Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2024 – 07:24 PM EDT

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
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:

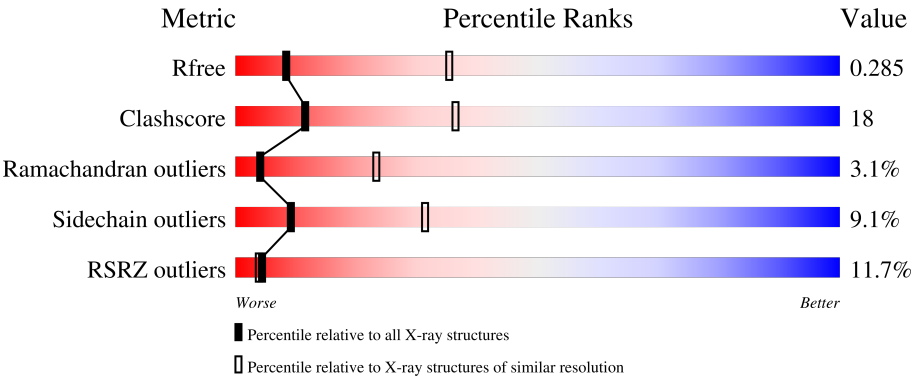
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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 <=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	7% 64% 26% 5%
1	B	640	16% 67% 25% 6%

2 Entry composition (i)

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.

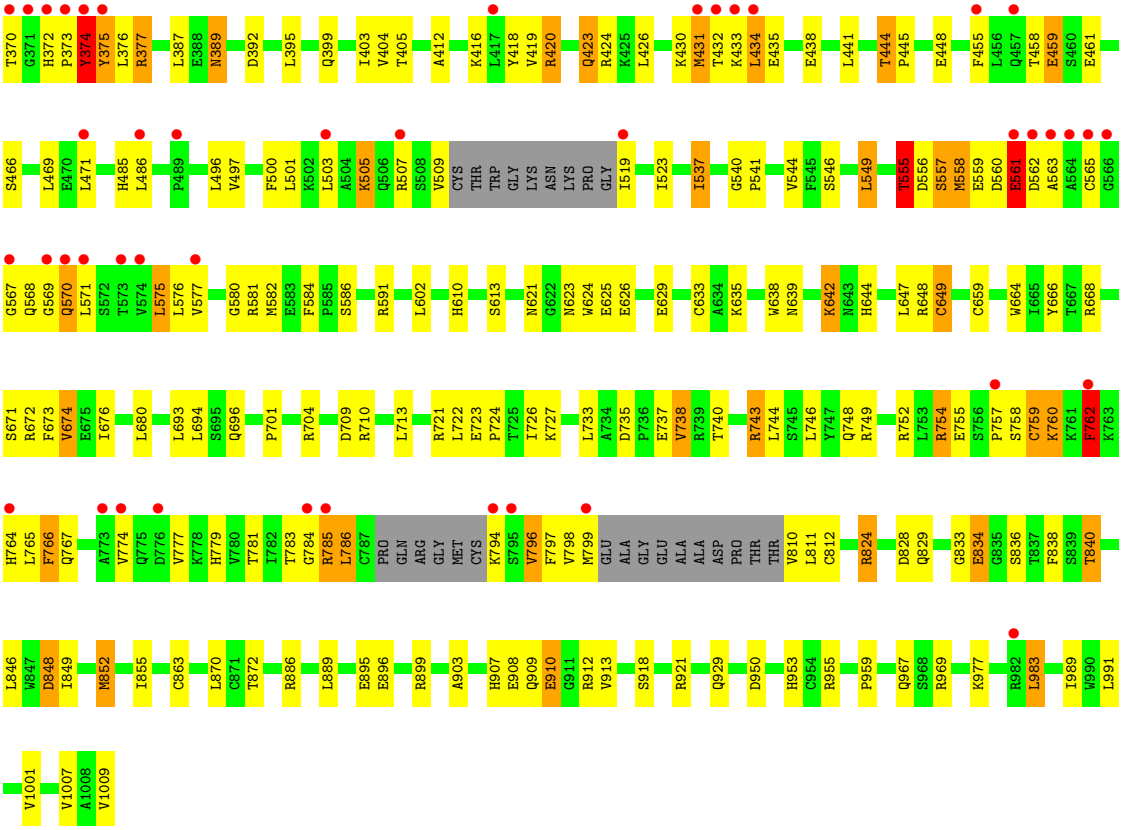
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	615	Total	C	N	O	S	0	0	0
			4944	3147	880	890	27			
1	B	628	Total	C	N	O	S	0	0	0
			5037	3201	897	912	27			

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.

