



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:49 PM GMT

PDB ID : 4DG7  
Title : Low resolution structure of Drosophila Translin  
Authors : Kumar, V.; Gupta, G.D.  
Deposited on : 2012-01-25  
Resolution : 4.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) 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

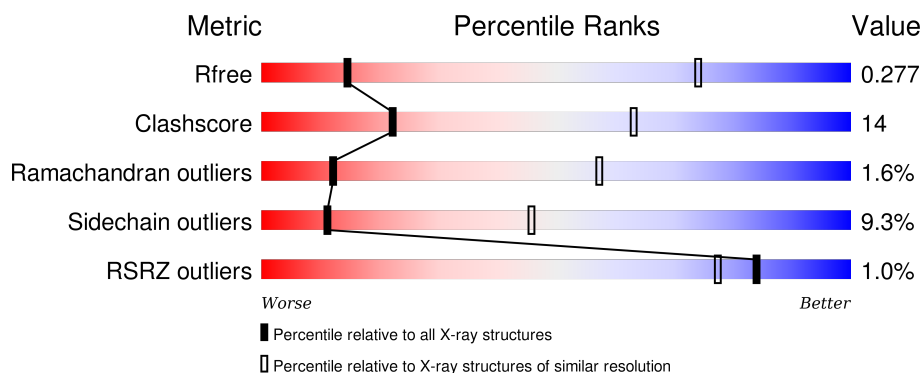
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 4.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1039 (4.80-3.60)
Clashscore	102246	1140 (4.80-3.60)
Ramachandran outliers	100387	1083 (4.80-3.60)
Sidechain outliers	100360	1067 (4.80-3.60)
RSRZ outliers	91569	1042 (4.80-3.60)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	255	<div> <div>50%</div> <div>27%</div> <div>5%</div> <div>17%</div> </div>
1	B	255	<div> <div>52%</div> <div>28%</div> <div>•</div> <div>16%</div> </div>
1	C	255	<div> <div>53%</div> <div>26%</div> <div>•</div> <div>17%</div> </div>
1	D	255	<div> <div>56%</div> <div>24%</div> <div>•</div> <div>16%</div> </div>
1	E	255	<div> <div>2%</div> <div>55%</div> <div>25%</div> <div>•</div> <div>15%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	255	<div><div><div>%</div><div><div></div><div>54%</div><div>27%</div><div>•</div><div>16%</div></div></div></div>
1	G	255	<div><div><div>%</div><div><div></div><div>53%</div><div>26%</div><div>5%</div><div>16%</div></div></div></div>
1	H	255	<div><div><div>2%</div><div><div></div><div>53%</div><div>28%</div><div>•</div><div>15%</div></div></div></div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 13931 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 GM27569p.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	212	Total	C	N	O	S	0	0	0
			1727	1108	294	321	4			
1	B	213	Total	C	N	O	S	0	0	0
			1731	1108	295	324	4			
1	C	212	Total	C	N	O	S	0	0	0
			1727	1108	294	321	4			
1	D	214	Total	C	N	O	S	0	0	0
			1739	1114	296	325	4			
1	E	216	Total	C	N	O	S	0	0	0
			1757	1125	299	329	4			
1	F	215	Total	C	N	O	S	0	0	0
			1748	1120	298	326	4			
1	G	214	Total	C	N	O	S	0	0	0
			1739	1114	296	325	4			
1	H	217	Total	C	N	O	S	0	0	0
			1763	1129	301	329	4			

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP Q7JVK6
A	-18	GLY	-	EXPRESSION TAG	UNP Q7JVK6
A	-17	SER	-	EXPRESSION TAG	UNP Q7JVK6
A	-16	SER	-	EXPRESSION TAG	UNP Q7JVK6
A	-15	HIS	-	EXPRESSION TAG	UNP Q7JVK6
A	-14	HIS	-	EXPRESSION TAG	UNP Q7JVK6
A	-13	HIS	-	EXPRESSION TAG	UNP Q7JVK6
A	-12	HIS	-	EXPRESSION TAG	UNP Q7JVK6
A	-11	HIS	-	EXPRESSION TAG	UNP Q7JVK6
A	-10	HIS	-	EXPRESSION TAG	UNP Q7JVK6
A	-9	SER	-	EXPRESSION TAG	UNP Q7JVK6
A	-8	SER	-	EXPRESSION TAG	UNP Q7JVK6
A	-7	GLY	-	EXPRESSION TAG	UNP Q7JVK6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	LEU	-	EXPRESSION TAG	UNP Q7JVK6
A	-5	VAL	-	EXPRESSION TAG	UNP Q7JVK6
A	-4	PRO	-	EXPRESSION TAG	UNP Q7JVK6
A	-3	ARG	-	EXPRESSION TAG	UNP Q7JVK6
A	-2	GLY	-	EXPRESSION TAG	UNP Q7JVK6
A	-1	SER	-	EXPRESSION TAG	UNP Q7JVK6
A	0	HIS	-	EXPRESSION TAG	UNP Q7JVK6
B	-19	MET	-	EXPRESSION TAG	UNP Q7JVK6
B	-18	GLY	-	EXPRESSION TAG	UNP Q7JVK6
B	-17	SER	-	EXPRESSION TAG	UNP Q7JVK6
B	-16	SER	-	EXPRESSION TAG	UNP Q7JVK6
B	-15	HIS	-	EXPRESSION TAG	UNP Q7JVK6
B	-14	HIS	-	EXPRESSION TAG	UNP Q7JVK6
B	-13	HIS	-	EXPRESSION TAG	UNP Q7JVK6
B	-12	HIS	-	EXPRESSION TAG	UNP Q7JVK6
B	-11	HIS	-	EXPRESSION TAG	UNP Q7JVK6
B	-10	HIS	-	EXPRESSION TAG	UNP Q7JVK6
B	-9	SER	-	EXPRESSION TAG	UNP Q7JVK6
B	-8	SER	-	EXPRESSION TAG	UNP Q7JVK6
B	-7	GLY	-	EXPRESSION TAG	UNP Q7JVK6
B	-6	LEU	-	EXPRESSION TAG	UNP Q7JVK6
B	-5	VAL	-	EXPRESSION TAG	UNP Q7JVK6
B	-4	PRO	-	EXPRESSION TAG	UNP Q7JVK6
B	-3	ARG	-	EXPRESSION TAG	UNP Q7JVK6
B	-2	GLY	-	EXPRESSION TAG	UNP Q7JVK6
B	-1	SER	-	EXPRESSION TAG	UNP Q7JVK6
B	0	HIS	-	EXPRESSION TAG	UNP Q7JVK6
C	-19	MET	-	EXPRESSION TAG	UNP Q7JVK6
C	-18	GLY	-	EXPRESSION TAG	UNP Q7JVK6
C	-17	SER	-	EXPRESSION TAG	UNP Q7JVK6
C	-16	SER	-	EXPRESSION TAG	UNP Q7JVK6
C	-15	HIS	-	EXPRESSION TAG	UNP Q7JVK6
C	-14	HIS	-	EXPRESSION TAG	UNP Q7JVK6
C	-13	HIS	-	EXPRESSION TAG	UNP Q7JVK6
C	-12	HIS	-	EXPRESSION TAG	UNP Q7JVK6
C	-11	HIS	-	EXPRESSION TAG	UNP Q7JVK6
C	-10	HIS	-	EXPRESSION TAG	UNP Q7JVK6
C	-9	SER	-	EXPRESSION TAG	UNP Q7JVK6
C	-8	SER	-	EXPRESSION TAG	UNP Q7JVK6
C	-7	GLY	-	EXPRESSION TAG	UNP Q7JVK6
C	-6	LEU	-	EXPRESSION TAG	UNP Q7JVK6
C	-5	VAL	-	EXPRESSION TAG	UNP Q7JVK6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	PRO	-	EXPRESSION TAG	UNP Q7JVK6
C	-3	ARG	-	EXPRESSION TAG	UNP Q7JVK6
C	-2	GLY	-	EXPRESSION TAG	UNP Q7JVK6
C	-1	SER	-	EXPRESSION TAG	UNP Q7JVK6
C	0	HIS	-	EXPRESSION TAG	UNP Q7JVK6
D	-19	MET	-	EXPRESSION TAG	UNP Q7JVK6
D	-18	GLY	-	EXPRESSION TAG	UNP Q7JVK6
D	-17	SER	-	EXPRESSION TAG	UNP Q7JVK6
D	-16	SER	-	EXPRESSION TAG	UNP Q7JVK6
D	-15	HIS	-	EXPRESSION TAG	UNP Q7JVK6
D	-14	HIS	-	EXPRESSION TAG	UNP Q7JVK6
D	-13	HIS	-	EXPRESSION TAG	UNP Q7JVK6
D	-12	HIS	-	EXPRESSION TAG	UNP Q7JVK6
D	-11	HIS	-	EXPRESSION TAG	UNP Q7JVK6
D	-10	HIS	-	EXPRESSION TAG	UNP Q7JVK6
D	-9	SER	-	EXPRESSION TAG	UNP Q7JVK6
D	-8	SER	-	EXPRESSION TAG	UNP Q7JVK6
D	-7	GLY	-	EXPRESSION TAG	UNP Q7JVK6
D	-6	LEU	-	EXPRESSION TAG	UNP Q7JVK6
D	-5	VAL	-	EXPRESSION TAG	UNP Q7JVK6
D	-4	PRO	-	EXPRESSION TAG	UNP Q7JVK6
D	-3	ARG	-	EXPRESSION TAG	UNP Q7JVK6
D	-2	GLY	-	EXPRESSION TAG	UNP Q7JVK6
D	-1	SER	-	EXPRESSION TAG	UNP Q7JVK6
D	0	HIS	-	EXPRESSION TAG	UNP Q7JVK6
E	-19	MET	-	EXPRESSION TAG	UNP Q7JVK6
E	-18	GLY	-	EXPRESSION TAG	UNP Q7JVK6
E	-17	SER	-	EXPRESSION TAG	UNP Q7JVK6
E	-16	SER	-	EXPRESSION TAG	UNP Q7JVK6
E	-15	HIS	-	EXPRESSION TAG	UNP Q7JVK6
E	-14	HIS	-	EXPRESSION TAG	UNP Q7JVK6
E	-13	HIS	-	EXPRESSION TAG	UNP Q7JVK6
E	-12	HIS	-	EXPRESSION TAG	UNP Q7JVK6
E	-11	HIS	-	EXPRESSION TAG	UNP Q7JVK6
E	-10	HIS	-	EXPRESSION TAG	UNP Q7JVK6
E	-9	SER	-	EXPRESSION TAG	UNP Q7JVK6
E	-8	SER	-	EXPRESSION TAG	UNP Q7JVK6
E	-7	GLY	-	EXPRESSION TAG	UNP Q7JVK6
E	-6	LEU	-	EXPRESSION TAG	UNP Q7JVK6
E	-5	VAL	-	EXPRESSION TAG	UNP Q7JVK6
E	-4	PRO	-	EXPRESSION TAG	UNP Q7JVK6
E	-3	ARG	-	EXPRESSION TAG	UNP Q7JVK6

