



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:30 PM UTC

PDB ID : 3N6Q / pdb_00003n6q
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

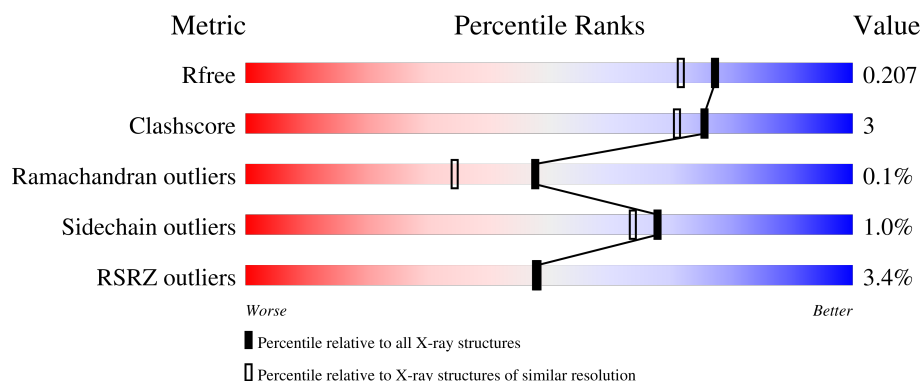
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	346	0% 86% 5% 9%
1	B	346	0% 85% 6% 9%
1	C	346	2% 86% • 10%
1	D	346	0% 85% 5% • 9%
1	E	346	5% 80% 8% • 11%

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Mol	Chain	Length	Quality of chain
1	F	346	% 85% 5% 10%
1	G	346	4% 84% 6% 10%
1	H	346	9% 79% 8% 12%

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 (CCD ID: MG) (formula: Mg).

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total 1	Mg 1	0	0
2	H	1	Total 1	Mg 1	0	0

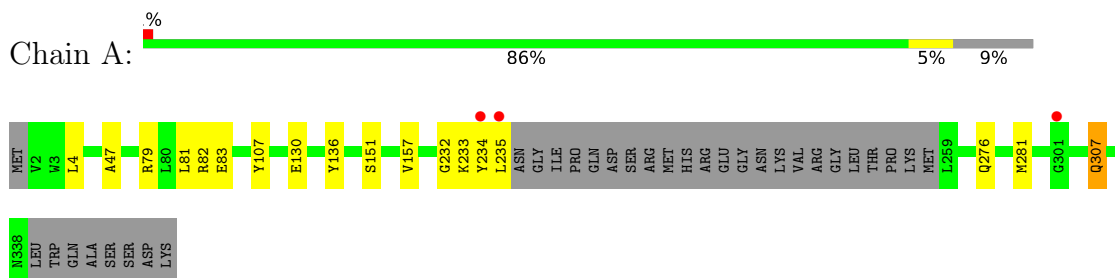
- Molecule 3 is water.

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

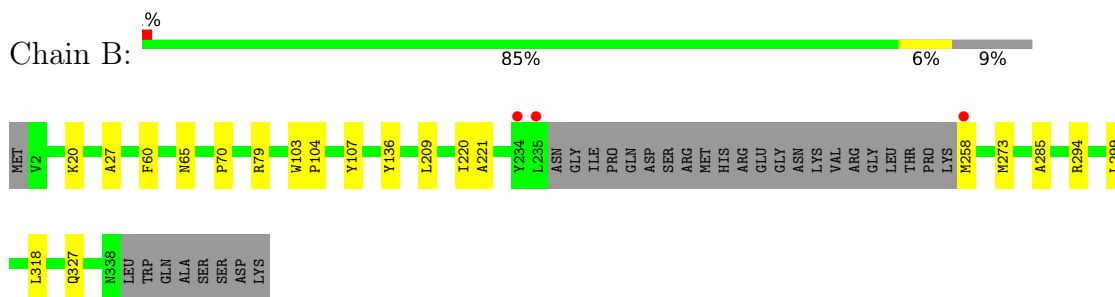
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

