Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 06:36 PM GMT

PDB ID	:	1BO1
Title	:	PHOSPHATIDYLINOSITOL PHOSPHATE KINASE TYPE II BETA
Authors	:	Rao, V.D.; Misra, S.; Boronenkov, I.V.; Anderson, R.A.; Hurley, J.H.
Deposited on	:	1998-08-02
Resolution	:	3.00 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:

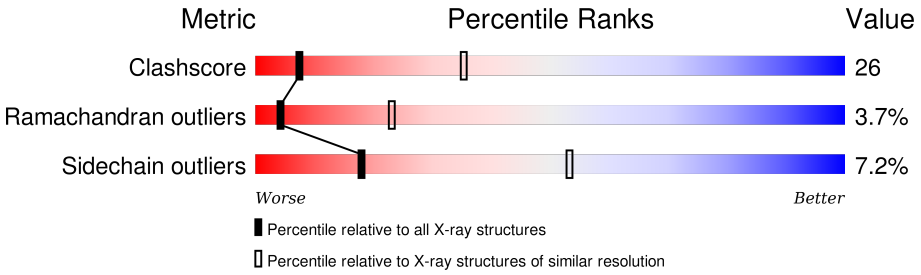
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)

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	416	40% 33% 5% 22%
1	B	416	36% 34% 6% 24%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5301 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 PROTEIN (PHOSPHATIDYLINOSITOL PHOSPHATE KINASE IIBETA).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	S	0	0	0
			2674	1695	454	511	14			
1	B	318	Total	C	N	O	S	0	0	0
			2608	1651	448	494	15			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	13	Total	O	0	0
			13	13		
2	B	6	Total	O	0	0
			6	6		

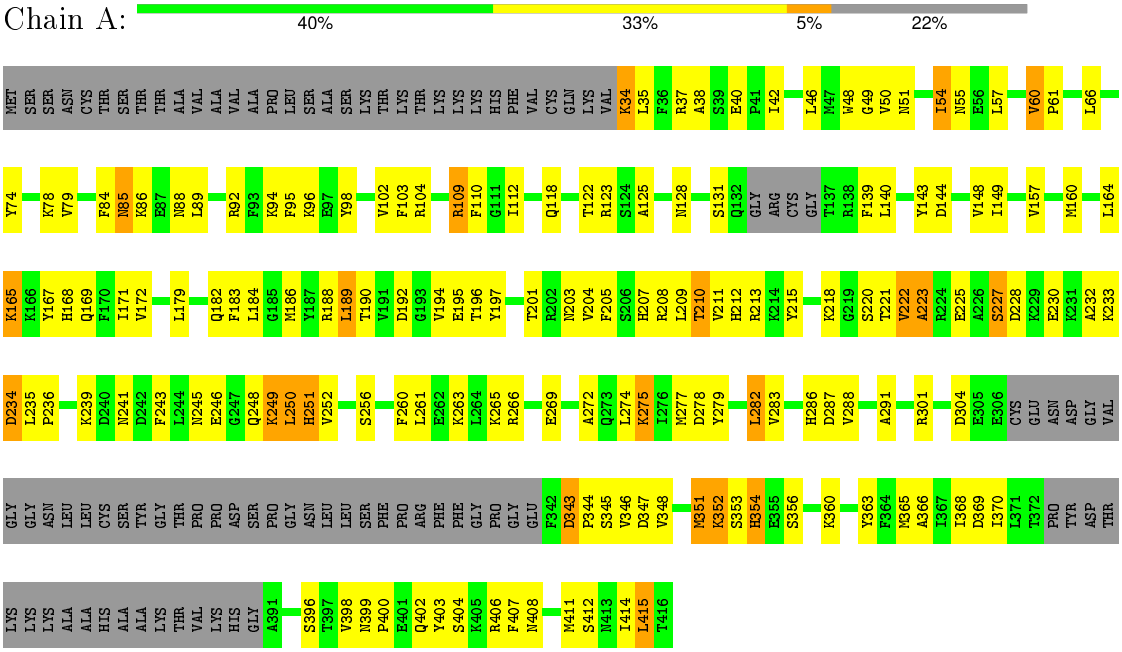
3 Residue-property plots (i)

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.

