Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:08 PM GMT

PDB ID	:	1S9I
Title	:	X-ray structure of the human mitogen-activated protein kinase kinase 2 (MEK2)in a complex with ligand and MgATP
Authors	:	Ohren, J.F.; Chen, H.; Pavlovsky, A.; Whitehead, C.; Yan, C.; McConnell, P.; Delaney, A.; Dudley, D.T.; Sebolt-Leopold, J.; Hasemann, C.A.
Deposited on	:	2004-02-04
Resolution	:	3.20 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 (1)) were used in the production of this report:

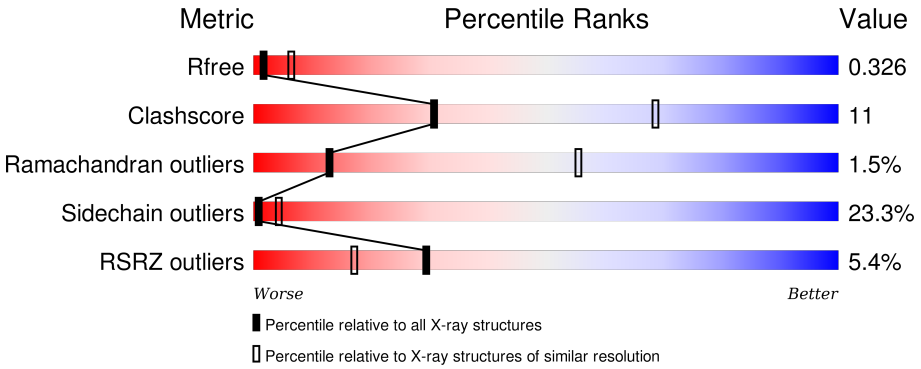
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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	354	3% 51% 27% 8% • 14%
1	B	354	6% 51% 26% 5% 18%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4812 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 Dual specificity mitogen-activated protein kinase kinase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	303	Total	C	N	O	S	0	0	0
			2385	1518	416	437	14			
1	B	291	Total	C	N	O	S	0	0	0
			2301	1466	399	422	14			

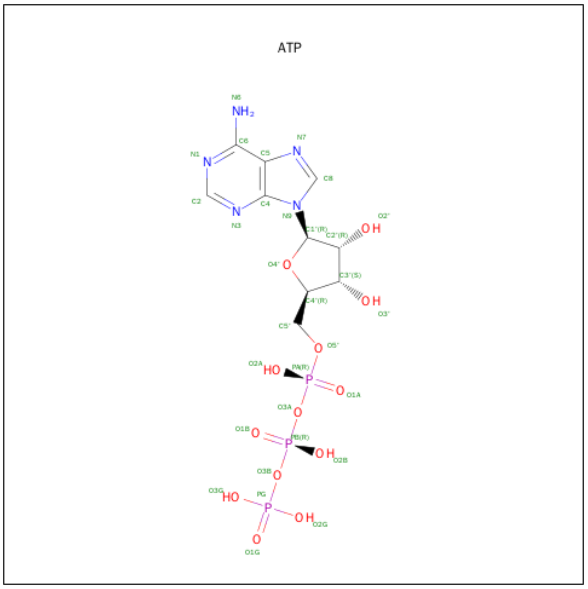
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	401	LEU	-	CLONING ARTIFACT	UNP P36507
A	402	GLU	-	CLONING ARTIFACT	UNP P36507
A	403	HIS	-	EXPRESSION TAG	UNP P36507
A	404	HIS	-	EXPRESSION TAG	UNP P36507
A	405	HIS	-	EXPRESSION TAG	UNP P36507
A	406	HIS	-	EXPRESSION TAG	UNP P36507
A	407	HIS	-	EXPRESSION TAG	UNP P36507
A	408	HIS	-	EXPRESSION TAG	UNP P36507
B	401	LEU	-	CLONING ARTIFACT	UNP P36507
B	402	GLU	-	CLONING ARTIFACT	UNP P36507
B	403	HIS	-	EXPRESSION TAG	UNP P36507
B	404	HIS	-	EXPRESSION TAG	UNP P36507
B	405	HIS	-	EXPRESSION TAG	UNP P36507
B	406	HIS	-	EXPRESSION TAG	UNP P36507
B	407	HIS	-	EXPRESSION TAG	UNP P36507
B	408	HIS	-	EXPRESSION TAG	UNP P36507

