Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 01:36 am BST

PDB ID	:	3GQ2
Title	:	Crystal Structure of the Dimer of the p115 Tether Globular Head Domain
Authors	:	An, Y.; Elsliger, M.A.; Wilson, I.A.
Deposited on	:	2009-03-23
Resolution	:	2.18 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 ⓘ) were used in the production of this report:

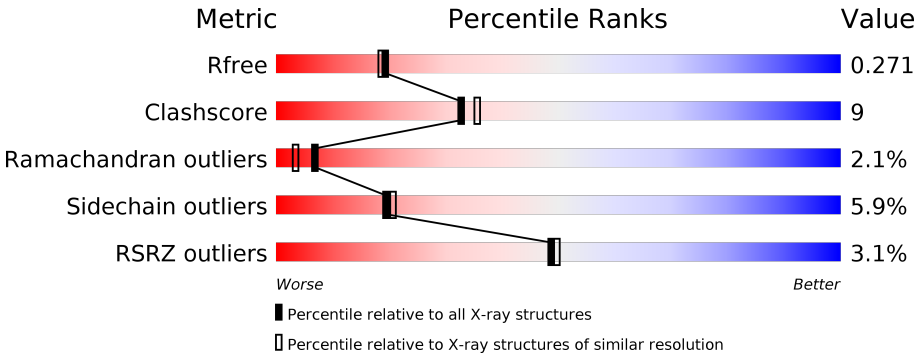
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.18 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	6864 (2.20-2.16)
Clashscore	141614	7689 (2.20-2.16)
Ramachandran outliers	138981	7564 (2.20-2.16)
Sidechain outliers	138945	7564 (2.20-2.16)
RSRZ outliers	127900	6738 (2.20-2.16)

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	651	3% 74% 17% • 6%
1	B	651	3% 77% 15% • 6%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 10300 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 General vesicular transport factor p115.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	614	Total	C	N	O	S	0	6	0
			4866	3075	832	932	27			
1	B	614	Total	C	N	O	S	0	2	0
			4827	3055	824	921	27			

- Molecule 2 is water.

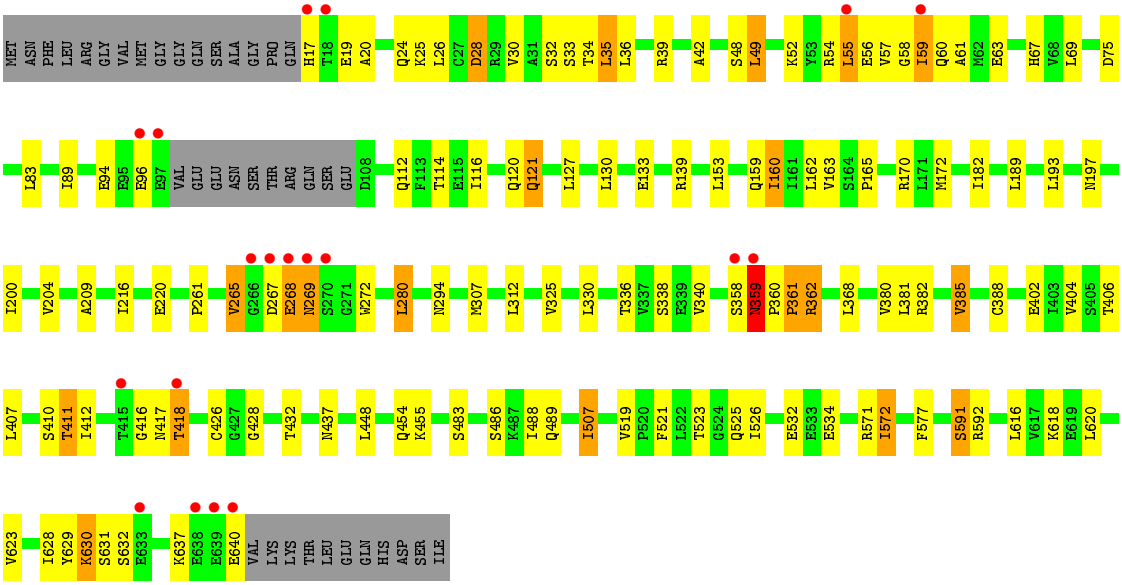
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	312	Total	O	0	0
			312	312		
2	B	295	Total	O	0	0
			295	295		

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.

