



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 07:50 AM UTC

PDB ID : 3QYE / pdb_00003qye
Title : Crystal Structure of Human TBC1D1 RabGAP domain
Authors : Park, S.Y.; Shoelson, S.E.
Deposited on : 2011-03-03
Resolution : 2.20 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

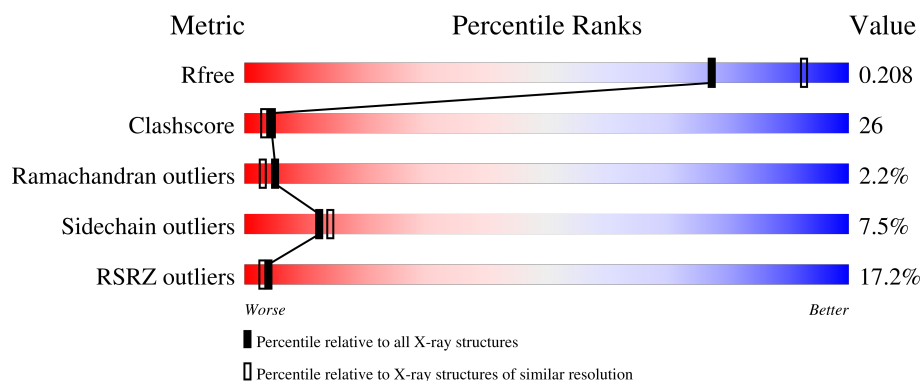
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	331	10% 68% 22% ...
1	B	331	23% 59% 28% 8% ...

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5609 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 TBC1 domain family member 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	317	Total	C	N	O	S	0	0	0
			2605	1698	432	460	15			
1	B	317	Total	C	N	O	S	0	0	0
			2606	1699	432	460	15			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	742	GLY	-	expression tag	UNP Q86TI0
A	743	SER	-	expression tag	UNP Q86TI0
A	744	HIS	-	expression tag	UNP Q86TI0
A	745	MET	-	expression tag	UNP Q86TI0
B	742	GLY	-	expression tag	UNP Q86TI0
B	743	SER	-	expression tag	UNP Q86TI0
B	744	HIS	-	expression tag	UNP Q86TI0
B	745	MET	-	expression tag	UNP Q86TI0

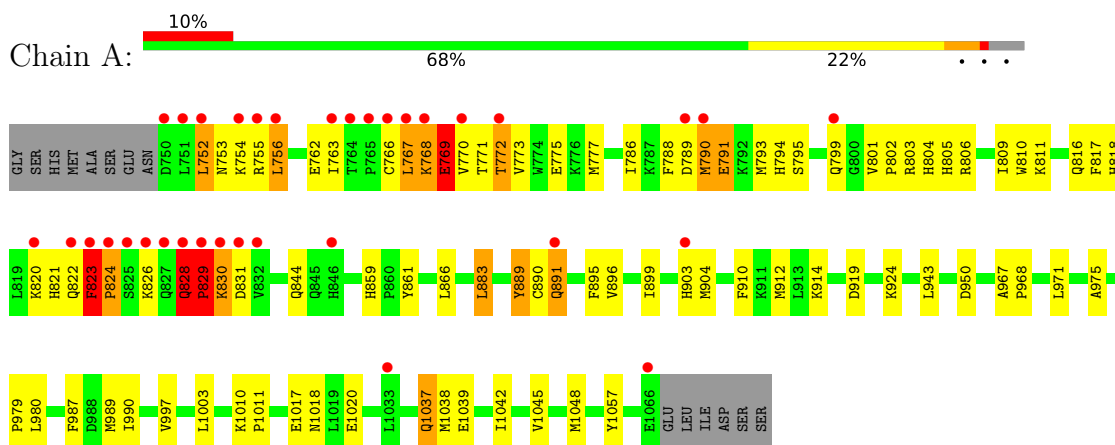
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	231	Total	O	0	0
			231	231		
2	B	167	Total	O	0	0
			167	167		

