Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 11:59 PM GMT

PDB ID	:	1ZBU
Title	:	crystal structure of full-length 3'-exonuclease
Authors	:	Cheng, Y.; Patel, D.J.
Deposited on	:	2005-04-08
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 (1)) were used in the production of this report:

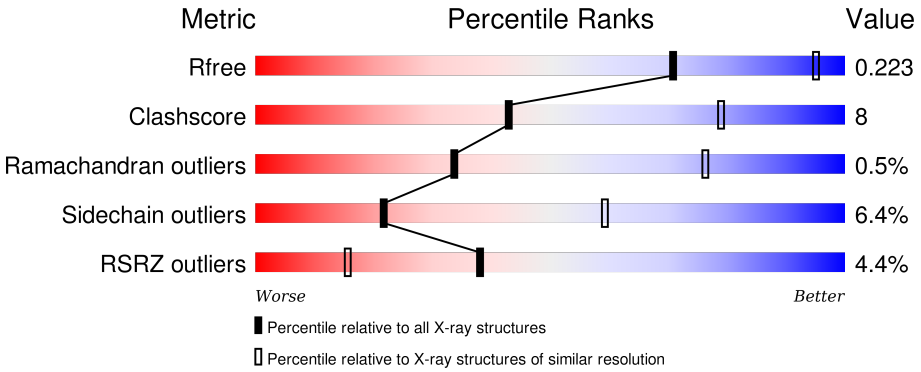
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

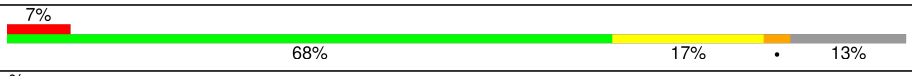
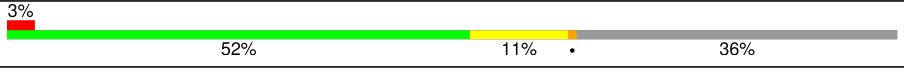
The reported resolution of this entry is 3.00 Å.

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))
R_{free}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (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.

Mol	Chain	Length	Quality of chain
1	A	349	
1	B	349	
1	C	349	
1	D	349	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MG	A	1001	-	-	-	X
2	MG	B	2001	-	-	-	X
2	MG	C	3001	-	-	-	X
3	AMP	A	1002	-	-	-	X
3	AMP	B	2002	-	-	-	X
3	AMP	C	3002	-	-	-	X
3	AMP	D	4002	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8084 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 3'-5' exonuclease ERI1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	225	Total	C	N	O	S	Se	0	0	0
			1827	1168	304	341	6	8			
1	B	304	Total	C	N	O	S	Se	0	0	0
			2467	1571	416	462	8	10			
1	C	225	Total	C	N	O	S	Se	0	0	0
			1827	1168	304	341	6	8			
1	D	225	Total	C	N	O	S	Se	0	0	0
			1826	1168	304	340	6	8			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	MODIFIED RESIDUE	UNP Q8IV48
A	79	MSE	MET	MODIFIED RESIDUE	UNP Q8IV48
A	116	MSE	MET	MODIFIED RESIDUE	UNP Q8IV48
A	213	LEU	TRP	CONFLICT	UNP Q8IV48
A	214	MSE	MET	MODIFIED RESIDUE	UNP Q8IV48
A	235	MSE	MET	MODIFIED RESIDUE	UNP Q8IV48
A	280	MSE	MET	MODIFIED RESIDUE	UNP Q8IV48
A	286	MSE	MET	MODIFIED RESIDUE	UNP Q8IV48
A	309	MSE	MET	MODIFIED RESIDUE	UNP Q8IV48
A	322	MSE	MET	MODIFIED RESIDUE	UNP Q8IV48
A	328	MSE	MET	MODIFIED RESIDUE	UNP Q8IV48
A	344	MSE	MET	MODIFIED RESIDUE	UNP Q8IV48
B	1	MSE	-	MODIFIED RESIDUE	UNP Q8IV48
B	79	MSE	MET	MODIFIED RESIDUE	UNP Q8IV48
B	116	MSE	MET	MODIFIED RESIDUE	UNP Q8IV48
B	213	LEU	TRP	CONFLICT	UNP Q8IV48
B	214	MSE	MET	MODIFIED RESIDUE	UNP Q8IV48
B	235	MSE	MET	MODIFIED RESIDUE	UNP Q8IV48
B	280	MSE	MET	MODIFIED RESIDUE	UNP Q8IV48
B	286	MSE	MET	MODIFIED RESIDUE	UNP Q8IV48
B	309	MSE	MET	MODIFIED RESIDUE	UNP Q8IV48

