



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:10 PM GMT

PDB ID : 1NSN  
Title : THE CRYSTAL STRUCTURE OF ANTIBODY N10-STAPHYLOCOCCAL  
NUCLEASE COMPLEX AT 2.9 ANGSTROMS RESOLUTION  
Authors : Sheriff, S.; Bossart-Whitaker, P.  
Deposited on : 1995-06-06  
Resolution : 2.80 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

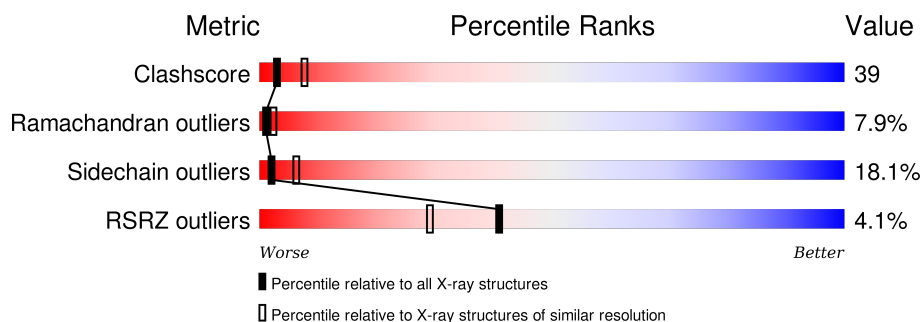
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	L	218	
2	H	210	
3	S	149	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4388 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 IGG FAB (IGG1, KAPPA).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	217	Total	C	N	O	S	0	0	0
			1694	1056	289	343	6			

- Molecule 2 is a protein called IGG FAB (IGG1, KAPPA).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	210	Total	C	N	O	S	0	0	0
			1587	997	261	322	7			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	29	ILE	VAL	CONFLICT	GB 1513182
H	32	ASP	GLU	CONFLICT	GB 1513182
H	48	MET	LEU	CONFLICT	GB 1513182
H	52	THR	ASN	CONFLICT	GB 1513182
H	56	THR	SER	CONFLICT	GB 1513182
H	70	SER	THR	CONFLICT	GB 1513182
H	80	MET	LEU	CONFLICT	GB 1513182
H	88	GLY	ALA	CONFLICT	GB 1513182
H	90	PHE	TYR	CONFLICT	GB 1513182
H	?	-	ALA	DELETION	GB 1513182
H	93	THR	ASP	CONFLICT	GB 1513182
H	?	-	SER	DELETION	GB 1513182
H	95	GLY	TRP	CONFLICT	GB 1513182
H	96	ASN	PHE	CONFLICT	GB 1513182
H	97	GLY	ALA	CONFLICT	GB 1513182
H	98	ASP	TYR	CONFLICT	GB 1513182
H	108	THR	LEU	CONFLICT	GB 1513182
H	109	LEU	VAL	CONFLICT	GB 1513182
H	113	SER	ALA	CONFLICT	GB 1513182
H	199	PRO	THR	CONFLICT	GB 1513182

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Chain	Residue	Modelled	Actual	Comment	Reference
H	200	ARG	TRP	CONFLICT	GB 1513182

- Molecule 3 is a protein called STAPHYLOCOCCAL NUCLEASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	S	138	Total	C	N	O	S	0	0	0
			1107	707	195	201	4			

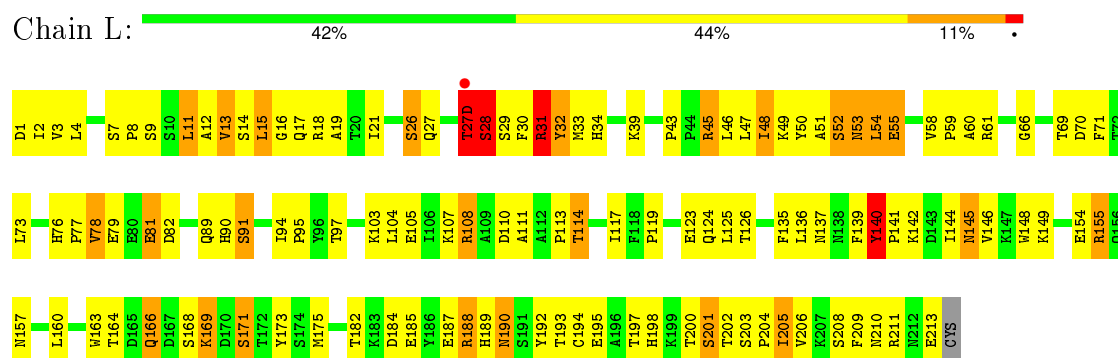
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	143	ASN	ASP	CONFLICT	UNP P00644
S	144	ASP	ASN	CONFLICT	UNP P00644