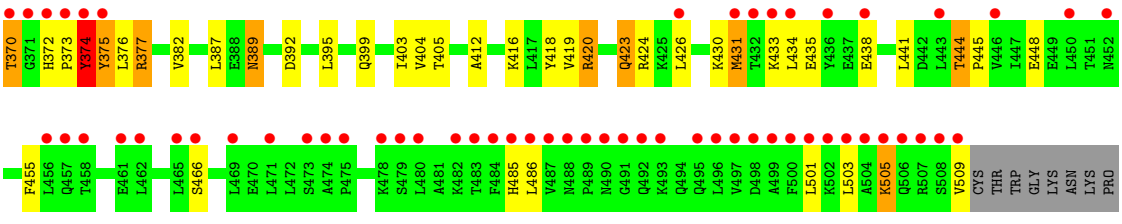
• Molecule 1: Fanconi-associated nuclease 1

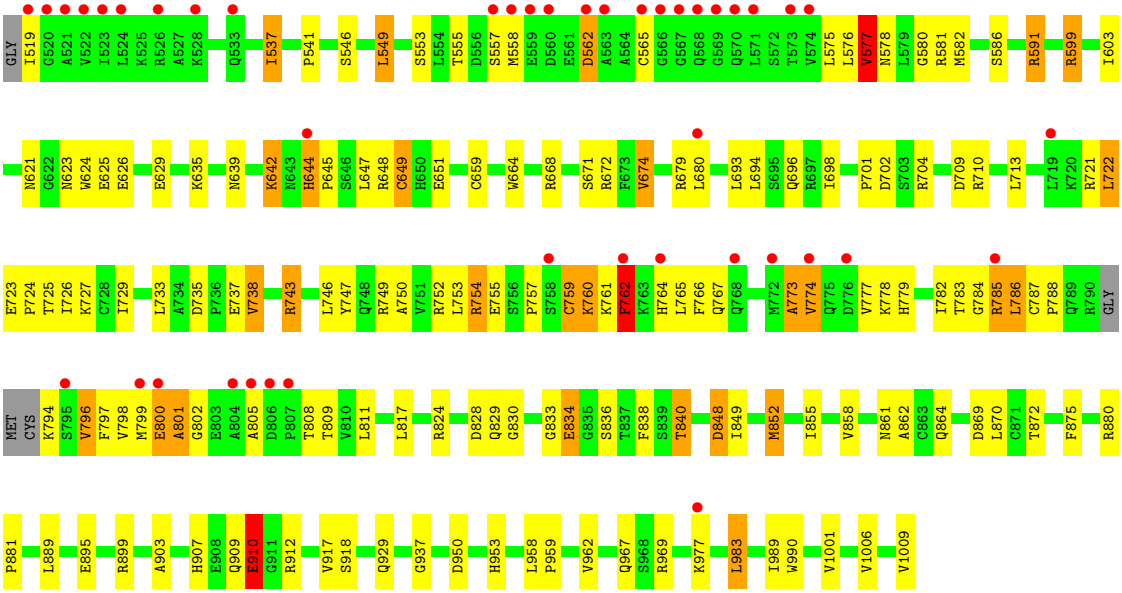
Chain A:



• Molecule 1: Fanconi-associated nuclease 1

Chain B:




GLY I519 G520 A521 V522 I523 L524 K525 R526 A527 K528 Q533 I537 P541 S546 L549 S553 L554 T555 D556 S557 M558 E559 D560 E561 D562 A563 A564 C565 G566 G567 Q568 G569 Q570 L571 S572 T573 V574 L575 L576 V577 N578 L579 G580 R581 M582 S586 R591 R599 I603
N621 G622 N623 W624 E625 E626 E629 K635 N639 K642 N643 H644 P645 S646 L647 R648 C649 H650 E651 C659 W664 R668 S671 R672 F673 V674 R679 L680 L693 L694 S695 Q696 R697 I698 P701 D702 S703 R704 D709 R710 L713 L719 K720 R721 L722
E723 P724 T725 I726 K727 G728 I729 L733 A734 D735 P736 E737 V738 R743 L746 Y747 Q748 R749 A750 V751 R752 L753 R754 E755 S756 P757 S758 C759 K760 K761 F762 K763 H764 L765 F766 Q767 Q768 M772 A773 V774 Q775 D776 V777 K778 H779 I782 T783 G784 R785 L786 C787 P788 Q789 R790 GLY
MET CYS K794 S795 V796 F797 V798 M799 E800 A801 G802 E803 A804 A805 D806 P807 T808 T809 V810 L811 L817 R824 D828 Q829 G830 G833 E834 G835 S836 T837 F838 S839 I840 D848 I849 M852 I855 V858 N861 A862 C863 Q864 D869 L870 C871 T872 F875 R880
P881 L889 E895 R899 A903 H907 E908 Q909 E910 G911 R912 V917 S918 Q929 G937 D950 H953 L958 P959 V962 Q967 S968 R969 K977 L983 I989 W990 V1001 V1006 V1009

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	1.03 (at 3.07Å)	Xtriage
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 (3.10%)	wwPDB-VP
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
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	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 $< |L| >$, $< L^2 >$ 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	0.45	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(^{o})	Ideal(^{o})
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: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
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: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: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:A:556:ASP:HB2	1:A:863:CYS:O	1.87	0.75
1:B:784:GLY:C	1:B:1009:VAL:HG21	2.06	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: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

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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: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: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:370:THR:HB	1:B:586:SER:OG	1.99	0.62
1:A:586:SER:HG	1:B:370:THR:N	1.97	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: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

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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: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: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:762:PHE:C	1:A:762:PHE:CD2	2.80	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

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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:A:624:TRP:HB2	1:A:680:LEU:HD21	1.89	0.54
1:B:762:PHE:C	1:B:762:PHE:CD2	2.80	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: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
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: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: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: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:757:PRO:C	1:A:759:CYS:H	2.14	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: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: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:B:773:ALA:C	1:B:774:VAL:HG23	2.33	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: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: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: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: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: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: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:O	1:A:799:MET:CG	2.64	0.45
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:576:LEU:O	1:B:577:VAL:C	2.55	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: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: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:505:LYS:C	1:A:505:LYS:HE2	2.38	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: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:403:ILE:HD12	1:A:544:VAL:HG21	1.99	0.44
1:A:762:PHE:C	1:A:762:PHE:HD2	2.19	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: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: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: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:A:896:GLU:CD	1:A:896:GLU:H	2.21	0.43
1:B:599:ARG:O	1:B:603:ILE:HG13	2.19	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:459:GLU:C	1:A:461:GLU:H	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:849:ILE:HG23	1:B:852:MET:HE2	1.99	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: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:505:LYS:C	1:B:505:LYS:HE2	2.41	0.41
1:B:648:ARG:O	1:B:649:CYS:C	2.57	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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:B:777:VAL:O	1:B:778:LYS:C	2.60	0.40
1:A:846:LEU:HA	1:A:886:ARG:NH1	2.37	0.40
1:A:991:LEU:HD22	1:A:1001:VAL:HB	2.03	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: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
1:A:784:GLY:O	1:A:1009:VAL:HG11	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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%)	4	24
1	B	622/640 (97%)	534 (86%)	68 (11%)	20 (3%)	4	22
All	All	1229/1280 (96%)	1065 (87%)	126 (10%)	38 (3%)	4	23

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 (i)

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%)	9	31
1	B	548/557 (98%)	498 (91%)	50 (9%)	9	31
All	All	1087/1114 (98%)	988 (91%)	99 (9%)	9	31