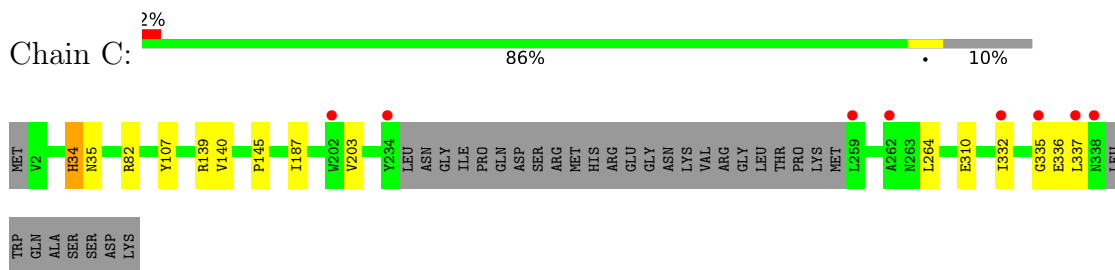
- Molecule 1: YghZ aldol-keto reductase



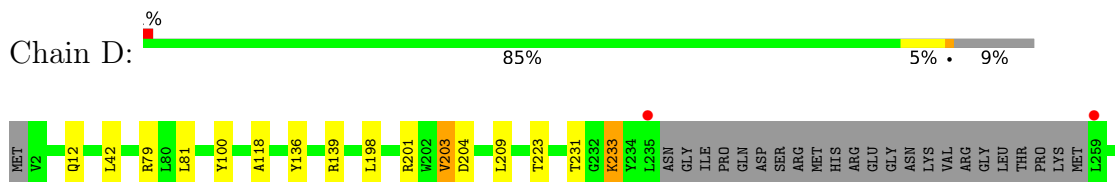
- Molecule 1: YghZ aldol-keto reductase

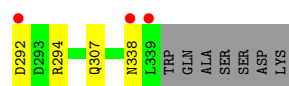


- Molecule 1: YghZ aldol-keto reductase

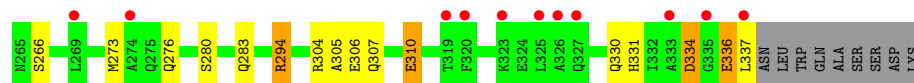
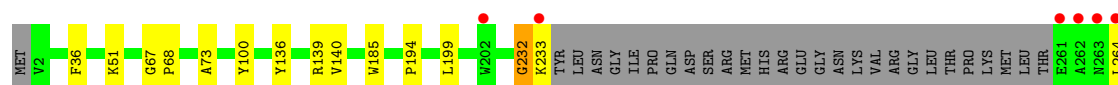
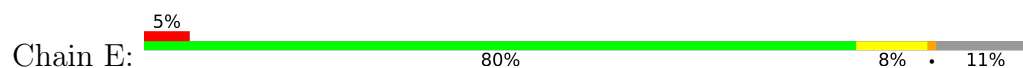


- Molecule 1: YghZ aldol-keto reductase

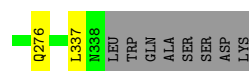
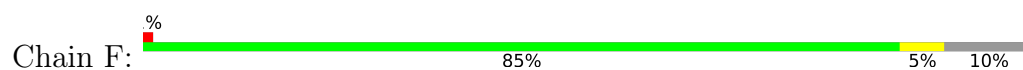




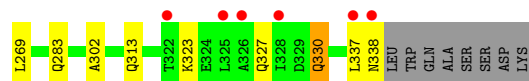
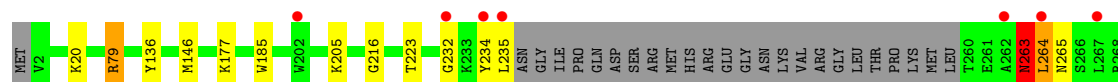
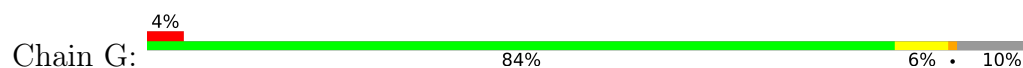
- Molecule 1: YghZ aldoketo reductase



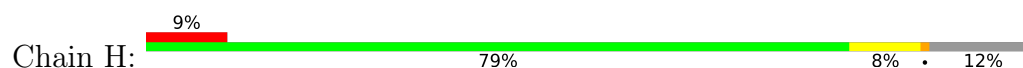
- Molecule 1: YghZ aldoketo reductase



- Molecule 1: YghZ aldoketo reductase



- Molecule 1: YghZ aldoketo reductase



4 Data and refinement statistics

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 94.07 – 1.80	Depositor EDS
% Data completeness (in resolution range)	96.2 (94.07-1.80) 96.2 (94.07-1.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ 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 (5.05%)	wwPDB-VP
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 , 46.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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	1.11	2/2649 (0.1%)	0.98	1/3582 (0.0%)
1	B	1.19	3/2629 (0.1%)	1.02	3/3557 (0.1%)
1	C	1.01	2/2554 (0.1%)	0.94	2/3457 (0.1%)
1	D	1.03	2/2552 (0.1%)	0.94	0/3456
1	E	0.87	0/2519	0.89	0/3408
1	F	1.12	2/2541 (0.1%)	0.98	0/3440
1	G	1.03	3/2552 (0.1%)	0.98	1/3455 (0.0%)
1	H	0.93	3/2497 (0.1%)	0.91	3/3381 (0.1%)
All	All	1.04	17/20493 (0.1%)	0.96	10/27736 (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	3
1	H	0	1
All	All	0	14