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	GLY	-	EXPRESSION TAG	UNP Q7JVK6
E	-1	SER	-	EXPRESSION TAG	UNP Q7JVK6
E	0	HIS	-	EXPRESSION TAG	UNP Q7JVK6
F	-19	MET	-	EXPRESSION TAG	UNP Q7JVK6
F	-18	GLY	-	EXPRESSION TAG	UNP Q7JVK6
F	-17	SER	-	EXPRESSION TAG	UNP Q7JVK6
F	-16	SER	-	EXPRESSION TAG	UNP Q7JVK6
F	-15	HIS	-	EXPRESSION TAG	UNP Q7JVK6
F	-14	HIS	-	EXPRESSION TAG	UNP Q7JVK6
F	-13	HIS	-	EXPRESSION TAG	UNP Q7JVK6
F	-12	HIS	-	EXPRESSION TAG	UNP Q7JVK6
F	-11	HIS	-	EXPRESSION TAG	UNP Q7JVK6
F	-10	HIS	-	EXPRESSION TAG	UNP Q7JVK6
F	-9	SER	-	EXPRESSION TAG	UNP Q7JVK6
F	-8	SER	-	EXPRESSION TAG	UNP Q7JVK6
F	-7	GLY	-	EXPRESSION TAG	UNP Q7JVK6
F	-6	LEU	-	EXPRESSION TAG	UNP Q7JVK6
F	-5	VAL	-	EXPRESSION TAG	UNP Q7JVK6
F	-4	PRO	-	EXPRESSION TAG	UNP Q7JVK6
F	-3	ARG	-	EXPRESSION TAG	UNP Q7JVK6
F	-2	GLY	-	EXPRESSION TAG	UNP Q7JVK6
F	-1	SER	-	EXPRESSION TAG	UNP Q7JVK6
F	0	HIS	-	EXPRESSION TAG	UNP Q7JVK6
G	-19	MET	-	EXPRESSION TAG	UNP Q7JVK6
G	-18	GLY	-	EXPRESSION TAG	UNP Q7JVK6
G	-17	SER	-	EXPRESSION TAG	UNP Q7JVK6
G	-16	SER	-	EXPRESSION TAG	UNP Q7JVK6
G	-15	HIS	-	EXPRESSION TAG	UNP Q7JVK6
G	-14	HIS	-	EXPRESSION TAG	UNP Q7JVK6
G	-13	HIS	-	EXPRESSION TAG	UNP Q7JVK6
G	-12	HIS	-	EXPRESSION TAG	UNP Q7JVK6
G	-11	HIS	-	EXPRESSION TAG	UNP Q7JVK6
G	-10	HIS	-	EXPRESSION TAG	UNP Q7JVK6
G	-9	SER	-	EXPRESSION TAG	UNP Q7JVK6
G	-8	SER	-	EXPRESSION TAG	UNP Q7JVK6
G	-7	GLY	-	EXPRESSION TAG	UNP Q7JVK6
G	-6	LEU	-	EXPRESSION TAG	UNP Q7JVK6
G	-5	VAL	-	EXPRESSION TAG	UNP Q7JVK6
G	-4	PRO	-	EXPRESSION TAG	UNP Q7JVK6
G	-3	ARG	-	EXPRESSION TAG	UNP Q7JVK6
G	-2	GLY	-	EXPRESSION TAG	UNP Q7JVK6
G	-1	SER	-	EXPRESSION TAG	UNP Q7JVK6

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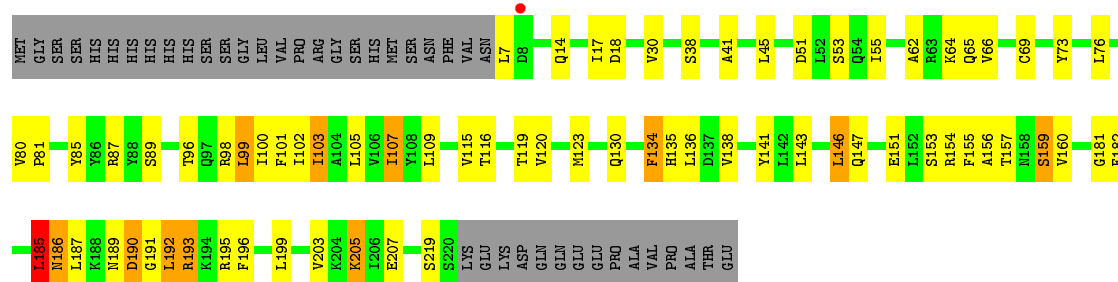
Chain	Residue	Modelled	Actual	Comment	Reference
G	0	HIS	-	EXPRESSION TAG	UNP Q7JVK6
H	-19	MET	-	EXPRESSION TAG	UNP Q7JVK6
H	-18	GLY	-	EXPRESSION TAG	UNP Q7JVK6
H	-17	SER	-	EXPRESSION TAG	UNP Q7JVK6
H	-16	SER	-	EXPRESSION TAG	UNP Q7JVK6
H	-15	HIS	-	EXPRESSION TAG	UNP Q7JVK6
H	-14	HIS	-	EXPRESSION TAG	UNP Q7JVK6
H	-13	HIS	-	EXPRESSION TAG	UNP Q7JVK6
H	-12	HIS	-	EXPRESSION TAG	UNP Q7JVK6
H	-11	HIS	-	EXPRESSION TAG	UNP Q7JVK6
H	-10	HIS	-	EXPRESSION TAG	UNP Q7JVK6
H	-9	SER	-	EXPRESSION TAG	UNP Q7JVK6
H	-8	SER	-	EXPRESSION TAG	UNP Q7JVK6
H	-7	GLY	-	EXPRESSION TAG	UNP Q7JVK6
H	-6	LEU	-	EXPRESSION TAG	UNP Q7JVK6
H	-5	VAL	-	EXPRESSION TAG	UNP Q7JVK6
H	-4	PRO	-	EXPRESSION TAG	UNP Q7JVK6
H	-3	ARG	-	EXPRESSION TAG	UNP Q7JVK6
H	-2	GLY	-	EXPRESSION TAG	UNP Q7JVK6
H	-1	SER	-	EXPRESSION TAG	UNP Q7JVK6
H	0	HIS	-	EXPRESSION TAG	UNP Q7JVK6