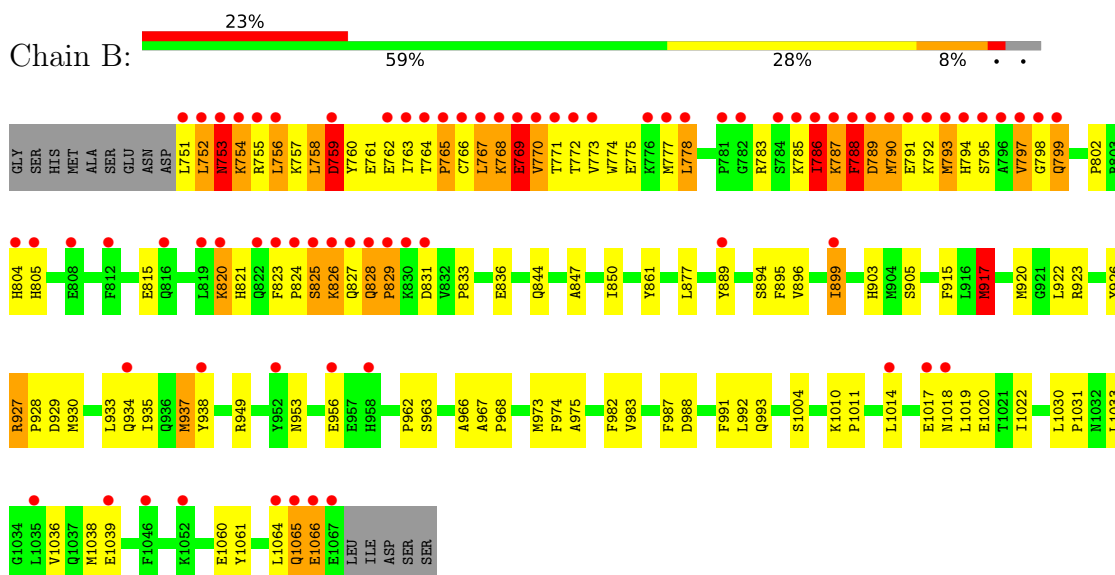
3 Residue-property plots

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: TBC1 domain family member 1



• Molecule 1: TBC1 domain family member 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	117.36Å 117.36Å 141.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 50.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.20) 99.6 (50.00-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.66 (at 2.20Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.199 , 0.239 0.219 , 0.208	Depositor DCC
R_{free} test set	2574 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	35.5	Xtriage
Anisotropy	0.245	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5609	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.50	0/2671	1.01	11/3606 (0.3%)
1	B	0.53	2/2672 (0.1%)	1.13	24/3607 (0.7%)
All	All	0.52	2/5343 (0.0%)	1.07	35/7213 (0.5%)

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	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	917	MET	SD-CE	-9.68	1.55	1.79
1	B	937	MET	SD-CE	-5.90	1.64	1.79

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	769	GLU	N-CA-C	10.77	124.94	111.69
1	B	764	THR	CA-C-N	10.76	133.28	119.84
1	B	764	THR	C-N-CA	10.76	133.28	119.84
1	A	824	PRO	N-CA-C	10.29	126.04	111.33
1	A	828	GLN	CA-C-N	-9.54	107.91	119.84
1	A	828	GLN	C-N-CA	-9.54	107.91	119.84
1	B	1019	LEU	N-CA-C	-9.19	101.16	111.82
1	B	762	GLU	N-CA-C	-8.97	99.07	110.19
1	A	823	PHE	CA-C-N	8.91	130.09	120.11
1	A	823	PHE	C-N-CA	8.91	130.09	120.11
1	A	771	THR	N-CA-C	-8.15	102.48	111.36
1	A	1017	GLU	N-CA-C	8.04	123.25	112.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	770	VAL	N-CA-C	-7.68	101.49	111.09
1	B	927	ARG	CA-C-N	7.62	127.16	119.24
1	B	927	ARG	C-N-CA	7.62	127.16	119.24
1	B	753	ASN	N-CA-C	-7.56	102.52	112.34
1	B	791	GLU	N-CA-C	-7.43	103.95	112.87
1	A	769	GLU	N-CA-C	7.39	119.97	111.11
1	B	829	PRO	N-CA-C	6.91	121.77	111.41
1	A	752	LEU	N-CA-C	-6.58	105.08	113.23
1	B	768	LYS	N-CA-C	6.44	124.52	110.80
1	B	759	ASP	CA-C-N	-6.29	111.76	122.33
1	B	759	ASP	C-N-CA	-6.29	111.76	122.33
1	B	772	THR	N-CA-C	-6.02	104.92	112.93
1	B	778	LEU	N-CA-C	-6.01	107.77	114.62
1	B	905	SER	N-CA-C	-6.00	102.80	110.53
1	B	758	LEU	N-CA-C	5.93	119.83	112.59
1	B	1066	GLU	N-CA-C	-5.89	104.55	110.97
1	B	797	VAL	N-CA-C	-5.57	105.07	110.42
1	B	1017	GLU	N-CA-C	5.47	121.73	114.12
1	A	786	ILE	N-CA-C	5.43	116.12	108.36
1	B	764	THR	N-CA-C	-5.39	97.90	109.81
1	B	988	ASP	N-CA-C	-5.35	105.34	111.07
1	A	767	LEU	N-CA-C	5.16	118.15	110.52
1	B	993	GLN	N-CA-C	5.13	119.64	113.17

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	823	PHE	Sidechain
1	A	889	TYR	Sidechain

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	2605	0	2627	106	0
1	B	2606	0	2629	175	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	231	0	0	7	0
2	B	167	0	0	1	0
All	All	5609	0	5256	274	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 26.

