Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 06:34 PM GMT

PDB ID	:	1BG5
Title	:	CRYSTAL STRUCTURE OF THE ANKYRIN BINDING DOMAIN OF ALPHA-NA,K-ATPASE AS A FUSION PROTEIN WITH GLUTATHIONE S-TRANSFERASE
Authors	:	Zhang, Z.; Devarajan, P.; Morrow, J.S.
Deposited on	:	1998-06-05
Resolution	:	2.60 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

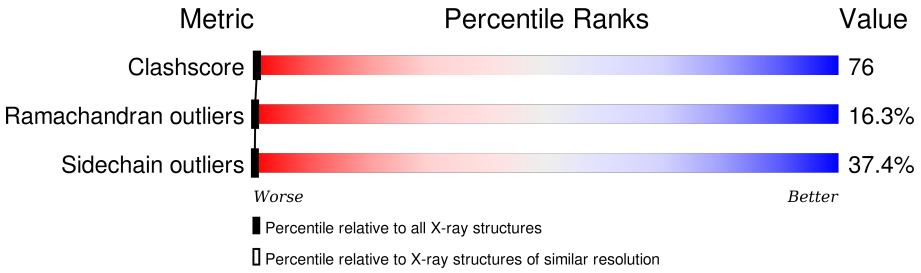
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.60 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))
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	254	16% 46% 32% 6%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2221 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 FUSION PROTEIN OF ALPHA-NA,K-ATPASE WITH GLUTATHIONE S-TRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	254	2074	1342	338	379	15	0	0	0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	147	147	147	0	0

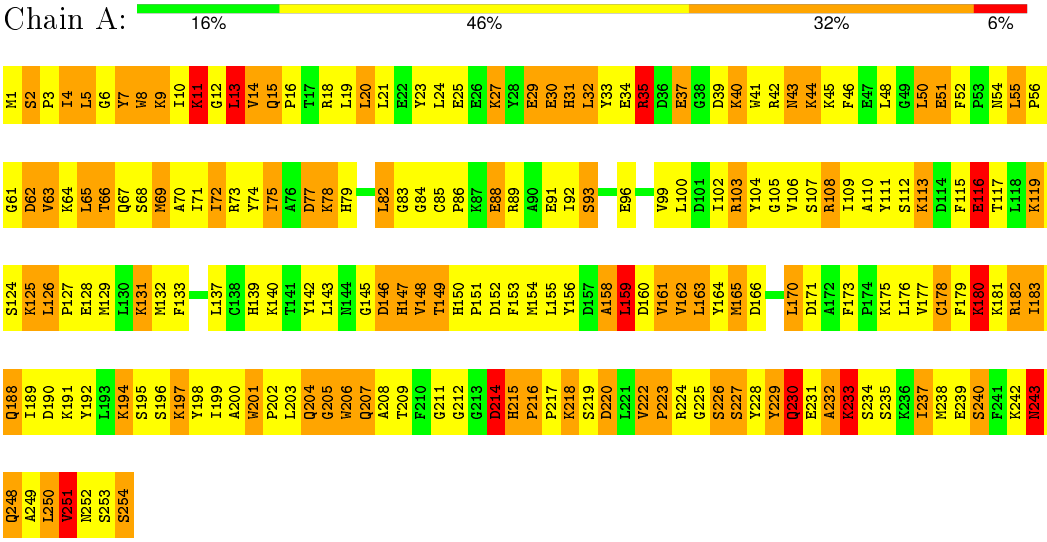
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

Note EDS was not executed.

• Molecule 1: FUSION PROTEIN OF ALPHA-NA,K-ATPASE WITH GLUTATHIONE S-TRANSFERASE

Chain A:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	92.17Å 92.17Å 57.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.60	Depositor
% Data completeness (in resolution range)	86.0 (8.00-2.60)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	0.10	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.193 , 0.359	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2221	wwPDB-VP
Average B, all atoms (Å^2)	10.0	wwPDB-VP

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	0.40	0/2128	0.68	0/2869

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	2074	0	2072	314	0
2	A	147	0	0	50	0
All	All	2221	0	2072	314	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 76.