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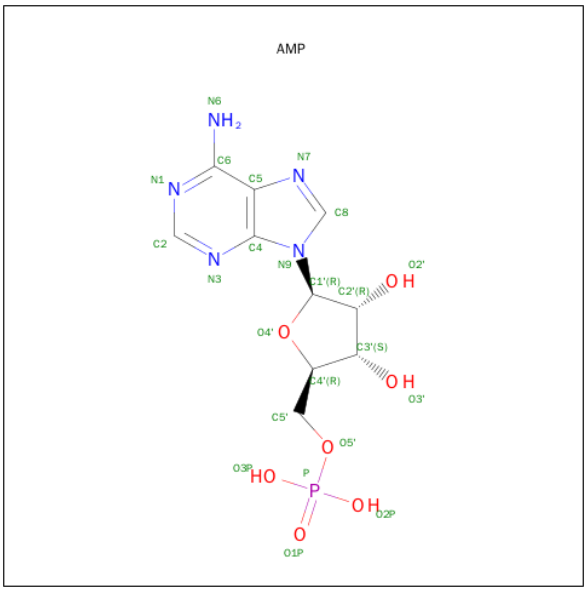
Chain	Residue	Modelled	Actual	Comment	Reference
B	322	MSE	MET	MODIFIED RESIDUE	UNP Q8IV48
B	328	MSE	MET	MODIFIED RESIDUE	UNP Q8IV48
B	344	MSE	MET	MODIFIED RESIDUE	UNP Q8IV48
C	1	MSE	-	MODIFIED RESIDUE	UNP Q8IV48
C	79	MSE	MET	MODIFIED RESIDUE	UNP Q8IV48
C	116	MSE	MET	MODIFIED RESIDUE	UNP Q8IV48
C	213	LEU	TRP	CONFLICT	UNP Q8IV48
C	214	MSE	MET	MODIFIED RESIDUE	UNP Q8IV48
C	235	MSE	MET	MODIFIED RESIDUE	UNP Q8IV48
C	280	MSE	MET	MODIFIED RESIDUE	UNP Q8IV48
C	286	MSE	MET	MODIFIED RESIDUE	UNP Q8IV48
C	309	MSE	MET	MODIFIED RESIDUE	UNP Q8IV48
C	322	MSE	MET	MODIFIED RESIDUE	UNP Q8IV48
C	328	MSE	MET	MODIFIED RESIDUE	UNP Q8IV48
C	344	MSE	MET	MODIFIED RESIDUE	UNP Q8IV48
D	1	MSE	-	MODIFIED RESIDUE	UNP Q8IV48
D	79	MSE	MET	MODIFIED RESIDUE	UNP Q8IV48
D	116	MSE	MET	MODIFIED RESIDUE	UNP Q8IV48
D	213	LEU	TRP	CONFLICT	UNP Q8IV48
D	214	MSE	MET	MODIFIED RESIDUE	UNP Q8IV48
D	235	MSE	MET	MODIFIED RESIDUE	UNP Q8IV48
D	280	MSE	MET	MODIFIED RESIDUE	UNP Q8IV48
D	286	MSE	MET	MODIFIED RESIDUE	UNP Q8IV48
D	309	MSE	MET	MODIFIED RESIDUE	UNP Q8IV48
D	322	MSE	MET	MODIFIED RESIDUE	UNP Q8IV48
D	328	MSE	MET	MODIFIED RESIDUE	UNP Q8IV48
D	344	MSE	MET	MODIFIED RESIDUE	UNP Q8IV48

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

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

- Molecule 3 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	D	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 4 is water.

