



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 01:59 AM UTC

PDB ID : 4F91 / pdb_00004f91
Title : Brr2 Helicase Region
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Deposited on : 2012-05-18
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

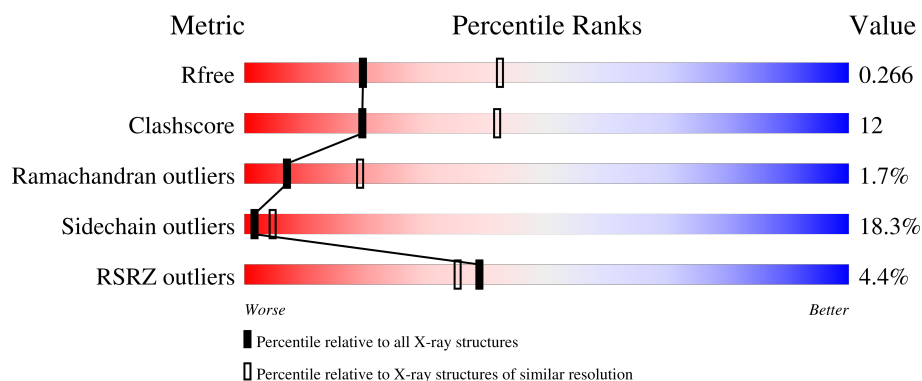
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	B	1724	4% 62% 29% 8%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13865 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 U5 small nuclear ribonucleoprotein 200 kDa helicase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	1724	Total	C	N	O	S	0	0	0
			13859	8857	2371	2559	72			

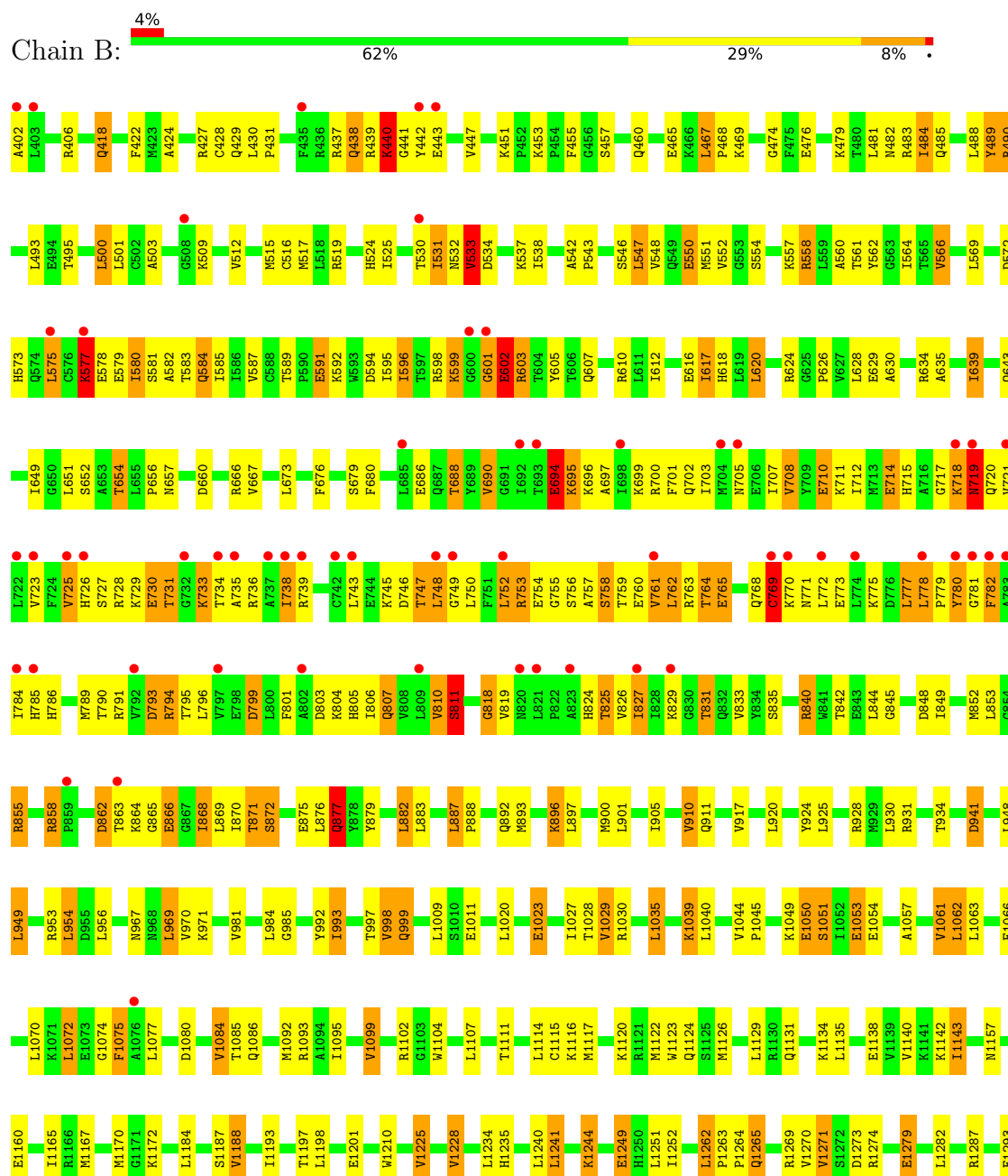
- Molecule 2 is water.