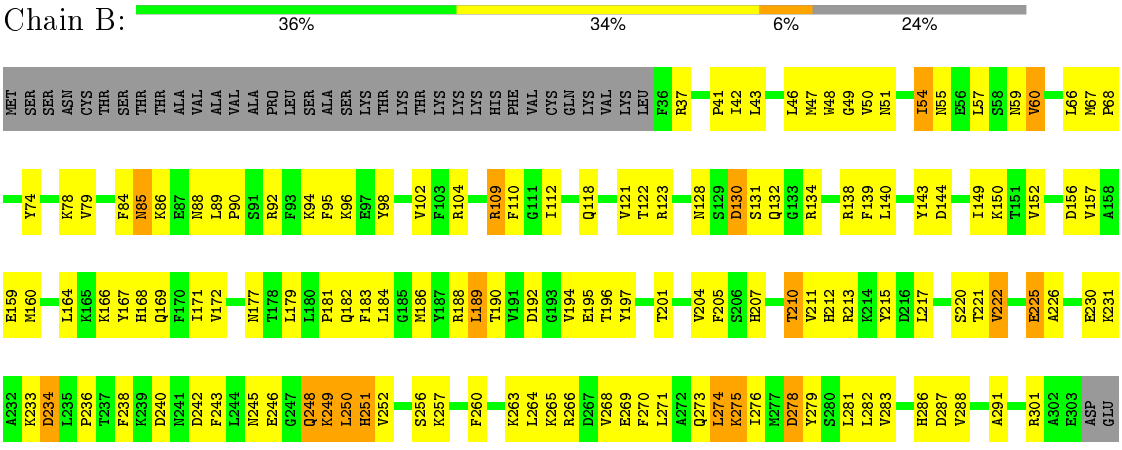
- Molecule 1: PROTEIN (PHOSPHATIDYLINOSITOL PHOSPHATE KINASE IIBETA)

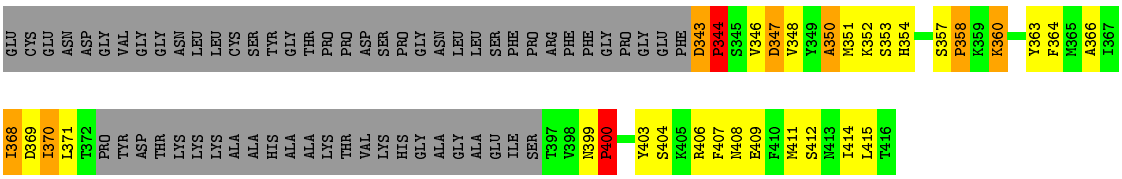
Chain A:



- Molecule 1: PROTEIN (PHOSPHATIDYLINOSITOL PHOSPHATE KINASE IIBETA)

Chain B:




GLU CYS GLU ASN ASP GLY VAL GLY GLY ASN LEU LEU CYS SER TYR GLY THR PRO PRO ASP SER PRO GLY ASN LEU LEU SER PHE PRO ARG PHE PHE GLY PRO GLY GLU PHE D343 P344 S345 V346 D347 V348 Y349 A350 M351 K352 S353 H354 S357 P358 K359 K360 Y363 F364 H365 A366 I367
I368 D369 I370 L371 T372 PRO TYR ASP THR LYS LYS LYS ALA ALA HIS ALA ALA LYS THR VAL LYS HIS GLY ALA GLY ALA GLU ILE SER T397 V398 N399 P400 Y403 S404 K405 R406 F407 N408 E409 F410 M411 S412 M413 I414 L415 T416

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	109.92Å 182.40Å 106.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 3.00	Depositor
% Data completeness (in resolution range)	94.9 (6.00-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.229 , 0.299	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5301	wwPDB-VP
Average B, all atoms (Å^2)	48.0	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	0.44	0/2726	0.68	1/3668 (0.0%)
1	B	0.43	0/2660	0.70	1/3580 (0.0%)
All	All	0.44	0/5386	0.69	2/7248 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	368	ILE	N-CA-C	6.23	127.81	111.00
1	A	368	ILE	N-CA-C	5.41	125.62	111.00

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	2674	0	2631	126	0
1	B	2608	0	2572	144	0
2	A	13	0	0	0	0
2	B	6	0	0	1	0
All	All	5301	0	5203	268	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 26.

