



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:19 PM GMT

PDB ID : 4RID
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

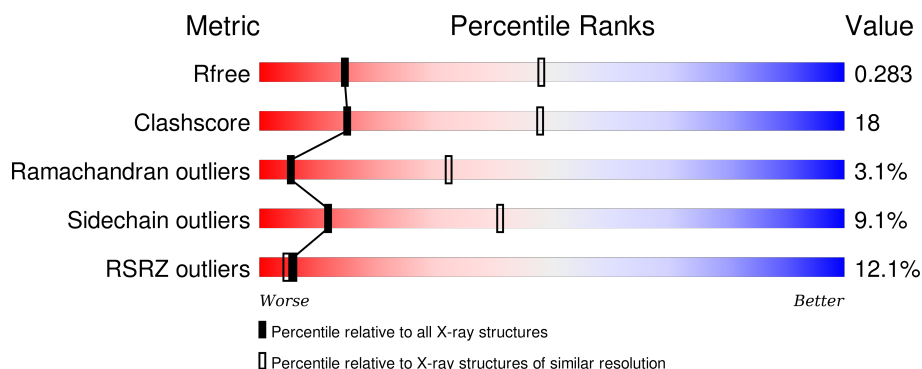
1 Overall quality at a glance

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}	91344	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	
1	B	640	

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.

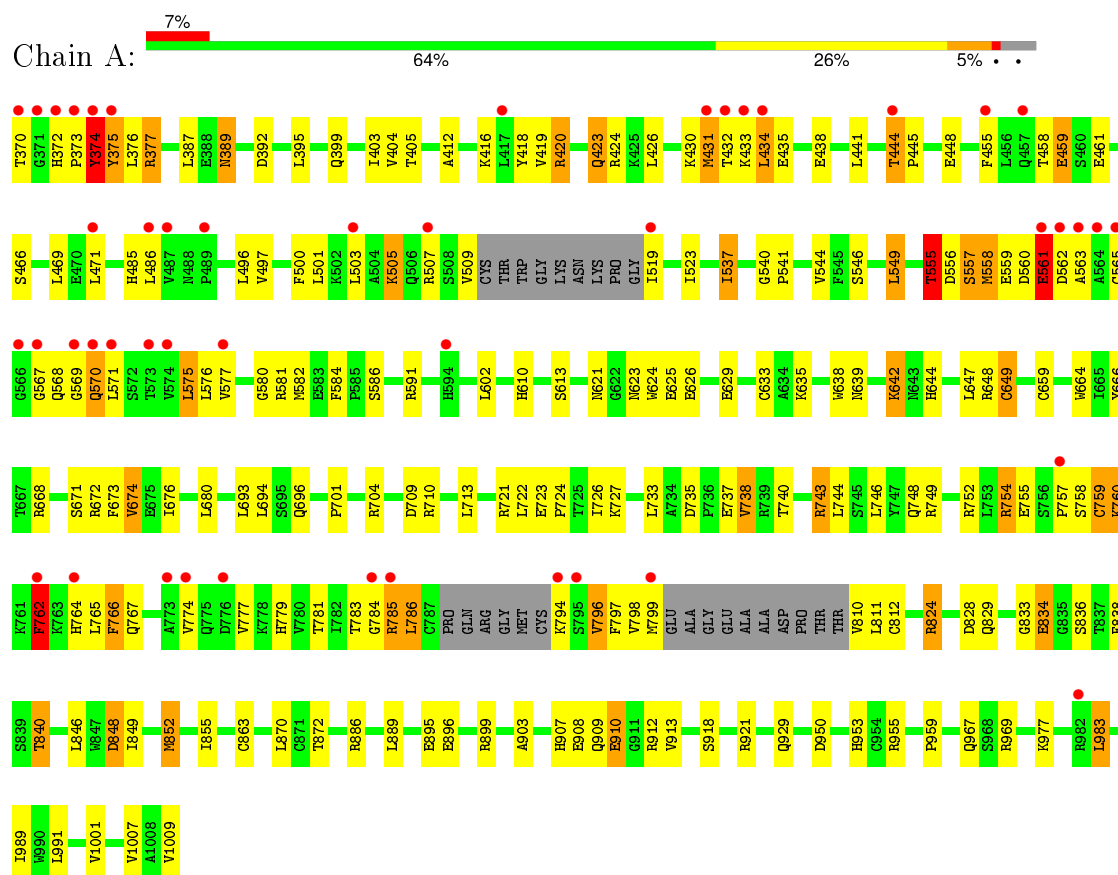
- Molecule 1 is a protein called Fanconi-associated nuclease 1.