All (314) 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:137:LEU:HD21	1:A:143:LEU:HD12	1.30	1.12
1:A:110:ALA:O	1:A:208:ALA:HB1	1.52	1.07
1:A:9:LYS:HE2	1:A:32:LEU:HD13	1.39	1.02
1:A:143:LEU:HB2	1:A:152:ASP:OD1	1.62	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:ARG:HE	1:A:82:LEU:HD21	1.24	0.97
1:A:4:ILE:HG13	1:A:59:ILE:HG23	1.47	0.95
1:A:43:ASN:HB2	1:A:44:LYS:HZ1	1.31	0.95
1:A:149:THR:HG22	2:A:354:HOH:O	1.68	0.93
1:A:149:THR:HB	1:A:151:PRO:HD2	1.53	0.91
1:A:148:VAL:HB	2:A:368:HOH:O	1.71	0.90
1:A:10:ILE:HG21	2:A:406:HOH:O	1.72	0.88
1:A:115:PHE:O	1:A:116:GLU:HB2	1.73	0.86
1:A:244:MET:O	1:A:245:VAL:HG12	1.75	0.85
1:A:2:SER:HB3	1:A:3:PRO:CD	2.05	0.85
1:A:58:TYR:OH	1:A:75:ILE:HD11	1.78	0.84
1:A:70:ALA:HB3	2:A:416:HOH:O	1.77	0.84
1:A:102:ILE:O	1:A:106:VAL:HG23	1.78	0.83
1:A:9:LYS:HG3	1:A:215:HIS:NE2	1.95	0.81
1:A:27:LYS:O	1:A:27:LYS:HD3	1.80	0.81
1:A:85:CYS:H	1:A:88:GLU:HB2	1.47	0.81
1:A:42:ARG:HG3	2:A:309:HOH:O	1.79	0.80
1:A:43:ASN:HB2	1:A:44:LYS:NZ	1.98	0.79
1:A:52:PHE:O	1:A:66:THR:HG21	1.83	0.78
1:A:100:LEU:HB3	1:A:104:TYR:CD1	2.20	0.77
1:A:73:ARG:NE	1:A:82:LEU:HD21	1.99	0.77
1:A:225:GLY:O	1:A:226:SER:HB2	1.85	0.76
1:A:50:LEU:HD11	1:A:57:TYR:HB2	1.67	0.76
1:A:99:VAL:HB	2:A:428:HOH:O	1.83	0.76
1:A:163:LEU:HD11	1:A:170:LEU:HB2	1.68	0.75
1:A:156:TYR:CG	1:A:183:ILE:HG21	2.22	0.74
1:A:72:ILE:HG23	2:A:333:HOH:O	1.87	0.74
1:A:233:LYS:HG3	1:A:234:SER:H	1.52	0.73
1:A:43:ASN:ND2	1:A:43:ASN:H	1.85	0.73
1:A:4:ILE:CG1	1:A:59:ILE:HG23	2.19	0.72
1:A:229:TYR:O	1:A:230:GLN:HB2	1.89	0.72
1:A:156:TYR:HA	1:A:159:LEU:HD11	1.72	0.71
1:A:1:MET:O	1:A:2:SER:HB2	1.90	0.71
1:A:103:ARG:HH21	1:A:161:VAL:HG11	1.55	0.71
1:A:7:TYR:HB2	1:A:56:PRO:HB3	1.73	0.70
1:A:9:LYS:HE3	1:A:34:GLU:OE2	1.92	0.70
1:A:2:SER:HB3	1:A:3:PRO:HD2	1.73	0.70
1:A:43:ASN:N	1:A:43:ASN:ND2	2.39	0.70
1:A:48:LEU:HD12	2:A:438:HOH:O	1.93	0.69
1:A:159:LEU:HA	1:A:162:VAL:HG23	1.72	0.69
1:A:13:LEU:HD22	2:A:308:HOH:O	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:SER:HB3	2:A:417:HOH:O	1.93	0.68
1:A:177:VAL:O	1:A:181:LYS:HG3	1.94	0.68
1:A:68:SER:O	1:A:72:ILE:HG22	1.94	0.68
1:A:126:LEU:N	1:A:127:PRO:CD	2.57	0.68
1:A:183:ILE:HA	2:A:427:HOH:O	1.93	0.68
1:A:126:LEU:H	1:A:127:PRO:CD	2.07	0.67
1:A:103:ARG:NH2	1:A:161:VAL:HG11	2.10	0.67
1:A:105:GLY:HA2	1:A:108:ARG:NE	2.09	0.67
1:A:245:VAL:N	1:A:246:PRO:HD3	2.10	0.67
1:A:202:PRO:HB3	1:A:212:GLY:O	1.94	0.67
1:A:204:GLN:NE2	1:A:204:GLN:HA	2.10	0.66
1:A:113:LYS:HD2	1:A:113:LYS:H	1.59	0.66
1:A:56:PRO:HD2	2:A:317:HOH:O	1.96	0.66
1:A:148:VAL:HG12	1:A:149:THR:N	2.12	0.65
1:A:103:ARG:HH21	1:A:161:VAL:HG21	1.62	0.65
1:A:126:LEU:O	1:A:129:MET:HG2	1.97	0.65
