



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 01:51 pm GMT

PDB ID : 3A8P  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

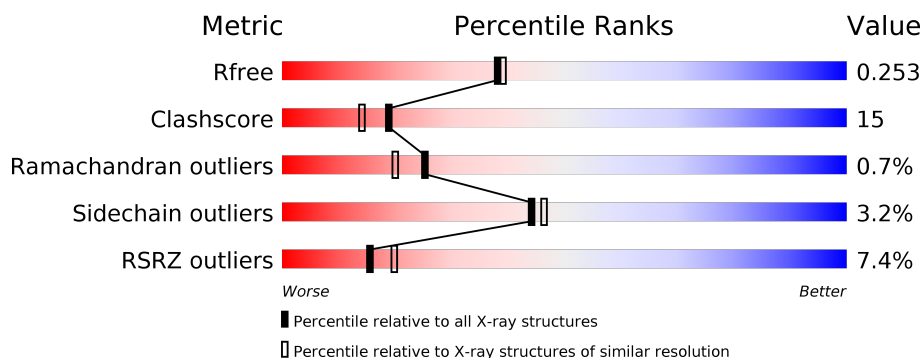
# 1 Overall quality at a glance

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))
$R_{free}$	100719	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	263	<div> <div>5%</div> <div> <div></div> <div>66%</div> <div>21%</div> <div>•</div> <div>12%</div> </div> </div>
1	B	263	<div> <div>5%</div> <div> <div></div> <div>65%</div> <div>21%</div> <div>•</div> <div>12%</div> </div> </div>
1	C	263	<div> <div>8%</div> <div> <div></div> <div>66%</div> <div>19%</div> <div>•</div> <div>13%</div> </div> </div>
1	D	263	<div> <div>8%</div> <div> <div></div> <div>62%</div> <div>24%</div> <div>•</div> <div>13%</div> </div> </div>

## 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			

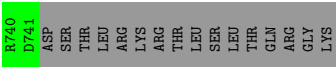
There are 20 discrepancies between the modelled and reference sequences:

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

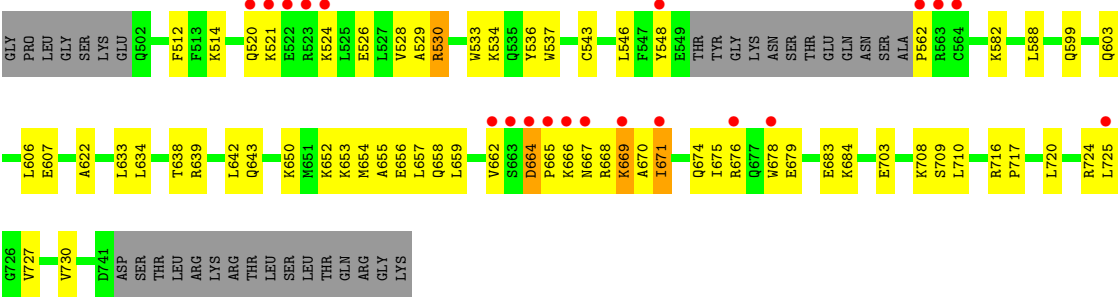
- Molecule 2 is water.

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





● 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, $\alpha$ , $\beta$ , $\gamma$	46.69Å 104.79Å 115.97Å 90.00° 80.55° 90.00°	Depositor
Resolution (Å)	29.81 – 2.10 37.76 – 2.08	Depositor EDS
% Data completeness (in resolution range)	98.7 (29.81-2.10) 97.7 (37.76-2.08)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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	6404 reflections (10.10%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.5	Xtriage
Anisotropy	0.546	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 53.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

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	0.35	0/1893	0.54	0/2548
1	B	0.34	0/1890	0.55	0/2544
1	C	0.33	0/1876	0.53	0/2525
1	D	0.33	0/1859	0.53	0/2500
All	All	0.34	0/7518	0.54	0/10117

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	49	0
1	B	1853	0	1901	62	0
1	C	1839	0	1892	49	0
1	D	1823	0	1875	62	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	219	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 15.



