



# Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 07:52 pm BST

PDB ID : 1KFQ  
Title : Crystal Structure of Exocytosis-Sensitive Phosphoprotein, pp63/parafusin (Phosphoglucomutase) from Paramecium. OPEN FORM  
Authors : Mueller, S.; Diederichs, K.; Breed, J.; Kissmehl, R.; Hauser, K.; Plattner, H.; Welte, W.  
Deposited on : 2001-11-22  
Resolution : 2.40 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](mailto: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.

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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
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

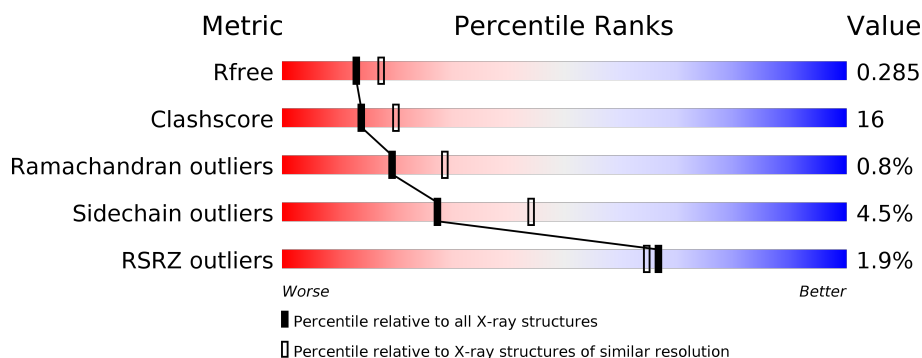
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 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	572	<div> <div>2%</div> <div> <div></div> <div>67%</div> <div>28%</div> <div>.</div> </div> </div>
1	B	572	<div> <div>2%</div> <div> <div></div> <div>73%</div> <div>25%</div> <div>.</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9056 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 phosphoglucomutase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	571	Total	C	N	O	S	0	0	0
			4499	2863	771	852	13			
1	B	571	Total	C	N	O	S	0	0	0
			4499	2863	771	852	13			

- 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		
2	A	1	Total	Ca	0	0
			1	1		

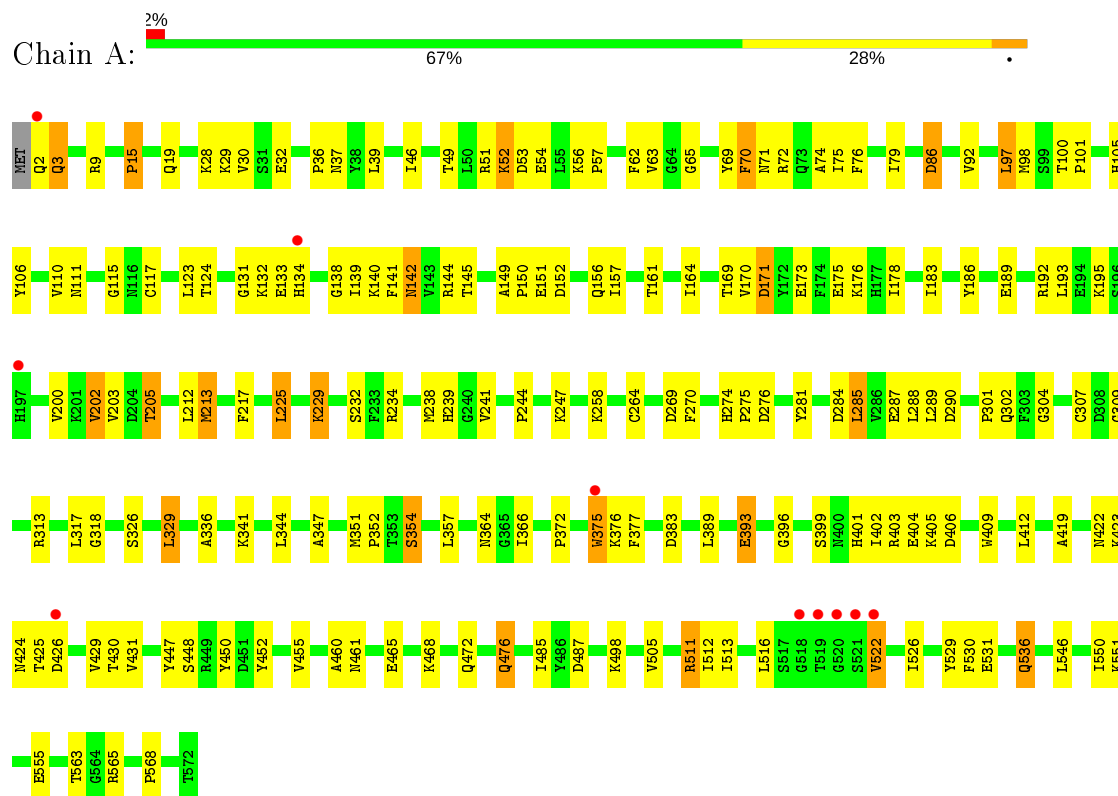
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	31	Total	O	0	0
			31	31		
3	B	25	Total	O	0	0
			25	25		