1:A:3:PRO:HD2	2:A:445:HOH:O	1.96	0.65
1:A:69:MET:HE1	1:A:154:MET:SD	2.36	0.65
1:A:131:LYS:HB2	1:A:173:PHE:CZ	2.32	0.64
1:A:192:TYR:O	1:A:195:SER:HB3	1.96	0.64
1:A:8:TRP:CD1	1:A:33:TYR:HB2	2.32	0.64
1:A:228:TYR:O	1:A:230:GLN:N	2.30	0.63
1:A:117:THR:HG22	2:A:335:HOH:O	1.97	0.63
1:A:215:HIS:HB3	1:A:216:PRO:HD2	1.79	0.63
1:A:62:ASP:O	1:A:63:VAL:HB	1.98	0.62
1:A:31:HIS:N	1:A:31:HIS:ND1	2.43	0.62
1:A:209:THR:HG23	2:A:327:HOH:O	1.98	0.62
1:A:214:ASP:OD1	1:A:217:PRO:HG3	2.00	0.62
1:A:248:GLN:HA	2:A:437:HOH:O	1.98	0.62
1:A:100:LEU:HB3	1:A:104:TYR:CE1	2.34	0.62
1:A:249:ALA:O	1:A:250:LEU:HB3	2.00	0.62
1:A:126:LEU:H	1:A:127:PRO:HD3	1.65	0.61
1:A:142:TYR:HB2	1:A:145:GLY:O	2.00	0.61
1:A:89:ARG:O	1:A:93:SER:HB2	2.00	0.61
1:A:43:ASN:CB	1:A:44:LYS:HZ1	2.08	0.61
1:A:230:GLN:HE22	1:A:232:ALA:HB3	1.64	0.61
1:A:159:LEU:HA	1:A:162:VAL:CG2	2.30	0.61
1:A:60:ASP:HA	2:A:395:HOH:O	1.99	0.60
1:A:5:LEU:O	1:A:57:TYR:O	2.19	0.60
1:A:111:TYR:HE1	1:A:205:GLY:HA3	1.65	0.60
1:A:7:TYR:CG	1:A:8:TRP:N	2.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:PHE:HB3	1:A:209:THR:HG21	1.84	0.60
1:A:11:LYS:HG2	1:A:12:GLY:N	2.16	0.60
1:A:240:SER:C	1:A:242:LYS:H	2.04	0.60
1:A:176:LEU:O	1:A:180:LYS:HB3	2.02	0.60
1:A:43:ASN:HD22	1:A:43:ASN:N	2.00	0.59
1:A:12:GLY:O	1:A:13:LEU:HB2	2.03	0.59
1:A:133:PHE:O	1:A:137:LEU:HG	2.03	0.59
1:A:245:VAL:HG13	1:A:245:VAL:O	2.03	0.59
1:A:105:GLY:HA2	1:A:108:ARG:HE	1.66	0.59
1:A:11:LYS:HG3	1:A:15:GLN:HG3	1.85	0.59
1:A:215:HIS:O	1:A:217:PRO:N	2.36	0.59
1:A:74:TYR:O	1:A:78:LYS:HG2	2.03	0.58
1:A:240:SER:C	1:A:242:LYS:N	2.55	0.58
1:A:14:VAL:HG13	1:A:14:VAL:O	2.02	0.58
1:A:173:PHE:O	1:A:177:VAL:HG23	2.04	0.58
1:A:230:GLN:NE2	1:A:232:ALA:HB3	2.18	0.58
1:A:11:LYS:NZ	1:A:199:ILE:O	2.37	0.58
1:A:251:VAL:HB	1:A:252:ASN:HD22	1.69	0.58
1:A:39:ASP:O	1:A:43:ASN:ND2	2.37	0.57
1:A:203:LEU:N	1:A:203:LEU:HD22	2.20	0.57
1:A:199:ILE:HB	2:A:336:HOH:O	2.04	0.57
1:A:30:GLU:O	1:A:30:GLU:HG3	2.04	0.57
1:A:55:LEU:HD23	1:A:57:TYR:HD2	1.70	0.57
1:A:115:PHE:O	1:A:116:GLU:CB	2.49	0.57
1:A:12:GLY:O	1:A:13:LEU:CB	2.53	0.57
1:A:129:MET:HA	1:A:132:MET:HG3	1.87	0.57
1:A:71:ILE:HG23	2:A:416:HOH:O	2.05	0.56
1:A:103:ARG:NH2	1:A:161:VAL:HG21	2.20	0.56
1:A:247:GLN:HE21	1:A:248:GLN:N	2.02	0.56
1:A:233:LYS:HB3	2:A:420:HOH:O	2.04	0.56
1:A:233:LYS:HG3	1:A:234:SER:N	2.21	0.56
1:A:6:GLY:HA2	1:A:31:HIS:ND1	2.20	0.56
1:A:201:TRP:O	1:A:215:HIS:HA	2.06	0.55
1:A:71:ILE:N	2:A:416:HOH:O	2.40	0.54
1:A:182:ARG:NH1	2:A:339:HOH:O	2.40	0.54
1:A:77:ASP:HB2	2:A:447:HOH:O	2.07	0.54
1:A:50:LEU:HB2	2:A:322:HOH:O	2.08	0.54
1:A:96:GLU:HA	2:A:428:HOH:O	2.06	0.54
1:A:102:ILE:HG23	1:A:126:LEU:CD1	2.38	0.54
