



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:20 AM GMT

PDB ID : 2WR5  
Title : STRUCTURE OF INFLUENZA H2 DUCK ONTARIO HEMAGGLUTININ  
Authors : Liu, J.; Stevens, D.J.; Haire, L.F.; Walker, P.A.; Coombs, P.J.; Russell, R.J.;  
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Deposited on : 2009-08-29  
Resolution : 2.65 Å(reported)

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

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

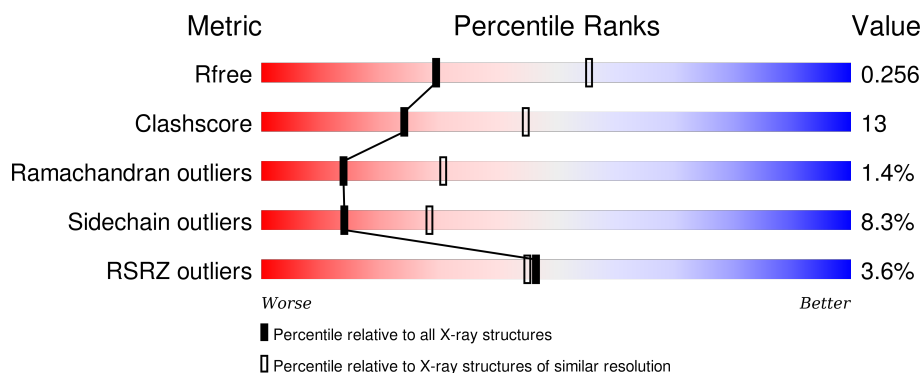
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.65 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	3152 (2.70-2.62)
Clashscore	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)
RSRZ outliers	91569	3161 (2.70-2.62)

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	507	<div> <div>4%</div> <div> <div></div> <div>71%</div> <div>20%</div> <div>• •</div> </div> </div>
1	B	507	<div> <div>2%</div> <div> <div></div> <div>71%</div> <div>21%</div> <div>• •</div> </div> </div>
1	C	507	<div> <div>4%</div> <div> <div></div> <div>67%</div> <div>25%</div> <div>• •</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11604 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 HEMAGGLUTININ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	485	Total	C	N	O	S	0	0	0
			3814	2396	654	742	22			
1	B	485	Total	C	N	O	S	0	0	0
			3814	2396	654	742	22			
1	C	485	Total	C	N	O	S	0	0	0
			3814	2396	654	742	22			

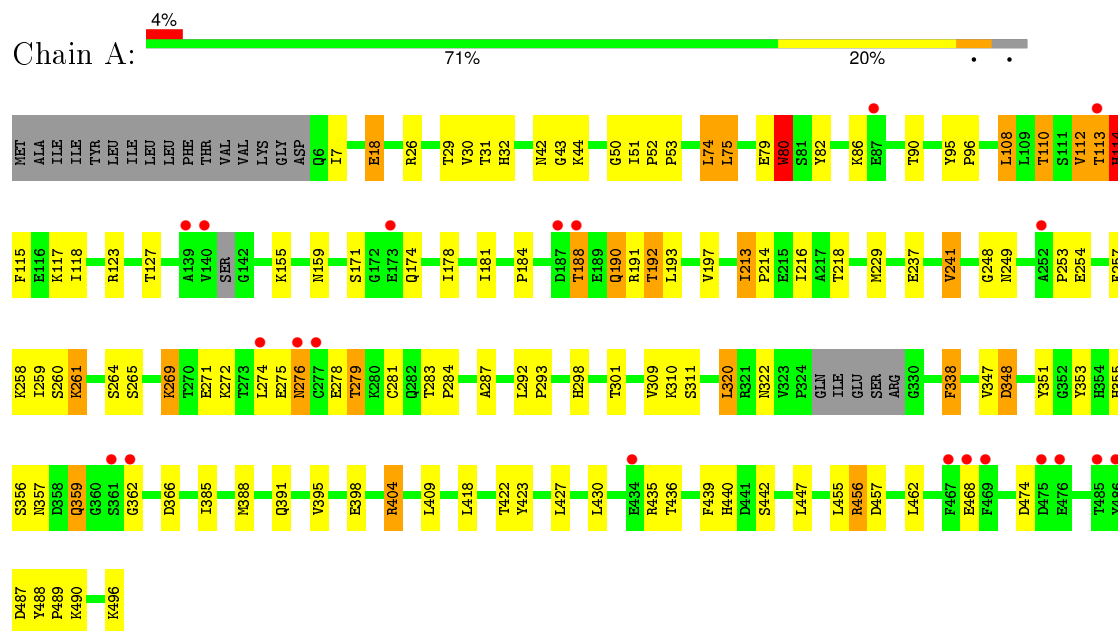
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	51	Total	O	0	0
			51	51		
2	B	61	Total	O	0	0
			61	61		
2	C	50	Total	O	0	0
			50	50		

