



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 10:31 PM GMT

PDB ID : 1RJ7  
Title : Crystal structure of EDA-A1  
Authors : Hymowitz, S.G.; Compaaan, D.M.; Yan, M.; Ackerly, H.; Dixit, V.M.; Starovasnik, M.A.; de Vos, A.M.  
Deposited on : 2003-11-18  
Resolution : 2.30 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

---

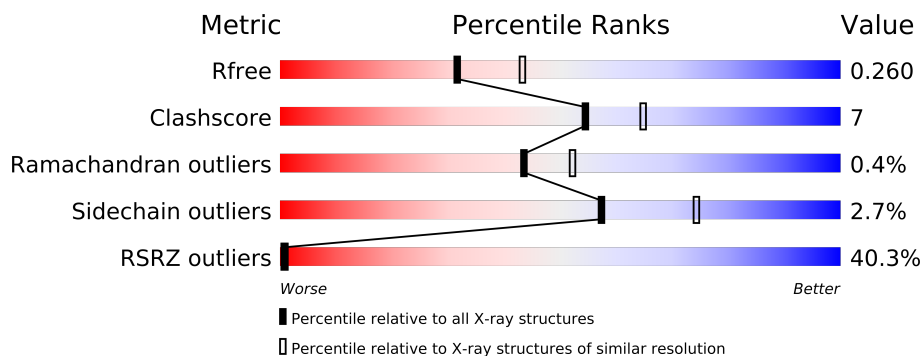
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.30 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))
$R_{free}$	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	163	
1	B	163	
1	D	163	
1	E	163	
1	F	163	
1	G	163	
1	H	163	
1	I	163	
1	J	163	
1	K	163	
1	L	163	
1	M	163	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13887 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Ectodysplasin A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	144	Total	C	N	O	S	0	0	0
			1124	719	190	209	6			
1	B	144	Total	C	N	O	S	0	0	0
			1124	719	190	209	6			
1	D	144	Total	C	N	O	S	0	0	0
			1125	720	190	209	6			
1	E	149	Total	C	N	O	S	0	0	0
			1168	743	200	219	6			
1	F	144	Total	C	N	O	S	0	0	0
			1129	722	191	210	6			
1	G	144	Total	C	N	O	S	0	0	0
			1125	720	190	209	6			
1	H	142	Total	C	N	O	S	0	0	0
			1113	712	188	207	6			
1	I	143	Total	C	N	O	S	0	0	0
			1124	719	190	209	6			
1	J	143	Total	C	N	O	S	0	0	0
			1118	715	189	208	6			
1	K	145	Total	C	N	O	S	0	0	0
			1136	725	192	213	6			
1	L	145	Total	C	N	O	S	0	0	0
			1133	724	192	211	6			
1	M	144	Total	C	N	O	S	0	0	0
			1129	722	191	210	6			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	229	GLY	-	CLONING ARTIFACT	UNP Q92838
A	230	SER	-	CLONING ARTIFACT	UNP Q92838
A	231	HIS	-	CLONING ARTIFACT	UNP Q92838
A	232	MET	-	CLONING ARTIFACT	UNP Q92838
B	229	GLY	-	CLONING ARTIFACT	UNP Q92838

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	230	SER	-	CLONING ARTIFACT	UNP Q92838
B	231	HIS	-	CLONING ARTIFACT	UNP Q92838
B	232	MET	-	CLONING ARTIFACT	UNP Q92838
D	229	GLY	-	CLONING ARTIFACT	UNP Q92838
D	230	SER	-	CLONING ARTIFACT	UNP Q92838
D	231	HIS	-	CLONING ARTIFACT	UNP Q92838
D	232	MET	-	CLONING ARTIFACT	UNP Q92838
E	229	GLY	-	CLONING ARTIFACT	UNP Q92838
E	230	SER	-	CLONING ARTIFACT	UNP Q92838
E	231	HIS	-	CLONING ARTIFACT	UNP Q92838
E	232	MET	-	CLONING ARTIFACT	UNP Q92838
F	229	GLY	-	CLONING ARTIFACT	UNP Q92838
F	230	SER	-	CLONING ARTIFACT	UNP Q92838
F	231	HIS	-	CLONING ARTIFACT	UNP Q92838
F	232	MET	-	CLONING ARTIFACT	UNP Q92838
G	229	GLY	-	CLONING ARTIFACT	UNP Q92838
G	230	SER	-	CLONING ARTIFACT	UNP Q92838
G	231	HIS	-	CLONING ARTIFACT	UNP Q92838
G	232	MET	-	CLONING ARTIFACT	UNP Q92838
H	229	GLY	-	CLONING ARTIFACT	UNP Q92838
H	230	SER	-	CLONING ARTIFACT	UNP Q92838
H	231	HIS	-	CLONING ARTIFACT	UNP Q92838
H	232	MET	-	CLONING ARTIFACT	UNP Q92838
I	229	GLY	-	CLONING ARTIFACT	UNP Q92838
I	230	SER	-	CLONING ARTIFACT	UNP Q92838
I	231	HIS	-	CLONING ARTIFACT	UNP Q92838
I	232	MET	-	CLONING ARTIFACT	UNP Q92838
J	229	GLY	-	CLONING ARTIFACT	UNP Q92838
J	230	SER	-	CLONING ARTIFACT	UNP Q92838
J	231	HIS	-	CLONING ARTIFACT	UNP Q92838
J	232	MET	-	CLONING ARTIFACT	UNP Q92838
K	229	GLY	-	CLONING ARTIFACT	UNP Q92838
K	230	SER	-	CLONING ARTIFACT	UNP Q92838
K	231	HIS	-	CLONING ARTIFACT	UNP Q92838
K	232	MET	-	CLONING ARTIFACT	UNP Q92838
L	229	GLY	-	CLONING ARTIFACT	UNP Q92838
L	230	SER	-	CLONING ARTIFACT	UNP Q92838
L	231	HIS	-	CLONING ARTIFACT	UNP Q92838
L	232	MET	-	CLONING ARTIFACT	UNP Q92838
M	229	GLY	-	CLONING ARTIFACT	UNP Q92838
M	230	SER	-	CLONING ARTIFACT	UNP Q92838
M	231	HIS	-	CLONING ARTIFACT	UNP Q92838

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
M	232	MET	-	CLONING ARTIFACT	UNP Q92838

- Molecule 2 is water.

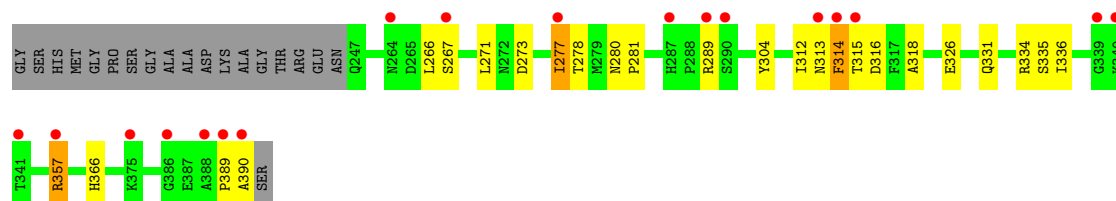
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	35	Total O 35 35	0	0
2	B	17	Total O 17 17	0	0
2	D	19	Total O 19 19	0	0
2	E	37	Total O 37 37	0	0
2	F	41	Total O 41 41	0	0
2	G	43	Total O 43 43	0	0
2	H	22	Total O 22 22	0	0
2	I	22	Total O 22 22	0	0
2	J	19	Total O 19 19	0	0
2	K	32	Total O 32 32	0	0
2	L	29	Total O 29 29	0	0
2	M	23	Total O 23 23	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

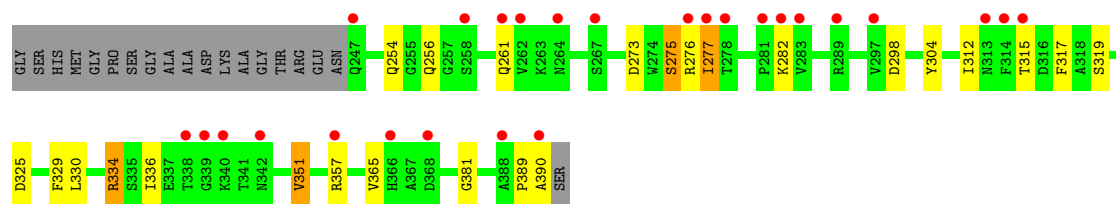
#### • Molecule 1: Ectodysplasin A

Chain A: 