1:A:4:ILE:HG22	1:A:30:GLU:HA	1.89	0.53
1:A:27:LYS:CD	1:A:27:LYS:H	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:TRP:CZ2	1:A:54:ASN:O	2.61	0.53
1:A:164:TYR:CD2	1:A:203:LEU:HD11	2.43	0.53
1:A:51:GLU:OE1	1:A:64:LYS:O	2.25	0.53
1:A:207:GLN:HE21	1:A:207:GLN:HA	1.74	0.53
1:A:11:LYS:HD2	1:A:203:LEU:HD13	1.91	0.53
1:A:113:LYS:CD	1:A:113:LYS:H	2.19	0.53
1:A:200:ALA:H	1:A:216:PRO:HD3	1.73	0.53
1:A:10:ILE:HD11	1:A:202:PRO:HG2	1.92	0.52
1:A:215:HIS:O	1:A:216:PRO:C	2.48	0.52
1:A:204:GLN:O	1:A:211:GLY:HA3	2.10	0.52
1:A:79:HIS:HE1	2:A:350:HOH:O	1.92	0.52
1:A:109:ILE:O	1:A:115:PHE:HB2	2.10	0.51
1:A:154:MET:HE2	2:A:428:HOH:O	2.10	0.51
1:A:207:GLN:NE2	1:A:207:GLN:HA	2.24	0.51
1:A:34:GLU:HB2	1:A:37:GLU:HB2	1.93	0.51
1:A:35:ARG:HG2	2:A:332:HOH:O	2.10	0.51
1:A:43:ASN:CB	1:A:44:LYS:NZ	2.72	0.51
1:A:18:ARG:HA	1:A:21:LEU:HD12	1.92	0.51
1:A:13:LEU:CD2	1:A:204:GLN:HE22	2.23	0.51
1:A:4:ILE:HG13	1:A:59:ILE:CG2	2.30	0.51
1:A:34:GLU:HB2	1:A:37:GLU:CB	2.41	0.51
1:A:9:LYS:CG	1:A:215:HIS:NE2	2.71	0.51
1:A:178:CYS:O	1:A:182:ARG:N	2.41	0.51
1:A:187:PRO:HB2	2:A:421:HOH:O	2.10	0.51
1:A:129:MET:HB3	2:A:362:HOH:O	2.11	0.51
1:A:37:GLU:C	1:A:39:ASP:H	2.13	0.51
1:A:131:LYS:HB2	1:A:173:PHE:CE1	2.46	0.51
1:A:239:GLU:HG2	2:A:352:HOH:O	2.11	0.51
1:A:148:VAL:CG1	1:A:149:THR:N	2.74	0.50
1:A:2:SER:HB3	1:A:3:PRO:HD3	1.91	0.50
1:A:180:LYS:HG3	1:A:180:LYS:O	2.10	0.50
1:A:215:HIS:CB	1:A:216:PRO:HD2	2.42	0.50
1:A:92:ILE:HG22	1:A:92:ILE:O	2.12	0.50
1:A:92:ILE:HG21	2:A:354:HOH:O	2.11	0.50
1:A:115:PHE:CD1	1:A:116:GLU:N	2.80	0.50
1:A:58:TYR:CZ	1:A:75:ILE:HD11	2.46	0.50
1:A:164:TYR:CE2	1:A:203:LEU:HD11	2.47	0.49
1:A:91:GLU:C	1:A:93:SER:H	2.15	0.49
1:A:99:VAL:HG21	1:A:155:LEU:HB2	1.94	0.49
1:A:92:ILE:O	1:A:96:GLU:HB2	2.11	0.49
1:A:23:TYR:HD1	1:A:24:LEU:HD12	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:ILE:HD12	1:A:189:ILE:HG12	1.93	0.49
1:A:11:LYS:HZ1	1:A:200:ALA:HA	1.78	0.49
1:A:233:LYS:O	1:A:235:SER:N	2.39	0.49
1:A:184:GLU:HB2	2:A:432:HOH:O	2.11	0.49
1:A:137:LEU:HD21	1:A:143:LEU:CD1	2.22	0.49
1:A:137:LEU:CD2	1:A:143:LEU:HD12	2.22	0.49
1:A:115:PHE:CZ	1:A:119:LYS:HB3	2.48	0.49
1:A:74:TYR:HA	2:A:447:HOH:O	2.12	0.49
1:A:85:CYS:O	1:A:88:GLU:HB2	2.12	0.49
1:A:106:VAL:HG11	1:A:161:VAL:HG12	1.94	0.49
1:A:7:TYR:O	1:A:55:LEU:HD13	2.12	0.49
1:A:45:LYS:HD3	1:A:46:PHE:CE1	2.48	0.49
1:A:61:GLY:C	1:A:63:VAL:H	2.16	0.49
1:A:161:VAL:O	1:A:161:VAL:HG12	2.12	0.48
1:A:182:ARG:CZ	2:A:339:HOH:O	2.60	0.48
1:A:44:LYS:NZ	1:A:44:LYS:N	2.62	0.48
1:A:155:LEU:O	1:A:158:ALA:HB3	2.13	0.48
1:A:20:LEU:O	1:A:20:LEU:HD22	2.13	0.48
1:A:55:LEU:HD23	1:A:57:TYR:CD2	2.48	0.48
1:A:233:LYS:CG	1:A:234:SER:H	2.23	0.48