All (219) 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: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:A:590:ASN:HD21	1:A:594:ASP:HB2	1.53	0.72
1:B:725:LEU:HD23	1:B:725:LEU:O	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
1:D:703:GLU:CD	1:D:703:GLU:H	1.93	0.70
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:A:504:VAL:N	1:A:541:LYS:HZ2	1.94	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:C:520:GLN:HG3	1:C:521:LYS:N	2.07	0.64
1:A:654:MET:HE1	1:A:657:LEU:HD23	1.80	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: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: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:HG2	1:A:530:ARG:O	2.00	0.60
1:B:662:VAL:HG13	1:B:668:ARG:HH11	1.63	0.60
1:D:725:LEU:C	1:D:725:LEU:HD23	2.21	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:520:GLN:CG	1:C:521:LYS:N	2.65	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: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:657:LEU:H	1:C:657:LEU:HD22	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: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
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:HD3	1:A:524:LYS:H	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:B:523:ARG:HH22	1:B:741:ASP:C	2.10	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:654:MET:CE	1:A:654:MET:HA	2.37	0.55
1:A:716:ARG:HB2	1:A:717:PRO:HD3	1.89	0.55
1:D:724:ARG:HH11	1:D:724:ARG:HG3	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:C:669:LYS:HA	1:C:672:GLU:CG	2.37	0.54
1:C:725:LEU:HD23	1:C:725:LEU:C	2.26	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:A:654:MET:HE2	1:A:654:MET:HA	1.89	0.53
1:D:671:ILE:O	1:D:671:ILE:HD13	2.08	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: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:530:ARG:HD3	1:C:530:ARG:C	2.29	0.52
1:A:579:HIS:O	1:B:719:LYS:HE2	2.09	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:HD2	1:B:563:ARG:N	2.26	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:D:671:ILE:C	1:D:671:ILE:HD13	2.30	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:CG	1:A:530:ARG:O	2.59	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:B:549:GLU:HA	1:B:549:GLU:OE1	2.12	0.50
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: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: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:A:520:GLN:HG3	1:A:526:GLU:CD	2.32	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:662:VAL:O	1:D:662:VAL:HG13	2.13	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:647:MET:HA	1:C:647:MET:CE	2.43	0.48
1:C:652:LYS:O	1:C:656:GLU:HG2	2.13	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:C:725:LEU:O	1:C:725:LEU:HD23	2.14	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:B:588:LEU:HD23	1:B:588:LEU:C	2.34	0.47
1:D:716:ARG:HB3	1:D:717:PRO:HD3	1.95	0.47
1:A:674:GLN:HE21	1:A:678:TRP:HE1	1.62	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:B:531:ARG:C	1:B:531:ARG:HD2	2.35	0.46
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:C:659:LEU:O	1:C:659:LEU:HD13	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:B:606:LEU:C	1:B:606:LEU:HD23	2.36	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:D:606:LEU:HD23	1:D:606:LEU:C	2.37	0.45
1:C:515:PRO:HB2	1:C:528:VAL:HG21	1.97	0.45
1:C:588:LEU:C	1:C:588:LEU:HD23	2.37	0.45
1:A:667:ASN:HB3	2:A:270:HOH:O	2.16	0.45
1:D:622:ALA:HA	1:D:633:LEU:CD2	2.46	0.45
1:B:532:LYS:N	1:B:532:LYS:HD2	2.27	0.45
1:A:621:PHE:HZ	1:A:637:GLN:HE21	1.65	0.44
1:C:606:LEU:C	1:C:606:LEU:HD23	2.38	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:B:579:HIS:CE1	1:B:581:LYS:HG3	2.53	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:665:PRO:C	1:D:667:ASN:H	2.19	0.44
1:A:634:LEU:O	1:A:638:THR:HG23	2.18	0.44
1:D:537:TRP:HB3	1:D:548:TYR:HB2	2.00	0.43
1:B:654:MET:HE1	1:B:657:LEU:HD22	2.01	0.43
1:C:728:LEU:HD23	1:C:728:LEU:C	2.38	0.43
1:B:634:LEU:HB2	1:B:696:LEU:HD13	1.99	0.43
1:C:590:ASN:ND2	1:C:594:ASP:HB2	2.33	0.43
1:C:668:ARG:HH11	1:C:668:ARG:HG2	1.82	0.43
1:A:520:GLN:HG2	1:A:526:GLU:HG2	2.01	0.43
1:A:588:LEU:C	1:A:588:LEU:HD23	2.39	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:606:LEU:HD23	1:A:606:LEU:C	2.40	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:724:ARG:HG3	1:D:724:ARG:NH1	2.35	0.41
1:B:529:ALA:O	1:B:530:ARG:C	2.58	0.41
1:D:716:ARG:O	1:D:720:LEU:HD13	2.20	0.41
1:B:654:MET:CE	1:B:657:LEU:HD22	2.50	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:HH21	1:A:530:ARG:HG2	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

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:634:LEU:O	1:B:638:THR:HG23	2.21	0.41
1:B:531:ARG:CD	1:B:531:ARG:N	2.82	0.41
1:D:668:ARG:HG3	1:D:668:ARG:HH11	1.85	0.41
1:C:716:ARG:HB2	1:C:717:PRO:HD3	2.02	0.41
1:B:522:GLU:HA	1:B:522:GLU:OE2	2.21	0.40
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:A:647:MET:HE3	1:A:651:MET:CG	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:588:LEU:HD23	1:D:588:LEU:C	2.42	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

