



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:51 AM GMT

PDB ID : 3JXI  
Title : Crystal structure of the chicken TRPV4 ankyrin repeat domain  
Authors : Phelps, C.B.; Wang, R.R.; Gaudet, R.  
Deposited on : 2009-09-19  
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](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.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

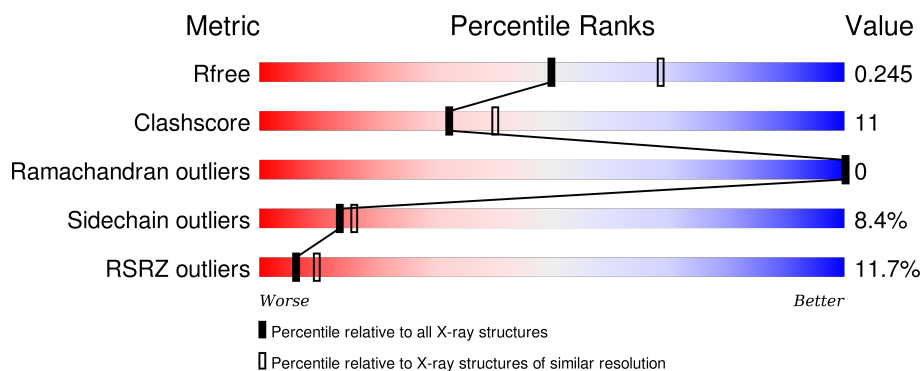
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	260	<div> <div>5%</div> <div>77%</div> <div>17%</div> <div>• •</div> </div>
1	B	260	<div> <div>7%</div> <div>75%</div> <div>19%</div> <div>5%</div> <div>•</div> </div>
1	C	260	<div> <div>4%</div> <div>72%</div> <div>20%</div> <div>• •</div> </div>
1	D	260	<div> <div>29%</div> <div>72%</div> <div>21%</div> <div>• •</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8556 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 Vanilloid receptor-related osmotically activated channel protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	253	Total 2017	C 1280	N 361	O 366	S 10	0	3	0
1	B	256	Total 2033	C 1289	N 368	O 367	S 9	0	0	0
1	C	249	Total 1990	C 1262	N 364	O 355	S 9	0	1	0
1	D	249	Total 1982	C 1257	N 361	O 355	S 9	0	0	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	132	MET	-	EXPRESSION TAG	UNP Q9DFS3
A	383	ALA	-	EXPRESSION TAG	UNP Q9DFS3
A	384	ALA	-	EXPRESSION TAG	UNP Q9DFS3
A	385	ALA	-	EXPRESSION TAG	UNP Q9DFS3
A	386	HIS	-	EXPRESSION TAG	UNP Q9DFS3
A	387	HIS	-	EXPRESSION TAG	UNP Q9DFS3
A	388	HIS	-	EXPRESSION TAG	UNP Q9DFS3
A	389	HIS	-	EXPRESSION TAG	UNP Q9DFS3
A	390	HIS	-	EXPRESSION TAG	UNP Q9DFS3
A	391	HIS	-	EXPRESSION TAG	UNP Q9DFS3
B	132	MET	-	EXPRESSION TAG	UNP Q9DFS3
B	383	ALA	-	EXPRESSION TAG	UNP Q9DFS3
B	384	ALA	-	EXPRESSION TAG	UNP Q9DFS3
B	385	ALA	-	EXPRESSION TAG	UNP Q9DFS3
B	386	HIS	-	EXPRESSION TAG	UNP Q9DFS3
B	387	HIS	-	EXPRESSION TAG	UNP Q9DFS3
B	388	HIS	-	EXPRESSION TAG	UNP Q9DFS3
B	389	HIS	-	EXPRESSION TAG	UNP Q9DFS3
B	390	HIS	-	EXPRESSION TAG	UNP Q9DFS3
B	391	HIS	-	EXPRESSION TAG	UNP Q9DFS3
C	132	MET	-	EXPRESSION TAG	UNP Q9DFS3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	383	ALA	-	EXPRESSION TAG	UNP Q9DFS3
C	384	ALA	-	EXPRESSION TAG	UNP Q9DFS3
C	385	ALA	-	EXPRESSION TAG	UNP Q9DFS3
C	386	HIS	-	EXPRESSION TAG	UNP Q9DFS3
C	387	HIS	-	EXPRESSION TAG	UNP Q9DFS3
C	388	HIS	-	EXPRESSION TAG	UNP Q9DFS3
C	389	HIS	-	EXPRESSION TAG	UNP Q9DFS3
C	390	HIS	-	EXPRESSION TAG	UNP Q9DFS3
C	391	HIS	-	EXPRESSION TAG	UNP Q9DFS3
D	132	MET	-	EXPRESSION TAG	UNP Q9DFS3
D	383	ALA	-	EXPRESSION TAG	UNP Q9DFS3
D	384	ALA	-	EXPRESSION TAG	UNP Q9DFS3
D	385	ALA	-	EXPRESSION TAG	UNP Q9DFS3
D	386	HIS	-	EXPRESSION TAG	UNP Q9DFS3
D	387	HIS	-	EXPRESSION TAG	UNP Q9DFS3
D	388	HIS	-	EXPRESSION TAG	UNP Q9DFS3
D	389	HIS	-	EXPRESSION TAG	UNP Q9DFS3
D	390	HIS	-	EXPRESSION TAG	UNP Q9DFS3
D	391	HIS	-	EXPRESSION TAG	UNP Q9DFS3