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

Sometimes 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 monosaccharides 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, 95^{th} 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%)	0.42	44 (7%) 15 15	69, 97, 161, 189	0
1	B	628/640 (98%)	0.94	102 (16%) 1 2	65, 116, 221, 266	0
All	All	1243/1280 (97%)	0.68	146 (11%) 4 4	65, 104, 200, 266	0

All (146) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	491	GLY	16.2
1	B	506	GLN	14.1
1	B	372	HIS	13.5
1	B	503	LEU	12.5
1	A	795	SER	10.9
1	A	373	PRO	10.4
1	B	485	HIS	9.5
1	B	806	ASP	9.3
1	B	795	SER	9.1
1	A	764	HIS	9.0
1	A	774	VAL	8.9
1	A	372	HIS	8.6
1	A	566	GLY	8.5
1	B	497	VAL	8.3
1	B	519	ILE	8.2
1	B	373	PRO	8.2
1	A	565	CYS	8.0
1	B	573	THR	7.6
1	B	524	LEU	7.6
1	B	509	VAL	7.2
1	B	500	PHE	7.1
1	A	486	LEU	7.0
1	B	499	ALA	7.0
1	B	486	LEU	7.0

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Mol	Chain	Res	Type	RSRZ
1	A	370	THR	7.0
1	B	370	THR	6.9
1	B	764	HIS	6.9
1	B	496	LEU	6.8
1	B	522	VAL	6.7
1	B	461	GLU	6.7
1	B	502	LYS	6.5
1	B	492	GLN	6.5
1	B	431	MET	6.5
1	B	566	GLY	6.4
1	B	807	PRO	6.3
1	B	432	THR	5.9
1	B	568	GLN	5.9
1	B	434	LEU	5.6
1	B	504	ALA	5.6
1	B	507	ARG	5.5
1	A	564	ALA	5.4
1	B	520	GLY	5.3
1	B	774	VAL	5.2
1	A	371	GLY	5.2
1	B	462	LEU	5.2
1	A	571	LEU	5.1
1	B	374	TYR	5.0
1	B	483	THR	5.0
1	B	498	ASP	4.9
1	B	487	VAL	4.9
1	B	482	LYS	4.9
1	A	374	TYR	4.9
1	B	804	ALA	4.8
1	B	495	GLN	4.8
1	B	776	ASP	4.7
1	A	785	ARG	4.7
1	B	493	LYS	4.6
1	B	371	GLY	4.6
1	B	465	LEU	4.6
1	B	469	LEU	4.6
1	B	565	CYS	4.4
1	B	571	LEU	4.4
1	B	558	MET	4.4
1	B	375	TYR	4.4
1	B	489	PRO	4.2
1	B	785	ARG	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	375	TYR	4.1
1	A	573	THR	4.1
1	B	557	SER	4.1
1	B	505	LYS	4.0
1	B	528	LYS	4.0
1	B	533	GLN	4.0
1	B	508	SER	4.0
1	A	433	LYS	4.0
1	B	570	GLN	3.9
1	B	433	LYS	3.9
1	A	776	ASP	3.8
1	A	503	LEU	3.6
1	A	563	ALA	3.6
1	A	507	ARG	3.5
1	A	431	MET	3.5
1	B	523	ILE	3.5
1	B	450	LEU	3.4
1	B	479	SER	3.3
1	B	800	GLU	3.3
1	B	501	LEU	3.3
1	B	559	GLU	3.2
1	A	784	GLY	3.2
1	A	574	VAL	3.1
1	A	562	ASP	3.1
1	A	799	MET	3.0
1	A	794	LYS	2.9
1	B	443	LEU	2.9
1	B	490	ASN	2.9
1	B	458	THR	2.9
1	B	446	VAL	2.8
1	B	644	HIS	2.8
1	A	489	PRO	2.8
1	B	526	ARG	2.8
1	B	799	MET	2.8
1	B	438	GLU	2.7
1	A	567	GLY	2.7
1	B	456	LEU	2.7
1	B	562	ASP	2.7
1	A	457	GLN	2.7
1	B	484	PHE	2.7
1	B	563	ALA	2.7
1	B	521	ALA	2.6

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