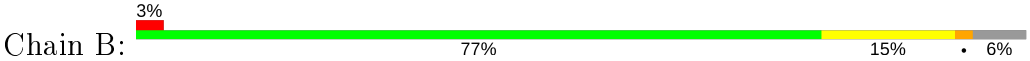
- Molecule 1: General vesicular transport factor p115

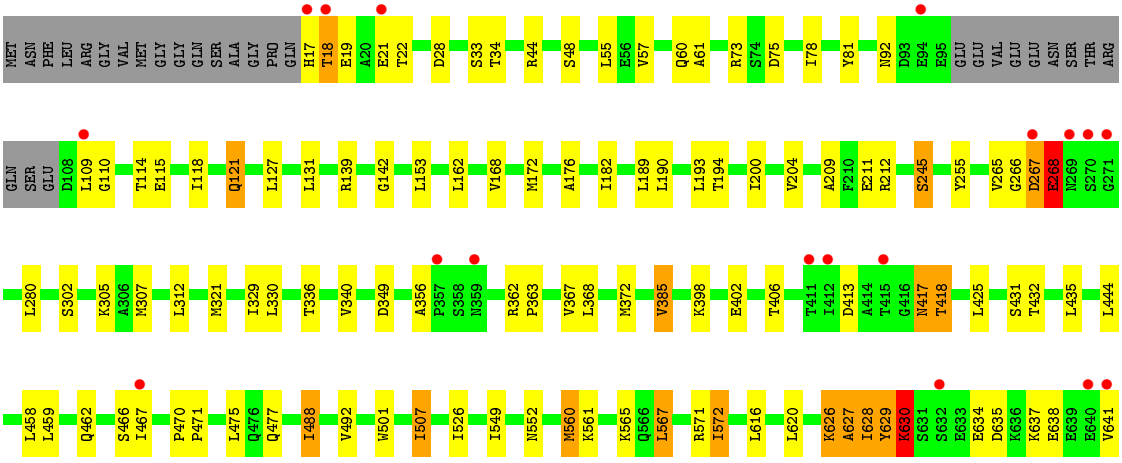
Chain A:

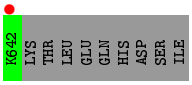


- Molecule 1: General vesicular transport factor p115

Chain B:






K642
LYS
THR
LEU
GLU
GLN
HIS
ASP
SER
ILE

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	78.16Å 159.82Å 81.45Å 90.00° 115.13° 90.00°	Depositor
Resolution (Å)	20.00 – 2.18 19.98 – 2.18	Depositor EDS
% Data completeness (in resolution range)	87.2 (20.00-2.18) 87.3 (19.98-2.18)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	1.40 (at 2.19Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.199 , 0.254 0.216 , 0.271	Depositor DCC
R_{free} test set	8222 reflections (10.03%)	wwPDB-VP
Wilson B-factor (Å^2)	38.2	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 24.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.044 for l,-k,h	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10300	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.18% 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

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	0.59	1/4941 (0.0%)	0.66	0/6688
1	B	0.58	0/4902	0.67	0/6637
All	All	0.59	1/9843 (0.0%)	0.66	0/13325

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	A	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	591	SER	CB-OG	-5.07	1.35	1.42

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	267	ASP	Peptide
1	A	268	GLU	Peptide
1	A	359	ASN	Peptide

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	4866	0	4924	95	0
1	B	4827	0	4900	75	0
2	A	312	0	0	19	0
2	B	295	0	0	9	0
All	All	10300	0	9824	170	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 9.