All (274) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:826:LYS:HG3	1:B:769:GLU:OE1	1.33	1.26
1:B:786:ILE:HG21	1:B:788:PHE:CE2	1.80	1.16
1:B:982:PHE:HB2	1:B:1038:MET:HE3	1.27	1.12
1:A:788:PHE:HB2	1:A:793:MET:HE3	1.17	1.10
1:B:786:ILE:HG21	1:B:788:PHE:CD2	1.86	1.09
1:B:786:ILE:HG23	1:B:787:LYS:N	1.66	1.06
1:B:799:GLN:HE21	1:B:799:GLN:CA	1.69	1.06
1:A:826:LYS:HE3	1:B:769:GLU:HG3	1.34	1.04
1:B:799:GLN:HE21	1:B:799:GLN:HA	0.96	1.04
1:B:789:ASP:HB2	1:B:792:LYS:HE2	1.42	1.02
1:A:979:PRO:HG2	1:A:1038:MET:HE1	1.41	1.01
1:A:826:LYS:HE3	1:B:769:GLU:CG	1.92	0.98
1:B:799:GLN:HA	1:B:799:GLN:NE2	1.78	0.97
1:A:793:MET:HE1	1:A:816:GLN:HG3	1.48	0.93
1:B:759:ASP:CG	1:B:759:ASP:O	2.13	0.92
1:B:797:VAL:HG21	1:B:992:LEU:HD22	1.51	0.90
1:A:828:GLN:OE1	1:A:829:PRO:HD3	1.71	0.90
1:A:823:PHE:CZ	1:A:919:ASP:O	2.26	0.89
1:B:786:ILE:O	1:B:787:LYS:HG2	1.72	0.89
1:B:786:ILE:HG23	1:B:787:LYS:H	1.34	0.89
1:B:752:LEU:HD23	1:B:753:ASN:N	1.88	0.88
1:B:823:PHE:CD2	1:B:824:PRO:HD2	2.08	0.88
1:A:767:LEU:HB3	1:A:768:LYS:HD2	1.54	0.88
1:B:824:PRO:O	1:B:826:LYS:N	2.08	0.87
1:A:766:CYS:SG	1:A:802:PRO:HA	2.16	0.85
1:B:763:ILE:HD13	1:B:1038:MET:HE2	1.60	0.84
1:A:823:PHE:CE2	1:A:919:ASP:HA	2.12	0.84
1:B:786:ILE:HG21	1:B:788:PHE:HE2	1.39	0.84
1:B:774:TRP:HA	1:B:777:MET:HB3	1.57	0.83
1:A:826:LYS:CG	1:B:769:GLU:OE1	2.25	0.82
1:A:788:PHE:CB	1:A:793:MET:HE3	2.07	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:752:LEU:O	1:B:755:ARG:HG2	1.80	0.82
1:B:760:TYR:OH	1:B:903:HIS:HE1	1.63	0.80
1:B:751:LEU:O	1:B:754:LYS:N	2.12	0.80
1:A:823:PHE:CE2	1:A:919:ASP:O	2.36	0.79
1:B:920:MET:HE1	1:B:991:PHE:HD1	1.48	0.78
1:A:828:GLN:OE1	1:A:828:GLN:HA	1.85	0.77
1:B:788:PHE:C	1:B:792:LYS:HE3	2.07	0.77
1:B:787:LYS:HE3	1:B:790:MET:HE1	1.65	0.76
1:B:774:TRP:O	1:B:778:LEU:HG	1.85	0.76
1:B:786:ILE:HD13	1:B:788:PHE:CE2	2.19	0.76
1:B:1061:TYR:CE2	1:B:1065:GLN:OE1	2.39	0.75
1:A:793:MET:HE1	1:A:816:GLN:CG	2.17	0.75
1:A:826:LYS:CE	1:B:769:GLU:HG3	2.16	0.75
1:B:752:LEU:HD12	1:B:755:ARG:HH21	1.51	0.74
1:A:859:HIS:HD2	1:A:861:TYR:H	1.33	0.74
1:A:768:LYS:HG2	1:A:769:GLU:H	1.52	0.74
1:B:917:MET:HE3	1:B:922:LEU:HD23	1.69	0.74
1:B:774:TRP:CA	1:B:777:MET:HB3	2.18	0.74
1:A:829:PRO:O	1:A:830:LYS:CB	2.35	0.73
1:A:990:ILE:HD13	1:A:997:VAL:HB	1.70	0.73
1:A:979:PRO:CG	1:A:1038:MET:HE1	2.17	0.73
1:B:795:SER:O	1:B:799:GLN:N	2.21	0.73
1:B:786:ILE:CG2	1:B:788:PHE:CD2	2.69	0.72
1:B:938:TYR:OH	1:B:1060:GLU:CD	2.33	0.72
1:A:788:PHE:HB2	1:A:793:MET:CE	2.09	0.71
1:A:768:LYS:HZ2	1:A:768:LYS:HB3	1.55	0.71
1:B:786:ILE:HG21	1:B:788:PHE:HD2	1.52	0.71
1:A:788:PHE:H	1:A:816:GLN:HE22	1.40	0.70
1:A:762:GLU:HG3	1:A:803:ARG:NH1	2.06	0.70
1:B:753:ASN:C	1:B:753:ASN:OD1	2.35	0.69
1:A:896:VAL:O	1:A:899:ILE:HG22	1.92	0.69
1:B:920:MET:HE1	1:B:991:PHE:CD1	2.28	0.69
1:A:793:MET:CE	1:A:816:GLN:HG3	2.21	0.68
1:B:771:THR:O	1:B:775:GLU:HG3	1.94	0.68
1:B:795:SER:O	1:B:799:GLN:CB	2.42	0.68
1:A:811:LYS:O	1:A:811:LYS:HD3	1.93	0.67
1:A:883:LEU:C	1:A:883:LEU:HD23	2.20	0.67
1:B:786:ILE:CG2	1:B:787:LYS:N	2.44	0.67
