



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:45 PM GMT

PDB ID : 1YI5  
Title : Crystal structure of the  $\alpha$ -cobratoxin-AChBP complex  
Authors : Bourne, Y.; Talley, T.T.; Hansen, S.B.; Taylor, P.; Marchot, P.  
Deposited on : 2005-01-11  
Resolution : 4.20 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

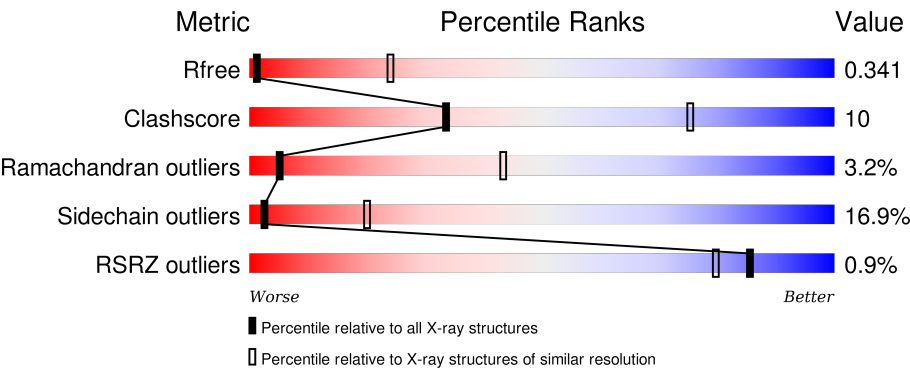
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.20 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 <sub>free</sub>	91344	1039 (4.80-3.60)
Clashscore	102246	1140 (4.80-3.60)
Ramachandran outliers	100387	1083 (4.80-3.60)
Sidechain outliers	100360	1067 (4.80-3.60)
RSRZ outliers	91569	1042 (4.80-3.60)

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	210	<div><div></div><div><div></div><div>61%</div><div>31%</div><div></div><div></div></div><div></div></div>
1	B	210	<div><div></div><div><div></div><div>%</div><div>61%</div><div>32%</div><div></div><div></div></div><div></div></div>
1	C	210	<div><div></div><div><div></div><div>63%</div><div>28%</div><div>6%</div><div></div></div><div></div></div>
1	D	210	<div><div></div><div><div></div><div>60%</div><div>31%</div><div>5%</div><div></div></div><div></div></div>
1	E	210	<div><div></div><div><div></div><div>59%</div><div>33%</div><div></div><div></div></div><div></div></div>

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Mol	Chain	Length	Quality of chain
2	F	71	<div><div></div><div>46%42%6% . .</div></div>
2	G	71	<div>%<div><div></div><div>48%39%8% .</div></div></div>
2	H	71	<div><div></div><div>44%45%6% . .</div></div>
2	I	71	<div>6%<div><div></div><div>41%45%8%6%</div></div></div>
2	J	71	<div>%<div><div></div><div>46%39%10% .</div></div></div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10648 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 Acetylcholine-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	202	Total	C	N	O	S	0	0	0
			1612	1010	276	321	5			
1	B	204	Total	C	N	O	S	0	0	0
			1627	1018	279	325	5			
1	C	203	Total	C	N	O	S	0	0	0
			1623	1016	280	322	5			
1	D	205	Total	C	N	O	S	0	0	0
			1636	1023	280	328	5			
1	E	203	Total	C	N	O	S	0	0	0
			1620	1014	278	323	5			

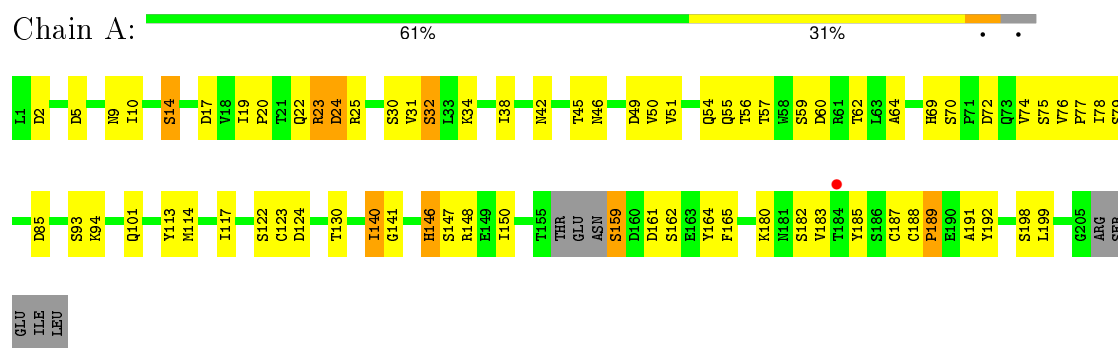
- Molecule 2 is a protein called Long neurotoxin 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	68	Total	C	N	O	S	0	0	0
			507	312	88	97	10			
2	G	68	Total	C	N	O	S	0	0	0
			507	312	88	97	10			
2	H	68	Total	C	N	O	S	0	0	0
			507	312	88	97	10			
2	I	67	Total	C	N	O	S	0	0	0
			502	309	87	96	10			
2	J	68	Total	C	N	O	S	0	0	0
			507	312	88	97	10			

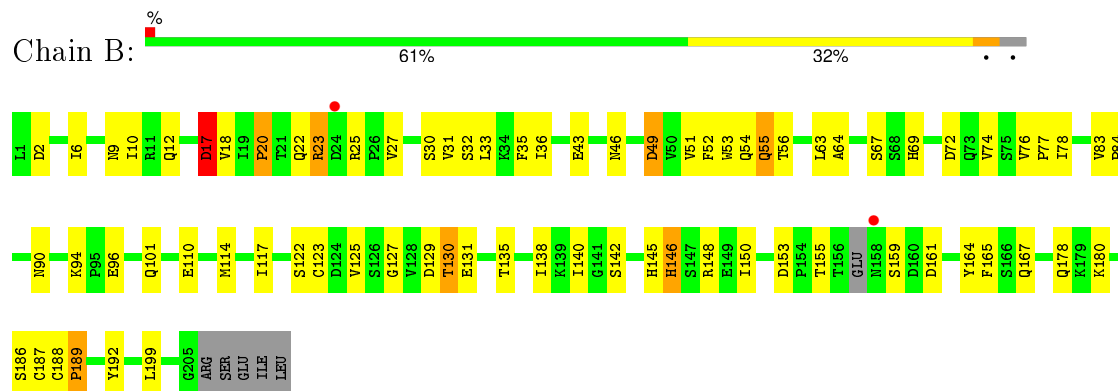
### 3 Residue-property plots

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.

