.01	0.41
1:A:375:TYR:CZ	1:A:420:ARG:HG2	2.56	0.40
1:A:722:LEU:HD23	1:A:722:LEU:HA	1.93	0.40
1:B:880:ARG:N	1:B:881:PRO:CD	2.84	0.40
1:B:977:LYS:HA	1:B:977:LYS:HD3	1.76	0.40
1:A:444:THR:O	1:A:448:GLU:HB2	2.20	0.40
1:A:673:PHE:HA	1:A:676:ILE:HD12	2.03	0.40
1:A:840:THR:HG21	1:A:918:SER:H	1.84	0.40
1:B:989:ILE:HD13	1:B:989:ILE:HA	1.92	0.40
1:A:373:PRO:HD2	1:A:376:LEU:HB3	2.04	0.40
1:A:458:THR:HG22	1:A:459:GLU:N	2.36	0.40
1:B:375:TYR:CE2	1:B:420:ARG:HG2	2.57	0.40
1:A:764:HIS:C	1:A:767:GLN:HG3	2.46	0.40
1:A:846:LEU:HA	1:A:886:ARG:NH1	2.37	0.40
1:A:849:ILE:HG23	1:A:852:MET:HE3	2.01	0.40
1:A:991:LEU:HD22	1:A:1001:VAL:HB	2.03	0.40
1:B:764:HIS:O	1:B:767:GLN:NE2	2.55	0.40
1:A:374:TYR:CE1	1:A:576:LEU:CD2	2.93	0.40
1:A:784:GLY:O	1:A:1009:VAL:HG11	2.22	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	607/640 (95%)	531 (88%)	58 (10%)	18 (3%)	3	20
1	B	622/640 (97%)	534 (86%)	68 (11%)	20 (3%)	3	19
All	All	1229/1280 (96%)	1065 (87%)	126 (10%)	38 (3%)	3	20

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	557	SER
1	A	649	CYS
1	A	766	PHE
1	A	785	ARG
1	A	910	GLU
1	B	649	CYS
1	B	766	PHE
1	B	774	VAL
1	B	785	ARG
1	B	800	GLU
1	B	801	ALA
1	A	374	TYR
1	A	760	LYS
1	A	834	GLU
1	B	374	TYR
1	B	760	LYS
1	B	788	PRO
1	B	834	GLU
1	B	910	GLU
1	A	561	GLU
1	A	569	GLY
1	A	852	MET
1	B	599	ARG
1	A	435	GLU
1	A	555	THR
1	A	762	PHE
1	B	435	GLU
1	B	762	PHE
1	B	773	ALA
1	B	937	GLY
1	A	758	SER
1	B	702	ASP
1	B	852	MET

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Mol	Chain	Res	Type
1	A	558	MET
1	A	644	HIS
1	A	540	GLY
1	B	577	VAL
1	B	644	HIS

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	539/557 (97%)	484 (90%)	55 (10%)	7	26
1	B	548/557 (98%)	494 (90%)	54 (10%)	7	27
All	All	1087/1114 (98%)	978 (90%)	109 (10%)	7	27

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	374	TYR
1	A	375	TYR
1	A	389	ASN
1	A	405	THR
1	A	423	GLN
1	A	424	ARG
1	A	425	LYS
1	A	431	MET
1	A	432	THR
1	A	438	GLU
1	A	441	LEU
1	A	444	THR
1	A	486	LEU
1	A	487	VAL
1	A	503	LEU
1	A	505	LYS
1	A	537	ILE
1	A	546	SER

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Mol	Chain	Res	Type
1	A	549	LEU
1	A	555	THR
1	A	558	MET
1	A	560	ASP
1	A	561	GLU
1	A	570	GLN
1	A	571	LEU
1	A	575	LEU
1	A	577	VAL
1	A	591	ARG
1	A	642	LYS
1	A	674	VAL
1	A	721	ARG
1	A	722	LEU
1	A	738	VAL
1	A	743	ARG
1	A	754	ARG
1	A	759	CYS
1	A	762	PHE
1	A	777	VAL
1	A	778	LYS
1	A	782	ILE
1	A	783	THR
1	A	786	LEU
1	A	794	LYS
1	A	796	VAL
1	A	824	ARG
1	A	840	THR
1	A	848	ASP
1	A	852	MET
1	A	870	LEU
1	A	872	THR
1	A	889	LEU
1	A	910	GLU
1	A	967	GLN
1	A	969	ARG
1	A	983	LEU
1	B	370	THR
1	B	374	TYR
1	B	375	TYR
1	B	389	ASN
1	B	405	THR

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Mol	Chain	Res	Type
1	B	413	THR
1	B	424	ARG
1	B	425	LYS
1	B	431	MET
1	B	432	THR
1	B	438	GLU
1	B	441	LEU
1	B	444	THR
1	B	486	LEU
1	B	487	VAL
1	B	503	LEU
1	B	505	LYS
1	B	537	ILE
1	B	546	SER
1	B	549	LEU
1	B	558	MET
1	B	562	ASP
1	B	565	CYS
1	B	575	LEU
1	B	577	VAL
1	B	591	ARG
1	B	642	LYS
1	B	674	VAL
1	B	721	ARG
1	B	722	LEU
1	B	738	VAL
1	B	743	ARG
1	B	754	ARG
1	B	759	CYS
1	B	762	PHE
1	B	777	VAL
1	B	778	LYS
1	B	782	ILE
1	B	783	THR
1	B	786	LEU
1	B	794	LYS
1	B	796	VAL
1	B	808	THR
1	B	809	THR
1	B	824	ARG
1	B	840	THR
1	B	848	ASP

