Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 06:12 am BST

PDB ID	:	4WIT
Title	:	TMEM16 lipid scramblase in crystal form 2
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Deposited on	:	2014-09-26
Resolution	:	3.40 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 following versions of software and data (see references ①) were used in the production of this report:

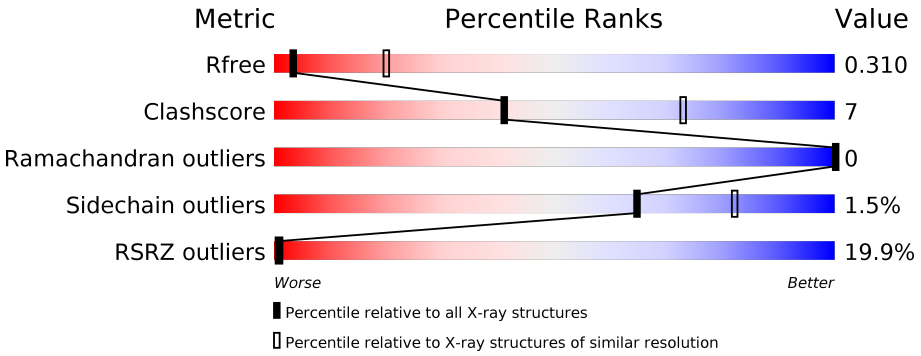
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 3.40 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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 on 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	735	20% 74% 15% • 11%
1	B	735	15% 73% 15% • 11%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 10574 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 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).

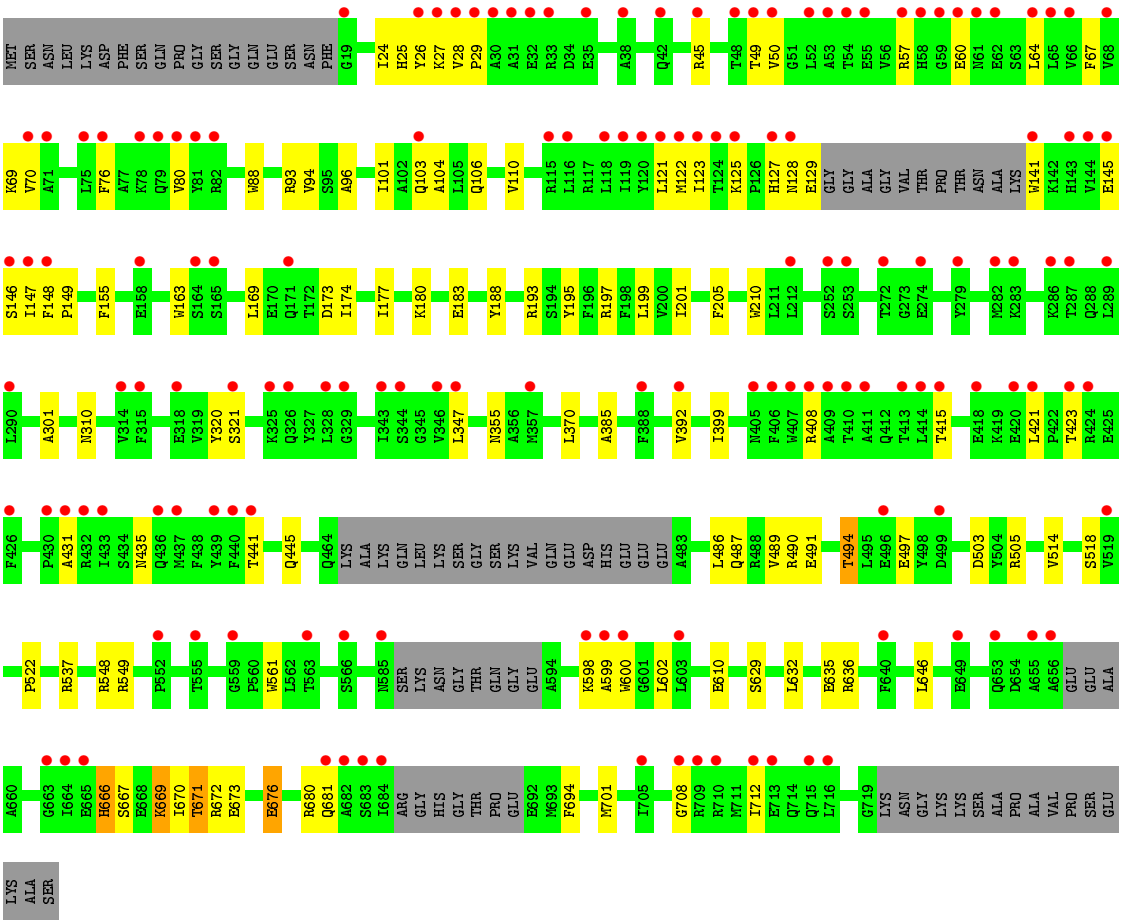
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Ca	0	0
			2	2		
2	A	2	Total	Ca	0	0
			2	2		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