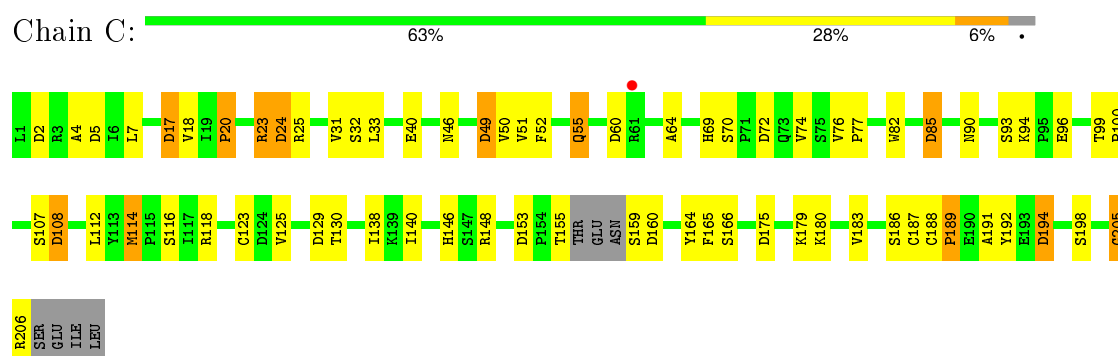
#### • Molecule 1: Acetylcholine-binding protein



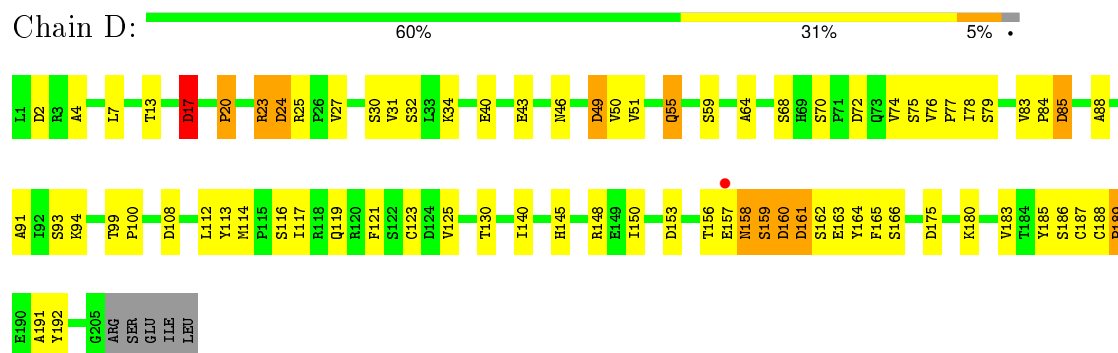
#### • Molecule 1: Acetylcholine-binding protein



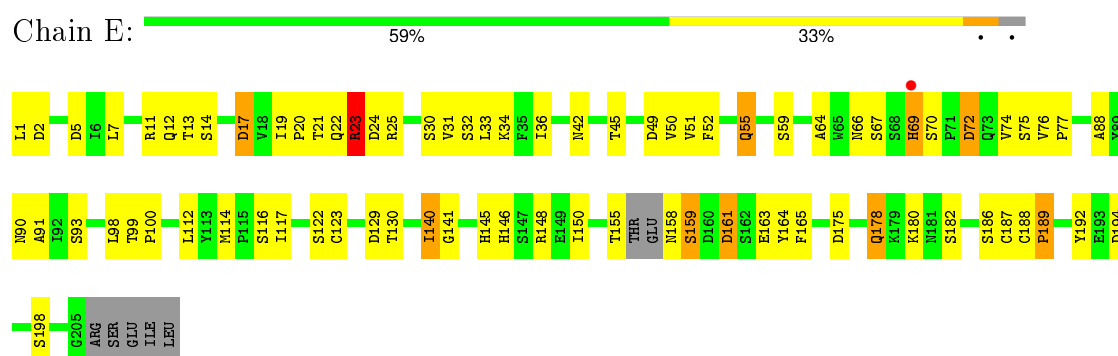
#### • Molecule 1: Acetylcholine-binding protein



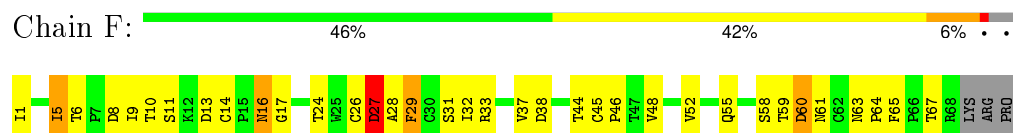
- Molecule 1: Acetylcholine-binding protein



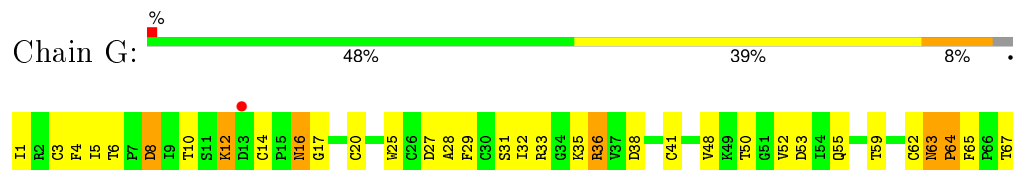
- Molecule 1: Acetylcholine-binding protein



