Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:51 AM GMT

PDB ID	:	3N6Q
Title	:	Crystal structure of YghZ from E. coli
Authors	:	Zubieta, C.; Totir, M.; Echols, N.; May, A.; Alber, T.
Deposited on	:	2010-05-26
Resolution	:	1.80 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:

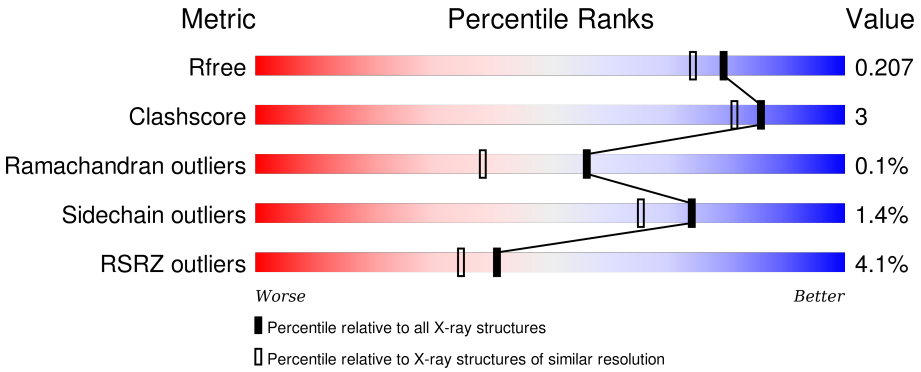
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.80 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	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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	346	% 85% 5% 9%
1	B	346	% 86% 5% 9%
1	C	346	3% 86% • 10%
1	D	346	% 85% 6% • 9%
1	E	346	8% 80% 9% • 11%

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Mol	Chain	Length	Quality of chain
1	F	346	2% 85% 5% 10%
1	G	346	6% 84% 6% 10%
1	H	346	8% 81% 7% 12%

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	B	401	-	-	-	X
2	MG	C	401	-	-	-	X
2	MG	D	401	-	-	-	X
2	MG	F	401	-	-	-	X
2	MG	G	401	-	-	-	X
2	MG	H	401	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22603 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 YghZ aldo-keto reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	314	Total	C	N	O	S	0	14	0
			2556	1624	445	476	11			
1	B	315	Total	C	N	O	S	0	10	0
			2547	1618	445	473	11			
1	C	313	Total	C	N	O	S	0	4	0
			2491	1575	438	468	10			
1	D	315	Total	C	N	O	S	0	2	0
			2495	1580	436	469	10			
1	E	309	Total	C	N	O	S	0	4	0
			2457	1553	434	460	10			
1	F	313	Total	C	N	O	S	0	3	0
			2481	1569	436	466	10			
1	G	313	Total	C	N	O	S	0	4	0
			2489	1574	439	466	10			
1	H	306	Total	C	N	O	S	0	3	0
			2436	1544	429	453	10			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Mg	0	0
			1	1		
2	D	2	Total	Mg	0	0
			2	2		
2	E	1	Total	Mg	0	0
			1	1		
2	H	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		

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

- Molecule 3 is water.

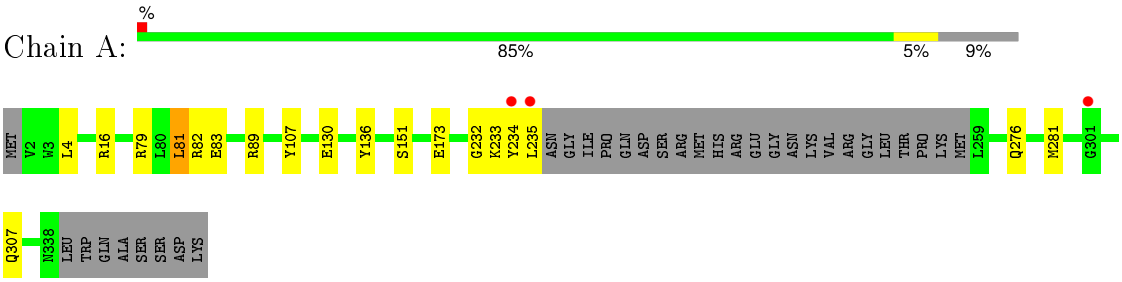
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	444	Total O 444 444	0	0
3	B	382	Total O 382 382	0	0
3	C	298	Total O 298 298	0	0
3	D	343	Total O 343 343	0	0
3	E	254	Total O 254 254	0	0
3	F	362	Total O 362 362	0	0
3	G	323	Total O 323 323	0	0
3	H	236	Total O 236 236	0	0

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.

