Full wwPDB X-ray Structure Validation Report (i)

Aug 28, 2023 – 01:24 AM EDT

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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

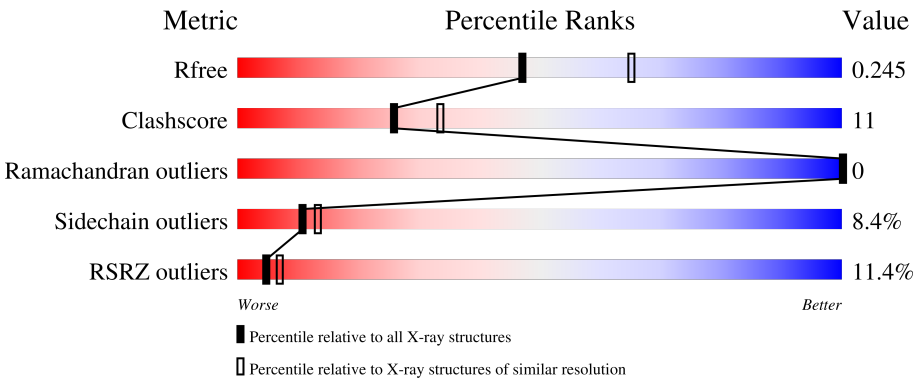
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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 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 <=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	5%, 77%, 17%, • •
1	B	260	7%, 75%, 19%, 5% •
1	C	260	4%, 72%, 20%, • •
1	D	260	29%, 72%, 21%, • •

2 Entry composition (i)

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

Continued on next page...

Continued from previous page...

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.

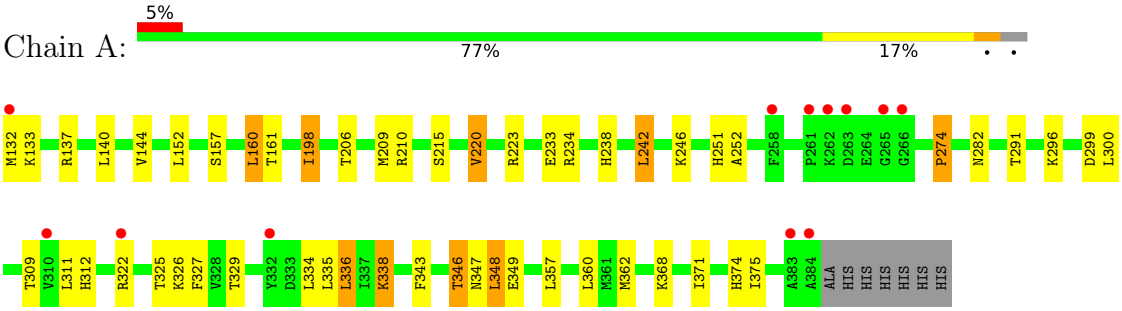
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	171	171	171	0	0
			Total	O		
2	B	178	178	178	0	0
			Total	O		
2	C	124	124	124	0	0
			Total	O		
2	D	61	61	61	0	0

3 Residue-property plots (i)

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.

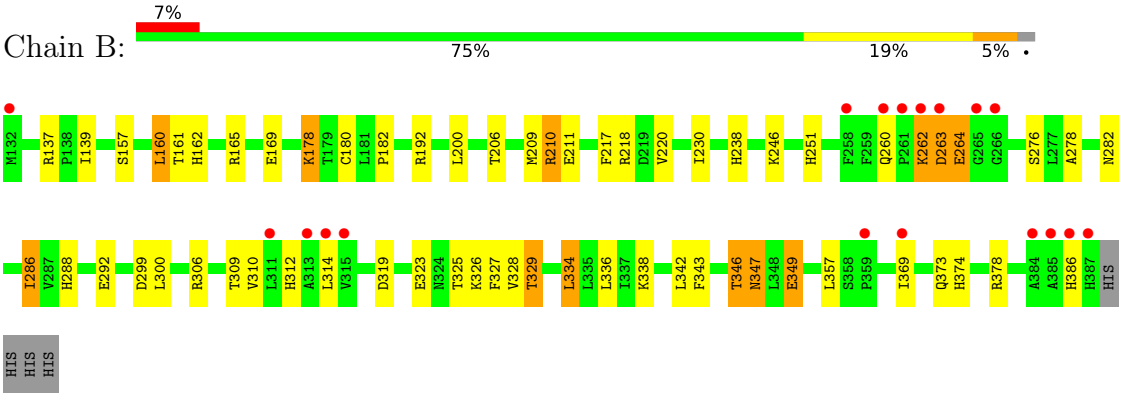
• Molecule 1: Vanilloid receptor-related osmotically activated channel protein

