



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2018 – 09:21 pm GMT

PDB ID : 3E4Z  
Title : Crystal structure of human insulin degrading enzyme in complex with insulin-like growth factor II  
Authors : Guo, Q.; Manolopoulou, M.; Tang, W.-J.  
Deposited on : 2008-08-12  
Resolution : 2.28 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

<https://www.wwpdb.org/validation/2017/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  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

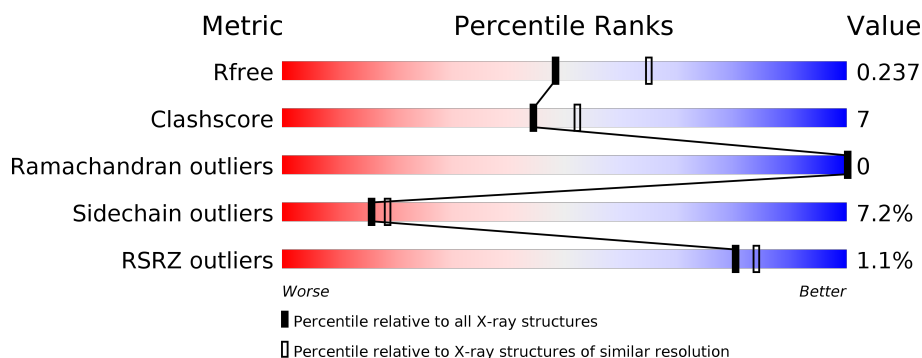
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.28 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))
$R_{free}$	111664	6121 (2.30-2.26)
Clashscore	122126	6842 (2.30-2.26)
Ramachandran outliers	120053	6755 (2.30-2.26)
Sidechain outliers	120020	6755 (2.30-2.26)
RSRZ outliers	108989	5992 (2.30-2.26)

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	990	<div> <div></div> <div>79%15% . .</div> </div>
1	B	990	<div> <div></div> <div>78%16% . .</div> </div>
2	C	67	<div> <div>4%10% . .</div> <div>87%</div> </div>
2	D	67	<div> <div>4%9% .</div> <div>87%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16411 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 Insulin-degrading enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	953	Total	C	N	O	S	0	0	0
			7783	5014	1306	1441	22			
1	B	952	Total	C	N	O	S	0	0	0
			7778	5011	1305	1440	22			

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	MET	-	EXPRESSION TAG	UNP Q5T5N2
A	31	HIS	-	EXPRESSION TAG	UNP Q5T5N2
A	32	HIS	-	EXPRESSION TAG	UNP Q5T5N2
A	33	HIS	-	EXPRESSION TAG	UNP Q5T5N2
A	34	HIS	-	EXPRESSION TAG	UNP Q5T5N2
A	35	HIS	-	EXPRESSION TAG	UNP Q5T5N2
A	36	HIS	-	EXPRESSION TAG	UNP Q5T5N2
A	37	ALA	-	EXPRESSION TAG	UNP Q5T5N2
A	38	ALA	-	EXPRESSION TAG	UNP Q5T5N2
A	39	GLY	-	EXPRESSION TAG	UNP Q5T5N2
A	40	ILE	-	EXPRESSION TAG	UNP Q5T5N2
A	41	PRO	-	EXPRESSION TAG	UNP Q5T5N2
A	110	LEU	CYS	ENGINEERED	UNP Q5T5N2
A	111	GLN	GLU	ENGINEERED	UNP Q5T5N2
A	171	SER	CYS	ENGINEERED	UNP Q5T5N2
A	178	ALA	CYS	ENGINEERED	UNP Q5T5N2
A	257	VAL	CYS	ENGINEERED	UNP Q5T5N2
A	414	LEU	CYS	ENGINEERED	UNP Q5T5N2
A	573	ASN	CYS	ENGINEERED	UNP Q5T5N2
A	590	SER	CYS	ENGINEERED	UNP Q5T5N2
A	789	SER	CYS	ENGINEERED	UNP Q5T5N2
A	812	ALA	CYS	ENGINEERED	UNP Q5T5N2
A	819	ALA	CYS	ENGINEERED	UNP Q5T5N2
A	904	SER	CYS	ENGINEERED	UNP Q5T5N2
A	908	TYR	TRP	ENGINEERED	UNP Q5T5N2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	30	MET	-	EXPRESSION TAG	UNP Q5T5N2
B	31	HIS	-	EXPRESSION TAG	UNP Q5T5N2
B	32	HIS	-	EXPRESSION TAG	UNP Q5T5N2
B	33	HIS	-	EXPRESSION TAG	UNP Q5T5N2
B	34	HIS	-	EXPRESSION TAG	UNP Q5T5N2
B	35	HIS	-	EXPRESSION TAG	UNP Q5T5N2
B	36	HIS	-	EXPRESSION TAG	UNP Q5T5N2
B	37	ALA	-	EXPRESSION TAG	UNP Q5T5N2
B	38	ALA	-	EXPRESSION TAG	UNP Q5T5N2
B	39	GLY	-	EXPRESSION TAG	UNP Q5T5N2
B	40	ILE	-	EXPRESSION TAG	UNP Q5T5N2
B	41	PRO	-	EXPRESSION TAG	UNP Q5T5N2
B	110	LEU	CYS	ENGINEERED	UNP Q5T5N2
B	111	GLN	GLU	ENGINEERED	UNP Q5T5N2
B	171	SER	CYS	ENGINEERED	UNP Q5T5N2
B	178	ALA	CYS	ENGINEERED	UNP Q5T5N2
B	257	VAL	CYS	ENGINEERED	UNP Q5T5N2
B	414	LEU	CYS	ENGINEERED	UNP Q5T5N2
B	573	ASN	CYS	ENGINEERED	UNP Q5T5N2
B	590	SER	CYS	ENGINEERED	UNP Q5T5N2
B	789	SER	CYS	ENGINEERED	UNP Q5T5N2
B	812	ALA	CYS	ENGINEERED	UNP Q5T5N2
B	819	ALA	CYS	ENGINEERED	UNP Q5T5N2
B	904	SER	CYS	ENGINEERED	UNP Q5T5N2
B	908	TYR	TRP	ENGINEERED	UNP Q5T5N2