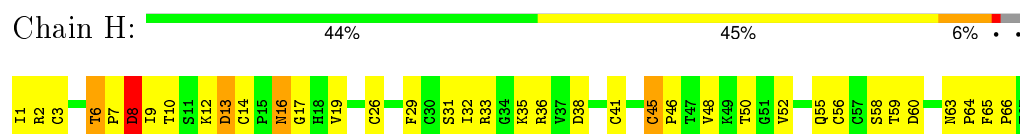
- Molecule 2: Long neurotoxin 1



- Molecule 2: Long neurotoxin 1

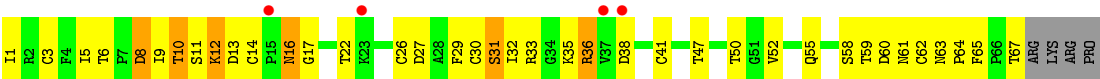


- Molecule 2: Long neurotoxin 1



- Molecule 2: Long neurotoxin 1





● Molecule 2: Long neurotoxin 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	162.60Å 313.42Å 106.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 4.20 156.71 – 4.20	Depositor EDS
% Data completeness (in resolution range)	94.9 (30.00-4.20) 94.5 (156.71-4.20)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.71 (at 4.15Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.331 , 0.378 0.290 , 0.341	Depositor DCC
$R_{free}$ test set	1040 reflections (5.70%)	DCC
Wilson B-factor (Å <sup>2</sup> )	75.2	Xtriage
Anisotropy	1.208	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , -2.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 20335 reflections	Xtriage
$F_o, F_c$ correlation	0.82	EDS
Total number of atoms	10648	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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	0.56	0/1647	0.87	10/2246 (0.4%)
1	B	0.58	0/1662	0.86	6/2267 (0.3%)
1	C	0.57	0/1658	0.87	13/2260 (0.6%)
1	D	0.56	0/1672	0.87	7/2282 (0.3%)
1	E	0.56	0/1655	0.88	6/2257 (0.3%)
2	F	0.63	0/518	0.98	5/706 (0.7%)
2	G	0.67	0/518	0.95	3/706 (0.4%)
2	H	0.72	0/518	1.01	5/706 (0.7%)
2	I	0.67	0/513	1.01	5/699 (0.7%)
2	J	0.65	0/518	0.98	2/706 (0.3%)
All	All	0.59	0/10879	0.90	62/14835 (0.4%)

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
2	F	0	1
2	G	0	1
2	H	0	1
2	I	0	1
2	J	0	1
All	All	0	5

There are no bond length outliers.

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	2	ASP	CB-CG-OD2	7.40	124.96	118.30
2	H	8	ASP	CB-CG-OD2	6.85	124.47	118.30
2	H	38	ASP	CB-CG-OD2	6.80	124.42	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	17	ASP	CB-CG-OD2	6.66	124.29	118.30
2	F	38	ASP	CB-CG-OD2	6.59	124.23	118.30
1	E	72	ASP	CB-CG-OD2	6.54	124.18	118.30
1	C	85	ASP	CB-CG-OD2	6.31	123.98	118.30
2	I	38	ASP	CB-CG-OD2	6.31	123.98	118.30
1	C	72	ASP	CB-CG-OD2	6.26	123.93	118.30
2	F	17	GLY	N-CA-C	-6.21	97.58	113.10
1	D	72	ASP	CB-CG-OD2	6.18	123.86	118.30
1	E	49	ASP	CB-CG-OD2	6.17	123.85	118.30
1	B	49	ASP	CB-CG-OD2	6.15	123.84	118.30
2	I	60	ASP	CB-CG-OD2	6.04	123.73	118.30
1	A	72	ASP	CB-CG-OD2	6.00	123.70	118.30
1	A	60	ASP	CB-CG-OD2	5.98	123.69	118.30
2	J	17	GLY	N-CA-C	-5.93	98.28	113.10
1	A	161	ASP	CB-CG-OD2	5.89	123.60	118.30
1	E	17	ASP	CB-CG-OD2	5.88	123.60	118.30
1	A	17	ASP	CB-CG-OD2	5.83	123.54	118.30
2	I	17	GLY	N-CA-C	-5.82	98.54	113.10
2	G	17	GLY	N-CA-C	-5.81	98.58	113.10
2	H	13	ASP	CB-CG-OD2	5.80	123.52	118.30
2	H	60	ASP	CB-CG-OD2	5.78	123.50	118.30
1	D	49	ASP	CB-CG-OD2	5.77	123.49	118.30
1	A	49	ASP	CB-CG-OD2	5.74	123.47	118.30
2	H	17	GLY	N-CA-C	-5.70	98.86	113.10
1	B	2	ASP	CB-CG-OD2	5.68	123.41	118.30
2	I	13	ASP	CB-CG-OD2	5.57	123.31	118.30
1	A	85	ASP	CB-CG-OD2	5.56	123.30	118.30
1	A	2	ASP	CB-CG-OD2	5.55	123.30	118.30
2	F	27	ASP	CB-CG-OD2	5.52	123.27	118.30
1	C	5	ASP	CB-CG-OD2	5.50	123.25	118.30
2	G	8	ASP	CB-CG-OD2	5.48	123.23	118.30
2	I	8	ASP	CB-CG-OD2	5.44	123.20	118.30
2	J	38	ASP	CB-CG-OD2	5.43	123.19	118.30
1	C	175	ASP	CB-CG-OD2	5.38	123.14	118.30
1	D	175	ASP	CB-CG-OD2	5.36	123.13	118.30
1	E	161	ASP	CB-CG-OD2	5.34	123.11	118.30
1	C	194	ASP	CB-CG-OD2	5.32	123.09	118.30
1	A	24	ASP	CB-CG-OD2	5.30	123.07	118.30
1	E	5	ASP	CB-CG-OD2	5.29	123.06	118.30
1	D	17	ASP	CB-CG-OD2	5.29	123.06	118.30
2	G	38	ASP	CB-CG-OD2	5.29	123.06	118.30
1	C	60	ASP	CB-CG-OD2	5.28	123.05	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	108	ASP	CB-CG-OD2	5.27	123.04	118.30
1	D	24	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	5	ASP	CB-CG-OD2	5.21	122.99	118.30
2	F	13	ASP	CB-CG-OD2	5.21	122.99	118.30
1	C	160	ASP	CB-CG-OD2	5.20	122.98	118.30
2	F	60	ASP	CB-CG-OD2	5.20	122.98	118.30
1	B	161	ASP	CB-CG-OD2	5.20	122.98	118.30
1	C	153	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	124	ASP	CB-CG-OD2	5.18	122.96	118.30
1	C	17	ASP	CB-CG-OD2	5.16	122.95	118.30
1	C	24	ASP	CB-CG-OD2	5.16	122.94	118.30
1	C	129	ASP	CB-CG-OD2	5.12	122.91	118.30
1	B	129	ASP	CB-CG-OD2	5.10	122.89	118.30
1	D	153	ASP	CB-CG-OD2	5.08	122.87	118.30
1	E	194	ASP	CB-CG-OD2	5.08	122.87	118.30
1	C	49	ASP	CB-CG-OD2	5.07	122.87	118.30
1	B	72	ASP	CB-CG-OD2	5.04	122.83	118.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	16	ASN	Peptide
2	G	16	ASN	Peptide
2	H	16	ASN	Peptide
2	I	16	ASN	Peptide
2	J	16	ASN	Peptide