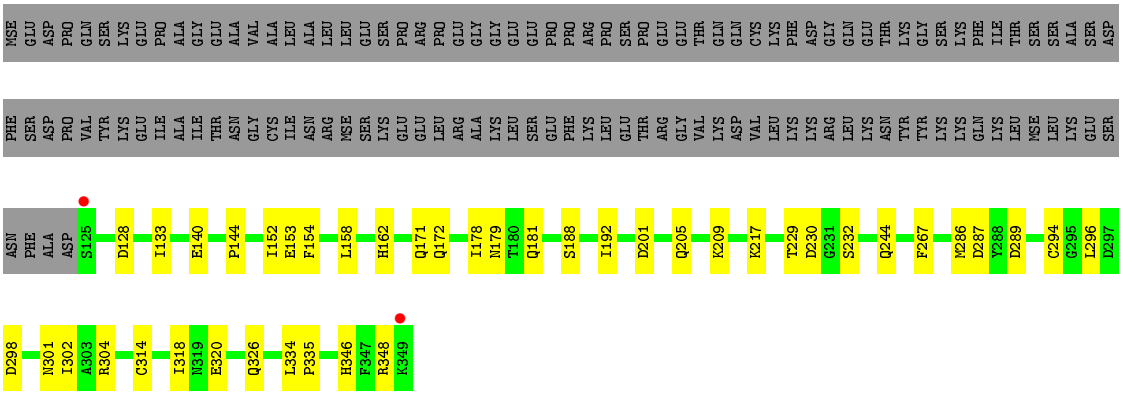
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	13	Total	O	1	0
			13	13		
4	B	13	Total	O	5	0
			13	13		
4	C	6	Total	O	2	0
			6	6		
4	D	5	Total	O	2	0
			5	5		

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.

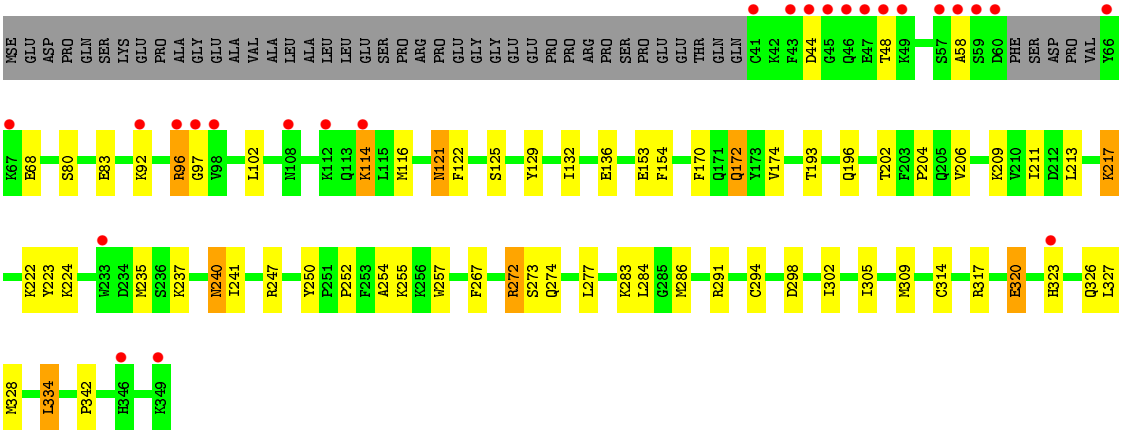
- Molecule 1: 3'-5' exonuclease ERI1

Chain A:



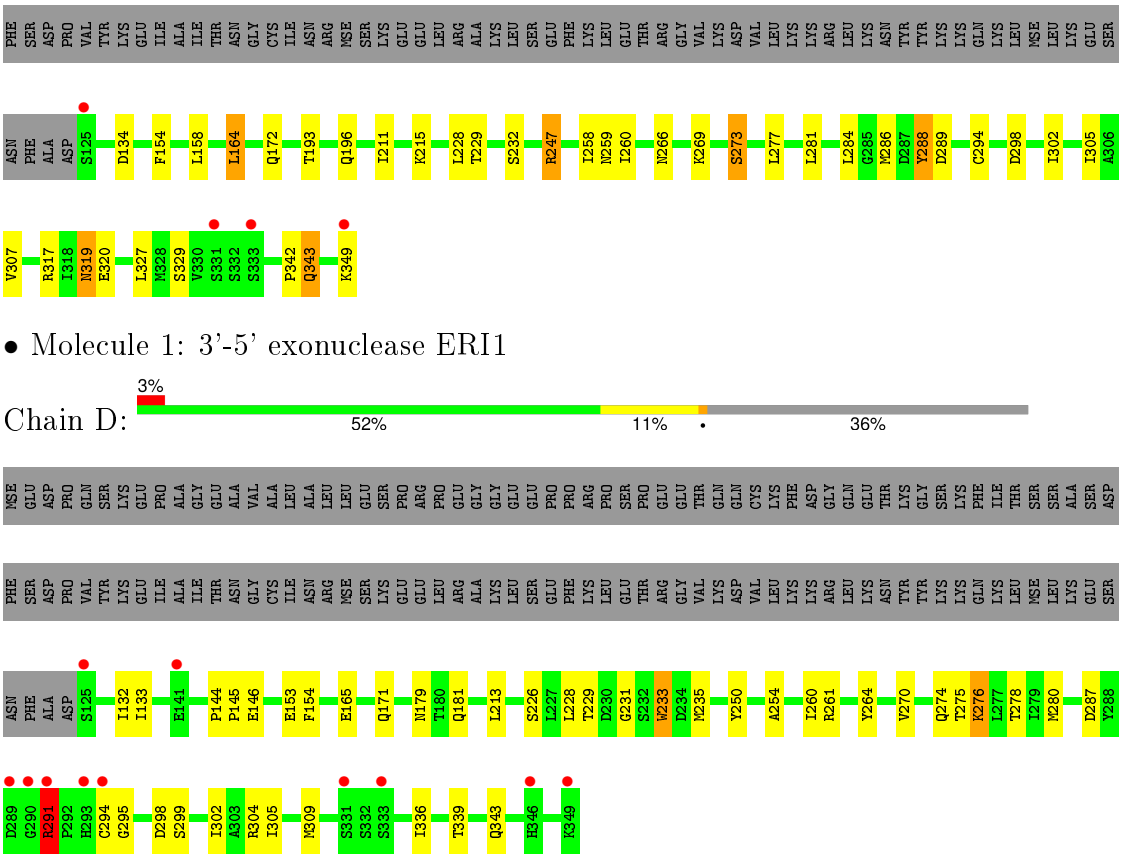
- Molecule 1: 3'-5' exonuclease ERI1

Chain B:



- Molecule 1: 3'-5' exonuclease ERI1

Chain C:



• Molecule 1: 3'-5' exonuclease ERI1

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	215.84Å 215.84Å 114.47Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.96 – 3.00 19.96 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.8 (19.96-3.00) 97.7 (19.96-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.98 (at 2.98Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.199 , 0.225 0.200 , 0.223	Depositor DCC
R_{free} test set	6227 reflections (11.54%)	DCC
Wilson B-factor (Å^2)	52.1	Xtriage
Anisotropy	0.188	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 46.8	EDS
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 61407 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	8084	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% 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: AMP, MG

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	0.56	0/1861	0.62	0/2501
1	B	0.51	0/2505	0.62	1/3348 (0.0%)
1	C	0.48	0/1861	0.60	0/2501
1	D	0.48	0/1860	0.55	0/2499
All	All	0.51	0/8087	0.60	1/10849 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	334	LEU	CA-CB-CG	9.00	135.99	115.30

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	1827	0	1827	21	0
1	B	2467	0	2496	42	0
1	C	1827	0	1827	33	0
1	D	1826	0	1827	37	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	23	0	12	0	0
3	B	23	0	12	0	0
3	C	23	0	12	0	0
3	D	23	0	12	0	0
4	A	13	0	0	0	1
4	B	13	0	0	0	1
4	C	6	0	0	0	0
4	D	5	0	0	0	0
All	All	8084	0	8025	131	1

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 8.

