



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:24 PM GMT

PDB ID : 4XMN  
Title : Structure of the yeast coat nucleoporin complex, space group P212121  
Authors : Stuwe, T.; Correia, A.R.; Lin, D.H.; Paduch, M.; Lu, V.T.; Kossiakoff, A.A.;  
Hoelz, A.  
Deposited on : 2015-01-14  
Resolution : 7.60 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.

---

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

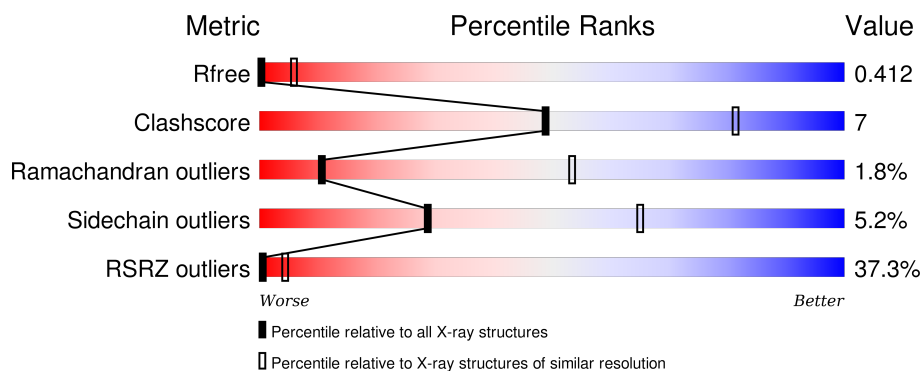
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 7.60 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	1015 (11.50-3.66)
Clashscore	102246	1064 (11.50-3.70)
Ramachandran outliers	100387	1036 (11.50-3.66)
Sidechain outliers	100360	1006 (11.50-3.66)
RSRZ outliers	91569	1014 (11.50-3.66)

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	297	<div> <div>49%</div> <div>66%</div> <div>24%</div> <div>8%</div> </div>
2	B	652	<div> <div>26%</div> <div>58%</div> <div>17%</div> <div>23%</div> </div>
3	F	454	<div> <div>28%</div> <div>70%</div> <div>19%</div> <div>8%</div> </div>
4	E	1045	<div> <div>27%</div> <div>73%</div> <div>12%</div> <div>14%</div> </div>
5	D	685	<div> <div>9%</div> <div>21%</div> <div>79%</div> </div>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	L	217	<div><div></div><div>41%</div><div></div><div>81%</div><div></div><div>13%</div><div></div><div></div></div>
7	H	267	<div><div></div><div>41%</div><div></div><div>68%</div><div></div><div>10%</div><div></div><div>19%</div></div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 19816 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 Protein transport protein SEC13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	0	0
			2160	1379	369	409	3			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	initiating methionine	UNP Q04491

- Molecule 2 is a protein called Nucleoporin NUP145.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	503	Total	C	N	O	S	Se	0	0	0
			3765	2393	640	722	6	4			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	61	MSE	-	initiating methionine	UNP P49687
B	62	GLY	-	expression tag	UNP P49687
B	63	SER	-	expression tag	UNP P49687
B	64	SER	-	expression tag	UNP P49687
B	65	HIS	-	expression tag	UNP P49687
B	66	HIS	-	expression tag	UNP P49687
B	67	HIS	-	expression tag	UNP P49687
B	68	HIS	-	expression tag	UNP P49687
B	69	HIS	-	expression tag	UNP P49687
B	70	HIS	-	expression tag	UNP P49687
B	71	SER	-	expression tag	UNP P49687
B	72	ASP	-	expression tag	UNP P49687
B	73	GLN	-	expression tag	UNP P49687
B	74	PRO	-	expression tag	UNP P49687

- Molecule 3 is a protein called Nucleoporin NUP84.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	F	419	Total	C	N	O	S	Se	0	0	0
			3404	2178	557	657	5	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-2	GLY	-	expression tag	UNP P52891
F	-1	PRO	-	expression tag	UNP P52891
F	0	HIS	-	expression tag	UNP P52891
F	1	MSE	-	expression tag	UNP P52891

- Molecule 4 is a protein called Nucleoporin NUP120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	896	Total	C	N	O	S	0	0	0
			6622	4232	1099	1275	16			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-7	MET	-	initiating methionine	UNP P35729
E	-6	HIS	-	expression tag	UNP P35729
E	-5	HIS	-	expression tag	UNP P35729
E	-4	HIS	-	expression tag	UNP P35729
E	-3	HIS	-	expression tag	UNP P35729
E	-2	HIS	-	expression tag	UNP P35729
E	-1	HIS	-	expression tag	UNP P35729
E	0	SER	-	expression tag	UNP P35729

- Molecule 5 is a protein called Nucleoporin NUP85.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	D	143	Total	C	N	O	0	0	0
			713	427	143	143			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	60	MSE	-	initiating methionine	UNP P46673
D	61	GLY	-	expression tag	UNP P46673
D	62	SER	-	expression tag	UNP P46673

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
D	63	SER	-	expression tag	UNP P46673
D	64	HIS	-	expression tag	UNP P46673
D	65	HIS	-	expression tag	UNP P46673
D	66	HIS	-	expression tag	UNP P46673
D	67	HIS	-	expression tag	UNP P46673
D	68	HIS	-	expression tag	UNP P46673
D	69	HIS	-	expression tag	UNP P46673
D	70	SER	-	expression tag	UNP P46673
D	71	ASP	-	expression tag	UNP P46673
D	72	GLN	-	expression tag	UNP P46673
D	744	MSE	-	expression tag	UNP P46673

- Molecule 6 is a protein called Antibody 87 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	L	209	Total	C	N	O	S	0	0	0
			1592	991	269	326	6			

- Molecule 7 is a protein called Antibody 87 heavy chain.

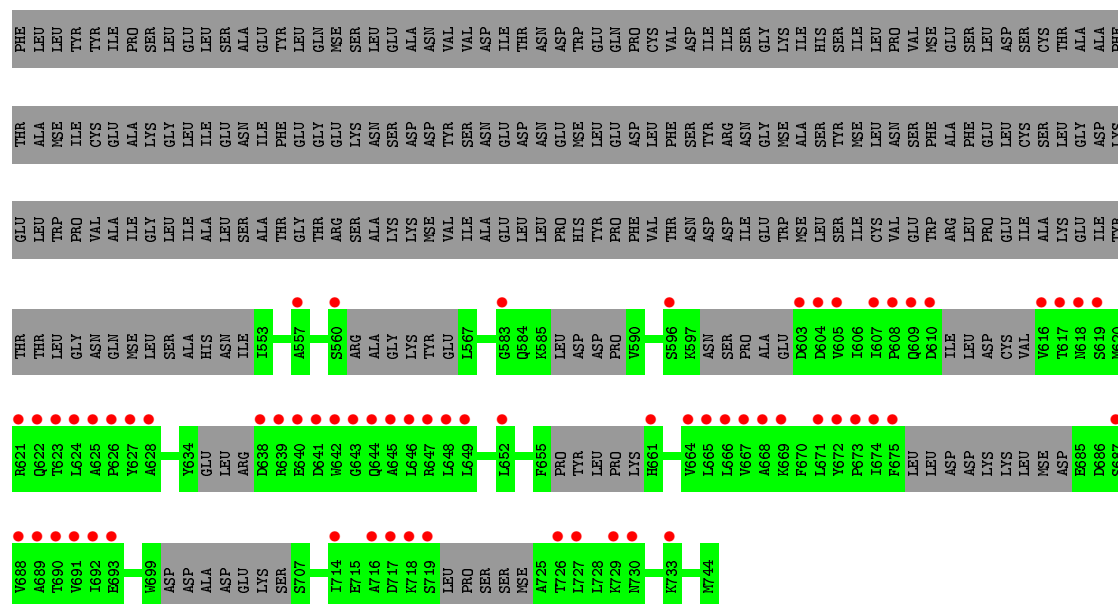
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	215	Total	C	N	O	S	0	0	0
			1560	977	265	312	6			