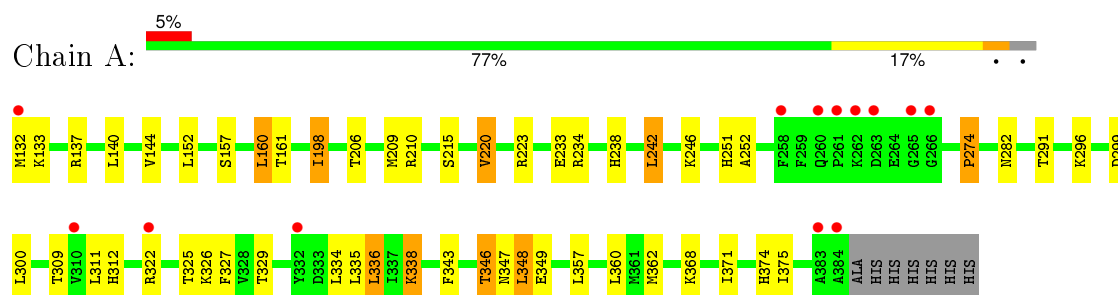
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	171	Total O 171 171	0	0
2	B	178	Total O 178 178	0	0
2	C	124	Total O 124 124	0	0
2	D	61	Total O 61 61	0	0

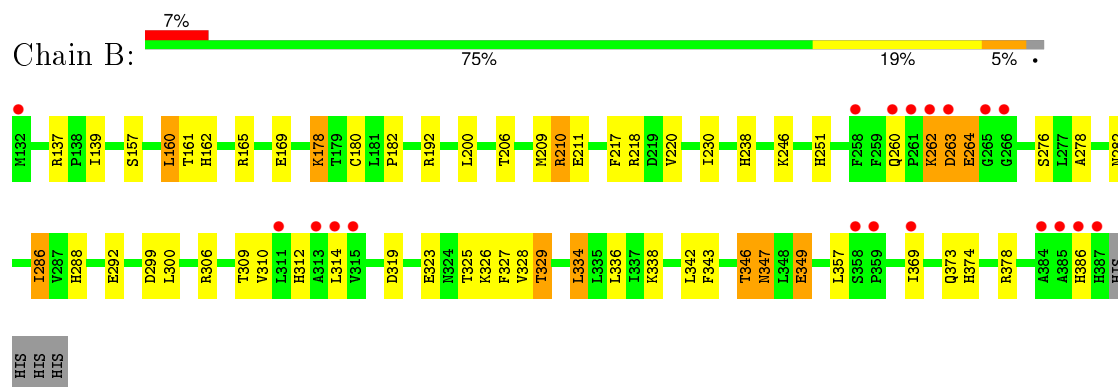
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

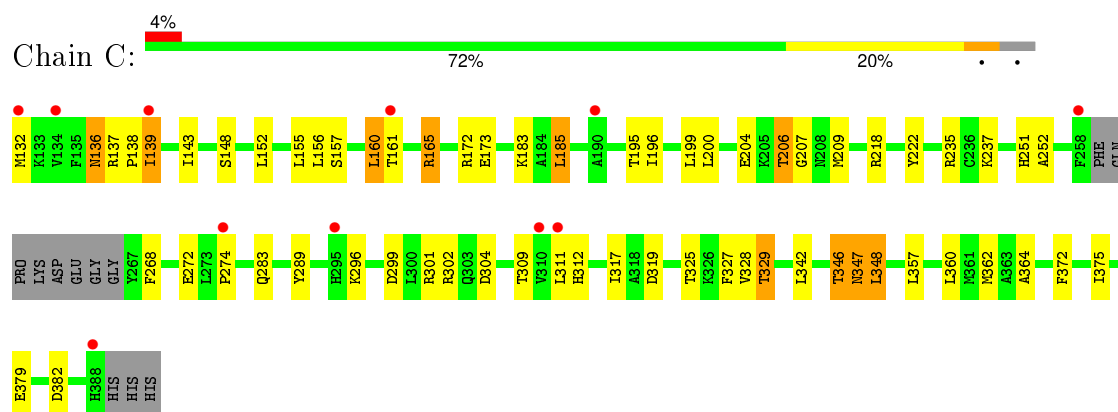
- Molecule 1: Vanilloid receptor-related osmotically activated channel protein