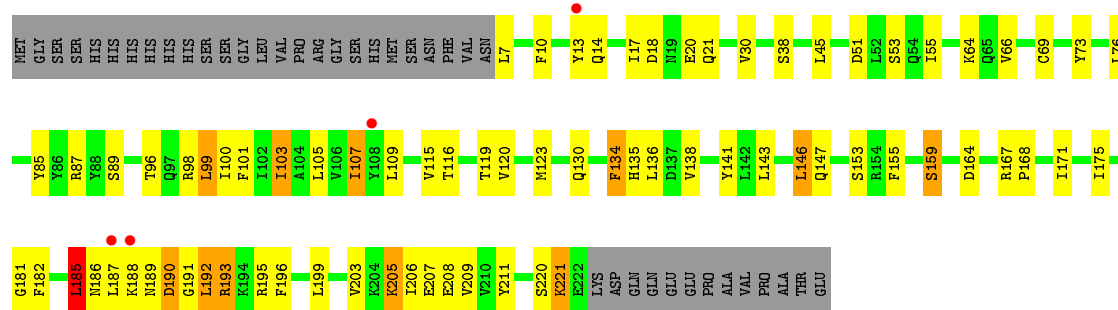
- Molecule 1: GM27569p

Chain D:  56% 24% • 16%



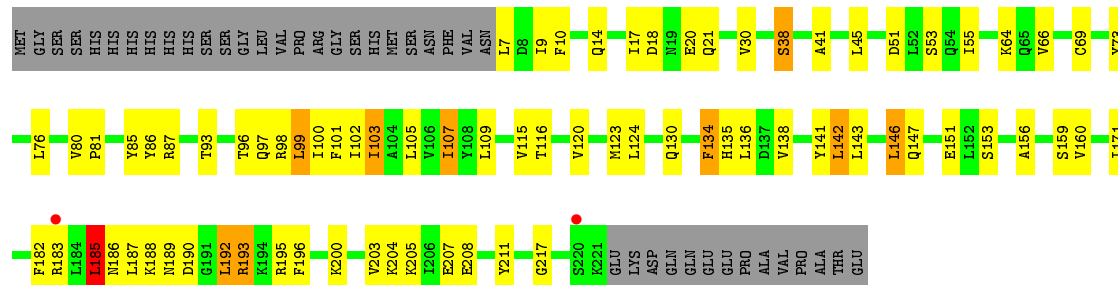
- Molecule 1: GM27569p

Chain E: 



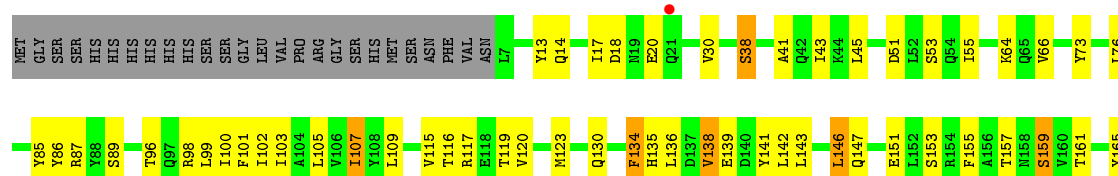
- Molecule 1: GM27569p

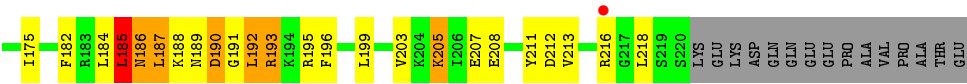
Chain F:  54% 27% 16%



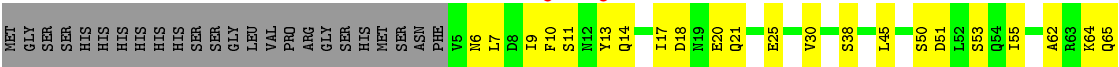
- Molecule 1: GM27569p

Chain G: 





● Molecule 1: GM27569p



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.05Å 131.20Å 96.40Å 90.00° 98.46° 90.00°	Depositor
Resolution (Å)	48.15 – 4.20 48.15 – 4.20	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.15-4.20) 99.4 (48.15-4.20)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.78 (at 4.14Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, $R_{free}$	0.237 , 0.292 0.220 , 0.277	Depositor DCC
$R_{free}$ test set	830 reflections (5.07%)	DCC
Wilson B-factor (Å <sup>2</sup> )	121.6	Xtriage
Anisotropy	0.534	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 119.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 16416 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	13931	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	183.0	wwPDB-VP

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

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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

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	0.57	1/1755 (0.1%)	0.65	0/2367
1	B	0.51	0/1759	0.63	1/2372 (0.0%)
1	C	0.51	0/1755	0.63	1/2367 (0.0%)
1	D	0.46	0/1767	0.59	0/2383
1	E	0.46	0/1785	0.62	0/2406
1	F	0.49	0/1776	0.62	1/2394 (0.0%)
1	G	0.54	0/1767	0.65	0/2383
1	H	0.51	0/1791	0.63	0/2415
All	All	0.51	1/14155 (0.0%)	0.63	3/19087 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	67	GLU	CG-CD	5.69	1.60	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	142	LEU	CA-CB-CG	-5.67	102.27	115.30
1	F	142	LEU	CA-CB-CG	-5.25	103.24	115.30
1	B	142	LEU	CA-CB-CG	-5.02	103.75	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	1727	0	1751	62	0
1	B	1731	0	1750	61	1
1	C	1727	0	1751	48	1
1	D	1739	0	1761	48	0
1	E	1757	0	1780	50	0
1	F	1748	0	1774	52	0
1	G	1739	0	1761	69	0
1	H	1763	0	1789	74	0
All	All	13931	0	14117	387	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 14.