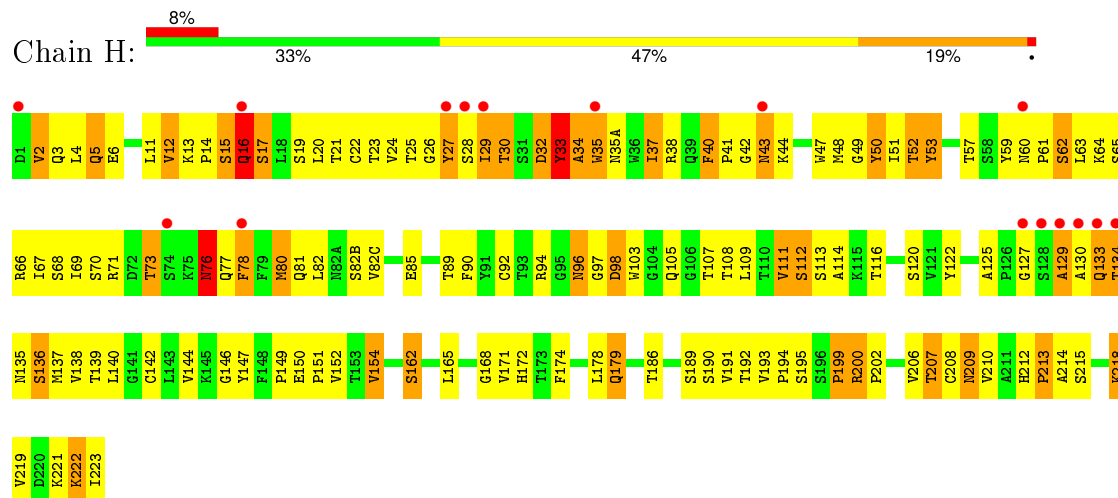
### 3 Residue-property plots

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.

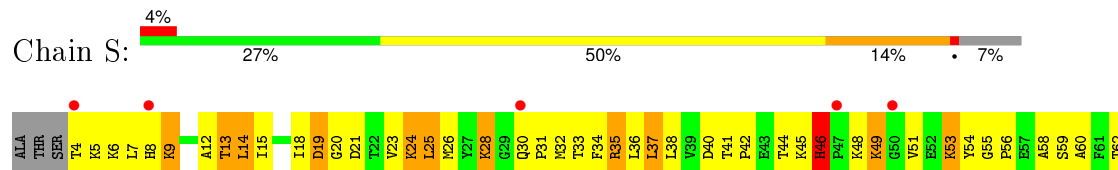
#### • Molecule 1: IGG FAB (IGG1, KAPPA)

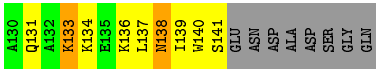
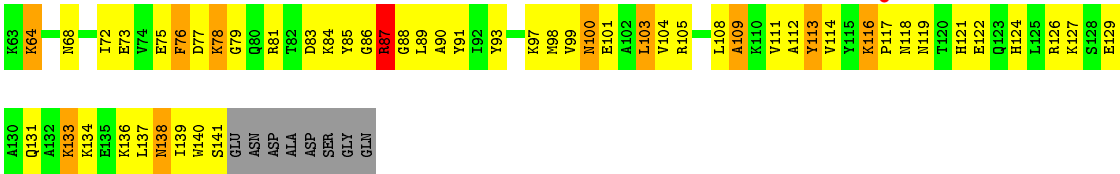


#### • Molecule 2: IGG FAB (IGG1, KAPPA)



#### • Molecule 3: STAPHYLOCOCCAL NUCLEASE





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	234.70 Å   43.50 Å   74.40 Å 90.00°   106.40°   90.00°	Depositor
Resolution (Å)	5.00 – 2.80 37.92 – 2.79	Depositor EDS
% Data completeness (in resolution range)	81.0 (5.00-2.80) 79.4 (37.92-2.79)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.85 (at 2.81 Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.195 , (Not available) 0.195 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	36.9	Xtriage
Anisotropy	0.194	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 97.7	EDS
Estimated twinning fraction	0.026 for -h-2*k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 14626 reflections	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	4388	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.45% 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	L	0.63	0/1736	0.92	2/2360 (0.1%)
2	H	0.62	0/1628	0.97	3/2228 (0.1%)
3	S	0.61	0/1128	0.91	3/1511 (0.2%)
All	All	0.62	0/4492	0.94	8/6099 (0.1%)

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	L	0	1
2	H	0	1
All	All	0	2

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	31	ARG	N-CA-C	-9.93	84.19	111.00
2	H	33	TYR	N-CA-C	-6.12	94.48	111.00
2	H	146	GLY	N-CA-C	6.08	128.30	113.10
3	S	14	LEU	CA-CB-CG	5.97	129.02	115.30
3	S	137	LEU	N-CA-C	5.68	126.34	111.00
3	S	25	LEU	CA-CB-CG	5.45	127.84	115.30
2	H	16	GLN	N-CA-C	5.24	125.15	111.00
1	L	205	ILE	N-CA-C	-5.12	97.17	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	50	TYR	Sidechain
1	L	140	TYR	Sidechain

## 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	L	1694	0	1615	117	0
2	H	1587	0	1543	139	0
3	S	1107	0	1151	100	0
All	All	4388	0	4309	339	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 39.