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	223	THR	CA-CB	7.65	1.59	1.52
1	A	157	VAL	CA-CB	6.25	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	307	GLN	CD-OE1	5.87	1.34	1.23
1	F	52	ALA	CA-CB	5.57	1.62	1.53
1	C	187	ILE	CA-CB	5.53	1.59	1.54
1	G	330	GLN	CD-OE1	5.48	1.33	1.23
1	C	34	HIS	ND1-CE1	5.45	1.38	1.32
1	G	223	THR	CA-CB	5.44	1.56	1.52
1	H	311	ASN	CG-OD1	5.33	1.33	1.23
1	B	27	ALA	CA-CB	5.32	1.62	1.53
1	H	263	ASN	CG-OD1	5.24	1.33	1.23
1	B	221	ALA	CA-CB	5.13	1.60	1.53
1	D	118	ALA	CA-CB	5.11	1.61	1.53
1	F	148	GLU	N-CA	5.09	1.52	1.46
1	A	47	ALA	CA-C	5.08	1.59	1.52
1	G	263	ASN	CG-OD1	5.08	1.33	1.23
1	B	285	ALA	CA-CB	5.04	1.61	1.53

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	302	ALA	N-CA-C	6.41	119.53	110.23
1	C	34	HIS	CB-CG-CD2	-6.39	122.89	131.20
1	B	65	ASN	N-CA-C	5.75	119.92	113.02
1	H	105	GLY	CA-C-N	5.66	125.76	119.87
1	H	105	GLY	C-N-CA	5.66	125.76	119.87
1	A	307	GLN	N-CA-C	-5.51	105.36	111.36
1	C	34	HIS	CB-CG-ND1	5.39	130.79	122.70
1	H	302	ALA	N-CA-C	5.37	118.01	110.23
1	B	318	LEU	CA-C-N	-5.02	115.17	122.65
1	B	318	LEU	C-N-CA	-5.02	115.17	122.65

There are no chirality outliers.