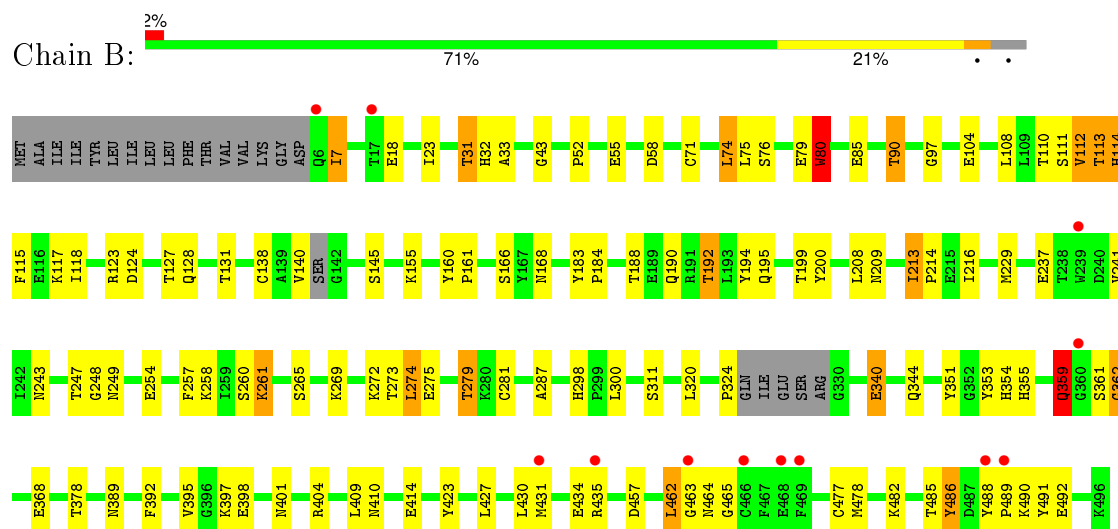
### 3 Residue-property plots

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.

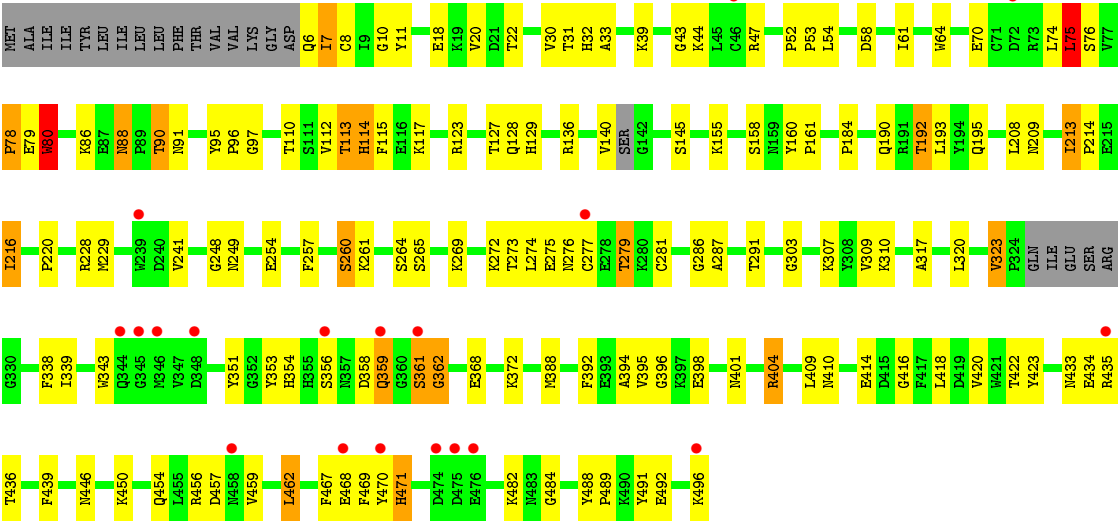
#### • Molecule 1: HEMAGGLUTININ



#### • Molecule 1: HEMAGGLUTININ



#### • Molecule 1: HEMAGGLUTININ



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.98Å 150.88Å 195.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.86 – 2.65 29.86 – 2.65	Depositor EDS
% Data completeness (in resolution range)	91.5 (29.86-2.65) 91.6 (29.86-2.65)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.26 (at 2.64Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.227 , 0.261 0.220 , 0.256	Depositor DCC
$R_{free}$ test set	3444 reflections (4.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	71.1	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 44.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 69042 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	11604	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% 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	0.40	0/3899	0.56	2/5284 (0.0%)
1	B	0.43	0/3899	0.59	2/5284 (0.0%)
1	C	0.40	0/3899	0.56	2/5284 (0.0%)
All	All	0.41	0/11697	0.57	6/15852 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	114	HIS	N-CA-C	7.21	130.45	111.00
1	A	114	HIS	N-CA-C	6.77	129.29	111.00
1	C	114	HIS	N-CA-C	6.37	128.19	111.00
1	A	113	THR	C-N-CA	5.42	135.24	121.70
1	B	113	THR	C-N-CA	5.35	135.07	121.70
1	C	113	THR	C-N-CA	5.06	134.34	121.70

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3814	0	3639	86	0
1	B	3814	0	3639	89	0
1	C	3814	0	3639	120	0
2	A	51	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	61	0	0	3	0
2	C	50	0	0	7	0
All	All	11604	0	10917	290	0

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 13.

