



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:12 AM UTC

PDB ID : 5WOA / pdb_00005woa
Title : Crystal Structure of Transient Receptor Potential (TRP) channel TRPV6* in the presence of Gadolinium
Authors : Singh, A.K.; Saotome, K.; Sobolevsky, A.I.
Deposited on : 2017-08-01
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 : 4-5-2 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

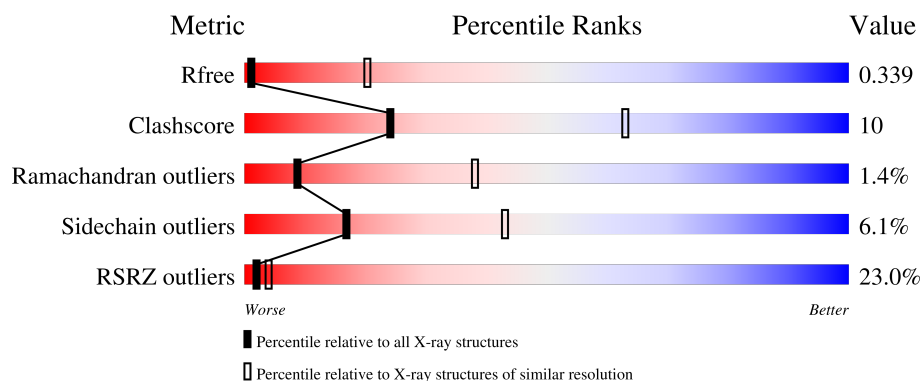
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1270 (4.10-3.70)
Clashscore	190562	1034 (4.08-3.72)
Ramachandran outliers	187476	1251 (4.10-3.70)
Sidechain outliers	187428	1243 (4.10-3.70)
RSRZ outliers	180081	1269 (4.10-3.70)

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	672	20% 66% 20% • 11%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4741 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 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	595	Total	C	N	O	S	0	0	0
			4739	3070	790	845	34			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	62	TYR	ILE	engineered mutation	UNP Q9R186
A	92	ASN	LEU	engineered mutation	UNP Q9R186
A	96	GLN	MET	engineered mutation	UNP Q9R186
A	670	VAL	-	expression tag	UNP Q9R186
A	671	PRO	-	expression tag	UNP Q9R186
A	672	ARG	-	expression tag	UNP Q9R186

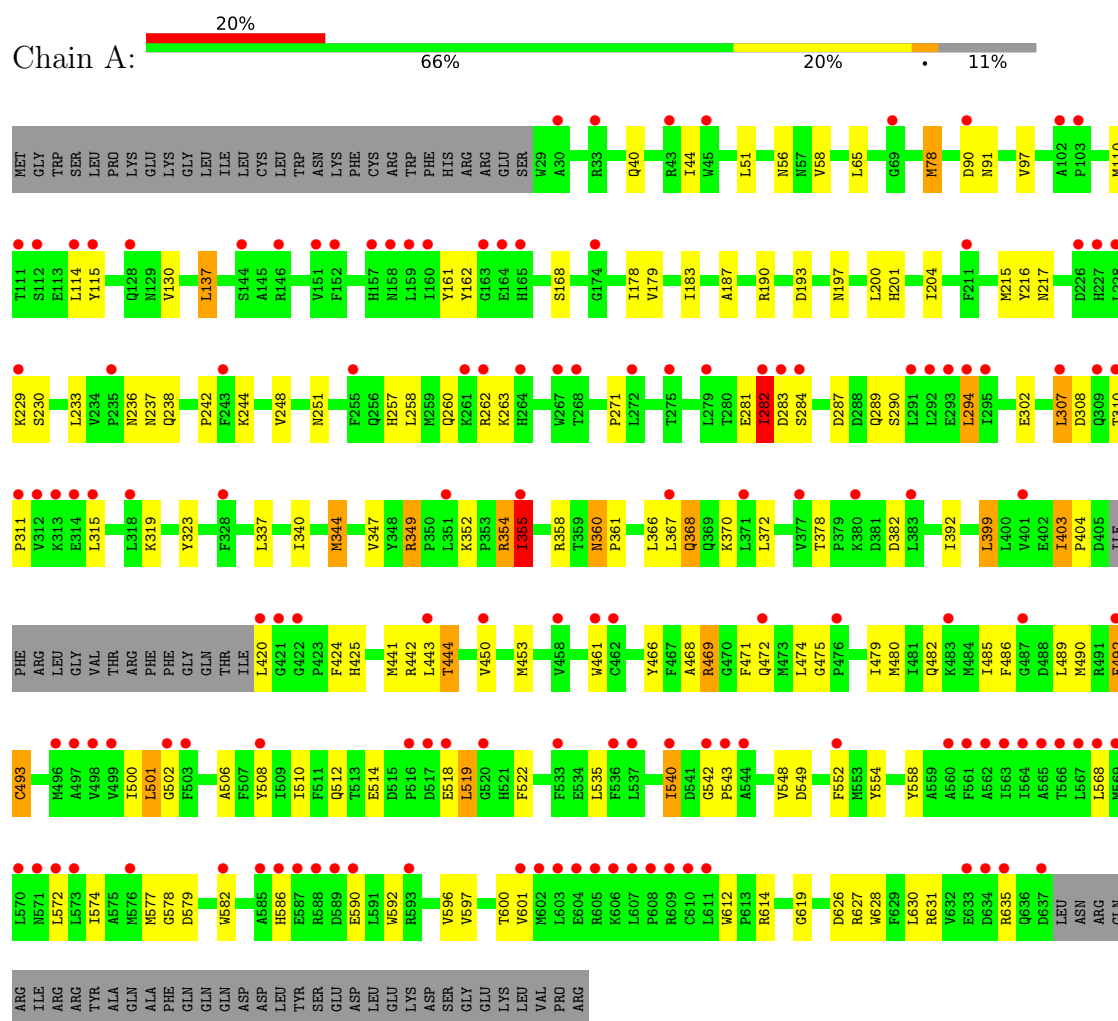
- Molecule 2 is GADOLINIUM ATOM (CCD ID: GD) (formula: Gd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Gd	0	0
			2	2		