1:A:37:GLU:O	1:A:40:LYS:HB3	2.13	0.48
1:A:24:LEU:HD23	1:A:79:HIS:ND1	2.29	0.48
1:A:190:ASP:O	1:A:194:LYS:HG3	2.13	0.48
1:A:222:VAL:HG23	1:A:223:PRO:N	2.29	0.48
1:A:29:GLU:O	1:A:30:GLU:HB3	2.13	0.47
1:A:83:GLY:HA3	1:A:89:ARG:HB3	1.95	0.47
1:A:126:LEU:O	1:A:126:LEU:HG	2.15	0.47
1:A:245:VAL:N	1:A:246:PRO:CD	2.76	0.47
1:A:106:VAL:HG21	2:A:312:HOH:O	2.13	0.47
1:A:131:LYS:HG2	1:A:131:LYS:O	2.15	0.47
1:A:10:ILE:CD1	1:A:202:PRO:HG2	2.44	0.47
1:A:156:TYR:O	1:A:159:LEU:HD12	2.14	0.47
1:A:194:LYS:HE3	2:A:405:HOH:O	2.14	0.46
1:A:16:PRO:HB3	1:A:154:MET:HA	1.97	0.46
1:A:35:ARG:HB3	2:A:332:HOH:O	2.14	0.46
1:A:126:LEU:C	1:A:128:GLU:H	2.18	0.46
1:A:196:SER:O	1:A:197:LYS:NZ	2.48	0.46
1:A:148:VAL:HG12	1:A:149:THR:H	1.79	0.46
1:A:178:CYS:HA	1:A:181:LYS:HE2	1.97	0.46
1:A:200:ALA:O	1:A:201:TRP:C	2.53	0.46
1:A:11:LYS:CG	1:A:15:GLN:HG3	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:ALA:O	1:A:162:VAL:HG22	2.16	0.46
1:A:207:GLN:CA	1:A:207:GLN:NE2	2.77	0.46
1:A:11:LYS:CG	1:A:12:GLY:N	2.77	0.46
1:A:59:ILE:HG12	1:A:59:ILE:O	2.14	0.46
1:A:179:PHE:C	1:A:181:LYS:N	2.67	0.46
1:A:249:ALA:O	1:A:250:LEU:CB	2.63	0.46
1:A:150:HIS:N	1:A:151:PRO:CD	2.79	0.46
1:A:15:GLN:N	1:A:16:PRO:CD	2.79	0.46
1:A:207:GLN:HB2	2:A:399:HOH:O	2.15	0.46
1:A:13:LEU:HD13	2:A:446:HOH:O	2.15	0.45
1:A:122:PHE:CD1	1:A:122:PHE:C	2.90	0.45
1:A:146:ASP:C	1:A:146:ASP:OD1	2.53	0.45
1:A:70:ALA:O	1:A:73:ARG:HB3	2.17	0.45
1:A:111:TYR:CE1	1:A:205:GLY:HA3	2.50	0.45
1:A:148:VAL:CG1	1:A:149:THR:H	2.30	0.45
1:A:253:SER:OG	1:A:254:SER:N	2.47	0.45
1:A:106:VAL:HG21	1:A:162:VAL:HG13	1.99	0.45
1:A:181:LYS:C	1:A:183:ILE:H	2.20	0.45
1:A:69:MET:HE2	1:A:96:GLU:HG2	1.97	0.45
1:A:215:HIS:O	1:A:217:PRO:CD	2.65	0.45
1:A:30:GLU:OE2	1:A:32:LEU:HD23	2.16	0.45
1:A:33:TYR:CD2	1:A:40:LYS:HD3	2.51	0.45
1:A:246:PRO:HG3	2:A:442:HOH:O	2.17	0.45
1:A:179:PHE:O	1:A:181:LYS:N	2.50	0.45
1:A:18:ARG:NH2	2:A:444:HOH:O	2.49	0.45
1:A:117:THR:O	1:A:120:VAL:O	2.35	0.45
1:A:42:ARG:NH2	2:A:373:HOH:O	2.48	0.44
1:A:215:HIS:C	1:A:217:PRO:HD3	2.38	0.44
1:A:91:GLU:C	1:A:93:SER:N	2.69	0.44
1:A:131:LYS:HB3	1:A:131:LYS:HE3	1.55	0.44
1:A:244:MET:O	1:A:245:VAL:CG1	2.57	0.44
1:A:231:GLU:O	1:A:232:ALA:HB2	2.18	0.44
1:A:7:TYR:CD2	1:A:8:TRP:N	2.84	0.44
1:A:24:LEU:HD23	1:A:79:HIS:CE1	2.52	0.44
1:A:2:SER:CB	1:A:3:PRO:CD	2.86	0.44
1:A:238:MET:HG2	1:A:243:ASN:HB3	1.99	0.44
1:A:126:LEU:C	1:A:128:GLU:N	2.70	0.44
1:A:121:ASP:O	1:A:125:LYS:HD2	2.18	0.44
1:A:116:GLU:OE1	1:A:116:GLU:HA	2.17	0.44
1:A:119:LYS:O	1:A:123:LEU:HB2	2.18	0.43
1:A:33:TYR:CE2	1:A:40:LYS:HD3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:GLN:HG2	1:A:188:GLN:H	1.41	0.43
1:A:222:VAL:HG23	1:A:223:PRO:HD2	2.00	0.43
