Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 12:39 AM GMT

PDB ID	:	2BAP
Title	:	Crystal structure of the N-terminal mDia1 Armadillo Repeat Region and Dimerisation Domain in complex with the mDia1 autoregulatory domain (DAD)
Authors	:	Lammers, M.; Rose, R.; Scrima, A.; Wittinghofer, A.
Deposited on	:	2005-10-14
Resolution	:	3.30 Å(reported)

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)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
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 3.30 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	Percentile Ranks	Value
Rfree		0.355
Clashscore		17
Ramachandran outliers		3.1%
Sidechain outliers		11.7%
RSRZ outliers		1.9%

Worse ← → *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
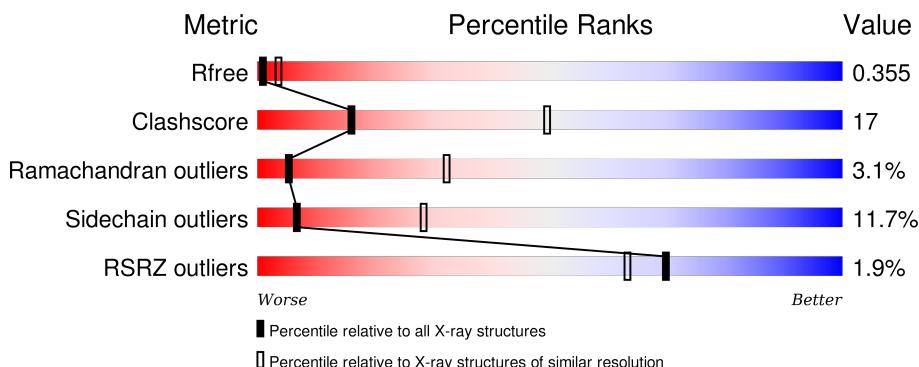
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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.

Mol	Chain	Length	Quality of chain
1	A	317	2% / 51% 35% 7% 7%
1	B	317	2% / 57% 32% • 7%
2	C	56	2% / 18% 11% 71%
2	D	56	23% 5% 71%
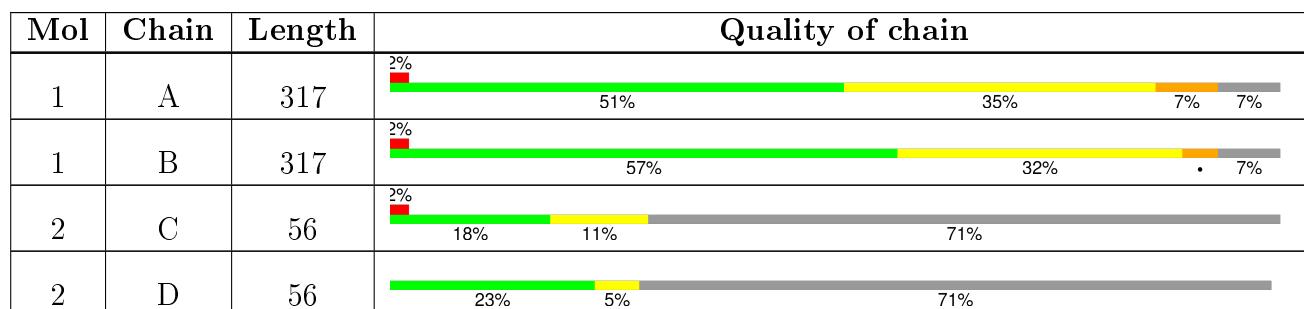
2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4960 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 Diaphanous protein homolog 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	294	Total 2363	C 1490	N 404	O 448	S 21	0	0	0
1	A	295	Total 2375	C 1499	N 405	O 450	S 21	0	0	0

- Molecule 2 is a protein called Diaphanous protein homolog 1.

| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	16	Total 111	C 70	N 17	O 23	S 1	0	0	0
2	C	16	Total 111	C 70	N 17	O 23	S 1	0	0	0

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 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.