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: Transient receptor potential cation channel subfamily V member 6



4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	146.08Å 146.08Å 116.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.18 – 3.90 47.18 – 3.90	Depositor EDS
% Data completeness (in resolution range)	93.0 (47.18-3.90) 93.8 (47.18-3.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 3.88Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.271 , 0.316 0.290 , 0.339	Depositor DCC
R_{free} test set	535 reflections (4.47%)	wwPDB-VP
Wilson B-factor (Å ²)	158.8	Xtriage
Anisotropy	0.316	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 152.5	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	0.83	EDS
Total number of atoms	4741	wwPDB-VP
Average B, all atoms (Å ²)	155.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.09% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

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	0.24	1/4849 (0.0%)	0.69	15/6590 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	501	LEU	CA-C	12.25	1.69	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	518	GLU	N-CA-C	29.47	142.97	111.14
1	A	471	PHE	N-CA-C	-15.17	84.17	108.90
1	A	472	GLN	N-CA-CB	-13.45	87.86	109.78
1	A	502	GLY	N-CA-C	12.59	127.73	112.49
1	A	471	PHE	CB-CA-C	10.63	129.16	109.71
1	A	501	LEU	CA-C-O	9.91	131.30	120.20
1	A	500	ILE	N-CA-C	-9.59	101.52	110.82
1	A	519	LEU	N-CA-C	-8.85	91.94	110.80
1	A	501	LEU	N-CA-C	7.21	120.98	111.75
1	A	472	GLN	N-CA-C	6.98	122.89	111.37
1	A	492	PHE	CB-CA-C	-6.75	96.99	110.42
1	A	493	CYS	N-CA-C	-6.58	105.26	113.55
1	A	486	PHE	N-CA-C	6.25	121.12	111.56
1	A	519	LEU	N-CA-CB	-5.44	101.29	110.49
1	A	444	THR	N-CA-C	-5.24	107.55	114.31

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	4739	0	4759	95	1
2	A	2	0	0	0	0
All	All	4741	0	4759	95	1

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 10.