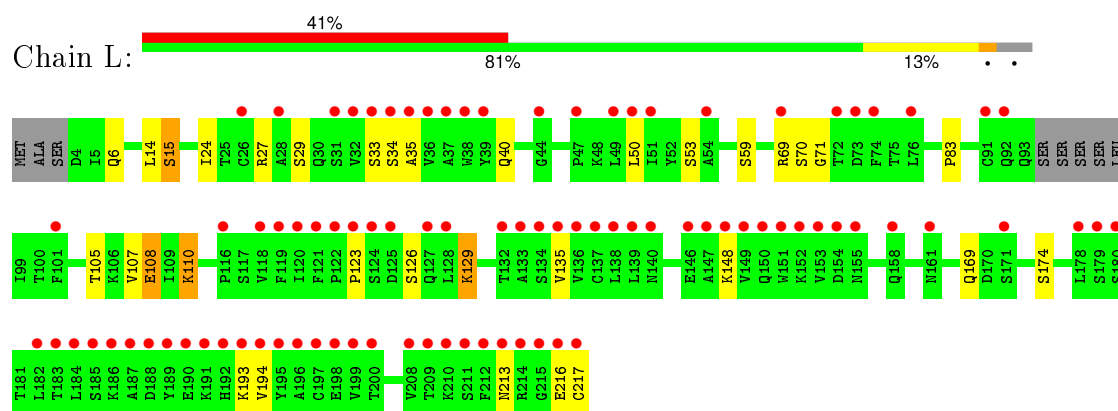




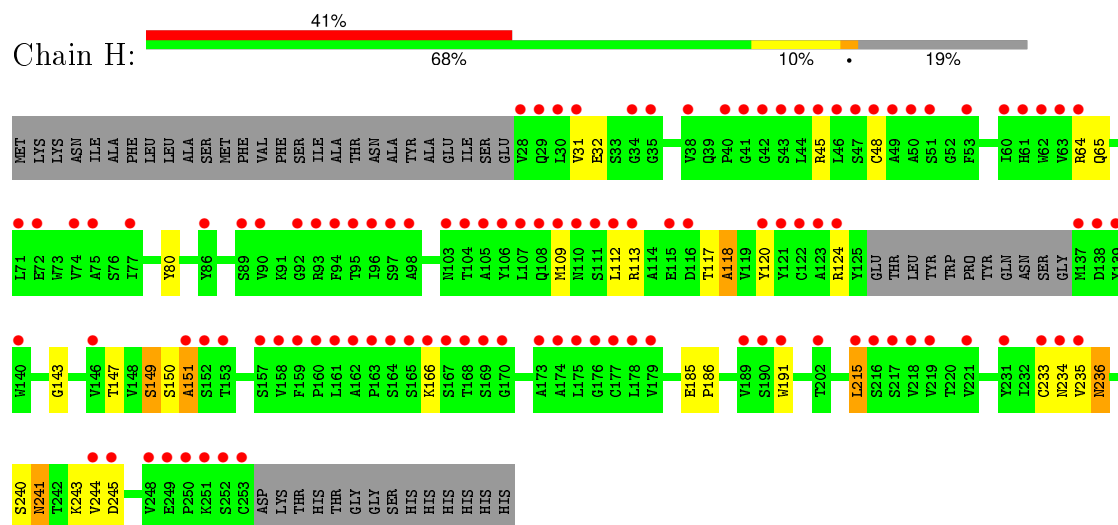
[illegible]



- Molecule 6: Antibody 87 light chain



- Molecule 7: Antibody 87 heavy chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	117.13Å 179.95Å 441.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.61 – 7.60 49.61 – 7.59	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.61-7.60) 99.6 (49.61-7.59)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.94 (at 7.37Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1809)	Depositor
R, $R_{free}$	0.318 , 0.347 0.396 , 0.412	Depositor DCC
$R_{free}$ test set	1205 reflections (11.13%)	DCC
Wilson B-factor (Å <sup>2</sup> )	597.7	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 705.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 12029 reflections	Xtriage
$F_o, F_c$ correlation	0.69	EDS
Total number of atoms	19816	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	536.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.34% 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	0.28	0/2220	0.58	0/3028
2	B	0.29	0/3813	0.58	0/5147
3	F	0.30	0/3465	0.59	0/4693
4	E	0.27	0/6730	0.49	1/9158 (0.0%)
5	D	0.18	0/700	0.34	0/958
6	L	0.31	0/1623	0.63	0/2199
7	H	0.31	0/1594	0.71	3/2172 (0.1%)
All	All	0.29	0/20145	0.56	4/27355 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	3
All	All	0	4

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	H	215	LEU	CA-CB-CG	5.90	128.88	115.30
4	E	818	PRO	N-CA-CB	5.82	110.29	103.30
7	H	185	GLU	C-N-CD	-5.39	108.75	120.60
7	H	245	ASP	N-CA-C	-5.18	97.00	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	41	GLU	Mainchain
2	B	368	GLU	Peptide
2	B	371	PHE	Peptide
2	B	392	TYR	Peptide

## 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	2160	0	2096	50	0
2	B	3765	0	3484	80	0
3	F	3404	0	3378	61	1
4	E	6622	0	5907	69	1
5	D	713	0	308	0	0
6	L	1592	0	1546	23	0
7	H	1560	0	1512	17	0
All	All	19816	0	18231	274	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 (274) 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)
4:E:451:ARG:HH12	6:L:69:ARG:HD3	1.27	0.97
4:E:325:ALA:HA	6:L:59:SER:HB2	1.50	0.94
3:F:314:ILE:HG22	3:F:315:LEU:HG	1.61	0.82
1:A:18:ASP:OD2	2:B:548:TYR:OH	1.97	0.80
4:E:293:LEU:HD13	4:E:297:LEU:HD12	1.63	0.79
4:E:113:VAL:HG23	4:E:114:GLU:H	1.51	0.76
4:E:404:VAL:HG11	4:E:438:GLU:HA	1.70	0.74
7:H:235:VAL:HB	7:H:244:VAL:HB	1.69	0.73
3:F:70:LEU:HD22	3:F:343:ILE:HD11	1.72	0.72
4:E:451:ARG:NH1	6:L:69:ARG:HD3	2.06	0.69
6:L:126:SER:O	6:L:129:LYS:HB3	1.92	0.69
3:F:62:VAL:HG12	3:F:66:LYS:HE3	1.75	0.69
6:L:193:LYS:HE3	6:L:213:ASN:HB3	1.74	0.68