All (268) 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:B:212:HIS:HD2	1:B:287:ASP:H	1.20	0.90
1:B:157:VAL:HG21	1:B:197:TYR:CD2	2.07	0.90
1:A:223:ALA:H	1:A:225:GLU:HG2	1.39	0.87
1:A:215:TYR:HB2	1:A:283:VAL:HB	1.60	0.83
1:B:215:TYR:HB2	1:B:283:VAL:HB	1.63	0.80
1:B:249:LYS:HB3	1:B:251:HIS:CE1	2.16	0.80
1:A:157:VAL:HG21	1:A:197:TYR:CD2	2.17	0.80
1:A:249:LYS:HB3	1:A:251:HIS:CE1	2.18	0.79
1:A:157:VAL:HA	1:A:186:MET:HE1	1.63	0.78
1:B:98:TYR:HD1	1:B:186:MET:HG2	1.49	0.78
1:A:98:TYR:HD1	1:A:186:MET:HG2	1.50	0.77
1:B:157:VAL:HA	1:B:186:MET:HE1	1.67	0.77
1:A:183:PHE:HA	1:A:201:THR:HG22	1.67	0.77
1:B:109:ARG:HH11	1:B:172:VAL:HA	1.48	0.76
1:B:183:PHE:HA	1:B:201:THR:HG22	1.68	0.76
1:A:343:ASP:HB2	1:A:344:PRO:HD3	1.68	0.76
1:A:66:LEU:HD13	1:A:102:VAL:HG22	1.66	0.75
1:B:243:PHE:HZ	1:B:414:ILE:HG23	1.49	0.74
1:A:109:ARG:NH1	1:A:172:VAL:HG22	2.02	0.74
1:B:131:SER:HB3	1:B:138:ARG:HA	1.68	0.74
1:A:352:LYS:HD3	1:A:366:ALA:HB2	1.70	0.72
1:B:252:VAL:HG12	1:B:256:SER:HB3	1.71	0.72
1:B:66:LEU:HD13	1:B:102:VAL:HG22	1.71	0.72
1:B:220:SER:HA	1:B:406:ARG:CZ	2.20	0.71
1:B:51:ASN:HB2	1:B:122:THR:HG21	1.72	0.71
1:B:260:PHE:CD2	1:B:415:LEU:HD11	2.26	0.71
1:A:51:ASN:HB2	1:A:122:THR:HG21	1.73	0.71
1:A:34:LYS:HA	1:B:59:ASN:HA	1.73	0.70
1:A:261:LEU:HD21	1:A:412:SER:HA	1.73	0.70
1:B:212:HIS:CD2	1:B:287:ASP:H	2.06	0.70
1:A:183:PHE:HZ	1:A:370:ILE:HG21	1.57	0.70
1:A:407:PHE:O	1:A:411:MET:HG2	1.91	0.70
1:B:268:VAL:HG13	1:B:279:TYR:OH	1.91	0.70
1:A:128:ASN:HA	1:A:140:LEU:HD23	1.72	0.69
1:A:54:ILE:HG21	1:A:118:GLN:HB2	1.74	0.69
1:A:37:ARG:HB2	1:A:88:ASN:HB3	1.75	0.69
1:A:415:LEU:HD23	1:A:415:LEU:H	1.57	0.69
1:A:123:ARG:HD3	1:A:143:TYR:OH	1.92	0.68
1:B:400:PRO:HA	1:B:403:TYR:HB2	1.76	0.67
1:B:407:PHE:O	1:B:411:MET:HG2	1.94	0.67
1:B:243:PHE:CD1	1:B:248:GLN:HG3	2.29	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:VAL:HG21	1:B:197:TYR:HD2	1.60	0.66
1:B:222:VAL:HA	1:B:225:GLU:OE1	1.95	0.66
1:B:98:TYR:CD1	1:B:186:MET:HG2	2.31	0.65
1:B:37:ARG:HB2	1:B:88:ASN:HB3	1.77	0.65
1:A:98:TYR:CD1	1:A:186:MET:HG2	2.32	0.65
1:B:46:LEU:HD21	1:B:149:ILE:HD13	1.78	0.65
1:B:54:ILE:HG21	1:B:118:GLN:HB2	1.78	0.65
1:A:212:HIS:HD2	1:A:287:ASP:H	1.44	0.64
1:A:46:LEU:HD21	1:A:149:ILE:HD13	1.81	0.62
1:A:275:LYS:HG2	1:A:275:LYS:O	1.96	0.62
1:B:139:PHE:CE2	1:B:150:LYS:HD2	2.35	0.62
1:B:128:ASN:HA	1:B:140:LEU:HD23	1.82	0.62