Chain A:



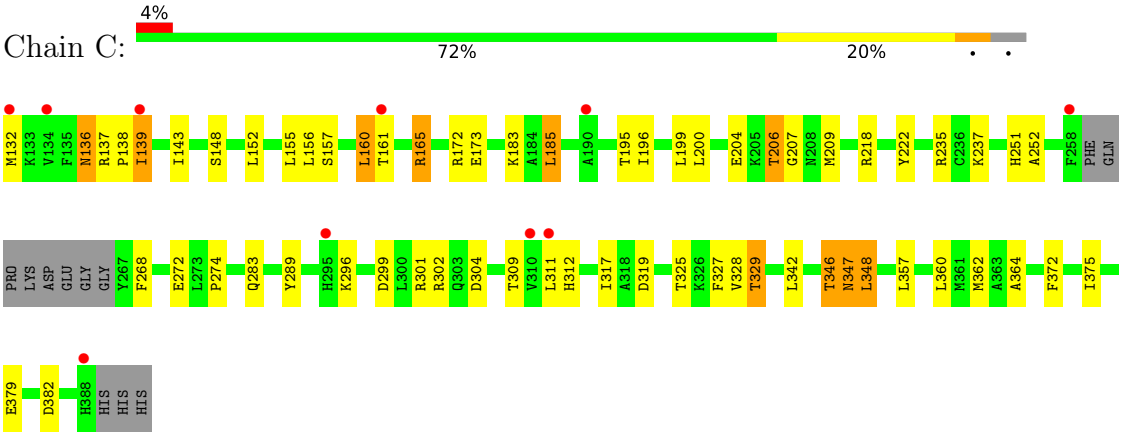
• Molecule 1: Vanilloid receptor-related osmotically activated channel protein

Chain B:



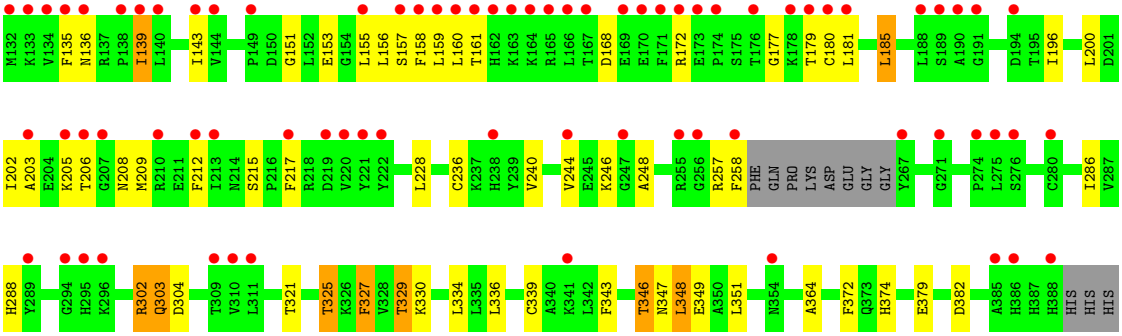
• Molecule 1: Vanilloid receptor-related osmotically activated channel protein

Chain C:



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

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	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 (2.04%)	wwPDB-VP
Wilson B-factor (Å^2)	37.4	Xtriage
Anisotropy	0.208	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 50.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8556	wwPDB-VP
Average B, all atoms (Å^2)	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.77	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(^{o})	Ideal(^{o})
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 (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	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

Continued on next page...

Continued from previous page...

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:HG2	1:C:218[B]:ARG:NH1	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:B:319:ASP:O	2:B:753:HOH:O	2.08	0.71
1:C:200:LEU:O	1:C:209:MET:HE3	1.89	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:A:238:HIS:HE1	2:A:779:HOH:O	1.83	0.62
1:C:218[B]:ARG:HH11	1:C:218[B]:ARG:HG3	1.62	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:A:329:THR:HG23	1:A:374:HIS:CE1	2.41	0.56
1:B:260:GLN:CB	1:B:264:GLU:HG2	2.35	0.56

Continued on next page...