All (131) 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:C:247:ARG:HH11	1:C:247:ARG:HG2	1.09	1.11
1:B:58:ALA:HA	1:B:116:MSE:HE3	1.33	1.04
1:D:305:ILE:HG22	1:D:309:MSE:CE	1.89	1.01
1:B:235:MSE:CE	1:B:254:ALA:HB1	1.92	0.98
1:D:235:MSE:CE	1:D:254:ALA:HB1	1.94	0.98
1:C:259:ASN:H	1:C:319:ASN:HD21	1.01	0.93
1:C:343:GLN:HA	1:C:343:GLN:HE21	1.35	0.90
1:C:215:LYS:NZ	1:C:343:GLN:HE22	1.69	0.88
1:D:233:TRP:HD1	1:D:233:TRP:H	1.22	0.87
1:C:215:LYS:HZ1	1:C:343:GLN:HE22	1.23	0.85
1:C:247:ARG:HG2	1:C:247:ARG:NH1	1.89	0.85
1:C:343:GLN:HA	1:C:343:GLN:NE2	1.91	0.85
1:D:235:MSE:HE1	1:D:254:ALA:HB1	1.60	0.80
1:B:170:PHE:HZ	1:B:172:GLN:HE21	1.29	0.80
1:C:247:ARG:HH11	1:C:247:ARG:CG	1.93	0.79
1:A:289:ASP:H	1:A:301:ASN:HD21	1.32	0.78
1:D:305:ILE:HG22	1:D:309:MSE:HE2	1.68	0.76
1:B:272:ARG:HH11	1:B:272:ARG:HG3	1.49	0.76
1:C:193:THR:H	1:C:196:GLN:HE21	1.32	0.76
1:B:235:MSE:HE1	1:B:254:ALA:HB1	1.69	0.74
1:D:233:TRP:CD1	1:D:233:TRP:N	2.55	0.74
1:D:291:ARG:NH1	1:D:294:CYS:HB3	2.04	0.73
1:B:272:ARG:HH11	1:B:272:ARG:CG	2.08	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:259:ASN:H	1:C:319:ASN:ND2	1.84	0.65
1:B:298:ASP:O	1:B:302:ILE:HG12	1.98	0.64
1:A:287:ASP:OD2	1:C:273:SER:HB2	1.98	0.63
1:B:193:THR:H	1:B:196:GLN:HE21	1.46	0.63
1:C:284:LEU:HB2	1:C:286:MSE:HE2	1.79	0.62
1:D:233:TRP:HD1	1:D:233:TRP:N	1.94	0.61
1:D:291:ARG:HH12	1:D:294:CYS:H	1.47	0.61
1:A:128:ASP:OD2	1:A:162:HIS:HE1	1.84	0.59
1:A:334:LEU:HB2	1:A:335:PRO:HD2	1.84	0.59
1:B:235:MSE:HE2	1:B:254:ALA:HB1	1.82	0.58
1:B:68:GLU:HB3	1:B:116:MSE:HE2	1.84	0.58
1:D:276:LYS:O	1:D:280:MSE:HG3	2.02	0.58
1:B:247:ARG:HH11	1:B:247:ARG:HG2	1.69	0.57
1:B:237:LYS:O	1:B:241:ILE:HG12	2.05	0.57
1:B:193:THR:H	1:B:196:GLN:NE2	2.03	0.57
1:D:305:ILE:CG2	1:D:309:MSE:HE2	2.34	0.57
1:C:286:MSE:HE1	1:C:305:ILE:HG12	1.86	0.57
1:D:153:GLU:OE2	1:D:295:GLY:HA3	2.05	0.57
1:B:58:ALA:CA	1:B:116:MSE:HE3	2.22	0.56
1:C:298:ASP:O	1:C:302:ILE:HG12	2.05	0.56
1:C:281:LEU:HD23	1:C:286:MSE:HE3	1.88	0.56
1:B:96:ARG:O	1:B:102:LEU:HD11	2.06	0.55
1:D:291:ARG:NH2	1:D:294:CYS:HB2	2.21	0.55
1:A:153:GLU:OE1	1:A:171:GLN:NE2	2.32	0.55
1:B:58:ALA:HB3	1:B:114:LYS:HB3	1.89	0.54
1:D:291:ARG:NH1	1:D:291:ARG:O	2.40	0.54
1:B:267:PHE:CE1	1:B:314:CYS:HB2	2.43	0.54
1:B:170:PHE:HZ	1:B:172:GLN:NE2	2.02	0.54
1:B:284:LEU:HB2	1:B:286:MSE:HE3	1.89	0.53
1:D:291:ARG:NH1	1:D:294:CYS:CB	2.72	0.53
1:C:232:SER:HB3	1:C:320:GLU:OE1	2.09	0.52
1:C:228:LEU:HD21	1:C:260:ILE:HB	1.92	0.52
1:C:215:LYS:HZ3	1:C:343:GLN:HE22	1.54	0.52
1:C:284:LEU:HD12	1:C:286:MSE:HE2	1.91	0.52
1:D:305:ILE:CG2	1:D:309:MSE:CE	2.76	0.52
1:D:261:ARG:HH12	1:D:276:LYS:HG3	1.74	0.52
1:D:305:ILE:HG22	1:D:309:MSE:HE1	1.88	0.52
1:A:178:ILE:HG22	1:A:179:ASN:N	2.25	0.51
1:D:228:LEU:HD11	1:D:260:ILE:HD12	1.91	0.51
1:B:174:VAL:HG22	1:B:206:VAL:HG21	1.93	0.51
1:D:287:ASP:O	1:D:304:ARG:NH2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:ASN:C	1:B:240:ASN:HD22	2.14	0.50