- Molecule 1: Diaphanous protein homolog 1
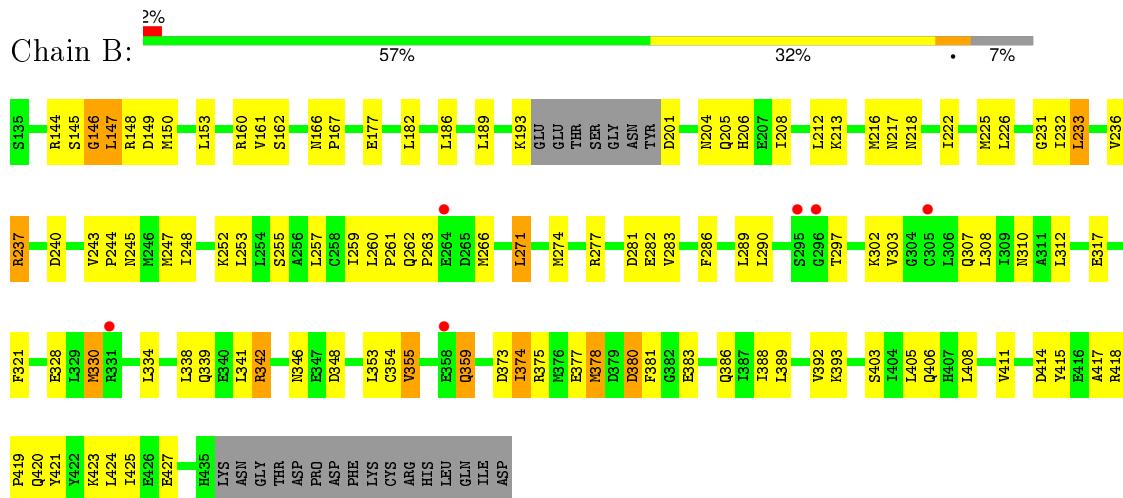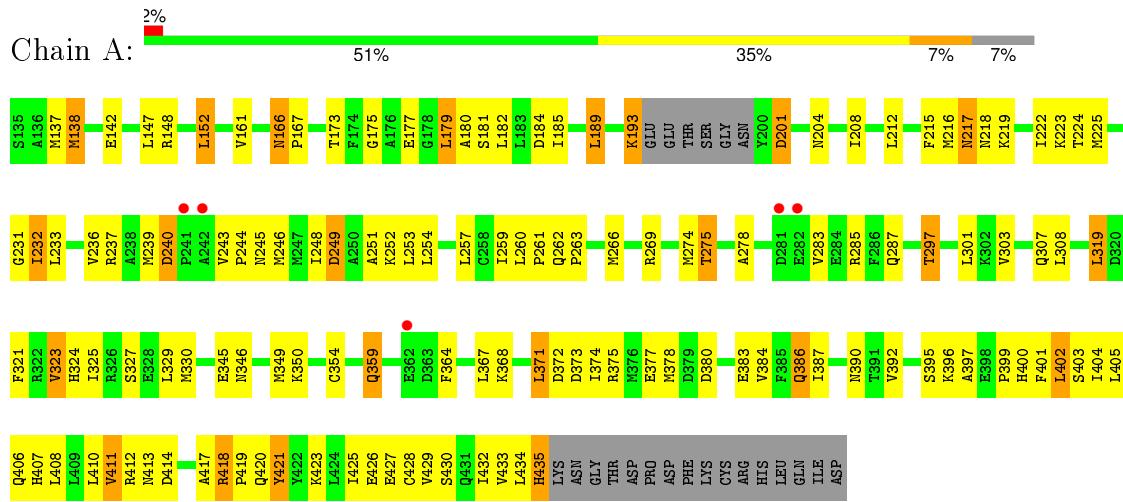
- Molecule 1: Diaphanous protein homolog 1

- Molecule 2: Diaphanous protein homolog 1

MET ARG ARG ALA LYS LEU ALA LYS GLU LYS ALA GLU GLU LYS ARG LEU GLU LYS GLN GLN LYS ARG GLU GLN LEU ILE ASP MET ASN ALA GLU GLY ASP GLU THR **G1180** **L1189** **G1192** **F1195** ARG ARG LYS ARG GLY