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			

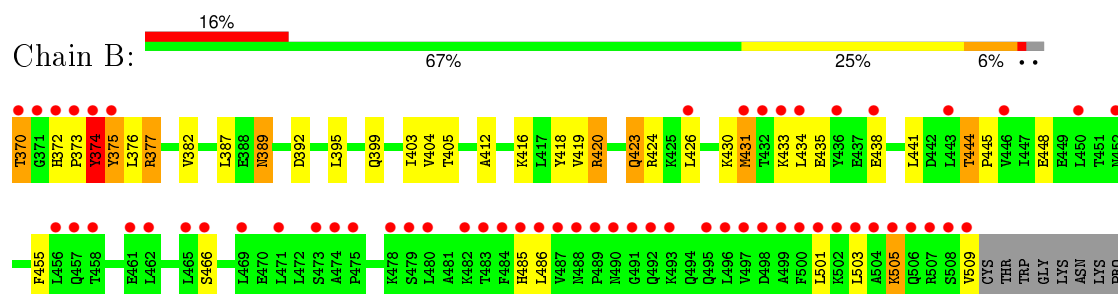
3 Residue-property plots

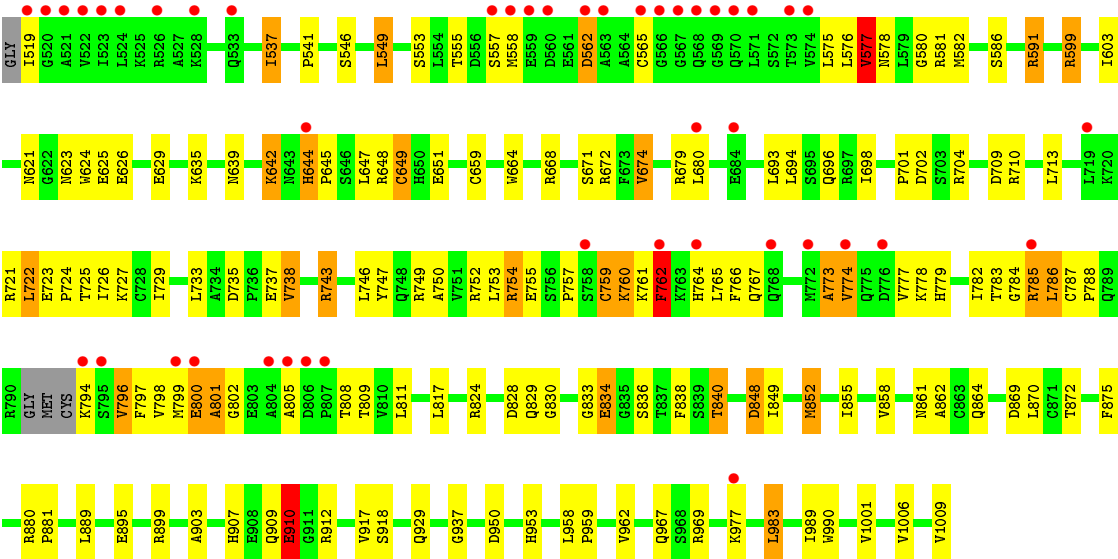
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 49.27 – 3.09	Depositor EDS
% Data completeness (in resolution range)	96.0 (30.00-3.30) 93.3 (49.27-3.09)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.03 (at 3.07Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.246 , 0.288 0.244 , 0.283	Depositor DCC
R_{free} test set	1120 reflections (3.34%)	DCC
Wilson B-factor (Å ²)	91.3	Xtriage
Anisotropy	0.402	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 70.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 43233 reflections	Xtriage
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