All (95) 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:A:468:ALA:HB1	1:A:474:LEU:CD1	1.48	1.41
1:A:468:ALA:HB1	1:A:474:LEU:HD13	1.25	1.17
1:A:492:PHE:CE1	1:A:568:LEU:O	2.11	1.03
1:A:492:PHE:HE1	1:A:568:LEU:O	1.45	1.00
1:A:468:ALA:CB	1:A:474:LEU:CD1	2.40	0.99
1:A:468:ALA:HB1	1:A:474:LEU:HD11	1.49	0.92
1:A:548:VAL:HG22	1:A:549:ASP:H	1.38	0.89
1:A:492:PHE:O	1:A:492:PHE:CG	2.28	0.86
1:A:577:MET:O	1:A:579:ASP:N	2.10	0.84
1:A:492:PHE:O	1:A:492:PHE:CD2	2.31	0.83
1:A:378:THR:HG23	1:A:378:THR:O	1.86	0.73
1:A:352:LYS:HB3	1:A:370:LYS:HA	1.69	0.73
1:A:490:MET:HA	1:A:493:CYS:SG	2.29	0.73
1:A:577:MET:C	1:A:579:ASP:H	2.00	0.70
1:A:468:ALA:CB	1:A:474:LEU:HD13	2.13	0.69
1:A:548:VAL:HG22	1:A:549:ASP:N	2.03	0.69
1:A:468:ALA:CB	1:A:474:LEU:HD11	2.14	0.67
1:A:378:THR:OG1	1:A:382:ASP:N	2.28	0.64
1:A:492:PHE:CE2	1:A:572:LEU:HD22	2.33	0.64
1:A:540:ILE:HG22	1:A:542:GLY:H	1.63	0.63
1:A:468:ALA:HB1	1:A:474:LEU:HD12	1.69	0.62
1:A:161:TYR:OH	1:A:193:ASP:OD2	2.18	0.61
1:A:479:ILE:HD13	1:A:592:TRP:HB2	1.84	0.60
1:A:490:MET:O	1:A:493:CYS:SG	2.58	0.60
1:A:619:GLY:N	1:A:627:ARG:O	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:ARG:HD3	1:A:453:MET:HE1	1.84	0.59
1:A:548:VAL:CG2	1:A:549:ASP:H	2.13	0.58
1:A:323:TYR:O	1:A:612:TRP:CZ3	2.56	0.58
1:A:230:SER:HB3	1:A:233:LEU:HD23	1.86	0.57
1:A:183:ILE:HD13	1:A:187:ALA:HB3	1.87	0.57
1:A:469:ARG:O	1:A:592:TRP:NE1	2.37	0.56
1:A:197:ASN:OD1	1:A:236:ASN:ND2	2.40	0.55
1:A:58:VAL:HG13	1:A:97:VAL:HG21	1.89	0.54
1:A:420:LEU:O	1:A:482:GLN:NE2	2.39	0.53
1:A:352:LYS:HD2	1:A:372:LEU:HB2	1.91	0.52
1:A:485:ILE:HG23	1:A:489:LEU:HD23	1.92	0.52
1:A:315:LEU:HG	1:A:319:LYS:HD2	1.92	0.52
1:A:378:THR:O	1:A:378:THR:CG2	2.58	0.51
1:A:201:HIS:HA	1:A:204:ILE:HD12	1.92	0.51
1:A:307:LEU:H	1:A:307:LEU:HD13	1.76	0.51
1:A:442:ARG:C	1:A:444:THR:H	2.18	0.51
1:A:574:ILE:HA	1:A:577:MET:HE2	1.93	0.51
1:A:450:VAL:HA	1:A:453:MET:HE3	1.92	0.50
1:A:260:GLN:HA	1:A:263:LYS:HE2	1.93	0.50
1:A:162:TYR:O	1:A:168:SER:OG	2.29	0.49
1:A:130:VAL:HG22	1:A:178:ILE:HD11	1.95	0.49
1:A:204:ILE:O	1:A:251:ASN:ND2	2.46	0.48
1:A:424:PHE:HB3	1:A:466:TYR:HB2	1.95	0.48
1:A:506:ALA:O	1:A:510:ILE:HG12	2.13	0.48
1:A:492:PHE:CD2	1:A:572:LEU:HD22	2.48	0.48
1:A:284:SER:HA	1:A:290:SER:HB3	1.95	0.48
1:A:403:ILE:HG22	1:A:404:PRO:HD3	1.96	0.47
1:A:475:GLY:O	1:A:479:ILE:HD12	2.14	0.47
1:A:474:LEU:HD12	1:A:474:LEU:C	2.39	0.47
1:A:262:ARG:HH12	1:A:281:GLU:HG3	1.79	0.47
1:A:282:ILE:HG22	1:A:283:ASP:H	1.80	0.47
1:A:40:GLN:O	1:A:44:ILE:HG12	2.15	0.46
1:A:354:ARG:HG2	1:A:368:GLN:HG3	1.97	0.46
1:A:490:MET:C	1:A:493:CYS:HG	2.19	0.46
1:A:110:MET:HB2	1:A:115:TYR:O	2.17	0.45
1:A:360:ASN:H	1:A:361:PRO:HD2	1.81	0.45
1:A:535:LEU:HD13	1:A:558:TYR:HE1	1.81	0.45
1:A:190:ARG:NH1	1:A:229:LYS:O	2.44	0.45
1:A:614:ARG:HD3	1:A:628:TRP:CE2	2.51	0.45
1:A:480:MET:HE2	1:A:480:MET:HB2	1.78	0.45
1:A:352:LYS:HE2	1:A:355:ILE:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:ARG:O	1:A:355:ILE:HG22	2.16	0.45
1:A:78:MET:HE1	1:A:114:LEU:HD12	2.00	0.44
1:A:586:HIS:O	1:A:590:GLU:HG2	2.18	0.44
1:A:344:MET:HA	1:A:347:VAL:HG22	2.00	0.44
1:A:179:VAL:HG21	1:A:215:MET:SD	2.57	0.43
1:A:358:ARG:HH12	1:A:367:LEU:HD12	1.82	0.43
1:A:442:ARG:HG3	1:A:443:LEU:H	1.84	0.43
1:A:399:LEU:HD12	1:A:399:LEU:HA	1.86	0.43
1:A:56:ASN:OD1	1:A:91:ASN:HB3	2.18	0.43
1:A:485:ILE:O	1:A:489:LEU:HB3	2.19	0.42
1:A:217:ASN:OD1	1:A:257:HIS:NE2	2.44	0.42
1:A:137:LEU:HD13	1:A:137:LEU:HA	1.89	0.42
1:A:236:ASN:OD1	1:A:237:ASN:N	2.52	0.42
1:A:244:LYS:HE3	1:A:244:LYS:HB2	1.91	0.42
1:A:543:PRO:O	1:A:554:TYR:OH	2.22	0.42
1:A:577:MET:C	1:A:579:ASP:N	2.67	0.41
1:A:354:ARG:HH22	1:A:367:LEU:HB2	1.85	0.41
1:A:392:ILE:HD13	1:A:392:ILE:HA	1.93	0.41
1:A:248:VAL:HG22	1:A:294:LEU:HB3	2.02	0.41
1:A:236:ASN:CG	1:A:238:GLN:HG2	2.46	0.41
1:A:466:TYR:O	1:A:469:ARG:HD2	2.21	0.41
1:A:596:VAL:O	1:A:600:THR:OG1	2.29	0.41
1:A:201:HIS:CE1	1:A:242:PRO:HD3	2.56	0.40
1:A:271:PRO:HB2	1:A:635:ARG:HG3	2.02	0.40
1:A:492:PHE:CD2	1:A:492:PHE:C	2.97	0.40
1:A:508:TYR:O	1:A:512:GLN:N	2.53	0.40
1:A:597:VAL:O	1:A:601:VAL:HG23	2.22	0.40
1:A:337:LEU:HA	1:A:340:ILE:HG22	2.03	0.40
1:A:200:LEU:HB3	1:A:216:TYR:HE2	1.85	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:TRP:CE2	1:A:501:LEU:CD2[3_1045]	2.09	0.11

