



# Full wwPDB X-ray Structure Validation Report

Nov 12, 2014 – 11:21 AM EST

PDB ID : 4WIS  
Title : Crystal structure of the lipid scramblase nhTMEM16 in crystal form 1  
Authors : Dutzler, R.; Brunner, J.D.; Lim, N.K.; Schenck, S.  
Deposited on : 2014-09-26  
Resolution : 3.30 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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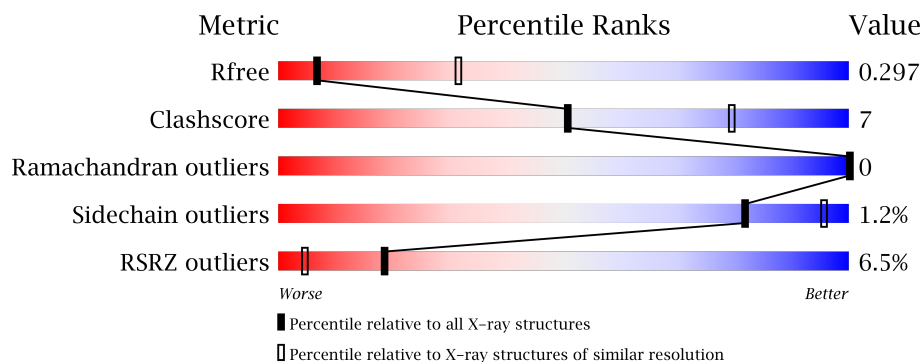
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1439  
EDS : stable24103  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.1.3  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable24103

# 1 Overall quality at a glance

The reported resolution of this entry is 3.30 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))
$R_{free}$	66092	1341 (3.40-3.20)
Clashscore	79885	1696 (3.40-3.20)
Ramachandran outliers	78287	1664 (3.40-3.20)
Sidechain outliers	78261	1662 (3.40-3.20)
RSRZ outliers	66119	1342 (3.40-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	735	
1	B	735	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

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

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10574 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Predicted protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	654	Total	C	N	O	S	0	0	0
			5285	3445	882	938	20			
1	B	654	Total	C	N	O	S	0	0	0
			5285	3445	882	938	20			

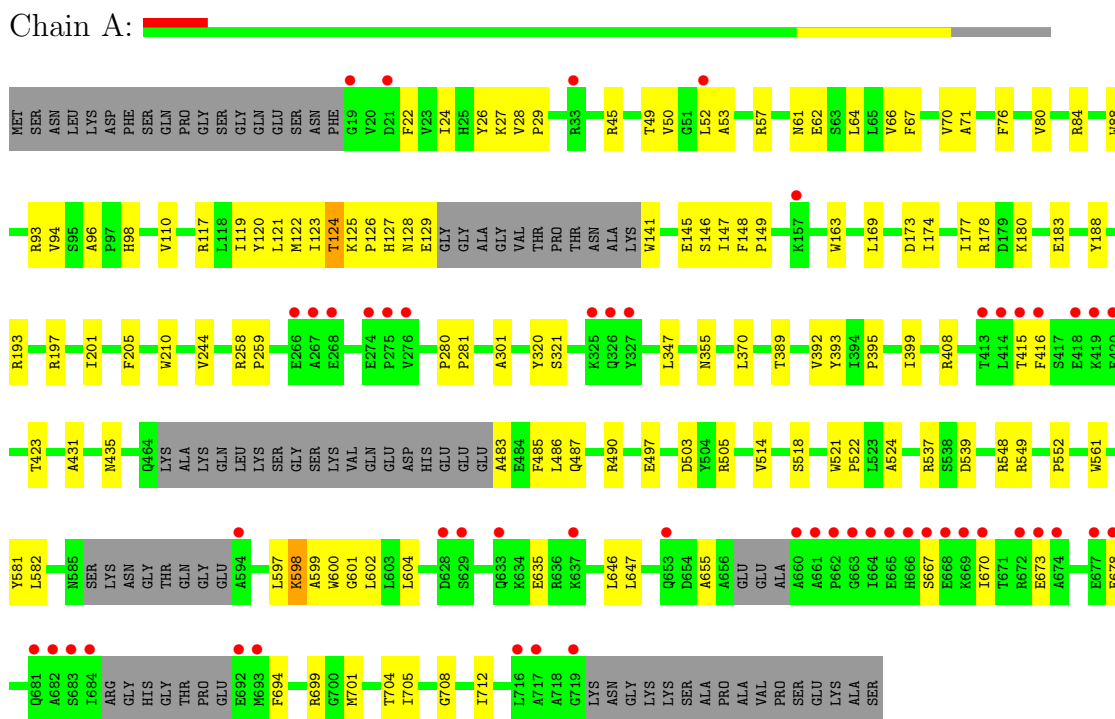
- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