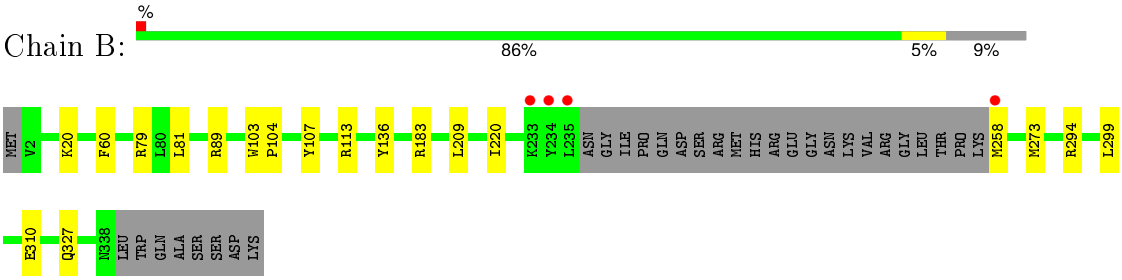
- Molecule 1: YghZ aldo-keto reductase

Chain A:



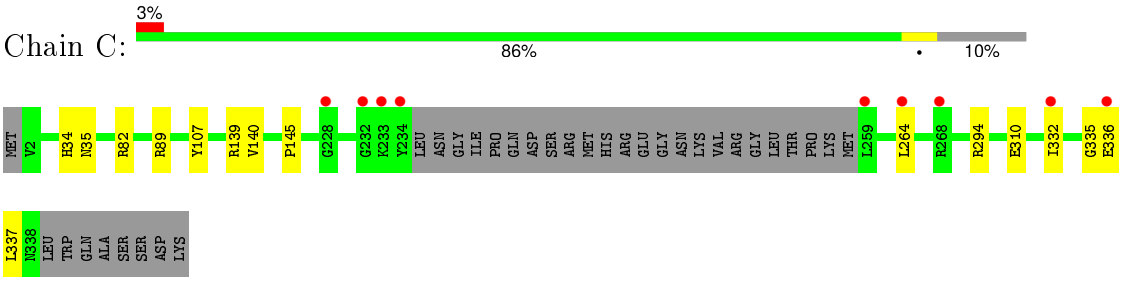
- Molecule 1: YghZ aldo-keto reductase

Chain B:



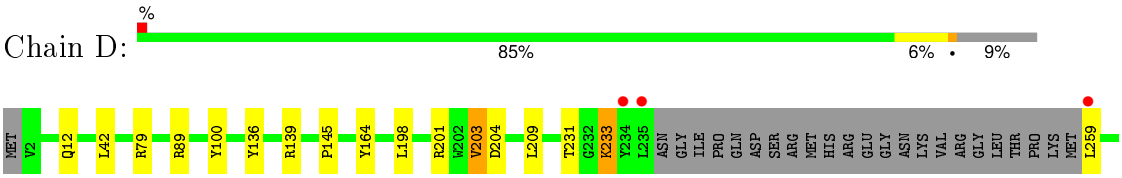
- Molecule 1: YghZ aldo-keto reductase

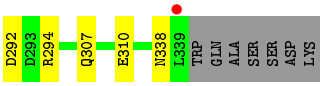
Chain C:



- Molecule 1: YghZ aldo-keto reductase

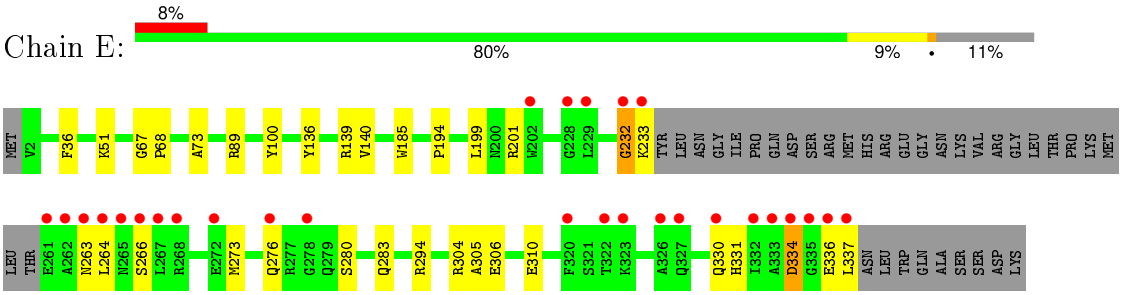
Chain D:





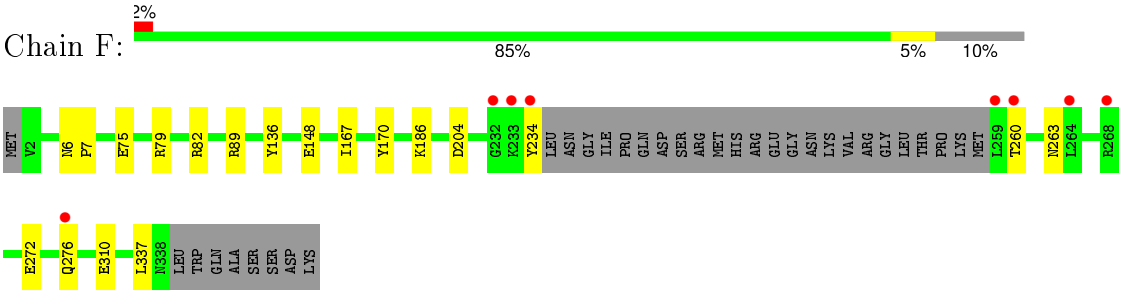
• Molecule 1: YghZ aldo-keto reductase

Chain E:



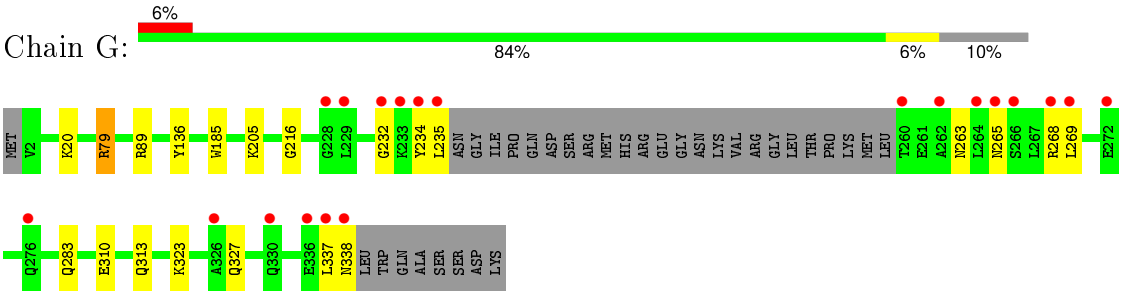
• Molecule 1: YghZ aldo-keto reductase

Chain F:



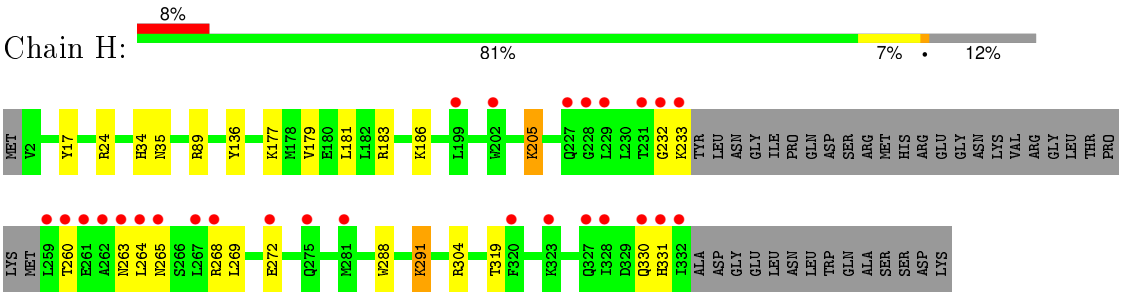
• Molecule 1: YghZ aldo-keto reductase

Chain G:



• Molecule 1: YghZ aldo-keto reductase

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	91.70Å 98.06Å 98.26Å 90.27° 92.97° 106.12°	Depositor
Resolution (Å)	94.07 – 1.80 67.37 – 1.80	Depositor EDS
% Data completeness (in resolution range)	96.2 (94.07-1.80) 95.6 (67.37-1.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.32 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.169 , 0.209 0.168 , 0.207	Depositor DCC
R_{free} test set	15375 reflections (5.53%)	DCC
Wilson B-factor (Å^2)	24.2	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 53.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 292748 reflections	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	22603	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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