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

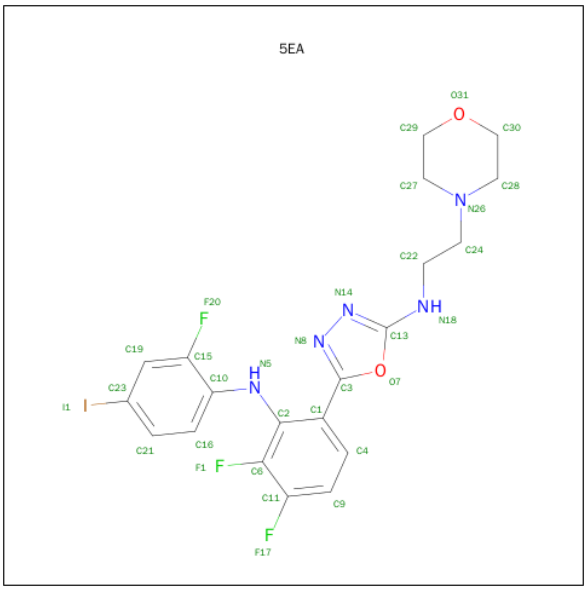
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 4 is 5-{3,4-DIFLUORO-2-[(2-FLUORO-4-IODOPHENYL)AMINO]PHENYL}-N-(2-MORPHOLIN-4-YLETHYL)-1,3,4-OXADIAZOL-2-AMINE (three-letter code: 5EA) (formula: $C_{20}H_{19}F_3IN_5O_2$).



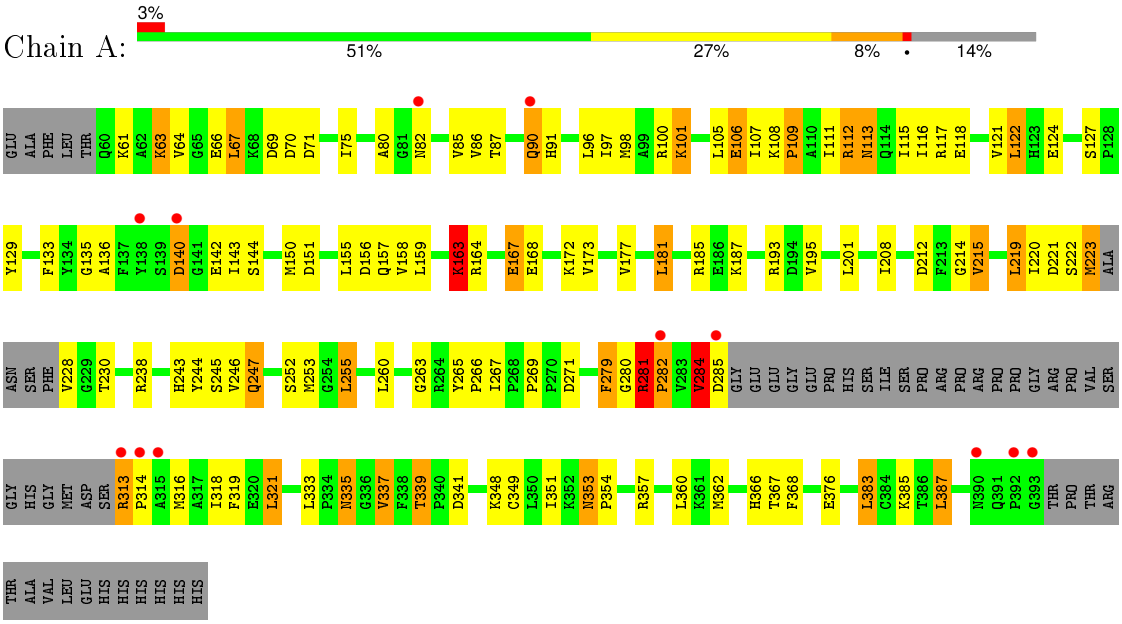
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	F	I	N	O	0	0
			31	20	3	1	5	2		
4	B	1	Total	C	F	I	N	O	0	0
			31	20	3	1	5	2		

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.