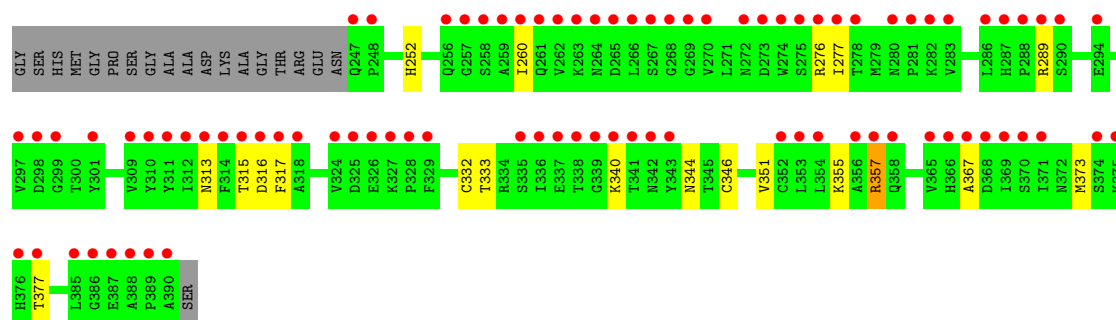
#### • Molecule 1: Ectodysplasin A

Chain B: 



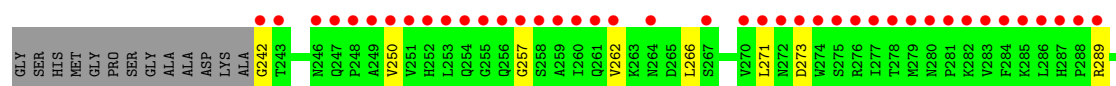
#### • Molecule 1: Ectodysplasin A

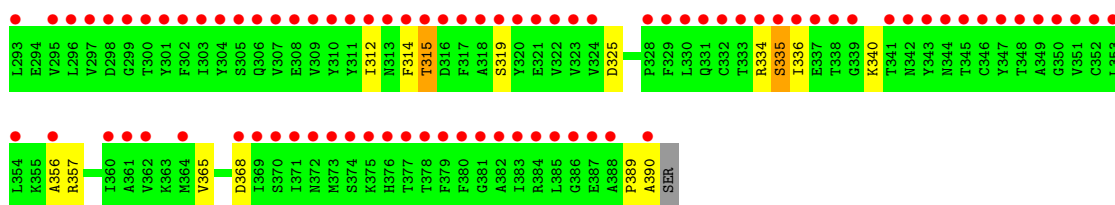
Chain D: 



#### • Molecule 1: Ectodysplasin A

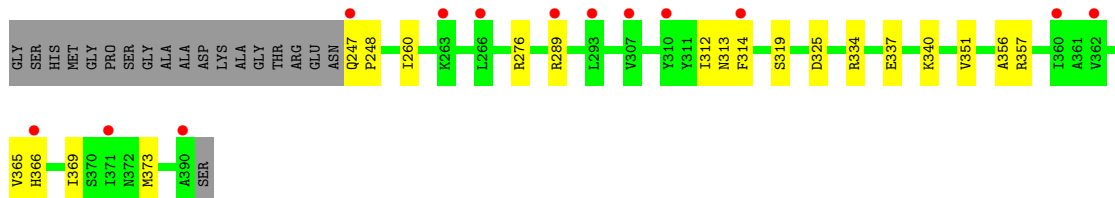
Chain E: 





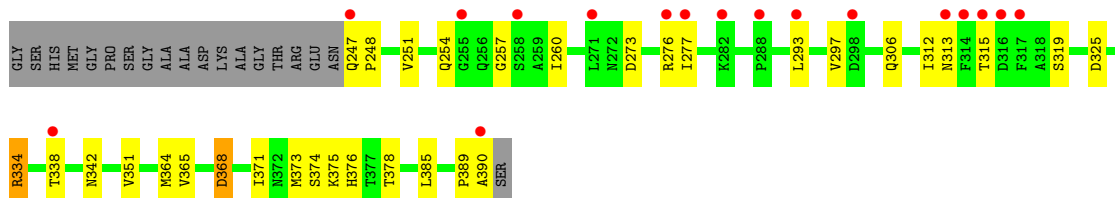
• Molecule 1: Ectodysplasin A

Chain F:



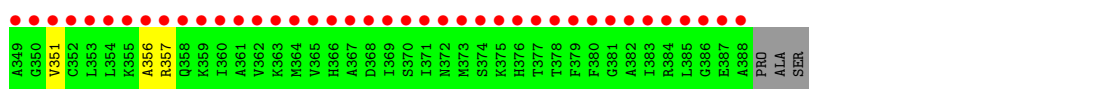
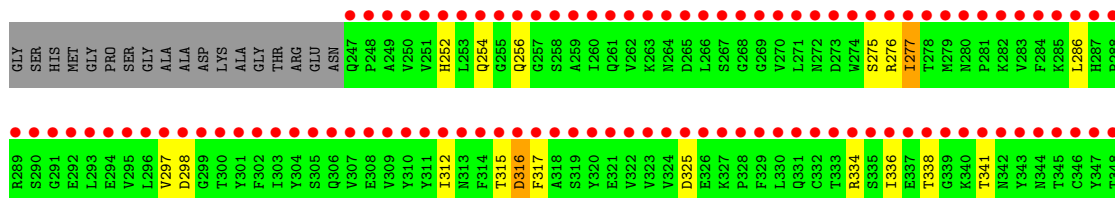
• Molecule 1: Ectodysplasin A

Chain G:



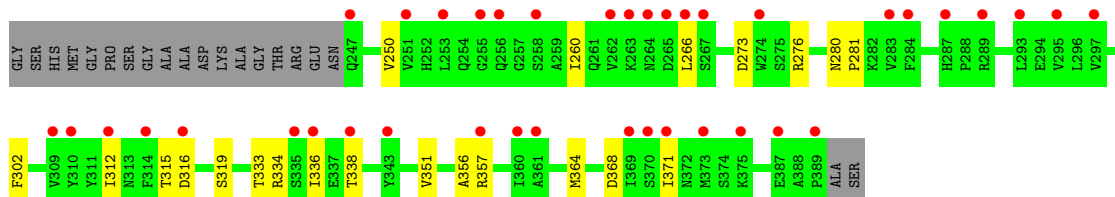
• Molecule 1: Ectodysplasin A

Chain H:



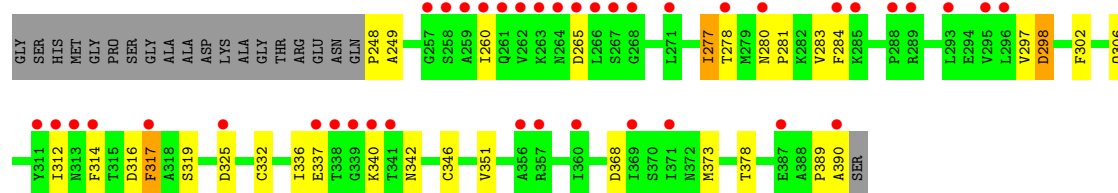
• Molecule 1: Ectodysplasin A

Chain I:



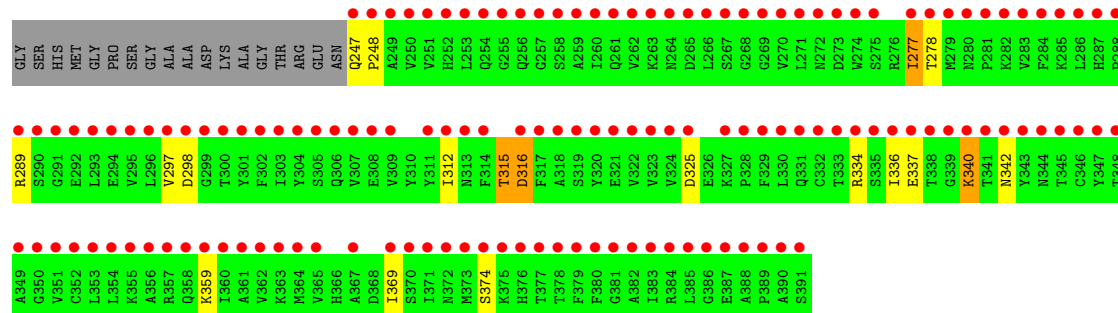
• Molecule 1: Ectodysplasin A

Chain J: 