Xtriage'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.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.45	0/5045	0.68	2/6818 (0.0%)
1	B	0.44	0/5141	0.67	1/6952 (0.0%)
All	All	0.44	0/10186	0.67	3/13770 (0.0%)

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 (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	983	LEU	CA-CB-CG	5.52	128.00	115.30
1	A	434	LEU	CA-CB-CG	5.08	126.98	115.30
1	A	983	LEU	CA-CB-CG	5.03	126.88	115.30

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	197	0
1	B	5037	0	5065	186	0
All	All	9981	0	10046	353	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 (353) 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:B:785:ARG:HB2	1:B:798:VAL:HB	1.28	1.15
1:A:784:GLY:O	1:A:1009:VAL:HG21	1.47	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
1:B:374:TYR:CE1	1:B:576:LEU:HD23	1.96	1.01
1:A:723:GLU:HB3	1:A:724:PRO:HD3	1.47	0.96
1:B:765:LEU:C	1:B:767:GLN:H	1.69	0.93
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:765:LEU:C	1:A:767:GLN:H	1.72	0.90
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:555:THR:HG21	1:B:861:ASN:OD1	1.82	0.80
1:B:785:ARG:CB	1:B:798:VAL:HB	2.11	0.79
1:B:786:LEU:CB	1:B:1009:VAL:HB	2.12	0.79
1:A:426:LEU:HD13	1:A:537:ILE:HG22	1.65	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:B:765:LEU:C	1:B:767:GLN:N	2.38	0.77
1:A:785:ARG:O	1:A:798:VAL:HG23	1.86	0.76
1:B:784:GLY:C	1:B:1009:VAL:HG21	2.06	0.75
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:A:765:LEU:C	1:A:767:GLN:N	2.40	0.75
1:B:785:ARG:O	1:B:798:VAL:HG23	1.87	0.74
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: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: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:568:GLN:CD	1:A:610:HIS:HB3	2.13	0.68
1:A:784:GLY:O	1:A:1009:VAL:CG2	2.34	0.68
1:A:777:VAL:O	1:A:779:HIS:HD2	1.77	0.68
1:B:765:LEU:HA	1:B:767:GLN:HG3	1.76	0.68
1:A:785:ARG:CA	1:A:1009:VAL:HG11	2.24	0.67
1:A:389:ASN:ND2	1:A:392:ASP:H	1.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:797:PHE:O	1:A:811:LEU:HA	1.96	0.66
1:A:565:CYS:O	1:A:613:SER:HB2	1.94	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:A:784:GLY:C	1:A:1009:VAL:HG21	2.15	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
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:586:SER:HG	1:B:370:THR:N	1.97	0.62
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: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:B:796:VAL:HG12	1:B:811:LEU:HB3	1.82	0.61
1:A:431:MET:HA	1:A:434:LEU:HD12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:509:VAL:C	1:A:519:ILE:N	2.58	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