All (170) 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:170[B]:ARG:HH11	1:A:170[B]:ARG:HG2	0.99	1.12
1:A:170[B]:ARG:HH11	1:A:170[B]:ARG:CG	1.79	0.96
1:A:170[B]:ARG:NH1	1:A:170[B]:ARG:HG2	1.82	0.90
1:B:162:LEU:HD13	1:B:200:ILE:CD1	2.08	0.83
1:B:18:THR:HA	1:B:22:THR:HG23	1.60	0.82
1:B:425:LEU:HD13	1:B:444:LEU:CD1	2.10	0.82
1:A:616:LEU:HD21	1:A:620:LEU:HD12	1.63	0.80
1:A:159:GLN:O	1:A:163:VAL:HG13	1.81	0.80
1:A:197:ASN:OD1	1:A:200:ILE:HD13	1.82	0.79
1:A:20:ALA:HB3	2:A:763:HOH:O	1.81	0.79
1:A:368:LEU:O	1:A:385:VAL:HG21	1.85	0.75
1:B:17:HIS:O	1:B:21:GLU:N	2.21	0.74
1:B:637:LYS:O	1:B:641:VAL:HG23	1.88	0.73
1:A:526:ILE:CG2	1:A:572:ILE:HD12	2.19	0.73
1:A:532:GLU:OE1	2:A:742:HOH:O	2.07	0.73
1:B:425:LEU:HD13	1:B:444:LEU:HD13	1.70	0.72
1:B:211:GLU:HG2	2:B:780:HOH:O	1.91	0.71
1:A:294[A]:ASN:OD1	2:A:887:HOH:O	2.08	0.70
1:A:114:THR:HG22	1:A:153:LEU:HD12	1.72	0.70
1:A:616:LEU:CD2	1:A:620:LEU:HD12	2.22	0.69
1:A:55:LEU:O	1:A:59:ILE:HG23	1.91	0.69
1:A:162:LEU:HD13	1:A:200:ILE:HD12	1.74	0.68
1:A:488:ILE:HD12	1:A:489:GLN:N	2.08	0.67
1:A:507:ILE:HD13	1:A:507:ILE:H	1.59	0.67
1:B:121:GLN:HA	2:B:724:HOH:O	1.92	0.67
1:A:20:ALA:CB	2:A:763:HOH:O	2.38	0.66
1:B:172:MET:HE1	1:B:204:VAL:HG22	1.77	0.66
1:A:526:ILE:HG22	1:A:572:ILE:HD12	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:616:LEU:O	1:A:616:LEU:HD23	1.97	0.65
1:A:361:PRO:O	1:A:362:ARG:HG3	1.97	0.65
1:A:572:ILE:HD11	1:A:577:PHE:HB2	1.79	0.65
1:A:261:PRO:O	2:A:748:HOH:O	2.14	0.64
1:A:170[B]:ARG:NH1	1:A:170[B]:ARG:CG	2.49	0.62
1:B:417:ASN:C	1:B:417:ASN:HD22	2.01	0.62
1:B:266:GLY:O	1:B:268:GLU:N	2.33	0.61
1:B:526:ILE:HG22	1:B:572:ILE:HG21	1.81	0.61
1:B:549:ILE:HD12	1:B:628:ILE:HD11	1.81	0.61
1:A:26:LEU:O	1:A:30:VAL:HG23	2.01	0.60
1:A:402:GLU:O	1:A:406:THR:HG23	2.02	0.60
1:B:92:ASN:HD21	1:B:110:GLY:HA3	1.66	0.59
1:A:338:SER:OG	1:A:388:CYS:HA	2.03	0.59
1:A:69:LEU:HD22	1:A:130:LEU:CD1	2.33	0.59
1:B:139:ARG:HG2	1:B:182:ILE:HD12	1.85	0.59
1:A:204:VAL:O	1:A:209:ALA:HB2	2.03	0.58
1:B:92:ASN:ND2	1:B:110:GLY:HA3	2.19	0.57
1:A:359:ASN:HB3	1:A:360:PRO:CD	2.35	0.57
1:B:616:LEU:HD21	1:B:620:LEU:HD12	1.87	0.57
1:A:418:THR:HG21	2:A:769:HOH:O	2.05	0.57
1:B:363:PRO:O	1:B:367:VAL:HG23	2.05	0.57
1:B:368:LEU:HD22	1:B:385:VAL:HG22	1.87	0.57
1:A:265:VAL:HG11	1:A:280:LEU:HD21	1.87	0.57
1:A:49:LEU:N	1:A:49:LEU:HD23	2.19	0.56
1:B:567:LEU:HD21	1:B:571[A]:ARG:NH2	2.21	0.56
1:B:417:ASN:N	2:B:661:HOH:O	2.37	0.56
1:A:55:LEU:O	1:A:59:ILE:CG2	2.53	0.56
1:B:616:LEU:C	1:B:616:LEU:HD23	2.27	0.56
1:B:168:VAL:HG21	1:B:200:ILE:HD12	1.88	0.55