- Molecule 2: Diaphanous protein homolog 1

Chain C:

2%

18% 11% 71%

MET ARG ARG ALA LYS LEU ALA LYS GLU LYS ALA GLU GLU LYS ARG LEU GLU LYS GLN GLN LYS ARG GLU GLN LEU ILE ASP MET ASN ALA GLU GLY ASP GLU THR **G1180** **V1181** **L1186** **E1187** **A1188** **L1189** **A1193** **A1194** **F1195** ARG ARG LYS ARG GLY

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	138.45Å 138.45Å 210.89Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.98 – 3.30 19.96 – 3.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.98-3.30) 100.0 (19.96-3.30)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.21 (at 3.29Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.288 , 0.364 0.285 , 0.355	Depositor DCC
R_{free} test set	925 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	89.0	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 58.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \lvert L \rvert > = 0.48, < L^2 > = 0.31$	Xtriage
Outliers	1 of 18489 reflections (0.005%)	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	4960	wwPDB-VP
Average B, all atoms (Å^2)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.93% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1] Intensities estimated from amplitudes.
[2] Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	0.63	1/2408 (0.0%)	0.65	1/3242 (0.0%)
1	B	0.40	0/2395	0.59	0/3224
2	C	0.41	0/111	0.67	0/148
2	D	0.40	0/111	0.52	0/148
All	All	0.52	1/5025 (0.0%)	0.62	1/6762 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	435	HIS	C-O	21.22	1.63	1.23

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	435	HIS	CA-C-O	-6.75	105.92	120.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	2375	0	2395	92	0
1	B	2363	0	2386	76	0
2	C	111	0	108	4	0
2	D	111	0	108	4	0
All	All	4960	0	4997	168	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 17.

All (168) 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:435:HIS:O	1:A:435:HIS:C	1.63	1.36
1:A:239:MET:CE	1:A:254:LEU:HD12	1.79	1.12
1:A:239:MET:HE1	1:A:254:LEU:HD12	1.30	1.11
1:A:421:TYR:HE1	1:A:425:ILE:HD11	1.12	1.06
1:A:402:LEU:O	1:A:406:GLN:HG3	1.65	0.95
1:A:421:TYR:CE1	1:A:425:ILE:HD11	2.02	0.94
1:B:263:PRO:HB2	1:B:266:MET:CE	1.98	0.93
1:B:263:PRO:HB2	1:B:266:MET:HE2	1.51	0.92
1:A:244:PRO:O	1:A:248:ILE:HG12	1.70	0.91
1:A:303:VAL:O	1:A:307:GLN:HB2	1.75	0.87
1:B:403:SER:HA	1:B:406:GLN:HE21	1.40	0.84
1:A:400:HIS:O	1:A:403:SER:OG	1.95	0.82
1:B:417:ALA:HA	1:B:420:GLN:OE1	1.87	0.75
1:A:421:TYR:HE1	1:A:425:ILE:CD1	1.97	0.74
1:A:346:ASN:HB3	1:A:349:MET:HB3	1.68	0.74
1:B:263:PRO:O	1:B:266:MET:HG2	1.87	0.73
1:B:380:ASP:HB2	1:B:383:GLU:HG2	1.71	0.72
1:A:378:MET:HG2	1:A:384:VAL:HG23	1.72	0.71
1:B:161:VAL:HG21	1:A:161:VAL:HG11	1.72	0.70
1:A:239:MET:CE	1:A:254:LEU:CD1	2.66	0.70
1:A:427:GLU:HA	1:A:430:SER:OG	1.92	0.69
1:B:263:PRO:HB2	1:B:266:MET:HE3	1.75	0.69
1:B:212:LEU:HB3	1:B:216:MET:HE3	1.73	0.68
1:A:182:LEU:HD22	1:A:208:ILE:HG23	1.77	0.65
1:B:213:LYS:HA	1:B:253:LEU:HD21	1.77	0.65
1:A:425:ILE:O	1:A:429:VAL:HG12	1.96	0.65
1:B:232:ILE:HD12	1:B:232:ILE:H	1.62	0.64
1:A:248:ILE:HD13	1:A:301:LEU:HA	1.80	0.63
1:B:182:LEU:HD22	1:B:208:ILE:HG23	1.80	0.62
1:B:380:ASP:HB3	1:B:383:GLU:H	1.65	0.61
1:A:396:LYS:O	1:A:399:PRO:HD2	1.99	0.61
1:A:418:ARG:N	1:A:419:PRO:HD2	2.14	0.61
1:A:239:MET:HE1	1:A:254:LEU:CD1	2.17	0.61
1:B:355:VAL:HG21	2:D:1195:PHE:CB	2.29	0.61
1:A:245:ASN:HA	1:A:248:ILE:HG13	1.82	0.61
1:B:420:GLN:O	1:B:424:LEU:HG	2.01	0.60
1:A:429:VAL:O	1:A:433:VAL:HG23	2.00	0.60