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:297:LEU:HD23	2:B:300:LEU:HD12	1.75	0.68
6:L:15:SER:HB3	6:L:110:LYS:HE3	1.75	0.68
2:B:178:THR:HG21	2:B:485:ALA:HB2	1.75	0.67
2:B:426:TYR:O	2:B:464:ARG:NH2	2.28	0.67
2:B:416:ASP:HA	2:B:443:THR:HG21	1.75	0.67
4:E:55:GLU:HB2	4:E:74:SER:HA	1.77	0.66
2:B:152:ALA:HB1	2:B:160:LEU:HD11	1.78	0.65
4:E:678:VAL:HG11	4:E:720:PHE:HA	1.79	0.65
1:A:12:ILE:HD12	2:B:170:GLY:HA3	1.79	0.65
2:B:300:LEU:HD23	2:B:388:LEU:HD21	1.78	0.65
2:B:292:ILE:H	2:B:292:ILE:HD12	1.61	0.65
3:F:8:GLN:C	3:F:10:GLU:H	2.00	0.64
4:E:335:VAL:HG13	4:E:352:ILE:HB	1.78	0.64
4:E:448:THR:OG1	6:L:71:GLY:N	2.26	0.64
3:F:71:GLU:OE1	3:F:75:TRP:NE1	2.29	0.64
7:H:149:SER:OG	7:H:150:SER:N	2.31	0.64
4:E:829:SER:HA	4:E:841:ALA:HB1	1.80	0.63
6:L:6:GLN:HB2	6:L:29:SER:HB3	1.81	0.62
2:B:367:PHE:O	2:B:369:GLY:N	2.30	0.62
2:B:209:PRO:HB3	2:B:532:LYS:HB2	1.82	0.62
4:E:609:GLY:O	4:E:613:ILE:HG22	1.99	0.61
6:L:14:LEU:HG	6:L:107:VAL:HG22	1.83	0.61
4:E:511:ARG:HD2	7:H:80:TYR:CE2	2.35	0.61
4:E:295:ASN:ND2	4:E:329:TRP:O	2.33	0.61
1:A:64:PRO:HB3	2:B:548:TYR:HB2	1.82	0.61
1:A:180:ASN:HA	1:A:207:VAL:HG23	1.83	0.61
2:B:184:PHE:HE2	2:B:225:MSE:HE3	1.64	0.61
3:F:410:SER:HA	3:F:436:LEU:HD11	1.82	0.60
2:B:483:GLU:CD	2:B:514:ARG:HH22	2.04	0.60
6:L:24:ILE:HG12	6:L:105:THR:HG21	1.82	0.60
1:A:227:GLN:HA	1:A:256:VAL:HG13	1.83	0.60
2:B:525:ASP:O	2:B:528:LEU:HB2	2.03	0.59
3:F:433:ALA:HB1	3:F:439:SER:OG	2.03	0.59
3:F:343:ILE:HD13	3:F:344:ARG:N	2.17	0.59
4:E:329:TRP:HB3	4:E:355:TRP:HB3	1.85	0.59
2:B:152:ALA:HB1	2:B:160:LEU:CD1	2.33	0.58
2:B:199:THR:HB	2:B:213:GLU:HB2	1.86	0.58
6:L:40:GLN:HB2	6:L:50:LEU:HD11	1.86	0.58
2:B:483:GLU:OE2	2:B:514:ARG:NH2	2.29	0.58
2:B:180:LEU:HD21	2:B:185:LEU:HD13	1.86	0.58
6:L:216:GLU:O	6:L:217:CYS:HB2	2.04	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:360:LYS:HG3	2:B:366:PRO:HA	1.85	0.57
4:E:101:SER:HA	4:E:123:LEU:HA	1.86	0.57
4:E:245:ILE:HB	4:E:255:GLN:HB2	1.87	0.57
6:L:15:SER:OG	6:L:108:GLU:OE1	2.22	0.57
2:B:389:THR:O	2:B:393:GLY:HA3	2.05	0.57
4:E:448:THR:HG21	6:L:70:SER:HA	1.85	0.56
4:E:342:LEU:HD13	4:E:379:ILE:HD12	1.85	0.56
2:B:433:GLU:OE1	2:B:467:SER:OG	2.20	0.56
2:B:359:TYR:CE2	3:F:210:MSE:HE1	2.40	0.56
4:E:63:SER:OG	4:E:112:GLU:OE1	2.23	0.56
1:A:49:LEU:HB3	1:A:82:TRP:CZ3	2.40	0.56
1:A:236:GLN:HB2	1:A:243:TRP:CE3	2.41	0.56
2:B:525:ASP:HA	2:B:528:LEU:HD12	1.88	0.55
4:E:200:ASN:O	4:E:200:ASN:ND2	2.39	0.55
3:F:34:ASP:HB3	3:F:35:PRO:HD3	1.88	0.55
1:A:217:LEU:HD22	1:A:218:LEU:H	1.71	0.55
3:F:237:ILE:HD11	3:F:240:HIS:HA	1.87	0.55
4:E:325:ALA:HA	6:L:59:SER:CB	2.32	0.55
7:H:64:ARG:HB3	7:H:120:TYR:CD2	2.42	0.55
4:E:58:ASN:HB3	4:E:70:TYR:CZ	2.42	0.54
2:B:519:LEU:O	2:B:529:ASN:ND2	2.40	0.54
2:B:305:VAL:HG13	3:F:314:ILE:HD11	1.89	0.54
1:A:205:ASP:HB3	1:A:227:GLN:HB3	1.88	0.54
3:F:341:HIS:CE1	3:F:343:ILE:HD12	2.42	0.54
2:B:492:LEU:HD12	2:B:508:ILE:HD13	1.89	0.54
4:E:511:ARG:HD2	7:H:80:TYR:HE2	1.73	0.54
1:A:117:LEU:HB2	1:A:153:TRP:NE1	2.22	0.54
2:B:180:LEU:HD11	2:B:478:PHE:HE1	1.71	0.54
4:E:125:ASP:OD1	4:E:127:SER:OG	2.19	0.54
2:B:359:TYR:HA	2:B:362:LEU:HD12	1.90	0.54
2:B:156:THR:HG22	2:B:514:ARG:HD2	1.90	0.54
3:F:13:THR:O	3:F:17:ASP:N	2.31	0.53
7:H:65:GLN:O	7:H:118:ALA:HB1	2.08	0.53
2:B:365:SER:HB3	2:B:368:GLU:HB2	1.90	0.53
4:E:119:VAL:HB	4:E:131:LEU:HB2	1.89	0.53
2:B:524:ASN:O	2:B:528:LEU:HG	2.09	0.53
1:A:178:ALA:HB1	1:A:206:TRP:CE2	2.43	0.53
7:H:31:VAL:O	7:H:48:CYS:HA	2.09	0.52
2:B:182:ARG:HD2	2:B:449:GLN:OE1	2.10	0.52
1:A:116:LEU:O	1:A:127:VAL:HA	2.10	0.52
4:E:508:LYS:O	4:E:512:THR:HG23	2.09	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:435:LEU:O	2:B:439:VAL:HG23	2.09	0.52
1:A:275:ASP:OD1	1:A:275:ASP:N	2.42	0.52
2:B:305:VAL:HG21	3:F:311:ASP:HB3	1.92	0.52
3:F:379:ILE:HG13	3:F:385:LEU:HD23	1.90	0.52
1:A:212:TRP:HA	1:A:222:LEU:HD23	1.92	0.52
1:A:154:ALA:HB2	1:A:212:TRP:CE3	2.45	0.51
1:A:117:LEU:HB2	1:A:153:TRP:HE1	1.75	0.51
2:B:159:MSE:SE	2:B:175:ARG:HH21	2.43	0.51
3:F:431:ILE:HD12	3:F:431:ILE:H	1.74	0.51
1:A:95:HIS:CE1	1:A:97:VAL:HG22	2.45	0.51
1:A:200:LEU:HD11	1:A:243:TRP:CD1	2.45	0.51
3:F:294:LEU:O	3:F:298:ILE:HD12	2.10	0.51
2:B:178:THR:HG22	2:B:180:LEU:H	1.75	0.51
1:A:261:SER:CB	2:B:153:LYS:HA	2.40	0.51
3:F:280:SER:HB2	3:F:284:SER:HB3	1.92	0.51
1:A:138:PRO:HB2	1:A:140:ILE:HD11	1.93	0.51
2:B:492:LEU:HD11	2:B:508:ILE:HG23	1.92	0.50
7:H:109:MET:HB3	7:H:112:LEU:HD21	1.92	0.50
4:E:400:LYS:HE3	4:E:736:ASN:HA	1.93	0.50
7:H:117:THR:O	7:H:118:ALA:HB2	2.11	0.50
1:A:62:ALA:HB2	1:A:107:TRP:CE2	2.46	0.50
2:B:281:ILE:HB	2:B:301:LEU:HD21	1.92	0.50
4:E:245:ILE:HG21	4:E:311:LEU:HD23	1.94	0.50
3:F:245:ARG:HG2	3:F:315:LEU:HB2	1.94	0.49
4:E:537:THR:HA	4:E:746:CYS:CB	2.42	0.49
4:E:102:MET:HB3	4:E:107:THR:HG21	1.94	0.49
4:E:448:THR:HG21	6:L:69:ARG:O	2.13	0.49
2:B:359:TYR:HE2	3:F:210:MSE:HE1	1.78	0.49
2:B:523:THR:HA	2:B:526:HIS:HB2	1.94	0.49
2:B:392:TYR:O	2:B:394:GLN:N	2.39	0.49
2:B:186:PHE:CD2	2:B:487:LEU:HD11	2.48	0.49
2:B:374:LYS:O	2:B:377:GLU:HB2	2.13	0.49
7:H:32:GLU:OE1	7:H:143:GLY:N	2.36	0.49
3:F:350:VAL:HG22	3:F:355:LEU:HD22	1.95	0.49
4:E:386:LEU:HD23	4:E:621:GLN:HA	1.95	0.49
3:F:106:GLU:O	3:F:110:MSE:HG2	2.13	0.49
4:E:522:ASN:O	4:E:526:ARG:HG3	2.12	0.49
2:B:270:THR:OG1	2:B:391:CYS:SG	2.71	0.49
1:A:181:LEU:HD23	1:A:201:GLU:HG2	1.95	0.48
4:E:70:TYR:HA	4:E:80:THR:O	2.12	0.48
3:F:293:ILE:HD11	3:F:327:VAL:HG21	1.95	0.48

