



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 01:47 PM GMT

PDB ID : 2PM9  
Title : Crystal structure of yeast Sec13/31 vertex element of the COPII vesicular coat  
Authors : Goldberg, J.; Fath, S.; Mancias, J.D.; Bi, X.  
Deposited on : 2007-04-20  
Resolution : 3.30 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>

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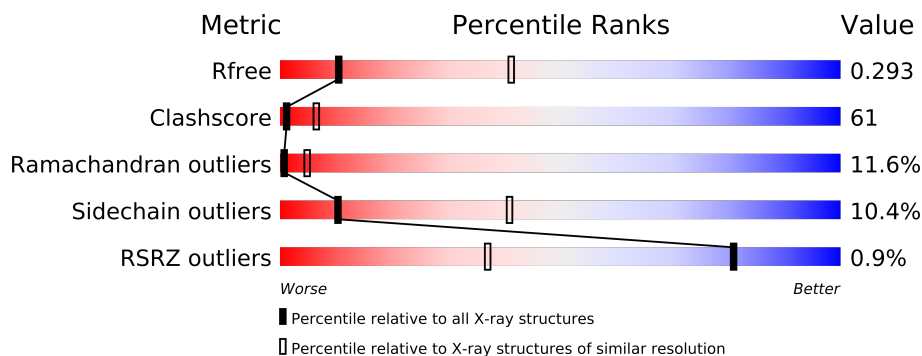
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 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 3.30 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	1341 (3.40-3.20)
Clashscore	79885	1696 (3.40-3.20)
Ramachandran outliers	78287	1664 (3.40-3.20)
Sidechain outliers	78261	1662 (3.40-3.20)
RSRZ outliers	66119	1342 (3.40-3.20)

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	416	
2	B	297	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5196 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 Protein transport protein SEC31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	384	Total	C	N	O	S	0	0	0
			2963	1862	506	588	7			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	CLONING ARTIFACT	UNP P38968
A	-3	ALA	-	CLONING ARTIFACT	UNP P38968
A	-2	MET	-	CLONING ARTIFACT	UNP P38968
A	-1	GLY	-	CLONING ARTIFACT	UNP P38968
A	0	SER	-	CLONING ARTIFACT	UNP P38968

- Molecule 2 is a protein called Protein transport protein SEC13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	280	Total	C	N	O	S	0	0	0
			2205	1402	376	418	9			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	11	MET	LEU	ENGINEERED	UNP Q04491
B	17	MET	LEU	ENGINEERED	UNP Q04491
B	24	MET	LEU	ENGINEERED	UNP Q04491
B	80	MET	LEU	ENGINEERED	UNP Q04491
B	115	MET	LEU	ENGINEERED	UNP Q04491
B	222	MET	LEU	ENGINEERED	UNP Q04491

- Molecule 3 is water.

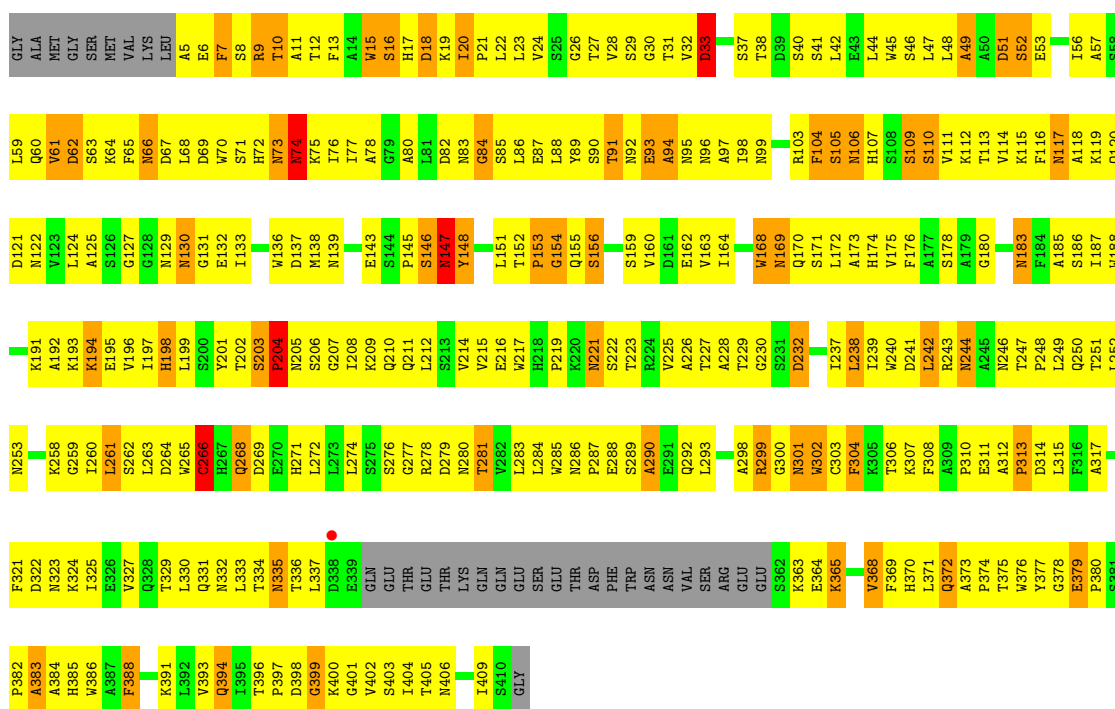
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	17	Total	O	0	0
			17	17		
3	B	11	Total	O	0	0
			11	11		

### 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.

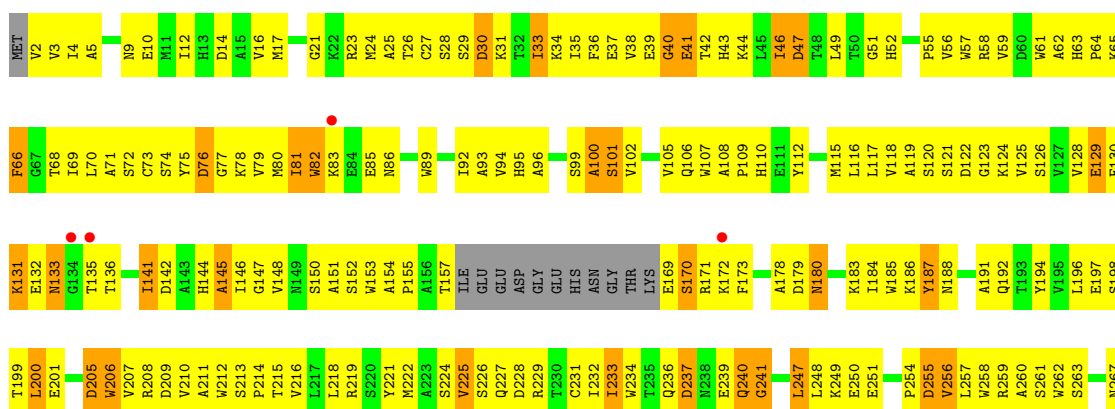
#### • Molecule 1: Protein transport protein SEC31

Chain A:



#### • Molecule 2: Protein transport protein SEC13

Chain B:



V268	L269	A270	L271	S272	G273	G274	D275	N276	K277	V278	T279	L280	W281	K282	E283	N284	L285	E286	G287	K288	W289	E290	P291	A292	GLY	GLU	VAL	HIS	GLN
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	155.16Å 155.16Å 59.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.30 37.95 – 3.30	Depositor EDS
% Data completeness (in resolution range)	86.9 (40.00-3.30) 86.9 (37.95-3.30)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.43 (at 3.32Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.251 , 0.305 0.242 , 0.293	Depositor DCC
$R_{free}$ test set	959 reflections (5.05%)	DCC
Wilson B-factor (Å <sup>2</sup> )	79.7	Xtriage
Anisotropy	0.326	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 37.4	EDS
Estimated twinning fraction	0.045 for h,-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 18996 reflections (0.005%)	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	5196	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% 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	0.48	0/3037	0.81	2/4140 (0.0%)
2	B	0.41	0/2265	0.67	0/3085
All	All	0.45	0/5302	0.75	2/7225 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	154	GLY	N-CA-C	5.10	125.85	113.10
1	A	156	SER	N-CA-C	5.09	124.75	111.00

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	2963	0	2842	384	0
2	B	2205	0	2132	254	0
3	A	17	0	0	2	0
3	B	11	0	0	3	0
All	All	5196	0	4974	623	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 61.



