



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:29 AM GMT

PDB ID : 3EUJ
Title : Crystal structure of MukE-MukF(residues 292-443)-MukB(head domain)-ATPgammaS complex, symmetric dimer
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Deposited on : 2008-10-10
Resolution : 3.10 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

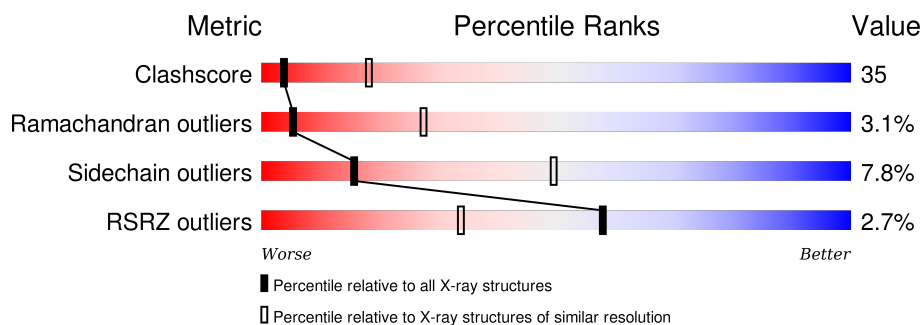
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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 $\leq 5\%$. 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	483	
2	B	152	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4224 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 Chromosome partition protein mukB, Linker.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	0	0	0
			3446	2178	608	646	14			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	GLY	-	EXPRESSION TAG	UNP Q7VL96
A	31	HIS	-	EXPRESSION TAG	UNP Q7VL96
A	32	MET	-	EXPRESSION TAG	UNP Q7VL96
A	160	THR	ALA	SEE REMARK 999	UNP Q7VL96
A	1347	ILE	VAL	SEE REMARK 999	UNP Q7VL96
A	1383	TYR	ASP	SEE REMARK 999	UNP Q7VL96
A	1435	GLN	GLU	ENGINEERED	UNP Q7VL96
A	1470	ARG	HIS	SEE REMARK 999	UNP Q7VL96

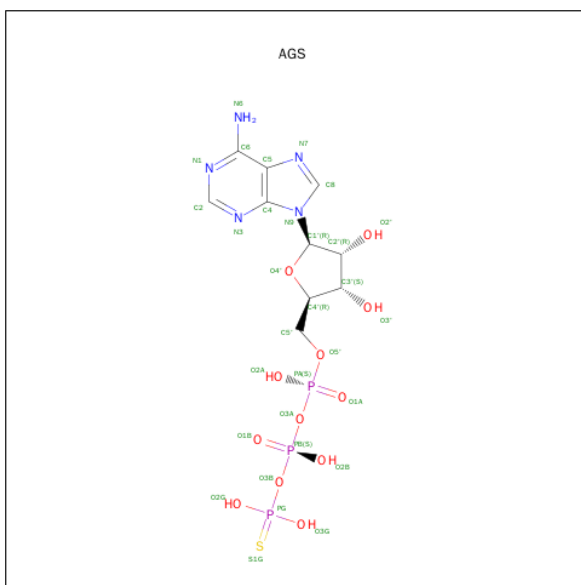
- Molecule 2 is a protein called Chromosome partition protein mukF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	90	Total	C	N	O	S	0	0	0
			716	452	128	135	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	372	ASN	ASP	SEE REMARK 999	UNP Q7VL94
B	384	GLN	ARG	SEE REMARK 999	UNP Q7VL94

- Molecule 3 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	23	Total O 23 23	0	0
5	B	7	Total O 7 7	0	0

A418	Y419	Y420	P421	V422	H423	Q424	P425	I426	D427	D428	F429	S430	A431	A432	V433	Q434	A435	H436	L437	I438	D439	Q440	Y441	D442	K443

4 Data and refinement statistics

Property	Value	Source
Space group	P 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	58.52Å 180.20Å 138.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.10 30.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	89.0 (30.00-3.10) 90.2 (30.00-3.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.01 (at 3.11Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.259 , 0.291 0.251 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	53.4	Xtriage
Anisotropy	0.518	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 59.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 24715 reflections	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	4224	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, AGS

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	0.43	1/3494 (0.0%)	0.67	1/4704 (0.0%)
2	B	0.37	0/731	0.62	0/996
All	All	0.42	1/4225 (0.0%)	0.66	1/5700 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	32	MET	SD-CE	6.39	2.13	1.77

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	107	GLY	N-CA-C	5.00	125.61	113.10

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	3446	0	3514	248	0
2	B	716	0	697	61	0
3	A	31	0	12	5	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	23	0	0	2	0
5	B	7	0	0	0	0
All	All	4224	0	4223	294	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 35.