## 5.2 Too-close contacts [i](#)

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	1612	0	1561	22	0
1	B	1627	0	1574	38	0
1	C	1623	0	1574	32	0
1	D	1636	0	1581	39	0
1	E	1620	0	1567	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	507	0	480	11	0
2	G	507	0	480	22	0
2	H	507	0	480	15	0
2	I	502	0	478	20	0
2	J	507	0	480	18	0
All	All	10648	0	10255	213	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 10.

All (213) 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:D:34:LYS:NZ	1:D:159:SER:OG	1.99	0.95
2:I:10:THR:O	2:I:12:LYS:NZ	2.10	0.83
1:D:186:SER:HB3	2:I:35:LYS:O	1.80	0.81
1:D:145:HIS:HE1	1:E:75:SER:HB2	1.45	0.81
1:D:186:SER:CB	2:I:35:LYS:O	2.30	0.80
1:B:33:LEU:H	1:B:178:GLN:HE22	1.28	0.79
2:H:31:SER:HB2	1:D:55:GLN:HE22	1.51	0.74
2:G:10:THR:O	2:G:12:LYS:NZ	2.20	0.73
2:J:59:THR:HB	2:J:62:CYS:HB3	1.73	0.71
1:C:186:SER:HB3	2:H:35:LYS:O	1.92	0.70
1:D:145:HIS:CE1	1:E:75:SER:HB2	2.27	0.69
1:C:192:TYR:OH	2:H:33:ARG:HD3	1.93	0.69
1:A:42:ASN:ND2	1:A:45:THR:OG1	2.28	0.67
2:H:10:THR:O	2:H:12:LYS:NZ	2.28	0.65
2:H:6:THR:HG23	2:H:7:PRO:HA	1.79	0.64
1:D:186:SER:OG	2:I:35:LYS:O	2.17	0.63
2:J:8:ASP:HB2	2:J:12:LYS:HZ1	1.61	0.63
1:C:99:THR:HB	1:C:100:PRO:CD	2.29	0.63
1:E:187:CYS:SG	1:E:188:CYS:N	2.72	0.62
2:G:32:ILE:CG2	1:C:112:LEU:HD13	2.29	0.62
2:G:32:ILE:HG21	1:C:112:LEU:HD13	1.81	0.62
1:B:187:CYS:SG	1:B:188:CYS:N	2.74	0.61
1:E:34:LYS:NZ	1:E:159:SER:OG	2.34	0.61
1:E:90:ASN:ND2	1:E:122:SER:O	2.34	0.60
1:E:22:GLN:O	1:E:25:ARG:HB2	2.01	0.60
1:B:33:LEU:H	1:B:178:GLN:NE2	2.00	0.59
1:D:187:CYS:SG	1:D:188:CYS:N	2.75	0.59
2:F:11:SER:HB3	2:F:61:ASN:HD21	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:SER:HB3	2:G:35:LYS:O	2.03	0.59
2:G:8:ASP:HB2	2:G:12:LYS:NZ	2.18	0.58
1:D:157:GLU:O	1:D:158:ASN:ND2	2.36	0.58
1:C:186:SER:CB	2:H:35:LYS:O	2.51	0.57
1:E:140:ILE:HG13	1:E:141:GLY:N	2.16	0.57
2:I:11:SER:HB3	2:I:61:ASN:HD21	1.68	0.57
1:B:164:TYR:O	1:B:165:PHE:C	2.42	0.57
2:G:5:ILE:HD12	2:G:12:LYS:HG3	1.87	0.57
1:E:164:TYR:O	1:E:165:PHE:C	2.42	0.57
1:C:187:CYS:SG	1:C:188:CYS:N	2.78	0.57
2:J:8:ASP:HB2	2:J:12:LYS:NZ	2.19	0.57
1:C:90:ASN:HD21	1:C:138:ILE:HA	1.69	0.56
2:H:31:SER:HB2	1:D:55:GLN:NE2	2.20	0.56
1:E:186:SER:OG	2:J:35:LYS:O	2.22	0.56
2:G:63:ASN:N	2:G:64:PRO:CD	2.68	0.55
1:D:76:VAL:HG12	1:D:77:PRO:HD2	1.89	0.55
1:C:99:THR:HG23	1:C:116:SER:HB3	1.89	0.55
1:A:164:TYR:O	1:A:165:PHE:C	2.44	0.55
1:E:186:SER:HB3	2:J:37:VAL:HG13	1.89	0.55
1:B:33:LEU:N	1:B:178:GLN:HE22	2.03	0.55
1:D:85:ASP:O	1:D:85:ASP:CG	2.44	0.54
1:E:186:SER:CB	2:J:35:LYS:O	2.55	0.54
1:B:145:HIS:HB2	1:B:150:ILE:HD12	1.88	0.54
1:D:164:TYR:O	1:D:165:PHE:C	2.46	0.54
1:B:145:HIS:CB	1:B:150:ILE:HD12	2.38	0.54
2:F:63:ASN:N	2:F:64:PRO:CD	2.71	0.54
1:B:83:VAL:HG12	1:B:84:PRO:HD2	1.90	0.54
1:C:55:GLN:HA	1:C:114:MET:HG3	1.88	0.53
1:A:187:CYS:SG	1:A:188:CYS:N	2.81	0.53
2:F:1:ILE:N	2:F:14:CYS:O	2.32	0.53
2:G:20:CYS:HB3	2:G:63:ASN:OD1	2.09	0.53
2:I:63:ASN:N	2:I:64:PRO:CD	2.71	0.53
1:B:186:SER:CB	2:G:35:LYS:O	2.56	0.53
2:I:30:CYS:SG	2:I:35:LYS:HA	2.48	0.53
2:H:8:ASP:HB2	2:H:12:LYS:NZ	2.24	0.52
2:H:63:ASN:N	2:H:64:PRO:CD	2.72	0.52
1:A:38:ILE:HD11	1:A:199:LEU:HD21	1.92	0.52
2:G:8:ASP:HB2	2:G:12:LYS:HZ1	1.73	0.52
1:E:31:VAL:HG12	1:E:32:SER:N	2.24	0.52
2:H:1:ILE:N	2:H:14:CYS:O	2.32	0.52