1:A:168:HIS:O	1:A:172:VAL:HG23	2.00	0.61
1:A:243:PHE:HZ	1:A:414:ILE:HG23	1.63	0.61
1:B:221:THR:H	1:B:406:ARG:NH1	1.99	0.61
1:A:40:GLU:HB3	1:A:42:ILE:HD12	1.80	0.61
1:A:160:MET:HE1	1:A:164:LEU:HD13	1.82	0.61
1:A:160:MET:O	1:A:164:LEU:HB2	2.01	0.61
1:B:233:LYS:HG2	1:B:234:ASP:H	1.64	0.61
1:B:278:ASP:HA	1:B:403:TYR:CE2	2.36	0.60
1:A:234:ASP:O	1:A:236:PRO:HD3	2.01	0.60
1:B:212:HIS:HD2	1:B:287:ASP:N	1.94	0.60
1:A:243:PHE:CZ	1:A:414:ILE:HG23	2.36	0.60
1:B:139:PHE:CZ	1:B:150:LYS:HD2	2.36	0.60
1:A:301:ARG:HH11	1:A:301:ARG:HG2	1.67	0.59
1:A:272:ALA:HB2	1:A:404:SER:OG	2.02	0.59
1:B:168:HIS:O	1:B:172:VAL:HG23	2.02	0.59
1:B:236:PRO:HB2	1:B:238:PHE:CZ	2.37	0.59
1:B:123:ARG:HD3	1:B:143:TYR:OH	2.02	0.59
1:A:144:ASP:O	1:A:207:HIS:HB2	2.02	0.59
1:A:249:LYS:HE3	1:A:249:LYS:H	1.67	0.59
1:A:347:ASP:O	1:A:351:MET:HB3	2.02	0.59
1:A:250:LEU:HG	1:A:414:ILE:HG22	1.85	0.58
1:B:192:ASP:O	1:B:194:VAL:HG23	2.04	0.58
1:B:204:VAL:HA	1:B:352:LYS:HD2	1.83	0.58
1:B:109:ARG:NH1	1:B:172:VAL:HA	2.19	0.58
1:A:251:HIS:O	1:A:356:SER:HA	2.04	0.58
1:B:213:ARG:HD3	1:B:215:TYR:OH	2.04	0.58
1:B:109:ARG:NH1	1:B:172:VAL:HG22	2.18	0.58
1:B:351:MET:O	1:B:352:LYS:HB2	2.02	0.58
1:B:160:MET:CE	1:B:164:LEU:HD13	2.34	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:PHE:CD1	1:A:248:GLN:HG3	2.39	0.57
1:A:225:GLU:O	1:A:241:ASN:HB2	2.04	0.57
1:B:243:PHE:CZ	1:B:414:ILE:HG23	2.37	0.57
1:B:110:PHE:CE1	1:B:182:GLN:HB3	2.40	0.57
1:A:78:LYS:HB3	1:B:78:LYS:HB3	1.85	0.57
1:B:131:SER:CB	1:B:138:ARG:HA	2.33	0.57
1:A:213:ARG:HD3	1:A:215:TYR:OH	2.05	0.56
1:B:249:LYS:H	1:B:249:LYS:HE3	1.70	0.56
1:A:109:ARG:HH11	1:A:172:VAL:HA	1.71	0.56
1:A:160:MET:CE	1:A:164:LEU:HD13	2.36	0.56
1:B:112:ILE:HD12	1:B:184:LEU:HD22	1.87	0.56
1:B:357:SER:HB3	1:B:358:PRO:HD3	1.88	0.55
1:B:353:SER:HG	1:B:364:PHE:HE2	1.54	0.55
1:B:189:LEU:HD12	1:B:189:LEU:H	1.71	0.55
1:B:210:THR:O	1:B:286:HIS:HD2	1.89	0.55
1:A:222:VAL:HA	1:A:225:GLU:HG3	1.87	0.55
1:B:251:HIS:HB3	2:B:417:HOH:O	2.07	0.55
1:B:268:VAL:CG1	1:B:404:SER:HA	2.37	0.55
1:B:233:LYS:HG2	1:B:234:ASP:N	2.21	0.54
1:A:123:ARG:HB3	1:A:143:TYR:CE2	2.43	0.54
1:A:208:ARG:NH1	1:A:209:LEU:HD21	2.23	0.54
1:B:160:MET:O	1:B:164:LEU:HB2	2.08	0.54
1:B:242:ASP:O	1:B:246:GLU:HG3	2.08	0.53
1:B:166:LYS:HD3	1:B:273:GLN:HE22	1.73	0.53
1:B:278:ASP:HA	1:B:403:TYR:HE2	1.71	0.53
1:B:301:ARG:HG2	1:B:301:ARG:HH11	1.74	0.53