1:B:789:ASP:CB	1:B:792:LYS:HE2	2.23	0.67
1:B:933:LEU:O	1:B:937:MET:HG2	1.95	0.66
1:A:820:LYS:HG3	1:A:821:HIS:CD2	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:829:PRO:O	1:A:830:LYS:HB2	1.93	0.66
1:B:825:SER:HA	1:B:828:GLN:HB2	1.76	0.66
1:B:826:LYS:C	1:B:828:GLN:H	2.04	0.65
1:B:766:CYS:SG	1:B:770:VAL:CG2	2.84	0.65
1:B:788:PHE:HD2	1:B:788:PHE:H	1.45	0.65
1:B:755:ARG:O	1:B:758:LEU:N	2.27	0.65
1:B:967:ALA:HB3	1:B:968:PRO:HD3	1.78	0.64
1:B:877:LEU:HD22	1:B:889:TYR:HE1	1.63	0.64
1:B:937:MET:HE2	1:B:963:SER:HA	1.78	0.64
1:B:766:CYS:SG	1:B:770:VAL:HG22	2.38	0.64
1:A:817:PHE:HA	1:A:820:LYS:NZ	2.12	0.64
1:B:775:GLU:OE1	1:B:805:HIS:HE1	1.80	0.64
1:B:795:SER:O	1:B:799:GLN:HB2	1.97	0.63
1:B:889:TYR:OH	1:B:894:SER:HB3	1.98	0.63
1:B:755:ARG:O	1:B:756:LEU:C	2.39	0.63
1:A:801:VAL:HG13	1:A:809:ILE:HD12	1.79	0.63
1:B:763:ILE:HD13	1:B:1038:MET:CE	2.28	0.63
1:B:799:GLN:CA	1:B:799:GLN:NE2	2.44	0.63
1:A:826:LYS:HE3	1:B:769:GLU:CD	2.24	0.62
1:A:769:GLU:O	1:A:772:THR:HB	1.98	0.62
1:A:820:LYS:HE2	1:A:821:HIS:NE2	2.15	0.61
1:B:1033:LEU:HB3	1:B:1038:MET:HG3	1.82	0.61
1:B:752:LEU:HD12	1:B:755:ARG:NH2	2.16	0.60
1:A:967:ALA:HB3	1:A:968:PRO:HD3	1.82	0.60
1:A:770:VAL:HG21	1:A:799:GLN:CB	2.31	0.60
1:A:768:LYS:HG2	1:A:769:GLU:N	2.16	0.60
1:B:751:LEU:O	1:B:754:LYS:HB3	2.01	0.60
1:B:915:PHE:HD2	1:B:920:MET:HE3	1.67	0.59
1:B:788:PHE:O	1:B:789:ASP:C	2.45	0.59
1:B:794:HIS:O	1:B:798:GLY:N	2.27	0.59
1:A:828:GLN:CD	1:A:829:PRO:HD3	2.26	0.59
1:A:1045:VAL:HA	1:A:1048:MET:HE3	1.84	0.59
1:A:943:LEU:HD13	1:A:1057:TYR:HE2	1.67	0.59
1:A:1010:LYS:HB3	1:A:1011:PRO:HD3	1.85	0.59
1:B:790:MET:C	1:B:792:LYS:N	2.60	0.59
1:A:823:PHE:CD2	1:A:919:ASP:HA	2.38	0.58
1:A:818:HIS:C	1:A:818:HIS:HD1	2.10	0.58
1:B:752:LEU:C	1:B:754:LYS:N	2.58	0.58
1:B:787:LYS:NZ	1:B:820:LYS:HB2	2.18	0.58
1:A:805:HIS:O	1:A:809:ILE:HG13	2.04	0.58
1:A:762:GLU:HG3	1:A:803:ARG:HH12	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:935:ILE:HG12	1:B:1061:TYR:CE2	2.39	0.57
1:B:754:LYS:O	1:B:757:LYS:HB2	2.05	0.57
1:B:763:ILE:CD1	1:B:1038:MET:HE2	2.33	0.57
1:B:770:VAL:CG1	1:B:799:GLN:HB3	2.34	0.57
1:B:786:ILE:HD13	1:B:788:PHE:CZ	2.39	0.57
1:A:788:PHE:H	1:A:816:GLN:NE2	2.02	0.56
1:B:820:LYS:HD2	1:B:821:HIS:CD2	2.40	0.56
1:A:766:CYS:SG	1:A:802:PRO:CA	2.93	0.56
1:B:917:MET:CE	1:B:922:LEU:HB3	2.35	0.56
1:B:755:ARG:O	1:B:757:LYS:N	2.39	0.56
1:A:793:MET:HE1	1:A:816:GLN:NE2	2.21	0.56
1:B:790:MET:C	1:B:792:LYS:H	2.14	0.56
1:B:899:ILE:O	1:B:903:HIS:HD2	1.87	0.56
1:B:787:LYS:NZ	1:B:820:LYS:CB	2.68	0.56
1:B:786:ILE:CG2	1:B:788:PHE:HD2	2.14	0.56
1:B:820:LYS:HD2	1:B:821:HIS:CE1	2.42	0.55
1:B:820:LYS:HD2	1:B:821:HIS:CG	2.42	0.55
1:A:793:MET:HE1	1:A:816:GLN:CD	2.32	0.55
1:B:917:MET:HE1	1:B:926:TYR:CE2	2.41	0.55
1:B:786:ILE:CG2	1:B:788:PHE:CE2	2.72	0.55
1:A:891:GLN:OE1	1:A:971:LEU:HD13	2.06	0.55
1:A:823:PHE:CE2	1:A:919:ASP:CA	2.89	0.55
1:A:1018:ASN:HD21	1:A:1020:GLU:HB3	1.72	0.54
1:B:825:SER:HA	1:B:828:GLN:CB	2.37	0.54
1:A:770:VAL:HG21	1:A:799:GLN:HB2	1.88	0.54
