Full wwPDB X-ray Structure Validation Report ⓘ

Dec 3, 2020 – 09:06 am GMT

PDB ID	:	6Z87
Title	:	human GTP cyclohydrolase I
Authors	:	Ebenhoch, R.; Nar, H.
Deposited on	:	2020-06-02
Resolution	:	2.56 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 following versions of software and data (see references ⓘ) were used in the production of this report:

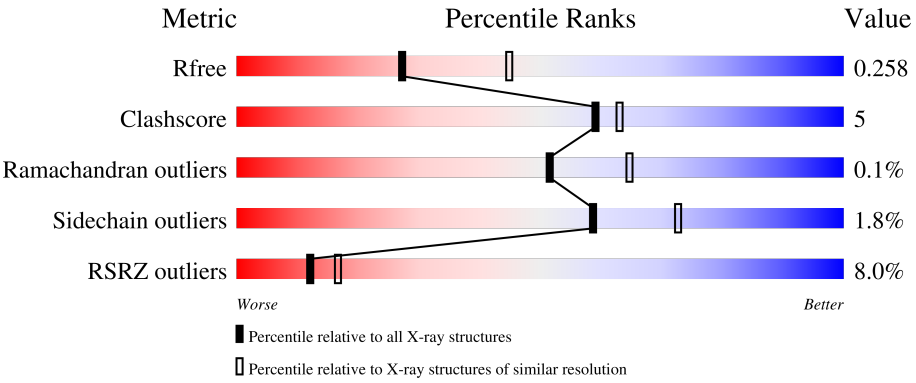
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

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 2.56 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}	130704	1279 (2.58-2.54)
Clashscore	141614	1327 (2.58-2.54)
Ramachandran outliers	138981	1312 (2.58-2.54)
Sidechain outliers	138945	1312 (2.58-2.54)
RSRZ outliers	127900	1269 (2.58-2.54)

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 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 <=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	224	4% 75% 8% • 16%
1	B	224	4% 75% 5% 19%
1	C	224	6% 76% 8% 16%
1	D	224	11% 73% 11% 16%
1	E	224	8% 73% 11% 16%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7457 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 GTP cyclohydrolase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	188	Total	C	N	O	S	0	0	0
			1482	935	259	278	10			
1	B	181	Total	C	N	O	S	0	0	0
			1427	901	253	263	10			
1	C	189	Total	C	N	O	S	0	0	0
			1493	941	263	279	10			
1	D	188	Total	C	N	O	S	0	0	0
			1482	935	259	278	10			
1	E	188	Total	C	N	O	S	0	0	0
			1482	935	259	278	10			

There are 70 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	MET	-	initiating methionine	UNP P30793
A	28	HIS	-	expression tag	UNP P30793
A	29	HIS	-	expression tag	UNP P30793
A	30	HIS	-	expression tag	UNP P30793
A	31	HIS	-	expression tag	UNP P30793
A	32	HIS	-	expression tag	UNP P30793
A	33	HIS	-	expression tag	UNP P30793
A	34	GLY	-	expression tag	UNP P30793
A	35	SER	-	expression tag	UNP P30793
A	36	ASP	-	expression tag	UNP P30793
A	37	ASP	-	expression tag	UNP P30793
A	38	ASP	-	expression tag	UNP P30793
A	39	ASP	-	expression tag	UNP P30793
A	40	LYS	-	expression tag	UNP P30793
B	27	MET	-	initiating methionine	UNP P30793
B	28	HIS	-	expression tag	UNP P30793
B	29	HIS	-	expression tag	UNP P30793
B	30	HIS	-	expression tag	UNP P30793
B	31	HIS	-	expression tag	UNP P30793