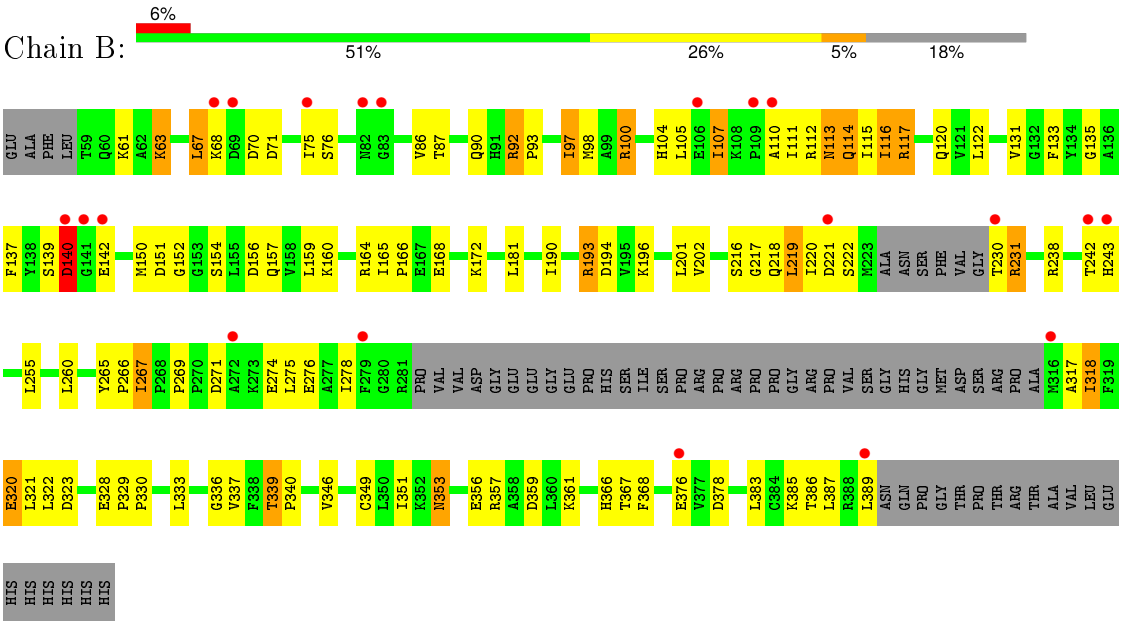
- Molecule 1: Dual specificity mitogen-activated protein kinase kinase 2

Chain A:



- Molecule 1: Dual specificity mitogen-activated protein kinase kinase 2

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	161.89Å 161.89Å 122.99Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	14.40 – 3.20 14.41 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (14.40-3.20) 99.9 (14.41-3.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.96 (at 3.18Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.290 , 0.364 0.267 , 0.326	Depositor DCC
R_{free} test set	802 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	72.8	Xtriage
Anisotropy	0.004	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 45.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 15951 reflections	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	4812	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 5EA, ATP

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	0.35	0/2432	0.68	9/3282 (0.3%)
1	B	0.34	0/2345	0.64	9/3161 (0.3%)
All	All	0.35	0/4777	0.66	18/6443 (0.3%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	71	ASP	CB-CG-OD2	5.87	123.58	118.30
1	B	323	ASP	CB-CG-OD2	5.84	123.56	118.30
1	A	151	ASP	CB-CG-OD2	5.84	123.56	118.30
1	A	341	ASP	CB-CG-OD2	5.83	123.55	118.30
1	A	140	ASP	CB-CG-OD2	5.80	123.52	118.30
1	A	70	ASP	CB-CG-OD2	5.56	123.31	118.30
1	A	212	ASP	CB-CG-OD2	5.54	123.28	118.30
1	A	221	ASP	CB-CG-OD2	5.41	123.17	118.30
1	B	378	ASP	CB-CG-OD2	5.33	123.10	118.30
1	A	69	ASP	CB-CG-OD2	5.29	123.07	118.30
1	B	194	ASP	CB-CG-OD2	5.28	123.05	118.30
1	A	156	ASP	CB-CG-OD2	5.25	123.03	118.30
1	B	151	ASP	CB-CG-OD2	5.20	122.98	118.30
1	B	140	ASP	CB-CG-OD2	5.13	122.91	118.30
1	B	221	ASP	CB-CG-OD2	5.08	122.88	118.30
1	B	71	ASP	CB-CG-OD2	5.05	122.85	118.30
1	B	70	ASP	CB-CG-OD2	5.03	122.83	118.30
1	B	271	ASP	CB-CG-OD2	5.03	122.83	118.30