All (387) 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:E:100:ILE:HD13	1:E:141:TYR:HA	1.46	0.97
1:G:100:ILE:HD13	1:G:141:TYR:HA	1.49	0.95
1:E:21:GLN:HE22	1:F:188:LYS:H	1.15	0.93
1:A:183:ARG:HB3	1:G:43:ILE:HG12	1.48	0.93
1:C:100:ILE:HD13	1:C:141:TYR:HA	1.50	0.91
1:D:100:ILE:HD13	1:D:141:TYR:HA	1.52	0.91
1:H:100:ILE:HD13	1:H:141:TYR:HA	1.52	0.90
1:A:100:ILE:HD13	1:A:141:TYR:HA	1.53	0.89
1:F:100:ILE:HD13	1:F:141:TYR:HA	1.53	0.88
1:B:100:ILE:HD13	1:B:141:TYR:HA	1.54	0.88
1:A:188:LYS:H	1:B:21:GLN:HE22	1.23	0.86
1:C:45:LEU:HD13	1:C:105:LEU:HD23	1.58	0.85
1:F:45:LEU:HD13	1:F:105:LEU:HD23	1.60	0.84
1:G:142:LEU:HD22	1:H:13:TYR:CE2	2.13	0.83
1:C:100:ILE:HD11	1:C:136:LEU:HD11	1.60	0.83
1:G:73:TYR:HH	1:G:96:THR:HG1	1.22	0.83
1:E:45:LEU:HD13	1:E:105:LEU:HD23	1.61	0.82
1:B:207:GLU:OE2	1:D:154:ARG:NH2	2.13	0.82
1:B:100:ILE:HD11	1:B:136:LEU:HD11	1.60	0.81
1:B:45:LEU:HD13	1:B:105:LEU:HD23	1.61	0.81
1:G:100:ILE:HD11	1:G:136:LEU:HD11	1.64	0.80
1:A:100:ILE:HD11	1:A:136:LEU:HD11	1.63	0.79
1:C:13:TYR:HD2	1:D:185:LEU:HD21	1.48	0.79
1:H:45:LEU:HD13	1:H:105:LEU:HD23	1.63	0.79
1:G:45:LEU:HD13	1:G:105:LEU:HD23	1.65	0.78
1:A:45:LEU:HD13	1:A:105:LEU:HD23	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:ARG:NH2	1:C:207:GLU:OE2	2.12	0.78
1:F:100:ILE:HD11	1:F:136:LEU:HD11	1.65	0.77
1:H:100:ILE:HD11	1:H:136:LEU:HD11	1.66	0.77
1:F:183:ARG:NH1	1:H:50:SER:HB2	1.98	0.77
1:A:73:TYR:HH	1:A:96:THR:HG1	1.33	0.77
1:E:100:ILE:HD11	1:E:136:LEU:HD11	1.67	0.76
1:B:43:ILE:HG23	1:H:183:ARG:HD2	1.67	0.76
1:D:45:LEU:HD13	1:D:105:LEU:HD23	1.69	0.75
1:D:100:ILE:HD11	1:D:136:LEU:HD11	1.71	0.73
1:A:66:VAL:HG11	1:A:103:ILE:HD11	1.69	0.73
1:C:73:TYR:HH	1:C:96:THR:HG1	1.34	0.72
1:G:66:VAL:HG11	1:G:103:ILE:HD11	1.71	0.72
1:B:73:TYR:HH	1:B:96:THR:HG1	1.38	0.72
1:B:66:VAL:HG11	1:B:103:ILE:HD11	1.72	0.72
1:E:73:TYR:HH	1:E:96:THR:HG1	1.37	0.70
1:D:73:TYR:HH	1:D:96:THR:HG1	1.35	0.69
1:F:200:LYS:HB2	1:H:161:THR:HG21	1.74	0.69
1:C:51:ASP:OD1	1:C:53:SER:OG	2.10	0.69
1:B:39:LYS:NZ	1:H:193:ARG:HH12	1.91	0.69
1:B:43:ILE:HG12	1:H:183:ARG:HD3	1.76	0.66
1:D:51:ASP:OD1	1:D:53:SER:OG	2.13	0.66
1:A:39:LYS:HE3	1:C:186:ASN:OD1	1.96	0.66
1:B:39:LYS:NZ	1:H:193:ARG:NH1	2.44	0.66
1:G:188:LYS:O	1:H:21:GLN:NE2	2.29	0.65
1:H:6:ASN:OD1	1:H:7:LEU:N	2.29	0.65
1:D:66:VAL:HG11	1:D:103:ILE:HD11	1.77	0.65
1:F:204:LYS:HD3	1:H:161:THR:HA	1.79	0.65
1:G:187:LEU:HB3	1:G:193:ARG:HG2	1.78	0.65
1:A:182:PHE:CE1	1:B:10:PHE:HE2	2.15	0.64
1:F:66:VAL:HG11	1:F:103:ILE:HD11	1.79	0.64
1:E:66:VAL:HG11	1:E:103:ILE:HD11	1.79	0.64
1:B:51:ASP:OD1	1:B:53:SER:OG	2.14	0.63
1:E:51:ASP:OD1	1:E:53:SER:OG	2.15	0.63
1:D:100:ILE:HG12	1:D:120:VAL:HG11	1.81	0.63
1:H:66:VAL:HG11	1:H:103:ILE:HD11	1.80	0.63
1:G:142:LEU:HD22	1:H:13:TYR:HE2	1.60	0.62
1:F:73:TYR:HH	1:F:96:THR:HG1	1.40	0.62
1:H:51:ASP:OD1	1:H:53:SER:OG	2.16	0.61
1:C:130:GLN:NE2	1:D:87:ARG:HH11	1.99	0.61
1:F:51:ASP:OD1	1:F:53:SER:OG	2.16	0.61
1:G:51:ASP:OD1	1:G:53:SER:OG	2.18	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:182:PHE:CE1	1:H:10:PHE:HE2	2.19	0.60
1:E:21:GLN:NE2	1:F:188:LYS:H	1.93	0.60
1:A:7:LEU:N	1:A:9:ILE:HD12	2.16	0.60
1:C:66:VAL:HG11	1:C:103:ILE:HD11	1.83	0.60
1:G:184:LEU:HD21	1:H:11:SER:HB3	1.84	0.60
1:H:143:LEU:HD22	1:H:195:ARG:HD2	1.84	0.60
1:B:39:LYS:HZ1	1:H:193:ARG:NH1	2.00	0.59
1:A:211:TYR:OH	1:G:212:ASP:OD2	2.16	0.59
1:A:51:ASP:OD1	1:A:53:SER:OG	2.14	0.59
1:F:100:ILE:HG12	1:F:120:VAL:HG11	1.86	0.58
1:B:100:ILE:HG12	1:B:120:VAL:HG11	1.84	0.58
1:C:100:ILE:HG12	1:C:120:VAL:HG11	1.86	0.57
1:A:100:ILE:HG12	1:A:120:VAL:HG11	1.86	0.57
1:F:7:LEU:N	1:F:9:ILE:HD12	2.19	0.57
1:A:188:LYS:NZ	1:B:25:GLU:OE2	2.32	0.57
1:H:6:ASN:HB3	1:H:9:ILE:HD11	1.87	0.57
1:G:182:PHE:O	1:G:185:LEU:HB2	2.04	0.57
1:E:100:ILE:HG12	1:E:120:VAL:HG11	1.87	0.56
1:H:55:ILE:HG23	1:H:109:LEU:HD13	1.87	0.56
1:A:183:ARG:CB	1:G:43:ILE:HG12	2.29	0.56
1:A:85:TYR:HE1	1:A:134:PHE:CE2	2.23	0.56
1:F:200:LYS:HE3	1:H:158:ASN:OD1	2.06	0.55
1:C:10:PHE:HE2	1:D:182:PHE:CD1	2.25	0.55
1:A:210:VAL:HG12	1:G:161:THR:OG1	2.07	0.55
1:A:130:GLN:HB3	1:A:135:HIS:CE1	2.41	0.55
1:C:187:LEU:HB3	1:C:193:ARG:HG2	1.89	0.54
1:B:85:TYR:HE1	1:B:134:PHE:CE2	2.25	0.54
1:E:220:SER:O	1:E:221:LYS:HB3	2.07	0.54
1:E:14:GLN:NE2	1:E:18:ASP:OD1	2.40	0.54
1:E:7:LEU:HD13	1:E:7:LEU:O	2.07	0.54
1:E:182:PHE:HB3	1:E:196:PHE:CE1	2.42	0.54
1:H:14:GLN:NE2	1:H:18:ASP:OD1	2.41	0.54
1:C:203:VAL:O	1:C:207:GLU:HG2	2.08	0.53
1:A:143:LEU:HD22	1:A:195:ARG:HD2	1.90	0.53
1:G:100:ILE:HG12	1:G:120:VAL:HG11	1.89	0.53
1:G:85:TYR:HE1	1:G:134:PHE:CE2	2.26	0.53
1:G:165:TYR:CD2	1:G:218:LEU:HB3	2.43	0.53
1:E:107:ILE:HG21	1:E:115:VAL:HB	1.90	0.53
1:C:86:TYR:CE2	1:D:87:ARG:HD2	2.45	0.52
1:B:187:LEU:HB3	1:B:193:ARG:HG2	1.90	0.52
1:A:14:GLN:NE2	1:A:18:ASP:OD1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:187:LEU:HB3	1:F:193:ARG:HG2	1.90	0.52
1:H:100:ILE:HG12	1:H:120:VAL:HG11	1.89	0.52
1:H:155:PHE:O	1:H:159:SER:HB2	2.10	0.52
1:F:107:ILE:HG21	1:F:115:VAL:HB	1.91	0.52
1:G:185:LEU:HA	1:H:14:GLN:HB2	1.90	0.52
1:G:130:GLN:HB3	1:G:135:HIS:CE1	2.44	0.52
1:E:85:TYR:HE1	1:E:134:PHE:CE2	2.27	0.52
1:E:13:TYR:HD2	1:F:185:LEU:HD21	1.73	0.52
1:F:183:ARG:HH12	1:H:50:SER:HB2	1.71	0.52
1:C:107:ILE:HG21	1:C:115:VAL:HB	1.92	0.51
1:A:185:LEU:HD21	1:B:13:TYR:HD2	1.75	0.51
1:G:142:LEU:HB2	1:H:13:TYR:OH	2.10	0.51
1:F:203:VAL:O	1:F:207:GLU:HG2	2.10	0.51
1:H:130:GLN:HB3	1:H:135:HIS:CE1	2.45	0.51
1:H:182:PHE:HB3	1:H:196:PHE:CE1	2.45	0.51
1:B:107:ILE:HG21	1:B:115:VAL:HB	1.92	0.51
1:D:143:LEU:HD22	1:D:195:ARG:HD2	1.93	0.51
1:B:157:THR:O	1:H:211:TYR:HD1	1.94	0.51
1:F:14:GLN:NE2	1:F:18:ASP:OD1	2.44	0.50
1:A:142:LEU:HD22	1:B:13:TYR:CE2	2.47	0.50
