



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:01 PM UTC

PDB ID : 3JXI / pdb_00003jxi
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 ⓘ 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

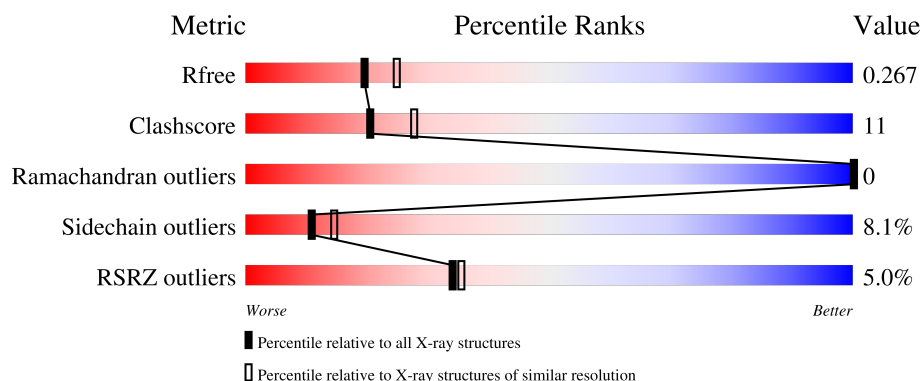
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 $\leq 5\%$. 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	
1	B	260	
1	C	260	
1	D	260	

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

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

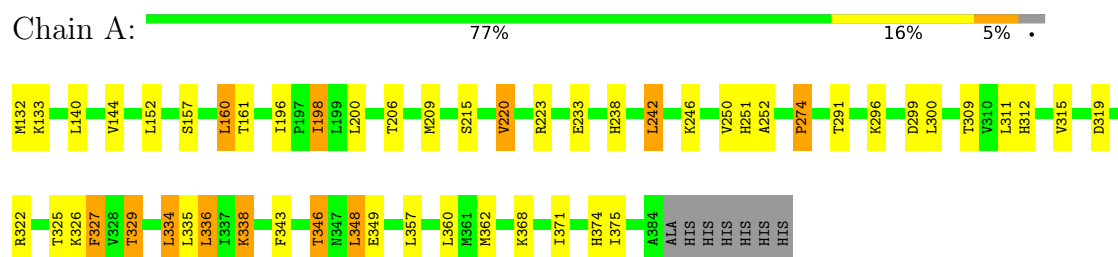
- Molecule 2 is water.

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

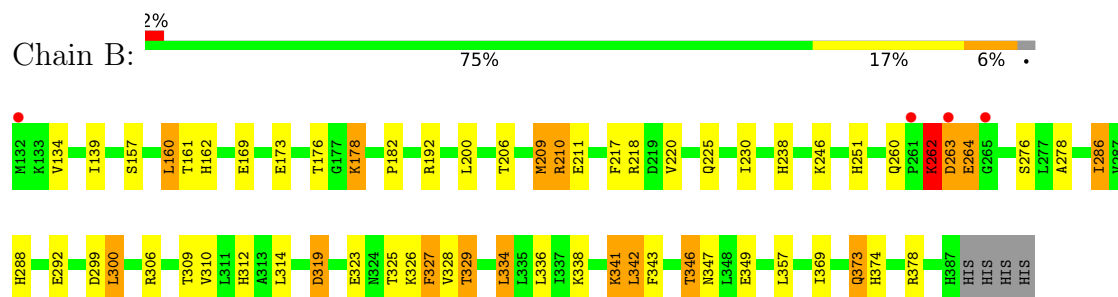
3 Residue-property plots

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.