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:380:ASP:O	1:B:381:PHE:HB2	2.02	0.60
1:A:378:MET:HG2	1:A:384:VAL:CG2	2.32	0.60
1:A:249:ASP:O	1:A:253:LEU:HB2	2.01	0.59
1:A:148:ARG:O	1:A:152:LEU:HB2	2.02	0.59
1:A:345:GLU:HA	1:A:350:LYS:NZ	2.17	0.59
1:B:359:GLN:HA	1:B:359:GLN:HE21	1.68	0.59
1:B:378:MET:HA	1:B:383:GLU:HB3	1.86	0.58
1:A:179:LEU:HG	1:A:215:PHE:CE2	2.40	0.57
1:B:257:LEU:HA	1:B:260:LEU:HD13	1.85	0.57
1:A:321:PHE:O	1:A:324:HIS:HB3	2.04	0.57
1:B:177:GLU:CD	1:B:177:GLU:H	2.09	0.56
1:A:217:ASN:ND2	2:C:1180:GLY:HA2	2.20	0.56
1:B:226:LEU:HD21	1:B:257:LEU:HD22	1.87	0.55
1:A:239:MET:HE2	1:A:251:ALA:HA	1.88	0.55
1:B:297:THR:OG1	1:B:302:LYS:HE3	2.06	0.55
2:C:1187:GLU:C	2:C:1189:LEU:H	2.10	0.55
1:B:144:ARG:HH22	1:B:177:GLU:HB3	1.72	0.55
1:A:142:GLU:O	1:A:147:LEU:HG	2.07	0.55
1:B:255:SER:HB3	1:B:308:LEU:HA	1.88	0.54
1:A:359:GLN:HE21	1:A:359:GLN:HA	1.74	0.53
1:B:233:LEU:O	1:B:237:ARG:HG2	2.07	0.53
1:A:372:ASP:HA	1:A:375:ARG:HG3	1.91	0.52
1:B:403:SER:HA	1:B:406:GLN:NE2	2.16	0.52
1:A:177:GLU:CD	1:A:177:GLU:H	2.13	0.52
1:A:166:ASN:HD22	1:A:167:PRO:HD2	1.76	0.51
1:B:374:ILE:HG23	1:B:378:MET:HE3	1.93	0.50
1:B:418:ARG:N	1:B:419:PRO:HD2	2.26	0.50
1:A:435:HIS:O	1:A:435:HIS:CA	2.56	0.50
1:B:330:MET:HE3	1:B:334:LEU:HD23	1.93	0.50
1:A:216:MET:O	1:A:218:ASN:N	2.40	0.50
1:A:367:LEU:HD23	1:A:434:LEU:HD23	1.93	0.50
1:A:420:GLN:O	1:A:423:LYS:HB3	2.12	0.50
1:A:407:HIS:HA	1:A:410:LEU:HD12	1.93	0.50
1:A:239:MET:O	1:A:240:ASP:HB3	2.11	0.50
1:B:240:ASP:H	1:B:247:MET:HB2	1.77	0.49
1:A:403:SER:HA	1:A:406:GLN:HE21	1.78	0.49
1:B:421:TYR:CE1	1:B:425:ILE:HG13	2.48	0.49
1:A:239:MET:HE3	1:A:254:LEU:HD12	1.84	0.49
1:B:415:TYR:CZ	1:B:417:ALA:HB3	2.48	0.49
1:B:339:GLN:O	1:B:342:ARG:HG3	2.13	0.48
1:A:405:LEU:HA	1:A:408:LEU:HD12	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:TYR:CD1	1:A:421:TYR:C	2.86	0.48
1:A:266:MET:SD	1:A:269:ARG:HD3	2.54	0.48
1:B:216:MET:CE	1:B:225:MET:HG2	2.44	0.48
1:B:289:LEU:HD21	1:B:308:LEU:HD23	1.96	0.48