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:B:373:PRO:HD3	1:B:416:LYS:HE2	1.87	0.56
1:A:840:THR:CG2	1:A:918:SER:H	2.17	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: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:B:773:ALA:O	1:B:774:VAL:CG2	2.53	0.55
1:A:458:THR:HG22	1:A:459:GLU:H	1.72	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:762:PHE:CD2	1:A:762:PHE:C	2.80	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:B:765:LEU:O	1:B:767:GLN:N	2.35	0.55
1:A:639:ASN:HA	1:A:642:LYS:HE2	1.88	0.55
1:B:444:THR:N	1:B:445:PRO:HD2	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:762:PHE:C	1:B:762:PHE:CD2	2.80	0.54
1:B:799:MET:HG3	1:B:799:MET:O	2.08	0.54
1:A:624:TRP:HB2	1:A:680:LEU:HD21	1.89	0.54
1:B:796:VAL:CG1	1:B:811:LEU:HB3	2.38	0.54
1:B:840:THR:CG2	1:B:918:SER:H	2.21	0.54
1:A:765:LEU:CA	1:A:767:GLN:HG3	2.38	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:A:668:ARG:O	1:A:672:ARG:HG2	2.08	0.53
1:B:581:ARG:N	1:B:581:ARG:HD2	2.22	0.52
1:A:777:VAL:O	1:A:779:HIS:CD2	2.61	0.52
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:B:764:HIS:O	1:B:765:LEU:HG	2.10	0.52
1:B:693:LEU:O	1:B:696:GLN:HG3	2.10	0.52
1:A:740:THR:HG21	1:A:953:HIS:O	2.10	0.52
1:A:785:ARG:O	1:A:798:VAL:N	2.44	0.51
1:A:372:HIS:O	1:A:377:ARG:HG2	2.11	0.51
1:A:848:ASP:OD1	1:A:848:ASP:N	2.44	0.51
1:B:374:TYR:HE1	1:B:576:LEU:HD23	1.66	0.51
1:A:642:LYS:HA	1:A:647:LEU:HD12	1.92	0.51
1:A:581:ARG:N	1:A:581:ARG:HD2	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:B:855:ILE:N	1:B:855:ILE:HD12	2.26	0.51
1:B:624:TRP:HB2	1:B:680:LEU:HD21	1.91	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: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:B:423:GLN:HE22	1:B:576:LEU:HD22	1.77	0.50
1:A:757:PRO:C	1:A:759:CYS:H	2.14	0.50
1:B:426:LEU:HD13	1:B:537:ILE:HG22	1.94	0.50
1:B:387:LEU:HD11	1:B:404:VAL:HG11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:LEU:HD13	1:A:503:LEU:HD21	1.94	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: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:773:ALA:C	1:B:774:VAL:HG23	2.33	0.48
1:A:912:ARG:NH2	1:B:377:ARG:HH22	2.12	0.48
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:838:PHE:HE2	1:A:959:PRO:HG2	1.79	0.48
1:A:485:HIS:H	1:A:485:HIS:CD2	2.31	0.48
1:A:733:LEU:O	1:A:743:ARG:NH2	2.47	0.48
1:B:509:VAL:C	1:B:519:ILE:N	2.67	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:B:777:VAL:O	1:B:779:HIS:CD2	2.63	0.48
1:B:578:ASN:O	1:B:582:MET:HG3	2.14	0.48
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:B:785:ARG:HA	1:B:1009:VAL:CG1	2.36	0.47