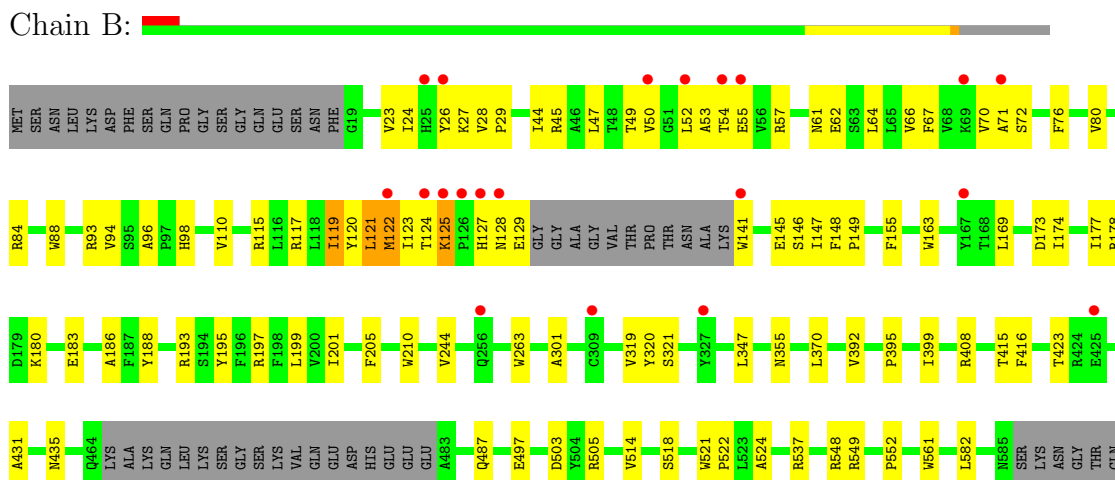
### 3 Residue-property plots

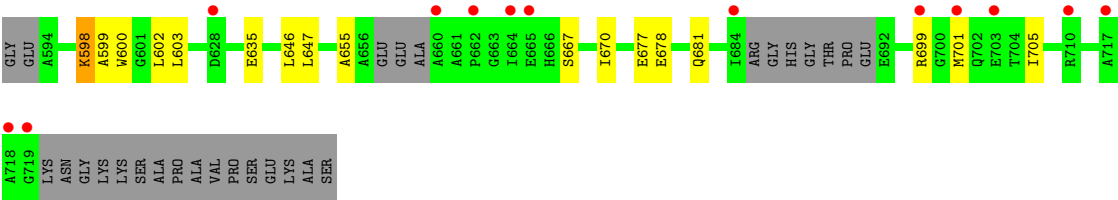
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Predicted protein



#### • Molecule 1: Predicted protein





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.48Å 113.69Å 235.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.98 – 3.30 48.98 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.2 (14.98-3.30) 99.2 (48.98-3.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.49 (at 3.33Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1760)	Depositor
R, $R_{free}$	0.237 , 0.285 0.252 , 0.297	Depositor DCC
$R_{free}$ test set	1954 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	115.7	Xtriage
Anisotropy	0.431	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 87.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 39477 reflections	Xtriage
$F_o, F_c$ correlation	0.83	EDS
Total number of atoms	10574	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	137.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 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	0.23	0/5423	0.40	0/7358
1	B	0.23	0/5423	0.41	0/7358
All	All	0.23	0/10846	0.40	0/14716

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5285	0	5248	85	0
1	B	5285	0	5248	83	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
All	All	10574	0	10496	156	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