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Chain	Residue	Modelled	Actual	Comment	Reference
B	32	HIS	-	expression tag	UNP P30793
B	33	HIS	-	expression tag	UNP P30793
B	34	GLY	-	expression tag	UNP P30793
B	35	SER	-	expression tag	UNP P30793
B	36	ASP	-	expression tag	UNP P30793
B	37	ASP	-	expression tag	UNP P30793
B	38	ASP	-	expression tag	UNP P30793
B	39	ASP	-	expression tag	UNP P30793
B	40	LYS	-	expression tag	UNP P30793
C	27	MET	-	initiating methionine	UNP P30793
C	28	HIS	-	expression tag	UNP P30793
C	29	HIS	-	expression tag	UNP P30793
C	30	HIS	-	expression tag	UNP P30793
C	31	HIS	-	expression tag	UNP P30793
C	32	HIS	-	expression tag	UNP P30793
C	33	HIS	-	expression tag	UNP P30793
C	34	GLY	-	expression tag	UNP P30793
C	35	SER	-	expression tag	UNP P30793
C	36	ASP	-	expression tag	UNP P30793
C	37	ASP	-	expression tag	UNP P30793
C	38	ASP	-	expression tag	UNP P30793
C	39	ASP	-	expression tag	UNP P30793
C	40	LYS	-	expression tag	UNP P30793
D	27	MET	-	initiating methionine	UNP P30793
D	28	HIS	-	expression tag	UNP P30793
D	29	HIS	-	expression tag	UNP P30793
D	30	HIS	-	expression tag	UNP P30793
D	31	HIS	-	expression tag	UNP P30793
D	32	HIS	-	expression tag	UNP P30793
D	33	HIS	-	expression tag	UNP P30793
D	34	GLY	-	expression tag	UNP P30793
D	35	SER	-	expression tag	UNP P30793
D	36	ASP	-	expression tag	UNP P30793
D	37	ASP	-	expression tag	UNP P30793
D	38	ASP	-	expression tag	UNP P30793
D	39	ASP	-	expression tag	UNP P30793
D	40	LYS	-	expression tag	UNP P30793
E	27	MET	-	initiating methionine	UNP P30793
E	28	HIS	-	expression tag	UNP P30793
E	29	HIS	-	expression tag	UNP P30793
E	30	HIS	-	expression tag	UNP P30793
E	31	HIS	-	expression tag	UNP P30793

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Chain	Residue	Modelled	Actual	Comment	Reference
E	32	HIS	-	expression tag	UNP P30793
E	33	HIS	-	expression tag	UNP P30793
E	34	GLY	-	expression tag	UNP P30793
E	35	SER	-	expression tag	UNP P30793
E	36	ASP	-	expression tag	UNP P30793
E	37	ASP	-	expression tag	UNP P30793
E	38	ASP	-	expression tag	UNP P30793
E	39	ASP	-	expression tag	UNP P30793
E	40	LYS	-	expression tag	UNP P30793

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Zn 1 1	0	0
2	A	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	E	1	Total Zn 1 1	0	0

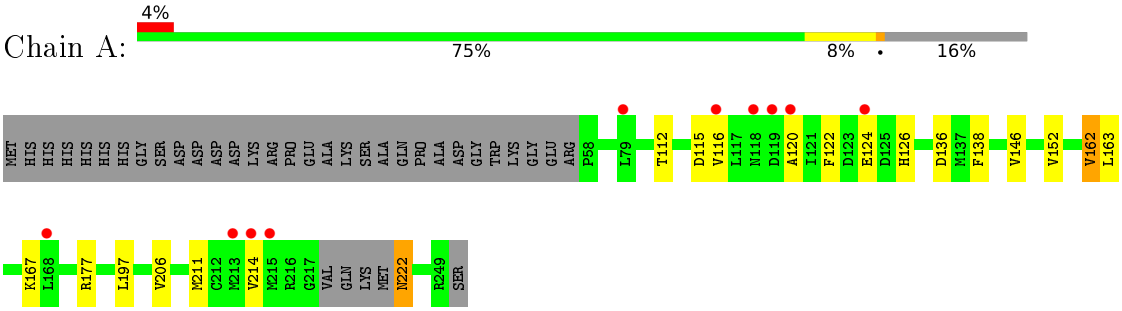
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	26	Total O 26 26	0	0
3	B	10	Total O 10 10	0	0
3	C	24	Total O 24 24	0	0
3	D	9	Total O 9 9	0	0
3	E	17	Total O 17 17	0	0