1:B:150:MET:SD	1:A:138:MET:HG3	2.53	0.48
1:A:275:THR:HG23	1:A:285:ARG:HD3	1.96	0.48
1:B:222:ILE:HG21	1:B:260:LEU:HD21	1.95	0.48
1:A:423:LYS:O	1:A:426:GLU:HB3	2.14	0.47
1:A:429:VAL:HA	1:A:432:ILE:HD12	1.96	0.47
1:B:271:LEU:HD22	1:B:312:LEU:HD22	1.96	0.47
1:A:185:ILE:O	1:A:189:LEU:HB2	2.15	0.47
1:A:257:LEU:O	1:A:260:LEU:HB2	2.15	0.47
1:B:334:LEU:O	1:B:338:LEU:HB2	2.15	0.47
1:A:243:VAL:HG12	1:A:243:VAL:O	2.15	0.47
1:A:236:VAL:HG11	1:A:274:MET:HA	1.97	0.46
1:A:177:GLU:O	1:A:180:ALA:HB3	2.14	0.46
1:A:201:ASP:OD2	1:A:204:ASN:ND2	2.48	0.46
1:A:248:ILE:CD1	1:A:301:LEU:HA	2.46	0.46
1:B:346:ASN:ND2	1:B:348:ASP:H	2.13	0.46
1:A:380:ASP:HB3	1:A:383:GLU:HG2	1.98	0.46
1:B:236:VAL:HG11	1:B:274:MET:HA	1.98	0.46
1:A:368:LYS:HD2	1:A:371:LEU:HD23	1.96	0.46
1:B:359:GLN:CA	1:B:359:GLN:HE21	2.30	0.45
1:A:216:MET:HB3	1:A:222:ILE:HG23	1.98	0.45
1:A:297:THR:HB	1:A:301:LEU:HD23	1.98	0.45
1:A:345:GLU:HA	1:A:350:LYS:HZ2	1.79	0.45
1:A:239:MET:HE3	1:A:254:LEU:CD1	2.44	0.45
1:A:395:SER:O	1:A:397:ALA:N	2.50	0.45
1:B:421:TYR:O	1:B:424:LEU:HB2	2.17	0.45
1:B:162:SER:O	1:B:166:ASN:ND2	2.44	0.45
1:B:378:MET:HG2	1:B:378:MET:O	2.17	0.45
1:B:204:ASN:H	1:B:204:ASN:HD22	1.63	0.45
1:A:193:LYS:N	1:A:193:LYS:HD3	2.32	0.45
1:A:392:VAL:HG11	1:A:401:PHE:CG	2.52	0.44
1:A:232:ILE:H	1:A:232:ILE:HG13	1.56	0.44
1:B:189:LEU:HD13	1:B:205:GLN:HB3	1.98	0.44
1:A:428:CYS:O	1:A:432:ILE:HG13	2.18	0.44
2:C:1186:LEU:O	2:C:1189:LEU:HB3	2.18	0.44
1:A:212:LEU:HB3	1:A:216:MET:HE2	1.99	0.44
1:A:218:ASN:HA	2:C:1181:VAL:HB	2.00	0.44
1:A:417:ALA:O	1:A:420:GLN:HB2	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:389:LEU:HA	1:B:393:LYS:HB2	2.00	0.43
1:B:405:LEU:HA	1:B:408:LEU:HD12	2.00	0.43
1:A:319:LEU:O	1:A:323:VAL:HG12	2.19	0.43
1:A:392:VAL:O	1:A:392:VAL:HG12	2.18	0.43
1:A:413:ASN:O	1:A:418:ARG:NH1	2.52	0.43
1:B:148:ARG:HD3	1:B:148:ARG:HA	1.76	0.43
1:B:147:LEU:O	1:B:148:ARG:NH1	2.52	0.43
1:A:321:PHE:O	1:A:325:ILE:HG13	2.18	0.43
1:B:160:ARG:HG3	1:B:161:VAL:H	1.84	0.43
1:B:216:MET:C	1:B:218:ASN:H	2.23	0.42