1:B:826:LYS:O	1:B:828:GLN:N	2.41	0.54
1:A:844:GLN:HE21	1:A:889:TYR:H	1.54	0.54
1:A:824:PRO:HA	2:A:170:HOH:O	2.08	0.54
1:A:821:HIS:O	1:A:822:GLN:C	2.49	0.53
1:B:949:ARG:HH12	1:B:953:ASN:HD21	1.54	0.53
1:B:937:MET:CE	1:B:963:SER:HA	2.38	0.53
1:A:768:LYS:HD2	1:A:768:LYS:N	2.23	0.53
1:B:752:LEU:O	1:B:755:ARG:N	2.41	0.53
1:B:755:ARG:C	1:B:757:LYS:N	2.65	0.53
1:B:937:MET:HE1	1:B:966:ALA:HB3	1.90	0.53
1:A:826:LYS:NZ	1:B:767:LEU:O	2.33	0.53
1:A:943:LEU:HG	1:A:1003:LEU:HD22	1.91	0.53
1:A:755:ARG:HD2	1:A:755:ARG:O	2.09	0.53
1:B:1030:LEU:HB3	1:B:1031:PRO:HD3	1.91	0.53
1:A:790:MET:O	1:A:790:MET:SD	2.67	0.52
1:B:789:ASP:O	1:B:792:LYS:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:890:CYS:SG	1:A:891:GLN:NE2	2.82	0.52
1:B:787:LYS:O	1:B:788:PHE:C	2.52	0.52
1:B:935:ILE:HG12	1:B:1061:TYR:CD2	2.44	0.52
1:B:773:VAL:O	1:B:777:MET:CB	2.58	0.52
1:A:810:TRP:CH2	1:A:903:HIS:ND1	2.78	0.51
1:B:917:MET:HE1	1:B:926:TYR:CD2	2.45	0.51
1:A:770:VAL:HG21	1:A:799:GLN:HB3	1.92	0.51
1:A:1018:ASN:ND2	1:A:1020:GLU:HB3	2.25	0.51
1:B:833:PRO:HG2	1:B:836:GLU:CG	2.42	0.50
1:B:759:ASP:O	1:B:759:ASP:OD1	2.27	0.50
1:B:774:TRP:CE3	1:B:777:MET:HG2	2.46	0.50
1:B:787:LYS:CE	1:B:790:MET:HE1	2.37	0.50
1:B:766:CYS:SG	1:B:770:VAL:HG21	2.50	0.50
1:B:775:GLU:OE1	1:B:805:HIS:CE1	2.64	0.50
1:B:802:PRO:HG2	1:B:805:HIS:HB2	1.94	0.50
1:B:795:SER:O	1:B:799:GLN:CG	2.60	0.50
1:B:777:MET:HG3	1:B:777:MET:O	2.11	0.49
1:B:789:ASP:N	1:B:792:LYS:CE	2.75	0.49
1:B:917:MET:HE2	1:B:923:ARG:N	2.28	0.49
1:B:828:GLN:NE2	1:B:829:PRO:HD2	2.27	0.49
1:B:917:MET:HE2	1:B:922:LEU:C	2.37	0.49
1:A:883:LEU:C	1:A:883:LEU:CD2	2.84	0.49
1:B:786:ILE:O	1:B:787:LYS:CG	2.55	0.49
1:B:949:ARG:NH1	1:B:953:ASN:HD21	2.10	0.49
1:A:883:LEU:HD23	1:A:883:LEU:O	2.12	0.49
1:B:774:TRP:C	1:B:777:MET:HB3	2.37	0.49
1:A:811:LYS:HD3	1:A:811:LYS:C	2.38	0.48
1:B:804:HIS:HB2	2:B:232:HOH:O	2.12	0.48
1:B:847:ALA:O	1:B:850:ILE:HG22	2.13	0.48
1:B:826:LYS:C	1:B:828:GLN:N	2.69	0.48
1:B:752:LEU:O	1:B:753:ASN:C	2.54	0.48
1:B:797:VAL:CG2	1:B:992:LEU:HD22	2.35	0.48
1:B:787:LYS:HZ2	1:B:820:LYS:CB	2.26	0.48
1:B:915:PHE:CD2	1:B:920:MET:HE3	2.49	0.48
1:A:756:LEU:CD1	1:A:861:TYR:HA	2.44	0.48
1:A:899:ILE:HG21	1:A:987:PHE:CZ	2.48	0.48
1:B:787:LYS:O	1:B:789:ASP:N	2.46	0.48
1:A:817:PHE:HA	1:A:820:LYS:HZ1	1.78	0.47
1:B:899:ILE:HG21	1:B:987:PHE:CZ	2.50	0.47
1:A:891:GLN:HE22	1:A:971:LEU:HD13	1.79	0.47
1:A:828:GLN:OE1	1:A:828:GLN:CA	2.60	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:828:GLN:HE21	1:B:829:PRO:HD2	1.78	0.47
1:B:752:LEU:HD23	1:B:752:LEU:C	2.39	0.47
1:B:917:MET:HE3	1:B:922:LEU:CD2	2.43	0.47
1:A:1037:GLN:HG2	2:A:293:HOH:O	2.14	0.47
1:B:786:ILE:CG2	1:B:787:LYS:H	2.04	0.47
1:A:791:GLU:OE2	1:A:791:GLU:HA	2.14	0.47
1:A:773:VAL:HG12	1:A:777:MET:HE2	1.96	0.47
1:A:818:HIS:C	1:A:818:HIS:ND1	2.71	0.47
1:B:789:ASP:N	1:B:792:LYS:HE3	2.30	0.47
1:A:924:LYS:HE3	2:A:228:HOH:O	2.14	0.46
1:A:806:ARG:HG2	1:A:903:HIS:ND1	2.31	0.46
1:A:817:PHE:HA	1:A:820:LYS:HZ3	1.80	0.46
1:A:795:SER:O	1:A:799:GLN:HG3	2.15	0.46