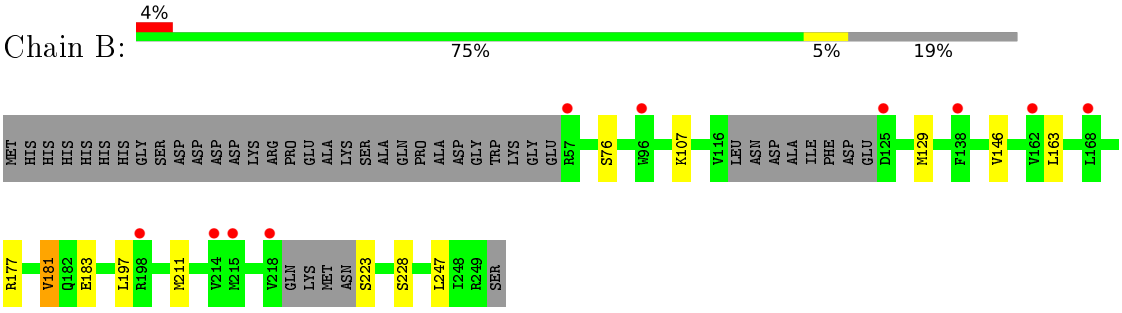
3 Residue-property plots (i)

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.

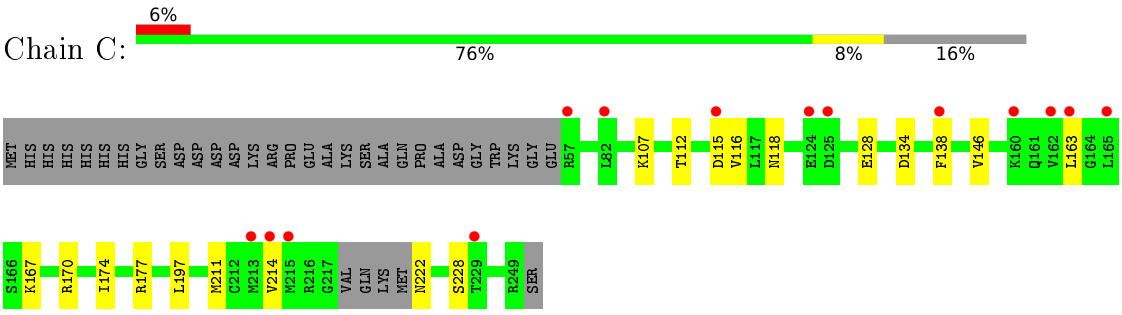
- Molecule 1: GTP cyclohydrolase 1



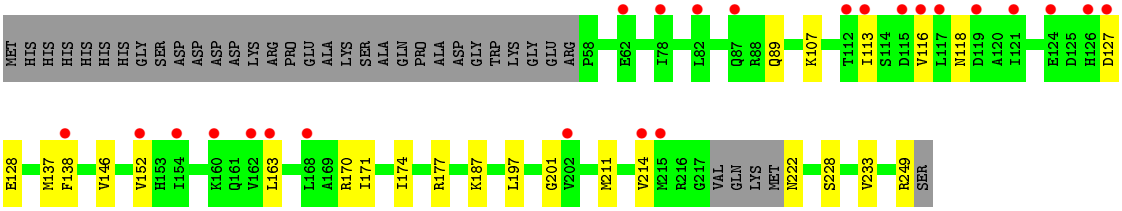
- Molecule 1: GTP cyclohydrolase 1



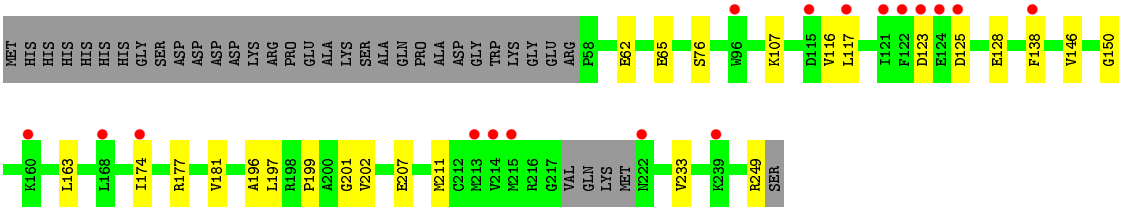
- Molecule 1: GTP cyclohydrolase 1



- Molecule 1: GTP cyclohydrolase 1



- Molecule 1: GTP cyclohydrolase 1



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	109.88Å 109.88Å 387.25Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	95.16 – 2.56 95.16 – 2.56	Depositor EDS
% Data completeness (in resolution range)	59.8 (95.16-2.56) 59.8 (95.16-2.56)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.88 (at 2.55Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.227 , 0.246 0.231 , 0.258	Depositor DCC
R_{free} test set	1370 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	60.9	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 64.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7457	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% 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, 0.333 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: ZN