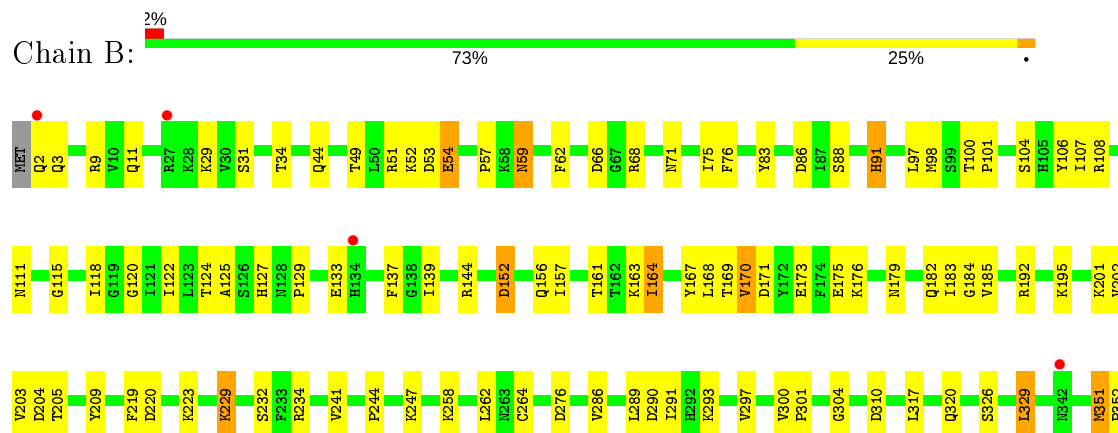
### 3 Residue-property plots

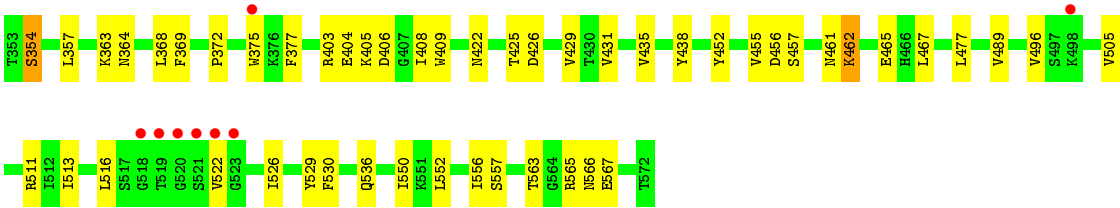
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: phosphoglucumutase 1



#### • Molecule 1: phosphoglucumutase 1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.90 Å 90.60 Å 212.00 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.40 20.03 – 2.43	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.40) 97.8 (20.03-2.43)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.96 (at 2.44 Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.233 , 0.284 0.226 , 0.285	Depositor DCC
$R_{free}$ test set	2344 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.7	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 38.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	9056	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.78 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.5225e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

<sup>2</sup> Theoretical 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: 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	0.39	0/4601	0.61	0/6219
1	B	0.39	0/4601	0.62	0/6219
All	All	0.39	0/9202	0.62	0/12438

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	4499	0	4393	158	0
1	B	4499	0	4393	125	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	31	0	0	4	0
3	B	25	0	0	3	0
All	All	9056	0	8786	280	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 16.