1:A:754:LYS:HD3	2:A:284:HOH:O	2.16	0.46
1:B:783:ARG:HH21	1:B:815:GLU:CD	2.23	0.46
1:B:788:PHE:HB2	1:B:793:MET:HE1	1.96	0.46
1:B:917:MET:HE2	1:B:922:LEU:HB3	1.97	0.45
1:B:765:PRO:O	1:B:767:LEU:HD23	2.16	0.45
1:B:975:ALA:HA	1:B:983:VAL:HG21	1.96	0.45
1:A:1038:MET:O	1:A:1042:ILE:HG12	2.17	0.45
1:B:752:LEU:HD23	1:B:753:ASN:H	1.76	0.45
1:A:883:LEU:HD11	1:A:914:LYS:HD2	1.99	0.45
1:B:774:TRP:O	1:B:778:LEU:N	2.50	0.45
1:B:789:ASP:O	1:B:792:LYS:CB	2.65	0.45
1:A:823:PHE:CE2	1:A:919:ASP:C	2.94	0.45
1:B:751:LEU:O	1:B:754:LYS:CB	2.65	0.45
1:B:760:TYR:O	1:B:761:GLU:C	2.60	0.45
1:A:950:ASP:N	1:A:950:ASP:OD1	2.50	0.44
1:B:769:GLU:O	1:B:773:VAL:HG23	2.17	0.44
1:B:937:MET:HE3	1:B:962:PRO:HB2	2.00	0.44
1:A:790:MET:SD	1:A:790:MET:C	3.01	0.44
1:B:1010:LYS:HG2	1:B:1011:PRO:HD3	1.99	0.44
1:B:917:MET:HE3	1:B:922:LEU:HB3	2.00	0.44
1:A:754:LYS:NZ	1:A:804:HIS:O	2.48	0.44
1:A:755:ARG:HD2	1:A:755:ARG:C	2.43	0.44
1:A:904:MET:HE1	1:A:912:MET:HG3	2.00	0.44
1:B:763:ILE:HG21	1:B:1038:MET:CE	2.47	0.44
1:B:896:VAL:O	1:B:899:ILE:CG2	2.66	0.43
1:A:820:LYS:CG	1:A:821:HIS:CD2	2.99	0.43
1:A:821:HIS:HB3	1:A:823:PHE:HD1	1.83	0.43
1:B:763:ILE:HG21	1:B:1038:MET:HE2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:820:LYS:HE3	2:A:166:HOH:O	2.19	0.43
1:B:1010:LYS:O	1:B:1014:LEU:HG	2.18	0.43
1:B:877:LEU:HD22	1:B:889:TYR:CE1	2.48	0.43
1:B:799:GLN:HE21	1:B:799:GLN:N	2.11	0.43
1:B:1036:VAL:O	1:B:1039:GLU:HG2	2.18	0.43
1:A:828:GLN:CD	1:A:829:PRO:CD	2.91	0.43
1:B:799:GLN:NE2	1:B:799:GLN:N	2.67	0.43
1:A:895:PHE:HB3	1:A:975:ALA:HB3	2.01	0.43
1:B:789:ASP:O	1:B:792:LYS:N	2.45	0.42
1:A:754:LYS:HE2	2:A:259:HOH:O	2.19	0.42
1:A:823:PHE:HE2	1:A:919:ASP:HA	1.77	0.42
1:B:753:ASN:OD1	1:B:754:LYS:N	2.52	0.42
1:B:949:ARG:HG3	1:B:949:ARG:HH11	1.84	0.42
1:A:794:HIS:HD2	2:A:19:HOH:O	2.01	0.42
1:B:927:ARG:HA	1:B:928:PRO:HD3	1.86	0.42
1:B:937:MET:HE3	1:B:962:PRO:C	2.45	0.42
1:B:917:MET:HB3	1:B:923:ARG:HB3	2.03	0.41
1:B:790:MET:H	1:B:790:MET:HG2	1.36	0.41
1:B:833:PRO:HG2	1:B:836:GLU:HG2	2.02	0.41
1:B:929:ASP:O	1:B:930:MET:HB2	2.20	0.41
1:B:1060:GLU:HG2	1:B:1064:LEU:HD12	2.02	0.41
1:B:773:VAL:O	1:B:777:MET:HB2	2.21	0.41
1:B:786:ILE:CG2	1:B:788:PHE:HE2	2.20	0.41
1:B:917:MET:CE	1:B:922:LEU:CB	2.98	0.41
1:B:788:PHE:C	1:B:792:LYS:CE	2.88	0.41
1:A:910:PHE:CZ	1:A:914:LYS:HD3	2.56	0.41
1:A:756:LEU:HD12	1:A:861:TYR:HD1	1.86	0.41
1:A:767:LEU:HD22	1:A:768:LYS:HE2	2.02	0.41
1:B:937:MET:HE3	1:B:963:SER:N	2.36	0.41
1:B:973:MET:O	1:B:974:PHE:HB2	2.20	0.41
1:A:763:ILE:HD12	1:A:1038:MET:SD	2.60	0.41
1:B:826:LYS:HA	1:B:826:LYS:HD2	1.14	0.41
1:B:895:PHE:O	1:B:899:ILE:HG22	2.21	0.41
1:B:844:GLN:HE21	1:B:889:TYR:H	1.67	0.40
1:B:757:LYS:HE2	1:B:861:TYR:CZ	2.57	0.40
1:A:989:MET:HE2	1:A:1042:ILE:HG23	2.03	0.40
1:B:917:MET:CE	1:B:922:LEU:CG	2.99	0.40
1:B:1018:ASN:O	1:B:1022:ILE:HD12	2.21	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	315/331 (95%)	300 (95%)	11 (4%)	4 (1%)	9	8
1	B	315/331 (95%)	288 (91%)	17 (5%)	10 (3%)	3	1
All	All	630/662 (95%)	588 (93%)	28 (4%)	14 (2%)	5	3

