Full wwPDB X-ray Structure Validation Report ⓘ

Sep 26, 2023 – 08:14 AM EDT

PDB ID	:	6BWM
Title	:	Crystal structure of the TRPV2 ion channel
Authors	:	Zubcevic, L.; Le, S.; Yang, H.; Lee, S.Y.
Deposited on	:	2017-12-15
Resolution	:	3.90 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:

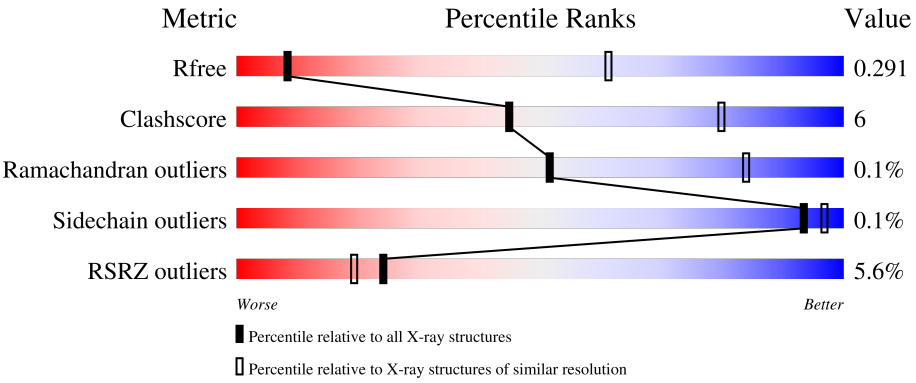
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.90 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	1002 (4.14-3.66)
Clashscore	141614	1004 (4.12-3.68)
Ramachandran outliers	138981	1021 (4.14-3.66)
Sidechain outliers	138945	1014 (4.14-3.66)
RSRZ outliers	127900	1275 (4.20-3.60)

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	776	4% 67% 11% 22%
1	B	776	5% 68% 10% 23%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CA	B	801	-	-	-	X

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8512 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 Transient receptor potential cation channel subfamily V member 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	606	Total	C	N	O	S	0	0	0
			4298	2758	742	776	22			
1	B	599	Total	C	N	O	S	0	0	0
			4213	2696	724	769	24			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	763	ASP	-	expression tag	UNP G1SNM3
A	764	TYR	-	expression tag	UNP G1SNM3
A	765	LYS	-	expression tag	UNP G1SNM3
A	766	ASP	-	expression tag	UNP G1SNM3
A	767	ASP	-	expression tag	UNP G1SNM3
A	768	ASP	-	expression tag	UNP G1SNM3
A	769	ASP	-	expression tag	UNP G1SNM3
A	770	LYS	-	expression tag	UNP G1SNM3
A	771	ALA	-	expression tag	UNP G1SNM3
A	772	HIS	-	expression tag	UNP G1SNM3
A	773	HIS	-	expression tag	UNP G1SNM3
A	774	HIS	-	expression tag	UNP G1SNM3
A	775	HIS	-	expression tag	UNP G1SNM3
A	776	HIS	-	expression tag	UNP G1SNM3
A	777	HIS	-	expression tag	UNP G1SNM3
B	763	ASP	-	expression tag	UNP G1SNM3
B	764	TYR	-	expression tag	UNP G1SNM3
B	765	LYS	-	expression tag	UNP G1SNM3
B	766	ASP	-	expression tag	UNP G1SNM3
B	767	ASP	-	expression tag	UNP G1SNM3
B	768	ASP	-	expression tag	UNP G1SNM3
B	769	ASP	-	expression tag	UNP G1SNM3
B	770	LYS	-	expression tag	UNP G1SNM3
B	771	ALA	-	expression tag	UNP G1SNM3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	772	HIS	-	expression tag	UNP G1SNM3
B	773	HIS	-	expression tag	UNP G1SNM3
B	774	HIS	-	expression tag	UNP G1SNM3
B	775	HIS	-	expression tag	UNP G1SNM3
B	776	HIS	-	expression tag	UNP G1SNM3
B	777	HIS	-	expression tag	UNP G1SNM3