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	0/1506	0.54	0/2033
1	B	0.34	0/1449	0.56	0/1954
1	C	0.34	0/1517	0.55	0/2048
1	D	0.34	0/1506	0.55	0/2033
1	E	0.36	0/1506	0.56	0/2033
All	All	0.35	0/7484	0.55	0/10101

There are no bond length outliers.

There are no bond angle outliers.

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	1482	0	1499	11	0
1	B	1427	0	1457	12	0
1	C	1493	0	1511	12	0
1	D	1482	0	1499	21	0
1	E	1482	0	1499	20	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1	0	0	0	0
2	E	1	0	0	0	0
3	A	26	0	0	0	0
3	B	10	0	0	0	0
3	C	24	0	0	0	0
3	D	9	0	0	0	0
3	E	17	0	0	0	0
All	All	7457	0	7465	70	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 5.

All (70) 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:107:LYS:NZ	1:B:177:ARG:HD2	1.85	0.91
1:B:107:LYS:HZ2	1:B:177:ARG:HD2	1.34	0.89
1:A:138:PHE:HB2	1:A:177:ARG:HH22	1.55	0.70
1:C:214:VAL:HG22	1:C:222:ASN:HA	1.73	0.70
1:C:138:PHE:HB2	1:C:177:ARG:HH22	1.57	0.69
1:D:116:VAL:HG21	1:D:174:ILE:HD11	1.75	0.69
1:D:138:PHE:HB2	1:D:177:ARG:HH22	1.57	0.69
1:B:107:LYS:NZ	1:B:177:ARG:HH21	1.92	0.67
1:E:138:PHE:HB2	1:E:177:ARG:HH22	1.59	0.66
1:B:181:VAL:HG13	1:B:183:GLU:OE1	1.95	0.66
1:E:117:LEU:HD13	1:E:196:ALA:HB2	1.78	0.66
1:E:107:LYS:HZ2	1:E:177:ARG:HD2	1.64	0.62
1:D:249:ARG:HH12	1:E:249:ARG:NH1	1.98	0.62
1:B:107:LYS:HZ1	1:B:177:ARG:HH21	1.46	0.61
1:E:146:VAL:HG12	1:E:211:MET:HB2	1.82	0.60
1:A:120:ALA:HB1	1:A:167:LYS:HG3	1.83	0.59
1:B:129:MET:HE1	1:B:247:LEU:HD12	1.85	0.58
1:E:107:LYS:HZ2	1:E:177:ARG:CD	2.16	0.58
1:D:146:VAL:HG12	1:D:211:MET:HB2	1.85	0.58
1:A:146:VAL:HG12	1:A:211:MET:HB2	1.85	0.58
1:B:146:VAL:HG12	1:B:211:MET:HB2	1.87	0.56
1:C:146:VAL:HG12	1:C:211:MET:HB2	1.87	0.56
1:A:214:VAL:HG22	1:A:222:ASN:HB3	1.87	0.56
1:C:116:VAL:HG21	1:C:174:ILE:HD11	1.87	0.56
1:A:138:PHE:HD2	1:A:177:ARG:HH12	1.55	0.55
1:D:107:LYS:HZ2	1:D:177:ARG:NE	2.04	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:228:SER:O	1:D:128:GLU:HB3	2.08	0.54
1:D:107:LYS:HZ2	1:D:177:ARG:HE	1.53	0.54
1:A:112:THR:HG23	1:A:115:ASP:HB2	1.90	0.54
1:D:107:LYS:HZ2	1:D:177:ARG:CD	2.22	0.53
1:A:120:ALA:CB	1:A:167:LYS:HG3	2.40	0.52
1:D:107:LYS:HZ2	1:D:177:ARG:HD2	1.74	0.52
1:A:163:LEU:HB2	1:A:197:LEU:HD21	1.91	0.51
1:D:138:PHE:HD2	1:D:177:ARG:HH12	1.57	0.51