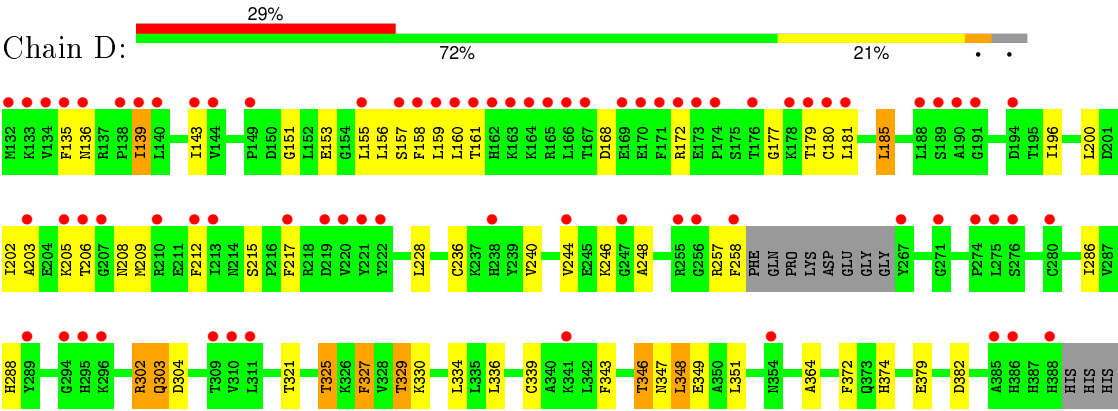
- Molecule 1: Vanilloid receptor-related osmotically activated channel protein



- Molecule 1: Vanilloid receptor-related osmotically activated channel protein



- Molecule 1: Vanilloid receptor-related osmotically activated channel protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.26Å 48.12Å 133.89Å 90.00° 101.89° 90.00°	Depositor
Resolution (Å)	29.51 – 2.30 29.51 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.7 (29.51-2.30) 97.6 (29.51-2.30)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.76 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.4.0066	Depositor
R, $R_{free}$	0.203 , 0.243 0.206 , 0.245	Depositor DCC
$R_{free}$ test set	1178 reflections (2.08%)	DCC
Wilson B-factor (Å <sup>2</sup> )	37.4	Xtriage
Anisotropy	0.208	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 50.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 57722 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8556	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.08 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.3910e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.77	0/2065	0.83	3/2788 (0.1%)
1	B	0.79	2/2074 (0.1%)	0.87	3/2799 (0.1%)
1	C	0.56	0/2032	0.70	1/2741 (0.0%)
1	D	0.46	0/2021	0.61	0/2727
All	All	0.66	2/8192 (0.0%)	0.76	7/11055 (0.1%)

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	2
1	C	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	180	CYS	CB-SG	-5.83	1.72	1.81
1	B	349	GLU	CB-CG	-5.29	1.42	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	378	ARG	NE-CZ-NH2	-7.01	116.80	120.30
1	B	378	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	A	137	ARG	NE-CZ-NH2	-6.13	117.24	120.30
1	A	137	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	B	137	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	A	234	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	C	172	ARG	NE-CZ-NH1	5.02	122.81	120.30



There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	262	LYS	Peptide
1	B	263	ASP	Peptide
1	C	207	GLY	Peptide

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2017	0	2049	39	0
1	B	2033	0	2053	41	0
1	C	1990	0	2019	44	0
1	D	1982	0	2006	48	0
2	A	171	0	0	6	0
2	B	178	0	0	7	0
2	C	124	0	0	6	0
2	D	61	0	0	5	0
All	All	8556	0	8127	170	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 11.