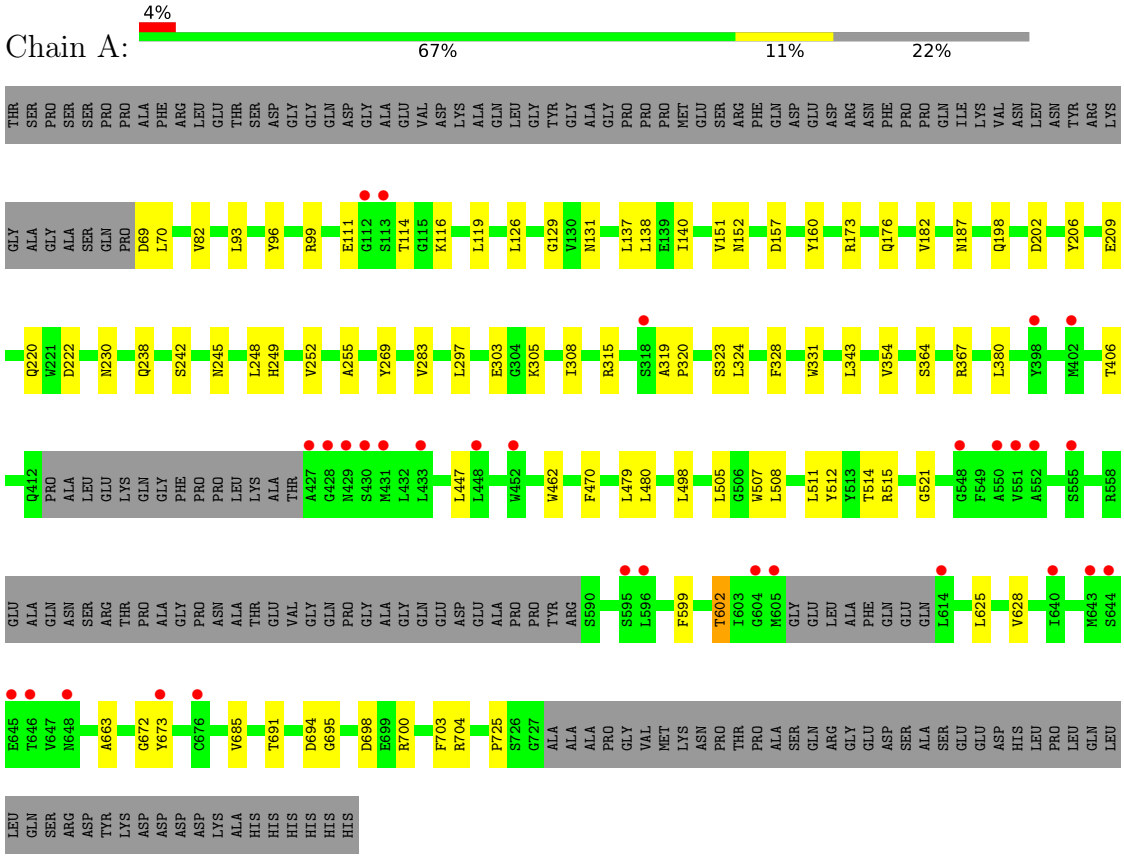
- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		

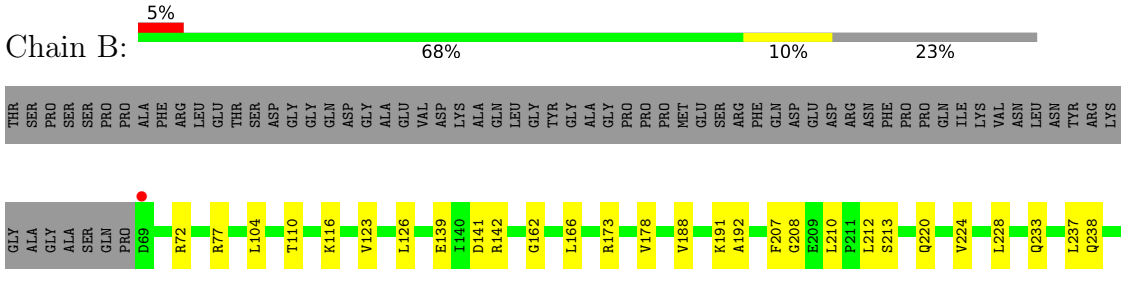
3 Residue-property plots (i)