1:C:281:LEU:HA	1:C:286:MSE:HE3	1.93	0.50
1:B:252:PRO:HA	1:B:255:LYS:HE2	1.93	0.50
1:D:291:ARG:CZ	1:D:294:CYS:HB2	2.42	0.50
1:A:286:MSE:HE1	1:A:304:ARG:HB3	1.93	0.50
1:C:215:LYS:NZ	1:C:343:GLN:NE2	2.50	0.50
1:A:301:ASN:ND2	1:A:304:ARG:NH1	2.59	0.50
1:B:44:ASP:HB3	1:B:122:PHE:CE1	2.47	0.49
1:D:264:TYR:CD2	1:D:275:THR:HG22	2.47	0.49
1:C:266:ASN:O	1:C:269:LYS:HE3	2.12	0.49
1:B:247:ARG:NH1	1:B:247:ARG:HG2	2.26	0.49
1:D:264:TYR:HD2	1:D:275:THR:HG22	1.78	0.49
1:B:272:ARG:NH1	1:B:272:ARG:CG	2.73	0.49
1:A:152:ILE:HD12	1:A:192:ILE:HD12	1.94	0.49
1:B:121:ASN:ND2	1:B:121:ASN:H	2.10	0.49
1:B:257:TRP:CZ2	1:B:320:GLU:HG2	2.48	0.49
1:B:284:LEU:CB	1:B:286:MSE:HE3	2.43	0.48
1:C:319:ASN:HD22	1:C:319:ASN:H	1.61	0.48
1:B:211:ILE:HG23	1:B:342:PRO:HB2	1.94	0.48
1:B:136:GLU:HB2	1:B:153:GLU:HB3	1.95	0.48
1:A:232:SER:HB3	1:A:320:GLU:OE2	2.14	0.48
1:B:222:LYS:HD3	1:B:223:TYR:CZ	2.48	0.48
1:D:231:GLY:HA3	1:D:233:TRP:HE1	1.79	0.48
1:B:170:PHE:CZ	1:B:172:GLN:HB2	2.48	0.47
1:D:291:ARG:HH12	1:D:294:CYS:HB3	1.77	0.47
1:B:235:MSE:HE3	1:B:250:TYR:OH	2.14	0.47
1:C:211:ILE:HG22	1:C:215:LYS:HD2	1.96	0.47
1:A:287:ASP:OD2	1:C:273:SER:CB	2.63	0.47
1:B:277:LEU:HD13	1:B:302:ILE:HD13	1.96	0.47
1:D:146:GLU:OE2	1:D:146:GLU:HA	2.14	0.47
1:A:301:ASN:HD22	1:A:304:ARG:NH1	2.13	0.45
1:D:299:SER:HA	1:D:302:ILE:HD12	1.98	0.45
1:C:215:LYS:HZ1	1:C:343:GLN:NE2	2.03	0.45
1:B:44:ASP:HB3	1:B:122:PHE:HE1	1.81	0.45
1:A:140:GLU:HB2	1:A:144:PRO:CD	2.46	0.45
1:C:288:TYR:C	1:C:288:TYR:CD2	2.91	0.44
1:B:125:SER:HB2	1:B:224:LYS:NZ	2.32	0.44
1:C:247:ARG:NH1	1:C:349:LYS:O	2.51	0.44
1:D:291:ARG:CZ	1:D:294:CYS:CB	2.96	0.44
1:D:144:PRO:HA	1:D:145:PRO:HD3	1.77	0.44
1:A:244:GLN:HA	1:A:348:ARG:HH12	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:291:ARG:HH22	1:D:294:CYS:N	2.16	0.43
1:A:171:GLN:HB2	1:A:296:LEU:HD22	2.00	0.43
1:A:133:ILE:O	1:A:229:THR:HG22	2.19	0.43
1:A:267:PHE:CE1	1:A:314:CYS:HB2	2.54	0.43
1:D:305:ILE:HG22	1:D:309:MSE:HE3	1.90	0.43
1:D:132:ILE:HG12	1:D:228:LEU:HD22	2.01	0.43
1:A:172:GLN:NE2	1:A:209:LYS:HD2	2.34	0.42
1:B:323:HIS:HB3	1:B:328:MSE:HE1	2.00	0.42
1:D:235:MSE:HE3	1:D:250:TYR:OH	2.19	0.42
1:B:129:TYR:OH	1:B:217:LYS:HE3	2.20	0.42
1:D:226:SER:HA	1:D:339:THR:HG1	1.85	0.42
1:C:193:THR:OG1	1:C:196:GLN:HG3	2.19	0.42
1:C:277:LEU:HD13	1:C:302:ILE:HD13	2.02	0.41
1:C:211:ILE:HD12	1:C:342:PRO:HB2	2.02	0.41
1:A:230:ASP:HB2	1:A:302:ILE:CD1	2.51	0.41
1:D:133:ILE:O	1:D:229:THR:HG22	2.20	0.41
1:B:305:ILE:O	1:B:309:MSE:HG3	2.20	0.41
1:B:80:SER:OG	1:B:83:GLU:HG3	2.20	0.41
1:D:226:SER:HA	1:D:339:THR:OG1	2.20	0.41
1:A:201:ASP:HB3	1:A:205:GLN:HB2	2.02	0.41
1:D:336:ILE:H	1:D:336:ILE:HD12	1.86	0.41
1:A:301:ASN:ND2	1:A:304:ARG:HH11	2.18	0.40
1:C:164:LEU:HG	1:C:307:VAL:HG13	2.03	0.40
1:C:258:ILE:HG12	1:C:317:ARG:C	2.42	0.40
1:B:202:THR:HB	1:B:204:PRO:HD2	2.04	0.40
1:B:172:GLN:HE22	1:B:209:LYS:HD2	1.86	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1003:HOH:O	4:B:2007:HOH:O[3_654]	1.39	0.81