All (290) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:THR:HG21	1:A:287:ALA:HB1	1.34	1.07
1:A:261:LYS:HZ3	1:A:261:LYS:HB2	1.34	0.91
1:A:113:THR:OG1	1:A:260:SER:HB2	1.71	0.90
1:B:279:THR:HG21	1:B:287:ALA:HB1	1.55	0.87
1:B:113:THR:OG1	1:B:260:SER:HB2	1.75	0.87
1:B:112:VAL:HG11	1:B:115:PHE:HB2	1.58	0.86
1:B:261:LYS:HB2	1:B:261:LYS:HZ3	1.42	0.84
1:B:118:ILE:HD11	1:B:258:LYS:HD2	1.57	0.84
1:B:359:GLN:H	1:B:359:GLN:HE21	1.25	0.83
1:C:155:LYS:NZ	1:C:195:GLN:HE21	1.77	0.82
1:A:112:VAL:HG11	1:A:115:PHE:HB2	1.59	0.80
1:A:178:ILE:O	1:A:253:PRO:HG3	1.80	0.79
1:A:123:ARG:HG3	1:A:254:GLU:OE2	1.83	0.78
1:A:79:GLU:HG3	1:A:113:THR:O	1.84	0.78
1:C:79:GLU:HG3	1:C:113:THR:O	1.83	0.78
1:A:7:ILE:HD11	1:A:353:TYR:HB3	1.66	0.76
1:C:359:GLN:HE21	1:C:359:GLN:N	1.84	0.76
1:A:118:ILE:HD11	1:A:258:LYS:HD3	1.67	0.75
1:A:279:THR:CG2	1:A:287:ALA:HB1	2.16	0.75
1:C:457:ASP:HB2	1:C:488:TYR:OH	1.88	0.74
1:C:7:ILE:HB	1:C:469:PHE:HE1	1.52	0.74
1:A:216:ILE:HD12	1:A:216:ILE:H	1.52	0.74
1:A:275:GLU:O	1:A:276:ASN:HB3	1.87	0.74
1:C:155:LYS:HD3	1:C:195:GLN:HG2	1.70	0.73
1:A:110:THR:CG2	1:A:265:SER:H	2.01	0.73
1:C:110:THR:HG21	1:C:265:SER:H	1.54	0.72
1:C:155:LYS:HZ2	1:C:195:GLN:HE21	1.33	0.72
1:B:324:PRO:HB3	1:B:344:GLN:NE2	2.05	0.71
1:C:279:THR:HG22	1:C:281:CYS:H	1.56	0.71
1:C:358:ASP:HB2	2:C:2034:HOH:O	1.91	0.71
1:A:31:THR:HG22	1:A:32:HIS:CG	2.27	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:SER:HB2	1:A:258:LYS:HD2	1.73	0.70
1:C:184:PRO:HG2	1:C:190:GLN:NE2	2.06	0.69
1:C:96:PRO:HB2	1:C:228:ARG:HD3	1.74	0.69
1:B:359:GLN:HE21	1:B:359:GLN:N	1.89	0.69
1:C:110:THR:CG2	1:C:265:SER:H	2.04	0.69
1:C:261:LYS:HB2	1:C:261:LYS:HZ3	1.58	0.69
1:B:188:THR:O	1:B:192:THR:HG22	1.93	0.69
1:A:118:ILE:HD11	1:A:258:LYS:CD	2.23	0.68
1:A:52:PRO:O	1:A:80:TRP:HA	1.94	0.67
1:B:279:THR:CG2	1:B:287:ALA:HB1	2.25	0.67
1:A:309:VAL:HG13	1:A:422:THR:HA	1.77	0.67
1:A:261:LYS:NZ	1:A:261:LYS:HB2	2.10	0.67
1:C:470:TYR:O	1:C:471:HIS:HB3	1.96	0.66
1:B:208:LEU:HG	1:B:209:ASN:N	2.11	0.66
1:A:455:LEU:O	1:A:456:ARG:HB2	1.94	0.66
1:A:108:LEU:HD23	1:A:261:LYS:HE3	1.77	0.66
1:C:6:GLN:HB3	1:C:356:SER:HB2	1.79	0.65
1:B:261:LYS:NZ	1:B:261:LYS:HB2	2.11	0.65
1:A:357:ASN:HD21	1:A:474:ASP:HA	1.60	0.65
1:C:269:LYS:HE2	1:C:398:GLU:OE1	1.96	0.65
1:C:128:GLN:HB3	1:C:161:PRO:HG2	1.79	0.65
1:C:310:LYS:HG3	1:C:418:LEU:HD21	1.79	0.65
1:C:248:GLY:O	1:C:249:ASN:HB2	1.96	0.65
1:B:184:PRO:HG2	1:B:190:GLN:NE2	2.13	0.64
1:A:188:THR:O	1:A:192:THR:HG22	1.98	0.63
1:C:7:ILE:HG22	1:C:467:PHE:HB2	1.81	0.62
1:B:18:GLU:HG2	1:B:33:ALA:HB3	1.80	0.62
1:B:128:GLN:HB3	1:B:161:PRO:HG2	1.81	0.62
1:A:43:GLY:O	1:A:272:LYS:HE2	2.00	0.62
1:A:184:PRO:HG2	1:A:190:GLN:HE21	1.65	0.62
1:A:75:LEU:O	1:A:75:LEU:HG	1.99	0.61
1:C:184:PRO:HG2	1:C:190:GLN:HE21	1.65	0.61
1:A:184:PRO:HG2	1:A:190:GLN:NE2	2.16	0.61
1:C:136:ARG:HD3	2:C:2016:HOH:O	2.00	0.61
1:C:18:GLU:HG2	1:C:33:ALA:HB3	1.83	0.61
1:B:155:LYS:HD2	1:B:195:GLN:HG2	1.82	0.60
1:C:274:LEU:HD23	1:C:275:GLU:N	2.16	0.60
1:A:359:GLN:N	1:A:359:GLN:HE21	1.99	0.60
1:C:117:LYS:HG3	1:C:257:PHE:CE2	2.37	0.60
1:B:79:GLU:HG3	1:B:113:THR:O	2.02	0.60