1:D:182:PHE:HB3	1:D:196:PHE:CE1	2.47	0.50
1:F:143:LEU:HD22	1:F:195:ARG:HD2	1.93	0.50
1:G:14:GLN:NE2	1:G:18:ASP:OD1	2.44	0.50
1:B:143:LEU:HD22	1:B:195:ARG:HD2	1.93	0.50
1:A:30:VAL:HG11	1:A:76:LEU:HB2	1.94	0.50
1:H:85:TYR:HE1	1:H:134:PHE:CE2	2.30	0.50
1:H:187:LEU:HB3	1:H:193:ARG:HG2	1.93	0.49
1:G:190:ASP:OD2	1:H:21:GLN:NE2	2.45	0.49
1:H:30:VAL:HG11	1:H:76:LEU:HB2	1.93	0.49
1:G:20:GLU:HG3	1:G:87:ARG:HH21	1.77	0.49
1:D:187:LEU:HB3	1:D:193:ARG:HG2	1.94	0.49
1:E:155:PHE:O	1:E:159:SER:HB2	2.12	0.49
1:H:62:ALA:O	1:H:65:GLN:HB2	2.13	0.49
1:E:203:VAL:O	1:E:207:GLU:HG2	2.12	0.49
1:B:43:ILE:HG23	1:H:183:ARG:CD	2.41	0.49
1:E:146:LEU:HG	1:E:182:PHE:CZ	2.48	0.49
1:D:119:THR:O	1:D:123:MET:HG3	2.13	0.49
1:G:203:VAL:O	1:G:207:GLU:HG2	2.12	0.49
1:G:182:PHE:HB3	1:G:196:PHE:CE1	2.48	0.49
1:E:187:LEU:HB3	1:E:193:ARG:HG2	1.95	0.48
1:H:203:VAL:O	1:H:207:GLU:HG2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:VAL:O	1:B:207:GLU:HG2	2.13	0.48
1:A:87:ARG:HH11	1:B:130:GLN:NE2	2.11	0.48
1:H:7:LEU:HD13	1:H:7:LEU:O	2.13	0.48
1:F:182:PHE:HB3	1:F:196:PHE:CE1	2.48	0.48
1:H:107:ILE:HG21	1:H:115:VAL:HB	1.94	0.48
1:G:30:VAL:HG11	1:G:76:LEU:HB2	1.95	0.48
1:E:119:THR:O	1:E:123:MET:HG3	2.14	0.48
1:F:116:THR:O	1:F:120:VAL:HG23	2.14	0.48
1:G:142:LEU:HB2	1:H:13:TYR:CZ	2.49	0.48
1:A:182:PHE:HB3	1:A:196:PHE:CE1	2.49	0.48
1:G:143:LEU:HD22	1:G:195:ARG:HD2	1.95	0.48
1:C:10:PHE:HD2	1:D:181:GLY:O	1.96	0.48
1:B:182:PHE:HB3	1:B:196:PHE:CE1	2.48	0.48
1:E:55:ILE:HG23	1:E:109:LEU:HD13	1.96	0.48
1:A:55:ILE:HG23	1:A:109:LEU:HD13	1.96	0.48
1:E:101:PHE:HB2	1:E:147:GLN:HB2	1.95	0.48
1:G:186:ASN:HB2	1:H:14:GLN:NE2	2.29	0.47
1:A:187:LEU:HB3	1:A:193:ARG:HG2	1.95	0.47
1:C:182:PHE:HB3	1:C:196:PHE:CE1	2.49	0.47
1:B:119:THR:O	1:B:123:MET:HG3	2.14	0.47
1:D:55:ILE:HG23	1:D:109:LEU:HD13	1.95	0.47
1:F:85:TYR:HE1	1:F:134:PHE:CE2	2.32	0.47
1:G:185:LEU:HD22	1:H:14:GLN:HB2	1.95	0.47
1:C:30:VAL:HG11	1:C:76:LEU:HB2	1.96	0.47
1:F:130:GLN:HB3	1:F:135:HIS:CE1	2.50	0.47
1:C:143:LEU:HD22	1:C:195:ARG:HD2	1.97	0.47
1:D:30:VAL:HG11	1:D:76:LEU:HB2	1.96	0.47
1:F:30:VAL:HG11	1:F:76:LEU:HB2	1.96	0.47
1:G:213:VAL:HG12	1:G:218:LEU:HD12	1.97	0.47
1:D:107:ILE:HG21	1:D:115:VAL:HB	1.95	0.47
1:E:30:VAL:HG11	1:E:76:LEU:HB2	1.97	0.47
1:C:85:TYR:HE1	1:C:134:PHE:CE2	2.32	0.47
1:G:87:ARG:HD2	1:H:86:TYR:CZ	2.49	0.47
1:C:205:LYS:HB3	1:C:205:LYS:HE2	1.58	0.47
1:A:146:LEU:HG	1:A:182:PHE:CZ	2.50	0.47
1:E:143:LEU:HD22	1:E:195:ARG:HD2	1.97	0.47
1:G:38:SER:HB2	1:G:99:LEU:CD2	2.45	0.47
1:A:164:ASP:OD2	1:A:167:ARG:HD2	2.15	0.47
1:C:13:TYR:CD2	1:D:185:LEU:HD21	2.39	0.46
1:E:87:ARG:HD2	1:F:86:TYR:CZ	2.50	0.46
1:C:14:GLN:NE2	1:C:18:ASP:OD1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:GLN:NE2	1:B:18:ASP:OD1	2.48	0.46
1:C:130:GLN:HB3	1:C:135:HIS:CE1	2.50	0.46
1:E:208:GLU:O	1:E:211:TYR:HB3	2.16	0.46
1:F:64:LYS:HA	1:F:64:LYS:HD3	1.80	0.46
1:B:116:THR:O	1:B:120:VAL:HG23	2.15	0.46
1:A:107:ILE:HG21	1:A:115:VAL:HB	1.98	0.46
1:D:156:ALA:O	1:D:160:VAL:HG23	2.16	0.46
1:D:14:GLN:NE2	1:D:18:ASP:OD1	2.48	0.46
1:C:156:ALA:HB2	1:C:171:ILE:HD12	1.97	0.46
1:A:203:VAL:O	1:A:207:GLU:HG2	2.14	0.46
1:H:73:TYR:OH	1:H:96:THR:OG1	2.08	0.46
1:B:130:GLN:HB3	1:B:135:HIS:CE1	2.50	0.46
1:G:192:LEU:O	1:G:192:LEU:HD12	2.16	0.46
1:C:84:GLN:NE2	1:D:130:GLN:NE2	2.64	0.46
1:G:13:TYR:HE1	1:H:138:VAL:HG13	1.80	0.46
1:E:116:THR:O	1:E:120:VAL:HG23	2.16	0.46
1:F:101:PHE:HB2	1:F:147:GLN:HB2	1.98	0.46
1:G:107:ILE:HG21	1:G:115:VAL:HB	1.97	0.46
1:D:85:TYR:HE1	1:D:134:PHE:CE2	2.34	0.46
1:C:55:ILE:HG23	1:C:109:LEU:HD13	1.98	0.45
1:G:188:LYS:HD3	1:H:25:GLU:OE2	2.16	0.45
1:D:130:GLN:HB3	1:D:135:HIS:CE1	2.50	0.45
1:B:30:VAL:HG11	1:B:76:LEU:HB2	1.97	0.45
1:B:20:GLU:HG3	1:B:87:ARG:HH21	1.82	0.45
1:C:10:PHE:HE2	1:D:182:PHE:CE1	2.34	0.45
1:G:41:ALA:HB3	1:G:102:ILE:HD13	1.99	0.45
1:A:182:PHE:O	1:A:185:LEU:HB2	2.16	0.45
1:A:155:PHE:O	1:A:159:SER:HB2	2.16	0.45
1:G:116:THR:O	1:G:120:VAL:HG23	2.17	0.45
1:D:105:LEU:HD13	1:D:151:GLU:HG2	1.99	0.45
1:G:86:TYR:CZ	1:H:87:ARG:HD2	2.52	0.45
1:C:130:GLN:HE22	1:D:87:ARG:HH11	1.61	0.45
1:E:13:TYR:CE2	1:F:142:LEU:HD22	2.51	0.45
1:G:205:LYS:HE2	1:G:205:LYS:HB3	1.66	0.45
1:F:156:ALA:O	1:F:160:VAL:HG23	2.16	0.45
1:B:185:LEU:HB3	1:B:186:ASN:H	1.46	0.45
1:B:55:ILE:HG23	1:B:109:LEU:HD13	1.98	0.45
1:E:69:CYS:SG	1:E:99:LEU:HD11	2.57	0.45
1:G:146:LEU:HG	1:G:182:PHE:CZ	2.52	0.45
1:G:213:VAL:HA	1:G:218:LEU:HD12	1.99	0.45
1:G:139:GLU:OE2	1:H:20:GLU:OE1	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:LYS:HB3	1:A:205:LYS:HE2	1.64	0.45
1:E:199:LEU:O	1:E:203:VAL:HG23	2.17	0.44
1:D:64:LYS:HA	1:D:64:LYS:HD3	1.77	0.44
1:A:64:LYS:HD3	1:A:64:LYS:HA	1.70	0.44
1:B:80:VAL:HA	1:B:81:PRO:HD3	1.84	0.44
1:B:182:PHE:O	1:B:185:LEU:HB2	2.17	0.44
1:G:185:LEU:CD2	1:H:14:GLN:HB2	2.47	0.44
1:D:69:CYS:SG	1:D:99:LEU:HD11	2.57	0.44
1:B:205:LYS:HE2	1:B:205:LYS:HB3	1.63	0.44
1:E:182:PHE:O	1:E:185:LEU:HB2	2.18	0.44
1:B:52:LEU:HD23	1:B:55:ILE:HD11	1.98	0.44
1:B:64:LYS:HA	1:B:64:LYS:HD3	1.77	0.44
1:G:190:ASP:HB2	1:G:191:GLY:H	1.59	0.44
1:F:156:ALA:HB2	1:F:171:ILE:HD12	2.00	0.44
1:A:116:THR:O	1:A:120:VAL:HG23	2.17	0.44
1:F:103:ILE:HD13	1:F:123:MET:SD	2.58	0.44
1:G:185:LEU:HD22	1:H:14:GLN:OE1	2.18	0.44
1:D:155:PHE:O	1:D:159:SER:HB2	2.17	0.44
1:A:156:ALA:O	1:A:160:VAL:HG23	2.17	0.44
1:H:146:LEU:HG	1:H:182:PHE:CZ	2.53	0.44
1:F:208:GLU:O	1:F:211:TYR:HB3	2.18	0.44
1:A:101:PHE:HB2	1:A:147:GLN:HB2	2.00	0.44
1:B:146:LEU:HG	1:B:182:PHE:CZ	2.52	0.44
1:A:86:TYR:CZ	1:B:87:ARG:HD2	2.53	0.44
1:C:41:ALA:HB3	1:C:102:ILE:HD13	2.00	0.44
1:E:181:GLY:O	1:F:10:PHE:HD2	2.01	0.44
1:F:38:SER:HB2	1:F:99:LEU:CD2	2.48	0.44
1:A:105:LEU:HD13	1:A:151:GLU:HG2	2.00	0.43