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	591/672 (88%)	528 (89%)	55 (9%)	8 (1%)	9 38

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	578	GLY
1	A	90	ASP
1	A	360	ASN
1	A	311	PRO
1	A	355	ILE
1	A	626	ASP
1	A	310	THR
1	A	282	ILE

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	510/584 (87%)	479 (94%)	31 (6%)	17 43

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	LEU
1	A	65	LEU
1	A	78	MET

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Mol	Chain	Res	Type
1	A	137	LEU
1	A	258	LEU
1	A	282	ILE
1	A	287	ASP
1	A	289	GLN
1	A	294	LEU
1	A	302	GLU
1	A	307	LEU
1	A	308	ASP
1	A	344	MET
1	A	349	ARG
1	A	354	ARG
1	A	355	ILE
1	A	366	LEU
1	A	368	GLN
1	A	399	LEU
1	A	403	ILE
1	A	425	HIS
1	A	441	MET
1	A	469	ARG
1	A	514	GLU
1	A	519	LEU
1	A	522	PHE
1	A	540	ILE
1	A	552	PHE
1	A	582	TRP
1	A	630	LEU
1	A	631	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	41	GLN
1	A	59	GLN
1	A	581	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](#)

Of 2 ligands modelled in this entry, 2 are 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, 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	595/672 (88%)	1.27	137 (23%) 2 4	103, 148, 218, 307	0

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	608	PRO	14.3
1	A	607	LEU	13.2
1	A	159	LEU	13.0
1	A	606	LYS	12.5
1	A	605	ARG	12.0
1	A	569	MET	10.7
1	A	633	GLU	8.9
1	A	570	LEU	8.5
1	A	158	ASN	8.4
1	A	573	LEU	8.2
1	A	565	ALA	7.4
1	A	568	LEU	7.3
1	A	609	ARG	7.3
1	A	462	CYS	7.2
1	A	292	LEU	7.0
1	A	421	GLY	7.0
1	A	151	VAL	6.9
1	A	355	ILE	6.4
1	A	283	ASP	6.3
1	A	564	ILE	6.1
1	A	499	VAL	6.0
1	A	635	ARG	5.9
1	A	492	PHE	5.9
1	A	602	MET	5.8
1	A	572	LEU	5.7
1	A	310	THR	5.4
1	A	603	LEU	5.4