All (623) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:22:LEU:HD11	1:A:94:ALA:HB1	1.30	1.13
2:B:256:VAL:HG12	2:B:257:LEU:H	1.11	1.12
1:A:93:GLU:HB2	1:A:96:ASN:HD22	1.16	1.07
2:B:24:MET:HG2	2:B:25:ALA:H	1.18	1.03
2:B:46:ILE:HG22	2:B:47:ASP:H	1.20	1.03
1:A:304:PHE:HD2	1:A:304:PHE:H	1.04	1.01
1:A:268:GLN:HE21	1:A:313:PRO:HD3	1.19	1.01
2:B:69:ILE:HD11	2:B:83:LYS:HE2	1.44	0.98
2:B:80:MET:HG2	2:B:94:VAL:HG23	1.43	0.98
1:A:154:GLY:O	1:A:155:GLN:HG2	1.61	0.97
2:B:69:ILE:HG12	2:B:83:LYS:HG2	1.45	0.96
2:B:233:ILE:H	2:B:233:ILE:HD12	1.33	0.94
1:A:299:ARG:HE	1:A:323:ASN:HB2	1.33	0.94
1:A:22:LEU:CD1	1:A:94:ALA:HB1	1.98	0.93
1:A:93:GLU:HB2	1:A:96:ASN:ND2	1.81	0.93
1:A:31:THR:HG22	1:A:32:VAL:H	1.33	0.93
1:A:125:ALA:HB2	1:A:168:TRP:CH2	2.05	0.92
1:A:72:HIS:CE1	1:A:118:ALA:HA	2.04	0.92
1:A:364:GLU:O	1:A:365:LYS:HB2	1.66	0.92
1:A:10:THR:HG23	1:A:28:VAL:HG12	1.50	0.92
1:A:368:VAL:O	1:A:370:HIS:N	2.02	0.91
1:A:202:THR:C	1:A:204:PRO:HD2	1.90	0.91
1:A:16:SER:O	1:A:310:PRO:HG3	1.69	0.91
1:A:244:ASN:HD21	1:A:246:ASN:ND2	1.70	0.90
2:B:249:LYS:HE3	2:B:251:GLU:HB2	1.54	0.90
1:A:106:ASN:HD22	1:A:106:ASN:N	1.70	0.89
1:A:268:GLN:HE21	1:A:313:PRO:CD	1.87	0.87
1:A:202:THR:O	1:A:204:PRO:HD2	1.74	0.86
1:A:75:LYS:NZ	1:A:94:ALA:H	1.74	0.85
1:A:10:THR:CG2	1:A:28:VAL:HG12	2.06	0.85
2:B:180:ASN:N	2:B:180:ASN:HD22	1.72	0.85
2:B:73:CYS:HB3	2:B:79:VAL:HG12	1.59	0.84
2:B:24:MET:CG	2:B:25:ALA:H	1.90	0.84
1:A:73:ASN:O	1:A:75:LYS:N	2.11	0.84
1:A:117:ASN:HD22	1:A:118:ALA:N	1.75	0.83
2:B:69:ILE:CD1	2:B:83:LYS:HE2	2.07	0.83
1:A:119:LYS:HB2	1:A:173:ALA:HB2	1.59	0.83
2:B:256:VAL:HG12	2:B:257:LEU:N	1.92	0.83
1:A:30:GLY:HA3	1:A:321:PHE:HE2	1.44	0.83
1:A:268:GLN:NE2	1:A:313:PRO:HD3	1.94	0.82
2:B:83:LYS:HG3	2:B:92:ILE:HD13	1.62	0.82
2:B:79:VAL:HG23	2:B:95:HIS:HB3	1.60	0.82

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:150:SER:OG	2:B:209:ASP:HA	1.79	0.82
1:A:74:ASN:N	1:A:74:ASN:HD22	1.77	0.82
1:A:313:PRO:HB2	1:A:376:TRP:CH2	2.16	0.81
1:A:221:ASN:HD22	1:A:222:SER:N	1.79	0.81
1:A:300:GLY:O	1:A:301:ASN:HB2	1.81	0.81
1:A:31:THR:HG22	1:A:32:VAL:N	1.95	0.81
1:A:133:ILE:HD11	1:A:163:VAL:HG21	1.62	0.81
1:A:75:LYS:HZ1	1:A:94:ALA:H	1.25	0.80
2:B:46:ILE:HG22	2:B:47:ASP:N	1.95	0.80
1:A:370:HIS:CG	1:A:371:LEU:H	1.99	0.80
2:B:24:MET:HG2	2:B:25:ALA:N	1.96	0.80
1:A:292:GLN:O	1:A:368:VAL:HG23	1.82	0.80
1:A:268:GLN:HG3	1:A:313:PRO:HG3	1.65	0.79
1:A:19:LYS:O	1:A:21:PRO:HD3	1.82	0.78
1:A:80:ALA:HB1	1:A:111:VAL:HG12	1.65	0.78
1:A:72:HIS:O	1:A:74:ASN:ND2	2.16	0.78
1:A:74:ASN:H	1:A:74:ASN:HD22	1.30	0.78
1:A:56:ILE:HD13	1:A:95:ASN:HA	1.65	0.77
1:A:250:GLN:NE2	1:A:251:THR:H	1.81	0.77
1:A:93:GLU:CB	1:A:96:ASN:HD22	1.97	0.77
2:B:37:GLU:HG2	2:B:46:ILE:HD11	1.65	0.77
2:B:154:ALA:HB2	2:B:212:TRP:CZ3	2.20	0.77
2:B:65:LYS:HD3	2:B:110:HIS:HB2	1.68	0.76
1:A:174:HIS:NE2	1:A:191:LYS:HB2	1.99	0.76
2:B:33:ILE:HB	2:B:49:LEU:HD12	1.67	0.76
1:A:80:ALA:HB2	1:A:114:VAL:HG23	1.67	0.76
2:B:71:ALA:HB2	2:B:81:ILE:HG22	1.67	0.76
1:A:202:THR:C	1:A:204:PRO:CD	2.55	0.75
1:A:151:LEU:HD12	1:A:152:THR:H	1.51	0.75
2:B:117:LEU:HD23	2:B:151:ALA:O	1.86	0.75
1:A:196:VAL:HG23	1:A:197:ILE:HG13	1.66	0.75
1:A:85:SER:HB2	1:A:104:PHE:O	1.88	0.74
1:A:133:ILE:CD1	1:A:163:VAL:HG21	2.17	0.74
1:A:372:GLN:HG3	1:A:372:GLN:O	1.86	0.73
1:A:31:THR:CG2	1:A:32:VAL:H	2.02	0.73
2:B:225:VAL:HG22	2:B:257:LEU:HB3	1.70	0.73
1:A:276:SER:OG	1:A:303:CYS:HB2	1.88	0.73
2:B:282:LYS:HA	3:B:298:HOH:O	1.87	0.73
1:A:93:GLU:CB	1:A:96:ASN:ND2	2.52	0.73
2:B:83:LYS:HG3	2:B:92:ILE:HG21	1.68	0.73
1:A:10:THR:HG23	1:A:28:VAL:CG1	2.18	0.73
1:A:78:ALA:CB	1:A:114:VAL:HG11	2.19	0.73