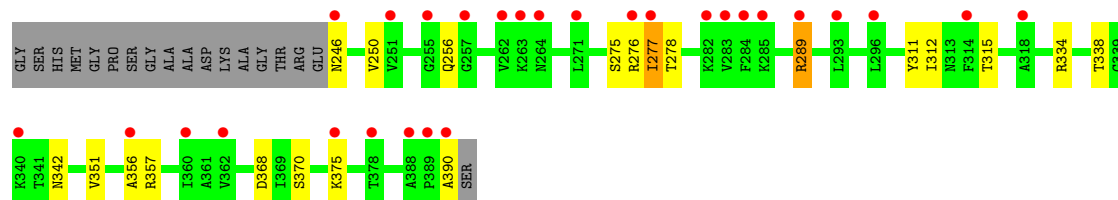
• Molecule 1: Ectodysplasin A

Chain K: 



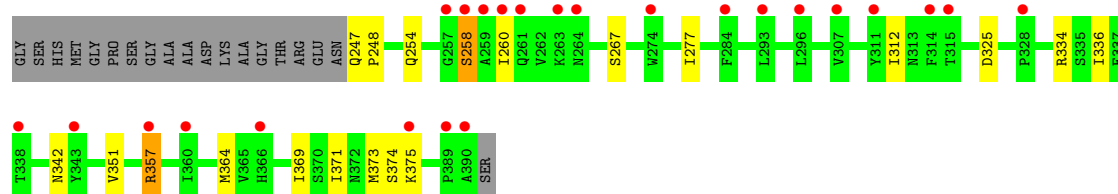
• Molecule 1: Ectodysplasin A

Chain L: 



• Molecule 1: Ectodysplasin A

Chain M: 





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	53.66Å 279.69Å 54.17Å 90.00° 91.36° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 19.99 – 2.30	Depositor EDS
% Data completeness (in resolution range)	94.3 (20.00-2.30) 94.4 (19.99-2.30)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.84 (at 2.30Å)	Xtriage
Refinement program	REFMAC 5.1.07	Depositor
R, $R_{free}$	0.194 , 0.260 0.198 , 0.260	Depositor DCC
$R_{free}$ test set	7099 reflections (12.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.4	Xtriage
Anisotropy	0.365	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 10.4	EDS
Estimated twinning fraction	0.000 for l,k,-h 0.046 for h,-k,-l 0.031 for l,-k,h	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 66279 reflections	Xtriage
$F_o, F_c$ correlation	0.77	EDS
Total number of atoms	13887	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	6.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.85% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 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	0.50	0/1148	0.77	2/1556 (0.1%)
1	B	0.50	0/1148	0.78	3/1556 (0.2%)
1	D	0.49	0/1149	0.74	1/1558 (0.1%)
1	E	0.54	0/1192	0.79	3/1615 (0.2%)
1	F	0.53	0/1153	0.76	1/1563 (0.1%)
1	G	0.53	0/1149	0.78	3/1558 (0.2%)
1	H	0.47	0/1136	0.74	2/1539 (0.1%)
1	I	0.46	0/1148	0.75	2/1556 (0.1%)
1	J	0.48	0/1141	0.76	6/1546 (0.4%)
1	K	0.52	0/1160	0.77	1/1571 (0.1%)
1	L	0.52	0/1157	0.76	1/1569 (0.1%)
1	M	0.50	0/1153	0.75	1/1563 (0.1%)
All	All	0.50	0/13834	0.76	26/18750 (0.1%)

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	325	ASP	CB-CG-OD2	7.22	124.80	118.30
1	B	273	ASP	CB-CG-OD2	6.67	124.30	118.30
1	E	273	ASP	CB-CG-OD2	6.43	124.08	118.30
1	M	325	ASP	CB-CG-OD2	6.40	124.06	118.30
1	F	325	ASP	CB-CG-OD2	6.21	123.89	118.30
1	I	273	ASP	CB-CG-OD2	6.10	123.79	118.30
1	J	248	PRO	N-CA-CB	6.07	110.59	103.30
1	A	273	ASP	CB-CG-OD2	5.79	123.51	118.30
1	H	316	ASP	CB-CG-OD2	5.75	123.48	118.30
1	H	325	ASP	CB-CG-OD2	5.55	123.30	118.30
1	A	357	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	E	325	ASP	CB-CG-OD2	5.38	123.14	118.30
1	G	273	ASP	CB-CG-OD2	5.38	123.14	118.30
1	G	368	ASP	CB-CG-OD2	5.33	123.09	118.30
1	L	368	ASP	CB-CG-OD2	5.32	123.09	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	368	ASP	CB-CG-OD2	5.28	123.05	118.30
1	J	325	ASP	CB-CG-OD2	5.27	123.04	118.30
1	G	325	ASP	CB-CG-OD2	5.26	123.04	118.30
1	J	316	ASP	CB-CG-OD2	5.26	123.04	118.30
1	E	368	ASP	CB-CG-OD2	5.22	123.00	118.30
1	J	298	ASP	CB-CG-OD2	5.20	122.98	118.30
1	B	298	ASP	CB-CG-OD2	5.20	122.98	118.30
1	B	325	ASP	CB-CG-OD2	5.19	122.97	118.30
1	J	368	ASP	CB-CG-OD2	5.13	122.92	118.30
1	J	265	ASP	CB-CG-OD2	5.09	122.88	118.30
1	D	316	ASP	CB-CG-OD2	5.07	122.86	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1124	0	1118	23	0
1	B	1124	0	1118	17	0
1	D	1125	0	1119	14	0
1	E	1168	0	1160	19	0
1	F	1129	0	1125	16	0
1	G	1125	0	1119	26	0
1	H	1113	0	1107	14	0
1	I	1124	0	1120	13	0
1	J	1118	0	1112	16	0
1	K	1136	0	1130	14	0
1	L	1133	0	1125	16	0
1	M	1129	0	1125	18	0
2	A	35	0	0	1	0
2	B	17	0	0	4	0
2	D	19	0	0	1	0
2	E	37	0	0	2	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	41	0	0	2	0
2	G	43	0	0	6	0
2	H	22	0	0	0	0
2	I	22	0	0	0	0
2	J	19	0	0	0	0
2	K	32	0	0	3	0
2	L	29	0	0	4	0
2	M	23	0	0	2	0
All	All	13887	0	13478	184	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