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:8:GLN:O	3:F:10:GLU:N	2.45	0.48
4:E:570:LEU:O	4:E:574:LEU:HB2	2.14	0.48
1:A:259:ARG:NH1	2:B:151:PHE:HB2	2.29	0.48
1:A:52:HIS:CE1	1:A:80:LEU:HD12	2.48	0.48
4:E:500:GLU:HB2	4:E:507:PHE:CZ	2.49	0.47
1:A:272:SER:OG	2:B:152:ALA:HB3	2.14	0.47
4:E:508:LYS:HG2	4:E:511:ARG:NH2	2.29	0.47
2:B:186:PHE:HD2	2:B:487:LEU:HD11	1.79	0.47
2:B:156:THR:HG22	2:B:514:ARG:CD	2.44	0.47
3:F:116:LEU:O	3:F:119:ILE:HB	2.15	0.47
1:A:16:VAL:HG21	1:A:59:VAL:O	2.14	0.47
4:E:531:LYS:HB3	4:E:553:ILE:HG12	1.96	0.47
2:B:393:GLY:O	2:B:394:GLN:HB2	2.13	0.47
1:A:9:ASN:HD22	1:A:9:ASN:HA	1.50	0.47
4:E:288:VAL:HG13	4:E:336:LEU:HD22	1.95	0.47
1:A:217:LEU:HD13	1:A:218:LEU:N	2.30	0.47
3:F:431:ILE:H	3:F:431:ILE:CD1	2.28	0.47
4:E:596:PHE:CZ	4:E:704:SER:HA	2.50	0.47
2:B:526:HIS:C	2:B:528:LEU:N	2.69	0.46
4:E:288:VAL:HG12	4:E:300:MET:HB3	1.97	0.46
1:A:174:VAL:HA	1:A:183:LYS:O	2.15	0.46
7:H:236:ASN:ND2	7:H:243:LYS:HD3	2.30	0.46
1:A:108:ALA:HB1	1:A:112:TYR:HD1	1.81	0.46
1:A:18:ASP:N	1:A:18:ASP:OD1	2.47	0.46
2:B:292:ILE:HA	2:B:295:ILE:HD12	1.98	0.46
3:F:431:ILE:N	3:F:431:ILE:HD12	2.30	0.46
7:H:236:ASN:HD21	7:H:243:LYS:HD3	1.80	0.46
3:F:194:ASP:HA	3:F:197:LEU:HD12	1.97	0.46
4:E:137:PHE:CD1	4:E:145:LEU:HD13	2.51	0.46
2:B:315:LYS:HG3	3:F:162:LEU:HB3	1.97	0.46
2:B:531:LEU:O	2:B:532:LYS:HG2	2.16	0.46
1:A:229:ARG:HH11	1:A:229:ARG:HB2	1.81	0.46
4:E:59:CYS:HB2	4:E:464:THR:OG1	2.15	0.46
3:F:382:LYS:HA	3:F:383:PRO:HD3	1.78	0.46
2:B:333:ILE:HD11	3:F:213:CYS:HB2	1.97	0.45
1:A:214:PRO:HG2	1:A:264:LEU:HA	1.98	0.45
4:E:436:HIS:CD2	4:E:438:GLU:H	2.34	0.45
3:F:227:ILE:C	3:F:229:ASN:H	2.20	0.45
4:E:111:GLN:HG3	4:E:168:TYR:CG	2.52	0.45
1:A:38:VAL:O	1:A:39:GLU:HG3	2.17	0.45
4:E:634:LEU:O	4:E:638:VAL:HG13	2.16	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:241:SER:O	3:F:245:ARG:HD2	2.17	0.44
6:L:33:SER:O	6:L:35:ALA:N	2.49	0.44
3:F:7:TYR:O	3:F:9:THR:N	2.50	0.44
1:A:227:GLN:OE1	1:A:256:VAL:HG11	2.18	0.44
3:F:385:LEU:O	3:F:389:VAL:HG23	2.16	0.44
4:E:53:GLY:HA2	4:E:73:SER:HA	1.98	0.44
1:A:9:ASN:OD1	1:A:12:ILE:HD11	2.18	0.44
4:E:354:LEU:HD21	4:E:460:ALA:HB1	1.99	0.44
4:E:382:VAL:HG21	4:E:495:TYR:CD1	2.52	0.44
6:L:169:GLN:HG2	6:L:174:SER:HA	1.99	0.44
4:E:91:LYS:NZ	4:E:142:ALA:O	2.34	0.44
3:F:86:ASN:C	3:F:88:ASP:H	2.20	0.44
3:F:86:ASN:OD1	3:F:400:ASN:ND2	2.50	0.44
4:E:24:VAL:HG11	4:E:143:ASN:HA	2.00	0.44
3:F:183:TYR:CE2	3:F:199:GLU:HG3	2.52	0.44
2:B:328:SER:HA	3:F:238:LYS:HE3	2.00	0.44
4:E:451:ARG:NH1	6:L:69:ARG:HH11	2.15	0.44
6:L:194:VAL:HG22	6:L:213:ASN:ND2	2.32	0.44
1:A:219:ARG:HB2	1:A:236:GLN:O	2.18	0.44
2:B:373:LEU:HB3	2:B:376:LEU:HD12	1.99	0.44
3:F:157:ASP:OD1	3:F:163:ARG:NH2	2.47	0.44
4:E:185:GLY:O	4:E:196:PRO:HA	2.18	0.44
2:B:393:GLY:O	2:B:394:GLN:CB	2.66	0.44
4:E:466:TYR:HB3	4:E:470:ILE:HB	2.00	0.44
3:F:8:GLN:C	3:F:10:GLU:N	2.68	0.44
2:B:526:HIS:C	2:B:530:ARG:HD2	2.38	0.44
2:B:297:LEU:O	2:B:300:LEU:HB2	2.18	0.43
3:F:143:LYS:HG3	3:F:144:TRP:N	2.33	0.43
3:F:349:SER:OG	3:F:358:VAL:HG21	2.18	0.43
2:B:315:LYS:HE3	3:F:162:LEU:HB3	2.00	0.43
1:A:191:ALA:C	1:A:193:THR:H	2.22	0.43
2:B:452:TRP:CD1	2:B:475:THR:HA	2.53	0.43
1:A:95:HIS:NE2	1:A:138:PRO:HB3	2.33	0.43
1:A:118:VAL:O	1:A:125:VAL:HA	2.18	0.43
6:L:108:GLU:OE2	6:L:169:GLN:NE2	2.51	0.43
4:E:427:LEU:HD13	4:E:442:TYR:CE1	2.53	0.43
2:B:321:VAL:HA	3:F:246:THR:HG21	2.00	0.43
4:E:678:VAL:HG11	4:E:720:PHE:CA	2.46	0.43
6:L:33:SER:C	6:L:35:ALA:H	2.22	0.43
4:E:53:GLY:HA3	4:E:71:HIS:HB3	2.01	0.43
4:E:241:CYS:HG	4:E:270:PHE:HE1	1.66	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:225:SER:OG	4:E:277:GLY:O	2.36	0.42
7:H:150:SER:HB2	7:H:151:ALA:H	1.59	0.42
3:F:433:ALA:O	3:F:435:PHE:N	2.44	0.42
3:F:264:TYR:O	3:F:268:SER:OG	2.31	0.42
3:F:267:LEU:O	3:F:295:GLN:NE2	2.52	0.42
1:A:280:LEU:HB2	1:A:292:ALA:O	2.19	0.42
2:B:341:LEU:HA	2:B:341:LEU:HD12	1.89	0.42
7:H:240:SER:O	7:H:241:ASN:C	2.58	0.42
2:B:273:ILE:HG23	2:B:383:LEU:HG	2.01	0.42
7:H:191:TRP:CZ3	7:H:233:CYS:HB3	2.55	0.42
3:F:77:LEU:HG	3:F:125:TRP:CD2	2.55	0.42
3:F:343:ILE:HD13	3:F:344:ARG:H	1.84	0.42
1:A:259:ARG:HB2	1:A:272:SER:HB2	2.02	0.42
4:E:190:ASP:OD2	4:E:191:GLY:N	2.52	0.42
1:A:181:LEU:HD22	1:A:199:THR:CG2	2.50	0.42
3:F:293:ILE:HD11	3:F:327:VAL:CG2	2.49	0.42
2:B:471:SER:O	2:B:475:THR:OG1	2.30	0.42
2:B:418:PRO:HB3	2:B:445:ALA:HB1	2.01	0.42
4:E:218:SER:OG	4:E:219:ASP:N	2.53	0.42
2:B:386:LEU:HA	2:B:407:HIS:CE1	2.55	0.42
2:B:536:GLN:HA	2:B:539:PHE:CE2	2.54	0.42
4:E:345:GLU:O	4:E:347:SER:N	2.53	0.42
1:A:209:ASP:OD1	1:A:259:ARG:HD3	2.20	0.41
4:E:233:TYR:CG	4:E:311:LEU:HD22	2.55	0.41
2:B:176:LEU:HA	2:B:177:PRO:HD2	1.86	0.41
3:F:94:MSE:HE2	3:F:108:LYS:HB2	2.02	0.41
3:F:363:VAL:HG11	3:F:408:ASP:OD1	2.20	0.41
2:B:431:ASN:HB2	2:B:434:LYS:HB3	2.01	0.41
4:E:297:LEU:HA	4:E:297:LEU:HD23	1.92	0.41
7:H:65:GLN:C	7:H:118:ALA:HB1	2.40	0.41
6:L:123:PRO:HD3	6:L:135:VAL:HG22	2.02	0.41
1:A:57:TRP:HD1	1:A:102:VAL:O	2.02	0.41
2:B:417:ASP:O	2:B:421:VAL:HG23	2.21	0.41
3:F:354:SER:O	3:F:358:VAL:HG23	2.21	0.41
1:A:284:ASN:OD1	1:A:286:GLU:HB2	2.21	0.41
2:B:492:LEU:CD1	2:B:508:ILE:HD13	2.50	0.41
1:A:16:VAL:HG23	1:A:59:VAL:HG23	2.01	0.41
3:F:81:LEU:HD12	3:F:350:VAL:HG12	2.03	0.41
1:A:59:VAL:HB	1:A:70:LEU:HD11	2.03	0.41
2:B:216:LEU:O	2:B:217:LEU:HD23	2.21	0.41
2:B:203:ARG:NE	2:B:210:GLN:HB2	2.36	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:102:ARG:NH2	3:F:308:VAL:HG22	2.36	0.40
4:E:659:TYR:OH	4:E:743:ASN:O	2.21	0.40
3:F:207:SER:HA	3:F:210:MSE:HE3	2.03	0.40
4:E:346:ALA:CB	4:E:369:ASN:HD22	2.35	0.40
4:E:258:ASP:OD1	4:E:260:VAL:HG22	2.20	0.40
2:B:526:HIS:O	2:B:528:LEU:N	2.54	0.40
3:F:50:ALA:HB1	3:F:69:GLU:HG3	2.03	0.40
2:B:340:GLN:HB2	3:F:206:ILE:HG21	2.03	0.40
2:B:263:LYS:HA	2:B:263:LYS:HD3	1.78	0.40
4:E:163:PRO:HA	4:E:178:LEU:HA	2.03	0.40
1:A:63:HIS:CD2	1:A:64:PRO:HD2	2.56	0.40
7:H:117:THR:HG23	7:H:147:THR:HA	2.03	0.40
2:B:155:SER:HB3	2:B:159:MSE:H	1.87	0.40
3:F:183:TYR:HE2	3:F:199:GLU:HG3	1.85	0.40
1:A:253:PHE:CD1	1:A:257:LEU:HD11	2.56	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)
3:F:329:ASN:OD1	4:E:204:TYR:OH[2_454]	1.97	0.23

## 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	270/297 (91%)	227 (84%)	37 (14%)	6 (2%)	<b>8</b> 49
2	B	485/652 (74%)	447 (92%)	28 (6%)	10 (2%)	<b>9</b> 50
3	F	413/454 (91%)	369 (89%)	33 (8%)	11 (3%)	<b>6</b> 45
4	E	858/1045 (82%)	797 (93%)	51 (6%)	10 (1%)	<b>16</b> 61

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	D	123/685 (18%)	123 (100%)	0	0	100	100
6	L	205/217 (94%)	195 (95%)	7 (3%)	3 (2%)	13	57
7	H	211/267 (79%)	198 (94%)	8 (4%)	5 (2%)	7	47
All	All	2565/3617 (71%)	2356 (92%)	164 (6%)	45 (2%)	11	53

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	158	SER
2	B	368	GLU
2	B	371	PHE
2	B	394	GLN
3	F	9	THR
3	F	11	ARG
3	F	138	ASN
3	F	165	ASN
7	H	118	ALA
1	A	218	LEU
2	B	180	LEU
2	B	348	GLY
2	B	429	ASN
2	B	527	ILE
3	F	8	GLN
3	F	55	ASN
3	F	141	THR
3	F	354	SER
3	F	434	THR
4	E	113	VAL
4	E	598	LYS
4	E	602	ILE
6	L	129	LYS
7	H	149	SER
3	F	440	ASP
4	E	346	ALA
6	L	34	SER
1	A	131	LYS
2	B	531	LEU
3	F	87	ALA
4	E	264	ASP
4	E	284	ASN
4	E	600	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
6	L	110	LYS
1	A	114	PRO
1	A	247	LEU
4	E	780	HIS
7	H	151	ALA
4	E	231	GLU
7	H	241	ASN
4	E	737	ILE
1	A	202	GLY
2	B	393	GLY
1	A	97	VAL
7	H	186	PRO