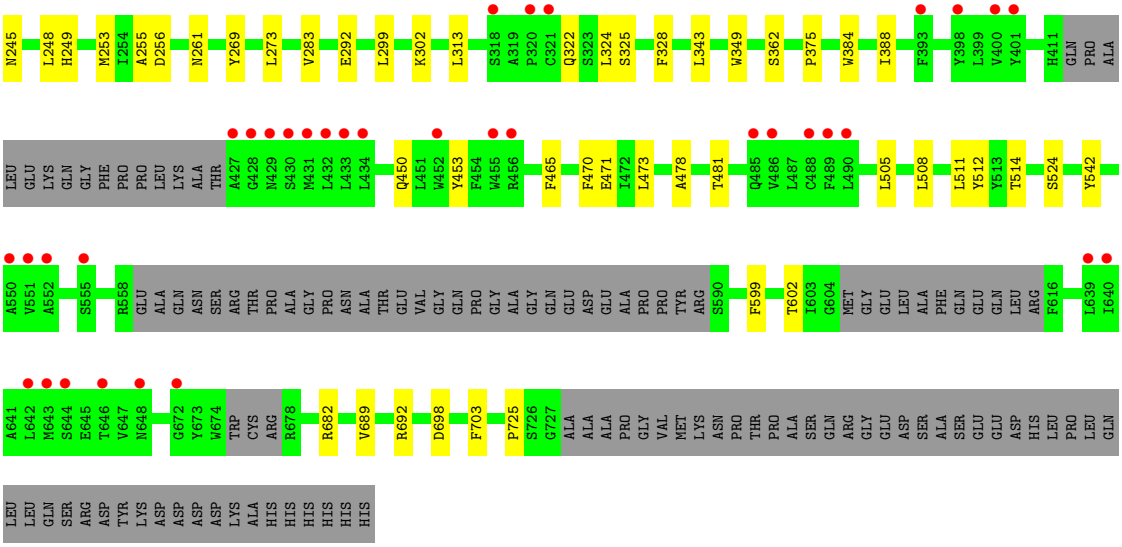
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Transient receptor potential cation channel subfamily V member 2



• Molecule 1: Transient receptor potential cation channel subfamily V member 2




N245 L248 H249 M253 I254 A255 D256 N261 Y269 L273 V283 E292 L299 K302 L313 S318 A319 P320 C321 Q322 S323 L324 S325 F328 L343 W349 S362 P375 W384 I388 F393 Y398 L399 V400 Y401 H411 GLN PRO ALA
LEU GLU LYS GLN GLY PHE PRO PRO LEU LYS ALA THR A427 G428 N429 S430 M431 L432 L433 L434 Q450 L451 W452 Y453 F454 W455 R456 F465 F470 E471 I472 L473 A478 T481 Q485 V486 L487 C488 F489 L490 L505 L508 L511 Y512 Y513 T514 S524 Y542
A550 V551 A552 S555 R558 GLU ALA GLN ASN SER ARG THR PRO ALA GLY PRO ASN ALA THR GLU VAL GLY GLN PRO GLY ALA GLY GLN GLU ASP GLU ALA PRO PRO TYR ARG S590 F599 T602 I603 G604 MET GLY GLU LEU ALA PHE GLN GLU GLN LEU ARG F616 L639 I640
A641 L642 M643 S644 E645 T646 V647 N648 G672 Y673 W674 TRP CYS ARG R678 R682 V689 R692 D698 F703 P725 S726 G727 ALA ALA ALA PRO GLY VAL MET LYS ASN PRO THR PRO ALA SER GLN ARG GLY GLU ASP SER ALA SER GLU GLU ASP HIS LEU PRO LEU GLN
LEU LEU GLN SER ARG ASP TYR LYS ASP ASP ASP ASP LYS ALA HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	92.03Å 122.36Å 187.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.85 – 3.90 39.85 – 3.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (39.85-3.90) 99.9 (39.85-3.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.83 (at 3.87Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.244 , 0.293 0.245 , 0.291	Depositor DCC
R_{free} test set	1058 reflections (5.32%)	wwPDB-VP
Wilson B-factor (Å^2)	89.7	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.23 , 65.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.82	EDS
Total number of atoms	8512	wwPDB-VP
Average B, all atoms (Å^2)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	0.25	0/4391	0.44	0/6013
1	B	0.25	0/4301	0.43	0/5890
All	All	0.25	0/8692	0.44	0/11903

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

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	4298	0	3785	54	0
1	B	4213	0	3682	52	0
2	B	1	0	0	0	0
All	All	8512	0	7467	103	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 6.