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	228/263 (87%)	225 (99%)	3 (1%)	0	100	100
1	B	227/263 (86%)	222 (98%)	3 (1%)	2 (1%)	20	14
1	C	225/263 (86%)	214 (95%)	9 (4%)	2 (1%)	20	14
1	D	224/263 (85%)	217 (97%)	5 (2%)	2 (1%)	20	14
All	All	904/1052 (86%)	878 (97%)	20 (2%)	6 (1%)	25	20

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%)	198 (97%)	6 (3%)	48	51
1	B	205/233 (88%)	199 (97%)	6 (3%)	48	51
1	C	203/233 (87%)	198 (98%)	5 (2%)	53	57
1	D	201/233 (86%)	192 (96%)	9 (4%)	32	30
All	All	813/932 (87%)	787 (97%)	26 (3%)	44	46

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	668	ARG
1	A	725	LEU
1	B	531	ARG
1	B	532	LYS
1	B	566	LEU
1	B	585	VAL
1	B	658	GLN
1	B	672	GLU
1	C	530	ARG
1	C	549	GLU
1	C	647	MET
1	C	657	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	664	ASP
1	D	530	ARG
1	D	543	CYS
1	D	582	LYS
1	D	642	LEU
1	D	657	LEU
1	D	658	GLN
1	D	664	ASP
1	D	669	LYS
1	D	671	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	574	GLN
1	A	658	GLN
1	A	667	ASN
1	A	673	ASN
1	A	674	GLN
1	A	680	GLN
1	B	574	GLN
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	C	686	HIS
1	D	574	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 [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	232/263 (88%)	0.32	14 (6%) 23 28	22, 32, 59, 72	0
1	B	231/263 (87%)	0.37	12 (5%) 28 34	20, 37, 66, 80	0
1	C	229/263 (87%)	0.51	22 (9%) 9 11	24, 37, 73, 88	0
1	D	228/263 (86%)	0.47	20 (8%) 11 14	22, 35, 68, 83	0
All	All	920/1052 (87%)	0.42	68 (7%) 15 20	20, 35, 68, 88	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	659	LEU	6.8
1	D	665	PRO	6.7
1	A	504	VAL	6.6
1	C	665	PRO	6.2
1	D	666	LYS	5.8
1	B	550	THR	5.5
1	C	669	LYS	5.5
1	C	530	ARG	4.9
1	A	665	PRO	4.7
1	C	522	GLU	4.7
1	D	563	ARG	4.6
1	B	551	TYR	4.4
1	B	531	ARG	4.2
1	A	666	LYS	4.2
1	C	504	VAL	4.2
1	A	530	ARG	4.1
1	D	522	GLU	4.0
1	C	666	LYS	3.9
1	D	521	LYS	3.9
1	D	663	SER	3.8
1	C	664	ASP	3.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	625	HIS	3.6
1	C	662	VAL	3.6
1	A	552	GLY	3.5
1	A	521	LYS	3.4
1	D	562	PRO	3.3
1	C	529	ALA	3.2
1	D	523	ARG	3.2
1	D	669	LYS	3.2
1	B	522	GLU	3.1
1	C	521	LYS	3.1
1	B	530	ARG	3.1
1	D	662	VAL	3.1
1	D	664	ASP	3.0
1	D	671	ILE	3.0
1	B	741	ASP	2.9
1	A	522	GLU	2.9
1	A	667	ASN	2.8
1	D	548	TYR	2.8
1	D	667	ASN	2.8
1	C	523	ARG	2.7
1	D	524	LYS	2.7
1	C	520	GLN	2.6
1	D	678	TRP	2.6
1	A	560	SER	2.5
1	D	725	LEU	2.5
1	B	523	ARG	2.5
1	B	560	SER	2.5
1	C	624	LYS	2.5
1	B	567	PHE	2.5
1	C	647	MET	2.5
1	A	505	VAL	2.4
1	B	563	ARG	2.4
1	C	561	ALA	2.4
1	D	564	CYS	2.4
1	A	664	ASP	2.4
1	D	676	ARG	2.3
1	B	561	ALA	2.3
1	C	673	ASN	2.3
1	B	725	LEU	2.3
1	A	529	ALA	2.3
1	D	520	GLN	2.2
1	C	626	GLY	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	520	GLN	2.2
1	C	676	ARG	2.1
1	C	670	ALA	2.0
1	A	710	LEU	2.0
1	C	724	ARG	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.