



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 01:37 PM UTC

PDB ID : 3A8P / pdb_00003a8p
Title : Crystal structure of the Tiam2 PHCCEX domain
Authors : Terawaki, S.; Kitano, K.; Mori, T.; Zhai, Y.; Higuchi, Y.; Itoh, N.; Watanabe, T.; Kaibuchi, K.; Hakoshima, T.
Deposited on : 2009-10-07
Resolution : 2.10 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

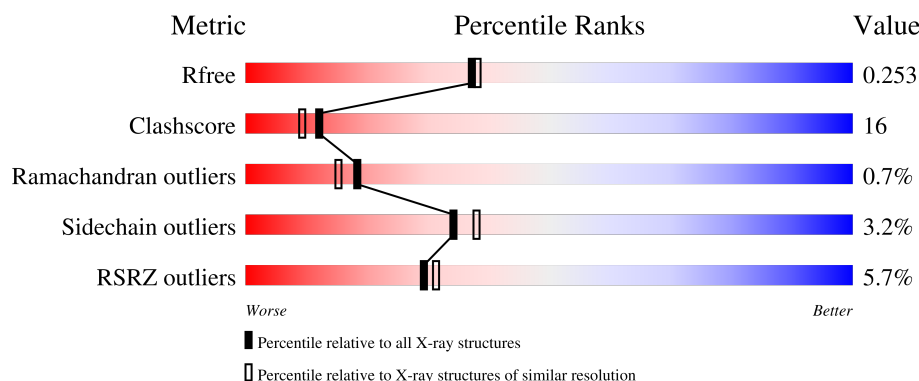
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	263	3% 63% 23% • 12%
1	B	263	5% 63% 21% • 12%
1	C	263	7% 65% 20% • 13%
1	D	263	5% 59% 25% • 13%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7754 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 T-lymphoma invasion and metastasis-inducing protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	232	Total	C	N	O	S	0	0	0
			1856	1184	331	329	12			
1	B	231	Total	C	N	O	S	0	0	0
			1853	1182	330	329	12			
1	C	229	Total	C	N	O	S	0	0	0
			1839	1175	328	324	12			
1	D	228	Total	C	N	O	S	0	0	0
			1823	1163	327	321	12			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	495	GLY	-	expression tag	UNP Q6ZPF3
A	496	PRO	-	expression tag	UNP Q6ZPF3
A	497	LEU	-	expression tag	UNP Q6ZPF3
A	498	GLY	-	expression tag	UNP Q6ZPF3
A	499	SER	-	expression tag	UNP Q6ZPF3
B	495	GLY	-	expression tag	UNP Q6ZPF3
B	496	PRO	-	expression tag	UNP Q6ZPF3
B	497	LEU	-	expression tag	UNP Q6ZPF3
B	498	GLY	-	expression tag	UNP Q6ZPF3
B	499	SER	-	expression tag	UNP Q6ZPF3
C	495	GLY	-	expression tag	UNP Q6ZPF3
C	496	PRO	-	expression tag	UNP Q6ZPF3
C	497	LEU	-	expression tag	UNP Q6ZPF3
C	498	GLY	-	expression tag	UNP Q6ZPF3
C	499	SER	-	expression tag	UNP Q6ZPF3
D	495	GLY	-	expression tag	UNP Q6ZPF3
D	496	PRO	-	expression tag	UNP Q6ZPF3
D	497	LEU	-	expression tag	UNP Q6ZPF3
D	498	GLY	-	expression tag	UNP Q6ZPF3
D	499	SER	-	expression tag	UNP Q6ZPF3

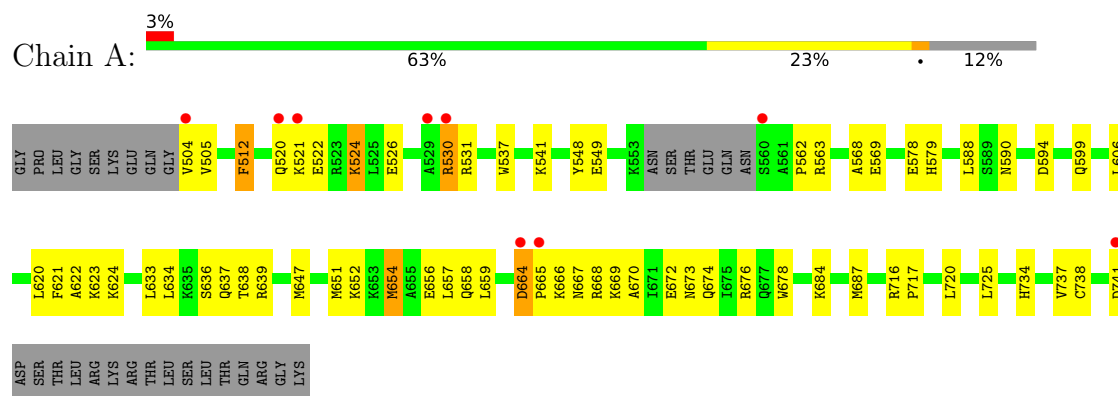
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	126	Total 126	O 126	0	0
2	B	75	Total 75	O 75	0	0
2	C	90	Total 90	O 90	0	0
2	D	92	Total 92	O 92	0	0