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:46:ILE:HD12	2:B:46:ILE:N	2.04	0.72
2:B:224:SER:HB2	2:B:234:TRP:HE1	1.53	0.72
1:A:202:THR:OG1	1:A:209:LYS:HD3	1.90	0.72
2:B:16:VAL:HG12	2:B:61:TRP:HD1	1.54	0.71
1:A:171:SER:O	1:A:172:LEU:HD23	1.90	0.71
2:B:196:LEU:HD11	2:B:198:SER:O	1.90	0.71
1:A:73:ASN:C	1:A:75:LYS:H	1.92	0.71
2:B:73:CYS:CB	2:B:79:VAL:HG12	2.20	0.71
1:A:331:GLN:OE1	1:A:333:LEU:HD21	1.91	0.70
1:A:69:ASP:OD2	1:A:116:PHE:HB2	1.90	0.70
1:A:164:ILE:HG12	1:A:180:GLY:HA2	1.74	0.70
1:A:304:PHE:CD2	1:A:304:PHE:N	2.52	0.70
2:B:154:ALA:HB2	2:B:212:TRP:CE3	2.26	0.70
2:B:82:TRP:O	2:B:89:TRP:HZ3	1.74	0.70
2:B:256:VAL:CG1	2:B:257:LEU:H	1.94	0.69
2:B:225:VAL:HG22	2:B:257:LEU:HD13	1.71	0.69
2:B:233:ILE:HD12	2:B:233:ILE:N	2.05	0.69
1:A:117:ASN:HD22	1:A:118:ALA:H	1.39	0.69
1:A:203:SER:O	1:A:205:ASN:N	2.26	0.69
1:A:28:VAL:HG22	1:A:29:SER:H	1.58	0.69
1:A:109:SER:O	1:A:110:SER:HB2	1.91	0.69
2:B:105:VAL:HG22	2:B:116:LEU:HD11	1.75	0.69
1:A:313:PRO:HB2	1:A:376:TRP:CZ2	2.28	0.69
2:B:29:SER:C	2:B:31:LYS:H	1.95	0.69
2:B:227:GLN:HA	2:B:256:VAL:HG13	1.75	0.68
1:A:185:ALA:HB3	1:A:199:LEU:HB2	1.75	0.68
1:A:212:LEU:HD13	1:A:227:THR:HG21	1.74	0.68
1:A:94:ALA:O	1:A:95:ASN:HB2	1.92	0.68
1:A:19:LYS:HD2	2:B:206:TRP:HE1	1.58	0.67
1:A:86:LEU:CD2	1:A:104:PHE:HB2	2.24	0.67
2:B:16:VAL:HG12	2:B:61:TRP:CD1	2.29	0.67
1:A:75:LYS:NZ	1:A:94:ALA:HB2	2.08	0.67
1:A:249:LEU:O	1:A:249:LEU:HD23	1.94	0.67
2:B:200:LEU:HB3	2:B:234:TRP:CZ3	2.30	0.67
1:A:107:HIS:ND1	1:A:111:VAL:HG22	2.09	0.67
2:B:144:HIS:HB2	2:B:147:GLY:O	1.95	0.67
2:B:75:TYR:CD1	2:B:101:SER:HB2	2.30	0.66
1:A:124:LEU:HG	1:A:125:ALA:N	2.10	0.66
2:B:153:TRP:O	2:B:212:TRP:HB3	1.95	0.66
1:A:96:ASN:HB2	3:A:420:HOH:O	1.96	0.66
1:A:289:SER:OG	1:A:290:ALA:N	2.24	0.66
2:B:225:VAL:CG2	2:B:257:LEU:HB3	2.26	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:75:LYS:NZ	1:A:94:ALA:N	2.44	0.65
1:A:30:GLY:HA3	1:A:321:PHE:CE2	2.30	0.65
1:A:250:GLN:HE21	1:A:251:THR:H	1.45	0.65
1:A:125:ALA:HB2	1:A:168:TRP:HH2	1.62	0.65
2:B:2:VAL:HG13	2:B:41:GLU:HA	1.79	0.64
2:B:207:VAL:HA	2:B:226:SER:HB2	1.78	0.64
1:A:124:LEU:HG	1:A:125:ALA:H	1.62	0.64
1:A:400:LYS:HE2	2:B:9:ASN:O	1.98	0.64
2:B:49:LEU:HD22	2:B:82:TRP:CD2	2.32	0.64
1:A:20:ILE:O	1:A:20:ILE:HG13	1.97	0.64
1:A:325:ILE:N	1:A:325:ILE:HD12	2.12	0.64
2:B:52:HIS:N	3:B:307:HOH:O	2.29	0.64
2:B:184:ILE:HD11	2:B:222:MET:CE	2.28	0.64
2:B:225:VAL:CG2	2:B:257:LEU:HD13	2.28	0.63
1:A:241:ASP:C	1:A:243:ARG:H	2.02	0.63
1:A:78:ALA:HB3	1:A:114:VAL:HG11	1.80	0.63
1:A:280:ASN:C	1:A:298:ALA:HB3	2.19	0.63
1:A:206:SER:O	1:A:208:ILE:HG13	1.98	0.63
1:A:239:ILE:HB	1:A:250:GLN:HB3	1.81	0.63
1:A:212:LEU:HD22	1:A:227:THR:CG2	2.28	0.63
2:B:224:SER:CB	2:B:234:TRP:HE1	2.11	0.62
2:B:233:ILE:H	2:B:233:ILE:CD1	2.09	0.62
1:A:106:ASN:H	1:A:106:ASN:HD22	1.45	0.62
2:B:105:VAL:CG2	2:B:116:LEU:HD11	2.28	0.62
1:A:193:LYS:O	1:A:194:LYS:HB3	1.99	0.62
2:B:69:ILE:HD11	2:B:83:LYS:CE	2.25	0.62
1:A:221:ASN:C	1:A:221:ASN:HD22	2.01	0.62
2:B:147:GLY:N	2:B:178:ALA:HB3	2.15	0.62
1:A:51:ASP:O	1:A:53:GLU:HG3	1.99	0.62
2:B:249:LYS:CE	2:B:251:GLU:HB2	2.28	0.62
1:A:268:GLN:HB2	1:A:376:TRP:CE3	2.35	0.62
1:A:192:ALA:O	1:A:194:LYS:HG2	2.00	0.62
1:A:370:HIS:CG	1:A:371:LEU:N	2.68	0.62
1:A:153:PRO:HB2	1:A:188:TRP:CZ3	2.35	0.61
2:B:118:VAL:O	2:B:125:VAL:HG13	2.00	0.61
2:B:27:CYS:HB2	2:B:56:VAL:HG11	1.82	0.61
2:B:23:ARG:HA	2:B:36:PHE:O	2.01	0.61
2:B:233:ILE:HD11	2:B:248:LEU:HD13	1.82	0.61
1:A:393:VAL:O	1:A:394:GLN:HB3	2.00	0.61
1:A:386:TRP:NE1	2:B:270:ALA:HB2	2.15	0.61
2:B:81:ILE:HD13	2:B:81:ILE:H	1.66	0.61
2:B:172:LYS:HA	2:B:185:TRP:O	2.01	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:78:ALA:HB1	1:A:114:VAL:HG11	1.84	0.60
2:B:106:GLN:O	2:B:116:LEU:HD12	2.01	0.60
1:A:402:VAL:CG1	1:A:403:SER:N	2.65	0.60
1:A:71:SER:O	1:A:73:ASN:N	2.34	0.60
2:B:247:LEU:HD13	2:B:249:LYS:O	2.02	0.60
1:A:92:ASN:O	1:A:93:GLU:HB2	2.02	0.60
1:A:244:ASN:ND2	1:A:246:ASN:ND2	2.47	0.60
2:B:115:MET:HG2	2:B:129:GLU:HB2	1.82	0.60
1:A:202:THR:O	1:A:202:THR:HG22	2.01	0.60
1:A:217:TRP:CD2	1:A:225:VAL:HG22	2.37	0.60
1:A:330:LEU:O	1:A:371:LEU:HD21	2.02	0.59
1:A:241:ASP:OD1	1:A:243:ARG:HB2	2.00	0.59
2:B:14:ASP:OD2	2:B:59:VAL:HG22	2.01	0.59
2:B:274:GLY:C	2:B:276:ASN:H	2.03	0.59
1:A:272:LEU:HD22	1:A:284:LEU:HD11	1.83	0.59
2:B:219:ARG:HG3	2:B:221:TYR:CE1	2.37	0.59
1:A:306:THR:HA	1:A:317:ALA:O	2.03	0.59
2:B:249:LYS:HG2	2:B:251:GLU:OE1	2.03	0.59
2:B:169:GLU:HG2	2:B:187:TYR:HD2	1.67	0.59
1:A:40:SER:OG	1:A:61:VAL:HG23	2.03	0.59
2:B:81:ILE:N	2:B:81:ILE:HD13	2.18	0.59
1:A:289:SER:O	1:A:290:ALA:HB2	2.03	0.59
1:A:112:LYS:HG3	1:A:164:ILE:HG22	1.85	0.59
1:A:227:THR:O	1:A:227:THR:HG22	2.02	0.59
2:B:225:VAL:HG22	2:B:257:LEU:CD1	2.32	0.59
2:B:147:GLY:H	2:B:178:ALA:HB3	1.66	0.59
2:B:28:SER:OG	2:B:29:SER:N	2.35	0.58
1:A:15:TRP:HB3	1:A:310:PRO:HD3	1.85	0.58
1:A:187:ILE:HG22	1:A:196:VAL:HG22	1.83	0.58
2:B:4:ILE:HD12	2:B:4:ILE:N	2.18	0.58
1:A:106:ASN:ND2	1:A:106:ASN:N	2.42	0.58
1:A:402:VAL:HG12	1:A:403:SER:N	2.18	0.58
1:A:88:LEU:HD13	1:A:138:MET:SD	2.43	0.58
1:A:268:GLN:HG3	1:A:313:PRO:CG	2.34	0.58
1:A:228:ALA:HB2	1:A:263:LEU:HD11	1.85	0.58
1:A:129:ASN:HA	1:A:162:GLU:HB3	1.84	0.58
2:B:37:GLU:HB2	2:B:44:LYS:HB3	1.85	0.58
1:A:228:ALA:HB1	1:A:260:ILE:HG21	1.85	0.58
1:A:146:SER:O	1:A:147:ASN:HB2	2.02	0.58
1:A:306:THR:O	1:A:307:LYS:HD3	2.04	0.58
2:B:196:LEU:HD12	2:B:197:GLU:H	1.66	0.58
2:B:187:TYR:CG	2:B:188:ASN:N	2.71	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:283:LEU:HD22	1:A:292:GLN:HE21	1.69	0.58
1:A:329:THR:HB	1:A:331:GLN:O	2.04	0.58
1:A:280:ASN:HB3	1:A:300:GLY:C	2.24	0.58
1:A:147:ASN:O	1:A:148:TYR:C	2.42	0.58
2:B:4:ILE:O	2:B:4:ILE:HG22	2.04	0.57
2:B:257:LEU:HD23	2:B:273:GLY:HA2	1.87	0.57
1:A:365:LYS:HD2	1:A:365:LYS:O	2.04	0.57
1:A:11:ALA:HB1	1:A:26:GLY:O	2.04	0.57