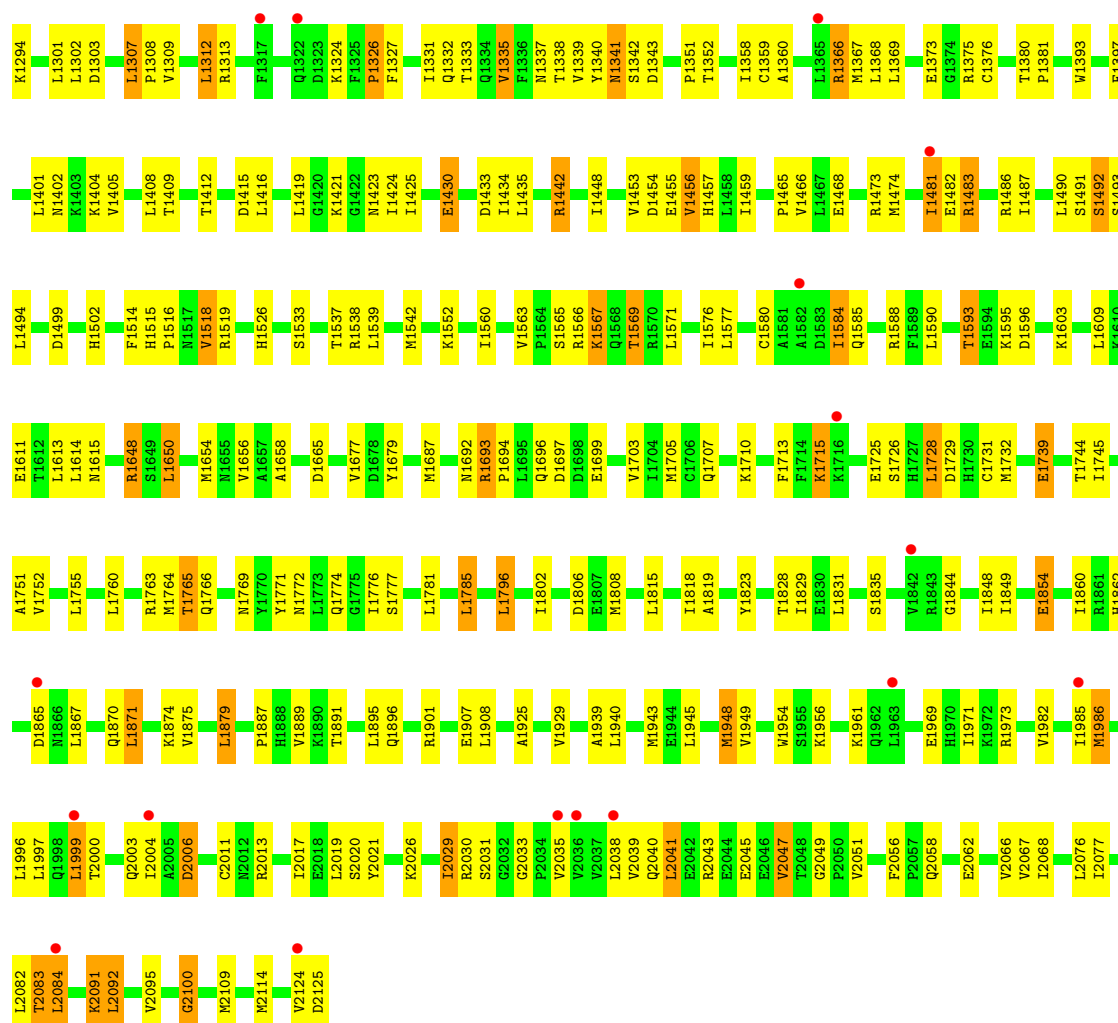
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	6	Total	O	0	0
			6	6		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: U5 small nuclear ribonucleoprotein 200 kDa helicase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	146.26Å 150.50Å 141.96Å 90.00° 120.21° 90.00°	Depositor
Resolution (Å)	48.39 – 2.70 48.39 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.3 (48.39-2.70) 98.3 (48.39-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.224 , 0.272 0.216 , 0.266	Depositor DCC
R_{free} test set	3656 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	65.0	Xtriage
Anisotropy	0.542	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 76.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for k,h,-1/2*h-1/2*k-l 0.000 for -k,-h,-1/2*h+1/2*k-l 0.007 for h,-k,-h-l	Xtriage
F_o , F_c correlation	0.95	EDS
Total number of atoms	13865	wwPDB-VP
Average B, all atoms (Å ²)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	B	0.58	1/14153 (0.0%)	0.98	38/19177 (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	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	910	VAL	CA-CB	6.88	1.63	1.54

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	877	GLN	N-CA-C	-7.84	103.72	113.28
1	B	430	LEU	CA-C-N	6.93	128.51	119.84
1	B	430	LEU	C-N-CA	6.93	128.51	119.84
1	B	440	LYS	N-CA-C	6.87	120.85	111.17
1	B	811	SER	N-CA-C	6.46	117.66	108.74
1	B	1563	VAL	CA-C-N	-6.33	113.25	119.64
1	B	1563	VAL	C-N-CA	-6.33	113.25	119.64
1	B	424	ALA	N-CA-C	-6.25	105.62	113.18
1	B	1693	ARG	CA-C-N	6.21	126.39	119.32
1	B	1693	ARG	C-N-CA	6.21	126.39	119.32
1	B	2047	VAL	N-CA-C	6.14	116.55	107.15
1	B	756	SER	N-CA-C	-6.13	104.87	113.20
1	B	503	ALA	CA-C-N	-6.12	113.97	120.03
1	B	503	ALA	C-N-CA	-6.12	113.97	120.03
1	B	778	LEU	N-CA-C	6.08	120.50	112.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	818	GLY	N-CA-C	6.08	120.55	112.77
1	B	1565	SER	N-CA-C	5.81	116.76	108.74
1	B	694	GLU	N-CA-C	5.78	117.57	108.96
1	B	1312	LEU	N-CA-C	-5.77	101.30	109.96
1	B	714	GLU	N-CA-C	-5.71	105.98	113.17
1	B	1054	GLU	N-CA-C	-5.65	103.63	110.13
1	B	771	ASN	N-CA-C	5.60	118.70	109.85
1	B	441	GLY	N-CA-C	-5.56	100.01	113.18
1	B	803	ASP	N-CA-C	-5.43	105.52	111.82
1	B	1044	VAL	CA-C-N	5.41	126.61	119.84
1	B	1044	VAL	C-N-CA	5.41	126.61	119.84
1	B	858	ARG	CA-C-N	5.32	126.49	119.84
1	B	858	ARG	C-N-CA	5.32	126.49	119.84
1	B	2056	PHE	CA-C-N	5.32	126.02	120.12
1	B	2056	PHE	C-N-CA	5.32	126.02	120.12
1	B	601	GLY	N-CA-C	-5.31	108.73	115.31
1	B	708	VAL	N-CA-C	5.26	115.47	110.42
1	B	1402	ASN	N-CA-C	5.24	119.25	112.86
1	B	2084	LEU	N-CA-C	5.11	119.64	113.41
1	B	1341	ASN	N-CA-C	5.10	118.33	112.57
1	B	998	VAL	CB-CA-C	-5.05	105.42	111.88
1	B	1875	VAL	CA-C-N	5.00	124.78	119.28
1	B	1875	VAL	C-N-CA	5.00	124.78	119.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	440	LYS	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	B	13859	0	14001	322	0
2	B	6	0	0	0	0
All	All	13865	0	14001	322	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 12.