1:B:162:LEU:HD13	1:B:200:ILE:HD13	1.88	0.55
1:A:507:ILE:HD13	1:A:507:ILE:N	2.21	0.55
1:B:115:GLU:HG2	1:B:153:LEU:HD11	1.89	0.55
1:A:572:ILE:HD11	1:A:577:PHE:CB	2.37	0.54
1:A:272:TRP:HZ3	1:A:280:LEU:HD23	1.73	0.54
1:B:634:GLU:O	1:B:638:GLU:HG2	2.07	0.54
1:A:525:GLN:NE2	2:A:926:HOH:O	2.39	0.54
1:B:626:LYS:O	1:B:627:ALA:C	2.45	0.54
1:A:526:ILE:HG21	1:A:572:ILE:HD12	1.89	0.53
1:A:189:LEU:C	1:A:189:LEU:HD23	2.28	0.53
1:A:197:ASN:CG	1:A:200:ILE:HD13	2.29	0.53
1:B:114:THR:O	1:B:118:ILE:HG23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:ARG:NH2	2:B:812:HOH:O	2.41	0.53
1:A:381:LEU:O	1:A:385:VAL:HG12	2.09	0.53
1:B:162:LEU:HB2	1:B:200:ILE:HD11	1.90	0.53
1:B:265:VAL:HG23	1:B:266:GLY:N	2.24	0.53
1:B:616:LEU:HD23	1:B:616:LEU:O	2.08	0.53
1:A:359:ASN:HB3	1:A:360:PRO:HD3	1.90	0.52
1:B:372:MET:HB2	1:B:385:VAL:CG1	2.40	0.52
1:B:417:ASN:HD22	1:B:418:THR:N	2.07	0.52
1:A:69:LEU:HD22	1:A:130:LEU:HD11	1.90	0.52
1:B:507:ILE:HD13	1:B:507:ILE:H	1.74	0.51
1:B:458:LEU:HD23	1:B:501:TRP:CH2	2.45	0.51
1:B:162:LEU:HD13	1:B:200:ILE:HD11	1.90	0.51
1:A:193:LEU:HG	1:A:200:ILE:HG21	1.92	0.51
1:B:18:THR:HG22	1:B:22:THR:CG2	2.41	0.51
1:B:245:SER:HB3	2:B:937:HOH:O	2.11	0.51
1:A:382:ARG:NH2	2:A:741:HOH:O	2.44	0.50
1:B:458:LEU:HD23	1:B:501:TRP:CZ2	2.47	0.50
1:A:35:LEU:HD12	1:A:36:LEU:N	2.27	0.49
1:B:459:LEU:CD2	1:B:475:LEU:HD22	2.42	0.49
1:B:118:ILE:HD13	1:B:153:LEU:HD12	1.94	0.49
1:B:18:THR:O	1:B:19:GLU:HG2	2.12	0.49
1:A:162:LEU:HD13	1:A:200:ILE:CD1	2.39	0.49
1:A:139:ARG:HD2	1:A:182:ILE:HD13	1.94	0.49
1:A:618:LYS:NZ	2:A:821:HOH:O	2.33	0.49
1:B:255:TYR:OH	2:B:749:HOH:O	2.06	0.48
1:B:307:MET:HG2	1:B:312:LEU:HD23	1.96	0.48
1:B:121:GLN:CA	2:B:724:HOH:O	2.56	0.48
1:B:368:LEU:CD2	1:B:385:VAL:HG22	2.44	0.48
1:A:121:GLN:HB2	2:A:850:HOH:O	2.13	0.48
1:A:120:GLN:O	1:A:121:GLN:C	2.51	0.48
1:B:193:LEU:HG	1:B:200:ILE:HG21	1.96	0.48
1:A:336:THR:O	1:A:340:VAL:HG23	2.13	0.47
1:A:57:VAL:O	1:A:61:ALA:HB3	2.14	0.47
1:A:507:ILE:CD1	1:A:507:ILE:H	2.22	0.47
1:B:57:VAL:O	1:B:61:ALA:HB3	2.15	0.47
1:A:519:VAL:O	1:A:523:THR:HG23	2.14	0.47
1:A:48:SER:C	1:A:49:LEU:HD23	2.35	0.47
1:A:60:GLN:HG2	2:A:740:HOH:O	2.14	0.47
1:B:402:GLU:O	1:B:406:THR:HG23	2.15	0.47
1:B:507:ILE:HD13	1:B:507:ILE:N	2.30	0.47
1:A:325:VAL:HB	1:A:330:LEU:HD13	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:488:ILE:HD13	2:A:781:HOH:O	2.14	0.46
1:B:211:GLU:CG	2:B:780:HOH:O	2.57	0.46
1:A:200:ILE:O	1:A:204:VAL:HG23	2.15	0.46
1:A:616:LEU:HD23	1:A:616:LEU:C	2.36	0.46
1:B:552:ASN:ND2	1:B:560:MET:O	2.48	0.46