1:A:205:PHE:CG	1:A:211:VAL:HG21	2.44	0.53
1:A:192:ASP:O	1:A:194:VAL:HG23	2.08	0.53
1:B:110:PHE:CD1	1:B:182:GLN:HB3	2.42	0.53
1:A:60:VAL:O	1:A:104:ARG:NH2	2.42	0.53
1:A:189:LEU:HD12	1:A:189:LEU:H	1.73	0.53
1:A:252:VAL:HG12	1:A:256:SER:HB3	1.90	0.53
1:A:210:THR:O	1:A:286:HIS:HD2	1.91	0.53
1:A:112:ILE:HD12	1:A:184:LEU:HD22	1.89	0.53
1:B:281:LEU:HB2	1:B:407:PHE:CZ	2.42	0.53
1:B:79:VAL:O	1:B:92:ARG:HA	2.09	0.53
1:B:408:ASN:O	1:B:412:SER:HB2	2.09	0.52
1:B:123:ARG:HB3	1:B:143:TYR:CE2	2.44	0.52
1:B:276:ILE:HD12	1:B:370:ILE:O	2.10	0.52
1:B:207:HIS:CE1	1:B:350:ALA:HB2	2.44	0.52
1:B:160:MET:HE1	1:B:164:LEU:HD13	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:VAL:O	1:A:92:ARG:HA	2.09	0.52
1:B:236:PRO:HB2	1:B:238:PHE:CE2	2.45	0.52
1:B:43:LEU:HD21	1:B:140:LEU:HD11	1.92	0.52
1:A:301:ARG:NH1	1:A:301:ARG:HG2	2.25	0.52
1:B:179:LEU:HB3	1:B:366:ALA:HA	1.91	0.51
1:B:264:LEU:HD11	1:B:407:PHE:HE2	1.75	0.51
1:A:279:TYR:HA	1:A:369:ASP:HB2	1.92	0.51
1:A:148:VAL:HG23	1:A:203:ASN:HB3	1.92	0.51
1:A:260:PHE:CE2	1:A:415:LEU:HD21	2.45	0.51
1:B:231:LYS:HG2	1:B:238:PHE:CE2	2.46	0.51
1:A:245:ASN:OD1	1:A:246:GLU:N	2.44	0.51
1:B:217:LEU:HD23	1:B:240:ASP:HA	1.92	0.51
1:A:277:MET:HG2	1:A:403:TYR:HD2	1.74	0.51
1:B:343:ASP:OD1	1:B:344:PRO:HD3	2.10	0.51
1:B:231:LYS:HG2	1:B:238:PHE:HE2	1.75	0.51
1:B:215:TYR:CD2	1:B:243:PHE:HB2	2.46	0.51
1:A:110:PHE:CE1	1:A:182:GLN:HB3	2.45	0.51
1:B:112:ILE:HD12	1:B:184:LEU:CD2	2.41	0.51
1:B:347:ASP:O	1:B:351:MET:HB3	2.11	0.50
1:A:408:ASN:O	1:A:412:SER:HB2	2.11	0.50
1:B:204:VAL:HA	1:B:352:LYS:CD	2.40	0.50
1:B:281:LEU:HB2	1:B:407:PHE:HZ	1.76	0.50
1:B:55:ASN:ND2	1:B:118:GLN:HE22	2.10	0.50
1:A:352:LYS:HD3	1:A:366:ALA:CB	2.38	0.49
1:B:48:TRP:CD1	1:B:89:LEU:HD11	2.46	0.49
1:A:204:VAL:HA	1:A:352:LYS:HD2	1.93	0.49
1:A:227:SER:HB3	1:A:230:GLU:HB2	1.93	0.49
1:A:157:VAL:HG21	1:A:197:TYR:HD2	1.74	0.49
1:A:346:VAL:HG12	1:A:348:VAL:CG1	2.42	0.49
1:A:167:TYR:O	1:A:171:ILE:HG12	2.13	0.49
1:B:265:LYS:O	1:B:269:GLU:HB2	2.12	0.49
1:B:221:THR:HG23	1:B:406:ARG:HH11	1.77	0.49
1:B:252:VAL:CG1	1:B:256:SER:HB3	2.42	0.49
1:A:222:VAL:HG13	1:A:241:ASN:HD21	1.78	0.49
1:A:265:LYS:O	1:A:269:GLU:HB2	2.12	0.49
1:B:51:ASN:HA	1:B:118:GLN:HE21	1.77	0.48
1:A:51:ASN:HA	1:A:118:GLN:HE21	1.78	0.48
1:B:188:ARG:HD2	1:B:195:GLU:OE2	2.14	0.48
1:B:264:LEU:HD11	1:B:407:PHE:CE2	2.49	0.48
1:A:179:LEU:HG	1:A:263:LYS:HG2	1.96	0.48