All (103) 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:B:542:TYR:OH	1:B:602:THR:HG21	1.38	1.20
1:B:542:TYR:CZ	1:B:602:THR:HG21	2.04	0.91
1:B:542:TYR:OH	1:B:602:THR:CG2	2.21	0.88
1:B:207:PHE:CD1	1:B:208:GLY:O	2.26	0.88
1:B:207:PHE:HD1	1:B:208:GLY:O	1.62	0.82
1:A:625:LEU:HA	1:B:599:PHE:CZ	2.15	0.81
1:A:198:GLN:HA	1:A:206:TYR:HD1	1.48	0.78
1:B:542:TYR:HH	1:B:602:THR:HG21	1.50	0.76
1:B:542:TYR:CE1	1:B:602:THR:HG21	2.21	0.75
1:A:138:LEU:HD22	1:A:151:VAL:HG22	1.77	0.67
1:A:480:LEU:HD22	1:A:498:LEU:HD11	1.78	0.66
1:B:255:ALA:O	1:B:261:ASN:ND2	2.29	0.66
1:A:198:GLN:HA	1:A:206:TYR:CD1	2.32	0.63
1:A:470:PHE:HE2	1:A:512:TYR:HB2	1.65	0.61
1:A:511:LEU:O	1:A:514:THR:HG22	2.01	0.61
1:A:343:LEU:HD11	1:A:703:PHE:HB2	1.83	0.60
1:A:114:THR:HA	1:A:157:ASP:HB2	1.83	0.59
1:B:343:LEU:HD11	1:B:703:PHE:HB2	1.84	0.59
1:A:255:ALA:HB3	1:A:305:LYS:HG2	1.84	0.59
1:A:69:ASP:O	1:A:96:TYR:HB2	2.03	0.59
1:A:70:LEU:O	1:A:99:ARG:NH1	2.37	0.58
1:B:212:LEU:HD21	1:B:237:LEU:HD23	1.86	0.58
1:B:453:TYR:CE2	1:B:471:GLU:HG2	2.39	0.57
1:A:173:ARG:HG2	1:A:220:GLN:NE2	2.19	0.56
1:A:447:LEU:HD11	1:A:479:LEU:HA	1.88	0.56
1:B:292:GLU:OE2	1:B:302:LYS:NZ	2.38	0.56
1:B:508:LEU:O	1:B:511:LEU:HB3	2.06	0.55
1:B:207:PHE:CE1	1:B:208:GLY:O	2.60	0.55
1:B:245:ASN:HB3	1:B:249:HIS:HB2	1.88	0.55
1:B:72:ARG:O	1:B:77:ARG:NH1	2.39	0.54
1:A:698:ASP:OD2	1:A:700:ARG:NH2	2.42	0.53
1:B:173:ARG:HG2	1:B:220:GLN:NE2	2.24	0.52
1:A:323:SER:HB3	1:A:691:THR:O	2.10	0.51
1:A:82:VAL:HG11	1:A:137:LEU:HD11	1.92	0.50
1:B:692:ARG:HE	1:B:698:ASP:HB3	1.76	0.49
1:A:252:VAL:HG22	1:A:308:ILE:HD13	1.94	0.49
1:A:628:VAL:CB	1:B:599:PHE:HZ	2.26	0.49
1:B:191:LYS:HG2	1:B:210:LEU:HD23	1.94	0.48
1:B:450:GLN:HE22	1:B:471:GLU:HG3	1.77	0.48
1:A:515:ARG:HA	1:A:521:GLY:HA2	1.95	0.48
1:B:110:THR:HA	1:B:116:LYS:O	2.14	0.48
1:B:256:ASP:HB3	1:B:261:ASN:HD22	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:473:LEU:HD11	1:B:505:LEU:HD11	1.95	0.47
1:A:406:THR:HG1	1:A:507:TRP:HE1	1.57	0.47
1:B:384:TRP:O	1:B:388:ILE:HG13	2.14	0.47
1:B:166:LEU:HD11	1:B:178:VAL:HG13	1.97	0.47
1:B:514:THR:HG23	1:B:524:SER:HB2	1.96	0.47
1:A:248:LEU:HB3	1:A:269:TYR:HE1	1.80	0.47
1:A:303:GLU:HB3	1:A:305:LYS:NZ	2.30	0.47
1:A:202:ASP:N	1:A:202:ASP:OD1	2.48	0.46
1:A:505:LEU:HD23	1:A:508:LEU:HD12	1.98	0.46
1:A:599:PHE:O	1:A:602:THR:HG22	2.14	0.46
1:B:104:LEU:HD12	1:B:141:ASP:HB2	1.96	0.46