All (280) 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:2:GLN:HG3	1:A:3:GLN:H	1.20	1.05
1:A:258:LYS:HD2	1:A:258:LYS:H	1.27	0.97
1:A:468:LYS:HE2	1:A:485:ILE:HD11	1.48	0.94
1:A:289:LEU:HD21	1:A:304:GLY:HA3	1.48	0.92
1:B:455:VAL:HG13	1:B:563:THR:HG23	1.52	0.91
1:A:229:LYS:H	1:A:229:LYS:HD3	1.34	0.91
1:A:51:ARG:HD2	1:A:53:ASP:OD2	1.74	0.88
1:A:258:LYS:N	1:A:258:LYS:HD2	1.92	0.84
1:B:403:ARG:O	1:B:404:GLU:HG2	1.78	0.84
1:A:422:ASN:HD21	1:A:429:VAL:H	1.22	0.83
1:B:44:GLN:HE21	1:B:167:TYR:HB2	1.44	0.81
1:A:111:ASN:HD21	1:A:117:CYS:H	1.27	0.80
1:B:563:THR:HG22	1:B:565:ARG:HG2	1.64	0.79
1:A:169:THR:HG22	1:A:170:VAL:H	1.47	0.79
1:B:183:ILE:HA	1:B:202:VAL:HG23	1.64	0.78
1:B:127:HIS:HB2	1:B:276:ASP:HB2	1.64	0.78
1:A:563:THR:HG22	1:A:565:ARG:HG2	1.65	0.78
1:B:2:GLN:HG3	1:B:3:GLN:H	1.49	0.77
1:A:326:SER:HB3	1:A:354:SER:HB3	1.65	0.77
1:A:52:LYS:HE2	1:A:52:LYS:H	1.50	0.76
1:B:51:ARG:HD2	1:B:53:ASP:OD1	1.85	0.76
1:B:513:ILE:HB	1:B:529:TYR:HB2	1.68	0.76
1:B:169:THR:HG22	1:B:170:VAL:H	1.51	0.75
1:A:455:VAL:HG13	1:A:563:THR:HG23	1.69	0.73
1:A:2:GLN:HG3	1:A:3:GLN:N	2.00	0.73
1:A:472:GLN:O	1:A:476:GLN:HG2	1.88	0.73
1:A:318:GLY:HA3	1:A:431:VAL:HG21	1.70	0.72
1:A:326:SER:CB	1:A:354:SER:HB3	2.20	0.72
1:A:403:ARG:O	1:A:404:GLU:HG2	1.89	0.71
1:A:498:LYS:HB2	1:A:498:LYS:NZ	2.05	0.71
1:A:318:GLY:HA3	1:A:431:VAL:CG2	2.20	0.71
1:B:229:LYS:HD3	1:B:229:LYS:H	1.54	0.70
1:A:289:LEU:HD21	1:A:304:GLY:CA	2.20	0.70
1:B:137:PHE:HE2	1:B:139:ILE:HD11	1.55	0.70
1:A:563:THR:CG2	1:A:565:ARG:HG2	2.22	0.69
1:A:183:ILE:HA	1:A:202:VAL:HG22	1.74	0.69
1:A:258:LYS:CD	1:A:258:LYS:H	2.05	0.69
1:A:229:LYS:N	1:A:229:LYS:HD3	2.06	0.68
1:A:111:ASN:ND2	1:A:117:CYS:H	1.92	0.68
1:B:182:GLN:O	1:B:202:VAL:HG21	1.94	0.67
1:B:247:LYS:HE3	1:B:264:CYS:O	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:LYS:HE2	1:A:485:ILE:CD1	2.23	0.67
1:B:219:PHE:O	1:B:223:LYS:HD3	1.95	0.67
1:B:59:ASN:ND2	1:B:88:SER:H	1.92	0.66
1:B:258:LYS:N	1:B:258:LYS:HD2	2.10	0.66
1:B:422:ASN:HD21	1:B:429:VAL:H	1.42	0.65
1:A:173:GLU:OE1	1:A:176:LYS:HD3	1.97	0.65
1:A:336:ALA:HB1	1:A:344:LEU:HD13	1.79	0.65
1:A:178:ILE:HD13	1:A:200:VAL:HG11	1.78	0.65
1:A:422:ASN:ND2	1:A:429:VAL:H	1.92	0.65
1:B:91:HIS:HD2	1:B:106:TYR:OH	1.80	0.65
1:A:157:ILE:O	1:A:161:THR:HG23	1.96	0.64
1:A:289:LEU:HD22	1:A:317:LEU:HB2	1.79	0.63
1:A:460:ALA:HB1	1:A:516:LEU:HD21	1.79	0.63
1:B:326:SER:CB	1:B:354:SER:HB3	2.28	0.63
1:B:461:ASN:O	1:B:465:GLU:HG2	1.98	0.63
1:B:54:GLU:CD	3:B:701:HOH:O	2.38	0.62
1:A:111:ASN:HD21	1:A:117:CYS:N	1.96	0.62
1:B:489:VAL:HG22	1:B:496:VAL:HG22	1.81	0.62
1:B:2:GLN:HG3	1:B:3:GLN:N	2.14	0.62
1:B:351:MET:HE1	1:B:513:ILE:HD12	1.81	0.61
1:B:290:ASP:OD2	1:B:293:LYS:HA	2.01	0.61
1:A:512:ILE:C	1:A:513:ILE:HD12	2.20	0.61
1:B:326:SER:HB3	1:B:354:SER:HB3	1.82	0.61
1:A:422:ASN:HD21	1:A:429:VAL:N	1.98	0.61
1:A:461:ASN:O	1:A:465:GLU:HG2	2.01	0.61
1:A:124:THR:O	1:A:138:GLY:HA3	2.01	0.60
1:A:336:ALA:CB	1:A:344:LEU:HD13	2.31	0.60
1:B:462:LYS:HE3	1:B:462:LYS:N	2.16	0.60
1:A:51:ARG:NH2	3:B:701:HOH:O	2.29	0.60