- Molecule 2 is a protein called Insulin-like growth factor II.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	9	Total	C	N	O	0	0	0
			62	39	10	13			
2	D	9	Total	C	N	O	0	0	0
			62	39	10	13			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		

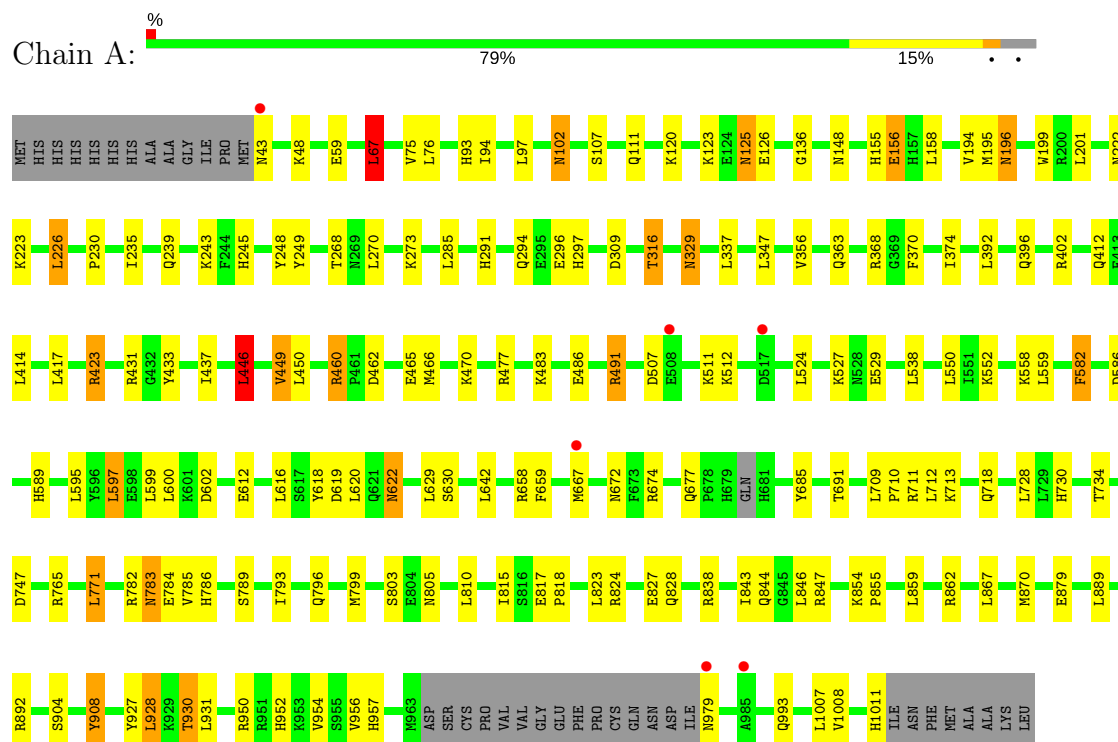
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	384	Total 384	O 384	0	0
4	B	338	Total 338	O 338	0	0
4	C	2	Total 2	O 2	0	0