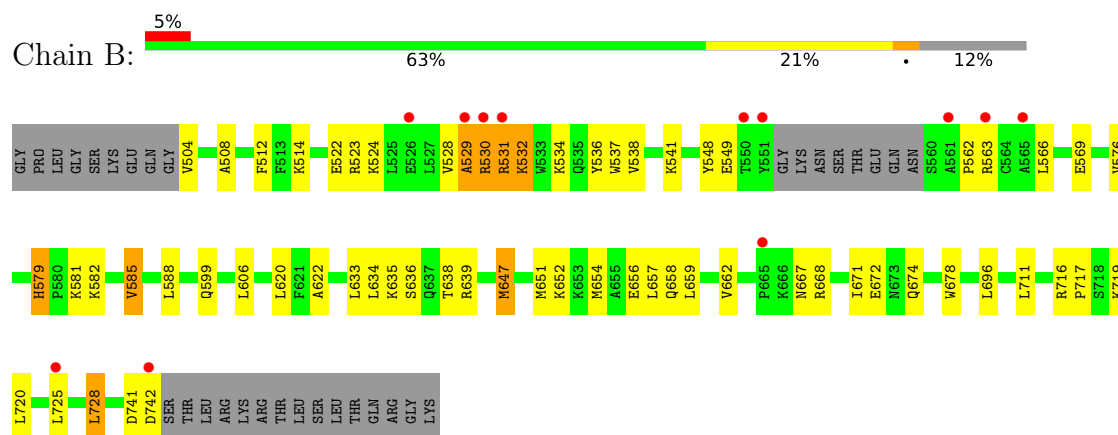
3 Residue-property plots

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.

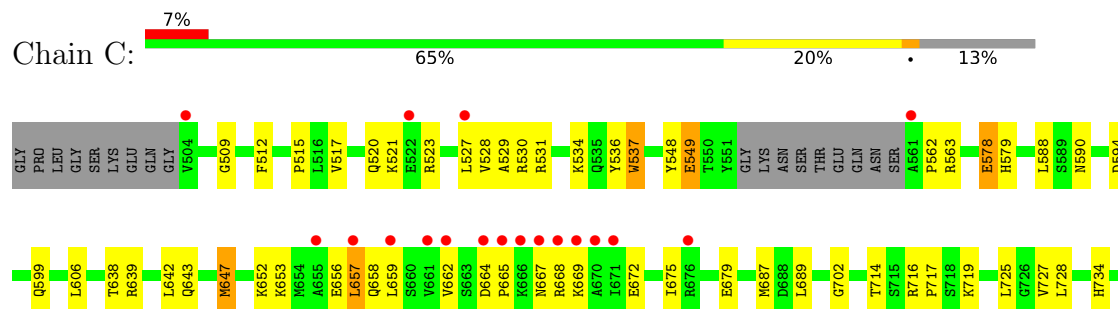
- Molecule 1: T-lymphoma invasion and metastasis-inducing protein 2