1:A:44:LEU:HD23	1:A:56:ILE:HB	1.86	0.57
1:A:221:ASN:ND2	1:A:223:THR:H	2.03	0.57
1:A:84:GLY:HA3	1:A:110:SER:H	1.68	0.57
1:A:396:THR:HB	1:A:397:PRO:CD	2.34	0.57
2:B:29:SER:O	2:B:31:LYS:N	2.37	0.57
1:A:382:PRO:HB2	2:B:278:VAL:HG23	1.86	0.57
1:A:113:THR:HG22	1:A:114:VAL:N	2.20	0.57
1:A:155:GLN:CB	1:A:195:GLU:HB3	2.35	0.57
2:B:130:PHE:HA	2:B:136:THR:HG22	1.86	0.57
1:A:262:SER:HB2	1:A:304:PHE:O	2.05	0.56
1:A:72:HIS:ND1	1:A:118:ALA:HA	2.19	0.56
1:A:145:PRO:O	1:A:147:ASN:N	2.39	0.56
1:A:75:LYS:HZ1	1:A:94:ALA:HB2	1.68	0.56
1:A:241:ASP:O	1:A:243:ARG:N	2.38	0.56
1:A:175:VAL:HG12	1:A:176:PHE:N	2.18	0.56
1:A:71:SER:HA	1:A:116:PHE:CG	2.40	0.56
1:A:21:PRO:HB2	1:A:47:LEU:HD11	1.86	0.56
1:A:74:ASN:ND2	1:A:74:ASN:N	2.50	0.56
2:B:80:MET:CG	2:B:94:VAL:HG23	2.27	0.56
1:A:280:ASN:HB3	1:A:300:GLY:O	2.06	0.56
1:A:377:TYR:HD2	2:B:57:TRP:CZ2	2.24	0.56
1:A:105:SER:C	1:A:107:HIS:H	2.09	0.56
2:B:155:PRO:HG2	2:B:214:PRO:HA	1.88	0.56
1:A:17:HIS:HB2	1:A:73:ASN:HB2	1.87	0.56
1:A:62:ASP:CG	1:A:103:ARG:HH12	2.08	0.56
1:A:12:THR:O	1:A:12:THR:HG23	2.06	0.56
2:B:25:ALA:HB1	2:B:70:LEU:HD21	1.86	0.55
2:B:81:ILE:HG12	2:B:92:ILE:HG13	1.88	0.55
1:A:260:ILE:CG2	1:A:261:LEU:N	2.69	0.55
2:B:239:GLU:N	3:B:304:HOH:O	2.38	0.55
1:A:120:GLN:HG3	1:A:122:ASN:OD1	2.06	0.55
2:B:74:SER:HB3	2:B:76:ASP:OD1	2.06	0.55
1:A:153:PRO:HB2	1:A:188:TRP:CE3	2.41	0.55
1:A:379:GLU:HG2	1:A:379:GLU:O	2.06	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:129:ASN:ND2	1:A:162:GLU:OE1	2.38	0.55
2:B:10:GLU:HG3	2:B:30:ASP:HB3	1.87	0.55
1:A:203:SER:N	1:A:204:PRO:CD	2.69	0.55
2:B:196:LEU:HG	2:B:197:GLU:N	2.20	0.55
2:B:39:GLU:O	2:B:41:GLU:N	2.33	0.55
1:A:80:ALA:HB2	1:A:114:VAL:CG2	2.36	0.55
2:B:29:SER:C	2:B:31:LYS:N	2.59	0.55
1:A:74:ASN:ND2	1:A:74:ASN:H	2.02	0.55
1:A:42:LEU:HD21	1:A:89:TYR:CD1	2.41	0.55
1:A:87:GLU:HG2	1:A:89:TYR:CE2	2.41	0.55
1:A:75:LYS:HZ1	1:A:94:ALA:N	2.01	0.55
1:A:74:ASN:O	1:A:76:ILE:HG12	2.06	0.55
2:B:150:SER:HB2	2:B:210:VAL:HG22	1.88	0.55
2:B:225:VAL:HG22	2:B:257:LEU:CB	2.37	0.55
1:A:312:ALA:CB	1:A:315:LEU:HD12	2.36	0.55
1:A:247:THR:CG2	1:A:248:PRO:HD2	2.37	0.55
2:B:236:GLN:HG2	2:B:237:ASP:N	2.22	0.55
2:B:283:GLU:HA	2:B:288:LYS:O	2.07	0.55
1:A:41:SER:O	1:A:42:LEU:HB3	2.07	0.55
1:A:199:LEU:HD13	1:A:240:TRP:CG	2.42	0.55
1:A:46:SER:HB2	1:A:56:ILE:HD11	1.90	0.54
2:B:59:VAL:HG12	2:B:72:SER:HA	1.89	0.54
1:A:365:LYS:NZ	1:A:371:LEU:HD22	2.21	0.54
2:B:183:LYS:HB2	2:B:185:TRP:HE1	1.72	0.54
2:B:155:PRO:CG	2:B:214:PRO:HA	2.37	0.54
1:A:38:THR:O	1:A:64:LYS:HE2	2.07	0.54
1:A:409:ILE:HD12	1:A:409:ILE:H	1.72	0.54
1:A:80:ALA:CB	1:A:111:VAL:HG12	2.37	0.54
1:A:162:GLU:O	1:A:164:ILE:HG23	2.06	0.54
1:A:62:ASP:OD2	1:A:62:ASP:N	2.36	0.54
1:A:59:LEU:HD22	1:A:98:ILE:HG12	1.90	0.54
1:A:292:GLN:O	1:A:368:VAL:CG2	2.53	0.54
1:A:178:SER:HB2	1:A:186:SER:HB2	1.89	0.54
1:A:394:GLN:HG3	1:A:403:SER:HB3	1.88	0.54
2:B:184:ILE:CG1	2:B:198:SER:HB2	2.38	0.54
1:A:399:GLY:O	2:B:12:ILE:HG13	2.07	0.54
2:B:17:MET:C	2:B:61:TRP:CD1	2.81	0.54
2:B:71:ALA:CB	2:B:81:ILE:HG22	2.37	0.54
1:A:364:GLU:O	1:A:365:LYS:CB	2.47	0.54
2:B:145:ALA:HB3	2:B:179:ASP:HB3	1.89	0.54
1:A:104:PHE:N	1:A:104:PHE:CD1	2.75	0.54
1:A:106:ASN:ND2	1:A:106:ASN:H	2.04	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:52:HIS:CE1	2:B:80:MET:HE3	2.43	0.54
2:B:229:ARG:HG2	2:B:256:VAL:HA	1.90	0.54
2:B:184:ILE:HG12	2:B:198:SER:HB2	1.88	0.54
2:B:208:ARG:H	2:B:226:SER:HA	1.72	0.53
1:A:48:LEU:O	1:A:49:ALA:O	2.25	0.53
2:B:92:ILE:HG13	2:B:93:ALA:H	1.73	0.53
2:B:2:VAL:O	2:B:2:VAL:HG12	2.07	0.53
1:A:7:PHE:O	1:A:324:LYS:HD3	2.09	0.53
1:A:66:ASN:N	1:A:80:ALA:O	2.39	0.53
1:A:90:SER:O	1:A:91:THR:HB	2.09	0.53
1:A:129:ASN:C	1:A:131:GLY:H	2.11	0.53
1:A:13:PHE:HA	1:A:24:VAL:O	2.09	0.53
2:B:25:ALA:HA	2:B:34:LYS:O	2.08	0.53
2:B:24:MET:CG	2:B:25:ALA:N	2.60	0.53
2:B:119:ALA:HB2	2:B:151:ALA:HB2	1.91	0.53
1:A:393:VAL:HG13	1:A:404:ILE:HD13	1.89	0.53
1:A:57:ALA:O	1:A:98:ILE:HG22	2.09	0.53
1:A:26:GLY:HA2	1:A:42:LEU:HA	1.89	0.53
2:B:46:ILE:CD1	2:B:46:ILE:N	2.71	0.53
2:B:184:ILE:HD11	2:B:222:MET:HE3	1.89	0.53
1:A:175:VAL:HG13	1:A:188:TRP:O	2.08	0.53
1:A:244:ASN:HD21	1:A:246:ASN:HD22	1.49	0.53
2:B:215:THR:O	2:B:215:THR:HG23	2.08	0.52
2:B:260:ALA:HA	2:B:271:LEU:HD12	1.89	0.52
2:B:78:LYS:HG2	2:B:96:ALA:CB	2.40	0.52
1:A:110:SER:OG	1:A:129:ASN:ND2	2.42	0.52
1:A:285:TRP:CZ3	1:A:292:GLN:HG3	2.44	0.52
2:B:108:ALA:HB2	2:B:153:TRP:CZ2	2.44	0.52
1:A:286:ASN:HB2	1:A:293:LEU:HD11	1.92	0.52
1:A:384:ALA:O	1:A:385:HIS:ND1	2.42	0.52
2:B:188:ASN:HB3	2:B:191:ALA:HB3	1.92	0.52
1:A:261:LEU:HB2	1:A:277:GLY:HA2	1.92	0.52
1:A:199:LEU:HD13	1:A:240:TRP:CD2	2.44	0.52
1:A:145:PRO:O	1:A:146:SER:C	2.48	0.52
1:A:252:LEU:HD13	1:A:285:TRP:CG	2.45	0.52
1:A:259:GLY:HA3	1:A:278:ARG:HH11	1.74	0.52
2:B:180:ASN:CG	2:B:205:ASP:O	2.49	0.51
1:A:137:ASP:OD1	1:A:139:ASN:HB2	2.10	0.51
2:B:123:GLY:HA2	2:B:147:GLY:HA2	1.92	0.51
1:A:22:LEU:CD1	1:A:94:ALA:CB	2.82	0.51
1:A:70:TRP:HD1	1:A:71:SER:O	1.94	0.51
1:A:72:HIS:HE1	1:A:118:ALA:HA	1.72	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:231:CYS:HB3	2:B:248:LEU:HD22	1.92	0.51
2:B:233:ILE:HG21	2:B:289:TRP:CZ2	2.45	0.51
2:B:63:HIS:ND1	2:B:64:PRO:HD2	2.26	0.51
2:B:259:ARG:HG3	2:B:259:ARG:HH11	1.76	0.51
1:A:396:THR:HB	1:A:397:PRO:HD2	1.92	0.51
2:B:65:LYS:CD	2:B:110:HIS:HB2	2.40	0.51
1:A:27:THR:HB	1:A:40:SER:CB	2.40	0.51
2:B:171:ARG:O	2:B:186:LYS:HA	2.11	0.51
2:B:69:ILE:CG1	2:B:83:LYS:HG2	2.32	0.51
1:A:155:GLN:HG3	1:A:194:LYS:HB2	1.92	0.51
1:A:212:LEU:HD13	1:A:227:THR:CG2	2.41	0.51
2:B:23:ARG:NH1	2:B:68:THR:CG2	2.74	0.51
1:A:15:TRP:HB3	1:A:310:PRO:CD	2.41	0.51
2:B:206:TRP:CD1	2:B:206:TRP:N	2.78	0.50
1:A:237:ILE:HB	1:A:252:LEU:HB2	1.93	0.50
1:A:172:LEU:C	1:A:174:HIS:H	2.13	0.50
1:A:378:GLY:O	1:A:380:PRO:HD2	2.11	0.50
1:A:333:LEU:HG	2:B:100:ALA:HA	1.93	0.50
2:B:99:SER:O	2:B:100:ALA:CB	2.58	0.50