All (294) 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:32:MET:SD	1:A:32:MET:CE	2.13	1.37
2:B:354:ASP:HB2	2:B:394:ARG:HD3	1.25	1.11
1:A:1435:GLN:HA	1:A:1435:GLN:HE21	1.16	1.03
1:A:1433:LEU:HB3	1:A:1460:ILE:HG22	1.47	0.93
1:A:1287:ASN:HD21	1:A:1303:LEU:H	1.14	0.93
1:A:131:ILE:HD13	1:A:210:LEU:HB3	1.49	0.92
1:A:253:GLU:HG2	1:A:1369:ARG:HH11	1.37	0.90
1:A:1435:GLN:HA	1:A:1435:GLN:NE2	1.89	0.88
1:A:1367:ASP:HB3	1:A:1370:ASN:HD22	1.40	0.85
1:A:1481:LEU:HD22	2:B:411:MET:HE1	1.58	0.85
1:A:169:GLU:HG3	1:A:178:LEU:HD22	1.62	0.82
1:A:83:ILE:HD11	1:A:230:ILE:HD12	1.63	0.80
1:A:1302:ARG:HG3	1:A:1385:TRP:CZ3	2.16	0.80
2:B:386:GLN:HG3	2:B:402:ILE:HD13	1.62	0.79
1:A:216:ARG:HH12	1:A:1420:MET:HE2	1.48	0.78
2:B:426:ILE:HG22	2:B:427:ASP:H	1.47	0.78
1:A:195:LYS:HD2	1:A:197:TYR:CE1	2.18	0.77
2:B:414:GLN:HA	2:B:417:GLN:HG2	1.66	0.76
1:A:1287:ASN:ND2	1:A:1303:LEU:H	1.82	0.76
1:A:131:ILE:CD1	1:A:210:LEU:HB3	2.14	0.76
2:B:394:ARG:O	2:B:398:VAL:HG23	1.86	0.75
1:A:45:ASN:O	1:A:113:LYS:HB2	1.86	0.75
1:A:123:THR:HG21	1:A:212:ILE:HG12	1.69	0.74
1:A:1411:GLN:NE2	1:A:1454:LEU:HD21	2.03	0.74
2:B:382:VAL:O	2:B:386:GLN:HG2	1.88	0.74
1:A:1441:ALA:HA	1:A:1444:ILE:HG22	1.71	0.72
1:A:1464:GLU:HG2	1:A:1465:ASN:N	2.04	0.72
1:A:247:ARG:HB2	1:A:251:LEU:HD22	1.72	0.72
1:A:1415:GLU:HG2	1:A:1418:ARG:CZ	2.19	0.72
1:A:1441:ALA:O	1:A:1444:ILE:HG22	1.90	0.72
1:A:1430:LEU:O	1:A:1431:LEU:HD12	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:LEU:HD13	1:A:1303:LEU:HD11	1.72	0.71
1:A:228:LYS:HE3	1:A:228:LYS:HA	1.71	0.71
2:B:391:PRO:C	2:B:393:SER:H	1.92	0.70
1:A:1302:ARG:NH2	1:A:1377:GLU:OE1	2.23	0.70
1:A:109:TYR:CE2	1:A:139:GLN:HB3	2.26	0.70
1:A:253:GLU:HG2	1:A:1369:ARG:NH1	2.06	0.69
1:A:1304:VAL:HG21	1:A:1377:GLU:OE2	1.92	0.69
1:A:125:ASN:ND2	1:A:210:LEU:O	2.23	0.69
2:B:391:PRO:O	2:B:393:SER:N	2.26	0.69
1:A:84:PRO:HB3	1:A:135:VAL:HG21	1.74	0.68
1:A:83:ILE:HD11	1:A:230:ILE:CD1	2.22	0.68
1:A:120:VAL:HG21	1:A:167:PHE:CE2	2.29	0.68
1:A:47:ASN:HA	1:A:113:LYS:HE2	1.75	0.68
1:A:135:VAL:HG13	1:A:149:ILE:HG23	1.75	0.67
1:A:125:ASN:HB2	1:A:129:GLN:HB2	1.76	0.66
1:A:47:ASN:HA	1:A:113:LYS:CE	2.26	0.66
1:A:42:THR:HA	1:A:52:ARG:O	1.96	0.65