1:H:103:ILE:HD13	1:H:123:MET:SD	2.58	0.43
1:E:130:GLN:HB3	1:E:135:HIS:CE1	2.52	0.43
1:G:155:PHE:O	1:G:159:SER:HB2	2.18	0.43
1:H:105:LEU:HD13	1:H:151:GLU:HG2	2.00	0.43
1:G:182:PHE:HE1	1:H:10:PHE:HE2	1.63	0.43
1:A:20:GLU:HG3	1:A:87:ARG:HH21	1.82	0.43
1:G:142:LEU:HD13	1:H:13:TYR:CE2	2.53	0.43
1:G:146:LEU:HA	1:G:146:LEU:HD23	1.61	0.43
1:A:143:LEU:HD21	1:A:192:LEU:HB2	2.00	0.43
1:B:156:ALA:O	1:B:160:VAL:HG23	2.19	0.43
1:E:146:LEU:HD23	1:E:146:LEU:HA	1.65	0.43
1:B:155:PHE:O	1:B:159:SER:HB2	2.18	0.43
1:G:55:ILE:HG23	1:G:109:LEU:HD13	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:105:LEU:HD13	1:F:151:GLU:HG2	2.00	0.43
1:A:142:LEU:HD22	1:B:13:TYR:CZ	2.53	0.43
1:A:7:LEU:HD21	1:B:184:LEU:HD22	2.01	0.43
1:D:80:VAL:HA	1:D:81:PRO:HD3	1.83	0.43
1:F:182:PHE:O	1:F:185:LEU:HB2	2.18	0.43
1:D:101:PHE:HB2	1:D:147:GLN:HB2	2.00	0.43
1:E:64:LYS:HD3	1:E:64:LYS:HA	1.78	0.43
1:C:101:PHE:HB2	1:C:147:GLN:HB2	2.00	0.43
1:G:175:ILE:HA	1:G:175:ILE:HD13	1.89	0.43
1:C:119:THR:O	1:C:123:MET:HG3	2.19	0.43
1:D:199:LEU:O	1:D:203:VAL:HG23	2.19	0.43
1:F:55:ILE:HG23	1:F:109:LEU:HD13	1.99	0.43
1:A:80:VAL:HA	1:A:81:PRO:HD3	1.86	0.43
1:H:101:PHE:HB2	1:H:147:GLN:HB2	1.99	0.43
1:G:105:LEU:HD13	1:G:151:GLU:HG2	2.01	0.43
1:C:84:GLN:HG2	1:D:130:GLN:HE22	1.83	0.43
1:C:190:ASP:HB2	1:C:191:GLY:H	1.59	0.43
1:E:205:LYS:HB3	1:E:205:LYS:HE2	1.75	0.43
1:G:64:LYS:HA	1:G:64:LYS:HD3	1.73	0.43
1:G:117:ARG:CZ	1:G:138:VAL:HG23	2.48	0.43
1:B:43:ILE:O	1:B:46:GLN:HB2	2.18	0.42
1:A:87:ARG:HH11	1:B:130:GLN:HE22	1.67	0.42
1:C:155:PHE:O	1:C:159:SER:HB2	2.19	0.42
1:H:190:ASP:HB2	1:H:191:GLY:H	1.63	0.42
1:D:41:ALA:HB3	1:D:102:ILE:HD13	2.00	0.42
1:C:13:TYR:CE2	1:D:185:LEU:HD11	2.54	0.42
1:G:119:THR:O	1:G:123:MET:HG3	2.19	0.42
1:H:189:ASN:HA	1:H:193:ARG:HG3	2.00	0.42
1:G:185:LEU:HD22	1:H:14:GLN:CA	2.50	0.42
1:G:85:TYR:CE1	1:G:134:PHE:CE2	3.07	0.42
1:E:10:PHE:HE2	1:F:182:PHE:CE1	2.37	0.42
1:B:101:PHE:HB2	1:B:147:GLN:HB2	2.01	0.42
1:E:221:LYS:HE3	1:E:221:LYS:HB3	1.85	0.42
1:A:190:ASP:HB2	1:A:191:GLY:H	1.63	0.42
1:D:205:LYS:HE2	1:D:205:LYS:HB3	1.71	0.42
1:A:208:GLU:O	1:A:211:TYR:HB3	2.20	0.42
1:A:138:VAL:HG11	1:B:16:TYR:CE2	2.54	0.42
1:C:199:LEU:O	1:C:203:VAL:HG23	2.19	0.42
1:A:73:TYR:OH	1:A:96:THR:OG1	2.14	0.42
1:D:143:LEU:HD21	1:D:192:LEU:HB2	2.02	0.42
1:H:208:GLU:O	1:H:211:TYR:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:ARG:HD2	1:B:86:TYR:CE2	2.55	0.42
1:H:64:LYS:HA	1:H:64:LYS:HD3	1.73	0.42
1:C:218:LEU:H	1:C:218:LEU:HG	1.60	0.42
1:G:103:ILE:HD13	1:G:123:MET:SD	2.60	0.42
1:G:185:LEU:O	1:G:186:ASN:ND2	2.53	0.42
1:D:203:VAL:O	1:D:207:GLU:HG2	2.20	0.42
1:D:62:ALA:O	1:D:65:GLN:HB2	2.19	0.42
1:A:17:ILE:HG23	1:A:21:GLN:OE1	2.20	0.42
1:D:146:LEU:HD23	1:D:146:LEU:HA	1.65	0.42
1:D:185:LEU:O	1:D:186:ASN:ND2	2.52	0.42
1:A:45:LEU:HD23	1:A:45:LEU:HA	1.91	0.42
1:B:157:THR:HG23	1:H:211:TYR:CD1	2.55	0.42
1:B:146:LEU:HA	1:B:146:LEU:HD23	1.67	0.42
1:H:199:LEU:O	1:H:203:VAL:HG23	2.20	0.42
1:F:143:LEU:HD21	1:F:192:LEU:HB2	2.02	0.42
1:C:164:ASP:OD2	1:C:167:ARG:HB2	2.20	0.42
1:H:216:ARG:HA	1:H:217:GLY:HA3	1.51	0.42
1:D:190:ASP:HB2	1:D:191:GLY:H	1.62	0.42
1:A:146:LEU:HD23	1:A:146:LEU:HA	1.67	0.41
1:F:69:CYS:SG	1:F:99:LEU:HD11	2.59	0.41
1:B:167:ARG:HB3	1:B:168:PRO:HD3	2.02	0.41
1:H:175:ILE:HA	1:H:175:ILE:HD13	1.93	0.41
1:F:120:VAL:O	1:F:124:LEU:HD12	2.20	0.41
1:F:146:LEU:HD23	1:F:146:LEU:HA	1.64	0.41
1:A:43:ILE:O	1:A:46:GLN:HB2	2.20	0.41
1:A:185:LEU:HD22	1:B:14:GLN:OE1	2.20	0.41
1:A:130:GLN:NE2	1:B:84:GLN:NE2	2.68	0.41
1:E:143:LEU:HD21	1:E:192:LEU:HB2	2.03	0.41
1:G:101:PHE:HB2	1:G:147:GLN:HB2	2.02	0.41
1:E:188:LYS:HB2	1:F:21:GLN:NE2	2.35	0.41
1:H:182:PHE:O	1:H:185:LEU:HB2	2.21	0.41
1:A:216:ARG:HG2	1:G:216:ARG:NH2	2.35	0.41
1:B:105:LEU:HD13	1:B:151:GLU:HG2	2.01	0.41
1:E:20:GLU:HG3	1:E:87:ARG:HH21	1.85	0.41
1:E:175:ILE:HD13	1:E:175:ILE:HA	1.93	0.41
1:C:185:LEU:O	1:C:186:ASN:ND2	2.49	0.41
1:F:146:LEU:HG	1:F:182:PHE:CZ	2.55	0.41
1:B:171:ILE:HG22	1:B:206:ILE:HG21	2.02	0.41
1:F:107:ILE:HA	1:F:107:ILE:HD12	1.79	0.41
1:C:25:GLU:HG3	1:C:28:ARG:HH12	1.85	0.41
1:E:190:ASP:HB2	1:E:191:GLY:H	1.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:117:ARG:CZ	1:H:138:VAL:HG23	2.51	0.41
1:C:164:ASP:OD2	1:C:167:ARG:HD2	2.21	0.41
1:A:179:ASN:OD1	1:A:199:LEU:HD23	2.21	0.41
1:A:69:CYS:SG	1:A:99:LEU:HD11	2.60	0.41
1:H:215:ILE:HA	1:H:215:ILE:HD12	1.87	0.41
1:G:208:GLU:O	1:G:211:TYR:HB3	2.21	0.41
1:C:116:THR:O	1:C:120:VAL:HG23	2.21	0.41
1:D:182:PHE:O	1:D:185:LEU:HB2	2.21	0.41
1:B:107:ILE:HD12	1:B:107:ILE:HA	1.79	0.41
1:E:181:GLY:O	1:F:10:PHE:CD2	2.74	0.41
1:C:212:ASP:O	1:C:215:ILE:HG22	2.21	0.41
1:C:105:LEU:HD13	1:C:151:GLU:HG2	2.03	0.40
1:D:146:LEU:HG	1:D:182:PHE:CZ	2.55	0.40
1:H:146:LEU:HA	1:H:146:LEU:HD23	1.65	0.40
1:D:116:THR:O	1:D:120:VAL:HG23	2.21	0.40
1:C:182:PHE:O	1:C:185:LEU:HB2	2.22	0.40
1:E:171:ILE:HG22	1:E:206:ILE:HG21	2.04	0.40
1:B:190:ASP:N	1:B:190:ASP:OD1	2.54	0.40
1:E:164:ASP:OD2	1:E:167:ARG:HD2	2.21	0.40
1:F:20:GLU:HG3	1:F:87:ARG:HH21	1.87	0.40
1:E:85:TYR:CE1	1:E:134:PHE:CE2	3.09	0.40
1:G:199:LEU:O	1:G:203:VAL:HG23	2.22	0.40
1:E:192:LEU:O	1:E:192:LEU:HD12	2.21	0.40
1:A:171:ILE:HG22	1:A:206:ILE:HG21	2.04	0.40
1:H:156:ALA:O	1:H:160:VAL:HG23	2.22	0.40
1:F:41:ALA:HB3	1:F:102:ILE:HD13	2.03	0.40
1:F:80:VAL:HA	1:F:81:PRO:HD3	1.87	0.40
1:C:20:GLU:HG3	1:C:87:ARG:HH21	1.86	0.40
1:G:182:PHE:CE1	1:H:10:PHE:CE2	3.06	0.40
1:B:190:ASP:HB2	1:B:191:GLY:H	1.58	0.40
1:H:205:LYS:HB3	1:H:205:LYS:HE2	1.70	0.40
1:E:168:PRO:HB3	1:E:209:VAL:HG12	2.03	0.40
1:F:93:THR:O	1:F:97:GLN:HG3	2.21	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)
1:B:127:LYS:NZ	1:C:132:GLU:O[2_645]	1.92	0.28