2:J:63:ASN:N	2:J:64:PRO:CD	2.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:186:SER:HB3	2:J:35:LYS:O	2.09	0.51
1:B:192:TYR:OH	2:G:33:ARG:HD3	2.10	0.51
1:A:54:GLN:O	1:A:56:THR:OG1	2.28	0.51
1:D:99:THR:HB	1:D:100:PRO:CD	2.41	0.51
1:C:99:THR:HB	1:C:100:PRO:HD2	1.92	0.51
1:D:183:VAL:O	1:D:191:ALA:HB1	2.11	0.51
1:E:21:THR:HG23	1:E:23:ARG:NH2	2.26	0.51
2:H:8:ASP:HB2	2:H:12:LYS:HZ1	1.76	0.50
1:E:188:CYS:O	1:E:189:PRO:C	2.50	0.50
1:D:99:THR:HG23	1:D:116:SER:HB2	1.93	0.50
1:A:22:GLN:O	1:A:25:ARG:HB2	2.12	0.50
1:D:31:VAL:HG12	1:D:32:SER:N	2.27	0.50
2:G:32:ILE:HD11	1:C:55:GLN:HG3	1.94	0.49
1:C:164:TYR:O	1:C:165:PHE:C	2.50	0.49
1:B:90:ASN:HD21	1:B:138:ILE:HA	1.77	0.49
1:A:188:CYS:O	1:A:189:PRO:C	2.51	0.49
1:C:188:CYS:O	1:C:189:PRO:C	2.51	0.49
1:E:19:ILE:HG23	1:E:19:ILE:O	2.13	0.49
2:F:27:ASP:CG	2:F:28:ALA:N	2.65	0.49
1:C:31:VAL:HG12	1:C:32:SER:N	2.27	0.49
1:E:50:VAL:HG22	1:E:51:VAL:N	2.27	0.49
2:I:31:SER:HB2	1:E:55:GLN:HE22	1.77	0.49
1:D:50:VAL:HG22	1:D:51:VAL:N	2.27	0.48
2:F:31:SER:HB3	1:B:55:GLN:HE22	1.78	0.48
2:I:31:SER:CB	1:E:55:GLN:HE22	2.26	0.48
2:H:3:CYS:HB2	2:H:41:CYS:HB3	1.95	0.48
1:B:188:CYS:O	1:B:189:PRO:C	2.52	0.48
1:D:192:TYR:OH	2:I:33:ARG:HD3	2.13	0.48
2:J:11:SER:CB	2:J:61:ASN:HD21	2.26	0.48
1:C:205:GLY:O	1:C:206:ARG:C	2.52	0.48
1:D:99:THR:HB	1:D:100:PRO:HD2	1.96	0.48
1:A:192:TYR:OH	2:F:33:ARG:HD3	2.13	0.48
1:D:188:CYS:O	1:D:189:PRO:C	2.52	0.48
2:I:22:THR:HB	2:I:55:GLN:HB3	1.96	0.48
1:B:146:HIS:HB3	1:B:192:TYR:CE2	2.49	0.48
1:D:88:ALA:HB3	1:D:91:ALA:HB2	1.96	0.48
1:B:18:VAL:HG11	1:C:4:ALA:HB2	1.96	0.48
1:B:55:GLN:HA	1:B:114:MET:HG3	1.96	0.48
1:C:96:GLU:HB3	1:C:118:ARG:HB3	1.96	0.48
2:G:3:CYS:HB2	2:G:41:CYS:HB3	1.96	0.47
1:A:75:SER:OG	1:E:145:HIS:CE1	2.67	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:31:SER:CB	1:B:55:GLN:HE22	2.27	0.47
1:C:50:VAL:HG22	1:C:51:VAL:N	2.29	0.47
1:A:146:HIS:CG	1:A:147:SER:N	2.81	0.47
2:I:59:THR:HB	2:I:62:CYS:HB3	1.97	0.47
1:D:83:VAL:HG12	1:D:84:PRO:HD2	1.96	0.47
1:A:10:ILE:O	1:A:14:SER:HB3	2.15	0.47
2:J:11:SER:HB2	2:J:61:ASN:HD21	1.80	0.47
1:D:185:TYR:OH	2:I:27:ASP:OD2	2.33	0.47
1:B:76:VAL:HG12	1:B:77:PRO:HD2	1.95	0.47
2:G:1:ILE:N	2:G:14:CYS:O	2.33	0.46
1:E:88:ALA:HB3	1:E:91:ALA:HB2	1.97	0.46
1:A:30:SER:OG	1:A:57:THR:HB	2.15	0.46
2:J:20:CYS:HB3	2:J:63:ASN:OD1	2.15	0.46
1:B:6:ILE:O	1:B:9:ASN:HB3	2.15	0.46
2:H:2:ARG:HG2	2:H:13:ASP:HA	1.97	0.46
1:D:76:VAL:HG12	1:D:77:PRO:CD	2.45	0.46
1:B:35:PHE:CD2	1:B:199:LEU:HD13	2.51	0.46
1:A:34:LYS:NZ	1:A:159:SER:OG	2.47	0.46
1:B:31:VAL:HG12	1:B:32:SER:N	2.31	0.46
2:I:5:ILE:O	2:I:8:ASP:O	2.34	0.46
1:C:76:VAL:HG12	1:C:77:PRO:HD2	1.97	0.46
1:B:17:ASP:O	1:C:7:LEU:HD13	2.16	0.45
1:B:35:PHE:CE2	1:B:199:LEU:HD22	2.51	0.45
1:B:125:VAL:HG12	1:B:125:VAL:O	2.16	0.45
1:A:31:VAL:HG12	1:A:32:SER:N	2.30	0.45
1:C:146:HIS:HB3	1:C:192:TYR:CE2	2.52	0.45
1:B:78:ILE:HG12	1:B:101:GLN:C	2.36	0.45
1:A:19:ILE:HD11	1:A:150:ILE:HG13	1.98	0.45
2:F:5:ILE:O	2:F:8:ASP:O	2.34	0.45
2:G:4:PHE:HB2	2:G:63:ASN:HD21	1.81	0.45
2:J:1:ILE:N	2:J:14:CYS:O	2.34	0.44
2:G:63:ASN:ND2	2:G:63:ASN:O	2.45	0.44
1:E:186:SER:HB3	2:J:37:VAL:CG1	2.48	0.44
1:B:46:ASN:HD22	1:B:125:VAL:HB	1.81	0.44
1:B:146:HIS:CD2	1:B:146:HIS:C	2.90	0.44
2:G:31:SER:CB	1:C:55:GLN:HE22	2.30	0.44
2:J:10:THR:O	2:J:12:LYS:NZ	2.50	0.44
1:A:51:VAL:HA	1:A:117:ILE:O	2.17	0.44
2:F:45:CYS:SG	2:F:46:PRO:HD2	2.57	0.44