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	0.97	1/2649 (0.0%)	0.83	2/3582 (0.1%)
1	B	1.03	0/2629	0.87	3/3557 (0.1%)
1	C	0.82	0/2554	0.76	1/3457 (0.0%)
1	D	0.88	1/2552 (0.0%)	0.76	1/3456 (0.0%)
1	E	0.73	0/2519	0.68	0/3408
1	F	0.95	1/2541 (0.0%)	0.82	0/3440
1	G	1.00	2/2552 (0.1%)	1.54	6/3455 (0.2%)
1	H	0.76	0/2497	0.72	0/3381
All	All	0.90	5/20493 (0.0%)	0.91	13/27736 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	3
1	C	0	1
1	D	0	1
1	E	0	2
1	F	0	1
1	G	0	1
1	H	0	1
All	All	0	12

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	79[A]	ARG	CD-NE	-18.10	1.15	1.46
1	G	79[B]	ARG	CD-NE	-18.10	1.15	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	148	GLU	CB-CG	5.70	1.62	1.52
1	D	164	TYR	CD1-CE1	5.30	1.47	1.39
1	A	173	GLU	CG-CD	5.00	1.59	1.51

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	79[A]	ARG	NE-CZ-NH2	-41.88	99.36	120.30
1	G	79[B]	ARG	NE-CZ-NH2	-41.88	99.36	120.30
1	G	79[A]	ARG	NE-CZ-NH1	35.72	138.16	120.30
1	G	79[B]	ARG	NE-CZ-NH1	35.72	138.16	120.30
1	G	79[A]	ARG	CG-CD-NE	11.46	135.86	111.80
1	G	79[B]	ARG	CG-CD-NE	11.46	135.86	111.80
1	A	16	ARG	NE-CZ-NH2	-6.05	117.27	120.30
1	D	259	LEU	CA-CB-CG	5.92	128.92	115.30
1	C	294	ARG	NE-CZ-NH2	-5.89	117.36	120.30
1	B	81	LEU	CA-CB-CG	5.49	127.92	115.30
1	A	81	LEU	CB-CG-CD1	-5.46	101.71	111.00
1	B	183	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	B	113	ARG	NE-CZ-NH1	-5.10	117.75	120.30

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	107	TYR	Sidechain
1	A	136	TYR	Peptide
1	B	107	TYR	Sidechain
1	B	136	TYR	Peptide
1	B	60	PHE	Sidechain
1	C	107	TYR	Sidechain
1	D	136	TYR	Peptide
1	E	136	TYR	Peptide
1	E	232	GLY	Peptide
1	F	136	TYR	Peptide
1	G	136	TYR	Peptide
1	H	136	TYR	Peptide

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	2556	0	2568	24	1
1	B	2547	0	2541	8	4
1	C	2491	0	2459	7	0
1	D	2495	0	2458	12	0
1	E	2457	0	2430	18	0
1	F	2481	0	2440	13	1
1	G	2489	0	2456	12	4
1	H	2436	0	2404	18	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	2	0	0	0	1
2	E	1	0	0	0	1
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	444	0	0	5	0
3	B	382	0	0	3	0
3	C	298	0	0	1	0
3	D	343	0	0	2	0
3	E	254	0	0	0	0
3	F	362	0	0	1	0
3	G	323	0	0	0	0
3	H	236	0	0	1	0
All	All	22603	0	19756	110	6

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 3.