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	223/349 (64%)	218 (98%)	5 (2%)	0	100 100
1	B	300/349 (86%)	285 (95%)	13 (4%)	2 (1%)	26 70
1	C	223/349 (64%)	214 (96%)	9 (4%)	0	100 100
1	D	223/349 (64%)	209 (94%)	11 (5%)	3 (1%)	15 53
All	All	969/1396 (69%)	926 (96%)	38 (4%)	5 (0%)	34 76

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	276	LYS
1	B	97	GLY
1	B	114	LYS
1	D	274	GLN
1	D	291	ARG

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	208/306 (68%)	198 (95%)	10 (5%)	31 71
1	B	279/306 (91%)	258 (92%)	21 (8%)	17 51
1	C	208/306 (68%)	193 (93%)	15 (7%)	18 53
1	D	208/306 (68%)	196 (94%)	12 (6%)	25 63
All	All	903/1224 (74%)	845 (94%)	58 (6%)	22 59

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	154	PHE
1	A	158	LEU
1	A	181	GLN

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Mol	Chain	Res	Type
1	A	188	SER
1	A	217	LYS
1	A	294	CYS
1	A	298	ASP
1	A	318	ILE
1	A	326	GLN
1	A	346	HIS
1	B	48	THR
1	B	92	LYS
1	B	96	ARG
1	B	121	ASN
1	B	132	ILE
1	B	154	PHE
1	B	172	GLN
1	B	213	LEU
1	B	217	LYS
1	B	240	ASN
1	B	272	ARG
1	B	273	SER
1	B	274	GLN
1	B	283	LYS
1	B	291	ARG
1	B	294	CYS
1	B	317	ARG
1	B	320	GLU
1	B	326	GLN
1	B	327	LEU
1	B	334	LEU
1	C	134	ASP
1	C	154	PHE
1	C	158	LEU
1	C	164	LEU
1	C	172	GLN
1	C	229	THR
1	C	247	ARG
1	C	273	SER
1	C	288	TYR
1	C	289	ASP
1	C	294	CYS
1	C	319	ASN
1	C	327	LEU
1	C	329	SER

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Mol	Chain	Res	Type
1	C	343	GLN
1	D	154	PHE
1	D	165	GLU
1	D	171	GLN
1	D	179	ASN
1	D	181	GLN
1	D	213	LEU
1	D	233	TRP
1	D	270	VAL
1	D	278	THR
1	D	291	ARG
1	D	298	ASP
1	D	343	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	162	HIS
1	A	172	GLN
1	A	301	ASN
1	B	121	ASN
1	B	172	GLN
1	B	196	GLN
1	B	240	ASN
1	B	244	GLN
1	B	326	GLN
1	B	343	GLN
1	C	143	ASN
1	C	171	GLN
1	C	172	GLN
1	C	179	ASN
1	C	196	GLN
1	C	319	ASN
1	C	343	GLN
1	D	301	ASN

5.3.3 RNA

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)

Of 12 ligands modelled in this entry, 8 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	$\#\|Z\| > 2$
3	AMP	A	1002	2	20,25,25	1.17	2 (10%)	22,38,38	2.33	3 (13%)
3	AMP	B	2002	2	20,25,25	1.13	1 (5%)	22,38,38	2.15	3 (13%)
3	AMP	C	3002	2	20,25,25	1.16	1 (5%)	22,38,38	2.14	4 (18%)
3	AMP	D	4002	2	20,25,25	1.19	1 (5%)	22,38,38	2.22	4 (18%)