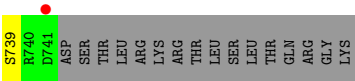


- Molecule 1: T-lymphoma invasion and metastasis-inducing protein 2

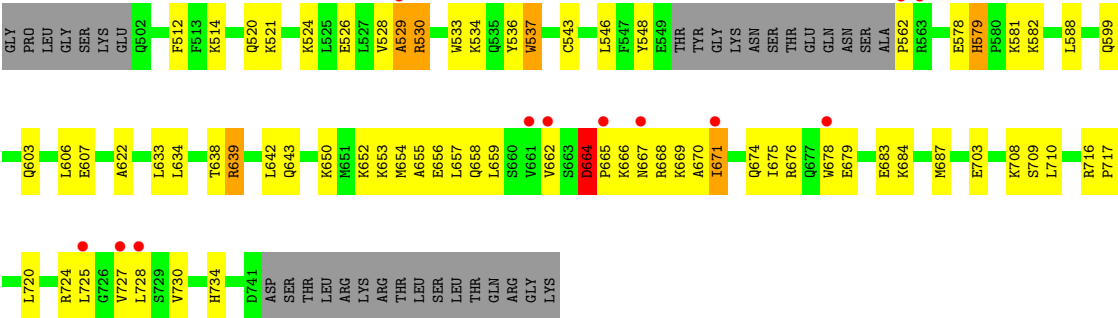


- Molecule 1: T-lymphoma invasion and metastasis-inducing protein 2





● Molecule 1: T-lymphoma invasion and metastasis-inducing protein 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	46.69Å 104.79Å 115.97Å 90.00° 80.55° 90.00°	Depositor
Resolution (Å)	29.81 – 2.10 29.81 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.7 (29.81-2.10) 98.7 (29.81-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 2.08Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.211 , 0.253 0.211 , 0.253	Depositor DCC
R_{free} test set	6524 reflections (10.11%)	wwPDB-VP
Wilson B-factor (Å ²)	30.5	Xtriage
Anisotropy	0.546	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 46.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.024 for h,-k,h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7754	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.22% 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	0.39	0/1893	0.81	3/2548 (0.1%)
1	B	0.38	0/1890	0.81	3/2544 (0.1%)
1	C	0.37	0/1876	0.81	3/2525 (0.1%)
1	D	0.37	0/1859	0.83	7/2500 (0.3%)
All	All	0.38	0/7518	0.82	16/10117 (0.2%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	664	ASP	CA-C-N	6.93	126.45	119.24
1	D	664	ASP	C-N-CA	6.93	126.45	119.24
1	A	537	TRP	N-CA-C	-6.50	98.62	108.96
1	B	537	TRP	N-CA-C	-6.00	98.95	108.73
1	B	579	HIS	CA-C-N	5.91	125.38	119.24
1	B	579	HIS	C-N-CA	5.91	125.38	119.24
1	D	537	TRP	N-CA-C	-5.74	98.39	108.20
1	D	579	HIS	CA-C-N	5.71	125.18	119.24
1	D	579	HIS	C-N-CA	5.71	125.18	119.24
1	D	529	ALA	N-CA-C	5.48	117.69	111.11
1	C	537	TRP	N-CA-C	-5.42	99.68	108.41
1	C	579	HIS	CA-C-N	5.25	124.88	119.05
1	C	579	HIS	C-N-CA	5.25	124.88	119.05
1	D	581	LYS	N-CA-C	5.22	119.92	113.50
1	A	512	PHE	N-CA-C	-5.08	101.43	109.96
1	A	568	ALA	N-CA-C	5.05	119.08	113.02

There are no chirality outliers.

There are no planarity outliers.

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	1856	0	1901	54	0
1	B	1853	0	1901	63	0
1	C	1839	0	1892	51	0
1	D	1823	0	1875	68	0
2	A	126	0	0	2	0
2	B	75	0	0	0	0
2	C	90	0	0	2	0
2	D	92	0	0	3	0
All	All	7754	0	7569	233	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 16.