All (322) 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:1049:LYS:O	1:B:1051:SER:N	2.09	0.85
1:B:700:ARG:HA	1:B:703:ILE:HD12	1.57	0.85
1:B:1940:LEU:HD22	1:B:2109:MET:HE3	1.62	0.82
1:B:753:ARG:NH1	1:B:779:PRO:O	2.12	0.81
1:B:2013:ARG:HE	1:B:2049:GLY:HA3	1.49	0.78
1:B:569:LEU:HD11	1:B:575:LEU:HD11	1.67	0.76
1:B:1819:ALA:HB2	1:B:1829:ILE:HG12	1.68	0.76
1:B:660:ASP:OD1	1:B:928:ARG:NH1	2.19	0.76
1:B:2043:ARG:HH11	1:B:2084:LEU:HD21	1.49	0.76
1:B:770:LYS:HD3	1:B:793:ASP:HB3	1.66	0.76
1:B:715:HIS:ND1	1:B:719:ASN:OD1	2.20	0.75
1:B:626:PRO:HG2	1:B:896:LYS:HG3	1.71	0.72
1:B:474:GLY:O	1:B:558:ARG:NH2	2.24	0.71
1:B:948:LEU:O	1:B:953:ARG:NH1	2.24	0.71
1:B:2068:ILE:HD11	1:B:2092:LEU:HD13	1.74	0.69
1:B:997:THR:OG1	1:B:1023:GLU:OE1	2.06	0.69
1:B:1901:ARG:HH12	1:B:1961:LYS:HE3	1.58	0.69
1:B:2066:VAL:HG23	1:B:2082:LEU:HD21	1.73	0.69
1:B:1765:THR:HG23	1:B:1781:LEU:HD13	1.73	0.69
1:B:701:PHE:O	1:B:705:ASN:ND2	2.25	0.69
1:B:735:ALA:HB2	1:B:810:VAL:HG11	1.74	0.69
1:B:1459:ILE:HD11	1:B:1468:GLU:HG3	1.75	0.69
1:B:1360:ALA:HB2	1:B:1490:LEU:HD11	1.75	0.68
1:B:720:GLN:NE2	1:B:801:PHE:O	2.27	0.68
1:B:1519:ARG:HH22	1:B:1692:ASN:HB2	1.60	0.67
1:B:438:GLN:HB3	1:B:440:LYS:HG2	1.77	0.67
1:B:1249:GLU:CD	1:B:1249:GLU:H	2.02	0.67
1:B:566:VAL:HB	1:B:585:ILE:HB	1.76	0.67
1:B:1729:ASP:HA	1:B:1732:MET:HE2	1.77	0.67
1:B:759:THR:OG1	1:B:760:GLU:N	2.28	0.66
1:B:1201:GLU:HB3	1:B:1251:LEU:HD11	1.78	0.66
1:B:785:HIS:HB3	1:B:811:SER:HB2	1.76	0.66
1:B:727:SER:HB3	1:B:729:LYS:CG	2.26	0.65
1:B:694:GLU:CD	1:B:695:LYS:H	2.05	0.65
1:B:777:LEU:HA	1:B:780:TYR:HE1	1.62	0.65
1:B:1351:PRO:HG3	1:B:1516:PRO:HA	1.80	0.64
1:B:738:ILE:HD11	1:B:782:PHE:CZ	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1815:LEU:HB3	1:B:1829:ILE:HD13	1.79	0.64
1:B:703:ILE:O	1:B:707:ILE:HG12	1.98	0.64
1:B:1456:VAL:HG23	1:B:1491:SER:HB2	1.78	0.64
1:B:1519:ARG:NH2	1:B:1692:ASN:HB2	2.13	0.63
1:B:2029:ILE:HD11	1:B:2035:VAL:HA	1.81	0.63
1:B:969:LEU:HD13	1:B:985:GLY:HA2	1.81	0.62
1:B:763:ARG:HD2	1:B:805:HIS:CE1	2.34	0.62
1:B:882:LEU:HG	1:B:887:LEU:HD12	1.82	0.62
1:B:1093:ARG:NH1	1:B:1273:ASP:OD2	2.32	0.61
1:B:550:GLU:HB2	1:B:818:GLY:O	2.01	0.61
1:B:1228:VAL:HG11	1:B:1264:PRO:HD2	1.81	0.61
1:B:793:ASP:OD1	1:B:793:ASP:N	2.33	0.60
1:B:905:ILE:HG22	1:B:981:VAL:HG22	1.82	0.60
1:B:1262:LEU:HD22	1:B:1263:PRO:HD2	1.83	0.60
1:B:577:LYS:HB2	1:B:579:GLU:HG2	1.84	0.60
1:B:781:GLY:O	1:B:807:GLN:N	2.33	0.60
1:B:1430:GLU:H	1:B:1430:GLU:CD	2.10	0.60
1:B:708:VAL:O	1:B:712:ILE:HG12	2.01	0.60
1:B:1901:ARG:NH2	1:B:1961:LYS:O	2.36	0.59
1:B:761:VAL:O	1:B:765:GLU:N	2.31	0.59
1:B:735:ALA:HB1	1:B:782:PHE:HE1	1.68	0.58
1:B:1210:TRP:HZ3	1:B:1241:LEU:HD13	1.69	0.58
1:B:824:HIS:HD2	1:B:825:THR:HG22	1.68	0.58
1:B:1405:VAL:HG22	1:B:1424:ILE:HB	1.84	0.58
1:B:482:ASN:HB3	1:B:485:GLN:CD	2.28	0.58
1:B:743:LEU:HA	1:B:747:THR:HA	1.85	0.58
1:B:768:GLN:HA	1:B:778:LEU:HD12	1.84	0.58
1:B:1123:TRP:HD1	1:B:1126:MET:HE3	1.69	0.58
1:B:2043:ARG:NH1	1:B:2084:LEU:HD21	2.19	0.57
1:B:871:THR:OG1	1:B:872:SER:N	2.35	0.57
1:B:1538:ARG:NH1	1:B:1665:ASP:OD2	2.38	0.57
1:B:738:ILE:HD11	1:B:782:PHE:HZ	1.69	0.57
1:B:763:ARG:HD2	1:B:805:HIS:NE2	2.20	0.56
1:B:1301:LEU:HD22	1:B:1518:VAL:HG22	1.88	0.56
1:B:1887:PRO:O	1:B:1891:THR:HG23	2.05	0.56
1:B:1188:VAL:HG12	1:B:1282:LEU:HD21	1.87	0.56
1:B:752:LEU:HD22	1:B:807:GLN:HB3	1.88	0.56
1:B:2051:VAL:HG22	1:B:2062:GLU:HG3	1.88	0.56
1:B:993:ILE:HD11	1:B:998:VAL:HG22	1.88	0.56
1:B:688:THR:HB	1:B:868:ILE:HG23	1.88	0.56
1:B:543:PRO:O	1:B:624:ARG:NH2	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2091:LYS:H	1:B:2091:LYS:HD2	1.71	0.55