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	2385	0	2418	62	0
1	B	2301	0	2335	43	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	31	0	12	0	0
3	B	31	0	12	0	0
4	A	31	0	19	1	0
4	B	31	0	19	2	0
All	All	4812	0	4815	105	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 11.

All (105) 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:313:ARG:HB3	1:A:314:PRO:CD	1.78	1.11
1:A:313:ARG:HB3	1:A:314:PRO:HD3	1.12	1.06
1:A:313:ARG:CB	1:A:314:PRO:HD3	2.01	0.88
1:A:108:LYS:N	1:A:109:PRO:HD3	2.02	0.75
1:B:92:ARG:HB3	1:B:93:PRO:HD3	1.76	0.66
1:A:366:HIS:HD2	1:A:368:PHE:H	1.44	0.65
1:A:177:VAL:O	1:A:181:LEU:HB2	1.97	0.65
1:A:214:GLY:HA3	1:A:220:ILE:HD11	1.79	0.64
1:B:265:TYR:CE2	1:B:267:ILE:HB	2.33	0.63
1:A:366:HIS:CD2	1:A:368:PHE:H	2.17	0.63
1:A:265:TYR:CE2	1:A:267:ILE:HB	2.36	0.61
1:B:75:ILE:HD11	1:B:90:GLN:HB2	1.83	0.60
1:B:349:CYS:O	1:B:357:ARG:HD2	2.01	0.60
1:A:353:ASN:HD22	1:A:354:PRO:HD2	1.68	0.58
1:A:349:CYS:O	1:A:357:ARG:HD2	2.04	0.58
1:B:100:ARG:HH21	1:B:137:PHE:HZ	1.51	0.58
1:A:281:ARG:N	1:A:282:PRO:CD	2.67	0.58
1:B:317:ALA:HB3	1:B:320:GLU:HB2	1.85	0.58
1:B:111:ILE:HA	1:B:114:GLN:HB2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:366:HIS:HD2	1:B:368:PHE:H	1.53	0.55
1:A:63:LYS:HD3	1:A:63:LYS:N	2.22	0.55
1:A:64:VAL:HG11	1:A:91:HIS:CE1	2.44	0.53
1:A:112:ARG:HA	1:A:115:ILE:HD12	1.90	0.52
1:A:105:LEU:HD21	1:A:222:SER:HB3	1.92	0.52
1:A:112:ARG:HE	1:A:113:ASN:HD22	1.57	0.51
1:A:219:LEU:O	1:A:223:MET:HG3	2.11	0.50
1:A:108:LYS:HG2	1:A:112:ARG:HD2	1.93	0.50
1:B:165:ILE:HD12	1:B:260:LEU:HD22	1.94	0.50
1:A:245:SER:OG	1:A:247:GLN:HG2	2.11	0.50
1:A:159:LEU:HD11	1:A:263:GLY:HA2	1.94	0.49
1:A:313:ARG:CB	1:A:314:PRO:CD	2.67	0.49
1:A:122:LEU:HB3	1:A:133:PHE:CD1	2.47	0.49
1:A:177:VAL:HG11	1:A:253:MET:HG3	1.93	0.49
1:A:281:ARG:N	1:A:282:PRO:HD3	2.26	0.49
1:B:333:LEU:HG	1:B:346:VAL:HG21	1.95	0.49
1:A:351:ILE:O	1:A:357:ARG:NH1	2.45	0.48
1:B:114:GLN:HG2	1:B:117:ARG:HH21	1.77	0.48
1:A:316:MET:HB2	1:A:321:LEU:HD23	1.95	0.48
1:A:159:LEU:HD22	1:A:260:LEU:HD23	1.94	0.48
1:B:154:SER:HB2	1:B:157:GLN:HG3	1.94	0.48
1:B:152:GLY:HA3	1:B:202:VAL:HG23	1.97	0.47
1:A:193:ARG:HA	1:A:244:TYR:CZ	2.50	0.47
1:B:231:ARG:HE	1:B:265:TYR:HB2	1.80	0.47
1:B:122:LEU:HD21	4:B:1002:5EA:H21	1.97	0.47
1:B:267:ILE:O	1:B:269:PRO:HD3	2.15	0.46
1:A:80:ALA:HB2	1:A:85:VAL:HG13	1.97	0.46
1:A:75:ILE:HD11	1:A:90:GLN:HB2	1.97	0.46
1:A:173:VAL:HA	1:A:208:ILE:HD13	1.96	0.46
1:A:280:GLY:HA2	1:A:281:ARG:HA	1.58	0.46
1:A:214:GLY:CA	1:A:220:ILE:HD11	2.46	0.46
1:A:150:MET:HG3	1:A:201:LEU:HD23	1.98	0.46