All (339) 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:L:15:LEU:HG	1:L:108:ARG:NH2	1.79	0.95
3:S:75:GLU:HB3	3:S:91:TYR:HB2	1.50	0.93
3:S:33:THR:HG23	3:S:87:ARG:HA	1.50	0.91
2:H:6:GLU:HG2	2:H:22:CYS:SG	2.16	0.86
2:H:57:THR:HB	2:H:69:ILE:HD11	1.57	0.85
2:H:24:VAL:HG11	2:H:35:TRP:HH2	1.41	0.85
1:L:149:LYS:HB2	1:L:193:THR:HB	1.59	0.84
2:H:35:TRP:NE1	2:H:78:PHE:HB2	1.94	0.83
1:L:15:LEU:HG	1:L:108:ARG:HH21	1.44	0.82
2:H:200:ARG:HD2	2:H:202:PRO:HA	1.60	0.82
3:S:46:HIS:HB3	3:S:48:LYS:O	1.80	0.81
1:L:135:PHE:CE2	2:H:190:SER:HB3	2.17	0.80
2:H:20:LEU:HD22	2:H:107:THR:HG21	1.65	0.79
2:H:24:VAL:HG11	2:H:35:TRP:CH2	2.17	0.78
3:S:40:ASP:HB2	3:S:112:ALA:HB2	1.64	0.78
2:H:125:ALA:HB2	2:H:223:ILE:HG22	1.65	0.76
2:H:4:LEU:HD23	2:H:24:VAL:HG12	1.69	0.75
2:H:28:SER:HA	2:H:76:ASN:OD1	1.87	0.74
3:S:40:ASP:HB2	3:S:112:ALA:CB	2.18	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:9:LYS:HB2	3:S:73:GLU:HB3	1.70	0.74
2:H:67:ILE:HG23	2:H:82:LEU:HD13	1.70	0.74
2:H:32:ASP:OD2	2:H:34:ALA:HB2	1.88	0.73
3:S:60:ALA:O	3:S:64:LYS:HG2	1.89	0.71
3:S:14:LEU:HA	3:S:25:LEU:HD22	1.71	0.71
2:H:96:ASN:HD21	3:S:105:ARG:HH11	1.37	0.71
2:H:137:MET:HA	2:H:195:SER:N	2.06	0.71
3:S:127:LYS:O	3:S:131:GLN:HG2	1.91	0.70
2:H:11:LEU:HD23	2:H:12:VAL:N	2.06	0.70
1:L:211:ARG:HH11	1:L:211:ARG:HG2	1.57	0.70
1:L:27(D):THR:CG2	1:L:28:SER:H	2.05	0.70
1:L:110:ASP:HB3	1:L:200:THR:HG21	1.74	0.70
1:L:27(D):THR:CG2	1:L:28:SER:N	2.55	0.69
2:H:94:ARG:HD2	2:H:96:ASN:N	2.09	0.68
2:H:200:ARG:NH1	2:H:202:PRO:HG3	2.09	0.67
1:L:144:ILE:HB	1:L:198:HIS:HD2	1.59	0.67
3:S:41:THR:HB	3:S:109:ALA:HB2	1.76	0.67
1:L:164:THR:HG23	2:H:174:PHE:CD2	2.29	0.67
3:S:15:ILE:HD11	3:S:26:MET:HB2	1.77	0.66
1:L:160:LEU:HD11	2:H:179:GLN:HB2	1.77	0.66
2:H:2:VAL:H	2:H:26:GLY:HA3	1.61	0.65
2:H:67:ILE:HG23	2:H:82:LEU:CD1	2.27	0.65
1:L:195:GLU:HB3	1:L:206:VAL:HB	1.78	0.65
1:L:43:PRO:HG3	2:H:105:GLN:NE2	2.11	0.65
2:H:35:TRP:HA	2:H:35:TRP:CE3	2.31	0.64
1:L:193:THR:HG23	1:L:208:SER:OG	1.98	0.64
3:S:76:PHE:CB	3:S:81:ARG:HH21	2.10	0.64
2:H:29:ILE:HG13	2:H:76:ASN:HD21	1.62	0.64
3:S:21:ASP:O	3:S:35:ARG:HA	1.97	0.64
1:L:61:ARG:HD2	1:L:77:PRO:O	1.97	0.64
2:H:80:MET:HE3	2:H:90:PHE:CD1	2.33	0.64
2:H:29:ILE:HB	2:H:73:THR:HG22	1.79	0.63
1:L:27(D):THR:HG22	1:L:28:SER:H	1.63	0.63
1:L:32:TYR:HD1	1:L:91:SER:HG	1.41	0.63
3:S:98:MET:HB3	3:S:101:GLU:HG2	1.81	0.63
1:L:18:ARG:HA	1:L:76:HIS:HA	1.79	0.63
1:L:27(D):THR:HG23	1:L:28:SER:N	2.15	0.62
2:H:137:MET:HA	2:H:195:SER:H	1.63	0.62
1:L:66:GLY:HA3	1:L:71:PHE:HA	1.81	0.62
3:S:32:MET:HG2	3:S:34:PHE:CE1	2.34	0.62
2:H:129:ALA:O	2:H:133:GLN:HG2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:18:ARG:HE	1:L:76:HIS:HD2	1.47	0.62
1:L:193:THR:HG23	1:L:208:SER:HG	1.65	0.62
2:H:96:ASN:HD21	3:S:105:ARG:NH1	1.97	0.61
1:L:184:ASP:O	1:L:188:ARG:HD3	1.99	0.61
3:S:15:ILE:HB	3:S:24:LYS:HD3	1.82	0.61
2:H:29:ILE:HG13	2:H:76:ASN:ND2	2.15	0.61
2:H:38:ARG:NH2	2:H:85:GLU:O	2.34	0.61
2:H:194:PRO:HB2	2:H:199:PRO:HD2	1.81	0.61
1:L:211:ARG:NH1	1:L:211:ARG:HG2	2.13	0.61
3:S:83:ASP:OD1	3:S:89:LEU:HD21	2.00	0.61
3:S:112:ALA:HB1	3:S:113:TYR:CD1	2.36	0.61
1:L:95:PRO:HA	2:H:47:TRP:CZ3	2.36	0.61
3:S:81:ARG:O	3:S:88:GLY:HA2	2.00	0.60
3:S:45:LYS:O	3:S:46:HIS:HB2	2.01	0.60
3:S:136:LYS:O	3:S:141:SER:HB3	2.02	0.60
1:L:47:LEU:HD22	1:L:58:VAL:HG11	1.83	0.60
1:L:182:THR:OG1	1:L:185:GLU:HG3	2.02	0.60
1:L:11:LEU:HD12	1:L:21:ILE:HG12	1.83	0.60
3:S:98:MET:SD	3:S:101:GLU:OE2	2.59	0.60
2:H:168:GLY:HA3	2:H:192:THR:OG1	2.02	0.60
2:H:112:SER:C	2:H:114:ALA:H	2.03	0.60
3:S:13:THR:HG23	3:S:26:MET:HB3	1.82	0.60
2:H:2:VAL:HG13	2:H:33:TYR:OH	2.02	0.60
1:L:12:ALA:HA	1:L:105:GLU:O	2.02	0.60