1:A:183:VAL:O	1:A:191:ALA:HB1	2.18	0.44
2:F:32:ILE:HD11	1:B:55:GLN:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:ILE:HG23	1:B:63:LEU:CD2	2.49	0.43
2:I:1:ILE:N	2:I:14:CYS:O	2.33	0.43
2:I:32:ILE:HG21	1:E:112:LEU:HD13	2.00	0.43
1:B:54:GLN:O	1:B:56:THR:OG1	2.28	0.43
2:J:21:TYR:HE2	2:J:42:ALA:HB2	1.83	0.43
1:D:123:CYS:O	1:D:125:VAL:HG23	2.19	0.43
2:G:59:THR:HB	2:G:62:CYS:HB3	2.00	0.43
2:I:3:CYS:HB2	2:I:41:CYS:HB3	2.00	0.43
2:G:31:SER:HB3	1:C:55:GLN:HE22	1.84	0.43
1:E:99:THR:HG23	1:E:116:SER:HB3	2.01	0.43
1:B:83:VAL:CG1	1:B:84:PRO:HD2	2.49	0.43
1:E:76:VAL:HG12	1:E:77:PRO:HD2	2.01	0.42
1:D:145:HIS:CB	1:D:150:ILE:HD12	2.49	0.42
1:B:76:VAL:HG12	1:B:77:PRO:CD	2.49	0.42
2:G:25:TRP:CZ2	2:G:36:ARG:NE	2.87	0.42
1:A:140:ILE:HG13	1:A:141:GLY:N	2.33	0.42
1:D:119:GLN:HB3	1:D:121:PHE:CE1	2.55	0.42
2:J:5:ILE:O	2:J:8:ASP:O	2.37	0.42
1:C:46:ASN:HD22	1:C:125:VAL:H	1.68	0.42
1:B:20:PRO:O	1:B:27:VAL:HG22	2.19	0.42
1:E:158:ASN:O	1:E:159:SER:CB	2.66	0.42
1:E:42:ASN:ND2	1:E:45:THR:OG1	2.53	0.42
1:A:50:VAL:HG22	1:A:51:VAL:N	2.35	0.42
1:C:33:LEU:HD13	1:C:52:PHE:CD1	2.55	0.42
1:E:69:HIS:CD2	1:E:69:HIS:H	2.38	0.42
2:J:27:ASP:CG	2:J:28:ALA:N	2.73	0.42
1:C:20:PRO:HD3	1:C:82:TRP:CG	2.55	0.42
2:I:32:ILE:HD11	1:E:55:GLN:HG3	2.01	0.41
1:D:40:GLU:HB2	1:D:49:ASP:CB	2.50	0.41
1:E:19:ILE:HD11	1:E:150:ILE:HG13	2.03	0.41
2:H:45:CYS:SG	2:H:46:PRO:HD2	2.59	0.41
1:D:17:ASP:O	1:E:7:LEU:HD13	2.21	0.41
1:E:188:CYS:HB3	1:E:189:PRO:HD2	2.01	0.41
1:E:98:LEU:N	1:E:98:LEU:HD23	2.36	0.41
1:C:18:VAL:HG11	1:D:4:ALA:HB2	2.01	0.41
1:C:17:ASP:O	1:D:7:LEU:HD13	2.20	0.41
2:I:32:ILE:CG2	1:E:112:LEU:HD13	2.50	0.41
2:H:32:ILE:CG2	1:D:112:LEU:HD13	2.50	0.41
1:E:146:HIS:HB3	1:E:192:TYR:CE2	2.56	0.41
1:E:33:LEU:H	1:E:178:GLN:HE22	1.69	0.41
1:B:127:GLY:O	1:B:130:THR:OG1	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:78:ILE:HG13	1:D:113:TYR:CZ	2.55	0.41
1:D:51:VAL:HA	1:D:117:ILE:O	2.21	0.41
1:B:36:ILE:HG12	1:B:52:PHE:HA	2.02	0.41
1:A:78:ILE:HG13	1:A:113:TYR:CZ	2.56	0.41
1:A:76:VAL:HG12	1:A:77:PRO:HD2	2.02	0.41
1:D:145:HIS:CE1	1:E:75:SER:CB	3.01	0.41
2:G:5:ILE:O	2:G:8:ASP:O	2.39	0.41
1:D:20:PRO:O	1:D:27:VAL:HG22	2.21	0.41
2:J:3:CYS:HB2	2:J:41:CYS:HB3	2.03	0.41
1:C:183:VAL:O	1:C:191:ALA:HB1	2.21	0.41
1:A:185:TYR:OH	2:F:29:PHE:HB3	2.21	0.41
1:D:46:ASN:HD22	1:D:125:VAL:HB	1.85	0.40
1:C:85:ASP:O	1:C:85:ASP:CG	2.59	0.40
1:E:99:THR:HB	1:E:100:PRO:HD2	2.03	0.40
1:E:36:ILE:HG12	1:E:52:PHE:HA	2.02	0.40
1:E:51:VAL:HA	1:E:117:ILE:O	2.22	0.40
1:B:51:VAL:HA	1:B:117:ILE:O	2.22	0.40
2:G:27:ASP:CG	2:G:28:ALA:N	2.74	0.40
1:C:40:GLU:HB2	1:C:49:ASP:HB2	2.02	0.40
1:D:183:VAL:HG11	2:I:36:ARG:CZ	2.51	0.40
1:B:36:ILE:HD11	1:B:53:TRP:CD2	2.57	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	198/210 (94%)	174 (88%)	19 (10%)	5 (2%)	7	48
1	B	200/210 (95%)	173 (86%)	22 (11%)	5 (2%)	7	48
1	C	199/210 (95%)	174 (87%)	19 (10%)	6 (3%)	5	45
1	D	203/210 (97%)	174 (86%)	21 (10%)	8 (4%)	4	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	199/210 (95%)	174 (87%)	19 (10%)	6 (3%)	5	45
2	F	66/71 (93%)	58 (88%)	6 (9%)	2 (3%)	5	45
2	G	66/71 (93%)	55 (83%)	8 (12%)	3 (4%)	3	34
2	H	66/71 (93%)	57 (86%)	6 (9%)	3 (4%)	3	34
2	I	65/71 (92%)	56 (86%)	7 (11%)	2 (3%)	5	44
2	J	66/71 (93%)	56 (85%)	8 (12%)	2 (3%)	5	45
All	All	1328/1405 (94%)	1151 (87%)	135 (10%)	42 (3%)	5	43