1:B:159:GLU:HB3	1:B:371:LEU:HD22	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:SER:HA	1:B:406:ARG:NE	2.27	0.48
1:B:110:PHE:CE2	1:B:182:GLN:HG2	2.48	0.48
1:B:167:TYR:O	1:B:171:ILE:HG12	2.13	0.48
1:A:282:LEU:O	1:A:365:MET:HA	2.14	0.48
1:A:60:VAL:O	1:A:60:VAL:HG22	2.13	0.48
1:B:74:TYR:CD1	1:B:96:LYS:HE3	2.49	0.48
1:A:218:LYS:CE	1:A:239:LYS:HD3	2.44	0.47
1:B:42:ILE:HD11	1:B:196:THR:HG21	1.96	0.47
1:A:74:TYR:CD1	1:A:96:LYS:HE3	2.50	0.47
1:B:50:VAL:O	1:B:54:ILE:HB	2.14	0.47
1:A:346:VAL:HG12	1:A:348:VAL:HG12	1.96	0.47
1:A:221:THR:HG23	1:A:406:ARG:HH11	1.79	0.47
1:B:230:GLU:O	1:B:236:PRO:HG3	2.15	0.47
1:B:275:LYS:HG2	1:B:275:LYS:O	2.14	0.47
1:B:57:LEU:HA	1:B:60:VAL:HG13	1.97	0.47
1:B:250:LEU:HD22	1:B:363:TYR:CE2	2.50	0.47
1:B:274:LEU:O	1:B:276:ILE:HG12	2.15	0.46
1:B:84:PHE:CE2	1:B:85:ASN:HB2	2.50	0.46
1:B:346:VAL:O	1:B:348:VAL:N	2.48	0.46
1:A:57:LEU:HA	1:A:60:VAL:HG13	1.97	0.46
1:B:130:ASP:O	1:B:132:GLN:NE2	2.48	0.46
1:A:34:LYS:O	1:A:35:LEU:HD23	2.16	0.46
1:A:50:VAL:O	1:A:54:ILE:HB	2.15	0.46
1:B:207:HIS:ND1	1:B:350:ALA:HB2	2.30	0.46
1:A:110:PHE:CD1	1:A:182:GLN:HB3	2.51	0.46
1:B:205:PHE:CG	1:B:211:VAL:HG21	2.51	0.46
1:A:370:ILE:O	1:A:370:ILE:HG12	2.16	0.46
1:A:103:PHE:HZ	1:A:160:MET:HE2	1.81	0.46
1:B:301:ARG:HG2	1:B:301:ARG:NH1	2.30	0.45
1:B:246:GLU:HB2	1:B:248:GLN:HG2	1.97	0.45
1:A:190:THR:HG22	1:A:195:GLU:HA	1.97	0.45
1:A:223:ALA:N	1:A:225:GLU:HG2	2.19	0.45
1:A:131:SER:HA	1:A:139:PHE:HB2	1.99	0.45
1:B:276:ILE:HA	1:B:276:ILE:HD13	1.86	0.45
1:B:144:ASP:O	1:B:207:HIS:HB2	2.16	0.45
1:A:277:MET:HG2	1:A:403:TYR:CD2	2.51	0.45
1:B:276:ILE:HG22	1:B:279:TYR:HD2	1.81	0.45
1:B:181:PRO:HG2	1:B:370:ILE:HG22	1.98	0.45
1:B:67:MET:HA	1:B:67:MET:CE	2.46	0.45
1:A:165:LYS:HA	1:A:165:LYS:HD2	1.73	0.44
1:A:55:ASN:ND2	1:A:118:GLN:HE22	2.14	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:MET:SD	1:B:68:PRO:HD2	2.57	0.44
1:A:38:ALA:HB2	1:A:125:ALA:CB	2.47	0.44
1:B:270:PHE:O	1:B:273:GLN:HB3	2.17	0.44
1:A:220:SER:HA	1:A:406:ARG:CZ	2.47	0.44
1:A:148:VAL:CG2	1:A:203:ASN:HB3	2.48	0.44
1:A:94:LYS:HB2	1:A:190:THR:OG1	2.17	0.44
1:A:360:LYS:HG2	1:A:360:LYS:O	2.17	0.44
1:A:354:HIS:ND1	1:A:365:MET:CE	2.81	0.44
1:B:260:PHE:CE2	1:B:415:LEU:HD11	2.52	0.44
1:B:177:ASN:HD21	1:B:263:LYS:HE2	1.83	0.44
1:A:84:PHE:CE2	1:A:85:ASN:HB2	2.53	0.44
1:A:103:PHE:HZ	1:A:160:MET:CE	2.30	0.43