1:B:616:LEU:CD2	1:B:620:LEU:HD12	2.46	0.46
1:B:75:ASP:O	1:B:78:ILE:HG22	2.16	0.46
1:B:477:GLN:OE1	1:B:477:GLN:HA	2.16	0.45
1:A:407:LEU:CD2	1:A:426:CYS:SG	3.04	0.45
1:A:637:LYS:HA	1:A:640:GLU:HB2	1.98	0.45
1:A:170[A]:ARG:NH2	2:A:885:HOH:O	2.48	0.45
1:A:380:VAL:HG22	2:A:724:HOH:O	2.17	0.45
1:A:56:GLU:O	2:A:740:HOH:O	2.21	0.45
1:A:294[B]:ASN:C	1:A:294[B]:ASN:OD1	2.54	0.45
1:A:272:TRP:CZ3	1:A:280:LEU:HD23	2.52	0.44
1:B:349:ASP:CG	1:B:398:LYS:HZ1	2.20	0.44
1:A:39:ARG:O	1:A:42:ALA:HB3	2.18	0.44
1:B:641:VAL:HG12	1:B:641:VAL:O	2.17	0.44
1:A:116:ILE:HG23	2:A:753:HOH:O	2.17	0.44
1:A:172:MET:SD	1:A:204:VAL:HG13	2.57	0.44
1:A:417:ASN:O	1:A:418:THR:HG22	2.17	0.44
1:A:410:SER:O	1:A:411:THR:CB	2.66	0.43
1:A:404:VAL:HG21	1:A:454:GLN:HB3	2.00	0.43
1:B:204:VAL:O	1:B:209:ALA:HB2	2.18	0.43
1:A:325:VAL:CG1	1:A:330:LEU:HD13	2.48	0.43
1:B:190:LEU:O	1:B:194:THR:HG23	2.18	0.43
1:A:361:PRO:O	1:A:362:ARG:CG	2.66	0.43
1:B:549:ILE:CD1	1:B:628:ILE:HD11	2.47	0.43
1:A:69:LEU:HD22	1:A:130:LEU:HD13	2.00	0.43
1:A:36:LEU:HD21	1:A:75:ASP:HB2	2.01	0.43
1:A:428:GLY:O	1:A:437:ASN:ND2	2.51	0.42
1:A:58:GLY:HA2	1:A:89:ILE:HD13	2.01	0.42
1:A:616:LEU:HD21	1:A:620:LEU:CD1	2.41	0.42
1:B:176:ALA:HB2	1:B:212[A]:ARG:NH2	2.35	0.42
1:B:629:TYR:O	1:B:630:LYS:O	2.38	0.42
1:A:448:LEU:HD22	1:A:455:LYS:HA	2.02	0.42
1:B:131:LEU:HD21	1:B:142:GLY:HA3	2.01	0.42
1:A:623:VAL:HG13	2:A:918:HOH:O	2.19	0.42
1:B:189:LEU:HD23	1:B:189:LEU:C	2.40	0.42
1:B:336:THR:O	1:B:340:VAL:HG23	2.18	0.42
1:A:483:SER:HB3	1:A:521:PHE:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:ARG:HD3	1:B:81:TYR:CE2	2.55	0.42
1:A:69:LEU:HD21	1:A:83:LEU:HG	2.02	0.42
1:B:462:GLN:NE2	2:B:808:HOH:O	2.52	0.42
1:A:216:ILE:O	1:A:220:GLU:HG2	2.19	0.41
1:B:268:GLU:OE1	1:B:268:GLU:HA	2.19	0.41
1:B:526:ILE:CG2	1:B:572:ILE:HG21	2.49	0.41
1:A:307:MET:HG2	1:A:312:LEU:HD23	2.02	0.41
1:A:571[B]:ARG:HA	1:A:571[B]:ARG:HD3	1.89	0.41
1:A:160:ILE:O	1:A:163:VAL:HG22	2.21	0.41
1:A:28:ASP:O	1:A:32:SER:N	2.38	0.41
1:A:629:TYR:O	1:A:630:LYS:CB	2.68	0.41
1:B:470:PRO:HA	1:B:471:PRO:HD3	1.96	0.41
1:B:488:ILE:O	1:B:492:VAL:HG23	2.21	0.41
1:B:75:ASP:HB3	1:B:78:ILE:HG22	2.02	0.41
1:A:623:VAL:N	2:A:918:HOH:O	2.52	0.41
1:B:321:MET:HE1	1:B:356:ALA:HA	2.03	0.41
1:A:25:LYS:HB2	2:A:766:HOH:O	2.22	0.40
1:B:329:ILE:HD13	1:B:329:ILE:HA	1.98	0.40
1:A:417:ASN:C	1:A:418:THR:HG22	2.42	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	616/651 (95%)	568 (92%)	32 (5%)	16 (3%)	5 2
1	B	612/651 (94%)	567 (93%)	35 (6%)	10 (2%)	9 6
All	All	1228/1302 (94%)	1135 (92%)	67 (6%)	26 (2%)	7 3