1:A:375:TRP:NE1	1:A:405:LYS:HG3	2.17	0.59
1:B:71:ASN:O	1:B:75:ILE:HG13	2.02	0.59
1:B:375:TRP:CE2	1:B:405:LYS:HG2	2.37	0.59
1:A:270:PHE:CG	1:A:275:PRO:HG3	2.37	0.59
1:A:183:ILE:HA	1:A:202:VAL:CG2	2.32	0.59
1:A:151:GLU:HB2	1:A:376:LYS:HZ2	1.68	0.58
1:A:289:LEU:CD2	1:A:317:LEU:HB2	2.33	0.58
1:A:396:GLY:HA3	1:A:405:LYS:HD2	1.84	0.58
1:B:422:ASN:ND2	1:B:429:VAL:H	2.00	0.58
1:A:476:GLN:HE21	1:A:476:GLN:HA	1.68	0.58
1:A:372:PRO:HB2	1:A:377:PHE:CE2	2.38	0.58
1:A:329:LEU:HD22	1:A:357:LEU:HD13	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:LEU:HD22	1:B:357:LEU:HD13	1.86	0.58
1:B:68:ARG:CZ	1:B:125:ALA:HB3	2.34	0.58
1:A:513:ILE:HB	1:A:529:TYR:HB2	1.84	0.58
1:B:59:ASN:HD22	1:B:59:ASN:H	1.53	0.57
1:A:2:GLN:CG	1:A:3:GLN:H	2.05	0.57
1:B:54:GLU:CG	1:B:144:ARG:HH21	2.18	0.57
1:A:487:ASP:OD1	1:A:498:LYS:HG3	2.04	0.57
1:B:209:TYR:OH	1:B:408:ILE:HB	2.04	0.56
1:A:15:PRO:HG3	1:A:164:ILE:O	2.05	0.56
1:B:467:LEU:HD21	1:B:557:SER:HB3	1.87	0.56
1:A:52:LYS:CE	1:A:52:LYS:H	2.17	0.56
1:B:54:GLU:CD	1:B:144:ARG:HH21	2.08	0.56
1:B:258:LYS:H	1:B:258:LYS:HD2	1.70	0.56
1:A:522:VAL:HG12	1:A:522:VAL:O	2.06	0.55
1:B:54:GLU:HG3	1:B:144:ARG:NH2	2.21	0.55
1:B:229:LYS:HD3	1:B:229:LYS:N	2.22	0.55
1:B:329:LEU:CD2	1:B:357:LEU:HD13	2.36	0.55
1:A:46:ILE:HG12	1:A:157:ILE:HD13	1.89	0.55
1:B:44:GLN:NE2	1:B:168:LEU:H	2.06	0.54
1:A:105:HIS:CD2	1:A:212:LEU:HD22	2.43	0.54
1:B:100:THR:HB	1:B:101:PRO:HD3	1.90	0.54
1:A:36:PRO:O	1:A:37:ASN:HB2	2.08	0.54
1:B:452:TYR:HB2	1:B:526:ILE:HB	1.90	0.54
1:A:241:VAL:O	1:A:244:PRO:HD2	2.09	0.53
1:A:364:ASN:HD22	1:A:364:ASN:N	2.06	0.53
1:A:234:ARG:O	1:A:304:GLY:HA2	2.08	0.53
1:B:34:THR:HG22	1:B:34:THR:O	2.09	0.53
1:A:383:ASP:OD2	1:A:403:ARG:NH1	2.42	0.53
1:A:141:PHE:C	1:A:142:ASN:HD22	2.12	0.53
1:A:289:LEU:HD12	1:A:289:LEU:N	2.24	0.52
1:A:192:ARG:HB2	1:A:195:LYS:O	2.10	0.52
1:A:247:LYS:HE2	1:A:264:CYS:O	2.10	0.52
1:A:455:VAL:CG1	1:A:563:THR:HG23	2.37	0.52
1:B:406:ASP:HB3	1:B:409:TRP:HB3	1.92	0.52
1:A:229:LYS:H	1:A:229:LYS:CD	2.13	0.52
1:A:393:GLU:HG3	1:A:447:TYR:OH	2.10	0.52
1:A:203:VAL:HG23	3:A:710:HOH:O	2.10	0.52
1:A:151:GLU:HB2	1:A:376:LYS:NZ	2.26	0.51
1:B:203:VAL:HG22	1:B:204:ASP:N	2.25	0.51
1:B:229:LYS:H	1:B:229:LYS:CD	2.23	0.51
1:A:49:THR:HG23	1:A:156:GLN:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:LYS:NZ	1:A:468:LYS:HB3	2.24	0.51
1:A:63:VAL:O	1:A:92:VAL:HG23	2.11	0.51
1:B:59:ASN:HD21	1:B:88:SER:H	1.59	0.51
1:A:551:LYS:O	1:A:555:GLU:HG3	2.10	0.50
1:A:9:ARG:NH2	1:A:171:ASP:OD2	2.38	0.50
1:A:241:VAL:HG12	1:A:309:GLY:O	2.12	0.50
1:B:137:PHE:CE2	1:B:139:ILE:HD11	2.43	0.50
1:B:467:LEU:HD21	1:B:557:SER:CB	2.41	0.50
1:B:241:VAL:HG12	1:B:310:ASP:HA	1.92	0.50
1:B:462:LYS:HE3	1:B:462:LYS:CA	2.42	0.50
1:A:56:LYS:HD2	1:A:56:LYS:N	2.27	0.50
1:A:111:ASN:ND2	1:A:117:CYS:HB3	2.26	0.49
1:A:364:ASN:N	1:A:364:ASN:ND2	2.59	0.49
1:B:289:LEU:HD22	1:B:317:LEU:HB2	1.94	0.49
1:A:288:LEU:C	1:A:290:ASP:H	2.15	0.49
1:B:83:TYR:CD1	1:B:170:VAL:HG21	2.47	0.49
1:A:431:VAL:HG22	3:A:702:HOH:O	2.13	0.49
1:A:511:ARG:NH1	1:A:531:GLU:OE2	2.41	0.49
1:A:111:ASN:HA	1:A:115:GLY:HA2	1.94	0.49