Continued from previous page...

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:A:311:LEU:CG	1:A:348:LEU:HD13	2.36	0.54
1:C:218[B]:ARG:CG	1:C:218[B]:ARG:NH1	2.43	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:157:SER:O	1:C:161:THR:HG23	2.08	0.53
1:C:317:ILE:HD11	1:C:328:VAL:HG22	1.90	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:A:312:HIS:HE1	1:A:357:LEU:O	1.92	0.52
1:D:321:THR:O	1:D:325:THR:CG2	2.56	0.52
1:C:237:LYS:NZ	1:C:289:TYR:HB2	2.25	0.52
1:A:334:LEU:HD23	1:A:334:LEU:C	2.30	0.52
1:D:179:THR:CG2	1:D:180:CYS:N	2.72	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:C:301:ARG:CD	1:C:346:THR:HG21	2.40	0.51
1:D:155:LEU:HD23	1:D:202:ILE:HD13	1.92	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: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:D:179:THR:HG22	1:D:181:LEU:H	1.75	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

Continued on next page...

Continued from previous page...

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: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:D:257:ARG:O	1:D:257:ARG:HG2	2.14	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:185:LEU:HD13	1:D:196:ILE:HD11	1.96	0.47
1:D:228:LEU:CD1	1:D:240:VAL:HG13	2.45	0.47
1:A:336:LEU:HD21	1:A:349:GLU:HG2	1.96	0.46
1:B:329:THR:HG23	1:B:374:HIS:CE1	2.50	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:A:152:LEU:HD12	1:A:198:ILE:HG12	1.99	0.45
1:C:251:HIS:HE1	1:C:299:ASP:H	1.64	0.45
1:D:179:THR:HG21	1:D:212:PHE:CD2	2.52	0.45
1:D:303:GLN:HE21	1:D:303:GLN:HB2	1.61	0.45
1:C:329:THR:CG2	2:C:18:HOH:O	2.64	0.45
1:B:278:ALA:HB1	1:B:286:ILE:HG13	1.99	0.45
1:D:155:LEU:HD23	1:D:202:ILE:CD1	2.47	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

Continued on next page...

Continued from previous page...

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:B:347:ASN:HD21	1:B:349:GLU:HB2	1.84	0.43
1:C:185:LEU:HD13	1:C:196:ILE:HD13	1.98	0.43
1:B:309:THR:H	1:B:312:HIS:CD2	2.34	0.42
1:B:217:PHE:CZ	1:B:230:ILE:HD11	2.54	0.42
1:D:185:LEU:HD13	1:D:196:ILE:CD1	2.49	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:B:278:ALA:HB2	1:B:286:ILE:HD11	2.01	0.42
1:D:240:VAL:HG21	1:D:286:ILE:HD13	2.01	0.42
1:A:300:LEU:HD21	1:A:335:LEU:HD23	2.02	0.42
1:B:200:LEU:O	1:B:209:MET:HE3	2.20	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:C:360:LEU:HD13	1:C:375:ILE:HB	2.01	0.41
1:D:209:MET:HE2	1:D:246:LYS:HB3	2.02	0.41
1:C:252:ALA:O	1:C:274:PRO:HD3	2.21	0.41
1:A:140:LEU:O	1:A:144:VAL:HG13	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: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:C:235:ARG:HA	1:C:283:GLN:OE1	2.21	0.40
1:D:325:THR:O	1:D:329:THR:HB	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%)	8	10
1	B	217/221 (98%)	197 (91%)	20 (9%)	9	11
1	C	213/221 (96%)	198 (93%)	15 (7%)	15	19
1	D	212/221 (96%)	195 (92%)	17 (8%)	12	15
All	All	860/884 (97%)	787 (92%)	73 (8%)	11	13

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

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Sometimes 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

Continued on next page...

Continued from previous page...