All (233) 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:C:520:GLN:HG3	1:C:521:LYS:H	1.30	0.94
1:A:664:ASP:HB2	1:A:667:ASN:HB2	1.51	0.93
1:D:650:LYS:O	1:D:653:LYS:HG2	1.78	0.82
1:B:662:VAL:HG13	1:B:668:ARG:NH1	1.95	0.80
1:C:520:GLN:CG	1:C:521:LYS:H	1.94	0.80
1:B:528:VAL:HB	1:B:531:ARG:HH11	1.46	0.79
1:A:654:MET:HE3	1:A:654:MET:HA	1.62	0.79
1:B:514:LYS:HG3	1:B:531:ARG:HD3	1.67	0.77
1:B:514:LYS:CG	1:B:531:ARG:HD3	2.16	0.76
1:B:532:LYS:H	1:B:532:LYS:HD2	1.50	0.75
1:D:703:GLU:CD	1:D:703:GLU:H	1.93	0.75
1:A:654:MET:HE2	1:A:658:GLN:HE21	1.52	0.73
1:A:590:ASN:HD21	1:A:594:ASP:HB2	1.53	0.72
1:B:725:LEU:O	1:B:725:LEU:HD23	1.90	0.72
1:B:522:GLU:HB3	1:B:524:LYS:HE3	1.70	0.71
1:D:530:ARG:H	1:D:530:ARG:NE	1.88	0.71
1:D:659:LEU:HA	1:D:662:VAL:HG12	1.73	0.71
1:C:638:THR:O	1:C:642:LEU:HD13	1.91	0.71
1:D:684:LYS:HE2	2:D:239:HOH:O	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:716:ARG:NH1	1:B:720:LEU:HD11	2.07	0.70
1:A:590:ASN:ND2	1:A:594:ASP:HB2	2.07	0.69
1:B:711:LEU:HD22	1:B:728:LEU:HD11	1.76	0.68
1:D:529:ALA:HB3	1:D:530:ARG:NH2	2.09	0.66
1:C:669:LYS:HA	1:C:672:GLU:HG2	1.77	0.66
1:C:664:ASP:CB	1:C:667:ASN:HB3	2.26	0.66
1:B:652:LYS:O	1:B:656:GLU:HG3	1.97	0.65
1:C:664:ASP:HB2	1:C:667:ASN:HB3	1.78	0.65
1:D:725:LEU:C	1:D:725:LEU:HD23	2.21	0.65
1:C:520:GLN:HG3	1:C:521:LYS:N	2.07	0.64
1:A:504:VAL:N	1:A:541:LYS:HZ2	1.96	0.64
1:D:528:VAL:HG13	1:D:530:ARG:HH11	1.62	0.64
1:D:674:GLN:HG3	1:D:678:TRP:CZ3	2.32	0.63
1:B:647:MET:HE2	1:B:651:MET:HG3	1.79	0.63
1:D:634:LEU:O	1:D:638:THR:HG23	1.99	0.63
1:D:524:LYS:HE2	1:D:526:GLU:OE2	1.99	0.63
1:D:725:LEU:HD22	1:D:727:VAL:H	1.65	0.62
1:C:664:ASP:HB2	1:C:667:ASN:HD22	1.65	0.61
1:B:647:MET:HE3	1:B:647:MET:HA	1.81	0.61
1:C:534:LYS:HD3	1:C:536:TYR:OH	2.00	0.61
1:A:716:ARG:O	1:A:720:LEU:HD13	2.01	0.60
1:A:673:ASN:HD22	1:A:676:ARG:NH1	1.99	0.60
1:A:530:ARG:O	1:A:530:ARG:HG2	2.00	0.60
1:B:523:ARG:HH22	1:B:741:ASP:C	2.10	0.60
1:B:662:VAL:HG13	1:B:668:ARG:HH11	1.63	0.60
1:C:725:LEU:HD23	1:C:725:LEU:C	2.26	0.59
1:D:671:ILE:O	1:D:675:ILE:HG12	2.02	0.59
1:D:669:LYS:HD3	1:D:670:ALA:H	1.67	0.59
1:B:654:MET:HE2	1:B:657:LEU:HD22	1.84	0.58
1:A:522:GLU:HB3	1:A:524:LYS:HD2	1.85	0.58
1:D:659:LEU:HA	1:D:662:VAL:CG1	2.33	0.58
1:B:582:LYS:HD3	1:B:599:GLN:NE2	2.18	0.58
1:D:548:TYR:CZ	1:D:562:PRO:HG3	2.39	0.58
1:C:520:GLN:CG	1:C:521:LYS:N	2.65	0.57
1:C:657:LEU:HD22	1:C:657:LEU:H	1.68	0.57
1:A:664:ASP:CB	1:A:667:ASN:HD22	2.17	0.57
1:A:664:ASP:HB3	1:A:667:ASN:HD22	1.70	0.57
1:C:647:MET:HA	1:C:647:MET:HE3	1.86	0.57
1:C:530:ARG:C	1:C:530:ARG:HD3	2.29	0.57
1:C:659:LEU:HD13	1:C:668:ARG:HH21	1.69	0.57