All (170) 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:D:257:ARG:O	1:D:258:PHE:CG	2.11	1.04
1:C:218[B]:ARG:HH11	1:C:218[B]:ARG:CG	1.71	1.03
1:D:158:PHE:HA	1:D:161:THR:HG22	1.44	0.97
1:C:218[B]:ARG:HH11	1:C:218[B]:ARG:HG2	1.24	0.97
1:D:257:ARG:O	1:D:258:PHE:CD2	2.24	0.90
1:D:155:LEU:HA	2:D:811:HOH:O	1.71	0.89
1:B:157:SER:O	1:B:161:THR:HG23	1.75	0.87
1:C:136:ASN:ND2	1:C:139:ILE:HG23	1.91	0.84
1:C:136:ASN:HD21	1:C:139:ILE:HG23	1.41	0.84
1:A:157:SER:O	1:A:161:THR:HG23	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:244:VAL:HA	1:D:248:ALA:HB3	1.65	0.78
1:A:209:MET:CE	2:A:623:HOH:O	2.31	0.77
1:C:218[B]:ARG:NH1	1:C:218[B]:ARG:HG2	2.00	0.76
1:A:209:MET:HE3	2:A:623:HOH:O	1.86	0.74
1:D:159:LEU:HD21	1:D:206:THR:HB	1.70	0.73
1:A:311:LEU:HG	1:A:348:LEU:HD13	1.70	0.72
1:A:360:LEU:HD13	1:A:375:ILE:CG2	2.20	0.71
1:C:200:LEU:O	1:C:209:MET:HE3	1.89	0.71
1:B:319:ASP:O	2:B:753:HOH:O	2.08	0.71
1:C:185:LEU:HD13	1:C:196:ILE:CD1	2.21	0.70
1:B:260:GLN:HB2	1:B:264:GLU:HG2	1.74	0.68
1:D:321:THR:O	1:D:325:THR:HG23	1.94	0.68
1:B:251:HIS:HE1	1:B:299:ASP:H	1.40	0.68
1:D:179:THR:HG21	1:D:212:PHE:CE2	2.29	0.68
1:C:206:THR:HG21	2:C:36:HOH:O	1.94	0.68
1:A:220:VAL:HG21	1:B:139:ILE:HG23	1.78	0.66
1:B:238:HIS:HB3	2:B:632:HOH:O	1.96	0.65
1:A:160:LEU:HD13	1:A:206:THR:HG22	1.79	0.65
1:C:165:ARG:HG2	1:C:206:THR:HG23	1.80	0.64
1:C:342:LEU:HD22	2:C:84:HOH:O	1.96	0.63
1:A:360:LEU:HD13	1:A:375:ILE:HG21	1.80	0.63
1:C:218[B]:ARG:HH11	1:C:218[B]:ARG:HG3	1.62	0.62
1:A:238:HIS:HE1	2:A:779:HOH:O	1.83	0.62
1:B:192:ARG:HG2	2:B:666:HOH:O	2.00	0.62
1:A:309:THR:H	1:A:312:HIS:HD2	1.48	0.61
1:A:209:MET:HE2	1:A:246:LYS:HD3	1.82	0.60
1:D:288:HIS:CE1	1:D:334:LEU:HD11	2.36	0.60
1:D:257:ARG:O	1:D:258:PHE:CD1	2.54	0.60
1:A:209:MET:HE1	2:A:623:HOH:O	1.99	0.60
1:D:168:ASP:HA	2:D:728:HOH:O	2.02	0.59
1:B:309:THR:H	1:B:312:HIS:HD2	1.49	0.59
1:D:329:THR:HG23	1:D:374:HIS:CE1	2.38	0.58
1:B:325:THR:O	1:B:329:THR:HB	2.02	0.58
1:B:209:MET:HE1	1:B:246:LYS:HD3	1.86	0.57
1:C:309:THR:H	1:C:312:HIS:HD2	1.52	0.57
1:A:209:MET:CE	1:A:246:LYS:HD3	2.35	0.57
1:C:311:LEU:HG	1:C:348:LEU:HD13	1.87	0.57
1:D:348:LEU:HD23	1:D:351:LEU:HD12	1.87	0.57
1:D:206:THR:HG23	1:D:208:ASN:HB2	1.87	0.57
1:B:260:GLN:CB	1:B:264:GLU:HG2	2.35	0.56
1:A:329:THR:HG23	1:A:374:HIS:CE1	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:362:MET:HE3	2:C:410:HOH:O	2.06	0.56
1:D:179:THR:CG2	1:D:212:PHE:CE2	2.88	0.56
1:A:209:MET:HE1	1:A:246:LYS:HE3	1.88	0.56
1:C:173:GLU:OE2	1:C:183:LYS:NZ	2.38	0.56
1:C:185:LEU:HD13	1:C:196:ILE:HD11	1.88	0.55
1:D:203:ALA:HA	1:D:206:THR:HG22	1.87	0.55
1:A:300:LEU:HD11	1:A:338:LYS:HD2	1.89	0.55
1:C:218[B]:ARG:NH1	1:C:218[B]:ARG:CG	2.43	0.54