All (110) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327[B]:GLN:NE2	3:B:572:HOH:O	1.62	1.28
1:A:79[B]:ARG:HH11	1:A:79[B]:ARG:CG	1.60	1.11
1:A:82[B]:ARG:HH11	1:A:82[B]:ARG:HG3	1.02	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79[B]:ARG:HH11	1:A:79[B]:ARG:HG3	1.27	0.96
1:A:82[B]:ARG:HH11	1:A:82[B]:ARG:CG	1.79	0.94
1:A:79[B]:ARG:NH1	1:A:83:GLU:OE1	2.01	0.94
1:E:294:ARG:HH11	1:E:294:ARG:HG2	1.37	0.90
1:A:79[B]:ARG:NH1	1:A:79[B]:ARG:CG	2.32	0.88
1:A:82[B]:ARG:HD3	3:A:818:HOH:O	1.73	0.88
1:A:79[B]:ARG:HH11	1:A:79[B]:ARG:HG2	1.40	0.85
1:A:82[B]:ARG:NH1	1:A:82[B]:ARG:HG3	1.84	0.83
1:F:79[B]:ARG:CD	1:F:82:ARG:HH21	1.94	0.80
1:A:79[B]:ARG:HG3	1:A:79[B]:ARG:NH1	1.92	0.76
1:F:79[B]:ARG:HD2	1:F:82:ARG:HH21	1.52	0.75
1:B:20[B]:LYS:HE3	3:B:841:HOH:O	1.88	0.73
1:E:336:GLU:O	1:E:337:LEU:HG	1.90	0.71
1:F:204:ASP:HB3	3:F:840:HOH:O	1.91	0.70
1:F:272:GLU:O	1:F:276[B]:GLN:HG3	1.93	0.69
1:A:232:GLY:HA2	1:A:235:LEU:HG	1.75	0.68
1:E:294:ARG:NH1	1:E:294:ARG:HG2	2.06	0.67
1:G:337:LEU:O	1:G:338:ASN:CG	2.32	0.67
1:H:232:GLY:O	1:H:233:LYS:HG2	1.94	0.67
1:A:307:GLN:HB2	3:A:756:HOH:O	1.96	0.66
1:E:199:LEU:HD22	1:E:336:GLU:HG3	1.79	0.63
1:B:258:MET:CE	1:B:258:MET:CG	2.77	0.63
1:G:232:GLY:HA2	1:G:235:LEU:HG	1.81	0.62
1:A:281[B]:MET:HE2	3:A:736:HOH:O	1.99	0.61
1:H:263:ASN:ND2	3:H:718:HOH:O	2.33	0.59
1:A:79[B]:ARG:CZ	1:A:83:GLU:OE1	2.45	0.59
1:D:201:ARG:HB3	1:D:204[B]:ASP:OD1	2.02	0.59
1:A:82[B]:ARG:CG	1:A:82[B]:ARG:NH1	2.46	0.58
1:E:264:LEU:H	1:E:264:LEU:HD12	1.69	0.57
1:F:79[B]:ARG:HD3	1:F:82:ARG:HH21	1.65	0.57
1:D:42:LEU:HD21	1:D:79:ARG:HD2	1.87	0.56
1:C:82:ARG:NH2	3:C:772:HOH:O	2.34	0.56
1:E:273:MET:O	1:E:276:GLN:HB2	2.06	0.56
1:A:79[B]:ARG:NH1	1:A:83:GLU:CD	2.60	0.55
1:E:304:ARG:HH11	1:E:306:GLU:HB2	1.72	0.55
1:A:151[B]:SER:OG	3:A:615:HOH:O	2.03	0.54
1:F:79[B]:ARG:CD	1:F:82:ARG:NH2	2.68	0.53
1:C:139[B]:ARG:HD2	1:C:140:VAL:O	2.08	0.53
1:G:20:LYS:HD3	1:G:216:GLY:HA3	1.90	0.53
1:H:34:HIS:O	1:H:35:ASN:HB2	2.08	0.53
1:A:79[B]:ARG:HH12	1:A:83:GLU:CD	2.13	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:LEU:HD13	1:B:294:ARG:HB3	1.91	0.52
1:A:130[A]:GLU:OE1	1:A:130[A]:GLU:HA	2.10	0.51
1:H:263:ASN:C	1:H:265:ASN:H	2.15	0.51
1:G:313[B]:GLN:OE1	1:G:313[B]:GLN:HA	2.11	0.51
1:H:179:VAL:O	1:H:183[B]:ARG:HG2	2.12	0.50
1:F:79[B]:ARG:HD2	1:F:82:ARG:NH2	2.22	0.50
1:E:280:SER:OG	1:E:283:GLN:HG3	2.12	0.49
1:E:51:LYS:HG2	1:E:305:ALA:HB1	1.94	0.49