1:B:785:HIS:CE1	1:B:794:ARG:HG3	2.42	0.55
1:B:1193:ILE:HB	1:B:1197:THR:HG23	1.88	0.55
1:B:577:LYS:HG3	1:B:580:ILE:HD13	1.88	0.54
1:B:707:ILE:HA	1:B:710:GLU:OE1	2.08	0.54
1:B:736:ARG:HA	1:B:739:ARG:HB3	1.89	0.54
1:B:864:LYS:HG3	1:B:865:GLY:H	1.72	0.54
1:B:1269:ARG:HD2	1:B:1279:GLU:OE2	2.08	0.54
1:B:548:VAL:HG13	1:B:587:VAL:HG12	1.88	0.54
1:B:1896:GLN:HB3	1:B:1954:TRP:HZ2	1.72	0.53
1:B:569:LEU:O	1:B:573:HIS:NE2	2.41	0.53
1:B:509:LYS:HE2	1:B:652:SER:O	2.07	0.53
1:B:781:GLY:HA3	1:B:807:GLN:HB2	1.89	0.53
1:B:734:THR:OG1	1:B:829:LYS:NZ	2.36	0.53
1:B:1739:GLU:HG3	1:B:1744:THR:HB	1.91	0.53
1:B:402:ALA:O	1:B:406:ARG:NH2	2.41	0.53
1:B:512:VAL:HA	1:B:515:MET:HE2	1.90	0.53
1:B:1533:SER:HA	1:B:1707:GLN:NE2	2.23	0.53
1:B:493:LEU:O	1:B:519:ARG:NH2	2.37	0.53
1:B:2020:SER:HB3	1:B:2040:GLN:HB2	1.92	0.53
1:B:727:SER:HB3	1:B:729:LYS:HG3	1.89	0.52
1:B:1456:VAL:CG2	1:B:1491:SER:HB2	2.39	0.52
1:B:2000:THR:HG23	1:B:2003:GLN:H	1.73	0.52
1:B:777:LEU:HA	1:B:780:TYR:CE1	2.44	0.52
1:B:1526:HIS:HB2	1:B:1703:VAL:HG22	1.90	0.52
1:B:1312:LEU:HD12	1:B:1340:TYR:CZ	2.45	0.52
1:B:840:ARG:NH2	1:B:842:THR:HG22	2.23	0.52
1:B:1560:ILE:HG13	1:B:1658:ALA:HB2	1.92	0.52
1:B:1157:ASN:HB3	1:B:1160:GLU:OE1	2.10	0.52
1:B:1728:LEU:HB3	1:B:1760:LEU:HD22	1.92	0.52
1:B:1925:ALA:O	1:B:1929:VAL:HG23	2.10	0.52
1:B:1796:LEU:HB3	1:B:1802:ILE:HG12	1.91	0.51
1:B:439:ARG:HB2	1:B:442:TYR:CZ	2.45	0.51
1:B:467:LEU:HB2	1:B:468:PRO:HD2	1.93	0.51
1:B:1057:ALA:O	1:B:1061:VAL:HG13	2.11	0.51
1:B:1648:ARG:HD3	1:B:1679:TYR:CE1	2.46	0.51
1:B:1650:LEU:O	1:B:1654:MET:HG3	2.10	0.51
1:B:796:LEU:HA	1:B:799:ASP:OD1	2.11	0.50
1:B:1945:LEU:HA	1:B:1948:MET:HG2	1.93	0.50
1:B:1066:PHE:CG	1:B:1085:THR:HG21	2.46	0.50
1:B:594:ASP:O	1:B:598:ARG:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:712:ILE:CD1	1:B:721:VAL:HG11	2.41	0.50
1:B:853:LEU:HD22	1:B:883:LEU:HD22	1.94	0.50
1:B:453:LYS:HB3	1:B:483:ARG:HH12	1.77	0.50
1:B:725:VAL:HG11	1:B:730:GLU:HG2	1.94	0.50
1:B:542:ALA:HB1	1:B:547:LEU:HD13	1.94	0.49
1:B:578:GLU:O	1:B:581:SER:HB3	2.12	0.49
1:B:753:ARG:C	1:B:755:GLY:H	2.20	0.49
1:B:552:VAL:HG13	1:B:566:VAL:HG22	1.94	0.49
1:B:1982:VAL:O	1:B:1986:MET:HG2	2.12	0.49
1:B:1035:LEU:O	1:B:1039:LYS:HG2	2.11	0.49
1:B:1338:THR:O	1:B:1342:SER:HB2	2.12	0.49
1:B:2031:SER:C	1:B:2033:GLY:H	2.21	0.49
1:B:516:CYS:SG	1:B:649:ILE:HG12	2.52	0.49
1:B:768:GLN:O	1:B:770:LYS:N	2.43	0.49
1:B:1986:MET:HE2	1:B:1986:MET:HA	1.95	0.49
1:B:538:ILE:HB	1:B:585:ILE:HG13	1.95	0.49
1:B:1939:ALA:O	1:B:1943:MET:HG3	2.13	0.49
1:B:690:VAL:HG13	1:B:870:ILE:HA	1.94	0.49
1:B:729:LYS:HB3	1:B:1075:PHE:CE1	2.47	0.49
1:B:853:LEU:HD12	1:B:853:LEU:N	2.28	0.48
1:B:723:VAL:HG22	1:B:827:ILE:HG23	1.95	0.48
1:B:1271:VAL:HG13	1:B:1279:GLU:HB2	1.96	0.48
1:B:484:ILE:HD11	1:B:680:PHE:HB3	1.94	0.48
1:B:531:ILE:HG12	1:B:562:TYR:O	2.13	0.48
1:B:603:ARG:O	1:B:607:GLN:HB2	2.13	0.48
1:B:876:LEU:HD22	1:B:879:TYR:CE1	2.48	0.48
1:B:1184:LEU:HD12	1:B:1270:VAL:HG11	1.96	0.48
1:B:1335:VAL:HG11	1:B:1359:CYS:SG	2.53	0.48
1:B:760:GLU:O	1:B:764:THR:HB	2.13	0.48
1:B:635:ALA:O	1:B:639:ILE:HD12	2.14	0.48
1:B:824:HIS:CD2	1:B:825:THR:HG22	2.48	0.48
1:B:941:ASP:OD1	1:B:941:ASP:N	2.32	0.48
1:B:1165:ILE:HG23	1:B:1167:MET:H	1.79	0.48
1:B:2006:ASP:OD1	1:B:2006:ASP:N	2.45	0.48
1:B:1332:GLN:CD	1:B:1358:ILE:HD11	2.39	0.48
1:B:1982:VAL:O	1:B:1985:ILE:HG13	2.13	0.48
1:B:1029:VAL:HG11	1:B:1053:GLU:O	2.14	0.48
1:B:1879:LEU:HD23	1:B:1889:VAL:HG13	1.97	0.47
1:B:626:PRO:HD3	1:B:892:GLN:HB2	1.96	0.47
1:B:794:ARG:HA	1:B:794:ARG:NE	2.29	0.47
1:B:967:ASN:HA	1:B:999:GLN:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1772:ASN:O	1:B:1774:GLN:NE2	2.46	0.47