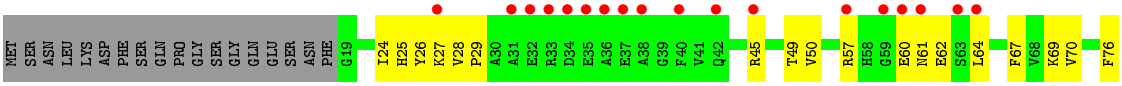
- Molecule 1: Predicted protein

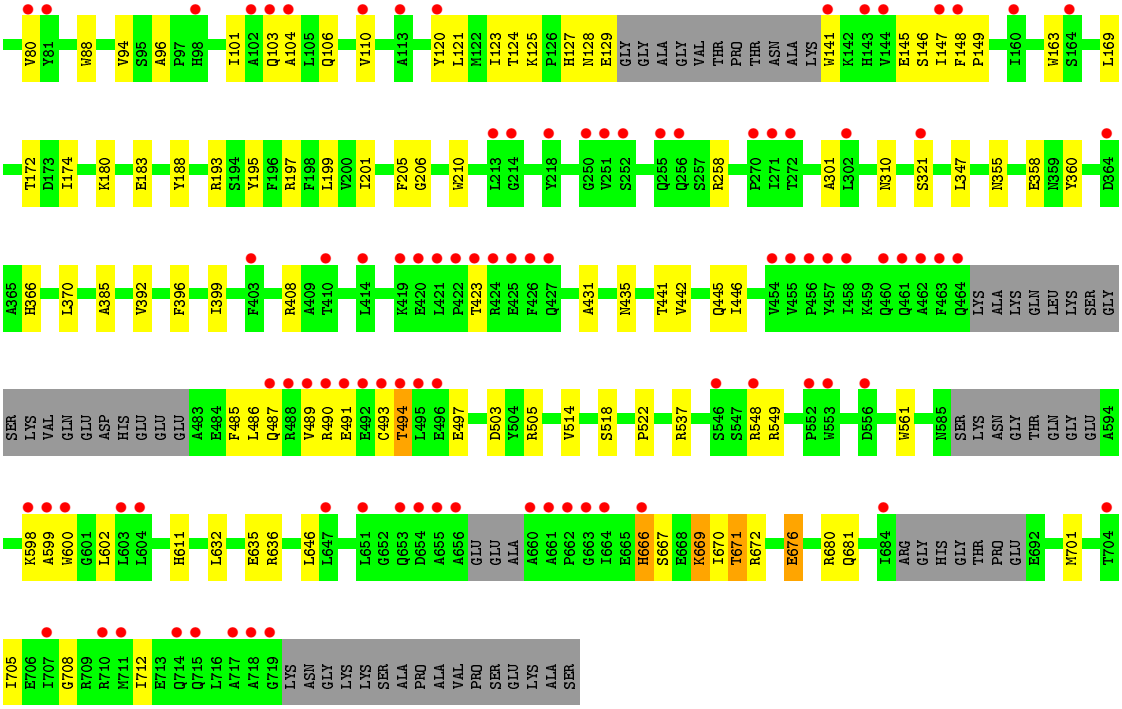
Chain A:



- Molecule 1: Predicted protein

Chain B:




V80 Y81 W88 V94 S95 A96 P97 H98 I101 A102 Q103 A104 L105 Q106 V110 A113 Y120 L121 M122 I123 T124 K125 P126 H127 N128 E129 GLY GLY ALA GLY VAL THR PRO THR ASN ALA LYS W141 K142 H143 V144 E145 S146 I147 F148 P149 I160 W163 S164 L169
T172 D173 I174 K180 E183 Y188 R193 S194 Y195 F196 R197 F198 L199 V200 I201 F205 G206 W210 L213 G214 Y218 G250 V251 S252 Q255 Q256 S257 R258 P270 I271 I272 A301 I302 N310 S321 L347 N355 E358 N359 Y360 D364
A365 H366 L370 A385 V392 F396 I399 F403 R408 A409 T410 L414 K419 E420 L421 P422 T423 R424 E425 F426 Q427 A431 N435 T441 V442 Q445 I446 V454 V455 P456 Y457 I458 K459 Q460 Q461 A462 F463 Q464 LYS ALA LYS GLN LEU LYS SER GLY
SER LYS VAL GLN GLU ASP HIS GLU GLU GLU A483 E484 F485 L486 Q487 R488 V489 R490 E491 E492 C493 T494 L495 E496 E497 D503 Y504 R505 V514 S518 P522 R537 S546 S547 R548 R549 P552 W553 D556 W561 N585 SER LYS ASN GLY THR GLN GLY GLU A594
K598 A599 W600 G601 L602 L603 L604 H611 L632 E635 R636 L646 L647 L651 G652 Q653 D654 A655 A656 GLU GLU ALA A660 A661 P662 G663 I664 E665 H666 S667 E668 K669 I670 T671 R672 E676 R680 Q681 I684 ARG GLY HIS GLY THR PRO GLU E692 M701 T704
I705 E706 I707 G708 R709 R710 M711 I712 E713 Q714 Q715 L716 A717 A718 G719 LYS ASN GLY LYS LYS SER ALA PRO ALA VAL PRO SER GLU LYS ALA SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	115.94Å 127.24Å 180.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.40 49.17 – 3.40	Depositor EDS
% Data completeness (in resolution range)	98.9 (15.00-3.40) 98.9 (49.17-3.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.65 (at 3.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1760)	Depositor
R, R_{free}	0.248 , 0.292 0.279 , 0.310	Depositor DCC
R_{free} test set	1618 reflections (4.38%)	wwPDB-VP
Wilson B-factor (Å^2)	134.6	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 106.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.82	EDS
Total number of atoms	10574	wwPDB-VP
Average B, all atoms (Å^2)	159.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% 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	0.22	0/5423	0.40	0/7358
1	B	0.22	0/5423	0.40	0/7358
All	All	0.22	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 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	5285	0	5248	77	0
1	B	5285	0	5248	81	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
All	All	10574	0	10496	150	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 7.