1:A:452:TYR:HB2	1:A:526:ILE:HB	1.95	0.49
1:A:145:THR:HG23	1:B:53:ASP:HB2	1.95	0.49
1:A:351:MET:N	1:A:352:PRO:HD2	2.28	0.48
1:B:363:LYS:C	1:B:364:ASN:HD22	2.16	0.48
1:B:52:LYS:H	1:B:52:LYS:CE	2.26	0.48
1:A:213:MET:HG3	1:A:412:LEU:HD13	1.95	0.48
1:A:289:LEU:HD22	1:A:317:LEU:CB	2.42	0.48
1:A:139:ILE:O	1:A:139:ILE:HG23	2.13	0.48
1:B:563:THR:CG2	1:B:565:ARG:HG2	2.39	0.48
1:A:106:TYR:O	1:A:110:VAL:HG23	2.13	0.48
1:A:30:VAL:HG11	1:A:132:LYS:HA	1.96	0.48
1:A:213:MET:CE	1:A:217:PHE:HE2	2.27	0.48
1:A:498:LYS:HB2	1:A:498:LYS:HZ3	1.76	0.48
1:B:184:GLY:H	1:B:202:VAL:HG23	1.79	0.48
1:B:202:VAL:HG23	1:B:202:VAL:O	2.13	0.48
1:B:375:TRP:HZ3	1:B:404:GLU:OE2	1.97	0.48
1:B:375:TRP:CZ2	1:B:405:LYS:CG	2.97	0.48
1:B:422:ASN:HD21	1:B:429:VAL:N	2.10	0.48
1:A:399:SER:HB3	1:A:401:HIS:HD2	1.79	0.47
1:B:192:ARG:HB2	1:B:195:LYS:O	2.14	0.47
1:B:59:ASN:ND2	1:B:59:ASN:H	2.11	0.47
1:A:425:THR:HG22	1:A:426:ASP:N	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:ASN:N	1:B:59:ASN:ND2	2.63	0.47
1:B:173:GLU:HB3	1:B:176:LYS:HG2	1.97	0.47
1:B:241:VAL:O	1:B:244:PRO:HD2	2.13	0.47
1:B:552:LEU:HD11	1:B:556:ILE:HD11	1.97	0.47
1:A:100:THR:HB	1:A:101:PRO:HD3	1.96	0.47
1:A:375:TRP:CE2	1:A:405:LYS:HG3	2.50	0.47
1:A:318:GLY:CA	1:A:431:VAL:HG21	2.43	0.47
1:B:289:LEU:HD21	1:B:304:GLY:N	2.30	0.47
1:A:225:LEU:HG	1:A:419:ALA:HA	1.97	0.47
1:A:318:GLY:HA3	1:A:431:VAL:HG22	1.95	0.47
1:B:425:THR:HG22	1:B:426:ASP:N	2.29	0.47
1:A:49:THR:HG23	1:A:156:GLN:CB	2.45	0.47
1:B:522:VAL:HG12	1:B:522:VAL:O	2.15	0.47
1:A:75:ILE:O	1:A:79:ILE:HG13	2.15	0.46
1:B:375:TRP:CZ2	1:B:405:LYS:HG2	2.50	0.46
1:B:44:GLN:NE2	1:B:167:TYR:HB2	2.23	0.46
1:B:52:LYS:H	1:B:52:LYS:HE2	1.79	0.46
1:A:133:GLU:HG3	1:A:134:HIS:H	1.80	0.46
1:A:140:LYS:NZ	1:A:142:ASN:HD21	2.14	0.46
1:A:186:TYR:HE1	1:A:202:VAL:HG13	1.80	0.46
1:A:536:GLN:N	1:A:536:GLN:CD	2.69	0.46
1:A:448:SER:HB3	1:A:546:LEU:CD2	2.46	0.46
1:A:62:PHE:CZ	1:A:98:MET:HG2	2.50	0.46
1:B:122:ILE:HG22	1:B:124:THR:HG22	1.98	0.46
1:B:220:ASP:HA	1:B:223:LYS:HE2	1.98	0.46
1:B:291:ILE:HD11	1:B:317:LEU:HD22	1.97	0.46
1:A:285:LEU:HD22	1:A:289:LEU:HD13	1.98	0.46
1:A:289:LEU:CD2	1:A:304:GLY:HA3	2.34	0.45
1:B:431:VAL:O	1:B:435:VAL:HG23	2.17	0.45
1:A:530:PHE:CE1	1:A:550:ILE:HA	2.51	0.45
1:B:59:ASN:HD22	1:B:59:ASN:N	2.11	0.45
1:A:169:THR:HG22	1:A:170:VAL:N	2.22	0.45
1:B:372:PRO:HB2	1:B:377:PHE:CE2	2.51	0.45
1:A:57:PRO:HB3	1:B:111:ASN:HB3	1.98	0.45
1:A:274:HIS:O	1:A:276:ASP:N	2.48	0.45
1:A:288:LEU:HB3	1:A:289:LEU:HD12	1.98	0.45
1:A:28:LYS:HD2	1:A:32:GLU:OE1	2.17	0.45
1:A:54:GLU:CD	1:A:144:ARG:HH21	2.19	0.45
1:A:307:CYS:HA	1:A:313:ARG:O	2.17	0.45
1:B:185:VAL:HG22	1:B:201:LYS:HG3	1.98	0.45
1:A:173:GLU:OE1	1:A:176:LYS:CD	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:PHE:CE2	1:A:175:GLU:HA	2.51	0.44
1:B:375:TRP:CZ3	1:B:404:GLU:OE2	2.70	0.44
1:B:49:THR:HG23	1:B:156:GLN:HB2	1.99	0.44
1:A:513:ILE:N	1:A:513:ILE:HD12	2.33	0.44
1:A:341:LYS:H	1:A:341:LYS:HG3	1.57	0.44
1:B:435:VAL:O	1:B:438:TYR:HB3	2.18	0.44
1:A:238:MET:O	1:A:239:HIS:HB2	2.18	0.44