1:A:245:ASN:OD1	1:A:246:GLU:HG3	2.18	0.43
1:B:160:MET:HG3	1:B:186:MET:HE3	2.00	0.43
1:A:112:ILE:HD12	1:A:184:LEU:CD2	2.47	0.43
1:A:399:ASN:ND2	1:A:402:GLN:H	2.16	0.43
1:B:288:VAL:O	1:B:291:ALA:HB3	2.19	0.43
1:B:249:LYS:HB3	1:B:251:HIS:HE1	1.75	0.43
1:A:250:LEU:HG	1:A:414:ILE:CG2	2.47	0.43
1:A:48:TRP:CD1	1:A:89:LEU:HD11	2.54	0.43
1:B:60:VAL:O	1:B:104:ARG:NH2	2.50	0.43
1:B:60:VAL:HG22	1:B:60:VAL:O	2.17	0.43
1:B:288:VAL:HB	1:B:360:LYS:HB3	1.99	0.43
1:A:215:TYR:O	1:A:282:LEU:HD23	2.18	0.43
1:A:415:LEU:HD23	1:A:415:LEU:N	2.29	0.43
1:A:188:ARG:HD2	1:A:195:GLU:OE2	2.19	0.42
1:B:160:MET:HE3	1:B:164:LEU:HD13	2.00	0.42
1:A:109:ARG:HH12	1:A:172:VAL:HG13	1.85	0.42
1:A:277:MET:HG3	1:A:400:PRO:HA	2.00	0.42
1:A:49:GLY:HA3	1:A:95:PHE:CZ	2.55	0.42
1:B:271:LEU:HB3	1:B:276:ILE:HB	2.01	0.42
1:A:60:VAL:HA	1:A:61:PRO:HD2	1.82	0.42
1:B:94:LYS:HB2	1:B:190:THR:OG1	2.20	0.42
1:B:205:PHE:CD1	1:B:211:VAL:HG21	2.54	0.42
1:B:169:GLN:O	1:B:172:VAL:HB	2.20	0.42
1:B:217:LEU:CD2	1:B:240:ASP:HA	2.50	0.42
1:B:190:THR:HG22	1:B:195:GLU:HA	2.02	0.42
1:A:234:ASP:HB3	1:A:235:LEU:H	1.77	0.42
1:A:169:GLN:O	1:A:172:VAL:HB	2.19	0.41
1:A:182:GLN:NE2	1:A:352:LYS:NZ	2.68	0.41
1:B:245:ASN:OD1	1:B:246:GLU:N	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:LYS:HE3	1:B:415:LEU:HB2	2.01	0.41
1:A:250:LEU:O	1:A:415:LEU:HA	2.19	0.41
1:A:278:ASP:N	1:A:403:TYR:HE2	2.17	0.41
1:B:215:TYR:CE2	1:B:243:PHE:HB2	2.55	0.41
1:A:157:VAL:HA	1:A:186:MET:CE	2.42	0.41
1:B:42:ILE:CD1	1:B:196:THR:HG21	2.50	0.41
1:A:398:VAL:HG21	1:A:406:ARG:NH1	2.36	0.41
1:A:353:SER:HA	1:A:363:TYR:O	2.21	0.41
1:A:208:ARG:HH22	1:A:345:SER:HA	1.85	0.41
1:A:278:ASP:N	1:A:403:TYR:CE2	2.89	0.41
1:A:399:ASN:HB2	1:A:400:PRO:HD2	2.02	0.41
1:B:41:PRO:HB3	1:B:90:PRO:HG3	2.02	0.41
1:B:47:MET:HG2	1:B:121:VAL:O	2.21	0.41
1:A:222:VAL:HA	1:A:225:GLU:CG	2.51	0.41
1:B:210:THR:O	1:B:286:HIS:CD2	2.71	0.41
1:A:288:VAL:O	1:A:291:ALA:HB3	2.21	0.41
1:B:152:VAL:HB	1:B:156:ASP:HB2	2.02	0.41
1:B:226:ALA:HA	1:B:242:ASP:OD2	2.21	0.40
1:B:215:TYR:HA	1:B:238:PHE:O	2.21	0.40
1:A:188:ARG:HA	1:A:196:THR:O	2.21	0.40
1:B:353:SER:OG	1:B:364:PHE:HE2	2.03	0.40
1:B:49:GLY:HA3	1:B:95:PHE:CZ	2.56	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	318/416 (76%)	268 (84%)	39 (12%)	11 (4%)	4	24
1	B	312/416 (75%)	266 (85%)	34 (11%)	12 (4%)	4	22
All	All	630/832 (76%)	534 (85%)	73 (12%)	23 (4%)	4	23