All (184) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:334:ARG:NH2	2:G:392:HOH:O	2.00	0.94
1:G:297:VAL:HB	2:G:426:HOH:O	1.69	0.92
1:F:260:ILE:HD12	1:F:373:MET:HG3	1.61	0.83
1:F:247:GLN:N	2:F:426:HOH:O	2.15	0.80
1:E:242:GLY:HA2	2:E:422:HOH:O	1.84	0.76
1:H:256:GLN:HG3	1:H:275:SER:HB2	1.67	0.75
1:E:314:PHE:O	1:E:315:THR:OG1	2.05	0.74
1:A:314:PHE:HB2	1:E:314:PHE:CD1	2.23	0.73
1:F:312:ILE:HG13	1:F:369:ILE:HG22	1.72	0.72
1:A:334:ARG:HH12	1:B:334:ARG:HE	1.38	0.70
1:H:312:ILE:HD12	1:H:336:ILE:HB	1.75	0.68
1:K:337:GLU:HB3	1:K:340:LYS:HE3	1.76	0.68
1:F:247:GLN:N	2:F:427:HOH:O	2.26	0.68
1:G:254:GLN:NE2	1:G:375:LYS:HG2	2.09	0.67
1:G:364:MET:SD	1:G:371:ILE:HD11	2.37	0.66
1:L:276:ARG:HD2	2:L:405:HOH:O	1.97	0.65
1:A:277:ILE:HG13	1:A:278:THR:H	1.62	0.65
1:B:365:VAL:HG13	2:B:7:HOH:O	1.97	0.65
1:A:312:ILE:HD12	1:A:336:ILE:HB	1.78	0.65
1:D:260:ILE:HD12	1:D:373:MET:HG3	1.78	0.64
1:L:277:ILE:HG23	1:L:278:THR:H	1.63	0.63
1:E:389:PRO:O	1:E:390:ALA:CB	2.46	0.62
1:L:256:GLN:NE2	2:L:407:HOH:O	2.33	0.62
1:K:247:GLN:HB3	1:K:248:PRO:HD3	1.82	0.61
1:H:315:THR:HG22	1:H:317:PHE:HB3	1.83	0.61
1:D:355:LYS:HE2	2:D:120:HOH:O	2.02	0.60
1:A:314:PHE:CD1	1:E:314:PHE:HB3	2.36	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:337:GLU:HB2	1:F:340:LYS:HE2	1.84	0.59
1:L:312:ILE:O	1:L:338:THR:O	2.21	0.59
1:K:312:ILE:CG2	1:K:315:THR:HG23	2.33	0.59
1:M:254:GLN:NE2	1:M:277:ILE:HD11	2.19	0.58
1:B:256:GLN:HG3	1:B:275:SER:HB2	1.86	0.57
1:F:312:ILE:CG1	1:F:369:ILE:HG22	2.34	0.57
1:J:340:LYS:HE3	1:J:342:ASN:HD21	1.68	0.57
1:E:312:ILE:HD12	1:E:336:ILE:HB	1.87	0.57
1:M:312:ILE:HD11	1:M:336:ILE:HB	1.86	0.57
1:A:334:ARG:NH1	1:B:334:ARG:HE	2.03	0.57
1:E:266:LEU:HD11	1:E:271:LEU:HD23	1.86	0.56
1:M:260:ILE:HD12	1:M:373:MET:HG3	1.88	0.55
1:M:260:ILE:HD12	1:M:373:MET:CG	2.37	0.55
1:H:252:HIS:HD2	1:H:277:ILE:HD11	1.71	0.55
1:B:312:ILE:HD12	1:B:336:ILE:HB	1.89	0.55
1:D:315:THR:HG21	1:D:367:ALA:HB1	1.88	0.54
1:G:312:ILE:O	1:G:312:ILE:HG13	2.07	0.54
1:M:312:ILE:HG23	1:M:369:ILE:HG12	1.89	0.54
1:H:254:GLN:HG3	1:H:277:ILE:HD11	1.90	0.54
1:I:302:PHE:HD1	1:I:351:VAL:HG22	1.73	0.54
1:M:312:ILE:CD1	1:M:336:ILE:HB	2.37	0.54
1:D:357:ARG:HH11	1:D:357:ARG:CG	2.21	0.53
1:B:365:VAL:CG1	2:B:7:HOH:O	2.54	0.53
1:A:314:PHE:CB	1:E:314:PHE:CD1	2.90	0.53
1:I:260:ILE:HD13	1:I:266:LEU:HD21	1.90	0.53
1:G:254:GLN:NE2	1:G:277:ILE:CD1	2.72	0.53
1:K:312:ILE:CD1	1:K:336:ILE:HB	2.39	0.53
1:B:282:LYS:HA	2:B:125:HOH:O	2.08	0.53
1:K:312:ILE:HD12	1:K:336:ILE:HB	1.90	0.53
1:A:335:SER:HB2	1:D:344:ASN:HD21	1.73	0.53
1:J:317:PHE:CE1	1:J:319:SER:HB2	2.43	0.52
1:H:276:ARG:HH11	1:H:286:LEU:HD23	1.74	0.52
1:D:357:ARG:HG3	1:D:357:ARG:NH1	2.23	0.52
1:G:389:PRO:O	1:G:390:ALA:CB	2.58	0.52
1:E:389:PRO:O	1:E:390:ALA:HB2	2.11	0.51
1:A:304:TYR:OH	1:B:351:VAL:HG23	2.11	0.51
1:B:389:PRO:O	1:B:390:ALA:HB3	2.10	0.51
1:K:337:GLU:HB3	1:K:340:LYS:CE	2.41	0.51
1:A:313:ASN:O	1:A:314:PHE:CD1	2.63	0.51
1:G:247:GLN:N	2:G:422:HOH:O	2.44	0.51
1:A:331:GLN:HB3	1:D:377:THR:HG22	1.93	0.50
1:G:251:VAL:HG11	1:G:293:LEU:HD21	1.93	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:364:MET:SD	1:I:371:ILE:HD11	2.52	0.50
1:M:248:PRO:HD2	2:M:169:HOH:O	2.09	0.50
1:M:254:GLN:NE2	1:M:375:LYS:O	2.44	0.50
1:A:314:PHE:CE1	1:E:314:PHE:O	2.65	0.50
1:E:334:ARG:HH12	1:F:334:ARG:NH1	2.09	0.50
1:L:356:ALA:O	1:L:357:ARG:HB2	2.12	0.50
1:I:312:ILE:HD12	1:I:336:ILE:HB	1.94	0.49
1:M:364:MET:CE	1:M:371:ILE:HD11	2.42	0.49
1:I:250:VAL:HG11	1:J:351:VAL:HG11	1.95	0.49
1:J:249:ALA:CB	1:J:283:VAL:HG21	2.42	0.49
1:D:357:ARG:HG3	1:D:357:ARG:HH11	1.76	0.49
1:A:357:ARG:CG	1:A:357:ARG:HH11	2.24	0.49
1:G:247:GLN:N	1:G:248:PRO:CD	2.76	0.49
1:L:390:ALA:HA	2:L:403:HOH:O	2.13	0.49
1:J:260:ILE:HD12	1:J:373:MET:HG3	1.95	0.48
1:M:357:ARG:HH11	1:M:357:ARG:HG3	1.78	0.48
1:M:357:ARG:NH1	1:M:357:ARG:HG3	2.28	0.48
1:L:250:VAL:HG11	1:M:351:VAL:HG21	1.96	0.48
1:A:366:HIS:ND1	1:A:366:HIS:C	2.67	0.48
1:A:314:PHE:HB2	1:E:314:PHE:CG	2.49	0.48
1:J:302:PHE:HD1	1:J:351:VAL:HG22	1.79	0.48
1:F:313:ASN:HB3	1:F:314:PHE:CD2	2.48	0.48
1:H:312:ILE:CD1	1:H:336:ILE:HB	2.44	0.47
1:B:317:PHE:CE1	1:B:319:SER:HB2	2.49	0.47
1:G:334:ARG:HH11	1:G:334:ARG:HG3	1.79	0.47
1:L:375:LYS:HG2	2:L:408:HOH:O	2.14	0.47
1:A:267:SER:HA	2:A:60:HOH:O	2.14	0.47
1:D:317:PHE:HE1	1:D:333:THR:HB	1.80	0.47
1:H:356:ALA:O	1:H:357:ARG:HB2	2.14	0.47
1:K:315:THR:HB	2:K:410:HOH:O	2.15	0.47