1:B:74:LEU:O	1:B:75:LEU:HB3	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:THR:HG21	1:A:265:SER:H	1.67	0.59
1:C:471:HIS:CE1	1:C:491:TYR:CD1	2.91	0.59
1:C:454:GLN:HB2	2:C:2047:HOH:O	2.03	0.58
1:B:110:THR:CG2	1:B:265:SER:H	2.15	0.58
1:C:95:TYR:CD2	1:C:96:PRO:HD2	2.39	0.58
1:B:261:LYS:CB	1:B:261:LYS:HZ3	2.16	0.58
1:C:155:LYS:HE2	1:C:192:THR:O	2.03	0.58
1:C:274:LEU:HD23	1:C:275:GLU:H	1.68	0.58
1:B:31:THR:HG22	1:B:32:HIS:ND1	2.18	0.58
1:B:166:SER:HB3	1:B:243:ASN:OD1	2.03	0.58
1:B:168:ASN:ND2	2:B:2029:HOH:O	2.33	0.58
1:B:353:TYR:CD1	1:B:482:LYS:HG2	2.38	0.58
1:C:279:THR:CG2	1:C:287:ALA:HB1	2.34	0.58
1:B:43:GLY:O	1:B:272:LYS:HE2	2.03	0.57
1:B:117:LYS:HG3	1:B:257:PHE:CE2	2.38	0.57
1:A:261:LYS:HZ3	1:A:261:LYS:CB	2.10	0.57
1:B:492:GLU:OE1	1:B:492:GLU:HA	2.04	0.57
1:A:279:THR:HB	1:A:281:CYS:H	1.70	0.56
1:B:359:GLN:H	1:B:359:GLN:NE2	1.99	0.56
1:C:64:TRP:CD1	1:C:74:LEU:HD12	2.40	0.56
1:C:44:LYS:O	1:C:286:GLY:HA2	2.05	0.56
1:C:462:LEU:HD21	1:C:468:GLU:HB2	1.87	0.56
1:B:188:THR:O	1:B:192:THR:CG2	2.53	0.56
1:A:26:ARG:NE	2:A:2004:HOH:O	2.39	0.56
1:C:279:THR:HG21	1:C:281:CYS:O	2.06	0.55
1:B:75:LEU:HG	1:B:75:LEU:O	2.07	0.55
1:A:488:TYR:HB3	1:A:489:PRO:HD3	1.88	0.55
1:B:58:ASP:HB2	1:B:90:THR:HG23	1.89	0.55
1:C:216:ILE:H	1:C:216:ILE:HD12	1.71	0.55
1:A:53:PRO:HG3	1:A:82:TYR:CZ	2.42	0.55
1:C:43:GLY:O	1:C:272:LYS:HE2	2.07	0.55
1:A:248:GLY:C	1:A:249:ASN:HD22	2.09	0.55
1:B:112:VAL:CG1	1:B:115:PHE:HB2	2.35	0.54
1:B:118:ILE:HD11	1:B:258:LYS:CD	2.33	0.54
1:A:74:LEU:O	1:A:75:LEU:HB3	2.07	0.54
1:B:488:TYR:HB3	1:B:489:PRO:HD3	1.89	0.54
1:B:112:VAL:HG11	1:B:115:PHE:CB	2.35	0.54
1:B:216:ILE:H	1:B:216:ILE:HD12	1.72	0.54
1:B:71:CYS:O	1:B:74:LEU:HB2	2.07	0.54
1:B:269:LYS:HE2	1:B:398:GLU:OE1	2.07	0.54
1:B:160:TYR:CZ	1:B:248:GLY:HA2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:TYR:CE1	1:B:214:PRO:HA	2.42	0.54
1:C:53:PRO:HD2	1:C:274:LEU:HD12	1.90	0.54
1:A:276:ASN:CG	1:A:276:ASN:O	2.46	0.54
1:C:457:ASP:O	1:C:470:TYR:HD1	1.91	0.53
1:C:303:GLY:HA2	1:C:392:PHE:CD1	2.43	0.53
1:B:279:THR:HB	1:B:281:CYS:H	1.74	0.53
1:C:248:GLY:C	1:C:249:ASN:HD22	2.12	0.53
1:B:423:TYR:CE1	1:C:388:MET:HE2	2.44	0.53
1:A:435:ARG:NH2	1:C:434:GLU:OE1	2.32	0.52
1:B:123:ARG:HG3	1:B:254:GLU:OE2	2.09	0.52
1:B:110:THR:HG23	1:B:265:SER:H	1.73	0.52
1:B:213:ILE:HD13	1:B:213:ILE:H	1.75	0.52
1:B:85:GLU:O	1:B:269:LYS:HA	2.10	0.52
1:B:124:ASP:N	1:B:124:ASP:OD2	2.42	0.52
1:A:31:THR:HG22	1:A:32:HIS:ND1	2.24	0.52
1:C:31:THR:CG2	2:C:2033:HOH:O	2.58	0.52
1:A:462:LEU:HD21	1:A:468:GLU:HB2	1.91	0.52
1:C:54:LEU:HB2	1:C:80:TRP:CG	2.44	0.52
1:C:97:GLY:HA3	1:C:229:MET:O	2.10	0.51
1:B:492:GLU:CD	2:B:2060:HOH:O	2.48	0.51
1:B:52:PRO:O	1:B:80:TRP:HA	2.11	0.51
1:C:279:THR:HG23	1:C:287:ALA:HB1	1.91	0.51
1:A:191:ARG:NH1	1:A:197:VAL:HG21	2.25	0.51
1:B:354:HIS:HA	1:B:362:GLY:O	2.11	0.51
1:A:455:LEU:O	1:A:456:ARG:CB	2.59	0.51
1:C:47:ARG:HB2	1:C:52:PRO:HA	1.93	0.50
1:B:184:PRO:HG2	1:B:190:GLN:HE21	1.75	0.50
1:B:491:TYR:C	2:B:2060:HOH:O	2.48	0.50
1:C:208:LEU:HG	1:C:209:ASN:N	2.26	0.50
1:C:64:TRP:HD1	1:C:74:LEU:HD12	1.75	0.50
1:C:75:LEU:HG	1:C:75:LEU:O	2.11	0.50