All (14) 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

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Mol	Chain	Res	Type	Group
1	E	232	GLY	Peptide
1	F	136	TYR	Peptide
1	G	136	TYR	Peptide
1	G	79[A]	ARG	Sidechain
1	G	79[B]	ARG	Sidechain
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	25	1
1	B	2547	0	2541	9	4
1	C	2491	0	2459	7	0
1	D	2495	0	2458	12	0
1	E	2457	0	2430	19	0
1	F	2481	0	2440	13	1
1	G	2489	0	2456	14	4
1	H	2436	0	2404	20	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	4	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	117	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 (117) 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:CG	1:A:79[B]:ARG:HH11	1.60	1.11
1:A:82[B]:ARG:HH11	1:A:82[B]:ARG:HG3	1.02	1.10
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:HG2	1:E:294:ARG:HH11	1.37	0.90
1:A:79[B]:ARG:CG	1:A:79[B]:ARG:NH1	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:HG3	1:A:82[B]:ARG:NH1	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:G:337:LEU:O	1:G:338:ASN:CG	2.32	0.72
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:HG2	1:E:294:ARG:NH1	2.06	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:79[B]:ARG:NH1	1:A:83:GLU:CD	2.60	0.60
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:A:79[B]:ARG:HH12	1:A:83:GLU:CD	2.13	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:H:263:ASN:C	1:H:265:ASN:H	2.15	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:281[B]:MET:HE2	3:A:736:HOH:O	2.08	0.53
1:F:79[B]:ARG:CD	1:F:82:ARG:NH2	2.68	0.53
1:E:232:GLY:O	1:E:233:LYS:C	2.51	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: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:G:313[B]:GLN:HA	1:G:313[B]:GLN:OE1	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: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:N	1:E:334:ASP:OD1	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:H:263:ASN:C	1:H:265:ASN:N	2.73	0.46
1:D:231:THR:OG1	1:D:233:LYS:HB2	2.16	0.46
1:G:232:GLY:C	1:G:234:TYR:H	2.24	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:C:336:GLU:OE1	1:C:336:GLU:HA	2.16	0.45
1:F:260:THR:O	1:F:263:ASN:HB2	2.16	0.45
1:G:205:LYS:HB3	1:G:205:LYS:HE2	1.69	0.45
1:H:17:TYR:CZ	1:H:24:ARG:HD2	2.52	0.45
1:H:273:MET:HE2	1:H:273:MET:HB3	1.83	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:G:146:MET:HE3	1:G:177:LYS:HG2	2.01	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:B:220:ILE:HD11	1:B:299:LEU:HG	2.02	0.42
1:G:265:ASN:O	1:G:269:LEU:HG	2.20	0.42
1:D:292:ASP:OD2	1:D:294:ARG:N	2.43	0.42
1:H:205:LYS:HD3	1:H:205:LYS:HA	1.79	0.42
1:D:100:TYR:CE1	1:D:139[B]:ARG:HD3	2.55	0.41
1:B:327[B]:GLN:CD	3:B:660:HOH:O	2.63	0.41
1:H:260:THR:O	1:H:263:ASN:HB2	2.20	0.41
1:E:310:GLU:OE1	1:E:310:GLU:C	2.64	0.41
1:F:234:TYR:CD1	1:F:234:TYR:N	2.88	0.41
1:G:263:ASN:O	1:G:264:LEU:C	2.63	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:A:4[B]:LEU:HD23	1:A:4[B]:LEU:HA	1.88	0.41
1:F:167:ILE:HD12	1:F:170:TYR:CG	2.56	0.41
1:G:283:GLN:NE2	1:G:313[B]:GLN:HB2	2.36	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:HD23	1:F:337:LEU:HA	1.89	0.41
1:H:288:TRP:O	1:H:291:LYS:HD3	2.22	0.40
1:D:198:LEU:HA	1:D:198:LEU:HD23	1.87	0.40
1:D:292:ASP:OD2	1:D:294:ARG:HB2	2.20	0.40
1:E:264:LEU:H	1:E:264:LEU:CD1	2.34	0.40
1:H:177:LYS:O	1:H:181:LEU:HG	2.21	0.40
1:H:306:GLU:H	1:H:306:GLU:CD	2.30	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%)	36	25
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%)	36	25
1	H	305/346 (88%)	292 (96%)	13 (4%)	0	100	100
All	All	2510/2768 (91%)	2425 (97%)	83 (3%)	2 (0%)	48	34

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%)	275 (100%)	0	100	100
1	B	272/290 (94%)	271 (100%)	1 (0%)	84	83
1	C	263/290 (91%)	260 (99%)	3 (1%)	65	60
1	D	262/290 (90%)	259 (99%)	3 (1%)	65	60
1	E	259/290 (89%)	252 (97%)	7 (3%)	39	27
1	F	260/290 (90%)	260 (100%)	0	100	100
1	G	262/290 (90%)	260 (99%)	2 (1%)	73	70
1	H	256/290 (88%)	252 (98%)	4 (2%)	55	47
All	All	2109/2320 (91%)	2089 (99%)	20 (1%)	68	67

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	70	PRO
1	C	203	VAL
1	C	264	LEU
1	C	310	GLU
1	D	81	LEU
1	D	203	VAL
1	D	233	LYS
1	E	194	PRO
1	E	294	ARG
1	E	307	GLN
1	E	310	GLU
1	E	330	GLN
1	E	334	ASP
1	E	336	GLU
1	G	264	LEU
1	G	330	GLN
1	H	264	LEU
1	H	291	LYS
1	H	319	THR
1	H	330	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	A	143	ASN
1	A	215	ASN
1	A	327	GLN
1	B	12	GLN
1	B	307	GLN
1	B	311	ASN
1	C	34	HIS
1	C	143	ASN
1	C	307	GLN
1	C	311	ASN
1	C	327	GLN
1	D	215	ASN
1	D	330	GLN
1	D	331	HIS
1	E	176	GLN
1	E	215	ASN
1	F	307	GLN
1	F	311	ASN
1	F	327	GLN
1	F	331	HIS
1	G	155	HIS
1	H	35	ASN
1	H	213	GLN
1	H	215	ASN
1	H	271	ASN
1	H	327	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 oligosaccharides 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, 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	314/346 (90%)	-0.64	3 (0%)	79 80	10, 18, 33, 61	14 (4%)
1	B	315/346 (91%)	-0.59	3 (0%)	79 80	10, 19, 34, 58	10 (3%)
1	C	313/346 (90%)	-0.07	8 (2%)	57 57	15, 26, 49, 70	4 (1%)
1	D	315/346 (91%)	-0.35	5 (1%)	70 71	14, 23, 40, 66	2 (0%)
1	E	309/346 (89%)	0.21	17 (5%)	30 29	16, 29, 67, 85	5 (1%)
1	F	313/346 (90%)	-0.34	5 (1%)	70 71	14, 22, 44, 70	6 (1%)
1	G	313/346 (90%)	-0.11	13 (4%)	40 40	13, 23, 60, 82	5 (1%)
1	H	306/346 (88%)	0.39	32 (10%)	11 10	19, 30, 65, 95	4 (1%)
All	All	2498/2768 (90%)	-0.19	86 (3%)	48 48	10, 24, 55, 95	50 (2%)