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	160	ASP
1	E	159	SER
1	A	55	GLN
1	A	64	ALA
2	F	16	ASN
1	B	55	GLN
1	B	64	ALA
2	G	16	ASN
1	C	64	ALA
1	C	205	GLY
2	H	16	ASN
1	D	55	GLN
1	D	64	ALA
1	D	161	ASP
2	I	16	ASN
1	E	55	GLN
1	E	64	ALA
2	J	16	ASN
1	A	189	PRO
1	B	23	ARG
2	G	29	PHE
1	C	55	GLN
2	I	29	PHE
1	A	23	ARG
2	F	29	PHE
1	B	189	PRO
1	C	23	ARG
1	C	189	PRO
2	H	29	PHE

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Mol	Chain	Res	Type
1	D	23	ARG
1	D	162	SER
1	D	189	PRO
1	E	23	ARG
2	J	29	PHE
1	B	20	PRO
1	A	20	PRO
1	C	20	PRO
1	D	20	PRO
1	E	20	PRO
1	E	189	PRO
2	G	64	PRO
2	H	66	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	188/196 (96%)	161 (86%)	27 (14%)	4	27
1	B	190/196 (97%)	162 (85%)	28 (15%)	4	26
1	C	189/196 (96%)	166 (88%)	23 (12%)	6	33
1	D	191/196 (97%)	162 (85%)	29 (15%)	3	25
1	E	189/196 (96%)	157 (83%)	32 (17%)	2	20
2	F	60/64 (94%)	43 (72%)	17 (28%)	0	4
2	G	60/64 (94%)	49 (82%)	11 (18%)	2	16
2	H	60/64 (94%)	45 (75%)	15 (25%)	1	7
2	I	60/64 (94%)	47 (78%)	13 (22%)	1	10
2	J	60/64 (94%)	44 (73%)	16 (27%)	0	5
All	All	1247/1300 (96%)	1036 (83%)	211 (17%)	2	20

All (211) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	14	SER
1	A	23	ARG
1	A	24	ASP
1	A	32	SER
1	A	46	ASN
1	A	59	SER
1	A	62	THR
1	A	69	HIS
1	A	70	SER
1	A	74	VAL
1	A	79	SER
1	A	93	SER
1	A	94	LYS
1	A	101	GLN
1	A	114	MET
1	A	122	SER
1	A	123	CYS
1	A	130	THR
1	A	140	ILE
1	A	146	HIS
1	A	148	ARG
1	A	159	SER
1	A	162	SER
1	A	180	LYS
1	A	182	SER
1	A	198	SER
2	F	5	ILE
2	F	6	THR
2	F	9	ILE
2	F	10	THR
2	F	24	THR
2	F	26	CYS
2	F	27	ASP
2	F	37	VAL
2	F	44	THR
2	F	48	VAL
2	F	52	VAL
2	F	55	GLN
2	F	58	SER
2	F	59	THR
2	F	60	ASP
2	F	65	PHE