1:B:248:ILE:HG22	1:B:252:LYS:HE2	2.01	0.42
1:A:222:ILE:HD12	1:A:223:LYS:N	2.33	0.42
1:B:286:PHE:CE1	1:B:328:GLU:HG2	2.55	0.42
1:A:248:ILE:HG12	1:A:248:ILE:H	1.71	0.42
1:B:310:ASN:ND2	1:B:355:VAL:HG12	2.34	0.42
1:A:386:GLN:O	1:A:390:ASN:ND2	2.52	0.42
1:A:260:LEU:HA	1:A:261:PRO:HD3	1.74	0.42
1:A:404:ILE:HG22	1:A:408:LEU:HD11	2.01	0.42
1:B:355:VAL:HG21	2:D:1195:PHE:HB3	2.01	0.42
1:B:260:LEU:HA	1:B:261:PRO:HD3	1.67	0.42
1:A:254:LEU:HA	1:A:257:LEU:HD12	2.02	0.41
1:A:421:TYR:C	1:A:421:TYR:HD1	2.23	0.41
1:A:243:VAL:HG11	1:A:246:MET:HE2	2.02	0.41
1:B:259:ILE:HD11	2:D:1189:LEU:HD21	2.02	0.41
1:B:341:LEU:O	1:B:353:LEU:HD11	2.20	0.41
1:B:243:VAL:O	1:B:243:VAL:HG12	2.19	0.41
1:B:355:VAL:HG21	2:D:1195:PHE:HB2	2.02	0.41
1:A:217:ASN:O	1:A:218:ASN:HB3	2.20	0.41
1:B:346:ASN:HD22	1:B:348:ASP:H	1.67	0.41
1:A:278:ALA:HB1	1:A:283:VAL:O	2.20	0.41
1:A:233:LEU:O	1:A:237:ARG:HG3	2.21	0.41
1:B:166:ASN:HB3	1:B:167:PRO:HD2	2.03	0.41
1:B:216:MET:HE1	1:B:225:MET:HG2	2.02	0.41
1:B:260:LEU:HB3	1:B:263:PRO:HD2	2.03	0.41
1:B:147:LEU:HB3	1:B:148:ARG:H	1.80	0.41
1:B:206:HIS:C	1:B:206:HIS:HD1	2.24	0.41
1:A:364:PHE:CD2	1:A:364:PHE:C	2.95	0.41
1:A:248:ILE:O	1:A:252:LYS:HG2	2.21	0.41
1:A:222:ILE:HD12	1:A:223:LYS:H	1.85	0.41
1:B:388:ILE:O	1:B:392:VAL:HB	2.21	0.41
1:B:290:LEU:HD13	1:B:290:LEU:HA	1.98	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:VAL:O	1:B:307:GLN:HB2	2.20	0.40
1:B:216:MET:O	1:B:222:ILE:HG13	2.20	0.40
1:B:144:ARG:C	1:B:146:GLY:H	2.25	0.40
1:B:373:ASP:C	1:B:375:ARG:H	2.23	0.40
1:A:260:LEU:HD23	1:A:263:PRO:CG	2.52	0.40
1:B:257:LEU:O	1:B:260:LEU:HB2	2.21	0.40
1:A:418:ARG:N	1:A:419:PRO:CD	2.84	0.40
1:B:421:TYR:HE1	1:B:425:ILE:HG13	1.86	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	291/317 (92%)	237 (81%)	47 (16%)	7 (2%)	7	38
1	B	290/317 (92%)	248 (86%)	32 (11%)	10 (3%)	5	29
2	C	14/56 (25%)	11 (79%)	2 (14%)	1 (7%)	1	11
2	D	14/56 (25%)	10 (71%)	3 (21%)	1 (7%)	1	11
All	All	609/746 (82%)	506 (83%)	84 (14%)	19 (3%)	5	32