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	222	VAL
1	A	232	ALA
1	A	396	SER
1	B	222	VAL
1	B	275	LYS
1	B	347	ASP
1	B	350	ALA
1	B	358	PRO
1	B	360	LYS
1	A	223	ALA
1	A	228	ASP
1	A	234	ASP
1	A	275	LYS
1	B	130	ASP
1	B	278	ASP
1	A	343	ASP
1	B	225	GLU
1	B	344	PRO
1	B	400	PRO
1	A	233	LYS
1	A	274	LEU
1	A	352	LYS
1	B	248	GLN

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	302/374 (81%)	283 (94%)	19 (6%)	22	60
1	B	295/374 (79%)	271 (92%)	24 (8%)	15	47
All	All	597/748 (80%)	554 (93%)	43 (7%)	18	53

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

Mol	Chain	Res	Type
1	A	34	LYS
1	A	54	ILE
1	A	60	VAL
1	A	85	ASN
1	A	86	LYS
1	A	109	ARG
1	A	165	LYS
1	A	189	LEU
1	A	210	THR
1	A	227	SER
1	A	249	LYS
1	A	250	LEU
1	A	251	HIS
1	A	266	ARG
1	A	282	LEU
1	A	304	ASP
1	A	351	MET
1	A	354	HIS
1	A	415	LEU
1	B	54	ILE
1	B	60	VAL
1	B	85	ASN
1	B	86	LYS
1	B	109	ARG
1	B	134	ARG
1	B	189	LEU
1	B	210	THR
1	B	234	ASP
1	B	249	LYS
1	B	250	LEU
1	B	251	HIS
1	B	266	ARG
1	B	274	LEU
1	B	282	LEU
1	B	343	ASP
1	B	344	PRO
1	B	354	HIS
1	B	368	ILE
1	B	369	ASP
1	B	370	ILE
1	B	399	ASN
1	B	400	PRO
1	B	409	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	55	ASN
1	A	81	ASN
1	A	85	ASN
1	A	118	GLN
1	A	119	ASN
1	A	169	GLN
1	A	212	HIS
1	A	241	ASN
1	A	259	ASN
1	A	286	HIS
1	A	399	ASN
1	B	51	ASN
1	B	55	ASN
1	B	81	ASN
1	B	85	ASN
1	B	118	GLN
1	B	119	ASN
1	B	132	GLN
1	B	212	HIS
1	B	251	HIS
1	B	273	GLN
1	B	286	HIS

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

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.