1:A:311:LEU:CG	1:A:348:LEU:HD13	2.36	0.54
1:B:160:LEU:HD13	1:B:206:THR:HG22	1.88	0.54
1:B:300:LEU:HD11	1:B:338:LYS:HG2	1.88	0.54
1:A:309:THR:H	1:A:312:HIS:CD2	2.25	0.53
1:C:325:THR:O	1:C:329:THR:HB	2.08	0.53
1:B:343:PHE:HB3	1:B:346:THR:HG23	1.90	0.53
1:C:317:ILE:HD11	1:C:328:VAL:HG22	1.90	0.53
1:C:157:SER:O	1:C:161:THR:HG23	2.08	0.53
1:D:156:LEU:HD21	1:D:205:LYS:HD3	1.90	0.53
1:A:251:HIS:HE1	1:A:299:ASP:H	1.57	0.53
1:A:251:HIS:CE1	1:A:299:ASP:H	2.27	0.53
1:D:321:THR:O	1:D:325:THR:CG2	2.56	0.52
1:A:312:HIS:HE1	1:A:357:LEU:O	1.92	0.52
1:C:237:LYS:NZ	1:C:289:TYR:HB2	2.25	0.52
1:D:179:THR:CG2	1:D:180:CYS:N	2.72	0.52
1:A:334:LEU:HD23	1:A:334:LEU:C	2.30	0.52
1:B:178:LYS:NZ	2:B:758:HOH:O	2.43	0.52
1:D:206:THR:HG23	1:D:208:ASN:CB	2.39	0.51
1:C:143:ILE:HG23	1:C:148:SER:O	2.10	0.51
1:C:222:TYR:OH	1:C:268:PHE:O	2.24	0.51
1:D:228:LEU:HD11	1:D:240:VAL:HG13	1.92	0.51
1:D:155:LEU:HD23	1:D:202:ILE:HD13	1.92	0.51
1:C:301:ARG:CD	1:C:346:THR:HG21	2.40	0.51
1:C:301:ARG:HD2	1:C:346:THR:HG21	1.93	0.50
1:D:200:LEU:HB3	1:D:209:MET:HE3	1.91	0.50
1:B:262:LYS:HB2	1:B:263:ASP:HB2	1.93	0.50
1:D:179:THR:HG22	1:D:181:LEU:H	1.75	0.50
1:B:209:MET:HE1	2:B:629:HOH:O	2.11	0.50
1:B:288:HIS:HD2	1:B:292:GLU:OE1	1.94	0.50
1:A:223:ARG:NE	2:A:755:HOH:O	2.35	0.49
1:B:210:ARG:HG3	1:B:211:GLU:OE2	2.12	0.49
1:A:343:PHE:HB3	1:A:346:THR:HG23	1.95	0.49
1:C:347:ASN:C	1:C:347:ASN:HD22	2.16	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:312:HIS:HE1	1:B:357:LEU:O	1.96	0.49
1:D:217:PHE:HA	2:D:772:HOH:O	2.12	0.49
1:D:364:ALA:HB2	1:D:372:PHE:CE1	2.48	0.49
1:A:252:ALA:O	1:A:274:PRO:HD3	2.13	0.48
1:A:242:LEU:CD2	1:A:246:LYS:HD2	2.44	0.48
1:D:257:ARG:O	1:D:257:ARG:HG2	2.14	0.48
1:A:325:THR:O	1:A:329:THR:HB	2.13	0.48
1:D:143:ILE:HD13	1:D:151:GLY:O	2.12	0.48
1:A:251:HIS:HD2	2:A:574:HOH:O	1.97	0.48
1:A:312:HIS:CA	1:A:362:MET:HE1	2.44	0.48
1:D:157:SER:O	1:D:160:LEU:N	2.46	0.48
1:D:135:PHE:CD1	1:D:139:ILE:HD11	2.49	0.47
1:B:314:LEU:HB3	1:B:328:VAL:HG13	1.96	0.47
1:C:156:LEU:HG	1:C:160:LEU:HD22	1.97	0.47
1:D:236:CYS:O	1:D:240:VAL:HG23	2.13	0.47
1:B:251:HIS:CE1	1:B:299:ASP:H	2.27	0.47
1:B:276:SER:HA	1:B:310:VAL:HG23	1.97	0.47
1:D:228:LEU:CD1	1:D:240:VAL:HG13	2.45	0.47
1:D:185:LEU:HD13	1:D:196:ILE:HD11	1.96	0.47
1:B:329:THR:HG23	1:B:374:HIS:CE1	2.50	0.46
1:A:336:LEU:HD21	1:A:349:GLU:HG2	1.96	0.46
1:C:272:GLU:OE1	1:C:304:ASP:HB2	2.15	0.46
1:B:178:LYS:HE2	2:B:715:HOH:O	2.15	0.46
1:D:177:GLY:O	2:D:772:HOH:O	2.21	0.46
1:D:302:ARG:HG2	2:D:785:HOH:O	2.16	0.46
1:A:311:LEU:CD1	1:A:348:LEU:HD13	2.46	0.46
1:C:204:GLU:HB2	1:C:209:MET:HE3	1.98	0.46
1:D:179:THR:HG22	1:D:180:CYS:N	2.30	0.46
1:D:343:PHE:O	1:D:346:THR:HG23	2.16	0.46
1:A:291:THR:OG1	1:A:338:LYS:CE	2.64	0.46