2:H:135:ASN:O	2:H:137:MET:N	2.36	0.59
1:L:52:SER:O	1:L:53:ASN:HB2	2.01	0.59
1:L:18:ARG:HE	1:L:76:HIS:CD2	2.22	0.58
2:H:25:THR:HG22	2:H:26:GLY:H	1.67	0.58
2:H:96:ASN:ND2	3:S:105:ARG:HD2	2.19	0.58
1:L:48:ILE:HD12	1:L:48:ILE:C	2.23	0.58
2:H:82(C):VAL:CG1	2:H:111:VAL:HG21	2.34	0.58
1:L:110:ASP:HB3	1:L:200:THR:CG2	2.33	0.58
1:L:144:ILE:HG22	1:L:163:TRP:CH2	2.39	0.57
1:L:189:HIS:HB2	1:L:192:TYR:OH	2.04	0.57
3:S:76:PHE:HB3	3:S:81:ARG:HH21	1.68	0.57
3:S:37:LEU:HB2	3:S:90:ALA:O	2.04	0.57
1:L:190:ASN:O	1:L:210:ASN:HA	2.03	0.57
1:L:15:LEU:HG	1:L:108:ARG:HH22	1.66	0.57
3:S:9:LYS:HD3	3:S:93:TYR:CE2	2.40	0.57
2:H:193:VAL:HG22	2:H:194:PRO:HD2	1.86	0.57
2:H:42:GLY:O	2:H:43:ASN:HB2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:89:GLN:HG2	1:L:90:HIS:N	2.19	0.57
2:H:35:TRP:NE1	2:H:78:PHE:CB	2.67	0.57
1:L:30:PHE:CD2	1:L:32:TYR:HD2	2.23	0.57
2:H:35:TRP:HA	2:H:35:TRP:HE3	1.70	0.57
1:L:16:GLY:H	1:L:78:VAL:HG12	1.67	0.57
2:H:24:VAL:CG1	2:H:35:TRP:HH2	2.15	0.56
3:S:108:LEU:O	3:S:109:ALA:HB2	2.05	0.56
2:H:207:THR:HG23	2:H:222:LYS:HB3	1.88	0.56
1:L:148:TRP:O	1:L:154:GLU:HA	2.06	0.56
3:S:53:LYS:HE2	3:S:54:TYR:H	1.71	0.56
2:H:33:TYR:HD2	2:H:35:TRP:CZ3	2.23	0.56
3:S:9:LYS:HD2	3:S:73:GLU:OE1	2.07	0.55
1:L:7:SER:HB3	1:L:8:PRO:HA	1.88	0.55
1:L:140:TYR:O	1:L:141:PRO:C	2.45	0.55
1:L:149:LYS:HD3	1:L:154:GLU:HG2	1.88	0.55
3:S:79:GLY:N	3:S:118:ASN:OD1	2.39	0.55
2:H:40:PHE:CD1	2:H:41:PRO:HD2	2.42	0.55
2:H:213:PRO:O	2:H:215:SER:N	2.40	0.55
2:H:14:PRO:O	2:H:15:SER:CB	2.55	0.54
2:H:35:TRP:HE1	2:H:78:PHE:HB2	1.67	0.54
2:H:194:PRO:O	2:H:199:PRO:HD2	2.08	0.54
2:H:67:ILE:HA	2:H:81:GLN:O	2.06	0.54
2:H:23:THR:HA	2:H:76:ASN:O	2.08	0.54
2:H:94:ARG:HD2	2:H:96:ASN:H	1.72	0.54
3:S:98:MET:HB3	3:S:101:GLU:CG	2.38	0.54
2:H:194:PRO:HB2	2:H:199:PRO:CD	2.37	0.54
1:L:168:SER:O	1:L:169:LYS:HE2	2.07	0.53
2:H:162:SER:H	2:H:209:ASN:ND2	2.06	0.53
1:L:15:LEU:CG	1:L:108:ARG:HH21	2.19	0.53
3:S:9:LYS:HD3	3:S:93:TYR:CD2	2.43	0.53
1:L:18:ARG:HB2	1:L:76:HIS:CD2	2.43	0.53
1:L:169:LYS:HE2	1:L:169:LYS:HA	1.90	0.53
1:L:119:PRO:HG3	1:L:209:PHE:CE1	2.44	0.53
1:L:90:HIS:CD2	1:L:97:THR:OG1	2.62	0.53
2:H:52:THR:OG1	2:H:53:TYR:N	2.41	0.53
3:S:14:LEU:HD13	3:S:15:ILE:N	2.24	0.53
1:L:2:ILE:HD11	1:L:90:HIS:CG	2.43	0.53
2:H:40:PHE:HB2	2:H:44:LYS:HE2	1.91	0.53
1:L:27:GLN:O	1:L:69:THR:HG22	2.08	0.53
2:H:154:VAL:HB	2:H:210:VAL:HG22	1.90	0.52
2:H:11:LEU:HD23	2:H:12:VAL:H	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:19:ASP:O	3:S:21:ASP:N	2.43	0.52
3:S:14:LEU:HA	3:S:25:LEU:CD2	2.37	0.52
3:S:21:ASP:HA	3:S:36:LEU:HB2	1.91	0.52
1:L:48:ILE:HD12	1:L:48:ILE:O	2.09	0.52
1:L:155:ARG:HD3	1:L:157:ASN:H	1.75	0.52
2:H:112:SER:O	2:H:114:ALA:N	2.43	0.52
3:S:33:THR:HG23	3:S:87:ARG:CA	2.31	0.51
1:L:17:GLN:O	1:L:78:VAL:HB	2.10	0.51
1:L:195:GLU:CB	1:L:206:VAL:HB	2.41	0.51
1:L:50:TYR:O	1:L:51:ALA:HB3	2.10	0.51
1:L:144:ILE:HG13	1:L:198:HIS:HB2	1.93	0.51
3:S:83:ASP:HB2	3:S:87:ARG:O	2.11	0.51
1:L:30:PHE:CG	1:L:32:TYR:HD2	2.28	0.51
1:L:15:LEU:CD2	1:L:79:GLU:HA	2.41	0.50
3:S:15:ILE:HG12	3:S:26:MET:H	1.77	0.50
1:L:43:PRO:HG3	2:H:105:GLN:HE21	1.74	0.50
1:L:117:ILE:CD1	1:L:208:SER:HA	2.41	0.50
2:H:35(A):ASN:OD1	2:H:50:TYR:HB3	2.12	0.50
1:L:135:PHE:C	1:L:136:LEU:HD12	2.31	0.50
3:S:93:TYR:HA	3:S:97:LYS:O	2.12	0.50
1:L:187:GLU:O	1:L:211:ARG:NH2	2.45	0.50
2:H:14:PRO:O	2:H:15:SER:HB2	2.12	0.50
2:H:59:TYR:HB2	2:H:64:LYS:HG3	1.94	0.50
2:H:35:TRP:CA	2:H:35:TRP:CE3	2.95	0.50
1:L:82:ASP:O	1:L:104:LEU:HD23	2.12	0.50
1:L:113:PRO:N	1:L:139:PHE:HB3	2.27	0.50
1:L:114:THR:O	1:L:114:THR:HG22	2.10	0.50
3:S:116:LYS:HG2	3:S:117:PRO:HA	1.94	0.50
1:L:123:GLU:O	1:L:126:THR:HB	2.12	0.50