1:B:1999:LEU:HB2	1:B:2004:ILE:HD11	1.96	0.47
1:B:2000:THR:HG22	1:B:2003:GLN:CD	2.40	0.47
1:B:853:LEU:HD12	1:B:853:LEU:H	1.78	0.47
1:B:1409:THR:H	1:B:1415:ASP:CG	2.21	0.47
1:B:524:HIS:HB3	1:B:532:ASN:HB2	1.95	0.47
1:B:591:GLU:H	1:B:591:GLU:HG2	1.44	0.47
1:B:930:LEU:HD23	1:B:949:LEU:HD22	1.96	0.47
1:B:712:ILE:HD12	1:B:721:VAL:HG11	1.97	0.47
1:B:917:VAL:HG13	1:B:953:ARG:HB2	1.95	0.47
1:B:579:GLU:O	1:B:583:THR:HG23	2.14	0.47
1:B:726:HIS:HB3	1:B:833:VAL:HG23	1.96	0.47
1:B:1340:TYR:O	1:B:1366:ARG:HG3	2.15	0.47
1:B:1481:ILE:O	1:B:1483:ARG:HD2	2.15	0.47
1:B:1577:LEU:HD11	1:B:1615:ASN:HB3	1.96	0.47
1:B:654:THR:HG21	1:B:676:PHE:O	2.14	0.46
1:B:1099:VAL:HG21	1:B:1107:LEU:HG	1.97	0.46
1:B:758:SER:O	1:B:762:LEU:HB2	2.16	0.46
1:B:1140:VAL:HA	1:B:1143:ILE:HG23	1.98	0.46
1:B:1986:MET:SD	1:B:2011:CYS:HB3	2.56	0.46
1:B:727:SER:HB3	1:B:729:LYS:HG2	1.97	0.46
1:B:707:ILE:O	1:B:711:LYS:HD3	2.15	0.46
1:B:1961:LYS:HG2	1:B:1971:ILE:HD11	1.98	0.46
1:B:1973:ARG:HB2	1:B:1997:LEU:HD11	1.97	0.46
1:B:542:ALA:O	1:B:589:THR:HA	2.16	0.46
1:B:858:ARG:H	1:B:862:ASP:HB2	1.81	0.46
1:B:1165:ILE:HG23	1:B:1167:MET:N	2.31	0.46
1:B:1416:LEU:HD21	1:B:1442:ARG:HD2	1.96	0.46
1:B:1710:LYS:O	1:B:1713:PHE:HB3	2.16	0.46
1:B:1870:GLN:O	1:B:1874:LYS:HD3	2.16	0.46
1:B:1337:ASN:O	1:B:1341:ASN:HB2	2.16	0.46
1:B:1419:LEU:HD22	1:B:1435:LEU:HD13	1.97	0.46
1:B:1648:ARG:HG2	1:B:1648:ARG:HH21	1.80	0.46
1:B:738:ILE:HD12	1:B:738:ILE:C	2.41	0.45
1:B:1760:LEU:HD11	1:B:1764:MET:HE3	1.99	0.45
1:B:599:LYS:HD2	1:B:599:LYS:HA	1.64	0.45
1:B:601:GLY:HA3	1:B:1537:THR:HG23	1.97	0.45
1:B:1308:PRO:HA	1:B:1327:PHE:HD1	1.80	0.45
1:B:481:LEU:HD22	1:B:485:GLN:HB3	1.98	0.45
1:B:869:LEU:HG	1:B:871:THR:HG22	1.98	0.45
1:B:579:GLU:C	1:B:582:ALA:H	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1116:LYS:O	1:B:1120:LYS:HB2	2.16	0.45
1:B:1343:ASP:OD2	1:B:1366:ARG:NE	2.50	0.45
1:B:726:HIS:CE1	1:B:831:THR:HA	2.52	0.45
1:B:743:LEU:HD21	1:B:750:LEU:HD13	1.99	0.45
1:B:848:ASP:O	1:B:852:MET:HG3	2.16	0.45
1:B:1225:VAL:HG13	1:B:1235:HIS:HB3	1.98	0.45
1:B:1307:LEU:H	1:B:1333:THR:HG21	1.82	0.45
1:B:1552:LYS:HE3	1:B:1552:LYS:HB2	1.66	0.45
1:B:1576:ILE:O	1:B:1580:CYS:HB2	2.17	0.45
1:B:777:LEU:HB3	1:B:782:PHE:HB3	2.00	0.44
1:B:1806:ASP:C	1:B:1808:MET:H	2.25	0.44
1:B:728:ARG:HB2	1:B:786:HIS:HB2	1.98	0.44
1:B:745:LYS:O	1:B:748:LEU:HD13	2.17	0.44
1:B:1351:PRO:CG	1:B:1516:PRO:HA	2.46	0.44
1:B:1457:HIS:ND1	1:B:1492:SER:HB2	2.32	0.44
1:B:1577:LEU:HD11	1:B:1615:ASN:CB	2.47	0.44
1:B:1373:GLU:HG2	1:B:1423:ASN:HD21	1.83	0.44
1:B:1120:LYS:HG3	1:B:1131:GLN:HG2	1.99	0.44
1:B:1593:THR:O	1:B:1596:ASP:HB2	2.18	0.44
1:B:1499:ASP:OD1	1:B:1766:GLN:HG3	2.17	0.44
1:B:628:LEU:HD23	1:B:628:LEU:HA	1.74	0.44
1:B:949:LEU:HD12	1:B:949:LEU:HA	1.89	0.44
1:B:769:CYS:HA	1:B:775:LYS:HE2	1.99	0.44
1:B:1381:PRO:HG2	1:B:1455:GLU:HB2	1.99	0.44
1:B:1648:ARG:HB2	1:B:1687:MET:CE	2.48	0.44
1:B:656:PRO:HB2	1:B:888:PRO:HA	1.99	0.44
1:B:1493:SER:OG	1:B:1514:PHE:O	2.21	0.44
1:B:1367:MET:SD	1:B:1376:CYS:HB2	2.58	0.43
1:B:753:ARG:C	1:B:755:GLY:N	2.76	0.43
1:B:949:LEU:O	1:B:953:ARG:HG3	2.18	0.43
1:B:1080:ASP:O	1:B:1084:VAL:HG13	2.18	0.43
1:B:1542:MET:HE2	1:B:1705:MET:HB3	1.98	0.43
1:B:1948:MET:HE3	1:B:1954:TRP:HA	1.99	0.43
1:B:877:GLN:O	1:B:877:GLN:HG2	2.18	0.43
1:B:1062:LEU:HA	1:B:1062:LEU:HD12	1.71	0.43
1:B:1715:LYS:HB3	1:B:1715:LYS:HE3	1.77	0.43
1:B:1049:LYS:HE3	1:B:1049:LYS:HB2	1.75	0.43
1:B:1228:VAL:HG13	1:B:1265:GLN:O	2.19	0.43
1:B:1763:ARG:HD2	1:B:1763:ARG:HA	1.86	0.43
1:B:1844:GLY:O	1:B:1848:ILE:HG13	2.19	0.43