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	19	GLU
1	A	268	GLU
1	A	269	ASN
1	A	358	SER
1	A	418	THR
1	A	630	LYS
1	A	631	SER
1	A	632	SER
1	B	362	ARG
1	B	418	THR
1	B	267	ASP
1	A	52	LYS
1	A	361	PRO
1	A	362	ARG
1	B	561	LYS
1	A	121	GLN
1	B	560	MET
1	B	629	TYR
1	B	630	LYS
1	A	165	PRO
1	A	411	THR
1	B	268	GLU
1	B	627	ALA
1	A	359	ASN
1	B	467	ILE
1	A	416	GLY

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	551/577 (96%)	520 (94%)	31 (6%)	21	23
1	B	547/577 (95%)	514 (94%)	33 (6%)	19	20
All	All	1098/1154 (95%)	1034 (94%)	64 (6%)	19	21

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	HIS
1	A	24	GLN
1	A	28	ASP
1	A	33	SER
1	A	34	THR
1	A	35	LEU
1	A	49	LEU
1	A	54	ARG
1	A	55	LEU
1	A	59	ILE
1	A	63	GLU
1	A	67	HIS
1	A	94	GLU
1	A	96	GLU
1	A	112	GLN
1	A	127	LEU
1	A	133	GLU
1	A	160	ILE
1	A	265	VAL
1	A	269	ASN
1	A	280	LEU
1	A	385	VAL
1	A	412	ILE
1	A	432	THR
1	A	486	SER
1	A	507	ILE
1	A	534	GLU
1	A	572	ILE
1	A	591	SER
1	A	592	ARG
1	A	628	ILE
1	B	18	THR
1	B	28	ASP
1	B	33	SER
1	B	34	THR
1	B	48	SER
1	B	55	LEU
1	B	60	GLN
1	B	109	LEU
1	B	121	GLN
1	B	127	LEU
1	B	245	SER
1	B	267	ASP