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	786	ILE
1	B	787	LYS
1	B	788	PHE
1	B	825	SER
1	B	827	GLN
1	A	829	PRO
1	A	830	LYS
1	B	789	ASP
1	B	768	LYS
1	B	831	ASP
1	B	756	LEU
1	B	765	PRO
1	A	823	PHE
1	A	828	GLN

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	286/298 (96%)	266 (93%)	20 (7%)	14	16
1	B	286/298 (96%)	263 (92%)	23 (8%)	11	13
All	All	572/596 (96%)	529 (92%)	43 (8%)	12	14

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	752	LEU
1	A	753	ASN
1	A	756	LEU
1	A	768	LYS
1	A	769	GLU
1	A	772	THR
1	A	775	GLU
1	A	789	ASP
1	A	790	MET
1	A	791	GLU
1	A	823	PHE
1	A	828	GLN
1	A	829	PRO
1	A	831	ASP
1	A	866	LEU
1	A	883	LEU
1	A	891	GLN
1	A	980	LEU
1	A	1037	GLN
1	A	1039	GLU
1	B	752	LEU
1	B	753	ASN
1	B	754	LYS
1	B	759	ASP
1	B	767	LEU
1	B	769	GLU
1	B	785	LYS
1	B	786	ILE
1	B	788	PHE
1	B	790	MET
1	B	793	MET
1	B	799	GLN
1	B	820	LYS
1	B	826	LYS
1	B	828	GLN