1:E:138:PHE:HD2	1:E:177:ARG:HH12	1.57	0.51
1:C:167:LYS:NZ	1:C:170:ARG:NH2	2.60	0.50
1:E:107:LYS:HZ2	1:E:177:ARG:NE	2.09	0.50
1:B:223:SER:HB3	1:C:134:ASP:HB2	1.93	0.50
1:E:107:LYS:NZ	1:E:177:ARG:HD2	2.26	0.50
1:D:107:LYS:NZ	1:D:177:ARG:HD2	2.26	0.50
1:A:122:PHE:HB2	1:A:162:VAL:HG12	1.92	0.50
1:C:138:PHE:HD2	1:C:177:ARG:HH12	1.60	0.49
1:D:214:VAL:HG22	1:D:222:ASN:HB2	1.95	0.49
1:E:107:LYS:HZ2	1:E:177:ARG:HE	1.62	0.48
1:A:124:GLU:OE1	1:A:126:HIS:ND1	2.47	0.48
1:D:163:LEU:HB2	1:D:197:LEU:HD21	1.96	0.48
1:D:107:LYS:NZ	1:D:177:ARG:CD	2.77	0.47
1:E:107:LYS:NZ	1:E:177:ARG:CD	2.77	0.47
1:D:113:ILE:HD11	1:D:171:ILE:HG12	1.97	0.47
1:B:228:SER:O	1:C:128:GLU:HB3	2.14	0.47
1:A:152:VAL:HG22	1:A:206:VAL:HG22	1.98	0.46
1:D:107:LYS:NZ	1:D:177:ARG:HE	2.12	0.46
1:E:107:LYS:NZ	1:E:177:ARG:HE	2.14	0.46
1:E:116:VAL:HG21	1:E:174:ILE:HD11	1.98	0.46
1:C:163:LEU:HB2	1:C:197:LEU:HD21	1.98	0.45
1:B:163:LEU:HB2	1:B:197:LEU:HD21	1.98	0.45
1:E:123:ASP:OD1	1:E:123:ASP:O	2.35	0.44
1:D:228:SER:O	1:E:128:GLU:HB3	2.18	0.44
1:E:163:LEU:HB2	1:E:197:LEU:HD21	1.99	0.44
1:D:187:LYS:HZ2	1:E:125:ASP:HB3	1.84	0.43
1:D:137:MET:HB2	1:D:152:VAL:HG23	2.02	0.42
1:B:107:LYS:HZ3	1:B:177:ARG:HD2	1.73	0.42
1:C:112:THR:OG1	1:C:115:ASP:HB2	2.19	0.42
1:D:201:GLY:HA3	1:D:233:VAL:HG12	2.01	0.41
1:E:201:GLY:HA3	1:E:233:VAL:HG12	2.02	0.41
1:E:199:PRO:HG2	1:E:202:VAL:HG12	2.03	0.41
1:E:150:GLY:HA3	1:E:207:GLU:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:LYS:NZ	1:B:177:ARG:NH2	2.65	0.40
1:C:167:LYS:HZ3	1:C:170:ARG:NH2	2.19	0.40
1:D:107:LYS:NZ	1:D:177:ARG:NE	2.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	184/224 (82%)	180 (98%)	4 (2%)	0	100 100
1	B	175/224 (78%)	172 (98%)	3 (2%)	0	100 100
1	C	185/224 (83%)	182 (98%)	3 (2%)	0	100 100
1	D	184/224 (82%)	177 (96%)	6 (3%)	1 (0%)	29 39
1	E	184/224 (82%)	180 (98%)	4 (2%)	0	100 100
All	All	912/1120 (81%)	891 (98%)	20 (2%)	1 (0%)	51 65

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	89	GLN

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	165/195 (85%)	161 (98%)	4 (2%)	49	63
1	B	159/195 (82%)	157 (99%)	2 (1%)	69	80
1	C	166/195 (85%)	164 (99%)	2 (1%)	71	81
1	D	165/195 (85%)	162 (98%)	3 (2%)	59	73
1	E	165/195 (85%)	161 (98%)	4 (2%)	49	63
All	All	820/975 (84%)	805 (98%)	15 (2%)	59	73