All (156) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:647:LEU:HD21	1:B:655:ALA:HB3	1.64	0.79
1:A:647:LEU:HD21	1:A:655:ALA:HB3	1.64	0.78
1:A:45:ARG:NH1	1:A:49:THR:OG1	2.19	0.75
1:B:45:ARG:NH1	1:B:49:THR:OG1	2.21	0.73
1:B:128:ASN:OD1	1:B:129:GLU:N	2.22	0.73
1:A:487:GLN:HA	1:A:490:ARG:HD3	1.70	0.72
1:A:646:LEU:HD11	1:B:646:LEU:HD11	1.70	0.72
1:A:128:ASN:OD1	1:A:129:GLU:N	2.22	0.72
1:A:174:ILE:HD11	1:A:193:ARG:HD3	1.72	0.71
1:A:678:GLU:OE1	1:A:699:ARG:NH1	2.27	0.68
1:B:169:LEU:O	1:B:197:ARG:NH2	2.27	0.68
1:B:174:ILE:HD11	1:B:193:ARG:HD3	1.76	0.68
1:A:120:TYR:O	1:A:124:THR:OG1	2.11	0.68
1:A:149:PRO:HB2	1:A:549:ARG:HD2	1.77	0.67
1:A:169:LEU:O	1:A:197:ARG:NH2	2.27	0.67
1:A:708:GLY:HA3	1:B:57:ARG:HH11	1.58	0.67
1:B:57:ARG:HG2	1:B:64:LEU:HD22	1.76	0.66
1:B:678:GLU:OE1	1:B:699:ARG:NH1	2.29	0.65
1:B:149:PRO:HB2	1:B:549:ARG:HD2	1.79	0.64
1:A:121:LEU:O	1:A:125:LYS:N	2.31	0.64
1:A:604:LEU:HD12	1:B:603:LEU:HD11	1.80	0.63
1:B:210:TRP:HB2	1:B:522:PRO:HG2	1.81	0.62
1:A:210:TRP:HB2	1:A:522:PRO:HG2	1.82	0.62
1:A:57:ARG:HG2	1:A:64:LEU:HD22	1.83	0.61
1:B:28:VAL:HG21	1:B:45:ARG:HH21	1.66	0.59
1:A:28:VAL:HG21	1:A:45:ARG:HH21	1.68	0.59
1:A:123:ILE:O	1:A:128:ASN:HB3	2.03	0.59
1:B:125:LYS:O	1:B:127:HIS:N	2.35	0.59
1:A:22:PHE:HA	1:A:485:PHE:HE1	1.69	0.57
1:B:70:VAL:HG11	1:B:76:PHE:HB2	1.85	0.57
1:A:70:VAL:HG11	1:A:76:PHE:HB2	1.86	0.56
1:A:392:VAL:HG13	1:A:399:ILE:HD11	1.88	0.56
1:A:514:VAL:HA	1:A:518:SER:HB3	1.87	0.56
1:B:497:GLU:HG2	1:B:548:ARG:HD2	1.89	0.55
1:A:183:GLU:N	1:A:183:GLU:OE1	2.40	0.55
1:B:119:ILE:HA	1:B:122:MET:HB2	1.89	0.55
1:B:514:VAL:HA	1:B:518:SER:HB3	1.87	0.55
1:B:392:VAL:HG13	1:B:399:ILE:HD11	1.88	0.54
1:A:188:TYR:CZ	1:A:503:ASP:HB3	2.43	0.54
1:A:667:SER:HA	1:A:670:ILE:HD12	1.90	0.54
1:A:94:VAL:HG11	1:A:244:VAL:HG13	1.89	0.54
1:B:183:GLU:OE1	1:B:183:GLU:N	2.39	0.53
1:A:121:LEU:HB3	1:A:125:LYS:HE2	1.90	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:121:LEU:HG	1:B:125:LYS:HG3	1.90	0.53
1:A:395:PRO:HB3	1:A:582:LEU:HB3	1.91	0.53
1:A:22:PHE:HA	1:A:485:PHE:CE1	2.44	0.52
1:A:497:GLU:HG2	1:A:548:ARG:HD2	1.90	0.52
1:B:188:TYR:CZ	1:B:503:ASP:HB3	2.45	0.52
1:A:88:TRP:CE2	1:A:96:ALA:HB2	2.45	0.52
1:B:26:TYR:CZ	1:B:149:PRO:HG3	2.45	0.52
1:A:26:TYR:OH	1:A:120:TYR:HB2	2.10	0.52
1:B:80:VAL:HG11	1:B:110:VAL:HG22	1.92	0.52
1:B:121:LEU:O	1:B:125:LYS:HB2	2.09	0.51
1:B:29:PRO:HD2	1:B:146:SER:O	2.10	0.51