3:S:15:ILE:HG12	3:S:26:MET:N	2.26	0.49
2:H:82(C):VAL:HG13	2:H:111:VAL:HG21	1.92	0.49
1:L:205:ILE:H	1:L:205:ILE:HD12	1.76	0.49
1:L:13:VAL:HG11	1:L:18:ARG:O	2.12	0.49
1:L:76:HIS:O	1:L:78:VAL:N	2.45	0.49
2:H:14:PRO:HG3	2:H:111:VAL:CG1	2.42	0.49
3:S:77:ASP:HB3	3:S:118:ASN:ND2	2.26	0.49
3:S:14:LEU:HD22	3:S:15:ILE:H	1.76	0.49
2:H:27:TYR:OH	3:S:127:LYS:HD3	2.12	0.49
1:L:166:GLN:NE2	1:L:173:TYR:OH	2.44	0.49
1:L:166:GLN:HE21	1:L:173:TYR:HE2	1.59	0.49
3:S:133:LYS:HG2	3:S:140:TRP:CE3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:3:GLN:HB3	2:H:25:THR:HB	1.93	0.49
3:S:53:LYS:O	3:S:54:TYR:HB2	2.13	0.49
3:S:9:LYS:CB	3:S:73:GLU:HB3	2.42	0.49
2:H:25:THR:HG22	2:H:26:GLY:N	2.26	0.49
2:H:40:PHE:CD1	2:H:41:PRO:N	2.80	0.49
3:S:62:THR:OG1	3:S:103:LEU:HD11	2.13	0.49
3:S:18:ILE:HD12	3:S:18:ILE:N	2.28	0.48
1:L:144:ILE:HG13	1:L:197:THR:O	2.14	0.48
1:L:185:GLU:O	1:L:188:ARG:HB2	2.14	0.48
2:H:135:ASN:O	2:H:195:SER:HB2	2.14	0.48
2:H:138:VAL:O	2:H:192:THR:HA	2.12	0.48
3:S:6:LYS:HB3	3:S:7:LEU:HD12	1.95	0.48
1:L:94:ILE:HG13	1:L:94:ILE:O	2.13	0.48
3:S:113:TYR:N	3:S:113:TYR:CD1	2.81	0.48
3:S:15:ILE:CD1	3:S:26:MET:HB2	2.42	0.48
1:L:113:PRO:HA	1:L:137:ASN:O	2.13	0.48
3:S:122:GLU:O	3:S:126:ARG:HG2	2.13	0.48
3:S:36:LEU:HD12	3:S:100:ASN:OD1	2.14	0.48
1:L:144:ILE:HB	1:L:198:HIS:CD2	2.44	0.48
3:S:26:MET:CE	3:S:31:PRO:HG3	2.43	0.47
3:S:58:ALA:HA	3:S:108:LEU:HD22	1.96	0.47
3:S:23:VAL:HG12	3:S:25:LEU:HG	1.97	0.47
2:H:24:VAL:HG23	2:H:24:VAL:O	2.15	0.47
3:S:76:PHE:HA	3:S:81:ARG:HE	1.79	0.47
2:H:71:ARG:HA	2:H:78:PHE:HD1	1.80	0.47
3:S:7:LEU:HD23	3:S:76:PHE:O	2.15	0.47
2:H:61:PRO:O	2:H:62:SER:C	2.53	0.47
2:H:133:GLN:HG3	2:H:134:THR:H	1.80	0.47
2:H:112:SER:C	2:H:114:ALA:N	2.68	0.47
1:L:90:HIS:HD2	1:L:97:THR:OG1	1.98	0.47
2:H:33:TYR:O	2:H:35:TRP:CE3	2.68	0.47
2:H:11:LEU:HD12	2:H:149:PRO:HD3	1.97	0.47
3:S:37:LEU:HD23	3:S:77:ASP:OD2	2.14	0.47
2:H:139:THR:OG1	2:H:192:THR:HG22	2.13	0.47
1:L:13:VAL:CG2	1:L:104:LEU:HD11	2.45	0.46
3:S:51:VAL:HG12	3:S:56:PRO:HD3	1.97	0.46
3:S:64:LYS:O	3:S:68:ASN:HB2	2.15	0.46
2:H:57:THR:HG21	2:H:69:ILE:HG13	1.98	0.46
1:L:189:HIS:O	1:L:211:ARG:NE	2.48	0.46
3:S:83:ASP:OD2	3:S:85:TYR:HD1	1.99	0.46
2:H:71:ARG:NH2	2:H:73:THR:OG1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:160:LEU:CD1	2:H:179:GLN:HB2	2.43	0.46
1:L:169:LYS:CE	1:L:169:LYS:HA	2.45	0.46
3:S:111:VAL:HG22	3:S:129:GLU:OE2	2.15	0.46
1:L:27(D):THR:HG21	3:S:64:LYS:HG3	1.97	0.46
2:H:97:GLY:O	2:H:98:ASP:O	2.34	0.46
1:L:39:LYS:NZ	1:L:81:GLU:O	2.49	0.46
3:S:35:ARG:HB2	3:S:87:ARG:CD	2.46	0.46
2:H:5:GLN:HE21	2:H:23:THR:HB	1.80	0.46
2:H:140:LEU:HD12	2:H:206:VAL:HG11	1.97	0.46
2:H:76:ASN:O	2:H:77:GLN:HG3	2.15	0.46
1:L:3:VAL:O	1:L:26:SER:OG	2.34	0.46
2:H:16:GLN:O	2:H:17:SER:O	2.34	0.45
2:H:68:SER:O	2:H:80:MET:HA	2.16	0.45
2:H:80:MET:O	2:H:80:MET:HG3	2.11	0.45
2:H:47:TRP:CZ2	2:H:49:GLY:HA2	2.51	0.45
2:H:13:LYS:HG2	2:H:114:ALA:HB2	1.98	0.45
1:L:4:LEU:HD11	1:L:97:THR:O	2.16	0.45
3:S:18:ILE:CD1	3:S:24:LYS:HB2	2.46	0.45
2:H:24:VAL:CG2	2:H:76:ASN:ND2	2.80	0.45
2:H:35:TRP:HB2	2:H:51:ILE:HG22	1.99	0.45
1:L:145:ASN:C	1:L:145:ASN:ND2	2.70	0.45
2:H:200:ARG:HB3	2:H:200:ARG:HH11	1.81	0.45
1:L:14:SER:HA	1:L:107:LYS:HG3	1.97	0.45
3:S:140:TRP:N	3:S:140:TRP:CD1	2.84	0.45
1:L:54:LEU:HD11	1:L:60:ALA:HA	1.99	0.45
1:L:108:ARG:HD2	1:L:171:SER:HB2	1.98	0.45
2:H:4:LEU:HD21	2:H:35:TRP:CH2	2.52	0.45
2:H:70:SER:O	2:H:78:PHE:HA	2.17	0.45
2:H:147:TYR:CE2	2:H:152:VAL:HG21	2.51	0.45
2:H:63:LEU:HD23	2:H:63:LEU:HA	1.75	0.45
2:H:40:PHE:HD1	2:H:41:PRO:N	2.15	0.44
3:S:108:LEU:O	3:S:109:ALA:CB	2.65	0.44
3:S:12:ALA:O	3:S:72:ILE:HB	2.17	0.44
1:L:31:ARG:NH2	1:L:52:SER:OG	2.51	0.44