1:A:828:ASP:OD2	1:A:829:GLN:HG2	2.14	0.47
1:B:373:PRO:HD2	1:B:376:LEU:HB3	1.97	0.47
1:B:738:VAL:O	1:B:743:ARG:NH1	2.48	0.47
1:B:786:LEU:H	1:B:1009:VAL:HB	1.80	0.47
1:A:912:ARG:NE	1:B:377:ARG:HH22	2.13	0.47
1:A:562:ASP:HB3	1:A:668:ARG:CZ	2.44	0.47
1:B:848:ASP:N	1:B:848:ASP:OD1	2.47	0.47
1:B:485:HIS:H	1:B:485:HIS:CD2	2.33	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:623:ASN:HB3	1:A:626:GLU:HB3	1.97	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:A:726:ILE:O	1:A:727:LYS:C	2.52	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:B:762:PHE:C	1:B:762:PHE:HD2	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:586:SER:H	1:B:370:THR:N	2.14	0.45
1:A:799:MET:CG	1:A:799:MET:O	2.64	0.45
1:A:796:VAL:HG12	1:A:811:LEU:HB3	1.98	0.45
1:B:576:LEU:O	1:B:577:VAL:C	2.55	0.45
1:A:855:ILE:HD12	1:A:855:ILE:N	2.30	0.45
1:B:399:GLN:HE22	1:B:403:ILE:HD11	1.81	0.45
1:A:556:ASP:O	1:A:557:SER:C	2.55	0.45
1:B:855:ILE:O	1:B:858:VAL:HG22	2.16	0.45
1:A:760:LYS:HA	1:A:762:PHE:CE2	2.52	0.45
1:A:722:LEU:O	1:A:723:GLU:C	2.56	0.45
1:B:830:GLY:HA2	1:B:962:VAL:O	2.16	0.45
1:A:581:ARG:HE	1:B:910:GLU:C	2.16	0.45
1:B:733:LEU:O	1:B:743:ARG:NH2	2.49	0.45
1:A:824:ARG:HB3	1:A:824:ARG:HE	1.44	0.45
1:A:907:HIS:CD2	1:B:374:TYR:HB2	2.53	0.44
1:A:567:GLY:HA3	1:A:570:GLN:HE22	1.83	0.44
1:B:419:VAL:O	1:B:423:GLN:HG3	2.17	0.44
1:B:757:PRO:C	1:B:759:CYS:H	2.20	0.44
1:A:505:LYS:HE2	1:A:505:LYS:C	2.38	0.44
1:A:395:LEU:HD13	1:A:602:LEU:HD22	2.00	0.44
1:B:786:LEU:N	1:B:1009:VAL:HG11	2.30	0.44
1:A:373:PRO:O	1:A:374:TYR:C	2.56	0.44
1:A:430:LYS:HD2	1:A:433:LYS:CG	2.47	0.44
1:A:762:PHE:HD2	1:A:762:PHE:C	2.19	0.44
1:A:909:GLN:HE22	1:B:370:THR:CA	2.22	0.44
1:A:403:ILE:HD12	1:A:544:VAL:HG21	1.99	0.44
1:B:760:LYS:HA	1:B:762:PHE:CE2	2.53	0.44
1:A:895:GLU:OE1	1:A:899:ARG:HD2	2.18	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: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:B:562:ASP:HA	1:B:668:ARG:HH22	1.83	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: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:A:896:GLU:CD	1:A:896:GLU:H	2.21	0.43
1:B:754:ARG:HG3	1:B:755:GLU:N	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:861:ASN:HB2	1:B:862:ALA:H	1.70	0.43
1:A:459:GLU:C	1:A:461:GLU:H	2.22	0.43
1:B:849:ILE:HG23	1:B:852:MET:HE2	1.99	0.43
1:A:503:LEU:HD23	1:A:523:ILE:HD11	2.00	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:A:757:PRO:C	1:A:759:CYS:N	2.73	0.42
1:B:726:ILE:O	1:B:727:LYS:C	2.57	0.42
1:A:785:ARG:O	1:A:798:VAL:CG2	2.62	0.42
1:A:582:MET:HG2	1:A:913:VAL:HG21	2.01	0.42