### 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	233/251 (93%)	224 (96%)	9 (4%)	39	72
2	B	367/584 (63%)	332 (90%)	35 (10%)	11	41
3	F	387/410 (94%)	365 (94%)	22 (6%)	25	62
4	E	639/980 (65%)	615 (96%)	24 (4%)	40	73
6	L	183/191 (96%)	177 (97%)	6 (3%)	45	76
7	H	173/223 (78%)	166 (96%)	7 (4%)	38	71
All	All	1982/2639 (75%)	1879 (95%)	103 (5%)	29	65

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	22	LYS
1	A	43	HIS
1	A	46	ILE
1	A	47	ASP
1	A	225	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	227	GLN
1	A	229	ARG
1	A	275	ASP
2	B	160	LEU
2	B	175	ARG
2	B	214	SER
2	B	216	LEU
2	B	225	MSE
2	B	234	LEU
2	B	251	THR
2	B	308	SER
2	B	319	LEU
2	B	328	SER
2	B	336	LEU
2	B	341	LEU
2	B	346	THR
2	B	349	CYS
2	B	351	ILE
2	B	368	GLU
2	B	370	LEU
2	B	371	PHE
2	B	400	LEU
2	B	402	SER
2	B	406	SER
2	B	408	LEU
2	B	412	SER
2	B	419	ILE
2	B	440	ARG
2	B	443	THR
2	B	456	GLN
2	B	464	ARG
2	B	467	SER
2	B	516	ILE
2	B	522	SER
2	B	524	ASN
2	B	531	LEU
2	B	539	PHE
2	B	547	ARG
3	F	17	ASP
3	F	26	GLN
3	F	58	ASP
3	F	71	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	F	77	LEU
3	F	86	ASN
3	F	88	ASP
3	F	94	MSE
3	F	118	GLN
3	F	166	THR
3	F	211	ILE
3	F	237	ILE
3	F	245	ARG
3	F	268	SER
3	F	274	GLN
3	F	284	SER
3	F	343	ILE
3	F	357	SER
3	F	365	MSE
3	F	403	SER
3	F	422	LEU
3	F	431	ILE
4	E	63	SER
4	E	72	PHE
4	E	127	SER
4	E	172	GLN
4	E	183	LEU
4	E	200	ASN
4	E	209	THR
4	E	230	HIS
4	E	270	PHE
4	E	280	LEU
4	E	305	VAL
4	E	314	THR
4	E	335	VAL
4	E	338	ARG
4	E	370	ASP
4	E	408	PHE
4	E	422	ARG
4	E	590	GLN
4	E	600	ASP
4	E	628	ARG
4	E	638	VAL
4	E	644	THR
4	E	703	ASP
4	E	706	ASN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
6	L	15	SER
6	L	27	ARG
6	L	53	SER
6	L	83	PRO
6	L	108	GLU
6	L	148	LYS
7	H	45	ARG
7	H	113	ARG
7	H	124	ARG
7	H	166	LYS
7	H	215	LEU
7	H	234	ASN
7	H	236	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	63	HIS
1	A	91	GLN
2	B	210	GLN
2	B	329	ASN
3	F	26	GLN
3	F	97	HIS
3	F	335	HIS
4	E	255	GLN
4	E	295	ASN
4	E	350	ASN
4	E	369	ASN
4	E	514	ASN
4	E	575	ASN
4	E	620	HIS
4	E	632	GLN
4	E	706	ASN
6	L	213	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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	274/297 (92%)	2.81	146 (53%) 0 4	579, 633, 655, 668	0
2	B	495/652 (75%)	1.80	168 (33%) 0 5	466, 557, 629, 666	0
3	F	412/454 (90%)	1.50	125 (30%) 1 5	455, 526, 597, 626	0
4	E	896/1045 (85%)	1.60	281 (31%) 1 5	424, 509, 574, 666	0
5	D	140/685 (20%)	2.33	65 (46%) 0 4	555, 634, 690, 699	0
6	L	209/217 (96%)	2.10	90 (43%) 0 4	422, 477, 527, 558	0
7	H	215/267 (80%)	2.47	109 (50%) 0 4	451, 495, 558, 613	0
All	All	2641/3617 (73%)	1.90	984 (37%) 0 4	422, 522, 644, 699	0

All (984) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	L	122	PRO	15.3
2	B	169	SER	14.3
1	A	104	SER	13.2
4	E	29	SER	12.9
6	L	123	PRO	12.7
2	B	170	GLY	12.7
1	A	224	SER	12.0
1	A	118	VAL	11.2
1	A	26	THR	10.9
1	A	209	ASP	10.8
5	D	618	ASN	10.3
1	A	25	ALA	10.3
4	E	28	VAL	10.3
1	A	119	ALA	10.2
1	A	103	ASN	10.0
1	A	293	GLY	9.9
4	E	292	PRO	9.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
7	H	97	SER	9.4
4	E	594	GLY	9.3
6	L	121	PHE	9.3
1	A	9	ASN	9.2
5	D	617	THR	9.1
7	H	162	ALA	8.9
1	A	141	ILE	8.7
1	A	105	VAL	8.7
1	A	150	SER	8.6
1	A	149	ASN	8.5
2	B	615	ASN	8.5
5	D	623	THR	8.5
7	H	160	PRO	8.5
5	D	719	SER	8.4
5	D	619	SER	8.4
2	B	613	SER	8.3
2	B	616	VAL	8.3
1	A	142	ASP	8.1
6	L	134	SER	8.0
4	E	291	LEU	8.0
2	B	633	THR	8.0
4	E	293	LEU	7.9
7	H	163	PRO	7.8
1	A	102	VAL	7.6
6	L	135	VAL	7.5
1	A	125	VAL	7.5
4	E	600	ASP	7.5
3	F	432	TYR	7.5
5	D	621	ARG	7.4
1	A	126	SER	7.4
4	E	207	SER	7.3
2	B	619	VAL	7.3
2	B	688	PRO	7.3
1	A	73	CYS	7.3
1	A	143	ALA	7.2
7	H	175	LEU	7.2
2	B	168	LYS	7.2
1	A	223	ALA	7.2
1	A	36	PHE	7.1
1	A	260	ALA	7.1
3	F	416	TYR	7.0
7	H	62	TRP	7.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
6	L	184	LEU	7.0
1	A	151	ALA	7.0
3	F	38	ILE	7.0
2	B	618	GLU	6.9
3	F	42	PHE	6.9
5	D	717	ASP	6.9
1	A	71	ALA	6.8
2	B	156	THR	6.8
2	B	175	ARG	6.8
1	A	101	SER	6.8
7	H	169	SER	6.8
2	B	167	GLY	6.8
4	E	264	ASP	6.7
7	H	176	GLY	6.7
3	F	391	HIS	6.7
4	E	296	GLY	6.7
4	E	266	ASP	6.6
2	B	617	PHE	6.6
2	B	635	ASP	6.6
1	A	120	SER	6.6
3	F	399	ILE	6.6
4	E	595	ILE	6.5
6	L	137	CYS	6.5
4	E	601	PHE	6.5
2	B	687	LEU	6.5
7	H	177	CYS	6.5
6	L	133	ALA	6.4
4	E	690	VAL	6.4
2	B	636	SER	6.4
7	H	116	ASP	6.4
6	L	215	GLY	6.4
1	A	100	ALA	6.4
3	F	395	CYS	6.4
6	L	32	VAL	6.4
7	H	96	ILE	6.3
5	D	616	VAL	6.3
4	E	433	ILE	6.3
4	E	98	PRO	6.3
2	B	686	GLU	6.3
6	L	120	ILE	6.2
2	B	151	PHE	6.2
1	A	148	VAL	6.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	B	163	LYS	6.1
3	F	35	PRO	6.1
1	A	12	ILE	6.1
7	H	161	LEU	6.1
2	B	171	VAL	6.1
2	B	631	GLN	6.1
7	H	174	ALA	6.1
5	D	622	GLN	6.1
5	D	624	LEU	6.0
1	A	72	SER	6.0
5	D	608	PRO	6.0
1	A	225	VAL	6.0
2	B	689	LEU	6.0
6	L	189	TYR	6.0
4	E	146	ASN	5.9
2	B	632	GLU	5.9
4	E	144	THR	5.9
6	L	212	PHE	5.8
1	A	155	PRO	5.8
2	B	614	ILE	5.8
4	E	846	SER	5.8
7	H	106	TYR	5.8
6	L	36	VAL	5.7
2	B	620	TYR	5.7
4	E	130	THR	5.7
4	E	149	TRP	5.7
6	L	213	ASN	5.7
4	E	206	LYS	5.7
4	E	259	MET	5.6
4	E	270	PHE	5.6
3	F	359	ILE	5.6
4	E	150	PHE	5.6
7	H	44	LEU	5.6
3	F	23	LYS	5.5
7	H	45	ARG	5.5
4	E	845	ILE	5.5
2	B	157	GLY	5.5
3	F	435	PHE	5.5
7	H	48	CYS	5.5
1	A	121	SER	5.5
2	B	158	SER	5.5
4	E	151	HIS	5.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
5	D	718	LYS	5.5
1	A	259	ARG	5.5
3	F	19	LEU	5.4
4	E	597	TRP	5.4
1	A	140	ILE	5.4
7	H	158	VAL	5.4
3	F	39	ILE	5.4
2	B	164	ASP	5.3
6	L	197	CYS	5.3
3	F	413	ILE	5.3
6	L	118	VAL	5.3
7	H	107	LEU	5.3
4	E	295	ASN	5.3
7	H	43	SER	5.3
3	F	393	ALA	5.3
1	A	265	SER	5.3
3	F	390	THR	5.2
1	A	200	LEU	5.2
1	A	79	VAL	5.2
3	F	394	ILE	5.2
4	E	265	SER	5.2
3	F	15	PHE	5.2
4	E	822	SER	5.2
3	F	36	PHE	5.2
5	D	604	ASP	5.2
6	L	147	ALA	5.2
6	L	33	SER	5.1
2	B	612	VAL	5.1
2	B	634	ILE	5.1
7	H	109	MET	5.1
4	E	849	ALA	5.1
4	E	153	GLN	5.1
7	H	251	LYS	5.1
4	E	685	GLU	5.1
4	E	263	SER	5.1
5	D	644	GLN	5.1
5	D	672	TYR	5.1
7	H	217	SER	5.1
1	A	98	HIS	5.1
1	A	156	ALA	5.1
2	B	152	ALA	5.1
7	H	252	SER	5.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	35	ILE	5.1
2	B	251	THR	5.0
4	E	192	VAL	5.0
4	E	145	LEU	5.0
6	L	195	TYR	5.0
1	A	8	HIS	5.0
4	E	842	LEU	5.0
2	B	149	TYR	5.0
4	E	596	PHE	5.0
7	H	64	ARG	5.0
2	B	150	THR	5.0
3	F	408	ASP	5.0
7	H	152	SER	5.0
7	H	168	THR	5.0
7	H	159	PHE	5.0
5	D	668	ALA	5.0
1	A	193	THR	5.0
4	E	267	PRO	5.0
2	B	200	ILE	5.0
1	A	95	HIS	4.9
3	F	157	ASP	4.9
7	H	46	LEU	4.9
7	H	94	PHE	4.9
1	A	234	TRP	4.9
3	F	434	THR	4.9
5	D	730	ASN	4.9
2	B	621	LEU	4.9
4	E	843	LYS	4.9
1	A	43	HIS	4.9
4	E	318	ASN	4.9
1	A	197	GLU	4.9
3	F	156	CYS	4.8
1	A	208	ARG	4.8
4	E	821	HIS	4.8
4	E	297	LEU	4.8
4	E	132	GLN	4.8
7	H	98	ALA	4.8
6	L	47	PRO	4.8
4	E	844	CYS	4.8
2	B	594	THR	4.8
6	L	183	THR	4.8
3	F	144	TRP	4.8