1:L:289:ARG:HH11	1:L:289:ARG:HB3	1.80	0.47
1:E:356:ALA:O	1:E:357:ARG:HB2	2.15	0.47
1:J:337:GLU:HB3	1:J:340:LYS:HE2	1.97	0.47
1:M:357:ARG:HH11	1:M:357:ARG:CG	2.28	0.47
1:D:276:ARG:O	1:D:276:ARG:HG3	2.15	0.47
1:J:332:CYS:SG	1:J:346:CYS:HB3	2.54	0.47
1:L:256:GLN:HG2	1:L:275:SER:HB2	1.96	0.47
1:B:357:ARG:HH11	1:B:357:ARG:CG	2.28	0.47
1:H:315:THR:O	1:H:316:ASP:HB2	2.15	0.46
1:I:315:THR:O	1:I:338:THR:HG22	2.15	0.46
1:F:356:ALA:O	1:F:357:ARG:HB2	2.15	0.46
1:B:254:GLN:HG3	1:B:277:ILE:HD11	1.98	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:254:GLN:NE2	1:G:277:ILE:HD11	2.30	0.46
1:I:312:ILE:CD1	1:I:336:ILE:HB	2.46	0.46
1:E:334:ARG:HH12	1:F:334:ARG:CZ	2.28	0.46
1:I:319:SER:OG	1:I:333:THR:HG22	2.14	0.46
1:D:332:CYS:SG	1:D:346:CYS:HB3	2.56	0.46
1:H:256:GLN:CG	1:H:275:SER:HB2	2.42	0.46
1:D:317:PHE:CE1	1:D:333:THR:HB	2.51	0.46
1:A:326:GLU:OE1	1:G:376:HIS:NE2	2.47	0.46
1:J:297:VAL:HG12	1:J:298:ASP:O	2.16	0.46
1:M:258:SER:HB2	2:M:141:HOH:O	2.15	0.46
1:K:316:ASP:C	1:K:316:ASP:OD1	2.55	0.45
1:D:252:HIS:O	1:D:277:ILE:HG22	2.16	0.45
1:K:369:ILE:HD12	2:K:411:HOH:O	2.17	0.45
1:J:283:VAL:HG23	1:J:284:PHE:CD2	2.52	0.45
1:L:334:ARG:HH12	1:M:334:ARG:CZ	2.30	0.45
1:G:368:ASP:HB2	2:G:413:HOH:O	2.16	0.45
1:L:342:ASN:HD22	1:L:342:ASN:HA	1.59	0.45
1:G:260:ILE:HD12	1:G:373:MET:HG3	1.98	0.45
1:J:280:ASN:HB3	1:J:283:VAL:HG22	1.98	0.44
1:E:340:LYS:HG3	2:E:392:HOH:O	2.17	0.44
1:H:334:ARG:HH12	1:I:334:ARG:CZ	2.30	0.44
1:B:261:GLN:HB3	2:B:3:HOH:O	2.16	0.44
1:G:247:GLN:N	1:G:248:PRO:HD2	2.33	0.44
1:J:280:ASN:HA	1:J:281:PRO:HD3	1.85	0.44
1:L:250:VAL:HB	1:M:351:VAL:HG11	1.99	0.44
1:H:357:ARG:HG3	1:H:357:ARG:HH11	1.82	0.44
1:D:252:HIS:O	1:D:277:ILE:CG2	2.66	0.44
1:G:276:ARG:HG2	2:G:408:HOH:O	2.18	0.44
1:J:312:ILE:HD11	1:J:336:ILE:O	2.18	0.44
1:K:334:ARG:HH12	1:L:334:ARG:CZ	2.32	0.43
1:G:315:THR:O	1:G:315:THR:HG23	2.17	0.43
1:A:312:ILE:HD11	1:A:318:ALA:HB2	2.00	0.43
1:B:312:ILE:HG22	1:B:315:THR:O	2.18	0.43
1:B:389:PRO:O	1:B:390:ALA:CB	2.66	0.43
1:A:315:THR:O	1:A:316:ASP:OD1	2.37	0.43
1:E:319:SER:O	1:E:365:VAL:HG22	2.19	0.43
1:I:280:ASN:HA	1:I:281:PRO:HD3	1.88	0.43
1:G:319:SER:O	1:G:365:VAL:HG22	2.19	0.43
1:G:313:ASN:HB3	1:G:368:ASP:HB3	2.01	0.42
1:F:366:HIS:O	1:F:366:HIS:CD2	2.72	0.42
1:J:306:GLN:O	1:J:378:THR:HA	2.19	0.42
1:K:337:GLU:HB2	1:K:342:ASN:ND2	2.34	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:306:GLN:O	1:G:378:THR:HA	2.20	0.42
1:A:389:PRO:O	1:A:390:ALA:HB3	2.19	0.42
1:J:389:PRO:O	1:J:390:ALA:CB	2.67	0.42
1:E:250:VAL:HG11	1:F:351:VAL:HG21	2.02	0.42
1:B:329:PHE:CD2	1:B:330:LEU:HG	2.55	0.42
1:L:315:THR:O	1:L:338:THR:HG22	2.20	0.42
1:I:316:ASP:HB2	1:I:336:ILE:O	2.20	0.42
1:K:297:VAL:HG12	1:K:298:ASP:O	2.19	0.42
1:M:247:GLN:OE1	1:M:247:GLN:HA	2.19	0.42
1:M:254:GLN:HB2	1:M:375:LYS:O	2.20	0.41
1:E:312:ILE:HD11	1:E:336:ILE:HD12	2.02	0.41
1:A:357:ARG:CG	1:A:357:ARG:NH1	2.83	0.41
1:G:312:ILE:O	1:G:338:THR:O	2.38	0.41
1:F:312:ILE:HG13	1:F:369:ILE:CG2	2.47	0.41
1:K:277:ILE:HG13	1:K:278:THR:N	2.34	0.41
1:I:356:ALA:O	1:I:357:ARG:HB2	2.21	0.41
1:F:319:SER:O	1:F:365:VAL:HG22	2.21	0.41
1:G:368:ASP:CB	2:G:413:HOH:O	2.68	0.41
1:B:304:TYR:CZ	1:B:381:GLY:HA3	2.55	0.41
1:L:311:TYR:HB3	1:L:370:SER:HB2	2.02	0.41
1:J:277:ILE:HG23	1:J:278:THR:O	2.20	0.41
1:F:276:ARG:HG2	1:F:276:ARG:H	1.76	0.41
1:A:280:ASN:HA	1:A:281:PRO:HD3	1.90	0.41
1:K:359:LYS:HE3	2:K:414:HOH:O	2.21	0.40
1:H:357:ARG:HG3	1:H:357:ARG:NH1	2.37	0.40
1:H:297:VAL:HG12	1:H:298:ASP:O	2.21	0.40
1:E:335:SER:OG	1:G:342:ASN:HB2	2.21	0.40
1:G:254:GLN:CD	1:G:277:ILE:HD12	2.40	0.40
1:A:266:LEU:HD11	1:A:271:LEU:HD23	2.04	0.40
1:I:357:ARG:CG	1:I:357:ARG:HH11	2.35	0.40
1:F:248:PRO:HG2	1:G:385:LEU:HB3	2.02	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	142/163 (87%)	132 (93%)	9 (6%)	1 (1%)	30	34
1	B	142/163 (87%)	132 (93%)	10 (7%)	0	100	100
1	D	142/163 (87%)	137 (96%)	5 (4%)	0	100	100
1	E	147/163 (90%)	138 (94%)	6 (4%)	3 (2%)	11	8
1	F	142/163 (87%)	132 (93%)	10 (7%)	0	100	100
1	G	142/163 (87%)	134 (94%)	7 (5%)	1 (1%)	30	34
1	H	140/163 (86%)	133 (95%)	7 (5%)	0	100	100
1	I	141/163 (86%)	136 (96%)	5 (4%)	0	100	100
1	J	141/163 (86%)	133 (94%)	8 (6%)	0	100	100
1	K	143/163 (88%)	137 (96%)	6 (4%)	0	100	100
1	L	143/163 (88%)	132 (92%)	10 (7%)	1 (1%)	30	34
1	M	142/163 (87%)	137 (96%)	5 (4%)	0	100	100
All	All	1707/1956 (87%)	1613 (94%)	88 (5%)	6 (0%)	43	52