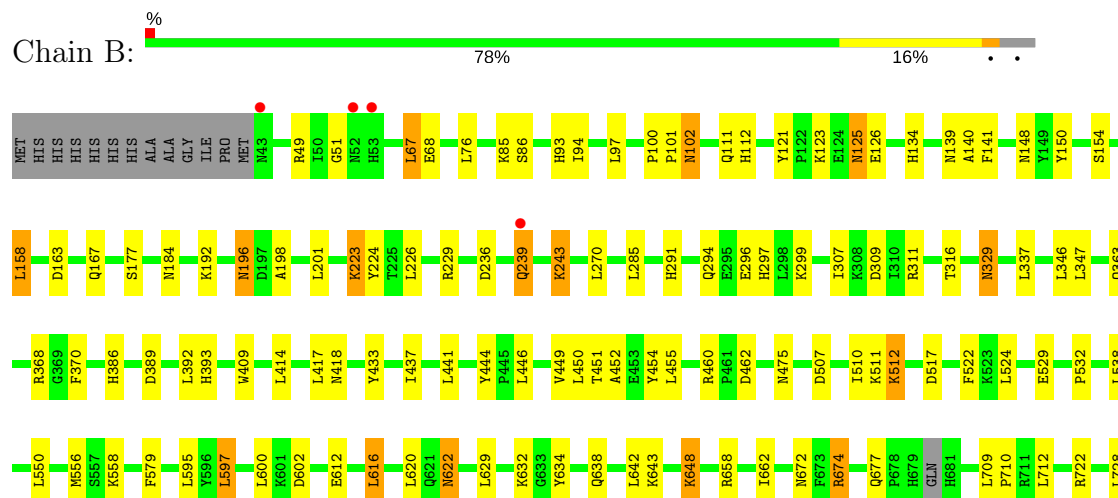
### 3 Residue-property plots

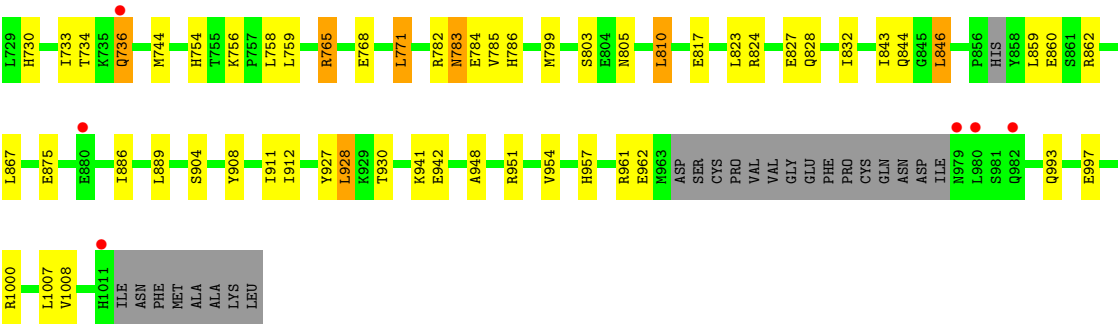
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Insulin-degrading enzyme

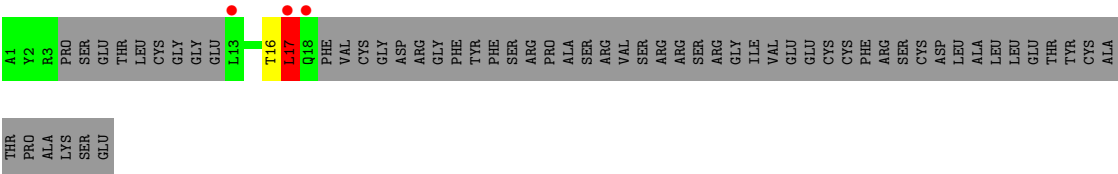


#### • Molecule 1: Insulin-degrading enzyme

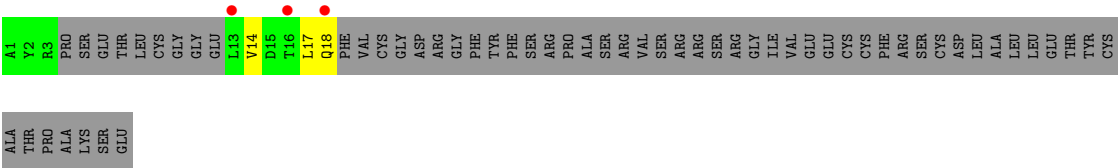




● Molecule 2: Insulin-like growth factor II



● Molecule 2: Insulin-like growth factor II



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	263.03Å 263.03Å 90.82Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.28 49.71 – 2.28	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.00-2.28) 99.7 (49.71-2.28)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.05 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.196 , 0.230 0.206 , 0.237	Depositor DCC
$R_{free}$ test set	8139 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.4	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 52.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	16411	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.86% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.59	1/7975 (0.0%)	0.68	6/10787 (0.1%)
1	B	0.57	0/7969	0.66	4/10777 (0.0%)
2	C	0.68	0/60	1.15	1/80 (1.2%)
2	D	0.61	0/60	0.79	0/80
All	All	0.58	1/16064 (0.0%)	0.67	11/21724 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	908	TYR	CD1-CE1	-5.36	1.31	1.39

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	67	LEU	CA-CB-CG	6.59	130.46	115.30
1	B	67	LEU	CA-CB-CG	6.34	129.88	115.30
1	B	311	ARG	NE-CZ-NH2	-5.75	117.42	120.30
2	C	17	LEU	CA-CB-CG	5.64	128.27	115.30
1	B	311	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	A	460	ARG	NE-CZ-NH2	-5.51	117.55	120.30
1	A	928	LEU	CA-CB-CG	5.40	127.73	115.30
1	A	908	TYR	CB-CG-CD1	-5.32	117.81	121.00
1	B	846	LEU	CA-CB-CG	5.19	127.24	115.30
1	A	460	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	A	446	LEU	CA-CB-CG	5.08	126.99	115.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7783	0	7721	106	1
1	B	7778	0	7718	111	0
2	C	62	0	60	4	0
2	D	62	0	60	4	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	384	0	0	30	0
4	B	338	0	0	23	0
4	C	2	0	0	0	0
All	All	16411	0	15559	221	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 7.