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Mol	Chain	Res	Type
1	B	870	LEU
1	B	872	THR
1	B	889	LEU
1	B	910	GLU
1	B	967	GLN
1	B	969	ARG
1	B	983	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	389	ASN
1	A	399	GLN
1	A	485	HIS
1	A	506	GLN
1	A	570	GLN
1	A	623	ASN
1	A	639	ASN
1	A	742	HIS
1	A	748	GLN
1	A	764	HIS
1	A	767	GLN
1	A	779	HIS
1	A	821	HIS
1	A	832	HIS
1	A	907	HIS
1	A	909	GLN
1	A	953	HIS
1	A	995	GLN
1	B	389	ASN
1	B	399	GLN
1	B	457	GLN
1	B	485	HIS
1	B	506	GLN
1	B	610	HIS
1	B	623	ASN
1	B	639	ASN
1	B	742	HIS
1	B	748	GLN
1	B	764	HIS
1	B	767	GLN
1	B	779	HIS

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Mol	Chain	Res	Type
1	B	821	HIS
1	B	832	HIS
1	B	909	GLN
1	B	953	HIS
1	B	985	HIS
1	B	995	GLN

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	615/640 (96%)	0.23	48 (7%) 19 14	69, 97, 161, 189	0
1	B	628/640 (98%)	0.56	77 (12%) 8 7	65, 116, 221, 266	0
All	All	1243/1280 (97%)	0.40	125 (10%) 12 10	65, 104, 200, 266	0

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	373	PRO	8.4
1	B	373	PRO	7.0
1	A	795	SER	6.3
1	B	372	HIS	6.3
1	A	764	HIS	6.1
1	A	765	LEU	6.0
1	A	374	TYR	5.9
1	A	375	TYR	5.8
1	B	503	LEU	5.7
1	B	374	TYR	5.4
1	A	372	HIS	5.2
1	B	486	LEU	5.1
1	B	370	THR	5.1
1	B	764	HIS	5.0
1	A	576	LEU	4.8
1	A	486	LEU	4.8
1	A	434	LEU	4.7
1	B	765	LEU	4.7
1	B	471	LEU	4.6
1	B	806	ASP	4.6
1	A	574	VAL	4.5
1	A	784	GLY	4.4
1	B	795	SER	4.4
1	A	507	ARG	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	558	MET	4.3
1	B	462	LEU	4.2
1	B	506	GLN	4.2
1	A	763	LYS	4.0
1	B	804	ALA	4.0
1	B	375	TYR	3.9
1	A	371	GLY	3.9
1	B	523	ILE	3.9
1	A	774	VAL	3.9
1	B	531	ALA	3.8
1	A	432	THR	3.8
1	B	574	VAL	3.7
1	B	575	LEU	3.7
1	A	564	ALA	3.7
1	B	576	LEU	3.6
1	B	768	GLN	3.6
1	A	799	MET	3.6
1	B	763	LYS	3.6
1	A	773	ALA	3.5
1	A	370	THR	3.5
1	A	762	PHE	3.5
1	B	519	ILE	3.5
1	B	500	PHE	3.4
1	B	557	SER	3.4
1	B	502	LYS	3.4
1	A	796	VAL	3.4
1	B	434	LEU	3.3
1	B	483	THR	3.3
1	B	371	GLY	3.3
1	B	504	ALA	3.3
1	B	507	ARG	3.3
1	B	480	LEU	3.3
1	B	509	VAL	3.3
1	A	766	PHE	3.2
1	B	784	GLY	3.2
1	A	571	LEU	3.1
1	A	519	ILE	3.1
1	B	563	ALA	3.1
1	A	575	LEU	3.1
1	A	433	LYS	3.1
1	B	450	LEU	3.0
1	B	799	MET	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	807	PRO	2.9
1	B	644	HIS	2.9
1	B	432	THR	2.9
1	B	649	CYS	2.9
1	B	766	PHE	2.9
1	B	559	GLU	2.9
1	B	800	GLU	2.9
1	A	794	LYS	2.8
1	B	484	PHE	2.8
1	A	562	ASP	2.8
1	A	559	GLU	2.8
1	A	785	ARG	2.8
1	A	565	CYS	2.8
1	B	501	LEU	2.8
1	A	594	HIS	2.7
1	B	835	GLY	2.7
1	B	469	LEU	2.7
1	B	431	MET	2.7
1	B	564	ALA	2.7
1	A	768	GLN	2.6
1	B	497	VAL	2.6
1	B	645	PRO	2.6
1	B	524	LEU	2.6
1	A	649	CYS	2.5
1	A	650	HIS	2.5
1	B	573	THR	2.5
1	B	521	ALA	2.5
1	B	646	SER	2.5
1	A	503	LEU	2.5
1	B	571	LEU	2.4
1	B	805	ALA	2.4
1	A	1009	VAL	2.4
1	B	975	GLU	2.4
1	A	787	CYS	2.4
1	B	465	LEU	2.4
1	B	775	GLN	2.4
1	B	762	PHE	2.4
1	B	461	GLU	2.4
1	A	645	PRO	2.4
1	B	520	GLY	2.3
1	A	563	ALA	2.3
1	B	499	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	431	MET	2.3
1	B	767	GLN	2.3
1	B	794	LYS	2.3
1	B	785	ARG	2.2
1	B	556	ASP	2.2
1	B	740	THR	2.2
1	B	774	VAL	2.2
1	A	435	GLU	2.2
1	B	532	GLY	2.2
1	A	644	HIS	2.2
1	B	808	THR	2.1
1	A	597	GLN	2.1
1	A	907	HIS	2.0
1	A	596	PHE	2.0
1	B	569	GLY	2.0
1	B	530	LEU	2.0
1	B	1009	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.