1:D:179:THR:HG21	1:D:212:PHE:CD2	2.52	0.45
1:C:251:HIS:HE1	1:C:299:ASP:H	1.64	0.45
1:A:152:LEU:HD12	1:A:198:ILE:HG12	1.99	0.45
1:D:303:GLN:HB2	1:D:303:GLN:HE21	1.61	0.45
1:C:329:THR:CG2	2:C:18:HOH:O	2.64	0.45
1:D:155:LEU:HD23	1:D:202:ILE:CD1	2.47	0.45
1:B:278:ALA:HB1	1:B:286:ILE:HG13	1.99	0.45
1:C:132:MET:SD	1:C:139:ILE:HD12	2.57	0.45
1:C:195:THR:O	1:C:199:LEU:HG	2.16	0.45
1:D:336:LEU:HD21	1:D:349:GLU:HG3	1.99	0.45
1:B:162:HIS:HD2	2:C:570:HOH:O	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:ARG:HB3	1:C:138:PRO:HD3	1.98	0.44
1:C:319:ASP:C	1:C:319:ASP:OD1	2.54	0.44
1:C:312:HIS:HE1	1:C:357:LEU:O	2.01	0.44
1:D:327:PHE:CD2	1:D:327:PHE:C	2.91	0.44
1:B:347:ASN:C	1:B:347:ASN:HD22	2.21	0.44
1:D:329:THR:HG22	1:D:330:LYS:N	2.32	0.44
1:C:364:ALA:HB2	1:C:372:PHE:CE1	2.53	0.44
1:B:306:ARG:NE	2:B:45:HOH:O	2.51	0.43
1:C:185:LEU:HD13	1:C:196:ILE:HD13	1.98	0.43
1:B:347:ASN:HD21	1:B:349:GLU:HB2	1.84	0.43
1:B:309:THR:H	1:B:312:HIS:CD2	2.34	0.42
1:D:185:LEU:HD13	1:D:196:ILE:CD1	2.49	0.42
1:B:217:PHE:CZ	1:B:230:ILE:HD11	2.54	0.42
1:C:136:ASN:HD21	1:C:139:ILE:CG2	2.23	0.42
1:A:291:THR:OG1	1:A:338:LYS:HE2	2.19	0.42
1:B:178:LYS:HG2	1:B:182:PRO:HB2	2.02	0.42
1:D:240:VAL:HG21	1:D:286:ILE:HD13	2.01	0.42
1:B:278:ALA:HB2	1:B:286:ILE:HD11	2.01	0.42
1:B:200:LEU:O	1:B:209:MET:HE3	2.20	0.42
1:A:300:LEU:HD21	1:A:335:LEU:HD23	2.02	0.42
1:C:152:LEU:HD22	1:C:155:LEU:HD22	2.02	0.42
1:B:369:ILE:O	1:B:373:GLN:HG3	2.20	0.41
1:D:209:MET:HE2	1:D:246:LYS:HB3	2.02	0.41
1:C:360:LEU:HD13	1:C:375:ILE:HB	2.01	0.41
1:C:252:ALA:O	1:C:274:PRO:HD3	2.21	0.41
1:B:260:GLN:CG	1:B:264:GLU:HG2	2.51	0.41
1:D:172:ARG:NH1	1:D:177:GLY:O	2.54	0.41
1:A:140:LEU:O	1:A:144:VAL:HG13	2.21	0.41
1:B:288:HIS:CE1	1:B:334:LEU:HD11	2.56	0.41
1:A:209:MET:HE1	1:A:246:LYS:CE	2.50	0.41
1:A:368:LYS:HB3	1:A:371:ILE:HG22	2.03	0.41
1:B:209:MET:CE	1:B:246:LYS:HD3	2.51	0.40
1:B:209:MET:HE2	1:B:246:LYS:HB3	2.04	0.40
1:D:325:THR:O	1:D:329:THR:HB	2.21	0.40
1:C:235:ARG:HA	1:C:283:GLN:OE1	2.21	0.40
1:A:220:VAL:HG22	1:B:139:ILE:HD12	2.04	0.40
1:C:329:THR:HG22	2:C:18:HOH:O	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	254/260 (98%)	246 (97%)	8 (3%)	0	100	100
1	B	254/260 (98%)	242 (95%)	12 (5%)	0	100	100
1	C	246/260 (95%)	235 (96%)	11 (4%)	0	100	100
1	D	245/260 (94%)	228 (93%)	17 (7%)	0	100	100
All	All	999/1040 (96%)	951 (95%)	48 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 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	218/221 (99%)	197 (90%)	21 (10%)	10	12
1	B	217/221 (98%)	197 (91%)	20 (9%)	11	13
1	C	213/221 (96%)	198 (93%)	15 (7%)	19	23
1	D	212/221 (96%)	195 (92%)	17 (8%)	15	18
All	All	860/884 (97%)	787 (92%)	73 (8%)	14	16