All (221) 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:A:908:TYR:HE1	4:A:1368:HOH:O	1.18	1.23
1:A:667:MET:HG3	4:A:1031:HOH:O	1.39	1.22
1:A:908:TYR:CE1	4:A:1368:HOH:O	1.94	1.10
4:A:1311:HOH:O	2:C:17:LEU:HB3	1.53	1.08
1:B:154:SER:HB3	4:B:1351:HOH:O	1.53	1.08
1:B:736:GLN:HG2	4:B:1223:HOH:O	1.68	0.93
1:B:93:HIS:HE1	1:B:368:ARG:HH21	1.21	0.88
2:C:16:THR:HB	2:C:17:LEU:HA	1.59	0.84
1:A:243:LYS:HG3	4:A:1121:HOH:O	1.76	0.84
1:A:309:ASP:H	1:A:672:ASN:HD21	1.26	0.83
1:B:329:ASN:HD21	1:B:363:GLN:HE22	1.26	0.81
1:A:854:LYS:HD2	1:A:855:PRO:HD2	1.61	0.80
1:B:875:GLU:HG2	4:B:1312:HOH:O	1.81	0.80
1:B:309:ASP:H	1:B:672:ASN:HD21	1.29	0.79
1:B:771:LEU:HD21	1:B:954:VAL:HG23	1.64	0.78
1:B:102:ASN:H	1:B:102:ASN:HD22	1.33	0.77
1:A:491:ARG:HG2	1:A:491:ARG:HH11	1.48	0.76
2:D:17:LEU:HD13	2:D:18:GLN:HG3	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:HIS:HE1	1:A:368:ARG:HH21	1.34	0.76
1:B:134:HIS:HB3	4:B:1351:HOH:O	1.86	0.75
1:A:582:PHE:CE2	1:A:718:GLN:HG2	2.22	0.75
1:B:441:LEU:HD23	1:B:449:VAL:HG11	1.69	0.75
1:B:294:GLN:H	1:B:297:HIS:HD2	1.35	0.74
1:A:296:GLU:HG3	4:A:1335:HOH:O	1.89	0.73
1:A:107:SER:HB3	4:A:1388:HOH:O	1.88	0.73
1:A:102:ASN:HD22	1:A:102:ASN:H	1.37	0.72
1:A:527:LYS:HD3	4:A:1033:HOH:O	1.90	0.71
1:B:579:PHE:HE2	1:B:765:ARG:HH12	1.37	0.71
1:B:658:ARG:NH2	4:B:1118:HOH:O	2.23	0.71
1:A:619:ASP:HB2	4:A:1352:HOH:O	1.91	0.71
1:A:294:GLN:H	1:A:297:HIS:HD2	1.37	0.71
1:A:771:LEU:HD21	1:A:954:VAL:HG23	1.71	0.71
1:A:527:LYS:HE3	4:A:1115:HOH:O	1.91	0.71
1:B:184:ASN:HD21	1:B:223:LYS:NZ	1.89	0.70
1:A:316:THR:CG2	4:A:1102:HOH:O	2.40	0.70
1:A:423:ARG:HG2	1:A:423:ARG:HH11	1.55	0.69
1:B:309:ASP:H	1:B:672:ASN:ND2	1.90	0.69
1:B:782:ARG:NH1	1:B:961:ARG:O	2.25	0.69
1:A:125:ASN:HD22	1:A:125:ASN:H	1.41	0.67
1:B:296:GLU:HG3	4:B:1263:HOH:O	1.95	0.67
1:B:783:ASN:ND2	1:B:785:VAL:H	1.94	0.66
1:B:93:HIS:CE1	1:B:368:ARG:HH21	2.09	0.66
1:A:316:THR:HG23	4:A:1102:HOH:O	1.96	0.66
1:A:550:LEU:HD11	1:A:558:LYS:HG3	1.78	0.65
1:A:582:PHE:CE2	1:A:718:GLN:CG	2.79	0.65
1:B:125:ASN:H	1:B:125:ASN:HD22	1.45	0.65
1:A:827:GLU:OE1	1:A:862:ARG:HD3	1.97	0.64
1:B:771:LEU:HD21	1:B:954:VAL:CG2	2.27	0.63
1:B:93:HIS:HE1	1:B:368:ARG:NH2	1.95	0.63
1:B:123:LYS:HB3	1:B:126:GLU:HB2	1.80	0.63
1:B:236:ASP:CG	1:B:239:GLN:HG2	2.19	0.62
1:B:134:HIS:HE1	4:B:1058:HOH:O	1.82	0.62
1:A:784:GLU:HB3	4:A:1269:HOH:O	2.00	0.62
1:A:783:ASN:ND2	1:A:786:HIS:H	1.98	0.61
1:A:1011:HIS:HD2	4:A:1379:HOH:O	1.83	0.61
1:A:93:HIS:CE1	1:A:368:ARG:HH21	2.18	0.61
1:A:423:ARG:CG	1:A:423:ARG:HH11	2.13	0.60
1:A:309:ASP:H	1:A:672:ASN:ND2	1.96	0.60
1:B:782:ARG:HH21	1:B:784:GLU:HG2	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:805:ASN:HD22	1:B:844:GLN:HE22	1.51	0.59
1:A:316:THR:HB	1:A:374:ILE:HG22	1.84	0.59
1:B:94:ILE:HB	4:B:1305:HOH:O	2.03	0.58
1:B:827:GLU:OE1	1:B:862:ARG:HD3	2.03	0.58
1:B:224:TYR:OH	1:B:229:ARG:NH1	2.37	0.58
1:A:538:LEU:HD13	1:A:734:THR:HG23	1.85	0.58
1:B:141:PHE:HB2	2:D:14:VAL:HG13	1.84	0.58
1:B:184:ASN:HD21	1:B:223:LYS:HZ3	1.51	0.58
1:B:783:ASN:ND2	1:B:786:HIS:H	2.02	0.58
1:A:431:ARG:CZ	4:A:1323:HOH:O	2.51	0.58
1:B:783:ASN:HD22	1:B:785:VAL:H	1.52	0.57
1:B:799:MET:HE3	1:B:1008:VAL:HG22	1.86	0.57
1:A:491:ARG:NH1	1:A:491:ARG:HG2	2.20	0.57
1:A:927:TYR:O	1:A:930:THR:HB	2.05	0.56