1:A:97:LEU:O	1:A:205:THR:HB	2.18	0.44
1:B:566:ASN:O	1:B:567:GLU:HG2	2.17	0.44
1:B:29:LYS:HG2	1:B:31:SER:H	1.83	0.43
1:A:30:VAL:HG21	1:A:131:GLY:O	2.18	0.43
1:A:536:GLN:N	1:A:536:GLN:OE1	2.45	0.43
1:B:76:PHE:CE1	1:B:175:GLU:HA	2.53	0.43
1:B:351:MET:HE2	1:B:513:ILE:HG13	2.00	0.43
1:B:234:ARG:HG3	1:B:262:LEU:HD11	2.01	0.43
1:A:269:ASP:O	1:A:270:PHE:HB2	2.18	0.43
1:A:396:GLY:CA	1:A:405:LYS:HD2	2.46	0.43
1:A:69:TYR:O	1:A:70:PHE:CB	2.67	0.43
1:A:111:ASN:HD21	1:A:117:CYS:HB3	1.83	0.43
1:A:406:ASP:HB3	1:A:409:TRP:HB3	2.00	0.43
1:A:213:MET:HE2	1:A:217:PHE:HE2	1.83	0.43
1:A:347:ALA:HA	1:A:389:LEU:O	2.18	0.43
1:A:65:GLY:HA2	1:A:123:LEU:O	2.19	0.43
1:B:104:SER:O	1:B:108:ARG:HG3	2.19	0.43
1:B:289:LEU:HD21	1:B:304:GLY:HA3	2.00	0.43
1:B:457:SER:HB2	1:B:522:VAL:C	2.39	0.42
1:A:149:ALA:HA	1:A:150:PRO:HD3	1.86	0.42
1:A:344:LEU:HD23	1:A:366:ILE:HG21	2.01	0.42
1:B:111:ASN:HA	1:B:115:GLY:HA2	2.01	0.42
1:B:289:LEU:HA	1:B:300:VAL:HG13	2.01	0.42
1:B:68:ARG:NH2	1:B:129:PRO:O	2.53	0.42
1:A:39:LEU:HD21	1:A:74:ALA:HA	2.01	0.42
1:A:54:GLU:CD	3:A:701:HOH:O	2.58	0.42
1:A:302:GLN:HE22	1:A:430:THR:HG22	1.85	0.42
1:B:66:ASP:OD2	1:B:68:ARG:HD2	2.20	0.42
1:A:133:GLU:HG3	1:A:134:HIS:N	2.35	0.42
1:B:351:MET:N	1:B:352:PRO:HD2	2.35	0.42
1:B:530:PHE:CG	1:B:550:ILE:HG12	2.55	0.42
1:B:258:LYS:H	1:B:258:LYS:CD	2.32	0.42
1:B:258:LYS:N	1:B:258:LYS:CD	2.81	0.42
1:B:455:VAL:HG12	1:B:456:ASP:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:ASP:HA	1:A:192:ARG:NH1	2.35	0.41
1:A:423:LYS:HG2	1:A:424:ASN:OD1	2.20	0.41
1:B:62:PHE:CZ	1:B:98:MET:HG2	2.55	0.41
1:A:111:ASN:HB3	1:B:57:PRO:HB3	2.02	0.41
1:A:536:GLN:H	1:A:536:GLN:CD	2.24	0.41
1:A:71:ASN:O	1:A:75:ILE:HG13	2.20	0.41
1:B:286:VAL:HG13	1:B:291:ILE:CG1	2.50	0.41
1:A:152:ASP:O	1:A:156:GLN:HG2	2.20	0.41
1:B:183:ILE:HA	1:B:202:VAL:CG2	2.44	0.41
1:B:290:ASP:O	1:B:320:GLN:HA	2.20	0.41
1:A:170:VAL:HG22	1:A:171:ASP:N	2.35	0.41
1:A:232:SER:OG	1:A:301:PRO:HA	2.20	0.41
1:A:52:LYS:HD3	3:A:725:HOH:O	2.19	0.41
1:B:52:LYS:H	1:B:52:LYS:NZ	2.19	0.41
1:A:19:GLN:HE21	1:A:161:THR:HB	1.86	0.41
1:B:232:SER:OG	1:B:301:PRO:HA	2.20	0.41
1:A:274:HIS:HB2	1:A:281:TYR:CD1	2.56	0.41
1:B:100:THR:N	1:B:101:PRO:CD	2.84	0.41
1:A:487:ASP:CG	1:A:498:LYS:HG3	2.41	0.41
1:B:49:THR:HG23	1:B:156:GLN:CB	2.51	0.41
1:B:157:ILE:O	1:B:161:THR:HG23	2.21	0.41
1:B:368:LEU:HD13	1:B:369:PHE:N	2.36	0.41
1:B:289:LEU:CD2	1:B:304:GLY:HA3	2.50	0.41
1:A:511:ARG:HG2	1:A:531:GLU:HB3	2.03	0.40
1:B:9:ARG:HH21	1:B:171:ASP:CG	2.24	0.40
1:A:288:LEU:C	1:A:290:ASP:N	2.74	0.40
1:A:450:TYR:CD1	1:A:568:PRO:HG3	2.56	0.40
1:B:118:ILE:HG22	1:B:144:ARG:NH2	2.35	0.40
1:B:169:THR:HG22	1:B:170:VAL:N	2.28	0.40
1:B:107:ILE:HD11	1:B:120:GLY:HA3	2.04	0.40
1:B:144:ARG:NH1	3:B:705:HOH:O	2.41	0.40
1:B:163:LYS:O	1:B:164:ILE:C	2.60	0.40
1:B:9:ARG:NH1	1:B:11:GLN:OE1	2.55	0.40
1:B:152:ASP:O	1:B:156:GLN:HG2	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	569/572 (100%)	523 (92%)	41 (7%)	5 (1%)	17	25
1	B	569/572 (100%)	529 (93%)	36 (6%)	4 (1%)	22	32
All	All	1138/1144 (100%)	1052 (92%)	77 (7%)	9 (1%)	19	29