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	AMP	A	1002	2	-	0/6/26/26	0/3/3/3
3	AMP	B	2002	2	-	0/6/26/26	0/3/3/3
3	AMP	C	3002	2	-	0/6/26/26	0/3/3/3
3	AMP	D	4002	2	-	0/6/26/26	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1002	AMP	C2-N3	2.03	1.35	1.32
3	B	2002	AMP	C5-C4	3.43	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3002	AMP	C5-C4	3.45	1.48	1.40
3	A	1002	AMP	C5-C4	3.46	1.48	1.40
3	D	4002	AMP	C5-C4	3.57	1.48	1.40

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	2002	AMP	N3-C2-N1	-7.88	122.86	128.89
3	C	3002	AMP	N3-C2-N1	-7.76	122.95	128.89
3	D	4002	AMP	N3-C2-N1	-7.61	123.07	128.89
3	A	1002	AMP	N3-C2-N1	-7.10	123.46	128.89
3	A	1002	AMP	C2'-C1'-N9	-6.48	104.39	114.29
3	D	4002	AMP	C2'-C1'-N9	-4.85	106.88	114.29
3	B	2002	AMP	C2'-C1'-N9	-3.94	108.27	114.29
3	C	3002	AMP	C2'-C1'-N9	-3.84	108.42	114.29
3	D	4002	AMP	C4-C5-N7	-2.91	106.80	109.48
3	B	2002	AMP	C4-C5-N7	-2.59	107.10	109.48
3	C	3002	AMP	C4-C5-N7	-2.54	107.14	109.48
3	A	1002	AMP	C4-C5-N7	-2.37	107.30	109.48
3	C	3002	AMP	C2-N1-C6	2.05	122.44	118.77
3	D	4002	AMP	O4'-C1'-N9	2.06	112.41	108.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

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	217/349 (62%)	-0.45	2 (0%) 85 64	11, 20, 30, 41	0
1	B	294/349 (84%)	0.01	25 (8%) 13 5	10, 20, 37, 57	0
1	C	217/349 (62%)	-0.29	4 (1%) 71 43	10, 20, 31, 37	0
1	D	217/349 (62%)	-0.08	11 (5%) 32 12	8, 19, 37, 50	0
All	All	945/1396 (67%)	-0.18	42 (4%) 38 16	8, 20, 34, 57	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	60	ASP	6.8
1	B	59	SER	5.6
1	B	41	CYS	5.5
1	D	349	LYS	5.3
1	B	48	THR	5.3
1	B	43	PHE	5.0
1	B	46	GLN	4.2
1	B	66	TYR	4.1
1	A	349	LYS	3.9
1	D	290	GLY	3.9
1	B	349	LYS	3.8
1	B	114	LYS	3.5
1	B	97	GLY	3.5
1	C	349	LYS	3.4
1	D	293	HIS	3.4
1	D	331	SER	3.3
1	B	98	VAL	3.2
1	D	333	SER	3.1
1	B	96	ARG	2.9
1	B	45	GLY	2.9
1	B	49	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	125	SER	2.9
1	B	67	LYS	2.9
1	B	323	HIS	2.8
1	B	44	ASP	2.8
1	B	47	GLU	2.8
1	D	289	ASP	2.7
1	B	112	LYS	2.7
1	D	294	CYS	2.7
1	D	291	ARG	2.6
1	B	92	LYS	2.6
1	C	333	SER	2.5
1	B	346	HIS	2.5
1	C	125	SER	2.4
1	B	58	ALA	2.4
1	A	125	SER	2.3
1	D	141	GLU	2.3
1	B	57	SER	2.2
1	B	108	ASN	2.1
1	D	346	HIS	2.1
1	B	233	TRP	2.1
1	C	331	SER	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
2	MG	B	2001	1/1	0.96	0.49	7.95	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	MG	C	3001	1/1	0.97	0.47	7.91	40,40,40,40	0
3	AMP	B	2002	23/23	0.89	0.38	6.11	57,60,64,65	0
2	MG	A	1001	1/1	0.99	0.37	5.26	42,42,42,42	0
3	AMP	C	3002	23/23	0.89	0.31	4.46	49,52,59,59	0
3	AMP	D	4002	23/23	0.70	0.53	3.86	83,86,90,91	0
3	AMP	A	1002	23/23	0.93	0.26	2.23	29,31,40,41	0
2	MG	D	4000	1/1	0.86	0.46	-	60,60,60,60	0
2	MG	D	4001	1/1	0.90	0.30	-	59,59,59,59	0
2	MG	C	3000	1/1	0.86	0.23	-	54,54,54,54	0
2	MG	B	2000	1/1	0.74	0.28	-	52,52,52,52	0
2	MG	A	1000	1/1	0.71	0.22	-	32,32,32,32	0

6.5 Other polymers (i)

There are no such residues in this entry.