1:B:299:LYS:HD2	1:B:510:ILE:HD13	1.87	0.56
1:B:622:ASN:HD22	1:B:622:ASN:H	1.54	0.56
1:A:222:ASN:O	1:A:226:LEU:HB2	2.05	0.56
1:B:451:THR:HB	1:B:455:LEU:HD12	1.88	0.56
1:A:771:LEU:HD21	1:A:954:VAL:CG2	2.35	0.56
1:B:460:ARG:NH1	1:B:462:ASP:OD1	2.40	0.55
1:A:524:LEU:HD12	4:A:1171:HOH:O	2.06	0.55
1:A:827:GLU:OE1	1:A:862:ARG:CD	2.55	0.55
1:B:927:TYR:O	1:B:930:THR:HB	2.07	0.55
1:A:67:LEU:HD23	1:A:75:VAL:HB	1.89	0.54
1:A:709:LEU:HB3	1:A:710:PRO:HD3	1.90	0.54
1:A:879:GLU:HG2	4:B:1074:HOH:O	2.07	0.54
1:B:86:SER:HB3	1:B:158:LEU:HG	1.90	0.53
1:B:239:GLN:O	1:B:243:LYS:HG2	2.07	0.53
1:B:309:ASP:N	1:B:672:ASN:HD21	2.05	0.53
1:B:475:ASN:HB3	4:B:1218:HOH:O	2.08	0.53
1:A:483:LYS:O	1:A:486:GLU:HB2	2.08	0.53
1:B:782:ARG:NH2	1:B:784:GLU:HG2	2.22	0.53
1:A:527:LYS:CD	4:A:1033:HOH:O	2.53	0.53
1:A:59:GLU:OE2	1:A:423:ARG:NH1	2.40	0.52
1:A:529:GLU:HG3	4:A:1382:HOH:O	2.09	0.52
1:B:307:ILE:O	1:B:674:ARG:NH2	2.42	0.52
1:A:446:LEU:O	1:A:449:VAL:HG22	2.09	0.52
1:B:658:ARG:O	1:B:662:ILE:HG12	2.09	0.52
1:B:538:LEU:HD23	1:B:734:THR:HG23	1.91	0.52
1:A:194:VAL:HG12	1:A:195:MET:CE	2.41	0.51
1:B:997:GLU:HG2	4:B:1039:HOH:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:597:LEU:HG	1:B:620:LEU:HG	1.93	0.50
1:B:803:SER:HA	1:B:927:TYR:CE2	2.46	0.50
1:A:815:ILE:HG22	1:A:870:MET:HG3	1.94	0.50
1:A:155:HIS:HD2	4:A:1280:HOH:O	1.94	0.50
1:B:722:ARG:HH21	1:B:756:LYS:HD3	1.77	0.50
1:B:507:ASP:O	1:B:511:LYS:HD3	2.11	0.50
1:A:552:LYS:HB3	1:A:559:LEU:HB3	1.94	0.49
1:B:329:ASN:ND2	1:B:363:GLN:HE22	2.03	0.49
1:A:460:ARG:NH1	1:A:462:ASP:OD1	2.45	0.49
1:B:730:HIS:HD2	1:B:904:SER:OG	1.96	0.49
1:A:805:ASN:HD22	1:A:844:GLN:HE22	1.60	0.49
1:B:192:LYS:HD2	1:B:832:ILE:HD11	1.95	0.49
1:A:783:ASN:ND2	1:A:785:VAL:H	2.10	0.49
1:B:196:ASN:ND2	1:B:198:ALA:H	2.11	0.49
1:A:622:ASN:H	1:A:622:ASN:HD22	1.61	0.49
1:A:470:LYS:HE2	4:A:1086:HOH:O	2.13	0.49
1:B:600:LEU:HD11	1:B:648:LYS:HB3	1.93	0.49
1:A:507:ASP:O	1:A:511:LYS:HD3	2.13	0.48
1:B:616:LEU:HD21	1:B:638:GLN:HG2	1.95	0.48
1:A:658:ARG:NH2	4:A:1297:HOH:O	2.45	0.48
1:B:602:ASP:OD1	1:B:658:ARG:HD3	2.12	0.48
1:A:582:PHE:CD2	1:A:718:GLN:HG3	2.49	0.48
1:B:643:LYS:HG2	1:B:744:MET:SD	2.54	0.48
1:A:799:MET:HG2	1:A:843:ILE:CD1	2.44	0.48
1:A:120:LYS:HE3	1:B:409:TRP:CD1	2.49	0.48
1:A:709:LEU:HG	1:A:713:LYS:HE3	1.96	0.48
1:A:783:ASN:HD22	1:A:785:VAL:H	1.62	0.48
1:B:291:HIS:CD2	1:B:370:PHE:HB2	2.49	0.48
1:A:230:PRO:HA	1:A:235:ILE:HD12	1.95	0.47
1:B:85:LYS:NZ	4:B:1238:HOH:O	2.46	0.47
1:B:121:TYR:HB3	1:B:126:GLU:HG2	1.95	0.47
1:A:291:HIS:CD2	1:A:370:PHE:HB2	2.48	0.47
1:B:140:ALA:HB1	4:B:1353:HOH:O	2.13	0.47
1:B:184:ASN:HD21	1:B:223:LYS:HZ1	1.61	0.47
1:B:550:LEU:HD11	1:B:558:LYS:HG3	1.95	0.47
1:A:136:GLY:O	1:A:892:ARG:NH1	2.48	0.47
1:A:433:TYR:O	1:A:437:ILE:HG12	2.14	0.47
1:A:793:ILE:O	1:A:847:ARG:HA	2.15	0.47
1:B:184:ASN:ND2	1:B:223:LYS:NZ	2.61	0.47
1:B:444:TYR:CD1	1:B:452:ALA:HB1	2.50	0.46
1:A:102:ASN:N	1:A:102:ASN:HD22	2.08	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:754:HIS:CD2	4:B:1341:HOH:O	2.69	0.46
1:A:309:ASP:N	1:A:672:ASN:HD21	2.05	0.46
1:A:950:ARG:HD2	4:A:1194:HOH:O	2.15	0.46
1:B:392:LEU:HD22	1:B:512:LYS:HE2	1.98	0.46
1:B:51:GLY:O	4:B:1241:HOH:O	2.20	0.46
1:B:930:THR:HG21	4:B:1326:HOH:O	2.16	0.46
1:B:294:GLN:H	1:B:297:HIS:CD2	2.23	0.46