1:B:298:HIS:CE1	1:B:300:LEU:HB2	2.46	0.50
1:C:353:TYR:CD1	1:C:482:LYS:HG2	2.46	0.50
1:B:200:TYR:CE2	1:B:247:THR:HG23	2.46	0.50
1:C:112:VAL:HG11	1:C:115:PHE:CB	2.42	0.50
1:A:112:VAL:CG1	1:A:115:PHE:HB2	2.38	0.50
1:C:459:VAL:HA	1:C:468:GLU:O	2.12	0.50
1:A:86:LYS:HE2	1:A:271:GLU:HG2	1.92	0.50
1:A:7:ILE:HD13	1:A:355:HIS:HB3	1.94	0.50
1:A:155:LYS:HE2	1:A:192:THR:O	2.12	0.50
1:C:338:PHE:CE1	1:C:339:ILE:HG13	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:470:TYR:O	1:C:471:HIS:CB	2.60	0.49
1:B:31:THR:CG2	1:B:32:HIS:ND1	2.76	0.49
1:A:117:LYS:HG3	1:A:257:PHE:CE2	2.48	0.49
1:A:95:TYR:CD2	1:A:96:PRO:HD2	2.47	0.48
1:C:7:ILE:HB	1:C:469:PHE:CE1	2.41	0.48
1:A:241:VAL:HG13	1:C:220:PRO:HG3	1.94	0.48
1:C:74:LEU:HA	1:C:74:LEU:HD23	1.69	0.48
1:B:248:GLY:O	1:B:249:ASN:HB2	2.12	0.48
1:A:366:ASP:OD1	1:A:447:LEU:HD11	2.14	0.48
1:C:274:LEU:CD2	1:C:276:ASN:H	2.27	0.48
1:B:490:LYS:HD2	1:B:491:TYR:CE2	2.49	0.48
1:B:97:GLY:HA3	1:B:229:MET:O	2.13	0.48
1:C:123:ARG:NH1	1:C:254:GLU:OE1	2.47	0.48
1:B:194:TYR:O	1:B:195:GLN:HB2	2.14	0.47
1:B:355:HIS:HB2	1:B:478:MET:CE	2.44	0.47
1:C:54:LEU:HD22	1:C:80:TRP:CZ2	2.49	0.47
1:A:436:THR:O	1:A:439:PHE:HB3	2.14	0.47
1:C:112:VAL:HG11	1:C:115:PHE:HB2	1.95	0.47
1:B:140:VAL:HG23	1:B:140:VAL:O	2.15	0.47
1:B:113:THR:HG23	1:B:260:SER:O	2.15	0.47
1:C:8:CYS:O	1:C:353:TYR:HA	2.15	0.47
1:A:110:THR:HG23	1:A:265:SER:H	1.80	0.46
1:A:284:PRO:HG2	1:A:298:HIS:CE1	2.49	0.46
1:C:484:GLY:HA2	2:C:2046:HOH:O	2.14	0.46
1:C:113:THR:OG1	1:C:260:SER:HB2	2.14	0.46
1:A:404:ARG:HB2	1:B:104:GLU:OE1	2.15	0.46
1:C:404:ARG:HA	1:C:404:ARG:HD2	1.64	0.46
1:B:74:LEU:O	1:B:74:LEU:HD13	2.15	0.46
1:C:54:LEU:HD22	1:C:80:TRP:CE2	2.51	0.46
1:C:58:ASP:HB2	1:C:90:THR:HG23	1.98	0.46
1:C:436:THR:O	1:C:439:PHE:HB3	2.16	0.46
1:A:112:VAL:HG13	1:A:114:HIS:O	2.16	0.46
1:C:86:LYS:C	1:C:88:ASN:H	2.20	0.46
1:C:110:THR:CG2	1:C:265:SER:N	2.77	0.46
1:A:50:GLY:N	1:A:278:GLU:OE1	2.45	0.46
1:B:7:ILE:HD11	1:B:353:TYR:HB3	1.99	0.45
1:C:31:THR:HG21	2:C:2033:HOH:O	2.14	0.45
1:B:274:LEU:HD23	1:B:275:GLU:H	1.79	0.45
1:A:213:ILE:HA	1:A:214:PRO:HD3	1.80	0.45
1:A:293:PRO:HG3	1:A:385:ILE:HA	1.98	0.45
1:A:423:TYR:CE2	1:A:427:LEU:HD22	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:THR:CG2	1:A:32:HIS:CE1	3.00	0.45
1:A:309:VAL:HG12	1:A:311:SER:H	1.81	0.45
1:B:168:ASN:OD1	1:B:168:ASN:C	2.55	0.45
1:A:29:THR:HG22	1:A:322:ASN:HB3	1.98	0.45
1:A:248:GLY:O	1:A:249:ASN:HB2	2.17	0.45
1:B:392:PHE:CD2	1:B:392:PHE:C	2.90	0.45
1:C:31:THR:HG22	1:C:32:HIS:CD2	2.51	0.45
1:B:463:GLY:O	1:B:465:GLY:N	2.50	0.45
1:A:487:ASP:OD1	1:A:490:LYS:HB2	2.17	0.45
1:A:110:THR:HG23	1:A:265:SER:HB3	1.98	0.45
1:C:446:ASN:O	1:C:450:LYS:HB2	2.17	0.45
1:A:174:GLN:HG3	1:A:237:GLU:OE2	2.17	0.45
1:C:394:ALA:O	1:C:396:GLY:N	2.50	0.44
1:C:372:LYS:O	1:C:372:LYS:HG2	2.17	0.44
1:C:309:VAL:HG13	1:C:422:THR:HA	2.00	0.44
1:C:54:LEU:HB2	1:C:80:TRP:CD2	2.52	0.44
1:B:113:THR:HG21	1:B:260:SER:HB3	1.97	0.44
1:C:488:TYR:N	1:C:489:PRO:HD2	2.32	0.44
1:C:8:CYS:N	1:C:354:HIS:O	2.50	0.44
1:A:348:ASP:N	1:A:348:ASP:OD1	2.50	0.44
1:C:155:LYS:CD	1:C:195:GLN:HG2	2.43	0.44
1:C:74:LEU:O	1:C:75:LEU:HB3	2.18	0.44