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	257	GLY
1	E	262	VAL
1	E	315	THR
1	G	257	GLY
1	A	277	ILE
1	L	277	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	123/136 (90%)	121 (98%)	2 (2%)	75	88
1	B	123/136 (90%)	118 (96%)	5 (4%)	41	55
1	D	123/136 (90%)	118 (96%)	5 (4%)	41	55
1	E	128/136 (94%)	126 (98%)	2 (2%)	75	88

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	124/136 (91%)	123 (99%)	1 (1%)	89	96
1	G	123/136 (90%)	120 (98%)	3 (2%)	61	79
1	H	122/136 (90%)	118 (97%)	4 (3%)	50	66
1	I	124/136 (91%)	123 (99%)	1 (1%)	89	96
1	J	122/136 (90%)	119 (98%)	3 (2%)	60	77
1	K	125/136 (92%)	119 (95%)	6 (5%)	35	46
1	L	124/136 (91%)	121 (98%)	3 (2%)	61	79
1	M	124/136 (91%)	119 (96%)	5 (4%)	42	56
All	All	1485/1632 (91%)	1445 (97%)	40 (3%)	57	74

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	289	ARG
1	A	314	PHE
1	B	275	SER
1	B	276	ARG
1	B	277	ILE
1	B	334	ARG
1	B	351	VAL
1	D	289	ARG
1	D	313	ASN
1	D	340	LYS
1	D	351	VAL
1	D	357	ARG
1	E	289	ARG
1	E	335	SER
1	F	289	ARG
1	G	334	ARG
1	G	351	VAL
1	G	374	SER
1	H	277	ILE
1	H	338	THR
1	H	341	THR
1	H	351	VAL
1	I	276	ARG
1	J	277	ILE
1	J	314	PHE
1	J	317	PHE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	K	277	ILE
1	K	289	ARG
1	K	315	THR
1	K	316	ASP
1	K	340	LYS
1	K	374	SER
1	L	246	ASN
1	L	289	ARG
1	L	351	VAL
1	M	258	SER
1	M	267	SER
1	M	342	ASN
1	M	357	ARG
1	M	374	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	254	GLN
1	B	342	ASN
1	D	313	ASN
1	F	366	HIS
1	F	376	HIS
1	G	254	GLN
1	H	376	HIS
1	I	254	GLN
1	J	342	ASN
1	K	254	GLN
1	L	342	ASN
1	M	254	GLN
1	M	342	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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	144/163 (88%)	0.87	18 (12%) 5 7	2, 5, 15, 21	0
1	B	144/163 (88%)	1.30	26 (18%) 2 3	2, 5, 14, 19	0
1	D	144/163 (88%)	2.48	86 (59%) 0 0	2, 5, 12, 16	0
1	E	149/163 (91%)	5.00	125 (83%) 0 0	2, 5, 16, 27	0
1	F	144/163 (88%)	0.98	13 (9%) 10 16	2, 5, 13, 24	0
1	G	144/163 (88%)	0.94	17 (11%) 5 8	2, 5, 15, 23	0
1	H	142/163 (87%)	9.67	142 (100%) 0 0	2, 5, 13, 18	0
1	I	143/163 (87%)	1.50	39 (27%) 1 1	2, 5, 14, 20	0
1	J	143/163 (87%)	1.47	40 (27%) 1 1	2, 5, 11, 16	0
1	K	145/163 (88%)	6.13	139 (95%) 0 0	2, 5, 14, 24	0
1	L	145/163 (88%)	1.15	28 (19%) 2 3	2, 5, 14, 22	0
1	M	144/163 (88%)	1.25	24 (16%) 2 4	2, 5, 14, 21	0
All	All	1731/1956 (88%)	2.73	697 (40%) 1 1	2, 5, 14, 27	0

All (697) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	380	PHE	18.5
1	H	383	ILE	18.0
1	H	333	THR	17.3
1	H	303	ILE	17.2
1	H	304	TYR	17.1
1	H	362	VAL	17.0
1	H	307	VAL	16.8
1	H	332	CYS	16.8
1	H	360	ILE	16.3
1	H	382	ALA	15.8
1	H	251	VAL	15.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	H	250	VAL	15.5
1	H	351	VAL	15.5
1	K	380	PHE	15.0
1	H	348	THR	15.0
1	H	350	GLY	14.6
1	H	322	VAL	14.6
1	H	301	TYR	14.5
1	H	309	VAL	14.5
1	H	302	PHE	14.4
1	H	349	ALA	14.4
1	H	320	TYR	13.9
1	K	383	ILE	13.8
1	H	286	LEU	13.6
1	H	346	CYS	13.6
1	H	364	MET	13.5
1	H	274	TRP	13.4
1	H	381	GLY	13.4
1	H	296	LEU	13.3
1	H	295	VAL	13.3
1	H	361	ALA	13.2
1	K	382	ALA	13.2
1	H	347	TYR	13.2
1	H	379	PHE	13.1
1	H	330	LEU	13.0
1	H	266	LEU	12.8
1	H	367	ALA	12.7
1	H	371	ILE	12.6
1	H	271	LEU	12.5
1	H	336	ILE	12.4
1	K	301	TYR	12.4
1	H	388	ALA	12.4
1	H	345	THR	12.4
1	H	369	ILE	12.3
1	H	279	MET	12.2
1	H	323	VAL	12.1
1	H	249	ALA	12.0
1	F	390	ALA	11.9
1	H	317	PHE	11.5
1	K	351	VAL	11.5
1	H	343	TYR	11.4
1	H	278	THR	11.3
1	E	380	PHE	11.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	H	352	CYS	11.2
1	H	293	LEU	11.2
1	H	329	PHE	11.2
1	K	360	ILE	11.2
1	H	318	ALA	11.1
1	K	350	GLY	11.1
1	K	271	LEU	11.1
1	K	381	GLY	11.1
1	B	390	ALA	10.9
1	H	331	GLN	10.9
1	K	362	VAL	10.7
1	H	252	HIS	10.6
1	H	385	LEU	10.6
1	H	305	SER	10.5
1	K	251	VAL	10.5
1	K	293	LEU	10.5
1	E	274	TRP	10.5
1	H	297	VAL	10.5
1	K	295	VAL	10.3
1	H	253	LEU	10.3
1	H	378	THR	10.3
1	H	306	GLN	10.3
1	H	284	PHE	10.2
1	K	304	TYR	10.2
1	K	303	ILE	10.2
1	E	371	ILE	10.1
1	E	283	VAL	10.1
1	H	314	PHE	10.0
1	K	385	LEU	10.0
1	K	352	CYS	10.0
1	K	302	PHE	10.0
1	H	312	ILE	10.0
1	K	332	CYS	10.0
1	K	388	ALA	10.0
1	K	353	LEU	9.9
1	H	335	SER	9.9
1	K	389	PRO	9.9
1	H	334	ARG	9.8
1	H	262	VAL	9.8
1	K	250	VAL	9.7
1	K	364	MET	9.6
1	H	310	TYR	9.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	H	281	PRO	9.5
1	E	309	VAL	9.5
1	E	383	ILE	9.4
1	E	351	VAL	9.3
1	H	376	HIS	9.3
1	E	373	MET	9.2
1	H	341	THR	9.2
1	H	248	PRO	9.2
1	H	373	MET	9.2
1	H	353	LEU	9.2
1	K	386	GLY	9.2
1	H	294	GLU	9.2
1	E	248	PRO	9.2
1	H	247	GLN	9.2
1	K	361	ALA	9.1
1	E	322	VAL	9.0
1	H	354	LEU	9.0
1	K	371	ILE	9.0
1	H	270	VAL	9.0
1	E	329	PHE	9.0
1	K	348	THR	9.0
1	K	323	VAL	8.9
1	K	349	ALA	8.9
1	E	390	ALA	8.9
1	K	379	PHE	8.9
1	H	283	VAL	8.9
1	K	390	ALA	8.8
1	E	251	VAL	8.8
1	K	369	ILE	8.8
1	E	330	LEU	8.8
1	H	338	THR	8.7
1	H	258	SER	8.7
1	H	273	ASP	8.7
1	H	384	ARG	8.7
1	E	379	PHE	8.6
1	K	300	THR	8.6
1	K	296	LEU	8.6
1	E	307	VAL	8.6
1	K	307	VAL	8.6
1	H	280	ASN	8.6
1	H	267	SER	8.5
1	H	344	ASN	8.5