2:H:40:PHE:CD1	2:H:41:PRO:CD	3.00	0.44
1:L:46:LEU:HD23	1:L:55:GLU:HG3	1.99	0.44
1:L:15:LEU:O	1:L:15:LEU:HD13	2.18	0.44
3:S:15:ILE:HG21	3:S:24:LYS:HD2	2.00	0.44
1:L:45:ARG:NH1	1:L:58:VAL:HG22	2.32	0.44
3:S:35:ARG:HB2	3:S:87:ARG:HD3	1.98	0.44
3:S:37:LEU:O	3:S:38:LEU:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:154:VAL:HA	2:H:209:ASN:O	2.18	0.44
2:H:218:LYS:HD3	2:H:219:VAL:N	2.33	0.44
3:S:6:LYS:HB2	3:S:7:LEU:H	1.67	0.44
2:H:14:PRO:HG3	2:H:111:VAL:HG12	2.00	0.44
2:H:165:LEU:O	2:H:171:VAL:HG21	2.18	0.44
3:S:139:ILE:HG22	3:S:140:TRP:CD1	2.53	0.44
2:H:16:GLN:NE2	2:H:16:GLN:HA	2.32	0.44
1:L:34:HIS:ND1	1:L:49:LYS:O	2.50	0.43
1:L:13:VAL:HG21	1:L:19:ALA:HB2	2.01	0.43
3:S:53:LYS:HA	3:S:53:LYS:CE	2.48	0.43
2:H:37:ILE:HG13	2:H:103:TRP:CZ3	2.53	0.43
2:H:65:SER:O	2:H:66:ARG:HG2	2.18	0.43
3:S:34:PHE:HA	3:S:88:GLY:O	2.18	0.43
1:L:201:SER:HB3	1:L:203:SER:O	2.17	0.43
3:S:116:LYS:HA	3:S:118:ASN:N	2.33	0.43
3:S:100:ASN:OD1	3:S:100:ASN:N	2.52	0.43
1:L:21:ILE:HD12	1:L:73:LEU:HD23	2.01	0.43
3:S:54:TYR:CZ	3:S:138:ASN:C	2.91	0.43
1:L:43:PRO:CG	2:H:105:GLN:HE21	2.32	0.43
3:S:15:ILE:CG1	3:S:26:MET:HB2	2.49	0.43
2:H:172:HIS:O	2:H:189:SER:HA	2.19	0.43
3:S:98:MET:SD	3:S:121:HIS:CD2	3.12	0.42
1:L:48:ILE:HD13	1:L:51:ALA:C	2.39	0.42
2:H:150:GLU:CB	2:H:151:PRO:HA	2.49	0.42
2:H:22:CYS:HB3	2:H:35:TRP:CZ2	2.54	0.42
1:L:160:LEU:HD21	2:H:186:THR:HB	2.02	0.42
1:L:54:LEU:HD11	1:L:59:PRO:O	2.20	0.42
3:S:28:LYS:HG3	3:S:28:LYS:O	2.19	0.42
1:L:111:ALA:H	1:L:140:TYR:HB3	1.85	0.42
1:L:107:LYS:HB3	1:L:140:TYR:OH	2.19	0.42
1:L:11:LEU:CD1	1:L:21:ILE:HG12	2.49	0.42
1:L:31:ARG:HH11	1:L:31:ARG:HG2	1.84	0.42
2:H:64:LYS:HB2	2:H:64:LYS:HE2	1.76	0.42
2:H:120:SER:HB3	2:H:122:TYR:CZ	2.55	0.42
2:H:35:TRP:CD1	2:H:78:PHE:CB	3.02	0.42
1:L:135:PHE:CD2	2:H:190:SER:HB3	2.53	0.42
2:H:30:THR:C	2:H:32:ASP:H	2.23	0.42
2:H:96:ASN:HD21	3:S:105:ARG:HD2	1.84	0.42
1:L:31:ARG:HB3	1:L:51:ALA:HB2	2.02	0.42
3:S:76:PHE:HE1	3:S:78:LYS:HA	1.85	0.42
3:S:78:LYS:O	3:S:117:PRO:CG	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:53:TYR:CD1	2:H:53:TYR:C	2.92	0.41
2:H:144:VAL:HG11	2:H:152:VAL:HG11	2.01	0.41
2:H:4:LEU:HD22	2:H:92:CYS:SG	2.60	0.41
1:L:76:HIS:HB3	1:L:77:PRO:CD	2.50	0.41
3:S:99:VAL:O	3:S:103:LEU:HD12	2.19	0.41
3:S:18:ILE:HD11	3:S:24:LYS:HB2	2.02	0.41
1:L:209:PHE:HE2	1:L:211:ARG:HA	1.84	0.41
1:L:203:SER:HB2	1:L:204:PRO:HD2	2.02	0.41
2:H:108:THR:O	2:H:109:LEU:HD13	2.21	0.41
3:S:18:ILE:HG22	3:S:19:ASP:N	2.36	0.41
2:H:140:LEU:HD21	2:H:200:ARG:HG3	2.02	0.41
2:H:140:LEU:HB2	2:H:191:VAL:CG1	2.50	0.41
1:L:144:ILE:HG22	1:L:163:TRP:CZ3	2.56	0.41
3:S:76:PHE:HB2	3:S:81:ARG:HE	1.86	0.41
2:H:194:PRO:O	2:H:199:PRO:HG2	2.21	0.41
1:L:140:TYR:CD1	1:L:140:TYR:C	2.92	0.41
2:H:32:ASP:OD1	2:H:34:ALA:N	2.53	0.41
3:S:54:TYR:CE1	3:S:138:ASN:HB3	2.56	0.41
2:H:50:TYR:CZ	3:S:97:LYS:NZ	2.88	0.41
2:H:48:MET:SD	2:H:90:PHE:HD1	2.44	0.41
2:H:111:VAL:O	2:H:111:VAL:HG12	2.21	0.41
2:H:212:HIS:HA	2:H:213:PRO:HD2	1.84	0.41
2:H:178:LEU:HG	2:H:178:LEU:O	2.20	0.41
2:H:89:THR:HA	2:H:107:THR:O	2.21	0.41
1:L:184:ASP:O	1:L:185:GLU:C	2.60	0.41
2:H:60:ASN:OD1	2:H:62:SER:N	2.54	0.40
3:S:5:LYS:HA	3:S:5:LYS:HD2	1.95	0.40
1:L:33:MET:O	1:L:51:ALA:N	2.54	0.40
2:H:135:ASN:OD1	2:H:136:SER:N	2.54	0.40
3:S:18:ILE:CD1	3:S:18:ILE:N	2.84	0.40
3:S:86:GLY:O	3:S:87:ARG:C	2.59	0.40
3:S:8:HIS:HD2	3:S:9:LYS:O	2.05	0.40
1:L:90:HIS:CD2	1:L:97:THR:H	2.39	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	L	215/218 (99%)	178 (83%)	30 (14%)	7 (3%)	5	16
2	H	208/210 (99%)	145 (70%)	41 (20%)	22 (11%)	0	1
3	S	136/149 (91%)	99 (73%)	22 (16%)	15 (11%)	0	1
All	All	559/577 (97%)	422 (76%)	93 (17%)	44 (8%)	1	2