1:A:366:HIS:HD2	1:A:368:PHE:HB3	1.81	0.46
1:A:281:ARG:H	1:A:282:PRO:HD3	1.80	0.46
1:A:67:LEU:HD11	1:A:135:GLY:HA3	1.98	0.46
1:B:339:THR:HG22	1:B:340:PRO:HD2	1.98	0.46
1:A:348:LYS:HA	1:A:351:ILE:HD12	1.98	0.45
1:B:156:ASP:HA	1:B:159:LEU:HB3	1.99	0.45
1:A:127:SER:C	1:A:129:TYR:H	2.19	0.45
1:A:108:LYS:N	1:A:109:PRO:CD	2.78	0.45
1:B:216:SER:OG	1:B:219:LEU:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:ILE:HA	1:B:166:PRO:HD3	1.81	0.45
1:A:255:LEU:HD11	1:A:267:ILE:HD11	1.98	0.45
1:B:366:HIS:CD2	1:B:368:PHE:H	2.35	0.44
1:A:163:LYS:H	1:A:163:LYS:HG2	1.59	0.44
1:A:279:PHE:CD1	1:A:279:PHE:N	2.84	0.44
1:B:86:VAL:HA	1:B:100:ARG:O	2.17	0.44
1:B:353:ASN:HD22	1:B:353:ASN:C	2.21	0.44
4:B:1002:5EA:H16	4:B:1002:5EA:C6	2.47	0.44
1:A:265:TYR:HA	1:A:266:PRO:HD3	1.81	0.44
1:B:113:ASN:HD22	1:B:117:ARG:HD3	1.81	0.44
1:A:177:VAL:HG12	1:A:181:LEU:HD22	2.00	0.43
1:B:116:ILE:O	1:B:120:GLN:HG2	2.18	0.43
1:B:67:LEU:HD11	1:B:135:GLY:HA3	1.99	0.43
1:A:195:VAL:HB	1:A:252:SER:HB3	1.99	0.43
1:B:193:ARG:HG2	1:B:193:ARG:H	1.55	0.43
1:A:118:GLU:O	1:A:121:VAL:HG22	2.18	0.43
1:B:63:LYS:HG2	1:B:63:LYS:H	1.45	0.43
1:B:318:ILE:H	1:B:318:ILE:HG13	1.52	0.43
1:B:351:ILE:HG21	1:B:356:GLU:HB3	1.99	0.43
1:A:167:GLU:OE1	1:A:339:THR:OG1	2.37	0.43
1:A:383:LEU:O	1:A:387:LEU:HB2	2.19	0.42
1:A:318:ILE:H	1:A:318:ILE:HD12	1.84	0.42
1:A:155:LEU:HA	1:A:155:LEU:HD23	1.83	0.42
1:B:353:ASN:HB3	1:B:356:GLU:HB2	2.00	0.42
1:B:265:TYR:CZ	1:B:267:ILE:HB	2.54	0.42
1:A:267:ILE:O	1:A:269:PRO:HD3	2.20	0.42
1:A:215:VAL:HG23	4:A:1001:5EA:F1	2.10	0.42
1:A:111:ILE:HD13	1:A:111:ILE:HA	1.92	0.42
1:A:319:PHE:CD1	1:B:322:LEU:HB3	2.55	0.42
1:B:97:ILE:HG13	1:B:97:ILE:H	1.47	0.42
1:A:86:VAL:HG22	1:A:101:LYS:HE2	2.02	0.42
1:B:107:ILE:HA	1:B:107:ILE:HD13	1.95	0.42
1:A:353:ASN:HD22	1:A:354:PRO:CD	2.31	0.41
1:B:122:LEU:HB3	1:B:133:PHE:CD1	2.55	0.41
1:B:265:TYR:HA	1:B:266:PRO:HD3	1.94	0.41
1:B:217:GLY:HA2	1:B:220:ILE:HD12	2.01	0.41
1:A:284:VAL:HB	1:A:285:ASP:H	1.63	0.41
1:B:154:SER:O	1:B:157:GLN:HB2	2.21	0.41
1:A:335:ASN:O	1:A:337:VAL:HG12	2.21	0.41
1:B:114:GLN:HA	1:B:117:ARG:HE	1.85	0.41
1:B:131:VAL:HG21	1:B:201:LEU:HD22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:ARG:HH12	1:A:243:HIS:CE1	2.39	0.41
1:B:150:MET:HG3	1:B:201:LEU:HB3	2.02	0.40
1:A:136:ALA:HA	1:A:144:SER:O	2.22	0.40
1:B:329:PRO:HA	1:B:330:PRO:HD3	1.84	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	297/354 (84%)	263 (89%)	28 (9%)	6 (2%)	9 48
1	B	285/354 (80%)	255 (90%)	27 (10%)	3 (1%)	17 62
All	All	582/708 (82%)	518 (89%)	55 (10%)	9 (2%)	13 55