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	132	MET
1	A	133	LYS

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Mol	Chain	Res	Type
1	A	160	LEU
1	A	198	ILE
1	A	210	ARG
1	A	215[A]	SER
1	A	215[B]	SER
1	A	220	VAL
1	A	233	GLU
1	A	242	LEU
1	A	274	PRO
1	A	282	ASN
1	A	296	LYS
1	A	322	ARG
1	A	326	LYS
1	A	327	PHE
1	A	336	LEU
1	A	338	LYS
1	A	346	THR
1	A	347	ASN
1	A	348	LEU
1	B	160	LEU
1	B	165	ARG
1	B	169	GLU
1	B	178	LYS
1	B	210	ARG
1	B	218	ARG
1	B	220	VAL
1	B	264	GLU
1	B	282	ASN
1	B	286	ILE
1	B	323	GLU
1	B	326	LYS
1	B	327	PHE
1	B	329	THR
1	B	334	LEU
1	B	336	LEU
1	B	342	LEU
1	B	346	THR
1	B	347	ASN
1	B	386	HIS
1	C	136	ASN
1	C	139	ILE
1	C	160	LEU

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Mol	Chain	Res	Type
1	C	165	ARG
1	C	185	LEU
1	C	206	THR
1	C	296	LYS
1	C	302	ARG
1	C	327	PHE
1	C	329	THR
1	C	346	THR
1	C	347	ASN
1	C	348	LEU
1	C	379	GLU
1	C	382	ASP
1	D	136	ASN
1	D	139	ILE
1	D	153	GLU
1	D	185	LEU
1	D	215	SER
1	D	302	ARG
1	D	303	GLN
1	D	304	ASP
1	D	325	THR
1	D	327	PHE
1	D	329	THR
1	D	339	CYS
1	D	346	THR
1	D	347	ASN
1	D	348	LEU
1	D	379	GLU
1	D	382	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	251	HIS
1	A	282	ASN
1	A	297	GLN
1	A	312	HIS
1	A	347	ASN
1	A	354	ASN
1	A	373	GLN
1	B	251	HIS
1	B	282	ASN

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Mol	Chain	Res	Type
1	B	297	GLN
1	B	312	HIS
1	B	347	ASN
1	B	354	ASN
1	B	387	HIS
1	C	136	ASN
1	C	208	ASN
1	C	251	HIS
1	C	253	GLN
1	C	282	ASN
1	C	297	GLN
1	C	312	HIS
1	C	320	ASN
1	C	347	ASN
1	C	354	ASN
1	C	373	GLN
1	D	225	GLN
1	D	282	ASN
1	D	303	GLN
1	D	320	ASN
1	D	347	ASN
1	D	354	ASN
1	D	373	GLN
1	D	386	HIS