1:D:679:GLU:O	1:D:683:GLU:HG3	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:521:LYS:O	1:A:522:GLU:HB3	2.06	0.56
1:A:504:VAL:HG12	1:A:505:VAL:N	2.21	0.56
1:A:524:LYS:H	1:A:524:LYS:HD3	1.71	0.56
1:B:576:VAL:HB	1:B:585:VAL:CG2	2.36	0.56
1:B:636:SER:HA	1:B:639:ARG:NH1	2.21	0.56
1:D:671:ILE:C	1:D:671:ILE:HD13	2.30	0.55
1:D:709:SER:HB2	2:D:141:HOH:O	2.06	0.55
1:A:673:ASN:HD22	1:A:676:ARG:HH12	1.54	0.55
1:A:716:ARG:HB2	1:A:717:PRO:HD3	1.89	0.55
1:D:724:ARG:HG3	1:D:724:ARG:HH11	1.70	0.55
1:B:531:ARG:CD	1:B:531:ARG:H	2.20	0.55
1:B:512:PHE:HB2	1:B:599:GLN:HB3	1.88	0.55
1:A:654:MET:HE1	1:A:657:LEU:HD23	1.88	0.54
1:C:669:LYS:HA	1:C:672:GLU:CG	2.37	0.54
1:B:531:ARG:HD2	1:B:531:ARG:N	2.21	0.54
1:D:665:PRO:HA	1:D:668:ARG:HG2	1.89	0.54
1:B:569:GLU:HG3	1:B:620:LEU:HD23	1.89	0.54
1:D:530:ARG:H	1:D:530:ARG:CD	2.19	0.54
1:B:534:LYS:HD3	1:B:536:TYR:OH	2.07	0.54
1:D:676:ARG:HG2	1:D:676:ARG:HH11	1.72	0.54
1:D:671:ILE:O	1:D:671:ILE:HD13	2.08	0.53
1:A:520:GLN:HG3	1:A:526:GLU:CD	2.32	0.53
1:A:668:ARG:O	1:A:672:GLU:HG3	2.08	0.53
1:A:521:LYS:O	1:A:522:GLU:CB	2.57	0.53
1:A:654:MET:HE2	1:A:658:GLN:NE2	2.21	0.53
1:B:528:VAL:HB	1:B:531:ARG:NH1	2.19	0.53
1:B:531:ARG:H	1:B:531:ARG:HD2	1.72	0.53
1:C:687:MET:HE3	1:C:734:HIS:HA	1.91	0.53
1:B:588:LEU:C	1:B:588:LEU:HD23	2.34	0.53
1:A:579:HIS:O	1:B:719:LYS:HE2	2.09	0.52
1:C:702:GLY:HA3	2:C:278:HOH:O	2.10	0.52
1:C:662:VAL:O	1:C:668:ARG:HD3	2.09	0.52
1:D:603:GLN:O	1:D:607:GLU:HG3	2.09	0.52
1:D:652:LYS:HE3	1:D:679:GLU:HG2	1.92	0.52
1:D:659:LEU:HB2	1:D:671:ILE:HD12	1.90	0.52
1:D:669:LYS:HD3	1:D:670:ALA:N	2.25	0.52
1:D:520:GLN:HG3	1:D:526:GLU:OE1	2.10	0.51
1:B:531:ARG:HD2	1:B:531:ARG:C	2.35	0.51
1:B:711:LEU:HD22	1:B:728:LEU:CD1	2.40	0.51
1:D:622:ALA:HA	1:D:633:LEU:HD23	1.92	0.51
1:A:665:PRO:HG2	1:A:666:LYS:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:710:LEU:HD23	1:D:730:VAL:HG22	1.91	0.51
1:B:504:VAL:N	1:B:541:LYS:HE3	2.26	0.51
1:B:563:ARG:N	1:B:563:ARG:HD2	2.26	0.51
1:B:606:LEU:C	1:B:606:LEU:HD23	2.36	0.51
1:C:578:GLU:OE2	1:D:708:LYS:HE2	2.11	0.51
1:C:656:GLU:OE2	1:C:656:GLU:HA	2.11	0.51
1:C:662:VAL:HG13	1:C:664:ASP:OD1	2.10	0.51
1:B:548:TYR:CZ	1:B:562:PRO:HG3	2.46	0.50
1:D:653:LYS:HG3	1:D:654:MET:N	2.26	0.50
1:A:530:ARG:O	1:A:530:ARG:CG	2.59	0.50
1:D:606:LEU:C	1:D:606:LEU:HD23	2.37	0.50
1:B:667:ASN:O	1:B:671:ILE:HG13	2.12	0.50
1:A:673:ASN:ND2	1:A:676:ARG:HH12	2.09	0.50
1:C:588:LEU:C	1:C:588:LEU:HD23	2.37	0.49
1:B:523:ARG:HH22	1:B:742:ASP:N	2.10	0.49
1:A:684:LYS:HD3	1:A:737:VAL:CG1	2.42	0.49
1:B:659:LEU:HA	1:B:662:VAL:HG12	1.94	0.49
1:C:509:GLY:HA2	1:C:537:TRP:CZ3	2.48	0.49