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Mol	Chain	Res	Type	RSRZ
1	A	560	ALA	5.3
1	A	160	ILE	5.2
1	A	152	PHE	5.2
1	A	272	LEU	5.0
1	A	314	GLU	5.0
1	A	634	ASP	4.9
1	A	115	TYR	4.5
1	A	566	THR	4.5
1	A	562	ALA	4.5
1	A	443	LEU	4.4
1	A	111	THR	4.3
1	A	33	ARG	4.2
1	A	498	VAL	4.1
1	A	157	HIS	4.1
1	A	279	LEU	4.0
1	A	164	GLU	4.0
1	A	567	LEU	4.0
1	A	537	LEU	3.8
1	A	496	MET	3.7
1	A	604	GLU	3.6
1	A	420	LEU	3.6
1	A	563	ILE	3.5
1	A	328	PHE	3.5
1	A	293	GLU	3.4
1	A	146	ARG	3.3
1	A	533	PHE	3.3
1	A	552	PHE	3.3
1	A	487	GLY	3.3
1	A	114	LEU	3.3
1	A	103	PRO	3.2
1	A	295	ILE	3.2
1	A	291	LEU	3.2
1	A	588	ARG	3.1
1	A	571	ASN	3.1
1	A	536	PHE	3.1
1	A	268	THR	3.1
1	A	90	ASP	3.1
1	A	422	GLY	3.1
1	A	544	ALA	3.1
1	A	503	PHE	3.1
1	A	261	LYS	3.0
1	A	315	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	542	GLY	3.0
1	A	243	PHE	3.0
1	A	610	CYS	3.0
1	A	601	VAL	3.0
1	A	227	HIS	2.9
1	A	586	HIS	2.9
1	A	450	VAL	2.9
1	A	229	LYS	2.9
1	A	377	VAL	2.8
1	A	380	LYS	2.8
1	A	585	ALA	2.8
1	A	576	MET	2.8
1	A	518	GLU	2.8
1	A	255	PHE	2.7
1	A	371	LEU	2.7
1	A	309	GLN	2.7
1	A	520	GLY	2.7
1	A	294	LEU	2.7
1	A	226	ASP	2.6
1	A	275	THR	2.6
1	A	112	SER	2.6
1	A	483	LYS	2.6
1	A	313	LYS	2.6
1	A	508	TYR	2.5
1	A	102	ALA	2.5
1	A	282	ILE	2.5
1	A	45	TRP	2.5
1	A	458	VAL	2.5
1	A	144	SER	2.4
1	A	561	PHE	2.4
1	A	307	LEU	2.4
1	A	383	LEU	2.4
1	A	264	HIS	2.4
1	A	516	PRO	2.4
1	A	540	ILE	2.4
1	A	611	LEU	2.4
1	A	69	GLY	2.3
1	A	174	GLY	2.3
1	A	235	PRO	2.3
1	A	543	PRO	2.3
1	A	312	VAL	2.3
1	A	472	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	165	HIS	2.3
1	A	43	ARG	2.3
1	A	262	ARG	2.3
1	A	401	VAL	2.2
1	A	30	ALA	2.2
1	A	587	GLU	2.2
1	A	590	GLU	2.2
1	A	163	GLY	2.2
1	A	311	PRO	2.2
1	A	228	LEU	2.2
1	A	284	SER	2.2
1	A	461	TRP	2.1
1	A	502	GLY	2.1
1	A	211	PHE	2.1
1	A	589	ASP	2.1
1	A	593	ARG	2.1
1	A	128	GLN	2.1
1	A	582	TRP	2.1
1	A	637	ASP	2.1
1	A	318	LEU	2.1
1	A	267	TRP	2.0
1	A	476	PRO	2.0
1	A	517	ASP	2.0
1	A	497	ALA	2.0
1	A	351	LEU	2.0
1	A	367	LEU	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 oligosaccharides 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, 95th 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($\text{\AA}^2$)	Q<0.9
2	GD	A	701	1/1	0.36	0.17	706,706,706,706	0
2	GD	A	702	1/1	0.96	0.07	30,30,30,30	1

6.5 Other polymers [i](#)

There are no such residues in this entry.