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	28	SER
1	L	29	SER
1	L	31	ARG
1	L	140	TYR
1	L	201	SER
2	H	15	SER
2	H	17	SER
2	H	30	THR
2	H	43	ASN
2	H	62	SER
2	H	96	ASN
2	H	98	ASP
2	H	130	ALA
2	H	133	GLN
2	H	136	SER
3	S	20	GLY
3	S	28	LYS
3	S	46	HIS
3	S	109	ALA
3	S	113	TYR
3	S	119	ASN
1	L	27(D)	THR
2	H	76	ASN
2	H	113	SER

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Mol	Chain	Res	Type
2	H	127	GLY
2	H	129	ALA
2	H	214	ALA
3	S	78	LYS
3	S	87	ARG
3	S	138	ASN
3	S	84	LYS
1	L	142	LYS
2	H	2	VAL
2	H	29	ILE
2	H	32	ASP
2	H	34	ALA
3	S	124	HIS
2	H	199	PRO
3	S	42	PRO
3	S	49	LYS
3	S	116	LYS
2	H	111	VAL
2	H	213	PRO
3	S	55	GLY

### 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	L	193/194 (100%)	156 (81%)	37 (19%)	2	5
2	H	186/186 (100%)	155 (83%)	31 (17%)	3	8
3	S	117/125 (94%)	95 (81%)	22 (19%)	2	6
All	All	496/505 (98%)	406 (82%)	90 (18%)	2	6