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 monosaccharides 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	253/260 (97%)	0.16	12 (4%)	31	38	9, 17, 28, 35	0
1	B	256/260 (98%)	0.19	18 (7%)	16	21	9, 18, 35, 64	0
1	C	249/260 (95%)	0.22	10 (4%)	38	45	16, 25, 32, 44	0
1	D	249/260 (95%)	1.63	75 (30%)	0	0	23, 39, 62, 70	0
All	All	1007/1040 (96%)	0.55	115 (11%)	5	7	9, 24, 51, 70	0

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	134	VAL	15.2
1	D	135	PHE	15.1
1	D	132	MET	10.8
1	D	258	PHE	10.7
1	D	139	ILE	10.5
1	D	207	GLY	10.1
1	D	159	LEU	9.4
1	D	163	LYS	8.2
1	D	165	ARG	7.5
1	D	171	PHE	7.4
1	D	166	LEU	7.3
1	D	138	PRO	6.9
1	C	132	MET	6.3
1	D	157	SER	6.3
1	B	263	ASP	5.9
1	D	164	LYS	5.6
1	D	210	ARG	5.1
1	A	132	MET	4.9
1	D	178	LYS	4.9
1	D	133	LYS	4.8
1	D	179	THR	4.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	132	MET	4.7
1	B	385	ALA	4.6
1	D	190	ALA	4.6
1	D	256	GLY	4.5
1	B	261	PRO	4.3
1	D	180	CYS	4.3
1	D	136	ASN	4.1
1	D	267	TYR	4.1
1	B	386	HIS	4.0
1	D	295	HIS	4.0
1	B	387	HIS	3.9
1	D	222	TYR	3.8
1	D	181	LEU	3.8
1	D	220	VAL	3.6
1	D	294	GLY	3.6
1	D	167	THR	3.6
1	D	161	THR	3.5
1	B	262	LYS	3.5
1	D	162	HIS	3.4
1	D	203	ALA	3.4
1	C	388	HIS	3.4
1	D	276	SER	3.3
1	D	354	ASN	3.3
1	D	388	HIS	3.2
1	A	258	PHE	3.2
1	D	189	SER	3.2
1	A	322	ARG	3.1
1	D	213	ILE	3.1
1	B	265	GLY	3.0
1	A	261	PRO	3.0
1	D	172	ARG	3.0
1	D	206	THR	2.9
1	D	275	LEU	2.9
1	A	265	GLY	2.9
1	D	341	LYS	2.9
1	D	244	VAL	2.9
1	C	190	ALA	2.9
1	D	173	GLU	2.8
1	D	217	PHE	2.8
1	B	266	GLY	2.8
1	D	160	LEU	2.8
1	B	311	LEU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	205	LYS	2.7
1	D	194	ASP	2.7
1	C	161	THR	2.7
1	D	176	THR	2.7
1	D	385	ALA	2.7
1	B	260	GLN	2.6
1	D	169	GLU	2.6
1	D	143	ILE	2.6
1	B	359	PRO	2.5
1	B	314	LEU	2.5
1	A	262	LYS	2.5
1	C	311	LEU	2.5
1	C	295	HIS	2.5
1	B	258	PHE	2.5
1	C	258	PHE	2.5
1	B	384	ALA	2.5
1	D	155	LEU	2.4
1	D	247	GLY	2.4
1	A	310	VAL	2.4
1	D	149	PRO	2.4
1	A	332	TYR	2.4
1	D	221	TYR	2.4
1	D	191	GLY	2.4
1	B	369	ILE	2.3
1	D	219	ASP	2.3
1	A	383	ALA	2.3
1	D	212	PHE	2.3
1	D	386	HIS	2.3
1	C	310	VAL	2.3
1	D	140	LEU	2.3
1	C	139	ILE	2.3
1	A	266	GLY	2.2
1	D	174	PRO	2.2
1	D	309	THR	2.2
1	C	134	VAL	2.2
1	D	296	LYS	2.2
1	D	238	HIS	2.2
1	D	311	LEU	2.2
1	D	158	PHE	2.2
1	D	255	ARG	2.2
1	D	280	CYS	2.2
1	B	315	VAL	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	170	GLU	2.1
1	D	188	LEU	2.1
1	D	274	PRO	2.1
1	B	313	ALA	2.1
1	D	144	VAL	2.1
1	D	310	VAL	2.1
1	D	271	GLY	2.1
1	D	289	TYR	2.1
1	A	263	ASP	2.0
1	A	384	ALA	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 monosaccharides 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.