1:A:271:HIS:O	1:A:272:LEU:HD23	2.12	0.50
1:A:274:LEU:HG	1:A:308:PHE:CZ	2.46	0.50
1:A:304:PHE:HD2	1:A:304:PHE:N	1.87	0.50
1:A:312:ALA:HB1	1:A:315:LEU:HD12	1.92	0.50
2:B:94:VAL:O	2:B:94:VAL:HG13	2.11	0.50
2:B:286:GLU:HG3	2:B:288:LYS:HD2	1.94	0.50
2:B:47:ASP:OD2	2:B:89:TRP:HB2	2.12	0.50
2:B:79:VAL:CG2	2:B:95:HIS:HB3	2.35	0.50
1:A:241:ASP:C	1:A:243:ARG:N	2.64	0.50
1:A:28:VAL:HG22	1:A:29:SER:N	2.26	0.50
2:B:27:CYS:HB2	2:B:56:VAL:CG1	2.41	0.50
1:A:283:LEU:HD13	1:A:292:GLN:NE2	2.26	0.50
2:B:131:LYS:HB3	2:B:132:GLU:OE2	2.12	0.50
1:A:57:ALA:O	1:A:98:ILE:CG2	2.60	0.49
1:A:268:GLN:HE21	1:A:313:PRO:CG	2.25	0.49
2:B:85:GLU:O	2:B:86:ASN:HB2	2.11	0.49
1:A:15:TRP:HZ3	1:A:307:LYS:O	1.96	0.49
1:A:11:ALA:HB3	1:A:325:ILE:HD11	1.93	0.49
1:A:325:ILE:N	1:A:325:ILE:CD1	2.76	0.49
2:B:59:VAL:HA	2:B:71:ALA:O	2.12	0.49
1:A:117:ASN:ND2	1:A:118:ALA:N	2.54	0.49
1:A:130:ASN:HB3	1:A:132:GLU:HG3	1.95	0.49
2:B:92:ILE:HG13	2:B:93:ALA:N	2.27	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:365:LYS:HZ3	1:A:371:LEU:HD22	1.78	0.49
2:B:29:SER:HA	2:B:55:PRO:HB3	1.93	0.49
1:A:335:ASN:OD1	2:B:99:SER:HB3	2.11	0.49
1:A:264:ASP:HB2	1:A:307:LYS:HD3	1.94	0.49
2:B:180:ASN:N	2:B:180:ASN:ND2	2.46	0.49
1:A:29:SER:HB2	1:A:82:ASP:OD1	2.13	0.49
2:B:259:ARG:HB2	2:B:272:SER:HB2	1.95	0.49
1:A:203:SER:C	1:A:205:ASN:H	2.17	0.49
2:B:274:GLY:C	2:B:276:ASN:N	2.67	0.49
1:A:19:LYS:C	1:A:21:PRO:HD3	2.33	0.49
2:B:52:HIS:ND1	2:B:74:SER:HB2	2.28	0.49
1:A:187:ILE:HB	1:A:197:ILE:HB	1.95	0.49
1:A:75:LYS:HZ1	1:A:94:ALA:CB	2.25	0.48
1:A:397:PRO:HA	2:B:276:ASN:HD21	1.78	0.48
1:A:109:SER:O	1:A:110:SER:CB	2.61	0.48
2:B:10:GLU:CG	2:B:30:ASP:HB3	2.43	0.48
2:B:75:TYR:C	2:B:77:GLY:H	2.17	0.48
2:B:78:LYS:HG2	2:B:96:ALA:HB1	1.94	0.48
2:B:24:MET:HB3	2:B:36:PHE:HB2	1.96	0.48
2:B:46:ILE:CG2	2:B:47:ASP:H	1.99	0.48
2:B:205:ASP:H	2:B:228:ASP:HB3	1.78	0.48
2:B:129:GLU:HG2	2:B:130:PHE:N	2.27	0.48
1:A:115:LYS:O	1:A:124:LEU:HD12	2.13	0.48
1:A:124:LEU:CG	1:A:125:ALA:H	2.24	0.48
2:B:52:HIS:CG	2:B:80:MET:HE1	2.48	0.48
1:A:196:VAL:C	1:A:197:ILE:HG13	2.32	0.48
1:A:19:LYS:HD2	2:B:206:TRP:NE1	2.27	0.48
1:A:42:LEU:CD2	1:A:98:ILE:HD11	2.44	0.48
2:B:95:HIS:CE1	2:B:128:VAL:HG21	2.48	0.48
1:A:31:THR:O	1:A:32:VAL:HG23	2.13	0.48
1:A:284:LEU:HD23	1:A:371:LEU:HD11	1.95	0.48
2:B:109:PRO:HD2	2:B:112:TYR:CD1	2.49	0.48
1:A:154:GLY:O	1:A:155:GLN:CG	2.48	0.48
2:B:157:THR:HB	2:B:170:SER:OG	2.14	0.48
1:A:186:SER:HB3	1:A:188:TRP:NE1	2.29	0.48
2:B:196:LEU:CG	2:B:197:GLU:N	2.77	0.48
1:A:33:ASP:OD1	1:A:37:SER:HB3	2.13	0.48
1:A:75:LYS:HD2	1:A:91:THR:HG22	1.95	0.48
1:A:114:VAL:HA	1:A:125:ALA:O	2.14	0.47
2:B:82:TRP:N	2:B:82:TRP:CD1	2.82	0.47
2:B:210:VAL:O	2:B:210:VAL:HG23	2.14	0.47
2:B:40:GLY:O	2:B:41:GLU:CG	2.62	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:102:VAL:HA	2:B:120:SER:HA	1.95	0.47
2:B:209:ASP:HB2	2:B:258:TRP:O	2.15	0.47
1:A:219:PRO:HG3	1:A:266:CYS:O	2.13	0.47
2:B:141:ILE:O	2:B:141:ILE:HD13	2.14	0.47
1:A:16:SER:HB2	1:A:18:ASP:OD1	2.14	0.47
1:A:10:THR:O	1:A:11:ALA:HB2	2.14	0.47
1:A:386:TRP:CG	2:B:263:SER:HA	2.49	0.47
2:B:24:MET:O	2:B:61:TRP:HZ2	1.97	0.47
1:A:115:LYS:O	1:A:168:TRP:HZ3	1.97	0.47
2:B:71:ALA:HB2	2:B:81:ILE:CG2	2.40	0.47
1:A:386:TRP:CZ2	2:B:280:LEU:HD22	2.50	0.47
1:A:73:ASN:C	1:A:75:LYS:N	2.59	0.47
2:B:31:LYS:HB3	2:B:52:HIS:O	2.15	0.47
1:A:271:HIS:CE1	1:A:288:GLU:OE2	2.67	0.47
2:B:108:ALA:HB3	2:B:115:MET:HB2	1.96	0.47
1:A:92:ASN:O	1:A:93:GLU:CB	2.62	0.47
1:A:402:VAL:CG1	1:A:403:SER:H	2.27	0.47
1:A:91:THR:O	1:A:91:THR:HG22	2.14	0.47
1:A:15:TRP:CZ3	1:A:317:ALA:N	2.83	0.47
1:A:172:LEU:C	1:A:174:HIS:N	2.69	0.47
1:A:404:ILE:HB	2:B:2:VAL:HB	1.97	0.47
2:B:124:LYS:HG2	2:B:142:ASP:OD1	2.15	0.47
2:B:216:VAL:HG12	2:B:216:VAL:O	2.15	0.46
1:A:124:LEU:CG	1:A:125:ALA:N	2.76	0.46
1:A:68:LEU:HA	1:A:78:ALA:O	2.15	0.46
2:B:23:ARG:NH1	2:B:68:THR:HG21	2.29	0.46
2:B:99:SER:O	2:B:100:ALA:HB2	2.15	0.46
2:B:131:LYS:HD2	2:B:135:THR:O	2.14	0.46
1:A:183:ASN:HA	1:A:211:GLN:HA	1.97	0.46
1:A:78:ALA:HB3	1:A:114:VAL:CG1	2.45	0.46
1:A:252:LEU:HD13	1:A:285:TRP:CB	2.46	0.46
2:B:194:TYR:HD1	2:B:194:TYR:H	1.63	0.46
1:A:312:ALA:O	1:A:314:ASP:N	2.48	0.46
2:B:247:LEU:HD23	2:B:247:LEU:HA	1.79	0.46
1:A:212:LEU:HD22	1:A:227:THR:HG22	1.98	0.46
2:B:152:SER:CB	2:B:211:ALA:HA	2.45	0.46
1:A:51:ASP:O	1:A:52:SER:C	2.54	0.46
2:B:118:VAL:HB	2:B:126:SER:OG	2.15	0.46
1:A:45:TRP:N	1:A:45:TRP:CD1	2.84	0.46
1:A:203:SER:C	1:A:205:ASN:N	2.69	0.46
1:A:127:GLY:HA2	1:A:132:GLU:O	2.16	0.46
1:A:202:THR:CG2	1:A:209:LYS:HD3	2.46	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:400:LYS:O	2:B:12:ILE:HD11	2.16	0.46
2:B:226:SER:OG	2:B:227:GLN:N	2.49	0.46
2:B:14:ASP:HB3	2:B:27:CYS:SG	2.55	0.46
2:B:59:VAL:HG12	2:B:72:SER:CB	2.46	0.46
1:A:404:ILE:O	1:A:405:THR:HG23	2.16	0.46
1:A:259:GLY:HA3	1:A:278:ARG:NH1	2.31	0.46
2:B:284:ASN:HB3	2:B:290:GLU:CD	2.36	0.46
1:A:221:ASN:C	1:A:221:ASN:ND2	2.69	0.46
2:B:85:GLU:HG2	2:B:86:ASN:ND2	2.31	0.46
1:A:42:LEU:HD23	1:A:98:ILE:HD11	1.96	0.46
1:A:331:GLN:HG2	1:A:371:LEU:HD23	1.96	0.46
2:B:75:TYR:O	2:B:77:GLY:N	2.49	0.46
1:A:260:ILE:HG23	1:A:261:LEU:N	2.31	0.46
2:B:120:SER:O	2:B:148:VAL:HG23	2.16	0.45
2:B:255:ASP:HB2	2:B:275:ASP:HB3	1.98	0.45
2:B:271:LEU:HA	2:B:271:LEU:HD12	1.57	0.45
1:A:212:LEU:HB3	1:A:227:THR:HG23	1.98	0.45
2:B:146:ILE:HB	2:B:178:ALA:HB3	1.96	0.45
1:A:409:ILE:HD12	1:A:409:ILE:N	2.31	0.45
1:A:63:SER:HB3	1:A:82:ASP:HB2	1.98	0.45
2:B:37:GLU:O	2:B:43:HIS:HA	2.15	0.45
2:B:200:LEU:HD13	2:B:234:TRP:CE3	2.51	0.45
1:A:371:LEU:O	1:A:372:GLN:C	2.55	0.45
1:A:15:TRP:CH2	1:A:317:ALA:HB2	2.52	0.45
1:A:133:ILE:HD11	1:A:163:VAL:CG2	2.41	0.45
1:A:151:LEU:CD1	1:A:152:THR:H	2.25	0.45
1:A:5:ALA:N	3:A:426:HOH:O	2.49	0.45
1:A:155:GLN:HB3	1:A:195:GLU:HB3	1.99	0.45
1:A:382:PRO:O	1:A:383:ALA:C	2.55	0.45
1:A:274:LEU:HD23	1:A:274:LEU:HA	1.69	0.45