1:B:248:LEU:HB3	1:B:269:TYR:HE1	1.79	0.46
1:B:188:VAL:HG22	1:B:233:GLN:NE2	2.30	0.46
1:B:349:TRP:CE3	1:B:682:ARG:HG3	2.50	0.46
1:A:328:PHE:HE2	1:A:700:ARG:HD2	1.81	0.46
1:B:302:LYS:HA	1:B:362:SER:HB3	1.98	0.46
1:A:315:ARG:NH1	1:A:324:LEU:O	2.29	0.45
1:B:139:GLU:OE1	1:B:142:ARG:NH2	2.43	0.45
1:B:208:GLY:O	1:B:213:SER:HB2	2.17	0.45
1:A:119:LEU:HD22	1:A:138:LEU:HD21	1.99	0.45
1:B:470:PHE:CE2	1:B:512:TYR:HB2	2.52	0.45
1:A:111:GLU:HB2	1:A:116:LYS:HB3	1.99	0.45
1:A:364:SER:O	1:A:367:ARG:HG3	2.17	0.45
1:A:126:LEU:HD23	1:A:131:ASN:HB2	1.99	0.44
1:A:206:TYR:OH	1:A:245:ASN:ND2	2.42	0.44
1:B:123:VAL:O	1:B:126:LEU:HG	2.17	0.44
1:A:182:VAL:HG11	1:A:230:ASN:HD22	1.82	0.44
1:A:222:ASP:OD1	1:A:222:ASP:N	2.49	0.44
1:B:542:TYR:OH	1:B:602:THR:CB	2.66	0.44
1:A:152:ASN:OD1	1:A:187:ASN:N	2.51	0.44
1:B:511:LEU:O	1:B:514:THR:HG22	2.18	0.44
1:B:470:PHE:CZ	1:B:512:TYR:HB2	2.53	0.43
1:B:238:GLN:NE2	1:B:283:VAL:HG21	2.33	0.43
1:B:162:GLY:HA3	1:B:192:ALA:HA	2.00	0.43
1:A:182:VAL:HG11	1:A:230:ASN:ND2	2.33	0.43
1:B:542:TYR:HH	1:B:602:THR:CG2	2.21	0.42
1:A:380:LEU:HD13	1:A:663:ALA:HB2	2.00	0.42
1:A:672:GLY:O	1:A:673:TYR:HB3	2.19	0.42
1:B:328:PHE:CZ	1:B:689:VAL:HG11	2.54	0.42
1:A:160:TYR:CE1	1:B:725:PRO:HG2	2.54	0.42
1:B:313:LEU:HB3	1:B:375:PRO:HG3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:322:GLN:O	1:B:325:SER:OG	2.38	0.42
1:A:319:ALA:HB1	1:A:320:PRO:HD2	2.02	0.41
1:B:253:MET:SD	1:B:299:LEU:HD21	2.60	0.41
1:A:93:LEU:HD23	1:A:140:ILE:HD13	2.02	0.41
1:A:685:VAL:HG21	1:A:704:ARG:HH12	1.84	0.41
1:A:245:ASN:HB3	1:A:249:HIS:HB2	2.01	0.41
1:A:297:LEU:HD22	1:A:354:VAL:HG21	2.03	0.41
1:A:173:ARG:HG2	1:A:220:GLN:HE21	1.86	0.41
1:A:238:GLN:HE21	1:A:283:VAL:HG11	1.84	0.41
1:A:238:GLN:HE21	1:A:283:VAL:HG21	1.85	0.41
1:A:331:TRP:CE3	1:A:725:PRO:HB3	2.56	0.41
1:B:478:ALA:O	1:B:481:THR:OG1	2.28	0.41
1:A:462:TRP:CG	1:A:462:TRP:O	2.74	0.41
1:A:694:ASP:OD1	1:A:695:GLY:N	2.53	0.41
1:B:450:GLN:NE2	1:B:471:GLU:HG3	2.35	0.41
1:A:129:GLY:HA3	1:A:176:GLN:NE2	2.36	0.40
1:A:209:GLU:OE2	1:A:242:SER:OG	2.33	0.40
1:A:248:LEU:HB3	1:A:269:TYR:CE1	2.57	0.40
1:B:273:LEU:HB3	1:B:324:LEU:HD13	2.03	0.40
1:B:224:VAL:O	1:B:228:LEU:HG	2.22	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	598/776 (77%)	582 (97%)	16 (3%)	0	100	100
1	B	589/776 (76%)	569 (97%)	19 (3%)	1 (0%)	47	79
All	All	1187/1552 (76%)	1151 (97%)	35 (3%)	1 (0%)	51	84