1:C:52:PRO:O	1:C:80:TRP:HA	2.18	0.44
1:C:488:TYR:HB3	1:C:489:PRO:HD3	1.99	0.44
1:B:199:THR:OG1	1:B:249:ASN:ND2	2.51	0.44
1:B:55:GLU:CD	1:B:274:LEU:HB2	2.38	0.44
1:C:32:HIS:CE1	2:C:2033:HOH:O	2.71	0.43
1:A:388:MET:HE2	1:C:423:TYR:CE1	2.53	0.43
1:C:113:THR:HG21	1:C:260:SER:HB2	2.00	0.43
1:C:457:ASP:O	1:C:470:TYR:CD1	2.70	0.43
1:C:160:TYR:CZ	1:C:248:GLY:HA2	2.53	0.43
1:C:10:GLY:HA3	1:C:343:TRP:CZ2	2.53	0.43
1:C:410:ASN:O	1:C:414:GLU:HG2	2.18	0.43
1:A:18:GLU:O	1:A:29:THR:HA	2.18	0.43
1:C:30:VAL:CG1	1:C:31:THR:N	2.79	0.43
1:A:42:ASN:O	1:A:44:LYS:HG3	2.18	0.43
1:B:340:GLU:HG3	1:B:464:ASN:HD22	1.84	0.43
1:C:115:PHE:CD1	1:C:115:PHE:C	2.91	0.43
1:B:462:LEU:HD22	1:B:462:LEU:HA	1.70	0.43
1:C:354:HIS:HA	1:C:362:GLY:O	2.18	0.43
1:B:423:TYR:CE2	1:B:427:LEU:HD22	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:430:LEU:HA	1:B:430:LEU:HD23	1.81	0.43
1:A:320:LEU:HB3	1:A:440:HIS:CG	2.54	0.43
1:B:361:SER:HA	1:B:362:GLY:HA3	1.68	0.43
1:A:7:ILE:O	1:A:7:ILE:HG23	2.19	0.42
1:A:309:VAL:CG1	1:A:422:THR:HA	2.47	0.42
1:C:10:GLY:HA3	1:C:343:TRP:CH2	2.54	0.42
1:B:138:CYS:O	1:B:145:SER:HB3	2.19	0.42
1:B:111:SER:HB2	1:B:265:SER:HB2	2.01	0.42
1:B:110:THR:HG23	1:B:111:SER:N	2.34	0.42
1:C:10:GLY:N	1:C:343:TRP:CH2	2.87	0.42
1:C:11:TYR:HE2	1:C:323:VAL:HG23	1.84	0.42
1:C:20:VAL:HG21	1:C:317:ALA:HB2	2.01	0.42
1:A:95:TYR:CD2	1:A:229:MET:HG3	2.54	0.42
1:A:404:ARG:HD2	1:A:404:ARG:HA	1.89	0.42
1:B:485:THR:O	1:B:486:TYR:C	2.57	0.42
1:C:213:ILE:HA	1:C:214:PRO:HD3	1.91	0.42
1:C:158:SER:O	1:C:195:GLN:HG3	2.20	0.42
1:A:430:LEU:HA	1:A:430:LEU:HD23	1.69	0.42
1:B:23:ILE:HD12	1:B:23:ILE:HG23	1.71	0.42
1:A:310:LYS:HG3	1:A:418:LEU:HD21	2.02	0.42
1:C:303:GLY:HA2	1:C:392:PHE:CE1	2.54	0.42
1:C:155:LYS:HZ3	1:C:195:GLN:HE21	1.62	0.42
1:A:51:ILE:HA	1:A:52:PRO:HD3	1.86	0.42
1:C:488:TYR:N	1:C:489:PRO:CD	2.82	0.41
1:C:489:PRO:O	1:C:492:GLU:HG2	2.20	0.41
1:C:274:LEU:HD23	1:C:276:ASN:H	1.84	0.41
1:C:22:THR:HG22	1:C:433:ASN:HB3	2.01	0.41
1:C:86:LYS:C	1:C:88:ASN:N	2.72	0.41
1:C:213:ILE:HD13	1:C:213:ILE:H	1.85	0.41
1:A:283:THR:HG22	1:A:301:THR:HG22	2.02	0.41
1:A:269:LYS:HE2	1:A:398:GLU:OE1	2.20	0.41
1:B:488:TYR:N	1:B:489:PRO:CD	2.83	0.41
1:B:431:MET:O	1:B:435:ARG:HG3	2.20	0.41
1:A:447:LEU:HD12	1:A:447:LEU:HA	1.91	0.41
1:A:338:PHE:C	1:A:338:PHE:CD1	2.93	0.41
1:C:140:VAL:HG22	1:C:145:SER:HB2	2.03	0.41
1:C:361:SER:HA	1:C:362:GLY:HA3	1.66	0.41
1:B:31:THR:CG2	1:B:32:HIS:CE1	3.04	0.41
1:C:30:VAL:HG13	1:C:31:THR:N	2.35	0.41
1:B:31:THR:HG22	1:B:32:HIS:N	2.35	0.41
1:A:462:LEU:HA	1:A:462:LEU:HD13	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:LEU:HA	1:A:293:PRO:HD3	1.87	0.41
1:C:70:GLU:HB3	1:C:91:ASN:ND2	2.35	0.41
1:B:410:ASN:O	1:B:414:GLU:HG2	2.21	0.41
1:C:416:GLY:O	1:C:420:VAL:HG23	2.20	0.41
1:C:113:THR:CG2	1:C:260:SER:HB2	2.51	0.41
1:C:273:THR:O	1:C:274:LEU:C	2.59	0.40
1:A:159:ASN:HA	1:A:159:ASN:HD22	1.70	0.40
1:B:111:SER:O	1:B:112:VAL:HG23	2.21	0.40
1:B:110:THR:HG21	1:B:265:SER:H	1.83	0.40
1:C:110:THR:HG23	1:C:265:SER:N	2.36	0.40
1:A:95:TYR:HA	1:A:96:PRO:HD3	1.96	0.40
1:C:78:PRO:O	1:C:114:HIS:HA	2.21	0.40
1:C:129:HIS:CE1	1:C:161:PRO:HD2	2.57	0.40