## 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	210/255 (82%)	193 (92%)	13 (6%)	4 (2%)	10	54
1	B	211/255 (83%)	193 (92%)	14 (7%)	4 (2%)	10	54
1	C	210/255 (82%)	193 (92%)	14 (7%)	3 (1%)	14	59
1	D	212/255 (83%)	195 (92%)	14 (7%)	3 (1%)	14	59
1	E	214/255 (84%)	193 (90%)	18 (8%)	3 (1%)	14	59
1	F	213/255 (84%)	195 (92%)	14 (7%)	4 (2%)	10	54
1	G	212/255 (83%)	191 (90%)	18 (8%)	3 (1%)	14	59
1	H	215/255 (84%)	197 (92%)	14 (6%)	4 (2%)	10	54
All	All	1697/2040 (83%)	1550 (91%)	119 (7%)	28 (2%)	12	57

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	185	LEU
1	A	186	ASN
1	A	189	ASN
1	B	185	LEU
1	B	186	ASN
1	B	189	ASN
1	C	185	LEU
1	C	186	ASN
1	C	189	ASN
1	D	185	LEU
1	D	186	ASN
1	D	189	ASN
1	E	185	LEU
1	E	186	ASN
1	E	189	ASN
1	F	185	LEU
1	F	186	ASN