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	465	PHE

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	367/666 (55%)	366 (100%)	1 (0%)	92 95
1	B	361/666 (54%)	361 (100%)	0	100 100
All	All	728/1332 (55%)	727 (100%)	1 (0%)	93 97

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	602	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	238	GLN
1	B	184	ASN
1	B	238	GLN
1	B	261	ASN
1	B	450	GLN

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)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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^{th} 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	606/776 (78%)	-0.02	31 (5%)	28	23	36, 91, 186, 217	0
1	B	599/776 (77%)	0.00	36 (6%)	21	16	41, 101, 183, 213	0
All	All	1205/1552 (77%)	-0.01	67 (5%)	24	19	36, 96, 185, 217	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	605	MET	9.5
1	A	430	SER	8.4
1	A	429	ASN	8.1
1	B	429	ASN	5.6
1	B	672	GLY	4.6
1	B	318	SER	4.5
1	B	489	PHE	4.4
1	B	646	THR	4.1
1	B	428	GLY	4.1
1	B	643	MET	4.0
1	A	452	TRP	3.9
1	B	430	SER	3.9
1	B	452	TRP	3.8
1	A	604	GLY	3.8
1	B	648	ASN	3.8
1	B	488	CYS	3.8
1	B	433	LEU	3.7
1	B	456	ARG	3.7
1	A	595	SER	3.7
1	A	646	THR	3.7
1	A	427	ALA	3.7
1	A	398	TYR	3.5
1	B	69	ASP	3.5
1	A	614	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	320	PRO	3.4
1	B	640	ILE	3.3
1	B	552	ALA	3.3
1	A	643	MET	3.3
1	B	427	ALA	3.2
1	B	321	CYS	3.1
1	A	551	VAL	3.1
1	B	642	LEU	3.1
1	A	676	CYS	3.1
1	A	550	ALA	3.0
1	B	550	ALA	3.0
1	A	428	GLY	2.9
1	B	551	VAL	2.8
1	A	548	GLY	2.8
1	A	640	ILE	2.8
1	A	645	GLU	2.7
1	B	486	VAL	2.7
1	B	431	MET	2.7
1	B	398	TYR	2.6
1	A	433	LEU	2.6
1	B	555	SER	2.5
1	B	432	LEU	2.5
1	A	431	MET	2.5
1	B	455	TRP	2.5
1	A	552	ALA	2.4
1	B	401	TYR	2.4
1	B	639	LEU	2.4
1	A	448	LEU	2.4
1	B	644	SER	2.4
1	A	673	TYR	2.3
1	B	393	PHE	2.3
1	A	648	ASN	2.3
1	B	434	LEU	2.2
1	A	644	SER	2.2
1	A	318	SER	2.2
1	A	113	SER	2.2
1	A	555	SER	2.1
1	B	490	LEU	2.1
1	A	596	LEU	2.1
1	A	402	MET	2.1
1	A	112	GLY	2.1
1	B	485	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	400	VAL	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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CA	B	801	1/1	0.75	1.10	145,145,145,145	1

6.5 Other polymers (i)

There are no such residues in this entry.