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
7	H	110	ASN	4.7
7	H	105	ALA	4.7
6	L	38	TRP	4.7
2	B	639	SER	4.7
7	H	50	ALA	4.7
7	H	95	THR	4.7
7	H	122	CYS	4.7
1	A	139	ILE	4.7
4	E	682	ASP	4.7
3	F	22	PHE	4.6
4	E	501	THR	4.6
4	E	689	GLY	4.6
7	H	108	GLN	4.6
4	E	284	ASN	4.6
4	E	27	TYR	4.6
7	H	111	SER	4.6
5	D	689	ALA	4.6
1	A	222	LEU	4.6
1	A	264	LEU	4.6
2	B	214	SER	4.6
2	B	622	LYS	4.6
4	E	546	THR	4.6
6	L	149	VAL	4.6
1	A	122	ASP	4.6
1	A	117	LEU	4.6
5	D	692	ILE	4.6
7	H	60	ILE	4.6
2	B	212	SER	4.5
5	D	560	SER	4.5
5	D	641	ASP	4.5
7	H	178	LEU	4.5
1	A	214	PRO	4.5
1	A	77	GLY	4.5
5	D	645	ALA	4.5
2	B	591	GLU	4.5
7	H	112	LEU	4.5
4	E	273	VAL	4.5
5	D	625	ALA	4.5
2	B	209	PRO	4.5
1	A	34	LYS	4.5
4	E	599	LYS	4.5
4	E	684	SER	4.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
3	F	412	LEU	4.5
4	E	642	LEU	4.5
2	B	281	ILE	4.5
2	B	252	ASP	4.4
1	A	198	SER	4.4
4	E	209	THR	4.4
4	E	2	ALA	4.4
1	A	24	LEU	4.4
4	E	402	GLY	4.4
2	B	466	PHE	4.4
6	L	91	CYS	4.4
4	E	271	ARG	4.4
7	H	250	PRO	4.4
4	E	194	TYR	4.4
4	E	978	ALA	4.4
5	D	647	ARG	4.3
3	F	431	ILE	4.3
2	B	623	LEU	4.3
3	F	398	ILE	4.3
4	E	442	TYR	4.3
7	H	189	VAL	4.3
7	H	216	SER	4.3
6	L	50	LEU	4.3
1	A	58	ARG	4.3
4	E	423	ALA	4.3
4	E	498	HIS	4.3
2	B	486	GLN	4.3
7	H	113	ARG	4.3
7	H	140	TRP	4.2
4	E	155	PRO	4.2
1	A	263	SER	4.2
2	B	165	ILE	4.2
2	B	211	ILE	4.2
4	E	401	THR	4.2
3	F	41	GLU	4.2
4	E	241	CYS	4.2
4	E	432	ILE	4.2
6	L	192	HIS	4.2
3	F	16	SER	4.2
7	H	47	SER	4.2
5	D	638	ASP	4.2
1	A	124	LYS	4.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	194	TYR	4.2
1	A	147	GLY	4.1
4	E	26	LEU	4.1
7	H	179	VAL	4.1
3	F	34	ASP	4.1
2	B	683	LYS	4.1
4	E	446	LEU	4.1
4	E	781	ASP	4.1
7	H	165	SER	4.1
2	B	638	ILE	4.1
1	A	46	ILE	4.1
4	E	848	SER	4.1
2	B	664	GLU	4.1
6	L	153	VAL	4.1
4	E	211	PHE	4.1
4	E	419	ILE	4.1
3	F	367	LEU	4.1
4	E	272	LYS	4.1
6	L	155	ASN	4.1
4	E	468	ASP	4.0
4	E	643	ASP	4.0
3	F	363	VAL	4.0
6	L	136	VAL	4.0
2	B	380	PHE	4.0
5	D	607	ILE	4.0
7	H	120	TYR	4.0
4	E	383	ASN	4.0
1	A	176	GLY	4.0
4	E	283	TYR	4.0
1	A	10	GLU	4.0
1	A	215	THR	4.0
6	L	214	ARG	4.0
1	A	116	LEU	4.0
5	D	667	VAL	4.0
4	E	97	LEU	4.0
1	A	144	HIS	4.0
2	B	178	THR	3.9
1	A	258	TRP	3.9
3	F	18	THR	3.9
4	E	131	LEU	3.9
4	E	299	GLN	3.9
4	E	701	TYR	3.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	45	LEU	3.9
4	E	646	ILE	3.9
3	F	170	ASP	3.9
4	E	706	ASN	3.9
1	A	99	SER	3.9
3	F	409	LYS	3.9
5	D	729	LYS	3.9
4	E	143	ASN	3.9
4	E	343	ASN	3.9
7	H	115	GLU	3.9
1	A	201	GLU	3.8
4	E	424	GLN	3.8
4	E	321	THR	3.8
7	H	123	ALA	3.8
4	E	152	LEU	3.8
6	L	39	TYR	3.8
6	L	154	ASP	3.8
6	L	139	LEU	3.8
4	E	683	SER	3.8
3	F	143	LYS	3.8
6	L	191	LYS	3.8
5	D	640	GLU	3.8
7	H	49	ALA	3.8
7	H	138	ASP	3.8
2	B	277	ILE	3.8
4	E	691	LYS	3.8
1	A	271	LEU	3.8
5	D	628	ALA	3.8
2	B	155	SER	3.8
7	H	53	PHE	3.7
4	E	333	ASP	3.7
2	B	637	LEU	3.7
5	D	671	LEU	3.7
7	H	51	SER	3.7
2	B	201	GLU	3.7
1	A	157	THR	3.7
1	A	286	GLU	3.7
1	A	107	TRP	3.7
6	L	138	LEU	3.7
4	E	129	LEU	3.7
4	E	191	GLY	3.7
5	D	669	LYS	3.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
6	L	92	GLN	3.7
2	B	595	LEU	3.7
6	L	54	ALA	3.7
2	B	285	ILE	3.7
1	A	177	GLY	3.7
7	H	93	ARG	3.7
3	F	71	GLU	3.7
7	H	63	VAL	3.7
1	A	19	TYR	3.7
5	D	716	ALA	3.7
4	E	128	PHE	3.7
6	L	182	LEU	3.7
3	F	381	ASP	3.7
4	E	210	ARG	3.7
4	E	543	SER	3.6
1	A	44	LYS	3.6
4	E	981	LEU	3.6
4	E	289	THR	3.6
6	L	127	GLN	3.6
5	D	726	THR	3.6
3	F	417	ILE	3.6
7	H	164	SER	3.6
2	B	592	LEU	3.6
2	B	184	PHE	3.6
4	E	381	SER	3.6
7	H	41	GLY	3.6
1	A	127	VAL	3.6
2	B	284	LYS	3.6
2	B	221	ALA	3.6
1	A	23	ARG	3.6
4	E	213	SER	3.6
4	E	598	LYS	3.6
2	B	162	THR	3.6
6	L	37	ALA	3.6
6	L	188	ASP	3.6
6	L	128	LEU	3.5
1	A	207	VAL	3.5
4	E	847	LYS	3.5
3	F	428	ASN	3.5
4	E	840	PHE	3.5
5	D	691	VAL	3.5
2	B	510	ARG	3.5