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Mol	Chain	Res	Type
2	F	67	THR
1	B	12	GLN
1	B	17	ASP
1	B	22	GLN
1	B	23	ARG
1	B	25	ARG
1	B	30	SER
1	B	43	GLU
1	B	49	ASP
1	B	67	SER
1	B	69	HIS
1	B	74	VAL
1	B	94	LYS
1	B	96	GLU
1	B	110	GLU
1	B	122	SER
1	B	123	CYS
1	B	130	THR
1	B	131	GLU
1	B	135	THR
1	B	140	ILE
1	B	142	SER
1	B	146	HIS
1	B	148	ARG
1	B	153	ASP
1	B	155	THR
1	B	159	SER
1	B	167	GLN
1	B	180	LYS
2	G	6	THR
2	G	12	LYS
2	G	36	ARG
2	G	48	VAL
2	G	50	THR
2	G	52	VAL
2	G	53	ASP
2	G	55	GLN
2	G	63	ASN
2	G	65	PHE
2	G	67	THR
1	C	2	ASP
1	C	23	ARG

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Mol	Chain	Res	Type
1	C	24	ASP
1	C	25	ARG
1	C	69	HIS
1	C	70	SER
1	C	74	VAL
1	C	93	SER
1	C	94	LYS
1	C	107	SER
1	C	108	ASP
1	C	114	MET
1	C	123	CYS
1	C	130	THR
1	C	140	ILE
1	C	148	ARG
1	C	155	THR
1	C	159	SER
1	C	166	SER
1	C	179	LYS
1	C	180	LYS
1	C	194	ASP
1	C	198	SER
2	H	6	THR
2	H	8	ASP
2	H	9	ILE
2	H	19	VAL
2	H	26	CYS
2	H	36	ARG
2	H	45	CYS
2	H	48	VAL
2	H	50	THR
2	H	52	VAL
2	H	55	GLN
2	H	56	CYS
2	H	58	SER
2	H	59	THR
2	H	65	PHE
1	D	13	THR
1	D	17	ASP
1	D	23	ARG
1	D	24	ASP
1	D	25	ARG
1	D	30	SER

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Mol	Chain	Res	Type
1	D	43	GLU
1	D	59	SER
1	D	68	SER
1	D	70	SER
1	D	74	VAL
1	D	75	SER
1	D	79	SER
1	D	85	ASP
1	D	93	SER
1	D	94	LYS
1	D	108	ASP
1	D	114	MET
1	D	130	THR
1	D	140	ILE
1	D	148	ARG
1	D	156	THR
1	D	158	ASN
1	D	159	SER
1	D	160	ASP
1	D	161	ASP
1	D	163	GLU
1	D	166	SER
1	D	180	LYS
2	I	6	THR
2	I	9	ILE
2	I	10	THR
2	I	12	LYS
2	I	26	CYS
2	I	31	SER
2	I	36	ARG
2	I	47	THR
2	I	50	THR
2	I	52	VAL
2	I	58	SER
2	I	65	PHE
2	I	67	THR
1	E	1	LEU
1	E	2	ASP
1	E	11	ARG
1	E	12	GLN
1	E	13	THR
1	E	14	SER

*Continued on next page...*

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Mol	Chain	Res	Type
1	E	17	ASP
1	E	23	ARG
1	E	24	ASP
1	E	30	SER
1	E	59	SER
1	E	66	ASN
1	E	67	SER
1	E	69	HIS
1	E	70	SER
1	E	72	ASP
1	E	74	VAL
1	E	93	SER
1	E	114	MET
1	E	123	CYS
1	E	129	ASP
1	E	130	THR
1	E	140	ILE
1	E	148	ARG
1	E	155	THR
1	E	161	ASP
1	E	163	GLU
1	E	175	ASP
1	E	178	GLN
1	E	180	LYS
1	E	182	SER
1	E	198	SER
2	J	5	ILE
2	J	6	THR
2	J	9	ILE
2	J	10	THR
2	J	11	SER
2	J	12	LYS
2	J	19	VAL
2	J	26	CYS
2	J	27	ASP
2	J	31	SER
2	J	37	VAL
2	J	44	THR
2	J	47	THR
2	J	48	VAL
2	J	60	ASP
2	J	65	PHE



Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	42	ASN
1	A	46	ASN
1	A	55	GLN
1	A	101	GLN
1	A	119	GLN
2	F	61	ASN
1	B	46	ASN
1	B	55	GLN
1	B	146	HIS
1	C	46	ASN
1	C	55	GLN
1	C	119	GLN
1	C	146	HIS
2	H	18	HIS
1	D	46	ASN
1	D	119	GLN
1	D	145	HIS
2	I	61	ASN
1	E	46	ASN
1	E	55	GLN
1	E	66	ASN
1	E	69	HIS
1	E	119	GLN
1	E	145	HIS
2	J	18	HIS
2	J	61	ASN

### 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	A	202/210 (96%)	0.19	1 (0%) 91 88	38, 39, 40, 42	0
1	B	204/210 (97%)	0.16	2 (0%) 84 77	38, 39, 40, 43	0
1	C	203/210 (96%)	0.20	1 (0%) 91 88	38, 39, 40, 41	0
1	D	205/210 (97%)	0.20	1 (0%) 91 88	38, 39, 40, 41	0
1	E	203/210 (96%)	0.17	1 (0%) 91 88	38, 39, 40, 41	0
2	F	68/71 (95%)	0.29	0 100 100	39, 39, 40, 40	0
2	G	68/71 (95%)	0.30	1 (1%) 76 67	39, 39, 40, 41	0
2	H	68/71 (95%)	0.20	0 100 100	39, 39, 40, 41	0
2	I	67/71 (94%)	0.34	4 (5%) 25 18	39, 39, 40, 40	0
2	J	68/71 (95%)	0.23	1 (1%) 76 67	39, 39, 40, 42	0
All	All	1356/1405 (96%)	0.20	12 (0%) 85 80	38, 39, 40, 43	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	23	LYS	3.0
1	D	157	GLU	2.9
1	B	158	ASN	2.9
2	I	37	VAL	2.7
1	B	24	ASP	2.6
2	J	37	VAL	2.5
2	I	38	ASP	2.4
2	G	13	ASP	2.3
1	C	61	ARG	2.3
1	E	69	HIS	2.1
1	A	184	THR	2.1
2	I	15	PRO	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.