1:B:765:LEU:N	1:B:767:GLN:HG3	2.35	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:A:496:LEU:O	1:A:500:PHE:HD2	2.03	0.42
1:B:762:PHE:HB2	1:B:764:HIS:HD2	1.84	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:759:CYS:SG	1:B:762:PHE:CE1	3.11	0.42
1:A:507:ARG:HH22	1:A:519:ILE:HD12	1.85	0.42
1:B:950:ASP:OD1	1:B:953:HIS:HD2	2.03	0.42
1:B:869:ASP:O	1:B:875:PHE:HB2	2.20	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:A:754:ARG:HG3	1:A:755:GLU:N	2.34	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:B:753:LEU:HG	1:B:759:CYS:SG	2.60	0.41
1:A:621:ASN:HB2	1:A:623:ASN:ND2	2.35	0.41
1:B:782:ILE:HG13	1:B:1006:VAL:HG22	2.02	0.41
1:A:977:LYS:HD3	1:A:977:LYS:HA	1.69	0.41
1:B:505:LYS:C	1:B:505:LYS:HE2	2.41	0.41
1:B:838:PHE:HE2	1:B:959:PRO:HG2	1.84	0.41
1:B:648:ARG:O	1:B:649:CYS:C	2.57	0.41
1:A:907:HIS:CG	1:B:374:TYR:HB2	2.55	0.41
1:B:722:LEU:O	1:B:723:GLU:C	2.59	0.41
1:A:370:THR:OG1	1:B:909:GLN:OE1	2.38	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:A:556:ASP:OD1	1:A:575:LEU:HD22	2.20	0.41
1:B:710:ARG:NH1	1:B:713:LEU:HD13	2.35	0.41
1:B:759:CYS:O	1:B:761:LYS:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:372:HIS:O	1:B:377:ARG:HG2	2.21	0.41
1:A:561:GLU:CB	1:A:955:ARG:HH22	2.33	0.41
1:B:709:ASP:HA	1:B:746:LEU:HD21	2.02	0.41
1:A:469:LEU:HB3	1:A:497:VAL:HG22	2.03	0.41
1:A:912:ARG:CZ	1:B:377:ARG:HH22	2.34	0.41
1:B:838:PHE:CD2	1:B:958:LEU:HD22	2.55	0.41
1:A:710:ARG:NH1	1:A:713:LEU:HD13	2.35	0.41
1:B:644:HIS:CG	1:B:645:PRO:HD2	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:B:623:ASN:HB3	1:B:626:GLU:HB3	2.02	0.41
1:A:989:ILE:HD13	1:A:989:ILE:HA	1.88	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:A:722:LEU:HA	1:A:722:LEU:HD23	1.93	0.40
1:A:375:TYR:CZ	1:A:420:ARG:HG2	2.56	0.40
1:A:555:THR:O	1:A:556:ASP:C	2.59	0.40
1:B:977:LYS:HA	1:B:977:LYS:HD3	1.76	0.40
1:B:880:ARG:N	1:B:881:PRO:CD	2.84	0.40
1:A:840:THR:HG21	1:A:918:SER:H	1.84	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:B:989:ILE:HD13	1:B:989:ILE:HA	1.92	0.40
1:B:375:TYR:CE2	1:B:420:ARG:HG2	2.57	0.40
1:A:373:PRO:HD2	1:A:376:LEU:HB3	2.04	0.40
1:B:777:VAL:O	1:B:778:LYS:C	2.60	0.40
1:A:458:THR:HG22	1:A:459:GLU:N	2.36	0.40
1:B:373:PRO:O	1:B:374:TYR:C	2.60	0.40
1:B:764:HIS:O	1:B:767:GLN:NE2	2.55	0.40
1:A:991:LEU:HD22	1:A:1001:VAL:HB	2.03	0.40
1:A:846:LEU:HA	1:A:886:ARG:NH1	2.37	0.40
1:A:784:GLY:O	1:A:1009:VAL:HG11	2.22	0.40
1:A:374:TYR:CE1	1:A:576:LEU:CD2	2.93	0.40
1:A:648:ARG:O	1:A:649:CYS:C	2.60	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%)	5	33
1	B	622/640 (97%)	534 (86%)	68 (11%)	20 (3%)	5	31
All	All	1229/1280 (96%)	1065 (87%)	126 (10%)	38 (3%)	5	32