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	116	VAL
1	A	136	ASP
1	A	162	VAL
1	A	222	ASN
1	B	76	SER
1	B	181	VAL
1	C	107	LYS
1	C	118	ASN
1	D	118	ASN
1	D	127	ASP
1	D	170	ARG
1	E	62	GLU
1	E	65	GLU
1	E	76	SER
1	E	181	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	222	ASN
1	D	118	ASN
1	D	222	ASN
1	E	118	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry

Of 5 ligands modelled in this entry, 5 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	188/224 (83%)	0.56	10 (5%) 26 33	39, 64, 112, 132	0
1	B	181/224 (80%)	0.70	10 (5%) 25 32	41, 62, 100, 113	0
1	C	189/224 (84%)	0.72	14 (7%) 14 19	39, 65, 108, 126	0
1	D	188/224 (83%)	0.92	24 (12%) 3 5	49, 82, 130, 143	0
1	E	188/224 (83%)	0.76	17 (9%) 9 13	38, 56, 107, 116	0
All	All	934/1120 (83%)	0.73	75 (8%) 12 17	38, 65, 113, 143	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	125	ASP	5.7
1	D	117	LEU	4.9
1	C	215	MET	4.8
1	E	214	VAL	4.8
1	E	160	LYS	4.6
1	D	87	GLN	4.5
1	B	138	PHE	4.4
1	D	119	ASP	4.3
1	E	117	LEU	4.2
1	A	124	GLU	4.1
1	A	215	MET	4.0
1	E	215	MET	3.9
1	E	123	ASP	3.9
1	A	214	VAL	3.9
1	C	214	VAL	3.8
1	D	82	LEU	3.7
1	D	116	VAL	3.7
1	D	138	PHE	3.7
1	C	213	MET	3.5
1	D	160	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	125	ASP	3.4
1	C	138	PHE	3.3
1	A	120	ALA	3.3
1	D	168	LEU	3.3
1	D	214	VAL	3.3
1	A	119	ASP	3.2
1	D	127	ASP	3.2
1	A	116	VAL	3.1
1	D	124	GLU	3.1
1	E	96	TRP	3.1
1	D	162	VAL	3.1
1	C	125	ASP	3.1
1	E	213	MET	3.0
1	E	122	PHE	3.0
1	D	215	MET	3.0
1	E	138	PHE	3.0
1	B	57	ARG	2.9
1	E	168	LEU	2.9
1	B	215	MET	2.8
1	E	121	ILE	2.8
1	B	96	TRP	2.8
1	E	124	GLU	2.8
1	A	168	LEU	2.8
1	E	222	ASN	2.7
1	D	163	LEU	2.7
1	E	239	LYS	2.7
1	D	154	ILE	2.6
1	C	82	LEU	2.6
1	D	112	THR	2.5
1	A	118	ASN	2.4
1	E	174	ILE	2.4
1	B	162	VAL	2.4
1	D	113	ILE	2.4
1	C	57	ARG	2.4
1	D	202	VAL	2.4
1	C	162	VAL	2.4
1	C	115	ASP	2.4
1	D	62	GLU	2.3
1	C	229	THR	2.3
1	B	214	VAL	2.3
1	B	168	LEU	2.3
1	D	126	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	124	GLU	2.3
1	A	79	LEU	2.2
1	D	115	ASP	2.2
1	C	160	LYS	2.2
1	D	78	ILE	2.2
1	D	121	ILE	2.2
1	E	115	ASP	2.1
1	D	152	VAL	2.1
1	A	213	MET	2.1
1	B	198	ARG	2.1
1	B	218	VAL	2.0
1	C	165	LEU	2.0
1	C	163	LEU	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 monosaccharides 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, 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	B-factors(Å^2)	Q<0.9
2	ZN	B	300	1/1	0.97	0.15	78,78,78,78	0
2	ZN	A	300	1/1	0.98	0.18	69,69,69,69	0
2	ZN	D	300	1/1	0.98	0.20	87,87,87,87	0
2	ZN	C	300	1/1	0.98	0.19	77,77,77,77	0
2	ZN	E	300	1/1	0.98	0.19	96,96,96,96	0

6.5 Other polymers (i)

There are no such residues in this entry.