1:B:273:MET:SD	1:B:327[B]:GLN:HG2	2.52	0.49
1:H:268:ARG:O	1:H:272:GLU:HG3	2.13	0.49
1:E:232:GLY:O	1:E:233:LYS:C	2.51	0.49
1:D:201:ARG:O	1:D:204[B]:ASP:OD1	2.32	0.48
1:E:266:SER:OG	1:E:331:HIS:O	2.25	0.48
1:H:260:THR:O	1:H:264:LEU:HG	2.14	0.48
1:G:79[B]:ARG:CZ	1:G:79[B]:ARG:HB2	2.44	0.48
1:E:334:ASP:OD1	1:E:334:ASP:N	2.47	0.47
1:H:288:TRP:CZ2	1:H:291:LYS:NZ	2.82	0.47
1:B:327[B]:GLN:NE2	3:B:660:HOH:O	2.48	0.47
1:D:231:THR:OG1	1:D:233:LYS:HB2	2.16	0.46
1:C:34:HIS:O	1:C:35:ASN:HB2	2.16	0.46
1:E:36:PHE:O	1:E:73:ALA:HA	2.16	0.46
1:G:185:TRP:CE2	1:H:186:LYS:HE3	2.51	0.46
1:C:332:ILE:HG23	1:C:337:LEU:HB2	1.97	0.46
1:H:288:TRP:CE2	1:H:291:LYS:NZ	2.80	0.45
1:A:233:LYS:HD3	1:A:234:TYR:CE2	2.51	0.45
1:A:79[B]:ARG:NH1	1:A:79[B]:ARG:HG2	2.16	0.45
1:F:260:THR:O	1:F:263:ASN:HB2	2.16	0.45
1:C:336:GLU:HA	1:C:336:GLU:OE1	2.16	0.45
1:G:205:LYS:HE2	1:G:205:LYS:HB3	1.69	0.45
1:H:17:TYR:CZ	1:H:24:ARG:HD2	2.52	0.45
1:C:335:GLY:O	1:C:336:GLU:HB2	2.17	0.44
1:D:203:VAL:HG23	1:D:209:LEU:HG	1.99	0.44
1:D:307:GLN:HB2	3:D:707:HOH:O	2.17	0.44
1:D:12:GLN:NE2	3:D:775:HOH:O	2.48	0.44
1:G:323:LYS:O	1:G:327:GLN:HB2	2.18	0.43
1:A:81:LEU:HD23	1:A:81:LEU:HA	1.85	0.43
1:D:42:LEU:CD2	1:D:79:ARG:HD2	2.47	0.43
1:E:67:GLY:HA3	1:E:68:PRO:HA	1.88	0.43
1:E:139[A]:ARG:HD2	1:E:140:VAL:O	2.19	0.43
1:B:103:TRP:HB2	1:B:104:PRO:HD2	2.01	0.42
1:H:269:LEU:HB3	1:H:331:HIS:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:263:ASN:C	1:H:265:ASN:N	2.73	0.42
1:H:34:HIS:O	1:H:35:ASN:CB	2.68	0.42
1:E:100:TYR:CE1	1:E:139[B]:ARG:HD3	2.55	0.42
1:G:265:ASN:O	1:G:269:LEU:HG	2.20	0.42
1:B:220:ILE:HD11	1:B:299:LEU:HG	2.02	0.42
1:D:292:ASP:OD2	1:D:294:ARG:N	2.43	0.42
1:H:205:LYS:HA	1:H:205:LYS:HD3	1.79	0.42
1:D:100:TYR:CE1	1:D:139[B]:ARG:HD3	2.55	0.41
1:H:260:THR:O	1:H:263:ASN:HB2	2.20	0.41
1:G:232:GLY:C	1:G:234:TYR:H	2.24	0.41
1:F:234:TYR:N	1:F:234:TYR:CD1	2.88	0.41
1:E:185:TRP:CE2	1:F:186:LYS:HE3	2.55	0.41
1:G:337:LEU:O	1:G:338:ASN:CB	2.67	0.41
1:G:283:GLN:NE2	1:G:313[B]:GLN:HB2	2.36	0.41
1:F:167:ILE:HD12	1:F:170:TYR:CG	2.56	0.41
1:A:4[B]:LEU:HD23	1:A:4[B]:LEU:HA	1.88	0.41
1:A:276:GLN:NE2	3:A:662:HOH:O	2.54	0.41
1:F:6:ASN:HA	1:F:7:PRO:HD3	1.98	0.41
1:F:337:LEU:HA	1:F:337:LEU:HD23	1.89	0.41
1:H:288:TRP:O	1:H:291:LYS:HD3	2.22	0.40
1:E:264:LEU:H	1:E:264:LEU:CD1	2.34	0.40
1:D:292:ASP:OD2	1:D:294:ARG:HB2	2.20	0.40
1:H:177:LYS:O	1:H:181:LEU:HG	2.21	0.40
1:D:198:LEU:HA	1:D:198:LEU:HD23	1.87	0.40