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

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Mol	Chain	Res	Type
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
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%)	490 (91%)	49 (9%)	12	41
1	B	548/557 (98%)	498 (91%)	50 (9%)	12	41
All	All	1087/1114 (98%)	988 (91%)	99 (9%)	12	41

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	374	TYR
1	A	375	TYR
1	A	377	ARG
1	A	389	ASN
1	A	405	THR
1	A	420	ARG
1	A	423	GLN
1	A	424	ARG
1	A	431	MET
1	A	432	THR

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Mol	Chain	Res	Type
1	A	438	GLU
1	A	441	LEU
1	A	444	THR
1	A	459	GLU
1	A	505	LYS
1	A	537	ILE
1	A	546	SER
1	A	549	LEU
1	A	555	THR
1	A	559	GLU
1	A	560	ASP
1	A	561	GLU
1	A	570	GLN
1	A	575	LEU
1	A	577	VAL
1	A	591	ARG
1	A	633	CYS
1	A	642	LYS
1	A	674	VAL
1	A	721	ARG
1	A	738	VAL
1	A	743	ARG
1	A	754	ARG
1	A	759	CYS
1	A	762	PHE
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	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

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Mol	Chain	Res	Type
1	B	377	ARG
1	B	389	ASN
1	B	405	THR
1	B	420	ARG
1	B	423	GLN
1	B	424	ARG
1	B	431	MET
1	B	438	GLU
1	B	441	LEU
1	B	444	THR
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	783	THR
1	B	786	LEU
1	B	787	CYS
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
1	B	870	LEU
1	B	872	THR
1	B	889	LEU

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Mol	Chain	Res	Type
1	B	910	GLU
1	B	967	GLN
1	B	969	ARG
1	B	983	LEU
1	B	990	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) 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	748	GLN
1	A	764	HIS
1	A	767	GLN
1	A	779	HIS
1	A	821	HIS
1	A	909	GLN
1	A	953	HIS
1	B	389	ASN
1	B	399	GLN
1	B	485	HIS
1	B	506	GLN
1	B	610	HIS
1	B	623	ASN
1	B	639	ASN
1	B	764	HIS
1	B	767	GLN
1	B	779	HIS
1	B	821	HIS
1	B	909	GLN
1	B	953	HIS
1	B	995	GLN

5.3.3 RNA ⓘ

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 carbohydrates 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%)	0.46	47 (7%) 17 14	69, 97, 161, 189	0
1	B	628/640 (98%)	0.98	104 (16%) 2 2	65, 116, 221, 266	0
All	All	1243/1280 (97%)	0.72	151 (12%) 6 4	65, 104, 200, 266	0

All (151) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	491	GLY	16.6
1	B	506	GLN	14.3
1	B	372	HIS	13.6
1	B	503	LEU	13.1
1	A	795	SER	11.2
1	A	373	PRO	10.7
1	B	485	HIS	9.8
1	B	806	ASP	9.6
1	B	795	SER	9.3
1	A	764	HIS	9.2
1	A	774	VAL	9.0
1	A	566	GLY	8.9
1	A	372	HIS	8.7
1	B	497	VAL	8.4
1	B	519	ILE	8.4
1	B	373	PRO	8.4
1	A	565	CYS	8.3
1	B	524	LEU	7.9
1	B	573	THR	7.9
1	B	486	LEU	7.4
1	B	509	VAL	7.3
1	B	500	PHE	7.3
1	A	486	LEU	7.2
1	B	370	THR	7.2