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Mol	Chain	Res	Type
1	B	899	ILE
1	B	917	MET
1	B	934	GLN
1	B	956	GLU
1	B	1004	SER
1	B	1020	GLU
1	B	1065	GLN
1	B	1066	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	753	ASN
1	A	794	HIS
1	A	799	GLN
1	A	816	GLN
1	A	844	GLN
1	A	859	HIS
1	A	875	ASN
1	A	934	GLN
1	A	958	HIS
1	A	1016	HIS
1	A	1018	ASN
1	A	1037	GLN
1	A	1055	GLN
1	B	799	GLN
1	B	805	HIS
1	B	828	GLN
1	B	840	GLN
1	B	844	GLN
1	B	875	ASN
1	B	903	HIS
1	B	948	HIS
1	B	953	ASN
1	B	1009	HIS
1	B	1016	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	317/331 (95%)	0.34	34 (10%) 11 8	20, 35, 81, 105	0
1	B	317/331 (95%)	1.03	75 (23%) 2 1	23, 47, 92, 102	0
All	All	634/662 (95%)	0.69	109 (17%) 4 3	20, 41, 89, 105	0

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	823	PHE	8.1
1	B	751	LEU	6.5
1	A	824	PRO	6.2
1	B	777	MET	6.0
1	A	825	SER	5.5
1	A	826	LYS	5.3
1	B	794	HIS	5.3
1	B	795	SER	5.2
1	B	825	SER	5.0
1	B	823	PHE	5.0
1	A	751	LEU	4.9
1	A	766	CYS	4.8
1	B	766	CYS	4.6
1	B	759	ASP	4.6
1	B	824	PRO	4.5
1	B	827	GLN	4.4
1	A	790	MET	4.3
1	B	778	LEU	4.3
1	B	793	MET	4.2
1	B	767	LEU	4.2
1	A	831	ASP	4.2
1	A	829	PRO	4.2
1	A	768	LYS	4.1
1	A	827	GLN	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	762	GLU	4.1
1	B	804	HIS	4.0
1	A	822	GLN	4.0
1	B	753	ASN	4.0
1	B	791	GLU	3.9
1	B	788	PHE	3.9
1	B	790	MET	3.9
1	B	770	VAL	3.9
1	B	752	LEU	3.9
1	B	755	ARG	3.8
1	B	787	LYS	3.8
1	B	786	ILE	3.6
1	B	763	ILE	3.6
1	A	770	VAL	3.6
1	B	819	LEU	3.6
1	B	776	LYS	3.5
1	B	782	GLY	3.4
1	A	820	LYS	3.4
1	A	767	LEU	3.3
1	B	765	PRO	3.3
1	B	796	ALA	3.3
1	A	799	GLN	3.3
1	A	830	LYS	3.3
1	B	1065	GLN	3.3
1	B	808	GLU	3.3
1	B	797	VAL	3.3
1	A	755	ARG	3.2
1	B	1014	LEU	3.2
1	A	828	GLN	3.1
1	B	754	LYS	3.1
1	B	889	TYR	3.1
1	B	829	PRO	3.1
1	A	750	ASP	3.0
1	A	1066	GLU	3.0
1	B	820	LYS	3.0
1	B	956	GLU	3.0
1	B	789	ASP	2.9
1	B	769	GLU	2.9
1	B	792	LYS	2.9
1	B	1067	GLU	2.9
1	B	830	LYS	2.8
1	B	771	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	816	GLN	2.7
1	B	784	SER	2.7
1	B	756	LEU	2.7
1	B	799	GLN	2.6
1	A	764	THR	2.6
1	B	1064	LEU	2.6
1	B	781	PRO	2.6
1	A	1033	LEU	2.6
1	B	899	ILE	2.6
1	B	938	TYR	2.6
1	B	1018	ASN	2.5
1	B	822	GLN	2.5
1	A	789	ASP	2.5
1	B	826	LYS	2.5
1	B	764	THR	2.5
1	B	805	HIS	2.5
1	B	1046	PHE	2.5
1	A	752	LEU	2.5
1	B	1039	GLU	2.4
1	A	765	PRO	2.4
1	A	832	VAL	2.4
1	B	828	GLN	2.4
1	B	934	GLN	2.3
1	B	785	LYS	2.3
1	B	812	PHE	2.3
1	B	1035	LEU	2.3
1	B	958	HIS	2.3
1	B	773	VAL	2.3
1	A	846	HIS	2.2
1	B	952	TYR	2.2
1	A	754	LYS	2.2
1	B	768	LYS	2.2
1	B	1052	LYS	2.2
1	A	763	ILE	2.2
1	A	756	LEU	2.1
1	B	1017	GLU	2.1
1	B	772	THR	2.1
1	A	891	GLN	2.1
1	A	903	HIS	2.1
1	B	831	ASP	2.1
1	B	798	GLY	2.1
1	B	1066	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	772	THR	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.