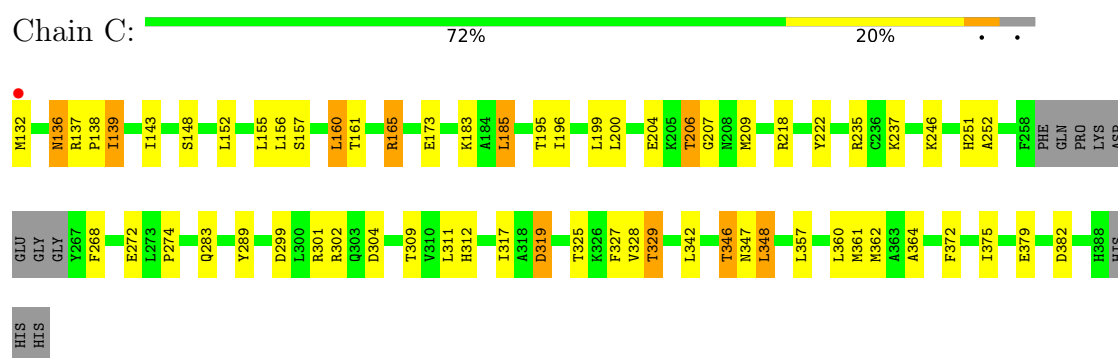
- Molecule 1: Vanilloid receptor-related osmotically activated channel protein



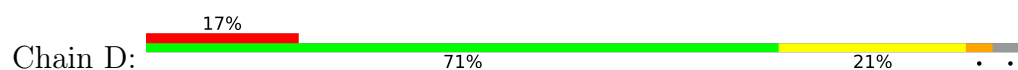
- Molecule 1: Vanilloid receptor-related osmotically activated channel protein

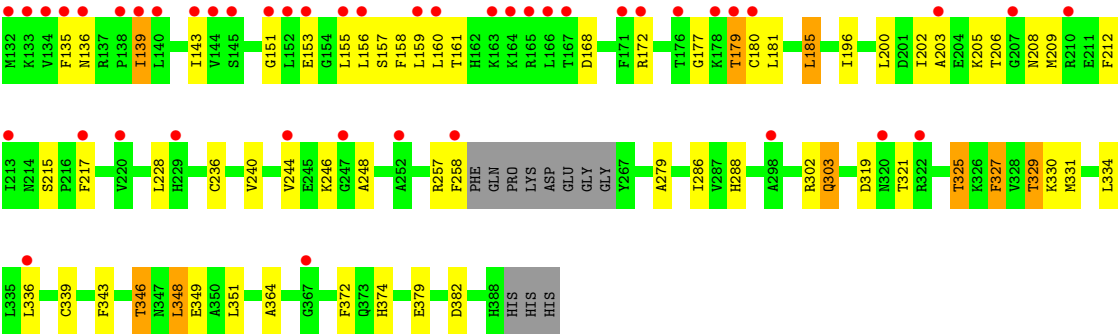


- Molecule 1: Vanilloid receptor-related osmotically activated channel protein



- 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, 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
$\langle I/\sigma(I) \rangle$ ¹	2.76 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.4.0066	Depositor
R, R_{free}	0.203 , 0.243 (Not available) , 0.267	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 , 53.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	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.*

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	1.00	2/2065 (0.1%)	1.03	1/2788 (0.0%)
1	B	0.99	0/2074	1.08	3/2799 (0.1%)
1	C	0.74	0/2032	0.92	1/2741 (0.0%)
1	D	0.66	0/2021	0.87	1/2727 (0.0%)
All	All	0.86	2/8192 (0.0%)	0.98	6/11055 (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	A	196	ILE	CA-CB	9.09	1.59	1.54
1	A	250	VAL	CA-CB	5.47	1.60	1.54

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	319	ASP	N-CA-C	-8.36	98.47	110.59
1	A	319	ASP	N-CA-C	-6.66	100.11	110.17
1	B	264	GLU	N-CA-C	6.30	120.69	113.19
1	C	319	ASP	N-CA-C	-6.12	100.44	109.81
1	B	319	ASP	N-CA-C	-5.73	101.70	109.95
1	B	209	MET	N-CA-C	5.13	116.56	111.07