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	123	GLY	3.5
7	H	245	ASP	3.5
4	E	99	ASN	3.5
7	H	92	GLY	3.5
1	A	60	ASP	3.5
6	L	196	ALA	3.5
1	A	267	ASN	3.5
4	E	708	ASN	3.5
6	L	119	PHE	3.5
1	A	277	LYS	3.4
3	F	26	GLN	3.4
3	F	169	LEU	3.4
4	E	519	THR	3.4
7	H	90	VAL	3.4
4	E	358	GLY	3.4
7	H	30	LEU	3.4
1	A	59	VAL	3.4
1	A	11	LEU	3.4
1	A	128	VAL	3.4
4	E	431	LYS	3.4
6	L	193	LYS	3.4
2	B	684	LEU	3.4
5	D	673	PRO	3.4
4	E	644	THR	3.4
3	F	279	TYR	3.4
4	E	499	SER	3.4
6	L	185	SER	3.4
2	B	198	VAL	3.4
1	A	272	SER	3.4
5	D	609	GLN	3.4
4	E	182	GLY	3.4
4	E	464	THR	3.4
3	F	99	TYR	3.3
1	A	257	LEU	3.3
2	B	624	VAL	3.3
7	H	139	TYR	3.3
2	B	166	VAL	3.3
2	B	668	LYS	3.3
4	E	705	LEU	3.3
1	A	266	GLY	3.3
4	E	841	ALA	3.3
1	A	210	VAL	3.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	B	417	ASP	3.3
6	L	199	VAL	3.3
4	E	16	GLU	3.3
6	L	211	SER	3.3
7	H	89	SER	3.3
2	B	382	TRP	3.3
4	E	420	PHE	3.3
4	E	608	ASP	3.3
7	H	233	CYS	3.3
3	F	95	GLU	3.3
3	F	360	HIS	3.3
6	L	194	VAL	3.3
6	L	148	LYS	3.3
6	L	124	SER	3.3
7	H	75	ALA	3.3
2	B	532	LYS	3.3
1	A	182	VAL	3.2
2	B	194	GLU	3.2
7	H	42	GLY	3.2
2	B	246	SER	3.2
4	E	852	SER	3.2
2	B	301	LEU	3.2
3	F	397	ASP	3.2
1	A	275	ASP	3.2
4	E	868	GLN	3.2
1	A	13	HIS	3.2
3	F	308	VAL	3.2
7	H	167	SER	3.2
1	A	47	ASP	3.2
3	F	255	GLY	3.2
4	E	290	LEU	3.2
2	B	593	LYS	3.2
3	F	146	ASN	3.2
2	B	559	LEU	3.2
6	L	51	ILE	3.2
7	H	74	VAL	3.2
4	E	240	ASN	3.2
4	E	467	GLY	3.2
7	H	34	GLY	3.2
7	H	71	LEU	3.2
4	E	201	ASP	3.2
4	E	514	ASN	3.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
4	E	839	GLU	3.2
6	L	132	THR	3.2
4	E	181	GLY	3.2
7	H	170	GLY	3.2
7	H	124	ARG	3.2
1	A	175	THR	3.2
3	F	97	HIS	3.2
4	E	77	THR	3.1
4	E	611	THR	3.1
2	B	590	ASN	3.1
7	H	218	VAL	3.1
1	A	61	TRP	3.1
1	A	243	TRP	3.1
4	E	615	SER	3.1
4	E	641	ASP	3.1
4	E	450	LEU	3.1
4	E	434	MET	3.1
4	E	183	LEU	3.1
2	B	181	GLN	3.1
5	D	610	ASP	3.1
3	F	140	PRO	3.1
4	E	1026	THR	3.1
2	B	250	LYS	3.1
4	E	230	HIS	3.1
4	E	637	PHE	3.1
2	B	485	ALA	3.1
4	E	427	LEU	3.1
6	L	216	GLU	3.1
7	H	249	GLU	3.1
4	E	496	ASN	3.1
4	E	205	LEU	3.1
4	E	338	ARG	3.1
4	E	400	LYS	3.1
6	L	190	GLU	3.1
5	D	675	PHE	3.1
6	L	150	GLN	3.1
4	E	156	TYR	3.0
4	E	180	ASP	3.0
6	L	217	CYS	3.0
3	F	362	SER	3.0
2	B	413	LEU	3.0
3	F	12	PHE	3.0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
4	E	734	HIS	3.0
6	L	151	TRP	3.0
1	A	40	GLY	3.0
7	H	244	VAL	3.0
4	E	133	LEU	3.0
6	L	152	LYS	3.0
4	E	212	PHE	3.0
4	E	612	SER	3.0
4	E	593	PRO	3.0
4	E	260	VAL	3.0
4	E	979	GLU	3.0
4	E	231	GLU	3.0
4	E	319	ILE	3.0
5	D	648	LEU	3.0
4	E	607	PHE	3.0
2	B	381	SER	3.0
1	A	196	LEU	3.0
2	B	300	LEU	3.0
2	B	224	TYR	3.0
4	E	545	THR	3.0
7	H	86	TYR	3.0
2	B	667	SER	3.0
5	D	605	VAL	3.0
5	D	674	ILE	3.0
3	F	404	VAL	3.0
4	E	502	ASP	3.0
4	E	320	PRO	3.0
2	B	318	HIS	3.0
7	H	35	GLY	3.0
2	B	414	PRO	2.9
3	F	8	GLN	2.9
4	E	96	HIS	2.9
7	H	61	HIS	2.9
5	D	690	THR	2.9
2	B	234	LEU	2.9
7	H	77	ILE	2.9
3	F	75	TRP	2.9
3	F	366	LEU	2.9
4	E	186	LEU	2.9
4	E	439	ASP	2.9
3	F	392	LEU	2.9
4	E	520	LEU	2.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
4	E	268	SER	2.9
4	E	542	ASP	2.9
1	A	232	ILE	2.9
4	E	111	GLN	2.9
1	A	273	GLY	2.9
2	B	531	LEU	2.9
1	A	226	SER	2.9
7	H	29	GLN	2.9
3	F	158	LEU	2.9
7	H	137	MET	2.9
1	A	97	VAL	2.9
2	B	341	LEU	2.9
3	F	442	LEU	2.9
7	H	146	VAL	2.9
2	B	514	ARG	2.9
4	E	18	PRO	2.9
6	L	116	PRO	2.9
4	E	850	GLU	2.9
1	A	138	PRO	2.9
4	E	445	ASN	2.9
2	B	235	TRP	2.9
2	B	199	THR	2.9
7	H	121	TYR	2.9
3	F	299	GLU	2.9
3	F	40	ARG	2.8
2	B	280	GLU	2.8
4	E	311	LEU	2.8
4	E	418	GLN	2.8
2	B	359	TYR	2.8
4	E	147	GLY	2.8
4	E	61	LEU	2.8
4	E	823	ALA	2.8
5	D	688	VAL	2.8
4	E	243	LEU	2.8
1	A	192	GLN	2.8
4	E	298	PHE	2.8
2	B	534	PRO	2.8
4	E	313	TYR	2.8
4	E	193	HIS	2.8
2	B	685	LEU	2.8
3	F	237	ILE	2.8
3	F	356	PRO	2.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
4	E	148	GLU	2.8
5	D	646	LEU	2.8
4	E	977	ALA	2.8
1	A	41	GLU	2.8
6	L	31	SER	2.8
3	F	378	ASP	2.8
7	H	235	VAL	2.8
1	A	199	THR	2.8
3	F	131	TYR	2.8
2	B	216	LEU	2.8
4	E	866	GLU	2.8
6	L	198	GLU	2.8
1	A	145	ALA	2.8
4	E	479	TYR	2.8
7	H	28	VAL	2.8
2	B	419	ILE	2.8
3	F	141	THR	2.8
4	E	733	SER	2.8
3	F	155	SER	2.8
5	D	693	GLU	2.8
4	E	838	GLN	2.8
1	A	203	HIS	2.8
3	F	387	ARG	2.8
3	F	389	VAL	2.8
4	E	184	LEU	2.8
7	H	202	THR	2.8
4	E	686	PHE	2.8
3	F	256	LEU	2.7
4	E	562	PHE	2.7
3	F	153	LEU	2.7
4	E	217	LYS	2.7
1	A	62	ALA	2.7
2	B	190	TYR	2.7
4	E	704	SER	2.7
4	E	540	LEU	2.7
2	B	597	GLU	2.7
3	F	205	ASN	2.7
4	E	262	GLN	2.7
2	B	558	ASN	2.7
6	L	69	ARG	2.7
2	B	528	LEU	2.7
1	A	14	ASP	2.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
4	E	544	MET	2.7
4	E	138	LEU	2.7
4	E	453	VAL	2.7
2	B	237	LEU	2.7
7	H	153	THR	2.7
7	H	191	TRP	2.7
6	L	74	PHE	2.7
1	A	195	VAL	2.7
2	B	555	GLU	2.7
7	H	231	TYR	2.7
4	E	707	SER	2.7
4	E	239	GLN	2.7
4	E	865	LYS	2.7
7	H	253	CYS	2.7
3	F	253	GLN	2.7
1	A	109	PRO	2.7
1	A	252	LYS	2.7
2	B	640	GLY	2.7
2	B	210	GLN	2.7
6	L	186	LYS	2.7
3	F	24	ILE	2.7
2	B	490	HIS	2.7
4	E	195	GLU	2.6
7	H	104	THR	2.6
5	D	733	LYS	2.6
4	E	204	TYR	2.6
2	B	529	ASN	2.6
3	F	125	TRP	2.6
4	E	709	VAL	2.6
5	D	639	ARG	2.6
2	B	330	ASP	2.6
6	L	178	LEU	2.6
6	L	209	THR	2.6
2	B	273	ILE	2.6
2	B	308	SER	2.6
2	B	560	LEU	2.6
3	F	194	ASP	2.6
5	D	727	LEU	2.6
7	H	248	VAL	2.6
7	H	234	ASN	2.6
6	L	125	ASP	2.6
7	H	151	ALA	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
4	E	222	SER	2.6
6	L	72	THR	2.6
3	F	14	LYS	2.6
2	B	323	ILE	2.6
1	A	57	TRP	2.6
4	E	535	ILE	2.6
3	F	257	ASP	2.6
1	A	239	GLU	2.6
2	B	324	SER	2.6
6	L	187	ALA	2.6
5	D	643	GLY	2.6
4	E	550	PHE	2.6
6	L	26	CYS	2.6
5	D	583	GLY	2.5
5	D	642	TRP	2.5
4	E	415	TYR	2.5
4	E	687	SER	2.5
2	B	297	LEU	2.5
3	F	177	ASP	2.5
7	H	72	GLU	2.5
4	E	95	ILE	2.5
3	F	68	TRP	2.5
5	D	687	SER	2.5
1	A	185	TRP	2.5
5	D	666	LEU	2.5
2	B	238	SER	2.5
3	F	45	ALA	2.5
4	E	269	HIS	2.5
3	F	230	GLU	2.5
2	B	349	CYS	2.5
4	E	766	SER	2.5
4	E	710	TYR	2.5
2	B	384	CYS	2.5
2	B	213	GLU	2.5
5	D	603	ASP	2.5
4	E	869	HIS	2.5
6	L	200	THR	2.5
3	F	37	ASN	2.5
4	E	275	ALA	2.5
2	B	533	ILE	2.5
5	D	557	ALA	2.5
4	E	628	ARG	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	B	371	PHE	2.4
3	F	74	PHE	2.4
6	L	101	PHE	2.4
3	F	396	LEU	2.4
2	B	383	LEU	2.4
4	E	469	GLU	2.4
6	L	146	GLU	2.4
4	E	980	VAL	2.4
1	A	240	GLN	2.4
1	A	63	HIS	2.4
3	F	129	ASN	2.4
6	L	140	ASN	2.4
3	F	20	LYS	2.4
2	B	173	ILE	2.4
2	B	422	ILE	2.4
3	F	191	GLY	2.4
4	E	203	SER	2.4
4	E	330	SER	2.4
4	E	3	CYS	2.4
7	H	190	SER	2.4
2	B	231	ASP	2.4
4	E	746	CYS	2.4
4	E	619	LEU	2.4
2	B	233	ASN	2.4
6	L	158	GLN	2.4
4	E	532	PHE	2.4
1	A	170	SER	2.4
5	D	649	LEU	2.4
4	E	175	VAL	2.4
4	E	726	SER	2.4
4	E	982	TYR	2.4
1	A	37	GLU	2.4
3	F	173	ASP	2.4
4	E	703	ASP	2.4
2	B	292	ILE	2.4
4	E	119	VAL	2.4
5	D	664	VAL	2.4
3	F	152	GLY	2.4
4	E	10	ASN	2.4
7	H	103	ASN	2.4
4	E	223	VAL	2.4
1	A	70	LEU	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
5	D	627	TYR	2.4
4	E	294	GLU	2.4
2	B	223	ASP	2.4
2	B	493	PHE	2.4
7	H	215	LEU	2.4
1	A	245	LYS	2.4
2	B	445	ALA	2.4
2	B	230	SER	2.3
3	F	147	SER	2.3
2	B	588	GLN	2.3
4	E	257	TYR	2.3
3	F	142	SER	2.3
1	A	276	ASN	2.3
2	B	497	PHE	2.3
4	E	825	TYR	2.3
2	B	430	GLU	2.3
1	A	15	ALA	2.3
2	B	177	PRO	2.3
6	L	34	SER	2.3
2	B	351	ILE	2.3
2	B	418	PRO	2.3
3	F	226	GLN	2.3
4	E	161	ARG	2.3
4	E	196	PRO	2.3
4	E	778	GLN	2.3
5	D	665	LEU	2.3
1	A	110	HIS	2.3
2	B	460	PHE	2.3
1	A	39	GLU	2.3
4	E	190	ASP	2.3
6	L	73	ASP	2.3
6	L	161	ASN	2.3
2	B	361	LEU	2.3
3	F	343	ILE	2.3
7	H	31	VAL	2.3
2	B	307	ALA	2.3
6	L	179	SER	2.3
3	F	433	ALA	2.3
2	B	222	LEU	2.3
2	B	282	GLU	2.3
4	E	323	LEU	2.3
2	B	358	ILE	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
4	E	435	ALA	2.3
4	E	200	ASN	2.3
3	F	400	ASN	2.3
3	F	406	GLU	2.3
2	B	185	LEU	2.2
2	B	320	SER	2.2
4	E	281	SER	2.2
2	B	416	ASP	2.2
4	E	339	PRO	2.2
4	E	337	THR	2.2
7	H	157	SER	2.2
2	B	589	ASN	2.2
2	B	208	TYR	2.2
4	E	465	LEU	2.2
3	F	52	ASP	2.2
4	E	112	GLU	2.2
4	E	224	ILE	2.2
3	F	236	GLY	2.2
4	E	202	ASN	2.2
4	E	440	GLU	2.2
4	E	63	SER	2.2
4	E	127	SER	2.2
7	H	219	VAL	2.2
4	E	398	VAL	2.2
1	A	202	GLY	2.2
1	A	89	TRP	2.2
3	F	96	LEU	2.2
4	E	411	LEU	2.2
5	D	714	ILE	2.2
6	L	208	VAL	2.2
3	F	150	SER	2.2
3	F	429	ILE	2.2
3	F	250	LEU	2.2
5	D	626	PRO	2.2
2	B	598	ILE	2.2
3	F	130	THR	2.2
3	F	414	THR	2.2
3	F	216	GLN	2.2
7	H	38	VAL	2.2
1	A	213	SER	2.2
4	E	711	ASN	2.2
4	E	872	TYR	2.2