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	1	ASP
1	L	9	SER

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Mol	Chain	Res	Type
1	L	11	LEU
1	L	13	VAL
1	L	15	LEU
1	L	26	SER
1	L	27(D)	THR
1	L	28	SER
1	L	31	ARG
1	L	32	TYR
1	L	45	ARG
1	L	48	ILE
1	L	52	SER
1	L	53	ASN
1	L	54	LEU
1	L	55	GLU
1	L	70	ASP
1	L	78	VAL
1	L	81	GLU
1	L	91	SER
1	L	103	LYS
1	L	108	ARG
1	L	114	THR
1	L	124	GLN
1	L	125	LEU
1	L	145	ASN
1	L	146	VAL
1	L	155	ARG
1	L	166	GLN
1	L	169	LYS
1	L	171	SER
1	L	175	MET
1	L	188	ARG
1	L	190	ASN
1	L	194	CYS
1	L	202	THR
1	L	213	GLU
2	H	5	GLN
2	H	12	VAL
2	H	16	GLN
2	H	19	SER
2	H	21	THR
2	H	27	TYR
2	H	33	TYR

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Mol	Chain	Res	Type
2	H	35	TRP
2	H	37	ILE
2	H	40	PHE
2	H	52	THR
2	H	53	TYR
2	H	73	THR
2	H	76	ASN
2	H	78	PHE
2	H	80	MET
2	H	82(B)	SER
2	H	112	SER
2	H	116	THR
2	H	134	THR
2	H	142	CYS
2	H	154	VAL
2	H	162	SER
2	H	179	GLN
2	H	200	ARG
2	H	207	THR
2	H	208	CYS
2	H	209	ASN
2	H	218	LYS
2	H	221	LYS
2	H	222	LYS
3	S	4	THR
3	S	9	LYS
3	S	13	THR
3	S	19	ASP
3	S	24	LYS
3	S	30	GLN
3	S	35	ARG
3	S	37	LEU
3	S	44	THR
3	S	46	HIS
3	S	49	LYS
3	S	53	LYS
3	S	59	SER
3	S	64	LYS
3	S	76	PHE
3	S	87	ARG
3	S	100	ASN
3	S	103	LEU

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Mol	Chain	Res	Type
3	S	104	VAL
3	S	114	VAL
3	S	133	LYS
3	S	134	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	38	GLN
1	L	53	ASN
1	L	76	HIS
1	L	90	HIS
1	L	138	ASN
1	L	145	ASN
1	L	166	GLN
1	L	212	ASN
2	H	39	GLN
2	H	76	ASN
2	H	77	GLN
2	H	96	ASN
2	H	105	GLN
2	H	209	ASN
3	S	8	HIS
3	S	123	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

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	L	217/218 (99%)	-0.41	1 (0%) 91 88	3, 14, 25, 36	0
2	H	210/210 (100%)	0.08	16 (7%) 17 9	4, 19, 35, 42	0
3	S	138/149 (92%)	-0.03	6 (4%) 39 27	10, 25, 33, 38	0
All	All	565/577 (97%)	-0.13	23 (4%) 41 29	3, 18, 32, 42	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	28	SER	6.0
2	H	29	ILE	5.2
3	S	47	PRO	5.1
3	S	4	THR	4.4
2	H	128	SER	4.1
2	H	130	ALA	3.9
3	S	117	PRO	3.9
2	H	74	SER	3.5
2	H	16	GLN	3.4
2	H	134	THR	3.3
2	H	43	ASN	3.1
2	H	129	ALA	3.0
2	H	133	GLN	2.8
2	H	78	PHE	2.8
3	S	8	HIS	2.4
2	H	127	GLY	2.4
3	S	30	GLN	2.4
2	H	27	TYR	2.3
2	H	1	ASP	2.3
2	H	60	ASN	2.2
2	H	35	TRP	2.2
3	S	50	GLY	2.1
1	L	27(D)	THR	2.1

## 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.