All (6) 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)
2:D:402:MG:MG	2:E:401:MG:MG[1_655]	1.28	0.92
1:A:79[B]:ARG:NH2	1:F:75:GLU:OE1[1_655]	1.52	0.68
1:B:79:ARG:NH2	1:G:79[B]:ARG:NH2[1_655]	2.00	0.20
1:B:79:ARG:CZ	1:G:79[B]:ARG:NH2[1_655]	2.04	0.16
1:B:79:ARG:NH1	1:G:79[B]:ARG:CZ[1_655]	2.08	0.12
1:B:79:ARG:NH1	1:G:79[B]:ARG:NH2[1_655]	2.09	0.11

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	324/346 (94%)	317 (98%)	7 (2%)	0	100	100
1	B	321/346 (93%)	311 (97%)	10 (3%)	0	100	100
1	C	313/346 (90%)	301 (96%)	12 (4%)	0	100	100
1	D	313/346 (90%)	304 (97%)	8 (3%)	1 (0%)	46	29
1	E	309/346 (89%)	296 (96%)	13 (4%)	0	100	100
1	F	312/346 (90%)	303 (97%)	9 (3%)	0	100	100
1	G	313/346 (90%)	301 (96%)	11 (4%)	1 (0%)	46	29
1	H	305/346 (88%)	292 (96%)	13 (4%)	0	100	100
All	All	2510/2768 (91%)	2425 (97%)	83 (3%)	2 (0%)	56	38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	338	ASN
1	G	263	ASN

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	275/290 (95%)	274 (100%)	1 (0%)	93	92
1	B	272/290 (94%)	270 (99%)	2 (1%)	88	86
1	C	263/290 (91%)	260 (99%)	3 (1%)	80	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	262/290 (90%)	257 (98%)	5 (2%)	65 52
1	E	259/290 (89%)	252 (97%)	7 (3%)	52 36
1	F	260/290 (90%)	258 (99%)	2 (1%)	86 83
1	G	262/290 (90%)	259 (99%)	3 (1%)	80 74
1	H	256/290 (88%)	250 (98%)	6 (2%)	58 42
All	All	2109/2320 (91%)	2080 (99%)	29 (1%)	74 65

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	ARG
1	B	89	ARG
1	B	310	GLU
1	C	89	ARG
1	C	264	LEU
1	C	310	GLU
1	D	89	ARG
1	D	145	PRO
1	D	203	VAL
1	D	233	LYS
1	D	310	GLU
1	E	89	ARG
1	E	194	PRO
1	E	201	ARG
1	E	263	ASN
1	E	310	GLU
1	E	330	GLN
1	E	334	ASP
1	F	89	ARG
1	F	310	GLU
1	G	89	ARG
1	G	268	ARG
1	G	310	GLU
1	H	89	ARG
1	H	205	LYS
1	H	291	LYS
1	H	304	ARG
1	H	319	THR
1	H	330	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	193	GLN

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 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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	314/346 (90%)	-0.36	3 (0%) 84 82	11, 18, 34, 61	0
1	B	315/346 (91%)	-0.43	4 (1%) 79 76	12, 19, 34, 58	0
1	C	313/346 (90%)	-0.17	9 (2%) 55 49	15, 26, 49, 70	0
1	D	315/346 (91%)	-0.37	4 (1%) 79 76	15, 23, 40, 66	0
1	E	309/346 (89%)	-0.00	28 (9%) 11 9	18, 29, 67, 85	1 (0%)
1	F	313/346 (90%)	-0.31	8 (2%) 59 54	14, 22, 44, 70	3 (0%)
1	G	313/346 (90%)	-0.09	20 (6%) 23 18	15, 24, 61, 82	1 (0%)
1	H	306/346 (88%)	0.13	27 (8%) 12 10	19, 30, 65, 95	1 (0%)
All	All	2498/2768 (90%)	-0.20	103 (4%) 41 35	11, 24, 55, 95	6 (0%)