1:B:529:GLU:HG3	4:B:1199:HOH:O	2.15	0.46
1:B:860:GLU:OE2	1:B:957:HIS:HE1	1.99	0.46
1:A:123:LYS:HB3	1:A:126:GLU:HB2	1.98	0.45
1:A:879:GLU:HB2	4:A:1167:HOH:O	2.16	0.45
1:A:730:HIS:HD2	1:A:904:SER:OG	1.99	0.45
1:B:824:ARG:O	1:B:828:GLN:HA	2.17	0.45
2:C:16:THR:HB	2:C:17:LEU:CA	2.38	0.45
2:C:16:THR:CB	2:C:17:LEU:HA	2.40	0.45
1:A:799:MET:HE3	1:A:1008:VAL:HG22	1.96	0.45
1:B:184:ASN:ND2	1:B:223:LYS:HZ3	2.15	0.45
1:A:618:TYR:HA	1:A:630:SER:O	2.17	0.45
1:A:862:ARG:HD2	4:A:1111:HOH:O	2.16	0.45
1:B:196:ASN:HD22	1:B:196:ASN:C	2.20	0.45
1:B:386:HIS:HD2	1:B:389:ASP:OD2	2.00	0.45
1:B:1000:ARG:NH1	4:B:1039:HOH:O	2.50	0.45
1:B:843:ILE:HG22	1:B:844:GLN:N	2.32	0.45
1:B:346:LEU:HA	1:B:522:PHE:CE2	2.52	0.44
1:B:948:ALA:HB3	1:B:951:ARG:HB2	1.99	0.44
1:A:239:GLN:O	1:A:243:LYS:HG2	2.17	0.44
1:A:477:ARG:HD3	4:A:1383:HOH:O	2.17	0.44
1:B:908:TYR:HE1	4:B:1316:HOH:O	2.00	0.44
1:A:602:ASP:OD1	1:A:658:ARG:HD3	2.17	0.44
1:B:722:ARG:HD2	4:B:1274:HOH:O	2.17	0.44
1:B:941:LYS:HE2	4:B:1245:HOH:O	2.16	0.44
1:A:599:LEU:HD21	1:A:659:PHE:HA	2.00	0.44
1:B:911:ILE:HG21	4:B:1316:HOH:O	2.18	0.44
1:A:194:VAL:HG12	1:A:195:MET:HE3	1.99	0.44
1:A:803:SER:HA	1:A:927:TYR:CE2	2.54	0.43
1:B:843:ILE:HG22	1:B:844:GLN:H	1.83	0.43
1:A:782:ARG:HD2	4:A:1373:HOH:O	2.18	0.43
1:B:444:TYR:CE1	1:B:452:ALA:HB1	2.53	0.43
1:A:156:GLU:HG2	1:A:156:GLU:H	1.66	0.43
1:A:796:GLN:HB3	1:A:952:HIS:HB2	1.99	0.43
1:A:586:ASP:OD1	1:A:589:HIS:HD2	2.02	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:ASN:N	1:B:102:ASN:HD22	2.08	0.43
1:B:433:TYR:O	1:B:437:ILE:HG12	2.19	0.43
1:B:961:ARG:HD2	1:B:962:GLU:OE1	2.19	0.43
1:A:48:LYS:HD3	4:A:1339:HOH:O	2.19	0.43
1:A:979:ASN:N	4:A:1089:HOH:O	2.52	0.42
1:A:94:ILE:HG13	1:A:248:TYR:HB3	2.01	0.42
1:B:49:ARG:HG2	1:B:68:GLU:HB3	2.01	0.42
1:A:67:LEU:HD11	1:A:268:THR:HG23	2.01	0.42
1:A:582:PHE:HE2	1:A:718:GLN:HG2	1.79	0.42
1:B:709:LEU:HB3	1:B:710:PRO:HD3	2.02	0.42
1:A:196:ASN:HD22	1:A:199:TRP:H	1.66	0.42
1:A:600:LEU:HD23	1:A:620:LEU:HD21	2.01	0.42
1:A:817:GLU:HB3	1:A:818:PRO:HD3	2.01	0.42
1:B:141:PHE:HB2	2:D:14:VAL:CG1	2.49	0.42
1:B:632:LYS:NZ	4:B:1104:HOH:O	2.52	0.42
1:B:886:ILE:HG23	1:B:928:LEU:HD13	2.01	0.42
1:B:532:PRO:HG3	1:B:634:TYR:CD2	2.54	0.42
1:A:465:GLU:HB2	4:A:1168:HOH:O	2.20	0.42
1:B:112:HIS:HA	2:D:17:LEU:HD23	2.02	0.42
1:A:597:LEU:HG	1:A:620:LEU:HG	2.01	0.41
1:B:163:ASP:O	1:B:167:GLN:HG2	2.20	0.41
1:B:418:ASN:ND2	1:B:454:TYR:O	2.53	0.41
1:A:402:ARG:NH2	4:A:1190:HOH:O	2.53	0.41
1:B:908:TYR:O	1:B:912:ILE:HG12	2.21	0.41
1:B:139:ASN:HB3	1:B:150:TYR:CZ	2.56	0.41
1:B:389:ASP:O	1:B:393:HIS:HD2	2.04	0.41
1:A:245:HIS:O	1:A:249:TYR:HB2	2.20	0.41
1:A:329:ASN:HD21	1:A:363:GLN:HE22	1.69	0.41
1:A:586:ASP:OD1	1:A:589:HIS:CD2	2.74	0.41
1:B:810:LEU:HG	1:B:928:LEU:HD21	2.03	0.41
1:A:824:ARG:O	1:A:828:GLN:HA	2.20	0.40
1:A:854:LYS:CD	1:A:855:PRO:HD2	2.43	0.40
1:A:392:LEU:O	1:A:396:GLN:HG3	2.21	0.40
1:A:685:TYR:HB2	1:A:956:VAL:HG11	2.03	0.40
1:B:236:ASP:OD2	1:B:239:GLN:HG2	2.21	0.40
1:B:100:PRO:HA	1:B:101:PRO:HD3	1.95	0.40
1:B:768:GLU:HB3	1:B:843:ILE:HG13	2.04	0.40
1:A:550:LEU:CD1	1:A:558:LYS:HG3	2.47	0.40
1:B:799:MET:HG2	1:B:843:ILE:CD1	2.51	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:A:460:ARG:NH2	1:A:747:ASP:OD1[3_655]	2.05	0.15