All (150) 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:169:LEU:O	1:A:197:ARG:NH2	2.12	0.83
1:A:60:GLU:HB3	1:A:490:ARG:HD2	1.62	0.82
1:B:169:LEU:O	1:B:197:ARG:NH2	2.14	0.80
1:B:60:GLU:HB3	1:B:490:ARG:HD2	1.62	0.79
1:B:28:VAL:HG21	1:B:45:ARG:HH21	1.51	0.76
1:A:28:VAL:HG21	1:A:45:ARG:HH21	1.53	0.73
1:A:45:ARG:NH1	1:A:49:THR:OG1	2.22	0.72
1:A:646:LEU:HD21	1:B:646:LEU:HD21	1.71	0.72
1:B:174:ILE:HD11	1:B:193:ARG:HD3	1.74	0.70
1:B:45:ARG:NH1	1:B:49:THR:OG1	2.27	0.67
1:B:149:PRO:HB2	1:B:549:ARG:HD2	1.77	0.67
1:A:497:GLU:HG2	1:A:548:ARG:HD2	1.77	0.67
1:B:666:HIS:O	1:B:669:LYS:HG3	1.95	0.66
1:A:666:HIS:O	1:A:669:LYS:HG3	1.95	0.65
1:A:174:ILE:HD11	1:A:193:ARG:HD3	1.78	0.64
1:B:101:ILE:HG13	1:B:104:ALA:H	1.63	0.64
1:A:149:PRO:HB2	1:A:549:ARG:HD2	1.80	0.63
1:A:101:ILE:HG13	1:A:104:ALA:H	1.64	0.63
1:A:392:VAL:HG13	1:A:399:ILE:HD11	1.83	0.61
1:B:497:GLU:HG2	1:B:548:ARG:HD2	1.83	0.61
1:A:669:LYS:HA	1:A:672:ARG:HE	1.66	0.60
1:A:128:ASN:OD1	1:A:129:GLU:N	2.35	0.60
1:B:392:VAL:HG13	1:B:399:ILE:HD11	1.84	0.59
1:B:80:VAL:HG11	1:B:110:VAL:HG22	1.84	0.59
1:B:210:TRP:HB2	1:B:522:PRO:HG2	1.84	0.59
1:B:669:LYS:HA	1:B:672:ARG:HE	1.68	0.58
1:A:210:TRP:HB2	1:A:522:PRO:HG2	1.86	0.58
1:A:441:THR:O	1:A:445:GLN:NE2	2.37	0.58
1:B:128:ASN:OD1	1:B:129:GLU:N	2.36	0.58
1:B:28:VAL:HG11	1:B:45:ARG:HE	1.69	0.57
1:A:598:LYS:HE2	1:A:602:LEU:HD22	1.87	0.56
1:B:514:VAL:HA	1:B:518:SER:HB3	1.87	0.56
1:A:514:VAL:HA	1:A:518:SER:HB3	1.87	0.56
1:A:57:ARG:HH22	1:B:705:ILE:HG12	1.72	0.55
1:A:60:GLU:HB3	1:A:490:ARG:CD	2.35	0.55
1:B:667:SER:O	1:B:671:THR:OG1	2.26	0.54
1:A:28:VAL:HG11	1:A:45:ARG:HE	1.73	0.54
1:A:431:ALA:O	1:A:435:ASN:ND2	2.36	0.54
1:A:669:LYS:HB3	1:A:672:ARG:HH21	1.73	0.54
1:B:125:LYS:O	1:B:127:HIS:N	2.39	0.54
1:A:667:SER:O	1:A:671:THR:OG1	2.22	0.54
1:B:669:LYS:HB3	1:B:672:ARG:HH21	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:431:ALA:O	1:B:435:ASN:ND2	2.31	0.54
1:B:598:LYS:HE2	1:B:602:LEU:HD22	1.90	0.53
1:A:599:ALA:HA	1:B:600:TRP:HB3	1.90	0.53
1:B:441:THR:O	1:B:445:GLN:NE2	2.41	0.53
1:B:27:LYS:HD2	1:B:489:VAL:HG13	1.91	0.53
1:A:80:VAL:HG11	1:A:110:VAL:HG22	1.89	0.53
1:A:26:TYR:CZ	1:A:149:PRO:HG3	2.44	0.52
1:A:188:TYR:CZ	1:A:503:ASP:HB3	2.43	0.52
1:B:29:PRO:HD2	1:B:146:SER:O	2.09	0.52