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	262	ALA	8.4
1	H	228	GLY	7.9
1	E	261	GLU	6.3
1	H	260	THR	6.3
1	B	258	MET	6.1
1	G	234	TYR	6.1
1	G	235	LEU	6.0
1	H	259	LEU	5.8
1	H	261	GLU	5.3
1	F	259	LEU	5.3
1	C	232	GLY	5.1
1	F	234	TYR	5.0
1	D	339	LEU	4.7
1	H	264	LEU	4.5
1	G	232	GLY	4.4
1	E	264	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
1	H	328	ILE	4.1
1	D	235	LEU	4.0
1	F	233	LYS	4.0
1	E	268	ARG	3.9
1	H	268	ARG	3.9
1	H	332	ILE	3.7
1	G	337	LEU	3.7
1	H	229	LEU	3.7
1	E	333	ALA	3.6
1	H	267	LEU	3.6
1	C	264	LEU	3.6
1	G	262	ALA	3.6
1	E	323	LYS	3.6
1	C	259	LEU	3.5
1	H	232	GLY	3.5
1	D	234	TYR	3.4
1	G	336	GLU	3.4
1	H	272	GLU	3.4
1	H	233	LYS	3.4
1	H	320	PHE	3.3
1	A	234	TYR	3.3
1	G	260	THR	3.3
1	B	235	LEU	3.2
1	H	199	LEU	3.2
1	E	278	GLY	3.2
1	C	332	ILE	3.1
1	D	259	LEU	3.1
1	E	327	GLN	3.1
1	B	234	TYR	3.1
1	E	265	ASN	3.0
1	H	327	GLN	3.0
1	C	233	LYS	3.0
1	G	228	GLY	2.9
1	H	263	ASN	2.9
1	E	276	GLN	2.9
1	E	320	PHE	2.8
1	H	202[A]	TRP	2.8
1	G	264	LEU	2.8
1	E	337	LEU	2.7
1	F	268	ARG	2.7
1	E	228	GLY	2.7
1	G	276	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	232	GLY	2.6
1	E	233	LYS	2.6
1	E	266	SER	2.6
1	E	330	GLN	2.6
1	H	231	THR	2.6
1	H	262	ALA	2.5
1	A	235	LEU	2.5
1	G	272	GLU	2.5
1	H	275	GLN	2.5
1	C	234	TYR	2.5
1	E	326	ALA	2.5
1	E	336	GLU	2.5
1	E	267	LEU	2.5
1	G	265	ASN	2.4
1	E	335	GLY	2.4
1	G	233	LYS	2.4
1	E	272	GLU	2.4
1	G	268	ARG	2.4
1	G	326	ALA	2.4
1	H	330	GLN	2.4
1	H	331	HIS	2.4
1	G	229	LEU	2.4
1	F	264	LEU	2.4
1	G	269	LEU	2.4
1	C	336	GLU	2.3
1	F	276[A]	GLN	2.3
1	E	334	ASP	2.3
1	E	263	ASN	2.3
1	G	338	ASN	2.3
1	C	268	ARG	2.3
1	G	330	GLN	2.3
1	F	232	GLY	2.3
1	E	229	LEU	2.2
1	A	301	GLY	2.2
1	H	323	LYS	2.2
1	H	227	GLN	2.2
1	E	332	ILE	2.2
1	G	266	SER	2.2
1	H	265	ASN	2.1
1	H	281	MET	2.1
1	E	202	TRP	2.1
1	C	228	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	233	LYS	2.1
1	E	322	THR	2.0
1	F	260	THR	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	401	1/1	0.97	0.21	5.44	12,12,12,12	0
2	MG	F	401	1/1	0.98	0.17	3.87	10,10,10,10	0
2	MG	D	401	1/1	0.96	0.19	3.84	17,17,17,17	0
2	MG	H	401	1/1	0.95	0.20	3.77	13,13,13,13	0
2	MG	C	401	1/1	0.98	0.16	3.07	19,19,19,19	0
2	MG	G	401	1/1	0.96	0.19	2.09	12,12,12,12	0
2	MG	A	401	1/1	1.00	0.15	1.08	12,12,12,12	0
2	MG	D	402	1/1	0.99	0.10	0.60	54,54,54,54	0
2	MG	E	401	1/1	1.00	0.09	0.13	15,15,15,15	0

6.5 Other polymers (i)

There are no such residues in this entry.