1:A:43:LEU:HD22	1:A:46:TRP:CD2	2.32	0.64
1:A:216:ARG:HH22	1:A:1420:MET:HE3	1.63	0.64
1:A:1376:VAL:HG21	1:A:1405:ILE:HD12	1.79	0.64
1:A:80:THR:HG21	1:A:137:LEU:HD21	1.81	0.63
1:A:117:CYS:HB2	1:A:137:LEU:O	1.97	0.63
1:A:215:LYS:HG2	1:A:216:ARG:H	1.64	0.63
1:A:67:ASN:N	5:A:2015:HOH:O	2.32	0.63
1:A:249:TYR:O	1:A:1409:VAL:HG13	1.99	0.62
1:A:1441:ALA:HA	1:A:1444:ILE:CG2	2.29	0.62
1:A:1266:GLU:HG2	1:A:1318:LEU:O	2.00	0.62
1:A:88:LEU:HD23	1:A:227:TYR:CB	2.29	0.62
1:A:1379:LEU:HD12	1:A:1384:GLY:O	1.99	0.62
1:A:206:PHE:CZ	1:A:210:LEU:HD12	2.35	0.62
1:A:1272:LEU:O	1:A:1276:ILE:HG13	1.99	0.62
2:B:379:LEU:H	2:B:379:LEU:HD12	1.64	0.61
2:B:391:PRO:C	2:B:393:SER:N	2.54	0.61
1:A:1464:GLU:HG2	1:A:1465:ASN:H	1.63	0.61
1:A:246:LEU:HD22	1:A:250:LEU:HD12	1.81	0.61
1:A:1341:ALA:O	1:A:1345:LYS:HG3	2.01	0.61
1:A:169:GLU:CG	1:A:178:LEU:HD22	2.29	0.61
1:A:217:LEU:HD12	1:A:217:LEU:N	2.15	0.61
2:B:369:HIS:HA	2:B:372:ASN:ND2	2.16	0.60
1:A:141:ALA:O	1:A:143:ARG:N	2.35	0.60
1:A:144:ASP:CG	1:A:145:LYS:H	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:THR:HG23	3:A:2001:AGS:O1A	2.01	0.60
1:A:1467:SER:H	2:B:400:ARG:NH2	2.00	0.60
1:A:1376:VAL:HG11	1:A:1405:ILE:HD11	1.83	0.60
1:A:131:ILE:HD13	1:A:210:LEU:CB	2.29	0.59
1:A:1467:SER:N	2:B:400:ARG:NH2	2.49	0.59
2:B:366:GLU:O	2:B:369:HIS:HB3	2.02	0.59
1:A:1311:HIS:HB3	1:A:1371:TYR:CD2	2.37	0.59
1:A:1367:ASP:HB3	1:A:1370:ASN:ND2	2.13	0.59
2:B:426:ILE:HG22	2:B:427:ASP:N	2.16	0.59
1:A:1338:GLU:O	1:A:1341:ALA:HB3	2.03	0.59
1:A:1403:MET:HG2	1:A:1447:LEU:HD21	1.84	0.59
1:A:178:LEU:H	1:A:178:LEU:HD23	1.68	0.58
1:A:219:SER:HB3	1:A:222:ASP:OD1	2.04	0.58
1:A:109:TYR:O	1:A:139:GLN:NE2	2.37	0.58
1:A:1417:SER:HB2	1:A:1421:ARG:NH2	2.18	0.58
1:A:63:LEU:HD23	1:A:1474:TYR:HB2	1.85	0.58
1:A:1476:LEU:HD12	1:A:1476:LEU:N	2.19	0.58
1:A:1302:ARG:HG3	1:A:1385:TRP:CH2	2.39	0.58
1:A:1435:GLN:CA	1:A:1435:GLN:HE21	1.97	0.58
1:A:1295:PHE:CD2	1:A:1400:GLY:HA3	2.39	0.57
1:A:1422:ALA:HB3	1:A:1425:ILE:HD12	1.86	0.57
2:B:425:PRO:HA	2:B:431:ALA:O	2.05	0.57
1:A:240:SER:OG	1:A:244:LYS:HE3	2.03	0.57
1:A:155:GLN:O	1:A:156:ASN:HB2	2.04	0.57
1:A:230:ILE:HG23	1:A:1432:PHE:HE2	1.70	0.57
1:A:1273:ARG:C	1:A:1275:THR:H	2.08	0.57
1:A:1474:TYR:CE2	1:A:1491:GLY:HA3	2.40	0.56