1:B:2100:GLY:HA2	1:B:2125:ASP:CG	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1117:MET:HG2	1:B:1122:MET:O	2.18	0.43
1:B:543:PRO:HG3	1:B:616:GLU:HB2	2.01	0.43
1:B:548:VAL:O	1:B:552:VAL:HG23	2.18	0.43
1:B:845:GLY:O	1:B:849:ILE:HD12	2.18	0.43
1:B:1430:GLU:O	1:B:1434:ILE:HG22	2.18	0.43
1:B:1515:HIS:CG	1:B:1516:PRO:HD2	2.54	0.43
1:B:2041:LEU:HD13	1:B:2041:LEU:HA	1.86	0.43
1:B:418:GLN:HG3	1:B:422:PHE:HA	2.01	0.42
1:B:1095:ILE:HG22	1:B:1111:THR:HG21	2.00	0.42
1:B:1433:ASP:OD2	1:B:1473:ARG:NH2	2.52	0.42
1:B:533:VAL:O	1:B:584:GLN:NE2	2.52	0.42
1:B:801:PHE:HA	1:B:806:ILE:HB	2.00	0.42
1:B:1481:ILE:C	1:B:1483:ARG:H	2.27	0.42
1:B:1871:LEU:HD23	1:B:1871:LEU:HA	1.86	0.42
1:B:490:ARG:HE	1:B:490:ARG:HB2	1.71	0.42
1:B:617:ILE:HG22	1:B:651:LEU:O	2.20	0.42
1:B:618:HIS:C	1:B:620:LEU:H	2.26	0.42
1:B:1331:ILE:O	1:B:1335:VAL:HB	2.19	0.42
1:B:1697:ASP:HB3	1:B:1699:GLU:O	2.18	0.42
1:B:801:PHE:HD1	1:B:806:ILE:CG2	2.31	0.42
1:B:853:LEU:C	1:B:855:ARG:H	2.27	0.42
1:B:1339:VAL:HA	1:B:1486:ARG:HH22	1.84	0.42
1:B:1755:LEU:HD13	1:B:1785:LEU:HD12	2.01	0.42
1:B:745:LYS:HB2	1:B:748:LEU:HD22	2.00	0.42
1:B:1339:VAL:HA	1:B:1486:ARG:NH2	2.35	0.42
1:B:1077:LEU:HD12	1:B:1077:LEU:HA	1.84	0.42
1:B:1693:ARG:HA	1:B:1694:PRO:HD2	1.78	0.42
1:B:500:LEU:HB2	1:B:667:VAL:HG21	2.01	0.42
1:B:1244:LYS:H	1:B:1244:LYS:HG3	1.36	0.42
1:B:629:GLU:CD	1:B:924:TYR:HB3	2.45	0.42
1:B:719:ASN:HD22	1:B:719:ASN:HA	1.47	0.42
1:B:1120:LYS:HA	1:B:1120:LYS:HD2	1.89	0.42
1:B:455:PHE:CE1	1:B:460:GLN:HA	2.54	0.42
1:B:547:LEU:HD22	1:B:551:MET:HG2	2.01	0.42
1:B:554:SER:O	1:B:558:ARG:HG2	2.20	0.42
1:B:1393:TRP:O	1:B:1397:PHE:N	2.51	0.42
1:B:2062:GLU:O	1:B:2083:THR:HG22	2.20	0.42
1:B:1567:LYS:H	1:B:1567:LYS:CE	2.33	0.41
1:B:748:LEU:O	1:B:750:LEU:N	2.53	0.41
1:B:755:GLY:C	1:B:757:ALA:H	2.29	0.41
1:B:1099:VAL:HG22	1:B:1104:TRP:HE3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1093:ARG:HD2	1:B:1115:CYS:SG	2.61	0.41
1:B:560:ALA:C	1:B:562:TYR:H	2.28	0.41
1:B:440:LYS:HD2	1:B:440:LYS:HA	1.76	0.41
1:B:517:MET:HG2	1:B:538:ILE:HG21	2.03	0.41
1:B:1142:LYS:HD2	1:B:1142:LYS:HA	1.96	0.41
1:B:592:LYS:HE3	1:B:596:ILE:HD11	2.03	0.41
1:B:630:ALA:O	1:B:634:ARG:HB2	2.19	0.41
1:B:656:PRO:O	1:B:657:ASN:HB2	2.20	0.41
1:B:533:VAL:HG22	1:B:584:GLN:CD	2.45	0.41
1:B:954:LEU:HD23	1:B:954:LEU:HA	1.93	0.41
1:B:1725:GLU:HB3	1:B:1771:TYR:OH	2.20	0.41
1:B:1726:SER:OG	1:B:1728:LEU:HB2	2.21	0.41
1:B:1745:ILE:HD13	1:B:1751:ALA:HA	2.02	0.41
1:B:2000:THR:H	1:B:2003:GLN:HB2	1.86	0.41
1:B:532:ASN:O	1:B:534:ASP:N	2.53	0.41
1:B:727:SER:C	1:B:729:LYS:H	2.29	0.41
1:B:733:LYS:O	1:B:736:ARG:HB3	2.20	0.41
1:B:1040:LEU:HD11	1:B:1072:LEU:HD11	2.02	0.41
1:B:437:ARG:HD3	1:B:439:ARG:HH11	1.85	0.41
1:B:696:LYS:O	1:B:700:ARG:N	2.34	0.41
1:B:1381:PRO:HD3	1:B:1454:ASP:O	2.20	0.41
1:B:686:GLU:O	1:B:866:GLU:HA	2.21	0.40
1:B:731:THR:HG21	1:B:786:HIS:CD2	2.55	0.40
1:B:827:ILE:HD11	1:B:870:ILE:HD11	2.02	0.40
1:B:1309:VAL:HG23	1:B:1326:PRO:O	2.20	0.40
1:B:1566:ARG:O	1:B:1569:THR:HG22	2.21	0.40
1:B:1908:LEU:HD23	1:B:1908:LEU:HA	1.87	0.40
1:B:602:GLU:HA	1:B:605:TYR:CE2	2.56	0.40
1:B:1613:LEU:HD23	1:B:1613:LEU:HA	1.94	0.40
1:B:489:TYR:O	1:B:493:LEU:HB2	2.20	0.40
1:B:699:LYS:HA	1:B:702:GLN:HG2	2.04	0.40
1:B:827:ILE:HD11	1:B:870:ILE:CD1	2.51	0.40
1:B:1434:ILE:HD13	1:B:1823:TYR:HB2	2.02	0.40
1:B:2013:ARG:NE	1:B:2049:GLY:HA3	2.27	0.40
1:B:1828:THR:OG1	1:B:1854:GLU:OE2	2.37	0.40
1:B:617:ILE:O	1:B:617:ILE:HG13	2.21	0.40
1:B:718:LYS:HD3	1:B:719:ASN:N	2.37	0.40
1:B:831:THR:HG21	1:B:869:LEU:HD11	2.03	0.40
1:B:1567:LYS:H	1:B:1567:LYS:HE3	1.85	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	B	1722/1724 (100%)	1566 (91%)	126 (7%)	30 (2%)	7	19