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	163	LYS
1	A	284	VAL
1	A	109	PRO
1	A	106	GLU
1	B	110	ALA
1	B	336	GLY
1	B	140	ASP
1	A	281	ARG
1	A	282	PRO

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	262/305 (86%)	202 (77%)	60 (23%)	1 4
1	B	253/305 (83%)	193 (76%)	60 (24%)	1 4
All	All	515/610 (84%)	395 (77%)	120 (23%)	1 4

All (120) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	LYS
1	A	63	LYS
1	A	66	GLU
1	A	67	LEU
1	A	82	ASN
1	A	87	THR
1	A	90	GLN
1	A	96	LEU
1	A	97	ILE
1	A	98	MET
1	A	100	ARG
1	A	101	LYS
1	A	106	GLU
1	A	107	ILE
1	A	112	ARG
1	A	113	ASN
1	A	116	ILE
1	A	117	ARG
1	A	122	LEU
1	A	124	GLU
1	A	140	ASP
1	A	142	GLU
1	A	143	ILE
1	A	157	GLN
1	A	158	VAL
1	A	163	LYS
1	A	164	ARG

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Mol	Chain	Res	Type
1	A	167	GLU
1	A	168	GLU
1	A	172	LYS
1	A	181	LEU
1	A	185	ARG
1	A	187	LYS
1	A	215	VAL
1	A	219	LEU
1	A	223	MET
1	A	228	VAL
1	A	230	THR
1	A	238	ARG
1	A	246	VAL
1	A	247	GLN
1	A	255	LEU
1	A	271	ASP
1	A	279	PHE
1	A	281	ARG
1	A	284	VAL
1	A	313	ARG
1	A	321	LEU
1	A	333	LEU
1	A	335	ASN
1	A	337	VAL
1	A	339	THR
1	A	353	ASN
1	A	360	LEU
1	A	362	MET
1	A	367	THR
1	A	376	GLU
1	A	383	LEU
1	A	385	LYS
1	A	387	LEU
1	B	61	LYS
1	B	63	LYS
1	B	67	LEU
1	B	68	LYS
1	B	76	SER
1	B	87	THR
1	B	92	ARG
1	B	97	ILE
1	B	98	MET