1:A:45:ASN:HB3	1:A:117:CYS:SG	2.45	0.56
1:A:1441:ALA:C	1:A:1444:ILE:HG22	2.26	0.56
1:A:1415:GLU:HG2	1:A:1418:ARG:NH1	2.21	0.56
1:A:1440:ASP:OD2	1:A:1442:MET:HB3	2.05	0.56
1:A:153:SER:HB3	1:A:197:TYR:HE2	1.71	0.56
1:A:1441:ALA:CA	1:A:1444:ILE:HG22	2.35	0.56
1:A:1466:ILE:HG23	2:B:400:ARG:HH12	1.71	0.55
2:B:378:ASN:O	2:B:380:GLY:N	2.38	0.55
1:A:1469:GLU:OE2	1:A:1496:GLY:HA2	2.05	0.55
1:A:1490:VAL:HG11	2:B:403:VAL:HG13	1.88	0.55
1:A:215:LYS:HG2	1:A:216:ARG:N	2.21	0.55
1:A:1492:LEU:HD11	2:B:403:VAL:HG21	1.87	0.55
1:A:233:SER:HB3	1:A:1406:LEU:HD21	1.88	0.55
2:B:371:ARG:HA	2:B:441:TYR:CE2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:ILE:CD1	1:A:230:ILE:HD12	2.34	0.55
1:A:251:LEU:HD21	1:A:1372:LEU:HD22	1.88	0.55
2:B:373:THR:HG22	2:B:374:ALA:H	1.72	0.55
1:A:47:ASN:HB3	1:A:111:LYS:O	2.06	0.54
1:A:88:LEU:HD23	1:A:227:TYR:HB3	1.89	0.54
1:A:55:ASP:HB2	1:A:1474:TYR:OH	2.07	0.54
1:A:247:ARG:HD3	1:A:1369:ARG:O	2.07	0.54
1:A:135:VAL:CG1	1:A:149:ILE:HG23	2.37	0.54
1:A:251:LEU:HD23	1:A:1369:ARG:HA	1.90	0.54
1:A:209:ASP:C	1:A:211:GLY:H	2.11	0.54
1:A:45:ASN:ND2	1:A:113:LYS:HB3	2.24	0.53
1:A:1363:GLU:O	1:A:1363:GLU:HG2	2.08	0.53
2:B:354:ASP:HB2	2:B:394:ARG:CD	2.17	0.53
1:A:1435:GLN:HE22	1:A:1463:PRO:HB3	1.71	0.53
2:B:384:GLN:HA	2:B:426:ILE:HG21	1.90	0.53
1:A:169:GLU:OE1	1:A:176:ARG:HD3	2.10	0.52
1:A:73:THR:HG22	1:A:111:LYS:HZ2	1.75	0.52
1:A:1376:VAL:HG11	1:A:1405:ILE:CD1	2.40	0.52
1:A:54:PHE:HD2	1:A:1474:TYR:CD1	2.28	0.52
1:A:125:ASN:HB3	1:A:127:ARG:H	1.76	0.51
1:A:249:TYR:HB3	1:A:1409:VAL:HG13	1.93	0.51
1:A:1293:ILE:HG23	1:A:1294:ALA:N	2.26	0.51
1:A:1336:PHE:O	1:A:1339:ALA:HB3	2.10	0.51
1:A:1287:ASN:HD21	1:A:1303:LEU:N	1.95	0.51
1:A:1462:ALA:C	1:A:1464:GLU:N	2.65	0.51
1:A:1474:TYR:CD2	1:A:1491:GLY:HA3	2.46	0.51
1:A:1474:TYR:HD2	1:A:1491:GLY:CA	2.24	0.51
1:A:1294:ALA:H	1:A:1446:THR:HG21	1.75	0.51
1:A:1488:HIS:CD2	2:B:407:VAL:HG13	2.46	0.51
1:A:1446:THR:O	1:A:1450:LEU:HG	2.11	0.50
1:A:1293:ILE:HG12	1:A:1295:PHE:HE1	1.75	0.50
1:A:136:ARG:NH2	1:A:148:ASP:OD2	2.45	0.50
1:A:1474:TYR:CD2	1:A:1491:GLY:CA	2.94	0.50
1:A:1403:MET:CE	1:A:1431:LEU:HD23	2.41	0.50
1:A:1488:HIS:CD2	2:B:407:VAL:HG22	2.47	0.50