1:A:162:GLU:HG3	1:A:164:ILE:HG23	1.99	0.45
1:A:169:ASN:OD1	1:A:172:LEU:HB2	2.16	0.45
1:A:197:ILE:HG22	1:A:198:HIS:N	2.32	0.45
1:A:75:LYS:HZ2	1:A:94:ALA:N	2.14	0.45
2:B:224:SER:HB2	2:B:234:TRP:NE1	2.28	0.45
1:A:119:LYS:CB	1:A:173:ALA:HB2	2.41	0.45
1:A:374:PRO:O	1:A:377:TYR:HB2	2.17	0.45
1:A:279:ASP:OD2	1:A:281:THR:HG22	2.16	0.45
1:A:269:ASP:OD1	1:A:375:THR:HG23	2.16	0.45
1:A:219:PRO:HD3	1:A:265:TRP:CD1	2.51	0.45
1:A:68:LEU:HD22	1:A:77:ILE:HG22	1.98	0.45
1:A:86:LEU:HD21	1:A:104:PHE:HB2	1.99	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:289:SER:O	1:A:290:ALA:CB	2.65	0.45
1:A:27:THR:O	1:A:65:PHE:HB2	2.17	0.45
1:A:378:GLY:O	1:A:380:PRO:CD	2.65	0.45
2:B:72:SER:O	2:B:79:VAL:HA	2.17	0.44
2:B:233:ILE:HG21	2:B:289:TRP:HZ2	1.82	0.44
1:A:169:ASN:HB3	1:A:172:LEU:O	2.16	0.44
1:A:86:LEU:HD23	1:A:104:PHE:HB2	1.96	0.44
2:B:63:HIS:HB3	2:B:66:PHE:CE1	2.53	0.44
1:A:312:ALA:N	1:A:313:PRO:CD	2.80	0.44
2:B:121:SER:C	2:B:123:GLY:H	2.20	0.44
1:A:232:ASP:O	1:A:258:LYS:HA	2.17	0.44
1:A:268:GLN:HG3	1:A:313:PRO:CB	2.46	0.44
2:B:38:VAL:HA	2:B:42:THR:O	2.18	0.44
2:B:52:HIS:ND1	2:B:74:SER:CB	2.81	0.44
1:A:232:ASP:HA	1:A:259:GLY:H	1.83	0.44
1:A:24:VAL:CG2	1:A:70:TRP:CZ3	3.01	0.44
1:A:162:GLU:HG3	1:A:164:ILE:CG2	2.48	0.44
2:B:184:ILE:O	2:B:196:LEU:HD12	2.18	0.44
1:A:155:GLN:HB2	1:A:195:GLU:HB3	1.99	0.44
2:B:240:GLN:O	2:B:241:GLY:C	2.55	0.44
1:A:116:PHE:CE2	1:A:124:LEU:HD13	2.53	0.43
1:A:129:ASN:HA	1:A:162:GLU:CB	2.47	0.43
1:A:299:ARG:HD2	1:A:299:ARG:HA	1.86	0.43
1:A:272:LEU:HA	1:A:272:LEU:HD23	1.81	0.43
1:A:249:LEU:C	1:A:249:LEU:HD23	2.38	0.43
2:B:259:ARG:HG3	2:B:259:ARG:NH1	2.33	0.43
2:B:26:THR:O	2:B:33:ILE:HA	2.18	0.43
1:A:242:LEU:N	1:A:242:LEU:HD23	2.33	0.43
1:A:42:LEU:O	1:A:42:LEU:HG	2.18	0.43
1:A:193:LYS:O	1:A:194:LYS:CB	2.65	0.43
2:B:58:ARG:HB2	2:B:58:ARG:HE	1.60	0.43
1:A:204:PRO:HG2	1:A:208:ILE:O	2.18	0.43
1:A:232:ASP:HA	1:A:259:GLY:N	2.33	0.43
1:A:201:TYR:CD2	1:A:238:LEU:HD11	2.54	0.43
1:A:252:LEU:HD13	1:A:285:TRP:CD2	2.53	0.43
1:A:204:PRO:C	1:A:206:SER:H	2.19	0.43
1:A:223:THR:O	1:A:241:ASP:HA	2.19	0.43
2:B:39:GLU:HB2	2:B:42:THR:OG1	2.18	0.43
1:A:396:THR:HG23	1:A:401:GLY:O	2.19	0.43
1:A:211:GLN:O	1:A:229:THR:HA	2.19	0.43
1:A:93:GLU:O	1:A:94:ALA:C	2.57	0.43
1:A:22:LEU:HD21	1:A:95:ASN:ND2	2.34	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:105:SER:C	1:A:107:HIS:N	2.71	0.43
2:B:231:CYS:HB2	2:B:271:LEU:HD21	2.00	0.43
1:A:88:LEU:CD1	1:A:138:MET:SD	3.06	0.43
1:A:67:ASP:OD1	1:A:113:THR:HG23	2.18	0.42
2:B:49:LEU:HD22	2:B:82:TRP:CG	2.54	0.42
1:A:202:THR:O	1:A:202:THR:CG2	2.67	0.42
2:B:68:THR:HG22	2:B:89:TRP:CH2	2.54	0.42
2:B:201:GLU:O	2:B:234:TRP:HH2	2.02	0.42
1:A:204:PRO:HG3	1:A:210:GLN:HG3	2.00	0.42
2:B:219:ARG:CG	2:B:221:TYR:CE1	3.02	0.42
1:A:373:ALA:HA	1:A:374:PRO:HD2	1.85	0.42
1:A:331:GLN:NE2	2:B:75:TYR:CZ	2.88	0.42
1:A:15:TRP:HZ3	1:A:317:ALA:H	1.67	0.42
1:A:388:PHE:O	1:A:391:LYS:HG3	2.20	0.42
2:B:23:ARG:HD3	2:B:61:TRP:CH2	2.54	0.42
1:A:196:VAL:O	1:A:197:ILE:HG13	2.19	0.42
2:B:62:ALA:HB2	2:B:107:TRP:CE2	2.55	0.42
1:A:31:THR:OG1	1:A:321:PHE:HD2	2.03	0.42
2:B:213:SER:OG	2:B:214:PRO:HD2	2.19	0.42
2:B:3:VAL:HG12	2:B:5:ALA:N	2.34	0.42
1:A:237:ILE:N	1:A:237:ILE:HD12	2.35	0.42
1:A:27:THR:HB	1:A:40:SER:HB2	2.01	0.42
2:B:213:SER:OG	2:B:215:THR:HG22	2.20	0.42
1:A:120:GLN:C	1:A:122:ASN:H	2.22	0.42
1:A:7:PHE:N	1:A:7:PHE:CD1	2.87	0.42
2:B:33:ILE:HD13	2:B:72:SER:HB3	2.02	0.42
2:B:179:ASP:C	2:B:180:ASN:HD22	2.20	0.42
2:B:35:ILE:HG13	2:B:89:TRP:NE1	2.35	0.42
2:B:232:ILE:HG21	2:B:234:TRP:CZ2	2.55	0.42
1:A:393:VAL:HG12	1:A:394:GLN:H	1.84	0.42
1:A:117:ASN:C	1:A:117:ASN:HD22	2.17	0.41
1:A:6:GLU:OE2	1:A:324:LYS:HB2	2.20	0.41
1:A:215:VAL:HA	1:A:226:ALA:O	2.20	0.41
1:A:29:SER:OG	1:A:66:ASN:ND2	2.53	0.41
2:B:257:LEU:HA	2:B:257:LEU:HD23	1.80	0.41
1:A:302:TRP:CD1	1:A:321:PHE:CD1	3.07	0.41
2:B:250:GLU:C	2:B:251:GLU:OE1	2.58	0.41
1:A:152:THR:HA	1:A:153:PRO:HD3	1.81	0.41
1:A:375:THR:C	1:A:377:TYR:H	2.23	0.41
2:B:102:VAL:HG22	2:B:120:SER:HB2	2.02	0.41
1:A:229:THR:HG22	1:A:230:GLY:N	2.35	0.41
1:A:252:LEU:HB3	1:A:285:TRP:CE3	2.55	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:261:LEU:N	1:A:277:GLY:HA2	2.35	0.41
1:A:9:ARG:HA	1:A:324:LYS:HA	2.02	0.41
1:A:84:GLY:HA2	1:A:111:VAL:HG23	2.03	0.41
2:B:10:GLU:HG3	2:B:30:ASP:CA	2.51	0.41
1:A:83:ASN:O	1:A:84:GLY:C	2.59	0.41
2:B:233:ILE:HD11	2:B:248:LEU:CD1	2.48	0.41
2:B:247:LEU:C	2:B:249:LYS:N	2.74	0.41
1:A:127:GLY:HA3	1:A:163:VAL:HB	2.03	0.41
1:A:214:VAL:HB	1:A:228:ALA:HB3	2.03	0.41
1:A:96:ASN:O	1:A:97:ALA:HB2	2.21	0.41
2:B:206:TRP:O	2:B:226:SER:OG	2.23	0.41
1:A:70:TRP:C	1:A:71:SER:O	2.55	0.41
2:B:105:VAL:HG21	2:B:116:LEU:HD21	2.02	0.41
2:B:152:SER:O	2:B:173:PHE:HB2	2.21	0.41
1:A:41:SER:O	1:A:42:LEU:CB	2.67	0.41
1:A:385:HIS:O	1:A:393:VAL:HG23	2.21	0.41
2:B:194:TYR:CD1	2:B:194:TYR:N	2.88	0.41
2:B:262:TRP:HA	2:B:262:TRP:CE3	2.55	0.41
2:B:4:ILE:HG13	2:B:43:HIS:HB3	2.03	0.40
2:B:59:VAL:HG12	2:B:72:SER:CA	2.50	0.40
2:B:224:SER:O	2:B:231:CYS:HA	2.21	0.40
2:B:196:LEU:CD1	2:B:197:GLU:H	2.30	0.40
2:B:169:GLU:HG2	2:B:187:TYR:CD2	2.53	0.40
1:A:7:PHE:HB2	1:A:8:SER:H	1.51	0.40
1:A:23:LEU:HD12	1:A:23:LEU:HA	1.90	0.40
1:A:116:PHE:CD2	1:A:124:LEU:HD13	2.57	0.40
2:B:27:CYS:HB3	2:B:33:ILE:HG23	2.02	0.40
2:B:30:ASP:O	2:B:31:LYS:HB2	2.21	0.40
2:B:94:VAL:O	2:B:94:VAL:CG1	2.70	0.40
1:A:271:HIS:HB3	1:A:286:ASN:OD1	2.21	0.40
2:B:226:SER:HG	2:B:227:GLN:N	2.20	0.40
2:B:191:ALA:C	2:B:192:GLN:HG2	2.41	0.40
1:A:19:LYS:HD3	1:A:311:GLU:HG3	2.03	0.40
1:A:187:ILE:HD13	1:A:187:ILE:HA	1.88	0.40
2:B:269:LEU:O	2:B:280:LEU:HA	2.21	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	380/416 (91%)	259 (68%)	70 (18%)	51 (13%)	0	3
2	B	276/297 (93%)	214 (78%)	37 (13%)	25 (9%)	1	10
All	All	656/713 (92%)	473 (72%)	107 (16%)	76 (12%)	1	5