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Mol	Chain	Res	Type
1	B	268	GLU
1	B	280	LEU
1	B	302	SER
1	B	305	LYS
1	B	330	LEU
1	B	385	VAL
1	B	413	ASP
1	B	417	ASN
1	B	431	SER
1	B	432	THR
1	B	435	LEU
1	B	466	SER
1	B	488	ILE
1	B	507	ILE
1	B	565	LYS
1	B	567	LEU
1	B	572	ILE
1	B	626	LYS
1	B	628	ILE
1	B	630	LYS
1	B	635	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	158	GLN
1	A	159	GLN
1	A	269	ASN
1	B	92	ASN
1	B	159	GLN
1	B	417	ASN

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

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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	614/651 (94%)	-0.08	19 (3%) 49 50	15, 29, 53, 95	0
1	B	614/651 (94%)	-0.09	19 (3%) 49 50	11, 29, 52, 97	0
All	All	1228/1302 (94%)	-0.09	38 (3%) 49 50	11, 29, 53, 97	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	641	VAL	6.9
1	B	17	HIS	6.1
1	A	97	GLU	5.6
1	B	642	LYS	5.2
1	A	17	HIS	5.1
1	B	270	SER	4.2
1	A	269	ASN	3.7
1	B	359	ASN	3.7
1	B	411	THR	3.6
1	A	359	ASN	3.5
1	B	271	GLY	3.4
1	B	94	GLU	3.3
1	A	18	THR	3.1
1	A	270	SER	3.0
1	B	640	GLU	2.8
1	A	633	GLU	2.8
1	B	267	ASP	2.7
1	A	268	GLU	2.7
1	B	357	PRO	2.7
1	A	266	GLY	2.7
1	A	638	GLU	2.6
1	A	640	GLU	2.6
1	B	18	THR	2.6
1	A	639	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	358	SER	2.5
1	B	269	ASN	2.4
1	B	109	LEU	2.4
1	B	412	ILE	2.4
1	A	96	GLU	2.4
1	A	267	ASP	2.3
1	A	59	ILE	2.3
1	A	418	THR	2.2
1	B	467	ILE	2.1
1	B	415	THR	2.1
1	A	55	LEU	2.1
1	B	632	SER	2.1
1	B	21	GLU	2.1
1	A	415	THR	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.