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	K	322	VAL	8.5
1	E	377	THR	8.4
1	H	260	ILE	8.4
1	E	352	CYS	8.3
1	K	333	THR	8.3
1	H	368	ASP	8.3
1	H	377	THR	8.2
1	E	253	LEU	8.2
1	H	261	GLN	8.1
1	E	303	ILE	8.1
1	K	270	VAL	8.1
1	K	284	PHE	8.1
1	E	382	ALA	8.1
1	E	284	PHE	8.1
1	K	249	ALA	8.1
1	E	249	ALA	8.0
1	K	253	LEU	8.0
1	H	315	THR	8.0
1	E	332	CYS	7.9
1	K	320	TYR	7.8
1	K	384	ARG	7.8
1	H	272	ASN	7.8
1	H	321	GLU	7.8
1	K	317	PHE	7.8
1	H	291	GLY	7.8
1	E	385	LEU	7.7
1	E	374	SER	7.6
1	E	293	LEU	7.6
1	K	330	LEU	7.6
1	E	378	THR	7.6
1	K	252	HIS	7.6
1	H	311	TYR	7.5
1	H	277	ILE	7.5
1	K	274	TRP	7.5
1	E	346	CYS	7.5
1	E	333	THR	7.5
1	K	335	SER	7.5
1	E	282	LYS	7.5
1	E	362	VAL	7.4
1	H	319	SER	7.4
1	E	345	THR	7.4
1	K	354	LEU	7.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	H	370	SER	7.4
1	K	262	VAL	7.3
1	K	346	CYS	7.3
1	H	259	ALA	7.3
1	E	250	VAL	7.2
1	H	300	THR	7.2
1	H	357	ARG	7.2
1	E	302	PHE	7.2
1	H	359	LYS	7.2
1	E	259	ALA	7.1
1	M	258	SER	7.1
1	K	294	GLU	7.1
1	H	268	GLY	7.1
1	A	390	ALA	7.0
1	K	318	ALA	7.0
1	H	324	VAL	7.0
1	K	297	VAL	7.0
1	E	299	GLY	7.0
1	E	353	LEU	7.0
1	E	360	ILE	7.0
1	H	386	GLY	6.9
1	D	311	TYR	6.9
1	K	347	TYR	6.9
1	E	271	LEU	6.9
1	H	328	PRO	6.9
1	E	320	TYR	6.9
1	H	337	GLU	6.8
1	E	372	ASN	6.8
1	H	288	PRO	6.8
1	H	282	LYS	6.7
1	D	389	PRO	6.7
1	K	324	VAL	6.7
1	H	308	GLU	6.7
1	H	313	ASN	6.7
1	K	248	PRO	6.7
1	H	372	ASN	6.7
1	I	314	PHE	6.7
1	E	376	HIS	6.6
1	E	296	LEU	6.6
1	K	286	LEU	6.6
1	H	292	GLU	6.6
1	H	365	VAL	6.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	E	297	VAL	6.6
1	D	390	ALA	6.6
1	K	305	SER	6.6
1	E	300	THR	6.6
1	E	295	VAL	6.6
1	E	304	TYR	6.6
1	K	331	GLN	6.5
1	H	287	HIS	6.5
1	E	311	TYR	6.5
1	K	373	MET	6.4
1	K	329	PHE	6.4
1	H	339	GLY	6.4
1	H	255	GLY	6.4
1	E	310	TYR	6.4
1	E	334	ARG	6.4
1	H	363	LYS	6.3
1	E	305	SER	6.3
1	K	359	LYS	6.3
1	D	258	SER	6.3
1	H	276	ARG	6.3
1	H	257	GLY	6.2
1	E	354	LEU	6.2
1	H	269	GLY	6.2
1	M	390	ALA	6.2
1	E	252	HIS	6.1
1	K	309	VAL	6.1
1	E	317	PHE	6.1
1	E	347	TYR	6.1
1	E	279	MET	6.0
1	D	315	THR	6.0
1	K	334	ARG	6.0
1	H	366	HIS	5.9
1	E	260	ILE	5.9
1	D	314	PHE	5.9
1	K	269	GLY	5.9
1	H	254	GLN	5.8
1	H	275	SER	5.8
1	E	384	ARG	5.8
1	D	267	SER	5.8
1	K	345	THR	5.8
1	D	338	THR	5.8
1	H	265	ASP	5.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	E	247	GLN	5.7
1	H	298	ASP	5.7
1	D	312	ILE	5.7
1	H	356	ALA	5.7
1	E	254	GLN	5.7
1	H	316	ASP	5.7
1	K	306	GLN	5.6
1	J	259	ALA	5.6
1	K	263	LYS	5.6
1	K	266	LEU	5.6
1	K	367	ALA	5.5
1	E	381	GLY	5.5
1	K	291	GLY	5.5
1	K	312	ILE	5.5
1	H	289	ARG	5.5
1	H	290	SER	5.5
1	E	280	ASN	5.5
1	E	386	GLY	5.4
1	K	378	THR	5.4
1	E	286	LEU	5.4
1	E	348	THR	5.4
1	B	314	PHE	5.3
1	E	361	ALA	5.3
1	E	370	SER	5.3
1	E	323	VAL	5.3
1	K	298	ASP	5.3
1	D	341	THR	5.3
1	K	283	VAL	5.3
1	K	358	GLN	5.3
1	E	281	PRO	5.3
1	I	389	PRO	5.2
1	H	256	GLN	5.2
1	K	357	ARG	5.2
1	D	264	ASN	5.2
1	E	318	ALA	5.2
1	H	355	LYS	5.2
1	E	314	PHE	5.2
1	K	387	GLU	5.1
1	J	258	SER	5.1
1	G	390	ALA	5.1
1	L	390	ALA	5.1
1	K	292	GLU	5.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	E	306	GLN	5.0
1	E	344	ASN	5.0
1	K	319	SER	5.0
1	H	387	GLU	5.0
1	K	281	PRO	5.0
1	B	278	THR	4.9
1	E	369	ILE	4.9
1	K	363	LYS	4.9
1	H	374	SER	4.9
1	B	267	SER	4.9
1	H	342	ASN	4.8
1	H	358	GLN	4.8
1	K	356	ALA	4.8
1	K	355	LYS	4.8
1	K	308	GLU	4.8
1	E	301	TYR	4.8
1	E	255	GLY	4.8
1	H	285	LYS	4.7
1	K	279	MET	4.7
1	D	277	ILE	4.7
1	K	260	ILE	4.6
1	K	365	VAL	4.6
1	K	290	SER	4.6
1	D	289	ARG	4.6
1	A	339	GLY	4.6
1	D	259	ALA	4.6
1	D	310	TYR	4.6
1	K	299	GLY	4.6
1	K	377	THR	4.6
1	F	314	PHE	4.6
1	K	278	THR	4.6
1	K	336	ILE	4.5
1	H	327	LYS	4.5
1	K	344	ASN	4.5
1	B	281	PRO	4.5
1	D	337	GLU	4.4
1	K	247	GLN	4.4
1	E	278	THR	4.4
1	E	273	ASP	4.4
1	E	349	ALA	4.4
1	J	263	LYS	4.4
1	D	257	GLY	4.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	277	ILE	4.3
1	E	277	ILE	4.3
1	K	372	ASN	4.3
1	H	375	LYS	4.3
1	A	314	PHE	4.3
1	D	340	LYS	4.3
1	H	264	ASN	4.3
1	E	336	ILE	4.3
1	H	263	LYS	4.2
1	K	314	PHE	4.2
1	M	314	PHE	4.2
1	I	310	TYR	4.2
1	I	264	ASN	4.2
1	B	258	SER	4.2
1	K	268	GLY	4.2
1	J	390	ALA	4.2
1	D	247	GLN	4.2
1	E	375	LYS	4.2
1	D	388	ALA	4.1
1	K	321	GLU	4.1
1	D	335	SER	4.1
1	B	339	GLY	4.1
1	E	350	GLY	4.1
1	J	264	ASN	4.1
1	E	242	GLY	4.1
1	K	339	GLY	4.1
1	E	388	ALA	4.1
1	K	273	ASP	4.1
1	K	311	TYR	4.1
1	K	280	ASN	4.0
1	D	316	ASP	4.0
1	B	283	VAL	4.0
1	B	357	ARG	4.0
1	B	289	ARG	4.0
1	E	335	SER	4.0
1	E	257	GLY	4.0
1	D	336	ILE	4.0
1	E	343	TYR	4.0
1	K	277	ILE	4.0
1	E	341	THR	3.9
1	L	283	VAL	3.9
1	L	277	ILE	3.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	E	289	ARG	3.9
1	D	387	GLU	3.9
1	B	315	THR	3.9
1	E	324	VAL	3.8
1	E	258	SER	3.8
1	I	338	THR	3.8
1	K	289	ARG	3.8
1	K	340	LYS	3.8
1	I	289	ARG	3.8
1	K	287	HIS	3.8
1	F	360	ILE	3.8
1	A	389	PRO	3.7
1	J	296	LEU	3.7
1	L	389	PRO	3.7
1	K	341	THR	3.7
1	K	343	TYR	3.7
1	E	331	GLN	3.7
1	D	343	TYR	3.7
1	D	263	LYS	3.7
1	E	298	ASP	3.7
1	D	265	ASP	3.7
1	E	342	ASN	3.7
1	E	319	SER	3.6
1	J	341	THR	3.6
1	J	357	ARG	3.6
1	K	272	ASN	3.6
1	J	262	VAL	3.6
1	D	268	GLY	3.6
1	D	385	LEU	3.6
1	K	257	GLY	3.6
1	K	255	GLY	3.6
1	D	248	PRO	3.6
1	K	316	ASP	3.6
1	D	313	ASN	3.5
1	D	342	ASN	3.5
1	E	308	GLU	3.5
1	L	255	GLY	3.5
1	D	288	PRO	3.5
1	E	264	ASN	3.5
1	E	312	ILE	3.5
1	E	276	ARG	3.5
1	E	387	GLU	3.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	386	GLY	3.5
1	K	254	GLN	3.5
1	K	338	THR	3.4
1	K	288	PRO	3.4
1	K	370	SER	3.4
1	J	337	GLU	3.4
1	E	275	SER	3.4
1	J	278	THR	3.4
1	M	293	LEU	3.4
1	L	388	ALA	3.4
1	M	259	ALA	3.4
1	B	262	VAL	3.4
1	G	315	THR	3.4
1	I	247	GLN	3.4
1	E	246	ASN	3.4
1	G	255	GLY	3.4
1	J	338	THR	3.4
1	E	328	PRO	3.3
1	J	261	GLN	3.3
1	H	325	ASP	3.3
1	D	366	HIS	3.3
1	D	369	ILE	3.3
1	E	364	MET	3.3
1	K	267	SER	3.3
1	E	285	LYS	3.3
1	M	257	GLY	3.3
1	D	281	PRO	3.3
1	E	313	ASN	3.3
1	I	316	ASP	3.3
1	J	360	ILE	3.3
1	J	314	PHE	3.3
1	A	341	THR	3.2
1	E	262	VAL	3.2
1	I	336	ILE	3.2
1	D	256	GLN	3.2
1	D	297	VAL	3.2
1	J	369	ILE	3.2
1	D	261	GLN	3.2
1	H	340	LYS	3.2
1	J	267	SER	3.2
1	D	356	ALA	3.2
1	M	311	TYR	3.2