All (76) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	33	ASP
1	A	49	ALA
1	A	74	ASN
1	A	110	SER
1	A	143	GLU
1	A	146	SER
1	A	147	ASN
1	A	159	SER
1	A	203	SER
1	A	242	LEU
1	A	290	ALA
1	A	301	ASN
1	A	313	PRO
1	A	335	ASN
1	A	336	THR
1	A	365	LYS
1	A	369	PHE
1	A	372	GLN
1	A	388	PHE
2	B	76	ASP
2	B	100	ALA
2	B	131	LYS
1	A	10	THR
1	A	84	GLY
1	A	105	SER
1	A	160	VAL
1	A	194	LYS

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Mol	Chain	Res	Type
1	A	238	LEU
1	A	266	CYS
1	A	322	ASP
1	A	332	ASN
1	A	337	LEU
1	A	399	GLY
2	B	30	ASP
2	B	41	GLU
2	B	133	ASN
2	B	241	GLY
2	B	254	PRO
2	B	256	VAL
2	B	273	GLY
1	A	16	SER
1	A	52	SER
1	A	60	GLN
1	A	93	GLU
1	A	121	ASP
1	A	153	PRO
1	A	204	PRO
1	A	299	ARG
1	A	363	LYS
1	A	394	GLN
2	B	40	GLY
2	B	47	ASP
2	B	101	SER
2	B	145	ALA
2	B	240	GLN
2	B	291	PRO
1	A	91	THR
1	A	148	TYR
1	A	302	TRP
1	A	368	VAL
1	A	383	ALA
2	B	46	ILE
2	B	218	LEU
2	B	267	ASN
2	B	274	GLY
1	A	9	ARG
1	A	94	ALA
1	A	109	SER
1	A	207	GLY