## 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	947/990 (96%)	924 (98%)	23 (2%)	0	100	100
1	B	944/990 (95%)	925 (98%)	19 (2%)	0	100	100
2	C	5/67 (8%)	3 (60%)	2 (40%)	0	100	100
2	D	5/67 (8%)	5 (100%)	0	0	100	100
All	All	1901/2114 (90%)	1857 (98%)	44 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	846/880 (96%)	783 (93%)	63 (7%)	15	17
1	B	846/880 (96%)	787 (93%)	59 (7%)	16	20
2	C	6/57 (10%)	5 (83%)	1 (17%)	2	2
2	D	6/57 (10%)	6 (100%)	0	100	100
All	All	1704/1874 (91%)	1581 (93%)	123 (7%)	16	19

All (123) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	43	ASN
1	A	67	LEU
1	A	76	LEU
1	A	97	LEU
1	A	102	ASN
1	A	111	GLN
1	A	125	ASN
1	A	148	ASN
1	A	156	GLU
1	A	158	LEU
1	A	196	ASN
1	A	201	LEU
1	A	223	LYS
1	A	226	LEU
1	A	270	LEU
1	A	273	LYS
1	A	285	LEU
1	A	316	THR
1	A	329	ASN
1	A	337	LEU
1	A	347	LEU
1	A	356	VAL
1	A	412	GLN
1	A	414	LEU
1	A	417	LEU
1	A	423	ARG
1	A	446	LEU
1	A	449	VAL
1	A	450	LEU
1	A	466	MET
1	A	491	ARG
1	A	512	LYS
1	A	582	PHE
1	A	595	LEU
1	A	597	LEU
1	A	612	GLU
1	A	616	LEU
1	A	622	ASN
1	A	629	LEU
1	A	642	LEU
1	A	674	ARG
1	A	677	GLN
1	A	691	THR