There are no symmetry-related clashes.

## 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	479/507 (94%)	430 (90%)	42 (9%)	7 (2%)	13	28
1	B	479/507 (94%)	437 (91%)	37 (8%)	5 (1%)	19	41
1	C	479/507 (94%)	429 (90%)	42 (9%)	8 (2%)	11	25
All	All	1437/1521 (94%)	1296 (90%)	121 (8%)	20 (1%)	14	31

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	80	TRP
1	A	348	ASP
1	C	80	TRP
1	A	276	ASN

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Mol	Chain	Res	Type
1	A	395	VAL
1	A	456	ARG
1	B	80	TRP
1	B	359	GLN
1	C	362	GLY
1	C	471	HIS
1	A	114	HIS
1	B	362	GLY
1	C	277	CYS
1	C	361	SER
1	C	395	VAL
1	A	362	GLY
1	B	486	TYR
1	C	75	LEU
1	C	456	ARG
1	B	395	VAL

### 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	415/445 (93%)	378 (91%)	37 (9%)	12	25
1	B	415/445 (93%)	380 (92%)	35 (8%)	14	27
1	C	415/445 (93%)	384 (92%)	31 (8%)	17	35
All	All	1245/1335 (93%)	1142 (92%)	103 (8%)	14	28

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

Mol	Chain	Res	Type
1	A	18	GLU
1	A	30	VAL
1	A	74	LEU
1	A	75	LEU
1	A	80	TRP
1	A	90	THR