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	431	PRO
1	B	457	SER
1	B	577	LYS
1	B	747	THR
1	B	1050	GLU
1	B	533	VAL
1	B	602	GLU
1	B	695	LYS
1	B	697	ALA
1	B	719	ASN
1	B	746	ASP
1	B	769	CYS
1	B	789	MET
1	B	1584	ILE
1	B	2100	GLY
1	B	428	CYS
1	B	749	GLY
1	B	754	GLU
1	B	791	ARG
1	B	804	LYS
1	B	875	GLU
1	B	1074	GLY
1	B	1303	ASP
1	B	561	THR
1	B	1075	PHE
1	B	1051	SER
1	B	1326	PRO
1	B	1465	PRO

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Mol	Chain	Res	Type
1	B	1045	PRO
1	B	717	GLY

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	B	1542/1542 (100%)	1260 (82%)	282 (18%)	2 5

All (282) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	418	GLN
1	B	427	ARG
1	B	429	GLN
1	B	438	GLN
1	B	440	LYS
1	B	443	GLU
1	B	447	VAL
1	B	451	LYS
1	B	465	GLU
1	B	467	LEU
1	B	469	LYS
1	B	476	GLU
1	B	479	LYS
1	B	484	ILE
1	B	488	LEU
1	B	489	TYR
1	B	490	ARG
1	B	495	THR
1	B	500	LEU
1	B	501	LEU
1	B	525	ILE
1	B	530	THR
1	B	531	ILE
1	B	533	VAL

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Mol	Chain	Res	Type
1	B	537	LYS
1	B	546	SER
1	B	547	LEU
1	B	550	GLU
1	B	557	LYS
1	B	558	ARG
1	B	564	ILE
1	B	566	VAL
1	B	572	ASP
1	B	575	LEU
1	B	577	LYS
1	B	580	ILE
1	B	584	GLN
1	B	591	GLU
1	B	595	ILE
1	B	596	ILE
1	B	599	LYS
1	B	602	GLU
1	B	603	ARG
1	B	610	ARG
1	B	612	ILE
1	B	617	ILE
1	B	620	LEU
1	B	639	ILE
1	B	643	GLN
1	B	654	THR
1	B	666	ARG
1	B	673	LEU
1	B	679	SER
1	B	688	THR
1	B	690	VAL
1	B	694	GLU
1	B	710	GLU
1	B	714	GLU
1	B	718	LYS
1	B	719	ASN
1	B	725	VAL
1	B	730	GLU
1	B	731	THR
1	B	733	LYS
1	B	738	ILE
1	B	748	LEU

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Mol	Chain	Res	Type
1	B	752	LEU
1	B	753	ARG
1	B	758	SER
1	B	761	VAL
1	B	762	LEU
1	B	764	THR
1	B	765	GLU
1	B	769	CYS
1	B	772	LEU
1	B	773	GLU
1	B	777	LEU
1	B	780	TYR
1	B	782	PHE
1	B	784	ILE
1	B	790	THR
1	B	793	ASP
1	B	794	ARG
1	B	795	THR
1	B	799	ASP
1	B	807	GLN
1	B	810	VAL
1	B	811	SER
1	B	819	VAL
1	B	825	THR
1	B	826	VAL
1	B	827	ILE
1	B	831	THR
1	B	835	SER
1	B	840	ARG
1	B	844	LEU
1	B	855	ARG
1	B	862	ASP
1	B	863	THR
1	B	866	GLU
1	B	868	ILE
1	B	871	THR
1	B	872	SER
1	B	877	GLN
1	B	882	LEU
1	B	887	LEU
1	B	893	MET
1	B	896	LYS

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Mol	Chain	Res	Type
1	B	897	LEU
1	B	900	MET
1	B	901	LEU
1	B	910	VAL
1	B	911	GLN
1	B	920	LEU
1	B	925	LEU
1	B	931	ARG
1	B	934	THR
1	B	941	ASP
1	B	949	LEU
1	B	954	LEU
1	B	956	LEU
1	B	969	LEU
1	B	970	VAL
1	B	971	LYS
1	B	984	LEU
1	B	992	TYR
1	B	993	ILE
1	B	999	GLN
1	B	1009	LEU
1	B	1011	GLU
1	B	1020	LEU
1	B	1023	GLU
1	B	1027	ILE
1	B	1028	THR
1	B	1029	VAL
1	B	1030	ARG
1	B	1035	LEU
1	B	1039	LYS
1	B	1050	GLU
1	B	1053	GLU
1	B	1061	VAL
1	B	1062	LEU
1	B	1063	LEU
1	B	1070	LEU
1	B	1072	LEU
1	B	1084	VAL
1	B	1086	GLN
1	B	1092	MET
1	B	1099	VAL
1	B	1102	ARG