1:C:658:GLN:O	1:C:662:VAL:HG23	2.12	0.49
1:B:529:ALA:O	1:B:531:ARG:N	2.45	0.49
1:B:534:LYS:HG3	1:B:536:TYR:CE2	2.47	0.49
1:C:606:LEU:HD23	1:C:606:LEU:C	2.38	0.49
1:C:664:ASP:HB3	1:C:667:ASN:HB3	1.93	0.49
1:D:659:LEU:HD13	1:D:671:ILE:HG23	1.93	0.49
1:C:714:THR:HG22	1:C:719:LYS:HG3	1.92	0.49
1:B:528:VAL:CB	1:B:531:ARG:HH11	2.20	0.49
1:B:549:GLU:OE1	1:B:549:GLU:HA	2.12	0.49
1:B:716:ARG:HH12	1:B:720:LEU:HD11	1.75	0.49
1:C:725:LEU:HD22	1:C:727:VAL:H	1.77	0.49
1:D:512:PHE:HB2	1:D:599:GLN:HB3	1.95	0.49
1:B:659:LEU:HA	1:B:662:VAL:CG1	2.42	0.49
1:C:653:LYS:O	1:C:657:LEU:HD22	2.13	0.49
1:D:665:PRO:C	1:D:667:ASN:H	2.19	0.49
1:C:652:LYS:O	1:C:656:GLU:HG2	2.13	0.48
1:D:662:VAL:O	1:D:662:VAL:HG13	2.13	0.48
1:A:647:MET:HE3	1:A:651:MET:CG	2.43	0.48
1:D:675:ILE:O	1:D:679:GLU:HG3	2.14	0.48
1:B:532:LYS:H	1:B:532:LYS:CD	2.24	0.48
1:D:708:LYS:NZ	2:D:107:HOH:O	2.47	0.48
1:A:588:LEU:C	1:A:588:LEU:HD23	2.39	0.48
1:C:725:LEU:HD23	1:C:725:LEU:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:728:LEU:C	1:C:728:LEU:HD23	2.38	0.47
1:D:548:TYR:CE1	1:D:562:PRO:HG3	2.49	0.47
1:B:716:ARG:HB3	1:B:717:PRO:HD3	1.95	0.47
1:D:528:VAL:CG1	1:D:530:ARG:HH11	2.28	0.47
1:A:548:TYR:CZ	1:A:562:PRO:HG3	2.49	0.47
1:A:659:LEU:HD11	1:A:668:ARG:HD3	1.97	0.47
1:C:647:MET:HA	1:C:647:MET:CE	2.43	0.47
1:D:716:ARG:HB3	1:D:717:PRO:HD3	1.95	0.47
1:A:654:MET:HA	1:A:654:MET:CE	2.37	0.47
1:A:674:GLN:HE21	1:A:678:TRP:HE1	1.62	0.47
1:A:606:LEU:C	1:A:606:LEU:HD23	2.40	0.47
1:B:662:VAL:HG13	1:B:668:ARG:HH12	1.79	0.47
1:D:668:ARG:HA	1:D:671:ILE:HG22	1.97	0.47
1:D:546:LEU:HD22	1:D:562:PRO:HG2	1.96	0.46
1:A:654:MET:CE	1:A:657:LEU:HD23	2.43	0.46
1:B:529:ALA:O	1:B:530:ARG:C	2.58	0.46
1:C:659:LEU:HD13	1:C:659:LEU:O	2.15	0.46
1:A:620:LEU:HD12	1:A:623:LYS:HE3	1.97	0.46
1:A:669:LYS:HG3	1:A:670:ALA:N	2.30	0.46
1:A:652:LYS:O	1:A:656:GLU:HG3	2.15	0.46
1:C:664:ASP:CB	1:C:667:ASN:HD22	2.28	0.46
1:D:652:LYS:O	1:D:656:GLU:HG3	2.16	0.46
1:A:569:GLU:OE2	1:A:624:LYS:HD2	2.15	0.46
1:C:549:GLU:OE2	1:C:563:ARG:NH1	2.49	0.46
1:D:659:LEU:HD13	1:D:671:ILE:CG2	2.46	0.45
1:C:515:PRO:HB2	1:C:528:VAL:HG21	1.97	0.45
1:A:667:ASN:HB3	2:A:270:HOH:O	2.16	0.45
1:D:588:LEU:HD23	1:D:588:LEU:C	2.42	0.45
1:D:622:ALA:HA	1:D:633:LEU:CD2	2.46	0.45
1:B:532:LYS:HD2	1:B:532:LYS:N	2.27	0.45
1:A:621:PHE:HZ	1:A:637:GLN:HE21	1.65	0.44
1:A:531:ARG:HA	2:A:311:HOH:O	2.16	0.44
1:A:622:ALA:HA	1:A:633:LEU:CD2	2.48	0.44
1:B:711:LEU:HD13	1:B:728:LEU:HD13	1.98	0.44
1:A:578:GLU:O	1:A:579:HIS:C	2.60	0.44
1:B:579:HIS:CE1	1:B:581:LYS:HG3	2.53	0.44
1:A:512:PHE:HB2	1:A:599:GLN:HB3	1.99	0.44
1:B:576:VAL:HB	1:B:585:VAL:HG23	1.99	0.44