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
4	E	679	LEU	2.2
6	L	180	SER	2.2
3	F	7	TYR	2.2
6	L	171	SER	2.2
3	F	388	ILE	2.2
6	L	210	LYS	2.2
3	F	214	GLY	2.1
7	H	173	ALA	2.1
2	B	446	LEU	2.1
3	F	259	TYR	2.1
6	L	49	LEU	2.1
1	A	178	ALA	2.1
4	E	999	CYS	2.1
5	D	596	SER	2.1
4	E	208	LEU	2.1
3	F	128	GLU	2.1
2	B	465	VAL	2.1
1	A	27	CYS	2.1
1	A	106	GLN	2.1
2	B	326	LEU	2.1
4	E	11	LEU	2.1
5	D	661	HIS	2.1
4	E	987	MET	2.1
4	E	853	LEU	2.1
6	L	44	GLY	2.1
5	D	652	LEU	2.1
4	E	702	ILE	2.1
6	L	28	ALA	2.1
4	E	449	ILE	2.1
4	E	735	LYS	2.1
2	B	278	GLY	2.1
2	B	344	TRP	2.1
4	E	971	ASN	2.1
4	E	886	LEU	2.1
7	H	166	LYS	2.1
2	B	423	PHE	2.1
3	F	122	VAL	2.1
4	E	616	LEU	2.1
1	A	76	ASP	2.1
3	F	204	ASP	2.1
4	E	879	PHE	2.1
2	B	272	TRP	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
3	F	405	GLU	2.1
3	F	11	ARG	2.1
3	F	172	LYS	2.1
1	A	183	LYS	2.1
3	F	168	VAL	2.1
3	F	43	ARG	2.1
4	E	518	SER	2.1
4	E	603	SER	2.1
2	B	172	SER	2.1
4	E	715	THR	2.1
3	F	386	LEU	2.0
4	E	285	ASN	2.0
2	B	337	ALA	2.0
6	L	35	ALA	2.0
1	A	216	VAL	2.0
1	A	227	GLN	2.0
3	F	403	SER	2.0
4	E	120	ASN	2.0
4	E	258	ASP	2.0
1	A	253	PHE	2.0
1	A	75	TYR	2.0
2	B	642	LYS	2.0
6	L	76	LEU	2.0
4	E	344	VAL	2.0
4	E	688	PHE	2.0
4	E	185	GLY	2.0
1	A	179	ASP	2.0
4	E	547	VAL	2.0
1	A	230	THR	2.0
3	F	109	LEU	2.0
4	E	640	PHE	2.0
4	E	647	PHE	2.0
4	E	745	GLU	2.0
7	H	221	VAL	2.0
2	B	325	TYR	2.0
4	E	443	LEU	2.0
4	E	618	SER	2.0
7	H	40	PRO	2.0
3	F	13	THR	2.0
2	B	355	ILE	2.0
4	E	280	LEU	2.0
2	B	488	HIS	2.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
4	E	878	HIS	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.