1:A:119:LYS:HE3	2:A:358:HOH:O	2.19	0.43
1:A:4:ILE:HA	1:A:29:GLU:O	2.19	0.43
1:A:178:CYS:SG	1:A:182:ARG:NH1	2.92	0.43
1:A:208:ALA:HB3	1:A:211:GLY:HA3	2.01	0.43
1:A:252:ASN:ND2	2:A:431:HOH:O	2.52	0.43
1:A:159:LEU:H	1:A:159:LEU:HG	1.56	0.43
1:A:119:LYS:HG3	1:A:120:VAL:N	2.34	0.43
1:A:119:LYS:HG3	1:A:120:VAL:H	1.83	0.42
1:A:92:ILE:HG12	1:A:149:THR:HG21	1.99	0.42
1:A:250:LEU:O	1:A:251:VAL:O	2.38	0.42
1:A:103:ARG:HH21	1:A:161:VAL:CG1	2.28	0.42
1:A:6:GLY:O	1:A:7:TYR:C	2.57	0.42
1:A:41:TRP:O	1:A:42:ARG:C	2.57	0.42
1:A:11:LYS:NZ	1:A:200:ALA:HA	2.33	0.42
1:A:39:ASP:OD1	1:A:39:ASP:O	2.37	0.42
1:A:85:CYS:O	1:A:88:GLU:N	2.31	0.42
1:A:198:TYR:N	2:A:417:HOH:O	2.53	0.42
1:A:79:HIS:CE1	2:A:350:HOH:O	2.70	0.42
1:A:7:TYR:HA	1:A:56:PRO:HA	2.00	0.42
1:A:82:LEU:O	1:A:92:ILE:HD12	2.20	0.42
1:A:228:TYR:C	1:A:230:GLN:N	2.72	0.42
1:A:110:ALA:HB3	1:A:204:GLN:HG2	2.02	0.42
1:A:159:LEU:HD13	1:A:180:LYS:HB2	2.01	0.42
1:A:147:HIS:HA	2:A:394:HOH:O	2.20	0.42
1:A:126:LEU:HA	1:A:129:MET:CE	2.49	0.41
1:A:226:SER:O	1:A:227:SER:C	2.58	0.41
1:A:238:MET:N	2:A:338:HOH:O	2.52	0.41
1:A:123:LEU:HD21	1:A:165:MET:HG2	2.02	0.41
1:A:72:ILE:HD11	1:A:150:HIS:HB2	2.01	0.41
1:A:78:LYS:HG2	1:A:78:LYS:H	1.64	0.41
1:A:187:PRO:HA	1:A:190:ASP:HB3	2.03	0.41
1:A:100:LEU:HD22	1:A:104:TYR:HE1	1.86	0.41
1:A:171:ASP:C	1:A:173:PHE:H	2.24	0.41
1:A:201:TRP:CD2	1:A:203:LEU:HD21	2.56	0.41
1:A:9:LYS:HB2	1:A:33:TYR:O	2.20	0.41
1:A:14:VAL:HG21	1:A:56:PRO:HB3	2.02	0.41
1:A:89:ARG:HG2	1:A:89:ARG:H	1.55	0.41
1:A:100:LEU:O	1:A:104:TYR:HB2	2.20	0.41
1:A:13:LEU:HD21	1:A:204:GLN:HE22	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:LEU:CD2	1:A:57:TYR:CD2	3.04	0.41
1:A:85:CYS:O	1:A:86:PRO:C	2.59	0.41
1:A:179:PHE:C	1:A:181:LYS:H	2.23	0.41
1:A:246:PRO:O	1:A:247:GLN:CB	2.68	0.41
1:A:228:TYR:C	1:A:230:GLN:H	2.23	0.41
1:A:18:ARG:O	1:A:21:LEU:HB2	2.21	0.41
1:A:204:GLN:HE21	1:A:204:GLN:HA	1.84	0.41
1:A:113:LYS:NZ	2:A:410:HOH:O	2.54	0.41
1:A:20:LEU:HD23	1:A:153:PHE:CE2	2.55	0.41
1:A:165:MET:HE2	1:A:165:MET:HB2	1.89	0.40
1:A:23:TYR:CD1	1:A:23:TYR:C	2.94	0.40
1:A:192:TYR:CE2	1:A:198:TYR:HD1	2.39	0.40
1:A:104:TYR:C	1:A:106:VAL:N	2.74	0.40
1:A:179:PHE:O	1:A:182:ARG:N	2.54	0.40
1:A:77:ASP:OD1	1:A:82:LEU:HG	2.20	0.40
1:A:250:LEU:HD13	1:A:250:LEU:C	2.42	0.40
1:A:43:ASN:C	1:A:44:LYS:NZ	2.74	0.40
1:A:240:SER:HB2	1:A:243:ASN:HB2	2.02	0.40
1:A:65:LEU:HD22	1:A:65:LEU:HA	1.79	0.40
1:A:162:VAL:O	1:A:165:MET:HB3	2.21	0.40
1:A:10:ILE:HD11	1:A:206:TRP:CE2	2.57	0.40
1:A:66:THR:O	1:A:67:GLN:HB2	2.21	0.40
1:A:232:ALA:O	1:A:233:LYS:O	2.40	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	252/254 (99%)	152 (60%)	59 (23%)	41 (16%)	0 0