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Mol	Chain	Res	Type
1	A	711	ARG
1	A	712	LEU
1	A	728	LEU
1	A	765	ARG
1	A	771	LEU
1	A	783	ASN
1	A	789	SER
1	A	810	LEU
1	A	823	LEU
1	A	838	ARG
1	A	846	LEU
1	A	859	LEU
1	A	867	LEU
1	A	889	LEU
1	A	928	LEU
1	A	930	THR
1	A	931	LEU
1	A	957	HIS
1	A	993	GLN
1	A	1007	LEU
1	B	67	LEU
1	B	76	LEU
1	B	97	LEU
1	B	102	ASN
1	B	111	GLN
1	B	125	ASN
1	B	148	ASN
1	B	158	LEU
1	B	177	SER
1	B	196	ASN
1	B	201	LEU
1	B	223	LYS
1	B	226	LEU
1	B	239	GLN
1	B	243	LYS
1	B	270	LEU
1	B	285	LEU
1	B	316	THR
1	B	329	ASN
1	B	337	LEU
1	B	347	LEU
1	B	414	LEU

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Mol	Chain	Res	Type
1	B	417	LEU
1	B	446	LEU
1	B	450	LEU
1	B	512	LYS
1	B	517	ASP
1	B	524	LEU
1	B	556	MET
1	B	595	LEU
1	B	597	LEU
1	B	612	GLU
1	B	616	LEU
1	B	622	ASN
1	B	629	LEU
1	B	642	LEU
1	B	648	LYS
1	B	674	ARG
1	B	677	GLN
1	B	712	LEU
1	B	728	LEU
1	B	733	ILE
1	B	736	GLN
1	B	758	LEU
1	B	759	LEU
1	B	765	ARG
1	B	771	LEU
1	B	783	ASN
1	B	810	LEU
1	B	817	GLU
1	B	823	LEU
1	B	846	LEU
1	B	859	LEU
1	B	867	LEU
1	B	889	LEU
1	B	928	LEU
1	B	942	GLU
1	B	993	GLN
1	B	1007	LEU
2	C	17	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	HIS
1	A	102	ASN
1	A	125	ASN
1	A	148	ASN
1	A	184	ASN
1	A	196	ASN
1	A	231	ASN
1	A	232	GLN
1	A	294	GLN
1	A	297	HIS
1	A	300	GLN
1	A	329	ASN
1	A	393	HIS
1	A	502	GLN
1	A	575	ASN
1	A	589	HIS
1	A	605	ASN
1	A	622	ASN
1	A	672	ASN
1	A	730	HIS
1	A	770	GLN
1	A	783	ASN
1	A	805	ASN
1	A	828	GLN
1	A	841	ASN
1	A	883	GLN
1	A	957	HIS
1	B	52	ASN
1	B	93	HIS
1	B	102	ASN
1	B	125	ASN
1	B	148	ASN
1	B	184	ASN
1	B	196	ASN
1	B	231	ASN
1	B	294	GLN
1	B	297	HIS
1	B	300	GLN
1	B	329	ASN
1	B	386	HIS
1	B	393	HIS
1	B	407	GLN
1	B	502	GLN

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Mol	Chain	Res	Type
1	B	575	ASN
1	B	589	HIS
1	B	605	ASN
1	B	622	ASN
1	B	672	ASN
1	B	730	HIS
1	B	770	GLN
1	B	783	ASN
1	B	788	ASN
1	B	805	ASN
1	B	828	GLN
1	B	883	GLN
1	B	922	ASN
1	B	957	HIS
1	B	979	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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 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 [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

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	953/990 (96%)	-0.27	6 (0%) 89 92	20, 32, 47, 62	0
1	B	952/990 (96%)	-0.22	10 (1%) 80 84	25, 37, 50, 71	0
2	C	9/67 (13%)	1.58	3 (33%) 0 0	37, 66, 67, 67	0
2	D	9/67 (13%)	1.27	3 (33%) 0 0	36, 73, 75, 75	0
All	All	1923/2114 (90%)	-0.23	22 (1%) 80 84	20, 35, 49, 75	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	979	ASN	4.0
1	B	43	ASN	3.6
2	C	17	LEU	3.1
2	C	18	GLN	3.0
1	B	52	ASN	2.9
1	B	53	HIS	2.8
1	A	979	ASN	2.8
1	B	736	GLN	2.7
1	B	239	GLN	2.4
2	D	18	GLN	2.4
1	B	880	GLU	2.3
2	C	13	LEU	2.3
1	B	980	LEU	2.3
2	D	13	LEU	2.2
1	A	667	MET	2.2
2	D	16	THR	2.2
1	B	1011	HIS	2.2
1	A	985	ALA	2.1
1	A	43	ASN	2.1
1	A	517	ASP	2.1
1	A	508	GLU	2.1
1	B	982	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](#)

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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
3	ZN	B	2	1/1	0.99	0.28	2,2,2,2	0
3	ZN	C	68	1/1	0.99	0.26	2,2,2,2	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.