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Mol	Chain	Res	Type
1	A	108	LEU
1	A	110	THR
1	A	112	VAL
1	A	114	HIS
1	A	127	THR
1	A	181	ILE
1	A	188	THR
1	A	190	GLN
1	A	192	THR
1	A	193	LEU
1	A	213	ILE
1	A	218	THR
1	A	241	VAL
1	A	259	ILE
1	A	261	LYS
1	A	264	SER
1	A	269	LYS
1	A	274	LEU
1	A	279	THR
1	A	320	LEU
1	A	338	PHE
1	A	347	VAL
1	A	351	TYR
1	A	356	SER
1	A	359	GLN
1	A	391	GLN
1	A	404	ARG
1	A	409	LEU
1	A	442	SER
1	A	457	ASP
1	A	496	LYS
1	B	7	ILE
1	B	31	THR
1	B	74	LEU
1	B	76	SER
1	B	80	TRP
1	B	90	THR
1	B	108	LEU
1	B	112	VAL
1	B	114	HIS
1	B	127	THR
1	B	131	THR

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Mol	Chain	Res	Type
1	B	192	THR
1	B	213	ILE
1	B	237	GLU
1	B	241	VAL
1	B	261	LYS
1	B	273	THR
1	B	274	LEU
1	B	279	THR
1	B	311	SER
1	B	320	LEU
1	B	340	GLU
1	B	351	TYR
1	B	359	GLN
1	B	368	GLU
1	B	378	THR
1	B	389	ASN
1	B	397	LYS
1	B	401	ASN
1	B	404	ARG
1	B	409	LEU
1	B	434	GLU
1	B	457	ASP
1	B	462	LEU
1	B	477	CYS
1	C	7	ILE
1	C	39	LYS
1	C	61	ILE
1	C	75	LEU
1	C	76	SER
1	C	78	PRO
1	C	80	TRP
1	C	88	ASN
1	C	90	THR
1	C	127	THR
1	C	192	THR
1	C	193	LEU
1	C	213	ILE
1	C	216	ILE
1	C	241	VAL
1	C	260	SER
1	C	264	SER
1	C	279	THR

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Mol	Chain	Res	Type
1	C	291	THR
1	C	307	LYS
1	C	320	LEU
1	C	323	VAL
1	C	351	TYR
1	C	359	GLN
1	C	368	GLU
1	C	401	ASN
1	C	404	ARG
1	C	409	LEU
1	C	435	ARG
1	C	462	LEU
1	C	496	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	GLN
1	A	159	ASN
1	A	190	GLN
1	A	249	ASN
1	A	359	GLN
1	A	391	GLN
1	B	125	GLN
1	B	129	HIS
1	B	174	GLN
1	B	190	GLN
1	B	249	ASN
1	B	344	GLN
1	B	359	GLN
1	B	389	ASN
1	B	391	GLN
1	C	32	HIS
1	C	129	HIS
1	C	159	ASN
1	C	190	GLN
1	C	195	GLN
1	C	196	ASN
1	C	249	ASN
1	C	359	GLN
1	C	389	ASN
1	C	454	GLN

### 5.3.3 RNA [i](#)

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	485/507 (95%)	0.05	21 (4%) 39 37	43, 81, 145, 205	0
1	B	485/507 (95%)	-0.07	12 (2%) 61 59	40, 70, 125, 207	0
1	C	485/507 (95%)	0.06	19 (3%) 43 41	42, 81, 139, 180	0
All	All	1455/1521 (95%)	0.01	52 (3%) 46 45	40, 77, 137, 207	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	476	GLU	5.1
1	C	475	ASP	4.5
1	B	468	GLU	3.7
1	A	276	ASN	3.5
1	A	485	THR	3.5
1	A	486	TYR	3.4
1	C	361	SER	3.3
1	C	46	CYS	3.2
1	A	476	GLU	3.1
1	B	360	GLY	3.1
1	B	488	TYR	3.1
1	C	496	LYS	3.0
1	A	469	PHE	3.0
1	A	87	GLU	3.0
1	A	475	ASP	2.9
1	C	468	GLU	2.8
1	B	466	CYS	2.7
1	A	467	PHE	2.7
1	B	435	ARG	2.7
1	A	188	THR	2.6
1	C	277	CYS	2.6
1	C	458	ASN	2.6
1	A	277	CYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	489	PRO	2.6
1	C	344	GLN	2.5
1	C	346	MET	2.5
1	C	474	ASP	2.5
1	C	356	SER	2.4
1	A	468	GLU	2.3
1	B	431	MET	2.3
1	B	469	PHE	2.3
1	B	463	GLY	2.3
1	A	173	GLU	2.3
1	C	72	ASP	2.3
1	B	239	TRP	2.3
1	A	140	VAL	2.2
1	A	434	GLU	2.2
1	C	435	ARG	2.2
1	B	6	GLN	2.2
1	A	274	LEU	2.1
1	C	470	TYR	2.1
1	A	187	ASP	2.1
1	A	252	ALA	2.1
1	C	348	ASP	2.1
1	A	362	GLY	2.1
1	A	113	THR	2.1
1	C	359	GLN	2.1
1	C	239	TRP	2.1
1	A	139	ALA	2.1
1	C	345	GLY	2.0
1	A	361	SER	2.0
1	B	17	THR	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 [i](#)

There are no such residues in this entry.