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	42	0
1	B	2033	0	2053	43	0
1	C	1990	0	2019	49	0
1	D	1982	0	2006	49	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	181	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 (181) 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:C:204:GLU:HB2	1:C:209:MET:HE3	1.65	0.79
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:HG2	1:C:218[B]:ARG:NH1	2.00	0.76
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: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:A:209:MET:HE2	1:A:246:LYS:HD3	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:209:MET:HE3	2:A:623:HOH:O	1.93	0.67
1:A:209:MET:HE1	2:A:623:HOH:O	1.91	0.66
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:D:279:ALA:HA	1:D:331:MET:HE3	1.80	0.62
1:B:192:ARG:HG2	2:B:666:HOH:O	2.00	0.62
1:B:209:MET:HE1	1:B:246:LYS:HD3	1.81	0.61
1:C:209:MET:HE1	1:C:246:LYS:NZ	2.15	0.61
1:A:309:THR:H	1:A:312:HIS:HD2	1.48	0.61
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: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: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:334:LEU:HD23	1:A:334:LEU:C	2.30	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:179:THR:CG2	1:D:212:PHE:CE2	2.88	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:C:347:ASN:C	1:C:347:ASN:HD22	2.16	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:341:LYS:HZ3	1:B:342:LEU:HD13	1.73	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:200:LEU:HB3	1:C:209:MET:HE2	1.91	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:209:MET:HE1	1:A:246:LYS:HE3	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:A:312:HIS:CA	1:A:362:MET:HE1	2.39	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: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:B:262:LYS:HB2	1:B:263:ASP:HB2	1.93	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:A:315:VAL:HB	1:A:362:MET:HE3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:319:ASP:C	1:C:319:ASP:OD1	2.54	0.49
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:327:PHE:C	1:D:327:PHE:CD2	2.91	0.49
1:B:347:ASN:C	1:B:347:ASN:HD22	2.21	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:C:209:MET:HE1	1:C:246:LYS:HZ3	1.79	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:C:362:MET:HE3	2:C:410:HOH:O	2.13	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:D:209:MET:HE1	1:D:246:LYS:HD3	1.97	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:200:LEU:HB3	1:D:209:MET:HE3	1.98	0.45
1:B:162:HIS:HD2	2:C:570:HOH:O	1.99	0.44
1:C:137:ARG:HB3	1:C:138:PRO:HD3	1.98	0.44
1:C:312:HIS:HE1	1:C:357:LEU:O	2.01	0.44
1:C:347:ASN:C	1:C:347:ASN:ND2	2.75	0.44
1:B:209:MET:HE1	2:B:629:HOH:O	2.18	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:200:LEU:O	1:B:209:MET:HE3	2.19	0.43
1:A:312:HIS:HA	1:A:362:MET:HE1	1.99	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:C:136:ASN:C	1:C:136:ASN:HD22	2.26	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:A:327:PHE:CD2	1:A:327:PHE:C	2.98	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:B:327:PHE:CD2	1:B:327:PHE:C	2.98	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:A:200:LEU:O	1:A:209:MET:HE3	2.20	0.41
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:B:173:GLU:OE1	1:B:176:THR:OG1	2.35	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:368:LYS:HB3	1:A:371:ILE:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:360:LEU:HD23	1:C:361:MET:HE3	2.02	0.40
1:B:209:MET:CE	1:B:246:LYS:HD3	2.51	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%)	198 (91%)	20 (9%)	8	11
1	B	217/221 (98%)	195 (90%)	22 (10%)	7	9
1	C	213/221 (96%)	200 (94%)	13 (6%)	17	24
1	D	212/221 (96%)	197 (93%)	15 (7%)	13	19
All	All	860/884 (97%)	790 (92%)	70 (8%)	11	14