1:B:94:VAL:HG11	1:B:244:VAL:HG13	1.91	0.51
1:B:431:ALA:O	1:B:435:ASN:ND2	2.31	0.51
1:A:50:VAL:HG21	1:B:701:MET:SD	2.51	0.51
1:A:52:LEU:HD12	1:A:53:ALA:HB2	1.92	0.51
1:A:29:PRO:HD2	1:A:146:SER:O	2.10	0.51
1:A:80:VAL:HG11	1:A:110:VAL:HG22	1.92	0.51
1:B:667:SER:HA	1:B:670:ILE:HD12	1.92	0.50
1:A:673:GLU:HG3	1:B:72:SER:HB2	1.93	0.50
1:B:88:TRP:CE2	1:B:96:ALA:HB2	2.47	0.50
1:B:94:VAL:HG12	1:B:635:GLU:HG2	1.92	0.50
1:B:44:ILE:HA	1:B:47:LEU:HB2	1.94	0.49
1:B:178:ARG:NH1	1:B:183:GLU:OE2	2.45	0.49
1:B:180:LYS:O	1:B:549:ARG:NH1	2.45	0.49
1:A:94:VAL:HG12	1:A:635:GLU:HG2	1.93	0.49
1:A:431:ALA:O	1:A:435:ASN:ND2	2.32	0.49
1:B:395:PRO:HB3	1:B:582:LEU:HB3	1.94	0.49
1:B:28:VAL:HG22	1:B:147:ILE:HG12	1.95	0.49
1:A:599:ALA:HA	1:B:600:TRP:HB3	1.94	0.48
1:A:125:LYS:O	1:A:127:HIS:N	2.44	0.48
1:A:180:LYS:O	1:A:549:ARG:NH1	2.46	0.48
1:A:28:VAL:HG21	1:A:45:ARG:NH2	2.29	0.48
1:A:126:PRO:C	1:A:127:HIS:HD1	2.16	0.48
1:B:123:ILE:O	1:B:128:ASN:HB3	2.14	0.47
1:B:28:VAL:HG21	1:B:45:ARG:NH2	2.29	0.47
1:B:701:MET:O	1:B:705:ILE:HG13	2.14	0.47
1:B:29:PRO:HG2	1:B:145:GLU:HB3	1.95	0.47
1:B:61:ASN:O	1:B:62:GLU:HG2	2.14	0.47
1:A:61:ASN:O	1:A:62:GLU:HG2	2.14	0.47
1:A:29:PRO:HG2	1:A:145:GLU:HB3	1.96	0.47
1:B:52:LEU:HD12	1:B:53:ALA:HB2	1.96	0.47
1:A:188:TYR:OH	1:A:539:ASP:OD2	2.25	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:117:ARG:HB2	1:B:552:PRO:HB2	1.97	0.47
1:A:708:GLY:HA3	1:B:57:ARG:NH1	2.29	0.47
1:A:26:TYR:CZ	1:A:149:PRO:HG3	2.50	0.46
1:B:163:TRP:O	1:B:537:ARG:NE	2.48	0.46
1:A:701:MET:HG3	1:B:50:VAL:HG21	1.97	0.46
1:A:708:GLY:O	1:A:712:ILE:HG13	2.16	0.46
1:B:320:TYR:O	1:B:321:SER:HB3	2.16	0.46
1:A:117:ARG:HB2	1:A:552:PRO:HB2	1.98	0.46
1:A:26:TYR:CZ	1:A:120:TYR:HB2	2.51	0.46
1:A:27:LYS:HD3	1:A:148:PHE:CZ	2.51	0.46
1:A:163:TRP:O	1:A:537:ARG:NE	2.48	0.46
1:A:320:TYR:O	1:A:321:SER:HB3	2.16	0.46
1:B:119:ILE:O	1:B:123:ILE:HG13	2.16	0.46
1:A:408:ARG:HH21	1:A:423:THR:HG21	1.82	0.45
1:B:115:ARG:O	1:B:119:ILE:HG23	2.16	0.45
1:B:505:ARG:HB3	1:B:561:TRP:CH2	2.51	0.45
1:B:26:TYR:OH	1:B:120:TYR:HB2	2.16	0.45
1:A:505:ARG:HB3	1:A:561:TRP:CH2	2.51	0.45
1:B:598:LYS:HE2	1:B:602:LEU:HD22	1.98	0.45
1:A:701:MET:O	1:A:705:ILE:HG13	2.17	0.45
1:B:201:ILE:HG22	1:B:205:PHE:HE2	1.81	0.45
1:A:694:PHE:HB3	1:B:23:VAL:HG11	1.98	0.45
1:A:119:ILE:HA	1:A:122:MET:HG3	1.97	0.45
1:A:600:TRP:HB3	1:B:599:ALA:HA	1.99	0.45
1:A:201:ILE:HG22	1:A:205:PHE:HE2	1.81	0.44