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	J	266	LEU	3.1
1	A	289	ARG	3.1
1	K	374	SER	3.1
1	D	317	PHE	3.1
1	J	317	PHE	3.1
1	L	246	ASN	3.1
1	K	328	PRO	3.1
1	M	284	PHE	3.1
1	D	368	ASP	3.1
1	B	340	LYS	3.1
1	E	315	THR	3.1
1	D	352	CYS	3.1
1	K	282	LYS	3.1
1	K	376	HIS	3.1
1	D	266	LEU	3.1
1	K	285	LYS	3.1
1	D	286	LEU	3.0
1	D	375	LYS	3.0
1	I	370	SER	3.0
1	I	283	VAL	3.0
1	B	313	ASN	3.0
1	E	338	THR	3.0
1	E	261	GLN	3.0
1	B	366	HIS	3.0
1	F	289	ARG	3.0
1	E	316	ASP	3.0
1	D	269	GLY	3.0
1	L	257	GLY	3.0
1	D	276	ARG	3.0
1	A	267	SER	3.0
1	I	267	SER	3.0
1	I	274	TRP	3.0
1	E	272	ASN	3.0
1	J	257	GLY	3.0
1	D	309	VAL	2.9
1	L	289	ARG	2.9
1	D	273	ASP	2.9
1	D	278	THR	2.9
1	I	293	LEU	2.9
1	L	314	PHE	2.9
1	D	299	GLY	2.9
1	L	284	PHE	2.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	H	326	GLU	2.9
1	D	370	SER	2.9
1	D	357	ARG	2.9
1	J	339	GLY	2.9
1	G	316	ASP	2.8
1	M	261	GLN	2.8
1	I	265	ASP	2.8
1	L	293	LEU	2.8
1	K	391	SER	2.8
1	M	360	ILE	2.8
1	A	287	HIS	2.8
1	D	353	LEU	2.8
1	I	360	ILE	2.8
1	D	376	HIS	2.8
1	B	388	ALA	2.8
1	F	247	GLN	2.7
1	H	299	GLY	2.7
1	F	266	LEU	2.7
1	G	271	LEU	2.7
1	A	264	ASN	2.7
1	G	277	ILE	2.7
1	G	313	ASN	2.7
1	D	325	ASP	2.7
1	J	265	ASP	2.7
1	K	327	LYS	2.7
1	J	313	ASN	2.7
1	G	338	THR	2.7
1	F	371	ILE	2.7
1	M	375	LYS	2.7
1	I	256	GLN	2.7
1	D	329	PHE	2.7
1	G	314	PHE	2.7
1	B	264	ASN	2.7
1	D	275	SER	2.7
1	L	375	LYS	2.7
1	L	251	VAL	2.6
1	D	371	ILE	2.6
1	I	369	ILE	2.6
1	K	259	ALA	2.6
1	M	366	HIS	2.6
1	D	282	LYS	2.6
1	J	340	LYS	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	I	253	LEU	2.6
1	I	266	LEU	2.6
1	M	357	ARG	2.6
1	E	337	GLU	2.6
1	F	293	LEU	2.6
1	K	261	GLN	2.6
1	A	375	LYS	2.6
1	D	272	ASN	2.6
1	F	263	LYS	2.6
1	G	288	PRO	2.6
1	I	343	TYR	2.6
1	I	361	ALA	2.6
1	D	298	ASP	2.6
1	I	258	SER	2.6
1	M	263	LYS	2.6
1	E	356	ALA	2.6
1	L	263	LYS	2.6
1	E	339	GLY	2.6
1	G	247	GLN	2.5
1	I	312	ILE	2.5
1	K	264	ASN	2.5
1	I	255	GLY	2.5
1	D	354	LEU	2.5
1	L	362	VAL	2.5
1	A	388	ALA	2.5
1	G	317	PHE	2.5
1	I	357	ARG	2.5
1	K	342	ASN	2.5
1	A	277	ILE	2.5
1	D	318	ALA	2.5
1	K	375	LYS	2.5
1	L	276	ARG	2.5
1	M	260	ILE	2.5
1	I	387	GLU	2.5
1	M	307	VAL	2.5
1	D	358	GLN	2.5
1	D	386	GLY	2.5
1	B	297	VAL	2.5
1	A	357	ARG	2.5
1	E	256	GLN	2.5
1	F	362	VAL	2.5
1	J	293	LEU	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	E	287	HIS	2.5
1	G	298	ASP	2.5
1	J	268	GLY	2.4
1	D	324	VAL	2.4
1	A	313	ASN	2.4
1	A	340	LYS	2.4
1	D	339	GLY	2.4
1	D	270	VAL	2.4
1	L	340	LYS	2.4
1	K	325	ASP	2.4
1	L	271	LEU	2.4
1	L	356	ALA	2.4
1	J	289	ARG	2.4
1	A	290	SER	2.4
1	E	321	GLU	2.4
1	K	258	SER	2.4
1	D	294	GLU	2.4
1	I	309	VAL	2.4
1	I	371	ILE	2.4
1	E	270	VAL	2.3
1	L	262	VAL	2.3
1	D	290	SER	2.3
1	E	243	THR	2.3
1	J	285	LYS	2.3
1	G	276	ARG	2.3
1	D	365	VAL	2.3
1	M	328	PRO	2.3
1	D	326	GLU	2.3
1	G	282	LYS	2.3
1	I	284	PHE	2.3
1	G	258	SER	2.3
1	D	377	THR	2.3
1	I	251	VAL	2.3
1	I	262	VAL	2.3
1	D	283	VAL	2.3
1	D	328	PRO	2.3
1	F	310	TYR	2.3
1	B	247	GLN	2.3
1	D	260	ILE	2.3
1	K	313	ASN	2.3
1	B	282	LYS	2.3
1	D	327	LYS	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	374	SER	2.3
1	I	335	SER	2.3
1	K	256	GLN	2.3
1	E	368	ASP	2.2
1	J	260	ILE	2.2
1	K	337	GLU	2.2
1	I	375	LYS	2.2
1	L	318	ALA	2.2
1	L	378	THR	2.2
1	I	295	VAL	2.2
1	I	287	HIS	2.2
1	D	367	ALA	2.2
1	J	295	VAL	2.2
1	K	265	ASP	2.2
1	J	280	ASN	2.2
1	A	315	THR	2.2
1	D	262	VAL	2.2
1	J	311	TYR	2.2
1	J	284	PHE	2.2
1	J	371	ILE	2.1
1	L	285	LYS	2.1
1	M	338	THR	2.1
1	I	373	MET	2.1
1	B	261	GLN	2.1
1	B	276	ARG	2.1
1	L	282	LYS	2.1
1	J	312	ILE	2.1
1	E	267	SER	2.1
1	L	296	LEU	2.1
1	K	275	SER	2.1
1	J	356	ALA	2.1
1	G	293	LEU	2.1
1	M	296	LEU	2.1
1	F	366	HIS	2.1
1	B	342	ASN	2.1
1	D	280	ASN	2.1
1	M	264	ASN	2.1
1	L	360	ILE	2.1
1	M	315	THR	2.1
1	J	271	LEU	2.1
1	D	274	TRP	2.1
1	E	288	PRO	2.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	I	297	VAL	2.0
1	B	368	ASP	2.0
1	M	343	TYR	2.0
1	J	387	GLU	2.0
1	L	264	ASN	2.0
1	J	288	PRO	2.0
1	M	389	PRO	2.0
1	F	307	VAL	2.0
1	D	301	TYR	2.0
1	I	263	LYS	2.0
1	D	287	HIS	2.0
1	J	325	ASP	2.0
1	B	338	THR	2.0
1	M	274	TRP	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.