1:A:225:LYS:NZ	1:A:248:ASP:HB3	2.27	0.50
1:A:1287:ASN:OD1	1:A:1303:LEU:HB2	2.11	0.50
2:B:390:TYR:N	2:B:390:TYR:CD1	2.80	0.50
1:A:108:LEU:HD23	1:A:147:VAL:HG21	1.92	0.50
1:A:1298:VAL:HG21	1:A:1397:GLU:HB3	1.94	0.50
1:A:200:ILE:HG23	1:A:201:THR:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:403:VAL:O	2:B:407:VAL:HG23	2.13	0.49
1:A:79:VAL:HG21	1:A:234:LEU:HD11	1.94	0.49
2:B:372:ASN:O	2:B:373:THR:O	2.30	0.49
1:A:216:ARG:HH22	1:A:1420:MET:CE	2.26	0.49
2:B:379:LEU:H	2:B:379:LEU:CD1	2.25	0.49
1:A:1298:VAL:CG2	1:A:1397:GLU:HB3	2.42	0.49
2:B:397:ASP:O	2:B:401:ILE:HG13	2.12	0.49
1:A:253:GLU:CG	1:A:1369:ARG:NH1	2.75	0.49
1:A:110:GLY:HA3	3:A:2001:AGS:N1	2.27	0.49
1:A:261:PHE:HE1	1:A:1268:VAL:HG22	1.76	0.49
1:A:136:ARG:HD3	1:A:180:LEU:HG	1.93	0.49
1:A:1414:GLU:OE1	1:A:1429:ARG:NH1	2.46	0.49
2:B:416:HIS:CD2	2:B:416:HIS:N	2.81	0.49
1:A:1318:LEU:HD11	1:A:1340:LEU:HD21	1.94	0.49
2:B:376:PRO:HA	2:B:441:TYR:OH	2.11	0.49
1:A:207:MET:HB3	1:A:213:LEU:HD23	1.94	0.49
1:A:249:TYR:HB3	1:A:1409:VAL:CG1	2.43	0.49
1:A:1314:LEU:HD11	1:A:1365:LEU:HD13	1.94	0.48
1:A:217:LEU:N	1:A:217:LEU:CD1	2.76	0.48
1:A:93:ASN:HD22	1:A:95:THR:H	1.61	0.48
2:B:423:TRP:CD2	2:B:434:GLN:HB2	2.49	0.48
2:B:371:ARG:HE	2:B:371:ARG:C	2.17	0.48
2:B:413:SER:OG	2:B:414:GLN:N	2.46	0.48
1:A:1467:SER:HB2	1:A:1468:PRO:CD	2.43	0.48
1:A:1405:ILE:O	1:A:1409:VAL:HG23	2.13	0.48
1:A:46:TRP:CH2	1:A:77:GLY:HA2	2.48	0.48
2:B:409:LEU:HD12	2:B:409:LEU:N	2.29	0.48
1:A:1380:ARG:C	1:A:1382:ALA:H	2.17	0.48
1:A:1494:GLY:HA3	2:B:430:SER:O	2.14	0.48
1:A:35:ARG:NH1	1:A:1427:PRO:O	2.46	0.47
1:A:44:ILE:HB	1:A:118:TYR:HB2	1.95	0.47
1:A:216:ARG:NH1	1:A:216:ARG:HG3	2.29	0.47
1:A:1317:ALA:HA	1:A:1321:GLN:OE1	2.14	0.47
1:A:190:THR:HG22	1:A:191:ALA:N	2.30	0.47
1:A:167:PHE:CD1	1:A:183:LEU:HD11	2.50	0.47
1:A:190:THR:HG22	1:A:191:ALA:H	1.80	0.47
1:A:59:LEU:HD13	1:A:1452:GLU:HG2	1.97	0.47
1:A:1293:ILE:HG22	1:A:1299:LYS:C	2.34	0.47
2:B:399:ALA:O	2:B:403:VAL:HG23	2.14	0.47
1:A:246:LEU:HD22	1:A:250:LEU:CD1	2.43	0.46
1:A:1494:GLY:HA3	2:B:431:ALA:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1372:LEU:HD12	1:A:1372:LEU:N	2.30	0.46
1:A:1478:ARG:NH1	3:A:2001:AGS:H4'	2.31	0.46
1:A:1273:ARG:C	1:A:1275:THR:N	2.69	0.46