1:B:188:TYR:CZ	1:B:503:ASP:HB3	2.45	0.52
1:A:29:PRO:HD2	1:A:146:SER:O	2.10	0.51
1:A:29:PRO:HG2	1:A:145:GLU:HB3	1.92	0.51
1:B:60:GLU:HB3	1:B:490:ARG:CD	2.35	0.50
1:A:24:ILE:HG21	1:A:67:PHE:HD2	1.76	0.50
1:A:491:GLU:O	1:A:494:THR:OG1	2.28	0.50
1:A:600:TRP:HB3	1:B:599:ALA:HA	1.94	0.50
1:B:491:GLU:O	1:B:494:THR:OG1	2.28	0.50
1:A:70:VAL:HG11	1:A:76:PHE:HB2	1.94	0.49
1:B:26:TYR:CZ	1:B:149:PRO:HG3	2.46	0.49
1:A:505:ARG:HB3	1:A:561:TRP:CH2	2.48	0.49
1:B:29:PRO:HG2	1:B:145:GLU:HB3	1.94	0.49
1:B:70:VAL:HG11	1:B:76:PHE:HB2	1.94	0.49
1:A:708:GLY:O	1:A:712:ILE:HG13	2.13	0.49
1:A:694:PHE:HE1	1:B:485:PHE:HZ	1.60	0.48
1:A:27:LYS:HD2	1:A:489:VAL:HG13	1.94	0.48
1:B:505:ARG:HB3	1:B:561:TRP:CH2	2.48	0.48
1:B:24:ILE:HG21	1:B:67:PHE:HD2	1.78	0.48
1:B:88:TRP:CE2	1:B:96:ALA:HB2	2.49	0.48
1:A:163:TRP:O	1:A:537:ARG:NE	2.46	0.48
1:A:201:ILE:HG22	1:A:205:PHE:HE2	1.79	0.47
1:A:125:LYS:O	1:A:127:HIS:N	2.40	0.47
1:B:60:GLU:OE2	1:B:486:LEU:HB3	2.14	0.47
1:B:183:GLU:N	1:B:183:GLU:OE1	2.46	0.47
1:A:57:ARG:HG2	1:A:64:LEU:HD22	1.97	0.47
1:B:57:ARG:HG2	1:B:64:LEU:HD22	1.96	0.47
1:A:27:LYS:HD3	1:A:148:PHE:CZ	2.50	0.46
1:B:28:VAL:HG22	1:B:147:ILE:HG12	1.97	0.46
1:B:493:CYS:O	1:B:548:ARG:NH2	2.49	0.46
1:B:27:LYS:HD3	1:B:148:PHE:CZ	2.50	0.46
1:A:25:HIS:HB2	1:A:69:LYS:HA	1.97	0.46
1:B:101:ILE:HG21	1:B:104:ALA:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:TRP:O	1:B:537:ARG:NE	2.49	0.46
1:A:103:GLN:O	1:A:106:GLN:HG2	2.16	0.45
1:A:632:LEU:O	1:A:636:ARG:HG3	2.16	0.45
1:A:180:LYS:O	1:A:549:ARG:NH1	2.49	0.45
1:A:671:THR:HG1	1:A:671:THR:H	1.53	0.45
1:B:103:GLN:O	1:B:106:GLN:HG2	2.16	0.45
1:A:94:VAL:HG11	1:A:635:GLU:HG2	1.97	0.45
1:A:50:VAL:HG21	1:B:701:MET:SD	2.56	0.45
1:B:201:ILE:HG22	1:B:205:PHE:HE2	1.81	0.45
1:B:358:GLU:OE2	1:B:360:TYR:OH	2.24	0.45
1:B:676:GLU:O	1:B:680:ARG:HG2	2.17	0.45
1:B:121:LEU:O	1:B:125:LYS:N	2.48	0.45
1:A:121:LEU:O	1:A:125:LYS:N	2.49	0.45
1:B:301:ALA:HB3	1:B:347:LEU:HD11	1.99	0.45
1:A:676:GLU:O	1:A:680:ARG:HG2	2.17	0.44
1:A:701:MET:HG3	1:B:50:VAL:HG21	1.98	0.44
1:B:101:ILE:CG2	1:B:104:ALA:HB3	2.47	0.44
1:B:667:SER:HA	1:B:670:ILE:HD13	1.99	0.44
1:A:88:TRP:CE2	1:A:96:ALA:HB2	2.51	0.44
1:A:195:TYR:O	1:A:199:LEU:HB2	2.18	0.44
1:B:120:TYR:O	1:B:124:THR:OG1	2.29	0.44