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Mol	Chain	Res	Type
1	B	1114	LEU
1	B	1124	GLN
1	B	1129	LEU
1	B	1134	LYS
1	B	1135	LEU
1	B	1138	GLU
1	B	1143	ILE
1	B	1170	MET
1	B	1172	LYS
1	B	1187	SER
1	B	1188	VAL
1	B	1198	LEU
1	B	1225	VAL
1	B	1228	VAL
1	B	1234	LEU
1	B	1240	LEU
1	B	1241	LEU
1	B	1244	LYS
1	B	1249	GLU
1	B	1252	ILE
1	B	1262	LEU
1	B	1265	GLN
1	B	1271	VAL
1	B	1274	ARG
1	B	1279	GLU
1	B	1287	ARG
1	B	1293	GLU
1	B	1294	LYS
1	B	1302	LEU
1	B	1307	LEU
1	B	1313	ARG
1	B	1324	LYS
1	B	1335	VAL
1	B	1352	THR
1	B	1366	ARG
1	B	1368	LEU
1	B	1369	LEU
1	B	1375	ARG
1	B	1380	THR
1	B	1401	LEU
1	B	1404	LYS
1	B	1408	LEU

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Mol	Chain	Res	Type
1	B	1412	THR
1	B	1421	LYS
1	B	1425	ILE
1	B	1430	GLU
1	B	1442	ARG
1	B	1448	ILE
1	B	1453	VAL
1	B	1456	VAL
1	B	1466	VAL
1	B	1474	MET
1	B	1481	ILE
1	B	1482	GLU
1	B	1483	ARG
1	B	1487	ILE
1	B	1492	SER
1	B	1494	LEU
1	B	1502	HIS
1	B	1518	VAL
1	B	1539	LEU
1	B	1567	LYS
1	B	1569	THR
1	B	1571	LEU
1	B	1584	ILE
1	B	1585	GLN
1	B	1588	ARG
1	B	1590	LEU
1	B	1593	THR
1	B	1595	LYS
1	B	1603	LYS
1	B	1609	LEU
1	B	1611	GLU
1	B	1614	LEU
1	B	1648	ARG
1	B	1650	LEU
1	B	1656	VAL
1	B	1677	VAL
1	B	1696	GLN
1	B	1715	LYS
1	B	1728	LEU
1	B	1731	CYS
1	B	1739	GLU
1	B	1752	VAL

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Mol	Chain	Res	Type
1	B	1765	THR
1	B	1769	ASN
1	B	1776	ILE
1	B	1777	SER
1	B	1785	LEU
1	B	1796	LEU
1	B	1818	ILE
1	B	1831	LEU
1	B	1835	SER
1	B	1849	ILE
1	B	1854	GLU
1	B	1860	ILE
1	B	1862	HIS
1	B	1865	ASP
1	B	1867	LEU
1	B	1871	LEU
1	B	1879	LEU
1	B	1895	LEU
1	B	1907	GLU
1	B	1948	MET
1	B	1949	VAL
1	B	1956	LYS
1	B	1969	GLU
1	B	1986	MET
1	B	1996	LEU
1	B	1999	LEU
1	B	2006	ASP
1	B	2017	ILE
1	B	2019	LEU
1	B	2021	TYR
1	B	2026	LYS
1	B	2029	ILE
1	B	2030	ARG
1	B	2038	LEU
1	B	2039	VAL
1	B	2041	LEU
1	B	2045	GLU
1	B	2047	VAL
1	B	2058	GLN
1	B	2067	VAL
1	B	2076	LEU
1	B	2077	ILE

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Mol	Chain	Res	Type
1	B	2083	THR
1	B	2091	LYS
1	B	2092	LEU
1	B	2095	VAL
1	B	2114	MET
1	B	2124	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	418	GLN
1	B	425	ASN
1	B	429	GLN
1	B	524	HIS
1	B	584	GLN
1	B	726	HIS
1	B	785	HIS
1	B	786	HIS
1	B	877	GLN
1	B	918	ASN
1	B	951	GLN
1	B	1528	GLN
1	B	1568	GLN
1	B	1674	HIS
1	B	1690	HIS
1	B	1692	ASN
1	B	1877	HIS
1	B	1924	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	B	1724/1724 (100%)	0.28	76 (4%) 39 35	45, 95, 166, 219	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	783	ALA	5.3
1	B	809	LEU	5.2
1	B	782	PHE	5.1
1	B	772	LEU	4.7
1	B	725	VAL	4.6
1	B	821	LEU	4.0
1	B	2084	LEU	3.9
1	B	732	GLY	3.7
1	B	575	LEU	3.6
1	B	774	LEU	3.5
1	B	1842	VAL	3.3
1	B	748	LEU	3.2
1	B	859	PRO	3.2
1	B	722	LEU	3.2
1	B	797	VAL	3.1
1	B	784	ILE	3.1
1	B	752	LEU	3.1
1	B	734	THR	3.1
1	B	402	ALA	3.1
1	B	823	ALA	3.0
1	B	742	CYS	3.0
1	B	737	ALA	3.0
1	B	1985	ILE	2.9
1	B	739	ARG	2.9
1	B	693	THR	2.9
1	B	705	ASN	2.9
1	B	743	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	508	GLY	2.8
1	B	749	GLY	2.8
1	B	1365	LEU	2.8
1	B	723	VAL	2.7
1	B	443	GLU	2.7
1	B	770	LYS	2.7
1	B	1481	ILE	2.6
1	B	785	HIS	2.6
1	B	698	ILE	2.5
1	B	802	ALA	2.5
1	B	769	CYS	2.4
1	B	442	TYR	2.4
1	B	1582	ALA	2.4
1	B	829	LYS	2.4
1	B	780	TYR	2.4
1	B	1317	PHE	2.4
1	B	1963	LEU	2.4
1	B	1716	LYS	2.4
1	B	403	LEU	2.3
1	B	721	VAL	2.3
1	B	685	LEU	2.3
1	B	601	GLY	2.2
1	B	781	GLY	2.2
1	B	2036	VAL	2.2
1	B	577	LYS	2.2
1	B	738	ILE	2.2
1	B	1322	GLN	2.2
1	B	2038	LEU	2.2
1	B	704	MET	2.2
1	B	1076	ALA	2.2
1	B	2035	VAL	2.2
1	B	435	PHE	2.2
1	B	827	ILE	2.2
1	B	863	THR	2.2
1	B	600	GLY	2.2
1	B	1999	LEU	2.2
1	B	820	ASN	2.1
1	B	761	VAL	2.1
1	B	792	VAL	2.1
1	B	530	THR	2.1
1	B	718	LYS	2.1
1	B	778	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	719	ASN	2.1
1	B	1865	ASP	2.1
1	B	692	ILE	2.1
1	B	726	HIS	2.0
1	B	2124	VAL	2.0
1	B	735	ALA	2.0
1	B	2004	ILE	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.