1:A:579:HIS:O	1:B:719:LYS:CE	2.66	0.44
1:C:639:ARG:O	1:C:643:GLN:HG3	2.18	0.44
1:A:634:LEU:O	1:A:638:THR:HG23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:703:GLU:CD	1:D:703:GLU:N	2.69	0.44
1:D:537:TRP:HB3	1:D:548:TYR:HB2	2.00	0.43
1:B:634:LEU:HB2	1:B:696:LEU:HD13	1.99	0.43
1:D:728:LEU:C	1:D:728:LEU:HD23	2.43	0.43
1:C:590:ASN:ND2	1:C:594:ASP:HB2	2.33	0.43
1:C:668:ARG:HG2	1:C:668:ARG:HH11	1.82	0.43
1:A:520:GLN:HG2	1:A:526:GLU:HG2	2.01	0.43
1:A:549:GLU:CD	1:A:563:ARG:HG3	2.44	0.43
1:D:520:GLN:HB2	1:D:524:LYS:HG3	2.00	0.43
1:D:725:LEU:HD22	1:D:727:VAL:N	2.32	0.43
1:B:674:GLN:HG3	1:B:678:TRP:CZ3	2.54	0.43
1:D:655:ALA:O	1:D:671:ILE:HD11	2.19	0.43
1:C:534:LYS:HD3	1:C:536:TYR:CZ	2.54	0.42
1:C:548:TYR:CZ	1:C:562:PRO:HG3	2.53	0.42
1:B:508:ALA:HA	1:B:538:VAL:O	2.19	0.42
1:B:674:GLN:HG3	1:B:678:TRP:CH2	2.55	0.42
1:A:687:MET:HE3	1:A:734:HIS:HA	2.02	0.42
1:C:523:ARG:HG2	1:C:739:SER:O	2.20	0.42
1:C:675:ILE:O	1:C:679:GLU:HG3	2.19	0.42
1:D:534:LYS:HE3	1:D:536:TYR:OH	2.20	0.42
1:A:738:CYS:HA	1:A:741:ASP:OD2	2.19	0.42
1:D:521:LYS:O	1:D:524:LYS:HG2	2.19	0.42
1:C:638:THR:HG23	1:C:689:LEU:HD11	2.01	0.42
1:C:512:PHE:HB2	1:C:599:GLN:HB3	2.02	0.41
1:D:687:MET:HE3	1:D:734:HIS:HA	2.02	0.41
1:D:724:ARG:HG3	1:D:724:ARG:NH1	2.35	0.41
1:D:664:ASP:O	1:D:664:ASP:CG	2.62	0.41
1:D:716:ARG:O	1:D:720:LEU:HD13	2.20	0.41
1:B:548:TYR:CE2	1:B:562:PRO:HG3	2.55	0.41
1:C:531:ARG:HB3	2:C:314:HOH:O	2.20	0.41
1:D:659:LEU:CA	1:D:662:VAL:HG12	2.46	0.41
1:B:635:LYS:O	1:B:639:ARG:HG3	2.21	0.41
1:A:530:ARG:HG2	1:A:530:ARG:HH21	1.86	0.41
1:A:654:MET:O	1:A:658:GLN:HG2	2.21	0.41
1:B:579:HIS:HE1	1:B:581:LYS:HG3	1.86	0.41
1:B:531:ARG:CD	1:B:531:ARG:N	2.82	0.41
1:B:634:LEU:O	1:B:638:THR:HG23	2.21	0.41
1:D:668:ARG:HH11	1:D:668:ARG:HG3	1.85	0.41
1:C:716:ARG:HB2	1:C:717:PRO:HD3	2.02	0.41
1:D:578:GLU:O	1:D:579:HIS:C	2.62	0.41
1:B:522:GLU:HA	1:B:522:GLU:OE2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:622:ALA:HA	1:B:633:LEU:HD23	2.03	0.40
1:A:636:SER:HA	1:A:639:ARG:CZ	2.51	0.40
1:B:622:ALA:HA	1:B:633:LEU:CD2	2.51	0.40
1:C:517:VAL:HG22	1:C:527:LEU:HD23	2.02	0.40
1:C:668:ARG:HD2	1:C:668:ARG:HA	1.91	0.40
1:D:639:ARG:O	1:D:643:GLN:HG3	2.21	0.40
1:D:655:ALA:HB3	1:D:675:ILE:HD11	2.04	0.40
1:D:514:LYS:HE3	1:D:533:TRP:CD1	2.57	0.40
1:D:728:LEU:C	1:D:728:LEU:CD2	2.95	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	228/263 (87%)	225 (99%)	3 (1%)	0	100	100
1	B	227/263 (86%)	222 (98%)	3 (1%)	2 (1%)	14	10
1	C	225/263 (86%)	214 (95%)	9 (4%)	2 (1%)	14	10
1	D	224/263 (85%)	217 (97%)	5 (2%)	2 (1%)	14	10
All	All	904/1052 (86%)	878 (97%)	20 (2%)	6 (1%)	18	15