1:A:1336:PHE:O	1:A:1339:ALA:N	2.49	0.46
1:A:1417:SER:HB2	1:A:1421:ARG:HH22	1.79	0.46
1:A:1309:ASP:O	1:A:1312:SER:HB3	2.15	0.46
1:A:1467:SER:N	2:B:400:ARG:HH22	2.13	0.45
1:A:97:ALA:C	1:A:99:SER:H	2.19	0.45
1:A:1299:LYS:HD2	1:A:1299:LYS:N	2.31	0.45
2:B:370:PHE:HB3	2:B:375:GLN:O	2.16	0.45
2:B:415:ASP:HA	2:B:436:HIS:ND1	2.31	0.45
1:A:1492:LEU:CD2	2:B:433:VAL:HG13	2.47	0.45
1:A:261:PHE:HZ	1:A:1336:PHE:CD2	2.34	0.45
1:A:208:PHE:CE2	1:A:216:ARG:HG2	2.51	0.45
1:A:68:GLY:HA2	3:A:2001:AGS:H5'1	1.99	0.45
1:A:70:GLY:HA2	3:A:2001:AGS:O1A	2.17	0.45
1:A:1419:ARG:C	1:A:1421:ARG:H	2.20	0.45
1:A:226:PHE:CE2	1:A:230:ILE:HD11	2.52	0.45
2:B:397:ASP:N	2:B:397:ASP:OD2	2.49	0.45
1:A:184:LYS:O	1:A:185:GLU:C	2.55	0.45
1:A:1298:VAL:C	1:A:1299:LYS:HD2	2.37	0.45
1:A:112:LEU:N	1:A:112:LEU:CD1	2.79	0.45
1:A:1464:GLU:CG	1:A:1465:ASN:N	2.79	0.45
1:A:131:ILE:CD1	1:A:210:LEU:HD13	2.47	0.45
1:A:144:ASP:CG	1:A:145:LYS:N	2.69	0.45
1:A:48:GLY:H	1:A:113:LYS:HE2	1.81	0.44
1:A:1340:LEU:HD23	1:A:1343:LEU:HD12	1.98	0.44
1:A:1335:SER:O	1:A:1338:GLU:HB3	2.17	0.44
1:A:137:LEU:HD12	1:A:137:LEU:N	2.32	0.44
2:B:404:ASP:O	2:B:408:LYS:HG3	2.17	0.44
1:A:1318:LEU:HD21	1:A:1343:LEU:CD1	2.47	0.44
1:A:78:PHE:CD2	1:A:78:PHE:C	2.90	0.44
1:A:1462:ALA:C	1:A:1464:GLU:H	2.21	0.44
1:A:162:SER:HA	5:A:2031:HOH:O	2.17	0.44
1:A:108:LEU:CD2	1:A:147:VAL:HG21	2.48	0.44
1:A:112:LEU:N	1:A:112:LEU:HD12	2.32	0.44
1:A:1416:GLU:O	1:A:1416:GLU:HG2	2.17	0.44
1:A:1303:LEU:HD23	1:A:1303:LEU:HA	1.78	0.43
1:A:84:PRO:HB2	1:A:149:ILE:HG21	2.00	0.43
1:A:1387:ARG:CZ	1:A:1387:ARG:HB2	2.49	0.43
1:A:100:THR:HG22	1:A:100:THR:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:386:GLN:HG3	2:B:402:ILE:CD1	2.42	0.43
1:A:1490:VAL:HG11	2:B:403:VAL:CG1	2.49	0.43
1:A:62:THR:HG21	1:A:1467:SER:CB	2.48	0.43
2:B:371:ARG:HB2	2:B:409:LEU:HD23	1.99	0.43
1:A:1481:LEU:HD22	2:B:411:MET:CE	2.38	0.43
1:A:218:ARG:HH11	1:A:218:ARG:HG2	1.82	0.43
1:A:209:ASP:C	1:A:211:GLY:N	2.72	0.43
1:A:1435:GLN:HE22	1:A:1463:PRO:CB	2.32	0.43
1:A:131:ILE:HD13	1:A:210:LEU:HD13	2.00	0.43
1:A:63:LEU:O	1:A:71:LYS:HD2	2.19	0.43
1:A:233:SER:HB3	1:A:1406:LEU:CD2	2.49	0.42
1:A:220:SER:OG	1:A:223:ARG:NH2	2.52	0.42