### 5.3.3 RNA [i](#)

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

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, 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	253/260 (97%)	0.22	13 (5%) 32 41	9, 17, 28, 35	0
1	B	256/260 (98%)	0.25	19 (7%) 17 25	9, 18, 35, 64	0
1	C	249/260 (95%)	0.28	11 (4%) 38 47	16, 25, 32, 44	0
1	D	249/260 (95%)	1.72	75 (30%) 1 1	23, 39, 62, 70	0
All	All	1007/1040 (96%)	0.61	118 (11%) 6 10	9, 24, 51, 70	0

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	134	VAL	15.7
1	D	135	PHE	15.5
1	D	132	MET	11.1
1	D	258	PHE	11.0
1	D	139	ILE	10.8
1	D	207	GLY	10.5
1	D	159	LEU	9.7
1	D	163	LYS	8.3
1	D	166	LEU	7.6
1	D	171	PHE	7.6
1	D	165	ARG	7.5
1	D	138	PRO	7.2
1	C	132	MET	6.5
1	D	157	SER	6.4
1	B	263	ASP	6.1
1	D	164	LYS	5.6
1	D	210	ARG	5.2
1	A	132	MET	5.0
1	D	178	LYS	5.0
1	D	179	THR	4.9
1	D	133	LYS	4.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	132	MET	4.8
1	D	190	ALA	4.8
1	B	385	ALA	4.8
1	D	256	GLY	4.7
1	D	180	CYS	4.5
1	B	261	PRO	4.5
1	D	136	ASN	4.3
1	D	267	TYR	4.2
1	D	295	HIS	4.1
1	B	386	HIS	4.1
1	B	387	HIS	4.1
1	D	181	LEU	4.0
1	D	222	TYR	3.9
1	D	220	VAL	3.8
1	D	161	THR	3.7
1	D	167	THR	3.7
1	D	294	GLY	3.7
1	D	162	HIS	3.6
1	B	262	LYS	3.5
1	D	203	ALA	3.5
1	C	388	HIS	3.5
1	D	276	SER	3.5
1	D	354	ASN	3.4
1	A	258	PHE	3.3
1	D	388	HIS	3.3
1	D	189	SER	3.3
1	A	322	ARG	3.2
1	B	265	GLY	3.2
1	D	213	ILE	3.2
1	A	261	PRO	3.1
1	D	275	LEU	3.1
1	D	172	ARG	3.1
1	D	206	THR	3.1
1	A	265	GLY	3.0
1	D	244	VAL	3.0
1	D	341	LYS	3.0
1	C	190	ALA	3.0
1	D	173	GLU	2.9
1	B	266	GLY	2.9
1	D	160	LEU	2.9
1	B	311	LEU	2.9
1	D	217	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	194	ASP	2.8
1	D	205	LYS	2.8
1	D	176	THR	2.8
1	C	161	THR	2.8
1	D	385	ALA	2.8
1	B	260	GLN	2.7
1	D	169	GLU	2.7
1	D	143	ILE	2.7
1	B	258	PHE	2.7
1	B	359	PRO	2.7
1	B	314	LEU	2.6
1	C	311	LEU	2.6
1	B	384	ALA	2.6
1	C	295	HIS	2.6
1	A	262	LYS	2.6
1	C	258	PHE	2.6
1	D	149	PRO	2.5
1	D	155	LEU	2.5
1	A	310	VAL	2.5
1	D	191	GLY	2.5
1	D	247	GLY	2.5
1	A	332	TYR	2.5
1	B	369	ILE	2.5
1	D	221	TYR	2.4
1	C	310	VAL	2.4
1	D	212	PHE	2.4
1	A	383	ALA	2.4
1	D	219	ASP	2.4
1	D	140	LEU	2.4
1	D	386	HIS	2.4
1	D	174	PRO	2.4
1	A	266	GLY	2.4
1	C	139	ILE	2.4
1	D	309	THR	2.4
1	C	134	VAL	2.4
1	D	158	PHE	2.3
1	D	311	LEU	2.3
1	D	238	HIS	2.3
1	D	280	CYS	2.3
1	D	255	ARG	2.3
1	B	315	VAL	2.3
1	D	188	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	296	LYS	2.2
1	D	170	GLU	2.2
1	B	313	ALA	2.2
1	D	310	VAL	2.2
1	D	274	PRO	2.2
1	D	144	VAL	2.2
1	D	289	TYR	2.2
1	D	271	GLY	2.2
1	A	263	ASP	2.2
1	A	384	ALA	2.1
1	B	358	SER	2.1
1	C	274	PRO	2.1
1	A	260	GLN	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.