1:A:60:GLU:OE2	1:A:486:LEU:HB3	2.17	0.44
1:B:180:LYS:O	1:B:549:ARG:NH1	2.50	0.44
1:A:28:VAL:HG22	1:A:147:ILE:HG12	1.99	0.44
1:B:632:LEU:O	1:B:636:ARG:HG3	2.18	0.44
1:A:183:GLU:N	1:A:183:GLU:OE1	2.48	0.43
1:A:415:THR:OG1	1:A:421:LEU:HD11	2.19	0.43
1:B:25:HIS:HB2	1:B:69:LYS:HA	1.99	0.43
1:B:321:SER:O	1:B:321:SER:OG	2.34	0.43
1:A:101:ILE:HG21	1:A:104:ALA:HB3	1.99	0.43
1:B:169:LEU:HA	1:B:169:LEU:HD23	1.92	0.43
1:A:667:SER:HA	1:A:670:ILE:HD13	2.00	0.43
1:A:301:ALA:HB3	1:A:347:LEU:HD11	1.99	0.43
1:B:28:VAL:HG21	1:B:45:ARG:NH2	2.28	0.43
1:B:123:ILE:O	1:B:128:ASN:HB3	2.19	0.42
1:B:408:ARG:HH21	1:B:423:THR:HG21	1.84	0.42
1:A:122:MET:HE2	1:A:122:MET:HB2	1.86	0.42
1:B:94:VAL:HG11	1:B:635:GLU:HG2	2.01	0.42
1:A:106:GLN:OE1	1:A:110:VAL:HG23	2.20	0.42
1:B:355:ASN:ND2	1:B:370:LEU:HB2	2.34	0.42
1:A:173:ASP:O	1:A:177:ILE:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:ASN:HD21	1:A:385:ALA:HA	1.85	0.42
1:B:121:LEU:HD13	1:B:121:LEU:HA	1.94	0.42
1:A:94:VAL:CG1	1:A:635:GLU:HG2	2.49	0.42
1:B:195:TYR:O	1:B:199:LEU:HB2	2.19	0.42
1:B:708:GLY:O	1:B:712:ILE:HG13	2.19	0.42
1:B:206:GLY:O	1:B:522:PRO:HB2	2.20	0.42
1:A:101:ILE:CG2	1:A:104:ALA:HB3	2.49	0.42
1:B:26:TYR:CZ	1:B:120:TYR:HB2	2.55	0.41
1:B:442:VAL:O	1:B:446:ILE:HG13	2.20	0.41
1:A:408:ARG:HH21	1:A:423:THR:HG21	1.84	0.41
1:A:320:TYR:O	1:A:321:SER:HB3	2.21	0.41
1:B:106:GLN:OE1	1:B:110:VAL:HG23	2.20	0.41
1:A:121:LEU:HA	1:A:121:LEU:HD13	1.92	0.41
1:A:629:SER:OG	1:A:632:LEU:HD12	2.20	0.41
1:B:310:ASN:HD21	1:B:385:ALA:HA	1.86	0.41
1:B:26:TYR:OH	1:B:120:TYR:HB2	2.20	0.41
1:A:155:PHE:CZ	1:A:180:LYS:HG3	2.56	0.41
1:B:258:ARG:HD2	1:B:366:HIS:HB2	2.02	0.41
1:B:396:PHE:HZ	1:B:598:LYS:HE3	1.86	0.41
1:B:94:VAL:CG1	1:B:635:GLU:HG2	2.51	0.40
1:A:123:ILE:O	1:A:128:ASN:HB3	2.21	0.40
1:A:355:ASN:ND2	1:A:370:LEU:HB2	2.37	0.40
1:A:669:LYS:HZ1	1:A:673:GLU:HG3	1.87	0.40
1:A:88:TRP:HA	1:A:93:ARG:HB3	2.03	0.40
1:A:610:GLU:OE2	1:B:611:HIS:NE2	2.55	0.40
1:B:61:ASN:O	1:B:62:GLU:HB3	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	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 (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	560/623 (90%)	552 (99%)	8 (1%)	67	83
1	B	560/623 (90%)	551 (98%)	9 (2%)	62	81
All	All	1120/1246 (90%)	1103 (98%)	17 (2%)	65	82