2:B:420:TYR:CD1	2:B:421:PRO:HD2	2.54	0.42
2:B:413:SER:C	2:B:415:ASP:H	2.22	0.42
1:A:1379:LEU:HD12	1:A:1384:GLY:C	2.39	0.42
2:B:378:ASN:O	2:B:381:ALA:N	2.52	0.42
1:A:1464:GLU:OE1	1:A:1466:ILE:HB	2.20	0.42
1:A:1293:ILE:HG12	1:A:1295:PHE:CE1	2.54	0.42
2:B:438:ILE:O	2:B:438:ILE:HG22	2.18	0.42
2:B:371:ARG:HG2	2:B:441:TYR:CD2	2.55	0.42
1:A:62:THR:HG21	1:A:1467:SER:HB2	2.02	0.42
1:A:1342:MET:O	1:A:1346:ARG:HG3	2.20	0.42
1:A:1313:ILE:O	1:A:1316:ASN:HB3	2.20	0.42
1:A:216:ARG:HD2	1:A:218:ARG:HH11	1.84	0.42
1:A:1464:GLU:CD	1:A:1466:ILE:HB	2.40	0.42
1:A:1302:ARG:HH21	1:A:1377:GLU:CD	2.20	0.42
2:B:417:GLN:O	2:B:418:ALA:HB3	2.20	0.42
1:A:80:THR:HA	1:A:89:LEU:HD11	2.01	0.42
1:A:1476:LEU:CD1	1:A:1476:LEU:N	2.83	0.41
1:A:1401:THR:O	1:A:1404:SER:HB2	2.20	0.41
1:A:1481:LEU:CD2	2:B:411:MET:HE1	2.41	0.41
1:A:240:SER:O	1:A:244:LYS:HG3	2.20	0.41
1:A:261:PHE:CE1	1:A:1268:VAL:HG22	2.54	0.41
1:A:108:LEU:HD23	1:A:109:TYR:N	2.35	0.41
1:A:196:PRO:O	1:A:196:PRO:HG2	2.20	0.41
1:A:228:LYS:CE	1:A:228:LYS:HA	2.44	0.41
1:A:1435:GLN:HE22	1:A:1463:PRO:CG	2.33	0.41
1:A:178:LEU:N	1:A:178:LEU:HD23	2.33	0.41
1:A:1296:GLY:HA3	1:A:1397:GLU:HG2	2.02	0.41
1:A:1363:GLU:HG3	1:A:1366:LEU:HD22	2.03	0.41
1:A:237:GLY:HA2	1:A:1399:ILE:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1380:ARG:O	1:A:1382:ALA:N	2.54	0.41
1:A:1287:ASN:ND2	1:A:1302:ARG:HB3	2.36	0.41
1:A:226:PHE:O	1:A:230:ILE:HG13	2.19	0.41
1:A:48:GLY:HA2	1:A:1485:GLU:O	2.21	0.41
2:B:405:GLN:O	2:B:409:LEU:HD13	2.21	0.41
1:A:1282:ARG:HE	1:A:1282:ARG:HB3	1.67	0.41
1:A:60:VAL:O	1:A:1471:GLY:HA3	2.21	0.41
1:A:1372:LEU:HD12	1:A:1372:LEU:H	1.85	0.41
1:A:1430:LEU:HA	1:A:1457:GLN:O	2.20	0.41
1:A:1295:PHE:O	1:A:1397:GLU:HG2	2.21	0.41
1:A:1431:LEU:HD22	1:A:1456:MET:SD	2.62	0.40
2:B:360:VAL:O	2:B:364:GLN:HG3	2.21	0.40
1:A:1407:LEU:HD23	1:A:1407:LEU:HA	1.92	0.40
1:A:106:LYS:HA	1:A:106:LYS:HD3	1.85	0.40
2:B:412:ALA:HB3	2:B:415:ASP:HB2	2.04	0.40
1:A:249:TYR:CD1	1:A:249:TYR:N	2.90	0.40
1:A:61:THR:O	1:A:1459:LEU:HA	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	429/483 (89%)	364 (85%)	55 (13%)	10 (2%)	8	35
2	B	88/152 (58%)	66 (75%)	16 (18%)	6 (7%)	1	8
All	All	517/635 (81%)	430 (83%)	71 (14%)	16 (3%)	5	27