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	147	LEU
1	B	411	VAL
1	A	217	ASN
1	A	219	LYS
1	A	231	GLY
1	B	262	GLN
1	B	145	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	282	GLU
2	D	1192	GLY
2	C	1188	ALA
1	B	217	ASN
1	B	231	GLY
1	A	411	VAL
1	A	175	GLY
1	A	259	ILE
1	B	146	GLY
1	B	244	PRO
1	B	374	ILE
1	A	240	ASP

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	267/287 (93%)	228 (85%)	39 (15%)	4	18
1	B	266/287 (93%)	240 (90%)	26 (10%)	10	37
2	C	11/45 (24%)	11 (100%)	0	100	100
2	D	11/45 (24%)	11 (100%)	0	100	100
All	All	555/664 (84%)	490 (88%)	65 (12%)	7	28

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	149	ASP
1	B	153	LEU
1	B	186	LEU
1	B	193	LYS
1	B	201	ASP
1	B	233	LEU
1	B	237	ARG
1	B	245	ASN
1	B	271	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	277	ARG
1	B	281	ASP
1	B	283	VAL
1	B	317	GLU
1	B	321	PHE
1	B	330	MET
1	B	342	ARG
1	B	354	CYS
1	B	355	VAL
1	B	359	GLN
1	B	377	GLU
1	B	378	MET
1	B	380	ASP
1	B	386	GLN
1	B	414	ASP
1	B	423	LYS
1	B	427	GLU
1	A	137	MET
1	A	138	MET
1	A	152	LEU
1	A	166	ASN
1	A	173	THR
1	A	179	LEU
1	A	181	SER
1	A	184	ASP
1	A	189	LEU
1	A	193	LYS
1	A	201	ASP
1	A	224	THR
1	A	225	MET
1	A	232	ILE
1	A	249	ASP
1	A	262	GLN
1	A	275	THR
1	A	287	GLN
1	A	297	THR
1	A	308	LEU
1	A	319	LEU
1	A	323	VAL
1	A	327	SER
1	A	329	LEU
1	A	330	MET

Continued from previous page...

Mol	Chain	Res	Type
1	A	354	CYS
1	A	359	GLN
1	A	371	LEU
1	A	373	ASP
1	A	374	ILE
1	A	377	GLU
1	A	386	GLN
1	A	387	ILE
1	A	402	LEU
1	A	411	VAL
1	A	412	ARG
1	A	414	ASP
1	A	418	ARG
1	A	421	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	172	GLN
1	B	190	HIS
1	B	324	HIS
1	B	346	ASN
1	B	359	GLN
1	B	406	GLN
1	A	166	ASN
1	A	190	HIS
1	A	205	GLN
1	A	346	ASN
1	A	359	GLN
1	A	406	GLN

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 (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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(Å²)	Q<0.9
1	A	295/317 (93%)	0.11	5 (1%)	73	67	29, 95, 108, 114	0
1	B	294/317 (92%)	-0.03	6 (2%)	68	62	29, 93, 105, 112	0
2	C	16/56 (28%)	0.24	1 (6%)	23	19	114, 116, 117, 118	0
2	D	16/56 (28%)	0.23	0	100	100	112, 115, 116, 117	0
All	All	621/746 (83%)	0.05	12 (1%)	70	63	29, 95, 113, 118	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	242	ALA	3.6
1	B	296	GLY	2.9
1	B	295	SER	2.4
1	A	282	GLU	2.4
1	B	331	ARG	2.3
1	A	241	PRO	2.2
1	B	358	GLU	2.2
1	A	281	ASP	2.1
1	B	305	CYS	2.1
1	B	264	GLU	2.1
1	A	362	GLU	2.1
2	C	1193	ALA	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.