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	141	TRP
1	A	487	GLN
1	A	494	THR
1	A	666	HIS
1	A	669	LYS
1	A	671	THR
1	A	676	GLU
1	A	681	GLN
1	B	141	TRP
1	B	172	THR
1	B	487	GLN
1	B	494	THR
1	B	666	HIS
1	B	669	LYS
1	B	671	THR
1	B	676	GLU
1	B	681	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	42	GLN

5.3.3 RNA

There are no RNA molecules 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.

No monomer is involved in short contacts.

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^{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	654/735 (88%)	1.11	148 (22%)	0	1	87, 145, 254, 325	0
1	B	654/735 (88%)	0.93	112 (17%)	1	2	87, 144, 268, 327	0
All	All	1308/1470 (88%)	1.02	260 (19%)	1	1	87, 144, 262, 327	0

All (260) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	662	PRO	17.1
1	B	660	ALA	16.8
1	A	414	LEU	14.4
1	B	661	ALA	12.5
1	B	421	LEU	11.9
1	B	656	ALA	11.1
1	B	654	ASP	10.8
1	B	655	ALA	9.6
1	A	19	GLY	9.3
1	B	103	GLN	9.2
1	A	421	LEU	9.2
1	B	420	GLU	9.2
1	A	413	THR	8.7
1	A	122	MET	8.3
1	A	29	PRO	8.0
1	A	49	THR	7.9
1	A	599	ALA	7.8
1	A	664	ILE	7.4
1	A	598	LYS	7.2
1	A	26	TYR	7.1
1	B	60	GLU	7.1
1	A	123	ILE	6.9
1	B	255	GLN	6.9
1	B	464	GLN	6.8