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	262	ALA	6.6
1	H	259	LEU	6.2
1	D	339	LEU	6.1
1	E	261	GLU	6.0
1	E	337	LEU	5.4
1	H	202[A]	TRP	5.0
1	C	259	LEU	4.6
1	D	259	LEU	4.5
1	H	332	ILE	4.4
1	G	337	LEU	3.9
1	B	258	MET	3.9
1	F	234	TYR	3.9
1	F	259	LEU	3.9
1	H	326	ALA	3.8
1	H	328	ILE	3.7
1	G	202	TRP	3.6

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Mol	Chain	Res	Type	RSRZ
1	H	262	ALA	3.6
1	G	235	LEU	3.6
1	H	199	LEU	3.5
1	G	338	ASN	3.5
1	E	264	LEU	3.5
1	H	325	LEU	3.5
1	H	269	LEU	3.4
1	H	270	LEU	3.4
1	C	337	LEU	3.3
1	H	229	LEU	3.2
1	H	301	GLY	3.1
1	E	326	ALA	3.1
1	E	202	TRP	3.1
1	H	322	THR	3.0
1	H	230	LEU	2.9
1	H	264	LEU	2.9
1	H	320	PHE	2.9
1	H	319	THR	2.8
1	E	320	PHE	2.8
1	E	333	ALA	2.8
1	G	264	LEU	2.8
1	H	273	MET	2.8
1	E	263	ASN	2.7
1	F	262	ALA	2.7
1	H	331	HIS	2.7
1	H	329	ASP	2.7
1	C	338	ASN	2.7
1	E	269	LEU	2.7
1	H	327	GLN	2.6
1	A	235	LEU	2.6
1	E	335	GLY	2.6
1	E	325	LEU	2.6
1	H	198	LEU	2.6
1	H	228	GLY	2.6
1	H	267	LEU	2.6
1	A	234	TYR	2.5
1	B	235	LEU	2.5
1	D	235	LEU	2.5
1	A	301	GLY	2.5
1	H	323	LYS	2.5
1	G	262	ALA	2.5
1	H	302	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	319	THR	2.5
1	C	234	TYR	2.5
1	H	233	LYS	2.5
1	F	204	ASP	2.5
1	H	288	TRP	2.4
1	H	260	THR	2.3
1	H	274	ALA	2.3
1	D	338	ASN	2.3
1	G	322	THR	2.3
1	C	335	GLY	2.3
1	G	325	LEU	2.3
1	G	232	GLY	2.2
1	E	323	LYS	2.2
1	H	330	GLN	2.2
1	C	202	TRP	2.2
1	G	234	TYR	2.2
1	E	274	ALA	2.2
1	D	292	ASP	2.2
1	B	234	TYR	2.1
1	C	332	ILE	2.1
1	G	267	LEU	2.1
1	G	326	ALA	2.1
1	G	328	ILE	2.1
1	E	233	LYS	2.1
1	F	232	GLY	2.1
1	E	327	GLN	2.0
1	C	262	ALA	2.0
1	H	285	ALA	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 oligosaccharides 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. 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	B-factors(Å ²)	Q<0.9
2	MG	B	401	1/1	0.96	0.09	12,12,12,12	0
2	MG	C	401	1/1	0.97	0.10	19,19,19,19	0
2	MG	F	401	1/1	0.97	0.07	10,10,10,10	0
2	MG	G	401	1/1	0.97	0.10	12,12,12,12	0
2	MG	D	401	1/1	0.98	0.11	17,17,17,17	0
2	MG	H	401	1/1	0.98	0.10	13,13,13,13	0
2	MG	D	402	1/1	0.99	0.07	54,54,54,54	0
2	MG	A	401	1/1	0.99	0.07	12,12,12,12	0
2	MG	E	401	1/1	1.00	0.03	15,15,15,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.