1:B:321:SER:O	1:B:321:SER:OG	2.34	0.44
1:A:71:ALA:CB	1:B:670:ILE:HG23	2.48	0.44
1:B:408:ARG:HH21	1:B:423:THR:HG21	1.82	0.44
1:B:667:SER:HA	1:B:670:ILE:HB	2.00	0.44
1:B:301:ALA:HB3	1:B:347:LEU:HD11	2.00	0.44
1:A:321:SER:OG	1:A:321:SER:O	2.35	0.43
1:B:521:TRP:HD1	1:B:524:ALA:HB2	1.83	0.43
1:B:120:TYR:O	1:B:124:THR:OG1	2.29	0.43
1:A:598:LYS:HE2	1:A:602:LEU:HD22	2.00	0.43
1:A:57:ARG:HG3	1:A:66:VAL:HG22	2.00	0.43
1:B:27:LYS:HD3	1:B:148:PHE:CZ	2.53	0.43
1:A:24:ILE:HG21	1:A:67:PHE:HD2	1.84	0.43
1:B:57:ARG:HG3	1:B:66:VAL:HG22	2.01	0.43
1:B:24:ILE:HG21	1:B:67:PHE:HD2	1.84	0.43
1:B:84:ARG:HD2	1:B:93:ARG:NH1	2.34	0.43
1:A:301:ALA:HB3	1:A:347:LEU:HD11	2.01	0.43
1:A:483:ALA:N	1:A:486:LEU:HD23	2.33	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:28:VAL:HG22	1:A:147:ILE:HG12	2.00	0.42
1:A:84:ARG:HD2	1:A:93:ARG:NH1	2.34	0.42
1:B:183:GLU:HA	1:B:186:ALA:HB3	2.01	0.42
1:A:415:THR:O	1:A:416:PHE:HB3	2.20	0.42
1:B:319:VAL:HG12	1:B:423:THR:HG23	2.02	0.42
1:A:280:PRO:HA	1:A:281:PRO:HD2	1.89	0.42
1:A:80:VAL:O	1:A:84:ARG:HG2	2.20	0.42
1:A:173:ASP:O	1:A:177:ILE:HG12	2.21	0.41
1:A:521:TRP:HD1	1:A:524:ALA:HB2	1.84	0.41
1:B:26:TYR:CZ	1:B:120:TYR:HB2	2.56	0.41
1:B:80:VAL:O	1:B:84:ARG:HG2	2.20	0.41
1:B:173:ASP:O	1:B:177:ILE:HG12	2.21	0.41
1:B:415:THR:O	1:B:416:PHE:HB3	2.20	0.41
1:A:178:ARG:NH1	1:A:183:GLU:OE2	2.54	0.41
1:B:193:ARG:HE	1:B:197:ARG:NH2	2.18	0.41
1:B:93:ARG:HE	1:B:93:ARG:HB3	1.75	0.41
1:A:389:THR:HA	1:A:393:TYR:HB3	2.02	0.41
1:B:155:PHE:CZ	1:B:180:LYS:HG3	2.56	0.41
1:A:148:PHE:HA	1:A:149:PRO:HD3	1.89	0.41
1:B:54:THR:OG1	1:B:71:ALA:HB2	2.21	0.41
1:A:581:TYR:OH	1:A:601:GLY:HA3	2.20	0.40
1:B:195:TYR:O	1:B:199:LEU:HB2	2.21	0.40
1:B:677:GLU:O	1:B:681:GLN:HG2	2.22	0.40
1:A:193:ARG:HE	1:A:197:ARG:NH2	2.19	0.40
1:A:704:THR:HG21	1:B:55:GLU:HG3	2.04	0.40
1:B:355:ASN:ND2	1:B:370:LEU:HB2	2.36	0.40
1:A:258:ARG:HA	1:A:259:PRO:HD3	1.97	0.40
1:A:355:ASN:ND2	1:A:370:LEU:HB2	2.35	0.40
1:A:597:LEU:HD13	1:A:600:TRP:HE1	1.86	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	642/735 (87%)	609 (95%)	33 (5%)	0	100	100
1	B	642/735 (87%)	610 (95%)	32 (5%)	0	100	100
All	All	1284/1470 (87%)	1219 (95%)	65 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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	560/623 (90%)	556 (99%)	4 (1%)	91	98
1	B	560/623 (90%)	551 (98%)	9 (2%)	75	94
All	All	1120/1246 (90%)	1107 (99%)	13 (1%)	82	95