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Mol	Chain	Res	Type	RSRZ
1	A	410	THR	6.7
1	B	663	GLY	6.7
1	A	430	PRO	6.7
1	A	146	SER	6.6
1	A	663	GLY	6.5
1	B	461	GLN	6.5
1	A	119	ILE	6.4
1	A	600	TRP	6.4
1	A	141	TRP	6.4
1	B	462	ALA	6.4
1	A	124	THR	6.4
1	B	463	PHE	6.3
1	B	61	ASN	6.3
1	A	656	ALA	6.3
1	B	600	TRP	6.3
1	A	28	VAL	6.1
1	A	712	ILE	6.1
1	A	57	ARG	6.1
1	A	325	LYS	6.0
1	B	37	GLU	6.0
1	B	271	ILE	6.0
1	A	713	GLU	6.0
1	A	61	ASN	5.9
1	A	418	GLU	5.9
1	B	546	SER	5.8
1	A	665	GLU	5.8
1	B	64	LEU	5.7
1	A	35	GLU	5.7
1	B	707	ILE	5.6
1	A	143	HIS	5.6
1	A	50	VAL	5.6
1	A	120	TYR	5.6
1	A	27	LYS	5.4
1	B	33	ARG	5.4
1	B	458	ILE	5.3
1	A	432	ARG	5.1
1	B	599	ALA	5.1
1	A	318	GLU	5.0
1	B	148	PHE	5.0
1	A	436	GLN	4.9
1	B	494	THR	4.9
1	B	427	GLN	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	52	LEU	4.9
1	A	440	PHE	4.8
1	B	57	ARG	4.7
1	B	495	LEU	4.7
1	A	682	ALA	4.6
1	A	653	GLN	4.6
1	B	490	ARG	4.6
1	A	283	LYS	4.6
1	B	38	ALA	4.6
1	A	48	THR	4.5
1	A	127	HIS	4.5
1	A	684	ILE	4.5
1	A	683	SER	4.5
1	B	251	VAL	4.5
1	B	711	MET	4.5
1	B	35	GLU	4.4
1	B	714	GLN	4.4
1	A	716	LEU	4.4
1	A	60	GLU	4.4
1	B	666	HIS	4.4
1	B	684	ILE	4.3
1	A	79	GLN	4.3
1	B	715	GLN	4.3
1	A	116	LEU	4.3
1	B	272	THR	4.3
1	B	36	ALA	4.3
1	B	143	HIS	4.2
1	A	286	LYS	4.2
1	B	553	TRP	4.2
1	B	34	ASP	4.2
1	B	664	ILE	4.2
1	A	585	ASN	4.2
1	B	256	GLN	4.1
1	A	433	ILE	4.1
1	B	718	ALA	4.1
1	A	424	ARG	4.1
1	A	655	ALA	4.0
1	A	681	GLN	4.0
1	B	653	GLN	3.9
1	A	407	TRP	3.9
1	A	147	ILE	3.9
1	B	59	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	63	SER	3.9
1	A	321	SER	3.8
1	A	709	ARG	3.8
1	B	717	ALA	3.8
1	B	426	PHE	3.8
1	A	125	LYS	3.8
1	B	460	GLN	3.8
1	B	321	SER	3.8
1	B	651	LEU	3.7
1	B	492	GLU	3.7
1	B	423	THR	3.7
1	A	347	LEU	3.6
1	B	42	GLN	3.6
1	B	32	GLU	3.6
1	A	121	LEU	3.6
1	A	519	VAL	3.6
1	A	563	THR	3.6
1	A	603	LEU	3.6
1	A	80	VAL	3.6
1	A	58	HIS	3.5
1	A	287	THR	3.5
1	A	326	GLN	3.5
1	B	493	CYS	3.5
1	B	419	LYS	3.5
1	A	420	GLU	3.4
1	B	548	ARG	3.4
1	A	53	ALA	3.4
1	A	423	THR	3.3
1	A	33	ARG	3.3
1	B	414	LEU	3.3
1	B	491	GLU	3.3
1	B	164	SER	3.3
1	A	388	PHE	3.3
1	A	405	ASN	3.3
1	B	147	ILE	3.2
1	A	45	ARG	3.2
1	B	364	ASP	3.2
1	A	75	LEU	3.1
1	A	71	ALA	3.1
1	A	82	ARG	3.1
1	A	145	GLU	3.1
1	A	426	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	148	PHE	3.1
1	A	70	VAL	3.1
1	A	78	LYS	3.1
1	A	552	PRO	3.1
1	B	218	TYR	3.0
1	B	141	TRP	3.0
1	B	455	VAL	3.0
1	B	302	LEU	3.0
1	B	598	LYS	3.0
1	A	32	GLU	3.0
1	B	457	TYR	3.0
1	A	54	THR	3.0
1	B	422	PRO	2.9
1	A	329	GLY	2.9
1	A	115	ARG	2.9
1	A	30	ALA	2.9
1	A	346	VAL	2.9
1	A	441	THR	2.9
1	A	715	GLN	2.9
1	B	31	ALA	2.9
1	A	411	ALA	2.9
1	A	274	GLU	2.9
1	B	704	THR	2.9
1	A	315	PHE	2.8
1	B	425	GLU	2.8
1	A	38	ALA	2.8
1	A	164	SER	2.8
1	A	68	VAL	2.8
1	A	289	LEU	2.8
1	A	31	ALA	2.8
1	B	214	GLY	2.8
1	A	640	PHE	2.8
1	A	65	LEU	2.8
1	A	64	LEU	2.7
1	A	566	SER	2.7
1	A	212	LEU	2.7
1	A	103	GLN	2.7
1	B	552	PRO	2.7
1	A	392	VAL	2.7
1	A	171	GLN	2.7
1	A	409	ALA	2.7
1	B	487	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	410	THR	2.7
1	A	344	SER	2.7
1	B	456	PRO	2.6
1	A	406	PHE	2.6
1	A	328	LEU	2.6
1	B	160	ILE	2.6
1	A	343	ILE	2.6
1	B	719	GLY	2.6
1	A	290	LEU	2.6
1	A	118	LEU	2.6
1	A	439	TYR	2.5
1	B	250	GLY	2.5
1	B	424	ARG	2.5
1	A	499	ASP	2.5
1	A	708	GLY	2.5
1	B	102	ALA	2.5
1	B	252	SER	2.5
1	B	556	ASP	2.5
1	A	415	THR	2.4
1	B	270	PRO	2.4
1	A	431	ALA	2.4
1	A	128	ASN	2.4
1	A	559	GLY	2.4
1	A	81	TYR	2.4
1	B	144	VAL	2.4
1	A	76	PHE	2.4
1	A	66	VAL	2.4
1	B	80	VAL	2.4
1	A	272	THR	2.4
1	A	59	GLY	2.4
1	A	55	GLU	2.4
1	B	489	VAL	2.3
1	A	144	VAL	2.3
1	A	253	SER	2.3
1	B	488	ARG	2.3
1	B	454	VAL	2.3
1	B	604	LEU	2.3
1	A	279	TYR	2.3
1	A	649	GLU	2.2
1	A	437	MET	2.2
1	A	314	VAL	2.2
1	B	104	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	158	GLU	2.2
1	B	603	LEU	2.2
1	B	120	TYR	2.2
1	B	40	PHE	2.2
1	B	113	ALA	2.2
1	A	710	ARG	2.2
1	A	496	GLU	2.2
1	B	710	ARG	2.2
1	B	45	ARG	2.1
1	B	110	VAL	2.1
1	B	647	LEU	2.1
1	B	98	HIS	2.1
1	A	705	ILE	2.1
1	B	403	PHE	2.1
1	B	213	LEU	2.1
1	A	357	MET	2.1
1	A	408	ARG	2.0
1	A	555	THR	2.0
1	A	252	SER	2.0
1	A	282	MET	2.0
1	A	62	GLU	2.0
1	B	496	GLU	2.0
1	A	42	GLN	2.0
1	A	165	SER	2.0
1	B	27	LYS	2.0
1	B	81	TYR	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 carbohydrates 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	A	802	1/1	0.92	0.21	147,147,147,147	0
2	CA	A	801	1/1	0.95	0.27	147,147,147,147	0
2	CA	B	802	1/1	0.98	0.21	141,141,141,141	0
2	CA	B	801	1/1	0.99	0.24	147,147,147,147	0

6.5 Other polymers (i)

There are no such residues in this entry.