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	141	ALA

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Mol	Chain	Res	Type
1	A	142	GLY
2	B	373	THR
2	B	379	LEU
2	B	439	ASP
1	A	104	ARG
1	A	186	LYS
1	A	1420	MET
2	B	392	GLN
1	A	1381	GLY
1	A	1422	ALA
1	A	185	GLU
2	B	372	ASN
1	A	256	GLY
2	B	355	VAL
1	A	236	GLY

5.3.2 Protein sidechains ⓘ

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	375/413 (91%)	351 (94%)	24 (6%)	22	57
2	B	75/129 (58%)	64 (85%)	11 (15%)	4	16
All	All	450/542 (83%)	415 (92%)	35 (8%)	16	49

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	MET
1	A	58	GLU
1	A	78	PHE
1	A	82	LEU
1	A	108	LEU
1	A	113	LYS
1	A	125	ASN
1	A	153	SER

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Mol	Chain	Res	Type
1	A	170	GLN
1	A	173	ASN
1	A	178	LEU
1	A	213	LEU
1	A	214	PRO
1	A	216	ARG
1	A	228	LYS
1	A	246	LEU
1	A	247	ARG
1	A	1277	GLN
1	A	1292	ASN
1	A	1293	ILE
1	A	1383	TYR
1	A	1435	GLN
1	A	1447	LEU
1	A	1476	LEU
2	B	371	ARG
2	B	390	TYR
2	B	394	ARG
2	B	395	HIS
2	B	397	ASP
2	B	416	HIS
2	B	422	VAL
2	B	427	ASP
2	B	433	VAL
2	B	439	ASP
2	B	440	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	ASN
1	A	93	ASN
1	A	155	GLN
1	A	1277	GLN
1	A	1280	GLN
1	A	1287	ASN
1	A	1291	GLN
1	A	1370	ASN
1	A	1411	GLN
1	A	1435	GLN
2	B	364	GLN

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Mol	Chain	Res	Type
2	B	372	ASN
2	B	405	GLN
2	B	416	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 ⓘ

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	AGS	A	2001	4	24,33,33	2.09	9 (37%)	28,52,52	1.64	5 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AGS	A	2001	4	-	0/15/38/38	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2001	AGS	PG-S1G	-4.70	1.81	1.90
3	A	2001	AGS	O4'-C4'	-2.82	1.38	1.45
3	A	2001	AGS	PG-O3G	-2.13	1.47	1.55
3	A	2001	AGS	O5'-C5'	-2.08	1.36	1.44
3	A	2001	AGS	C5-C4	2.30	1.45	1.40
3	A	2001	AGS	C2-N3	2.86	1.37	1.32
3	A	2001	AGS	C6-N6	3.58	1.46	1.34
3	A	2001	AGS	C4-N3	3.61	1.40	1.35
3	A	2001	AGS	C2-N1	3.73	1.41	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2001	AGS	N3-C2-N1	-3.94	125.88	128.89
3	A	2001	AGS	O3A-PA-O5'	-3.59	93.41	102.94
3	A	2001	AGS	C1'-N9-C4	-2.25	123.54	126.94
3	A	2001	AGS	C4'-O4'-C1'	2.73	112.72	109.72
3	A	2001	AGS	C4-C5-N7	3.31	112.52	109.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2001	AGS	5	0

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(Å ²)	Q<0.9
1	A	437/483 (90%)	-0.25	9 (2%) 67 44	15, 44, 106, 130	0
2	B	90/152 (59%)	0.01	5 (5%) 28 11	27, 62, 102, 123	0
All	All	527/635 (82%)	-0.21	14 (2%) 58 34	15, 46, 106, 130	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	259	GLN	4.3
1	A	1321	GLN	4.0
1	A	1338	GLU	3.4
1	A	262	GLN	3.2
2	B	443	LYS	3.2
1	A	261	PHE	3.2
2	B	354	ASP	3.0
1	A	1337	SER	2.8
2	B	366	GLU	2.7
2	B	358	GLN	2.5
1	A	1336	PHE	2.4
1	A	173	ASN	2.4
2	B	428	ASP	2.3
1	A	100	THR	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	LLDF	B-factors(\AA^2)	Q<0.9
3	AGS	A	2001	31/31	0.96	0.19	0.98	21,28,33,39	0
4	MG	A	2011	1/1	0.93	0.47	-	38,38,38,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.