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Mol	Chain	Res	Type
1	B	100	ARG
1	B	104	HIS
1	B	105	LEU
1	B	107	ILE
1	B	112	ARG
1	B	113	ASN
1	B	114	GLN
1	B	115	ILE
1	B	116	ILE
1	B	117	ARG
1	B	139	SER
1	B	140	ASP
1	B	142	GLU
1	B	160	LYS
1	B	164	ARG
1	B	168	GLU
1	B	172	LYS
1	B	181	LEU
1	B	190	ILE
1	B	193	ARG
1	B	196	LYS
1	B	218	GLN
1	B	219	LEU
1	B	222	SER
1	B	230	THR
1	B	231	ARG
1	B	238	ARG
1	B	242	THR
1	B	243	HIS
1	B	255	LEU
1	B	267	ILE
1	B	274	GLU
1	B	275	LEU
1	B	276	GLU
1	B	278	ILE
1	B	318	ILE
1	B	320	GLU
1	B	321	LEU
1	B	328	GLU
1	B	337	VAL
1	B	339	THR
1	B	353	ASN

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Mol	Chain	Res	Type
1	B	359	ASP
1	B	361	LYS
1	B	367	THR
1	B	376	GLU
1	B	383	LEU
1	B	385	LYS
1	B	386	THR
1	B	387	LEU
1	B	389	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	GLN
1	A	113	ASN
1	A	199	ASN
1	A	240	GLN
1	A	243	HIS
1	A	353	ASN
1	A	366	HIS
1	B	247	GLN
1	B	353	ASN
1	B	366	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 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
4	5EA	A	1001	-	29,34,34	2.70	5 (17%)	34,47,47	2.39	13 (38%)
3	ATP	A	535	2	24,33,33	1.04	1 (4%)	31,52,52	1.90	5 (16%)
4	5EA	B	1002	-	29,34,34	2.76	5 (17%)	34,47,47	2.40	13 (38%)
3	ATP	B	537	2	24,33,33	1.06	1 (4%)	31,52,52	1.84	6 (19%)

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
4	5EA	A	1001	-	-	0/9/22/22	0/3/4/4
3	ATP	A	535	2	-	0/18/38/38	0/3/3/3
4	5EA	B	1002	-	-	0/9/22/22	0/3/4/4
3	ATP	B	537	2	-	0/18/38/38	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1001	5EA	N8-N14	-3.25	1.31	1.37
4	B	1002	5EA	N8-N14	-3.20	1.31	1.37
3	A	535	ATP	C5-C4	3.22	1.47	1.40
3	B	537	ATP	C5-C4	3.29	1.47	1.40
4	A	1001	5EA	C11-C6	5.30	1.48	1.37
4	B	1002	5EA	C11-C6	5.65	1.49	1.37
4	A	1001	5EA	C1-C2	6.78	1.49	1.41
4	B	1002	5EA	C1-C2	6.91	1.49	1.41
4	A	1001	5EA	C2-C6	7.06	1.49	1.39
4	B	1002	5EA	C2-C6	7.30	1.49	1.39
4	A	1001	5EA	C10-C15	8.25	1.49	1.38
4	B	1002	5EA	C10-C15	8.33	1.49	1.38