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	11	LYS
1	A	35	ARG
1	A	63	VAL
1	A	121	ASP
1	A	148	VAL
1	A	160	ASP
1	A	214	ASP
1	A	216	PRO
1	A	218	LYS
1	A	229	TYR
1	A	230	GLN
1	A	233	LYS
1	A	245	VAL
1	A	246	PRO
1	A	251	VAL
1	A	7	TYR
1	A	13	LEU
1	A	59	ILE
1	A	116	GLU
1	A	219	SER
1	A	237	ILE
1	A	125	LYS
1	A	146	ASP
1	A	161	VAL
1	A	205	GLY
1	A	220	ASP
1	A	223	PRO
1	A	226	SER
1	A	232	ALA
1	A	180	LYS
1	A	247	GLN
1	A	30	GLU
1	A	207	GLN
1	A	227	SER
1	A	243	ASN
1	A	250	LEU
1	A	158	ALA
1	A	159	LEU
1	A	215	HIS
1	A	84	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	227/227 (100%)	142 (63%)	85 (37%)	0 0

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	5	LEU
1	A	8	TRP
1	A	9	LYS
1	A	11	LYS
1	A	13	LEU
1	A	14	VAL
1	A	15	GLN
1	A	19	LEU
1	A	20	LEU
1	A	25	GLU
1	A	27	LYS
1	A	29	GLU
1	A	31	HIS
1	A	32	LEU
1	A	35	ARG
1	A	37	GLU
1	A	40	LYS
1	A	43	ASN
1	A	44	LYS
1	A	50	LEU
1	A	51	GLU
1	A	55	LEU
1	A	62	ASP
1	A	65	LEU
1	A	66	THR
1	A	69	MET
1	A	72	ILE
1	A	75	ILE
1	A	77	ASP