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Mol	Chain	Res	Type
1	F	189	ASN
1	G	185	LEU
1	G	186	ASN
1	H	185	LEU
1	H	186	ASN
1	H	189	ASN
1	G	189	ASN
1	B	217	GLY
1	F	217	GLY
1	A	145	ILE
1	H	145	ILE

### 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	188/226 (83%)	170 (90%)	18 (10%)	10	44
1	B	189/226 (84%)	173 (92%)	16 (8%)	13	51
1	C	188/226 (83%)	169 (90%)	19 (10%)	9	41
1	D	190/226 (84%)	170 (90%)	20 (10%)	8	40
1	E	192/226 (85%)	174 (91%)	18 (9%)	11	45
1	F	191/226 (84%)	175 (92%)	16 (8%)	14	51
1	G	190/226 (84%)	173 (91%)	17 (9%)	12	48
1	H	193/226 (85%)	175 (91%)	18 (9%)	11	46
All	All	1521/1808 (84%)	1379 (91%)	142 (9%)	11	46

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	17	ILE
1	A	38	SER
1	A	89	SER

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Mol	Chain	Res	Type
1	A	98	ARG
1	A	99	LEU
1	A	103	ILE
1	A	107	ILE
1	A	134	PHE
1	A	138	VAL
1	A	146	LEU
1	A	157	THR
1	A	159	SER
1	A	185	LEU
1	A	190	ASP
1	A	192	LEU
1	A	193	ARG
1	A	205	LYS
1	B	17	ILE
1	B	38	SER
1	B	89	SER
1	B	98	ARG
1	B	107	ILE
1	B	134	PHE
1	B	138	VAL
1	B	146	LEU
1	B	153	SER
1	B	157	THR
1	B	159	SER
1	B	185	LEU
1	B	190	ASP
1	B	192	LEU
1	B	193	ARG
1	B	205	LYS
1	C	17	ILE
1	C	38	SER
1	C	89	SER
1	C	98	ARG
1	C	99	LEU
1	C	103	ILE
1	C	107	ILE
1	C	134	PHE
1	C	138	VAL
1	C	146	LEU
1	C	153	SER
1	C	157	THR

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Mol	Chain	Res	Type
1	C	159	SER
1	C	185	LEU
1	C	190	ASP
1	C	192	LEU
1	C	193	ARG
1	C	205	LYS
1	C	218	LEU
1	D	7	LEU
1	D	17	ILE
1	D	38	SER
1	D	89	SER
1	D	98	ARG
1	D	99	LEU
1	D	103	ILE
1	D	107	ILE
1	D	134	PHE
1	D	138	VAL
1	D	146	LEU
1	D	153	SER
1	D	157	THR
1	D	159	SER
1	D	185	LEU
1	D	190	ASP
1	D	192	LEU
1	D	193	ARG
1	D	205	LYS
1	D	219	SER
1	E	17	ILE
1	E	38	SER
1	E	89	SER
1	E	98	ARG
1	E	99	LEU
1	E	103	ILE
1	E	107	ILE
1	E	134	PHE
1	E	138	VAL
1	E	146	LEU
1	E	153	SER
1	E	159	SER
1	E	185	LEU
1	E	190	ASP
1	E	192	LEU

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Mol	Chain	Res	Type
1	E	193	ARG
1	E	205	LYS
1	E	221	LYS
1	F	17	ILE
1	F	38	SER
1	F	98	ARG
1	F	99	LEU
1	F	103	ILE
1	F	107	ILE
1	F	134	PHE
1	F	138	VAL
1	F	146	LEU
1	F	153	SER
1	F	159	SER
1	F	185	LEU
1	F	190	ASP
1	F	192	LEU
1	F	193	ARG
1	F	205	LYS
1	G	17	ILE
1	G	38	SER
1	G	89	SER
1	G	98	ARG
1	G	107	ILE
1	G	134	PHE
1	G	138	VAL
1	G	146	LEU
1	G	153	SER
1	G	157	THR
1	G	159	SER
1	G	185	LEU
1	G	187	LEU
1	G	190	ASP
1	G	192	LEU
1	G	193	ARG
1	G	205	LYS
1	H	17	ILE
1	H	38	SER
1	H	89	SER
1	H	98	ARG
1	H	99	LEU
1	H	103	ILE

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Mol	Chain	Res	Type
1	H	107	ILE
1	H	134	PHE
1	H	138	VAL
1	H	146	LEU
1	H	159	SER
1	H	185	LEU
1	H	190	ASP
1	H	192	LEU
1	H	193	ARG
1	H	205	LYS
1	H	218	LEU
1	H	221	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	130	GLN
1	B	21	GLN
1	B	130	GLN
1	C	21	GLN
1	C	130	GLN
1	D	14	GLN
1	D	130	GLN
1	E	21	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

There are no ligands in this entry.

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	212/255 (83%)	-0.20	1 (0%) 91 88	104, 163, 229, 309	0
1	B	213/255 (83%)	-0.30	1 (0%) 91 88	121, 178, 243, 382	0
1	C	212/255 (83%)	-0.26	0 100 100	106, 166, 239, 431	0
1	D	214/255 (83%)	-0.24	1 (0%) 91 88	110, 182, 245, 311	0
1	E	216/255 (84%)	-0.03	4 (1%) 70 60	127, 190, 265, 439	0
1	F	215/255 (84%)	-0.10	2 (0%) 85 80	121, 178, 247, 297	0
1	G	214/255 (83%)	-0.18	2 (0%) 85 80	105, 175, 237, 329	0
1	H	217/255 (85%)	0.01	6 (2%) 56 45	107, 181, 263, 360	0
All	All	1713/2040 (83%)	-0.16	17 (0%) 84 77	104, 178, 249, 439	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	187	LEU	4.0
1	H	10	PHE	3.9
1	H	188	LYS	3.7
1	E	187	LEU	3.5
1	E	188	LYS	3.5
1	G	216	ARG	2.8
1	F	183	ARG	2.8
1	H	13	TYR	2.6
1	B	13	TYR	2.4
1	E	13	TYR	2.4
1	A	8	ASP	2.3
1	H	189	ASN	2.2
1	F	220	SER	2.1
1	D	8	ASP	2.1
1	H	199	LEU	2.1
1	E	108	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	21	GLN	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.