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	535	ATP	N3-C2-N1	-7.15	123.42	128.89
3	B	537	ATP	N3-C2-N1	-6.90	123.61	128.89
3	A	535	ATP	PA-O3A-PB	-3.89	121.79	132.73
4	B	1002	5EA	C19-C15-C10	-3.58	119.85	123.40
4	A	1001	5EA	C19-C15-C10	-3.56	119.87	123.40
3	B	537	ATP	PB-O3B-PG	-3.42	121.20	132.67
3	B	537	ATP	PA-O3A-PB	-3.40	123.17	132.73
3	A	535	ATP	PB-O3B-PG	-3.36	121.39	132.67
3	B	537	ATP	C4-C5-N7	-2.76	106.94	109.48
3	B	537	ATP	C2'-C1'-N9	-2.69	110.17	114.29
3	A	535	ATP	C4-C5-N7	-2.65	107.04	109.48
4	A	1001	5EA	C22-C24-N26	-2.57	106.94	112.90
4	B	1002	5EA	C22-C24-N26	-2.38	107.37	112.90
3	A	535	ATP	C2'-C1'-N9	-2.34	110.71	114.29
4	A	1001	5EA	C24-N26-C28	2.01	116.41	111.27
3	B	537	ATP	O3G-PG-O2G	2.06	115.21	107.38
4	B	1002	5EA	C24-N26-C27	2.11	116.68	111.27
4	A	1001	5EA	C15-C19-C23	2.16	119.73	117.61
4	B	1002	5EA	C24-N26-C28	2.16	116.81	111.27
4	A	1001	5EA	C24-N26-C27	2.27	117.09	111.27
4	B	1002	5EA	C15-C19-C23	2.27	119.84	117.61
4	A	1001	5EA	C4-C9-C11	2.29	121.49	119.00
4	B	1002	5EA	C4-C9-C11	2.34	121.54	119.00
4	A	1001	5EA	F20-C15-C10	2.34	119.85	117.50
4	B	1002	5EA	F20-C15-C10	2.88	120.39	117.50
4	A	1001	5EA	C30-C28-N26	3.25	115.05	110.12
4	B	1002	5EA	C29-C27-N26	3.30	115.12	110.12
4	B	1002	5EA	C30-C28-N26	3.31	115.14	110.12
4	A	1001	5EA	C29-C27-N26	3.36	115.22	110.12
4	A	1001	5EA	O31-C29-C27	3.47	119.78	111.84
4	B	1002	5EA	O31-C30-C28	3.47	119.78	111.84
4	B	1002	5EA	O31-C29-C27	3.50	119.86	111.84
4	A	1001	5EA	O31-C30-C28	3.51	119.89	111.84
4	A	1001	5EA	C30-O31-C29	4.06	123.56	109.89
4	B	1002	5EA	C30-O31-C29	4.07	123.58	109.89
4	A	1001	5EA	C28-N26-C27	8.13	126.50	108.90
4	B	1002	5EA	C28-N26-C27	8.13	126.51	108.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1001	5EA	1	0
4	B	1002	5EA	2	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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	303/354 (85%)	0.01	12 (3%)	42	27	13, 34, 63, 68	2 (0%)
1	B	291/354 (82%)	0.19	20 (6%)	20	11	24, 46, 66, 68	2 (0%)
All	All	594/708 (83%)	0.10	32 (5%)	29	17	13, 40, 65, 68	4 (0%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	221	ASP	5.2
1	A	392	PRO	4.8
1	B	109	PRO	4.8
1	B	82	ASN	4.1
1	A	314	PRO	3.7
1	B	140	ASP	3.7
1	A	282	PRO	3.4
1	A	140	ASP	3.3
1	B	75	ILE	3.3
1	A	82	ASN	3.1
1	B	279	PHE	3.1
1	B	110	ALA	3.0
1	B	243	HIS	3.0
1	A	313	ARG	3.0
1	B	272	ALA	2.9
1	B	230	THR	2.9
1	A	90	GLN	2.9
1	B	242	THR	2.7
1	A	138	TYR	2.7
1	A	390	ASN	2.6
1	B	376	GLU	2.6
1	A	393	GLY	2.5
1	B	69	ASP	2.5
1	B	316	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	106	GLU	2.3
1	B	68	LYS	2.2
1	A	285	ASP	2.2
1	B	83	GLY	2.2
1	B	141	GLY	2.2
1	B	389	LEU	2.0
1	A	315	ALA	2.0
1	B	142	GLU	2.0

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, 95^{th} 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(Å^2)	Q<0.9
4	5EA	A	1001	31/31	0.92	0.20	-0.23	28,31,34,38	0
2	MG	B	538	1/1	0.87	0.21	-0.38	32,32,32,32	0
3	ATP	A	535	31/31	0.94	0.20	-0.43	46,47,48,49	0
4	5EA	B	1002	31/31	0.93	0.19	-0.48	33,33,40,46	0
3	ATP	B	537	31/31	0.94	0.17	-0.66	50,51,52,52	0
2	MG	A	536	1/1	0.96	0.21	-	18,18,18,18	0

6.5 Other polymers (i)

There are no such residues in this entry.