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Mol	Chain	Res	Type
1	A	78	LYS
1	A	82	LEU
1	A	88	GLU
1	A	93	SER
1	A	103	ARG
1	A	107	SER
1	A	108	ARG
1	A	112	SER
1	A	113	LYS
1	A	116	GLU
1	A	119	LYS
1	A	121	ASP
1	A	122	PHE
1	A	123	LEU
1	A	124	SER
1	A	126	LEU
1	A	131	LYS
1	A	139	HIS
1	A	140	LYS
1	A	147	HIS
1	A	149	THR
1	A	159	LEU
1	A	162	VAL
1	A	163	LEU
1	A	165	MET
1	A	166	ASP
1	A	170	LEU
1	A	175	LYS
1	A	178	CYS
1	A	180	LYS
1	A	182	ARG
1	A	183	ILE
1	A	186	ILE
1	A	188	GLN
1	A	191	LYS
1	A	194	LYS
1	A	197	LYS
1	A	201	TRP
1	A	204	GLN
1	A	206	TRP
1	A	214	ASP
1	A	218	LYS

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Mol	Chain	Res	Type
1	A	220	ASP
1	A	222	VAL
1	A	224	ARG
1	A	230	GLN
1	A	233	LYS
1	A	237	ILE
1	A	240	SER
1	A	243	ASN
1	A	245	VAL
1	A	247	GLN
1	A	248	GLN
1	A	251	VAL
1	A	254	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
1	A	79	HIS
1	A	204	GLN
1	A	207	GLN
1	A	247	GLN
1	A	252	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)

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

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.