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Mol	Chain	Res	Type	RSRZ
1	A	370	THR	7.2
1	B	499	ALA	7.1
1	B	764	HIS	7.0
1	B	496	LEU	6.9
1	B	522	VAL	6.9
1	B	461	GLU	6.8
1	B	502	LYS	6.8
1	B	431	MET	6.7
1	B	492	GLN	6.7
1	B	566	GLY	6.5
1	B	807	PRO	6.5
1	B	432	THR	6.0
1	B	568	GLN	6.0
1	B	434	LEU	5.8
1	B	507	ARG	5.8
1	B	504	ALA	5.7
1	A	564	ALA	5.6
1	B	520	GLY	5.4
1	B	774	VAL	5.4
1	B	462	LEU	5.3
1	A	371	GLY	5.3
1	B	374	TYR	5.2
1	A	571	LEU	5.2
1	A	374	TYR	5.1
1	B	498	ASP	5.1
1	B	483	THR	5.1
1	B	487	VAL	5.1
1	B	482	LYS	5.1
1	A	785	ARG	4.9
1	B	804	ALA	4.9
1	B	495	GLN	4.9
1	B	776	ASP	4.9
1	B	371	GLY	4.8
1	B	493	LYS	4.8
1	B	465	LEU	4.7
1	B	565	CYS	4.6
1	B	558	MET	4.6
1	B	469	LEU	4.6
1	B	375	TYR	4.6
1	B	571	LEU	4.4
1	B	489	PRO	4.3
1	A	375	TYR	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	785	ARG	4.3
1	B	505	LYS	4.3
1	A	573	THR	4.3
1	B	508	SER	4.2
1	B	557	SER	4.1
1	B	528	LYS	4.1
1	A	433	LYS	4.1
1	B	533	GLN	4.1
1	B	433	LYS	4.0
1	B	570	GLN	4.0
1	A	776	ASP	3.9
1	A	503	LEU	3.8
1	A	507	ARG	3.7
1	A	563	ALA	3.7
1	A	431	MET	3.6
1	B	523	ILE	3.6
1	B	450	LEU	3.5
1	B	501	LEU	3.4
1	B	800	GLU	3.4
1	B	479	SER	3.4
1	B	559	GLU	3.3
1	A	784	GLY	3.3
1	A	574	VAL	3.2
1	A	562	ASP	3.2
1	A	799	MET	3.1
1	B	443	LEU	3.0
1	A	794	LYS	3.0
1	B	490	ASN	3.0
1	B	458	THR	2.9
1	B	526	ARG	2.9
1	A	489	PRO	2.9
1	B	446	VAL	2.9
1	B	799	MET	2.9
1	B	644	HIS	2.9
1	B	438	GLU	2.8
1	A	567	GLY	2.8
1	B	456	LEU	2.8
1	B	562	ASP	2.8
1	B	569	GLY	2.8
1	A	457	GLN	2.7
1	B	563	ALA	2.7
1	B	521	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	436	TYR	2.7
1	B	484	PHE	2.7
1	B	805	ALA	2.7
1	B	426	LEU	2.7
1	B	471	LEU	2.6
1	A	762	PHE	2.6
1	A	519	ILE	2.6
1	B	768	GLN	2.6
1	B	567	GLY	2.6
1	A	432	THR	2.5
1	B	680	LEU	2.5
1	B	772	MET	2.5
1	B	475	PRO	2.5
1	A	773	ALA	2.5
1	B	457	GLN	2.5
1	A	561	GLU	2.4
1	B	560	ASP	2.4
1	B	474	ALA	2.4
1	A	417	LEU	2.4
1	B	466	SER	2.3
1	A	570	GLN	2.3
1	B	480	LEU	2.3
1	B	452	ASN	2.3
1	B	977	LYS	2.3
1	A	471	LEU	2.3
1	A	982	ARG	2.2
1	A	757	PRO	2.2
1	B	762	PHE	2.2
1	B	719	LEU	2.2
1	A	569	GLY	2.1
1	A	577	VAL	2.1
1	B	478	LYS	2.1
1	A	434	LEU	2.1
1	B	473	SER	2.1
1	B	758	SER	2.1
1	B	684	GLU	2.1
1	B	488	ASN	2.1
1	B	574	VAL	2.1
1	A	594	HIS	2.1
1	A	455	PHE	2.1
1	A	487	VAL	2.0
1	A	444	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	794	LYS	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 carbohydrates 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.