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	164	ILE
1	B	477	LEU
1	A	193	LEU
1	A	70	PHE
1	B	133	GLU
1	A	15	PRO
1	A	402	ILE
1	B	297	VAL
1	A	522	VAL

### 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	480/481 (100%)	455 (95%)	25 (5%)	23	38
1	B	480/481 (100%)	462 (96%)	18 (4%)	33	51
All	All	960/962 (100%)	917 (96%)	43 (4%)	27	44

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	29	LYS
1	A	52	LYS
1	A	72	ARG
1	A	86	ASP
1	A	97	LEU
1	A	142	ASN
1	A	171	ASP
1	A	189	GLU
1	A	202	VAL
1	A	205	THR
1	A	213	MET
1	A	225	LEU
1	A	229	LYS
1	A	284	ASP
1	A	285	LEU
1	A	287	GLU
1	A	329	LEU
1	A	354	SER
1	A	375	TRP
1	A	393	GLU
1	A	476	GLN
1	A	505	VAL
1	A	511	ARG
1	A	536	GLN
1	B	54	GLU
1	B	59	ASN
1	B	86	ASP
1	B	91	HIS
1	B	97	LEU
1	B	152	ASP
1	B	170	VAL
1	B	179	ASN
1	B	205	THR
1	B	229	LYS
1	B	329	LEU
1	B	351	MET
1	B	354	SER
1	B	462	LYS
1	B	505	VAL
1	B	511	ARG
1	B	516	LEU