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	98	HIS
1	A	124	THR
1	A	141	TRP
1	A	598	LYS
1	B	98	HIS
1	B	119	ILE
1	B	121	LEU
1	B	122	MET
1	B	125	LYS
1	B	141	TRP
1	B	263	TRP
1	B	487	GLN
1	B	598	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	291	GLN

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Mol	Chain	Res	Type
1	A	366	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 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.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	654/735 (88%)	0.31	52 (7%)	12 4	76, 129, 223, 279	0
1	B	654/735 (88%)	0.20	33 (5%)	28 6	76, 125, 199, 238	0
All	All	1308/1470 (88%)	0.26	85 (6%)	18 5	76, 127, 210, 279	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	681	GLN	7.1
1	A	669	LYS	6.5
1	A	663	GLY	6.4
1	A	684	ILE	6.4
1	A	662	PRO	6.3
1	A	419	LYS	6.0
1	A	682	ALA	5.8
1	A	666	HIS	5.6
1	A	268	GLU	5.4
1	A	414	LEU	5.0
1	A	267	ALA	5.0
1	A	275	PRO	4.9
1	A	661	ALA	4.8
1	A	673	GLU	4.7
1	A	664	ILE	4.4
1	A	670	ILE	4.3
1	B	710	ARG	4.2
1	A	668	GLU	4.2
1	A	416	PHE	4.1
1	A	678	GLU	4.1
1	B	127	HIS	4.1
1	A	693	MET	4.0
1	B	665	GLU	4.0
1	B	718	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	717	ALA	3.9
1	B	660	ALA	3.8
1	B	126	PRO	3.7
1	A	692	GLU	3.6
1	B	52	LEU	3.6
1	B	703	GLU	3.5
1	A	418	GLU	3.4
1	B	141	TRP	3.4
1	A	633	GLN	3.3
1	B	125	LYS	3.3
1	A	677	GLU	3.3
1	A	19	GLY	3.3
1	A	326	GLN	3.3
1	A	266	GLU	3.2
1	A	628	ASP	3.2
1	A	33	ARG	3.2
1	A	420	GLU	3.2
1	B	701	MET	3.2
1	A	660	ALA	3.1
1	A	325	LYS	3.0
1	A	274	GLU	3.0
1	B	256	GLN	3.0
1	A	276	VAL	2.9
1	B	684	ILE	2.9
1	B	26	TYR	2.9
1	B	25	HIS	2.8
1	B	54	THR	2.8
1	B	50	VAL	2.8
1	A	157	LYS	2.8
1	A	665	GLU	2.7
1	A	594	ALA	2.7
1	B	124	THR	2.6
1	A	667	SER	2.6
1	A	327	TYR	2.5
1	B	664	ILE	2.5
1	A	629	SER	2.5
1	A	653	GLN	2.5
1	B	719	GLY	2.5
1	A	717	ALA	2.5
1	B	71	ALA	2.4
1	B	628	ASP	2.4
1	B	55	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	413	THR	2.4
1	B	69	LYS	2.4
1	A	637	LYS	2.4
1	B	425	GLU	2.3
1	A	415	THR	2.3
1	B	309	CYS	2.3
1	B	662	PRO	2.3
1	A	52	LEU	2.3
1	B	122	MET	2.3
1	B	128	ASN	2.3
1	A	672	ARG	2.2
1	A	674	ALA	2.2
1	B	167	TYR	2.1
1	B	327	TYR	2.1
1	B	699	ARG	2.1
1	A	716	LEU	2.1
1	A	719	GLY	2.0
1	A	683	SER	2.0
1	A	21	ASP	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 carbohydrates in this entry.

## 6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	CA	B	801	1/1	0.25	3.38	104,104,104,104	0
2	CA	A	802	1/1	0.23	-0.05	113,113,113,113	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CA	A	801	1/1	0.20	-0.11	96,96,96,96	0
2	CA	B	802	1/1	0.14	-0.93	101,101,101,101	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.