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Mol	Chain	Res	Type
1	A	379	GLU
2	B	51	GLY
2	B	170	SER
2	B	187	TYR
2	B	21	GLY
2	B	287	GLY
1	A	287	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	331/359 (92%)	292 (88%)	39 (12%)	8	34
2	B	238/252 (94%)	218 (92%)	20 (8%)	16	55
All	All	569/611 (93%)	510 (90%)	59 (10%)	10	41

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	PHE
1	A	15	TRP
1	A	18	ASP
1	A	20	ILE
1	A	33	ASP
1	A	51	ASP
1	A	61	VAL
1	A	62	ASP
1	A	66	ASN
1	A	73	ASN
1	A	74	ASN
1	A	99	ASN
1	A	104	PHE
1	A	106	ASN
1	A	117	ASN
1	A	130	ASN
1	A	136	TRP
1	A	147	ASN

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Mol	Chain	Res	Type
1	A	156	SER
1	A	168	TRP
1	A	169	ASN
1	A	170	GLN
1	A	183	ASN
1	A	198	HIS
1	A	204	PRO
1	A	216	GLU
1	A	221	ASN
1	A	232	ASP
1	A	244	ASN
1	A	253	ASN
1	A	261	LEU
1	A	266	CYS
1	A	268	GLN
1	A	281	THR
1	A	304	PHE
1	A	327	VAL
1	A	334	THR
1	A	398	ASP
1	A	406	ASN
2	B	33	ILE
2	B	66	PHE
2	B	81	ILE
2	B	82	TRP
2	B	122	ASP
2	B	129	GLU
2	B	133	ASN
2	B	141	ILE
2	B	180	ASN
2	B	199	THR
2	B	200	LEU
2	B	205	ASP
2	B	206	TRP
2	B	225	VAL
2	B	233	ILE
2	B	237	ASP
2	B	247	LEU
2	B	255	ASP
2	B	261	SER
2	B	286	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	ASN
1	A	72	HIS
1	A	73	ASN
1	A	74	ASN
1	A	95	ASN
1	A	96	ASN
1	A	99	ASN
1	A	106	ASN
1	A	117	ASN
1	A	129	ASN
1	A	130	ASN
1	A	139	ASN
1	A	147	ASN
1	A	221	ASN
1	A	244	ASN
1	A	246	ASN
1	A	250	GLN
1	A	268	GLN
1	A	292	GLN
1	A	406	ASN
2	B	86	ASN
2	B	149	ASN
2	B	180	ASN
2	B	276	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	384/416 (92%)	-0.07	1 (0%)	91 63	27, 67, 129, 166	0
2	B	280/297 (94%)	0.11	5 (1%)	65 20	39, 85, 130, 176	0
All	All	664/713 (93%)	0.00	6 (0%)	81 37	27, 73, 130, 176	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	292	ALA	3.2
2	B	135	THR	2.6
1	A	338	ASP	2.3
2	B	83	LYS	2.2
2	B	134	GLY	2.2
2	B	172	LYS	2.1

### 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.