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Mol	Chain	Res	Type
1	B	536	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	37	ASN
1	A	94	GLN
1	A	105	HIS
1	A	111	ASN
1	A	142	ASN
1	A	214	GLN
1	A	263	ASN
1	A	302	GLN
1	A	320	GLN
1	A	335	ASN
1	A	337	ASN
1	A	364	ASN
1	A	401	HIS
1	A	422	ASN
1	A	437	GLN
1	A	440	GLN
1	A	476	GLN
1	A	500	GLN
1	A	548	ASN
1	B	19	GLN
1	B	37	ASN
1	B	44	GLN
1	B	59	ASN
1	B	85	ASN
1	B	91	HIS
1	B	94	GLN
1	B	142	ASN
1	B	179	ASN
1	B	211	GLN
1	B	214	GLN
1	B	239	HIS
1	B	263	ASN
1	B	283	HIS
1	B	314	ASN
1	B	320	GLN
1	B	335	ASN

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Mol	Chain	Res	Type
1	B	337	ASN
1	B	364	ASN
1	B	422	ASN
1	B	424	ASN
1	B	437	GLN
1	B	440	GLN
1	B	454	GLN
1	B	476	GLN
1	B	548	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 [i](#)

There are no carbohydrates 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

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	571/572 (99%)	-0.36	10 (1%) 68 66	6, 22, 50, 107	0
1	B	571/572 (99%)	-0.32	12 (2%) 63 61	6, 22, 50, 108	0
All	All	1142/1144 (99%)	-0.34	22 (1%) 66 64	6, 22, 50, 108	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	521	SER	7.4
1	B	522	VAL	7.3
1	A	519	THR	6.9
1	B	520	GLY	6.5
1	B	519	THR	6.1
1	B	523	GLY	5.1
1	A	521	SER	4.3
1	B	375	TRP	4.3
1	B	518	GLY	4.0
1	A	518	GLY	4.0
1	A	2	GLN	3.4
1	A	522	VAL	3.3
1	B	2	GLN	2.8
1	B	134	HIS	2.8
1	B	498	LYS	2.7
1	B	342	ASN	2.6
1	A	520	GLY	2.6
1	A	375	TRP	2.5
1	A	426	ASP	2.4
1	A	134	HIS	2.3
1	B	27	ARG	2.2
1	A	197	HIS	2.1

## 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<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	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CA	A	700	1/1	0.94	0.06	41,41,41,41	0
2	CA	B	700	1/1	0.98	0.07	39,39,39,39	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.