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	530	ARG
1	C	529	ALA
1	C	665	PRO
1	B	529	ALA
1	D	664	ASP
1	D	666	LYS

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	204/233 (88%)	199 (98%)	5 (2%)	42	48
1	B	205/233 (88%)	197 (96%)	8 (4%)	28	31
1	C	203/233 (87%)	199 (98%)	4 (2%)	48	56
1	D	201/233 (86%)	192 (96%)	9 (4%)	24	25
All	All	813/932 (87%)	787 (97%)	26 (3%)	34	38

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	524	LYS
1	A	530	ARG
1	A	654	MET
1	A	664	ASP
1	A	725	LEU
1	B	531	ARG
1	B	532	LYS
1	B	566	LEU
1	B	585	VAL
1	B	647	MET
1	B	658	GLN
1	B	672	GLU
1	B	728	LEU
1	C	549	GLU
1	C	578	GLU
1	C	647	MET
1	C	657	LEU
1	D	530	ARG
1	D	543	CYS
1	D	582	LYS
1	D	639	ARG
1	D	642	LEU
1	D	657	LEU
1	D	658	GLN

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Mol	Chain	Res	Type
1	D	664	ASP
1	D	671	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	658	GLN
1	A	667	ASN
1	A	673	ASN
1	A	674	GLN
1	A	677	GLN
1	A	680	GLN
1	B	579	HIS
1	B	599	GLN
1	B	637	GLN
1	B	658	GLN
1	B	667	ASN
1	B	673	ASN
1	C	637	GLN
1	C	667	ASN
1	C	674	GLN
1	C	680	GLN
1	D	599	GLN
1	D	643	GLN
1	D	686	HIS

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	A	232/263 (88%)	0.12	9 (3%) 43 45	22, 32, 59, 72	0
1	B	231/263 (87%)	0.35	12 (5%) 33 35	20, 37, 66, 80	0
1	C	229/263 (87%)	0.38	19 (8%) 17 18	24, 37, 73, 88	0
1	D	228/263 (86%)	0.25	12 (5%) 32 34	22, 35, 68, 83	0
All	All	920/1052 (87%)	0.27	52 (5%) 29 31	20, 35, 68, 88	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	550	THR	4.4
1	C	659	LEU	4.1
1	C	665	PRO	3.7
1	B	725	LEU	3.4
1	C	662	VAL	3.4
1	D	662	VAL	3.1
1	B	742	ASP	3.1
1	C	504	VAL	3.1
1	D	727	VAL	3.1
1	A	560	SER	3.1
1	A	504	VAL	3.0
1	D	678	TRP	2.9
1	D	725	LEU	2.9
1	C	661	VAL	2.9
1	B	531	ARG	2.8
1	B	529	ALA	2.8
1	D	671	ILE	2.8
1	C	671	ILE	2.8
1	C	561	ALA	2.7
1	C	664	ASP	2.7
1	A	665	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	522	GLU	2.7
1	C	741	ASP	2.6
1	B	565	ALA	2.6
1	C	670	ALA	2.5
1	D	529	ALA	2.5
1	C	657	LEU	2.5
1	D	728	LEU	2.5
1	A	741	ASP	2.4
1	B	530	ARG	2.3
1	C	666	LYS	2.3
1	B	526	GLU	2.3
1	D	661	VAL	2.3
1	B	551	TYR	2.3
1	B	665	PRO	2.3
1	D	665	PRO	2.3
1	D	563	ARG	2.2
1	B	563	ARG	2.2
1	D	562	PRO	2.2
1	B	561	ALA	2.2
1	C	527	LEU	2.2
1	A	529	ALA	2.2
1	C	668	ARG	2.2
1	A	664	ASP	2.2
1	C	667	ASN	2.1
1	A	530	ARG	2.1
1	A	521	LYS	2.1
1	C	669	LYS	2.1
1	C	655	ALA	2.1
1	A	520	GLN	2.0
1	C	676	ARG	2.0
1	D	667	ASN	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.