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	132	MET
1	A	133	LYS
1	A	160	LEU
1	A	198	ILE
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	296	LYS
1	A	322	ARG
1	A	326	LYS
1	A	327	PHE
1	A	329	THR
1	A	334	LEU
1	A	336	LEU
1	A	338	LYS
1	A	346	THR
1	A	348	LEU
1	B	134	VAL
1	B	160	LEU
1	B	169	GLU
1	B	178	LYS
1	B	210	ARG
1	B	218	ARG
1	B	220	VAL
1	B	225	GLN
1	B	262	LYS
1	B	286	ILE
1	B	300	LEU
1	B	323	GLU
1	B	326	LYS

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Mol	Chain	Res	Type
1	B	327	PHE
1	B	329	THR
1	B	334	LEU
1	B	336	LEU
1	B	341	LYS
1	B	342	LEU
1	B	346	THR
1	B	373	GLN
1	B	378	ARG
1	C	136	ASN
1	C	139	ILE
1	C	160	LEU
1	C	165	ARG
1	C	185	LEU
1	C	206	THR
1	C	302	ARG
1	C	327	PHE
1	C	329	THR
1	C	346	THR
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	179	THR
1	D	185	LEU
1	D	215	SER
1	D	303	GLN
1	D	325	THR
1	D	327	PHE
1	D	329	THR
1	D	339	CYS
1	D	346	THR
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 (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	162	HIS

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Mol	Chain	Res	Type
1	A	208	ASN
1	A	238	HIS
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	208	ASN
1	B	225	GLN
1	B	251	HIS
1	B	282	ASN
1	B	295	HIS
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	162	HIS
1	C	238	HIS
1	C	282	ASN
1	C	297	GLN
1	C	312	HIS
1	C	347	ASN
1	C	354	ASN
1	C	373	GLN
1	D	251	HIS
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 ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	253/260 (97%)	-0.23	0 100 100	9, 17, 28, 35	3 (1%)
1	B	256/260 (98%)	-0.29	4 (1%) 70 72	9, 18, 35, 64	0
1	C	249/260 (95%)	-0.22	1 (0%) 88 89	14, 25, 32, 44	1 (0%)
1	D	249/260 (95%)	1.14	45 (18%) 3 4	23, 39, 62, 70	0
All	All	1007/1040 (96%)	0.10	50 (4%) 34 35	9, 24, 51, 70	4 (0%)

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	207	GLY	6.6
1	D	135	PHE	5.4
1	D	134	VAL	5.3
1	D	159	LEU	5.0
1	D	203	ALA	4.7
1	D	139	ILE	4.6
1	D	213	ILE	4.0
1	D	178	LYS	3.9
1	D	138	PRO	3.9
1	D	244	VAL	3.8
1	D	171	PHE	3.6
1	D	166	LEU	3.6
1	D	156	LEU	3.5
1	D	247	GLY	3.4
1	D	165	ARG	3.3
1	C	132	MET	3.3
1	D	258	PHE	3.3
1	D	151	GLY	3.3
1	D	167	THR	3.0
1	D	179	THR	3.0
1	D	136	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	263	ASP	2.9
1	D	220	VAL	2.8
1	D	176	THR	2.8
1	D	140	LEU	2.8
1	D	133	LYS	2.7
1	D	160	LEU	2.7
1	D	322	ARG	2.6
1	B	132	MET	2.6
1	B	261	PRO	2.6
1	D	144	VAL	2.5
1	D	163	LYS	2.5
1	B	265	GLY	2.5
1	D	180	CYS	2.4
1	D	252	ALA	2.4
1	D	217	PHE	2.4
1	D	336	LEU	2.4
1	D	210	ARG	2.4
1	D	132	MET	2.3
1	D	153	GLU	2.3
1	D	320	ASN	2.3
1	D	367	GLY	2.2
1	D	229	HIS	2.1
1	D	172	ARG	2.1
1	D	143	ILE	2.1
1	D	145	SER	2.1
1	D	298	ALA	2.0
1	D	152	LEU	2.0
1	D	155	LEU	2.0
1	D	164	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.