



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:54 AM GMT

PDB ID : 2J1K  
Title : CAV-2 FIBRE HEAD IN COMPLEX WITH CAR D1  
Authors : Seiradake, E.; Lortat-Jacob, H.; Billet, O.; Kremer, E.J.; Cusack, S.  
Deposited on : 2006-08-14  
Resolution : 2.30 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

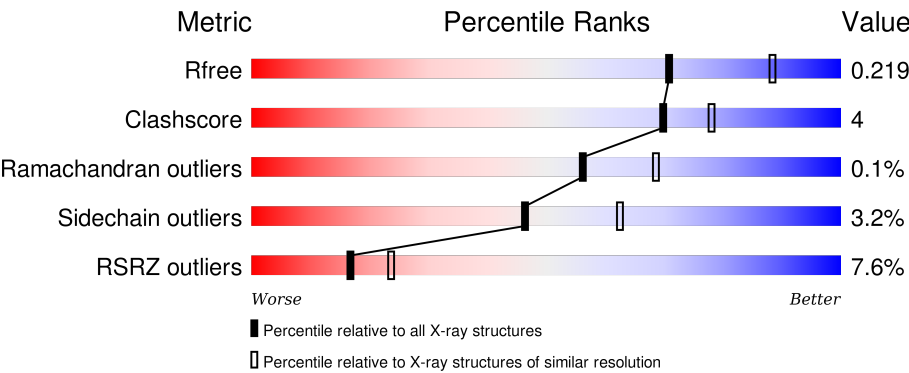
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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 <sub>free</sub>	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	128	<div><div>30%</div><div><div></div><div>75%</div><div>14%</div><div>•</div><div>9%</div></div></div>
1	B	128	<div><div>39%</div><div><div></div><div>63%</div><div>23%</div><div>•</div><div>12%</div></div></div>
1	G	128	<div><div>6%</div><div><div></div><div>80%</div><div>14%</div><div>•</div><div>•</div></div></div>
1	J	128	<div><div>5%</div><div><div></div><div>82%</div><div>13%</div><div>•</div><div>•</div></div></div>
1	K	128	<div><div>4%</div><div><div></div><div>82%</div><div>13%</div><div>•</div><div>•</div></div></div>

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Mol	Chain	Length	Quality of chain
1	O	128	
1	P	128	
1	T	128	
1	V	128	
1	X	128	
1	Y	128	
1	Z	128	
2	C	197	
2	D	197	
2	E	197	
2	F	197	
2	H	197	
2	I	197	
2	L	197	
2	M	197	
2	N	197	
2	Q	197	
2	R	197	
2	S	197	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 29978 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 COXSACKIEVIRUS AND ADENOVIRUS RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	117	Total	C	N	O	S	0	0	0
			914	581	147	183	3			
1	B	113	Total	C	N	O	S	0	0	0
			881	565	142	171	3			
1	G	123	Total	C	N	O	S	0	0	0
			959	611	156	189	3			
1	J	123	Total	C	N	O	S	0	0	0
			959	611	156	189	3			
1	K	123	Total	C	N	O	S	0	0	0
			963	615	156	189	3			
1	O	118	Total	C	N	O	S	0	0	0
			917	587	145	182	3			
1	P	123	Total	C	N	O	S	0	0	0
			959	611	156	189	3			
1	T	119	Total	C	N	O	S	0	0	0
			928	591	149	185	3			
1	V	121	Total	C	N	O	S	0	0	0
			944	600	154	187	3			
1	X	123	Total	C	N	O	S	0	0	0
			959	611	156	189	3			
1	Y	119	Total	C	N	O	S	0	0	0
			928	591	149	185	3			
1	Z	117	Total	C	N	O	S	0	0	0
			914	581	147	183	3			

- Molecule 2 is a protein called FIBER PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	182	Total	C	N	O	S	0	0	0
			1406	892	239	266	9			
2	D	182	Total	C	N	O	S	0	0	0
			1406	892	239	266	9			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	182	Total	C	N	O	S	0	0	0
			1406	892	239	266	9			
2	F	182	Total	C	N	O	S	0	0	0
			1406	892	239	266	9			
2	H	182	Total	C	N	O	S	0	0	0
			1406	892	239	266	9			
2	I	182	Total	C	N	O	S	0	0	0
			1406	892	239	266	9			
2	L	182	Total	C	N	O	S	0	0	0
			1406	892	239	266	9			
2	M	182	Total	C	N	O	S	0	0	0
			1406	892	239	266	9			
2	N	182	Total	C	N	O	S	0	0	0
			1406	892	239	266	9			
2	Q	182	Total	C	N	O	S	0	0	0
			1406	892	239	266	9			
2	R	182	Total	C	N	O	S	0	0	0
			1406	892	239	266	9			
2	S	182	Total	C	N	O	S	0	0	0
			1406	892	239	266	9			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	24	Total	O	0	0
			24	24		
3	B	15	Total	O	0	0
			15	15		
3	C	140	Total	O	0	0
			140	140		
3	D	127	Total	O	0	0
			127	127		
3	E	121	Total	O	0	0
			121	121		
3	F	129	Total	O	0	0
			129	129		
3	G	53	Total	O	0	0
			53	53		
3	H	135	Total	O	0	0
			135	135		
3	I	148	Total	O	0	0
			148	148		

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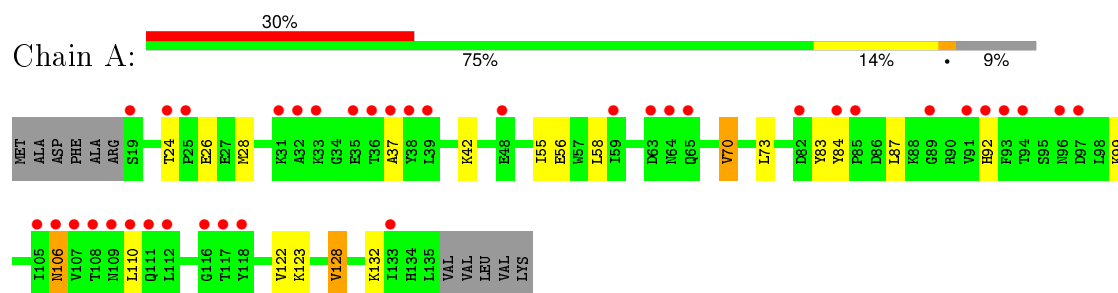
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	J	45	Total 45	O 45	0	0
3	K	45	Total 45	O 45	0	0
3	L	116	Total 116	O 116	0	0
3	M	134	Total 134	O 134	0	0
3	N	118	Total 118	O 118	0	0
3	O	31	Total 31	O 31	0	0
3	P	54	Total 54	O 54	0	0
3	Q	101	Total 101	O 101	0	0
3	R	111	Total 111	O 111	0	0
3	S	93	Total 93	O 93	0	0
3	T	32	Total 32	O 32	0	0
3	V	23	Total 23	O 23	0	0
3	X	50	Total 50	O 50	0	0
3	Y	23	Total 23	O 23	0	0
3	Z	13	Total 13	O 13	0	0

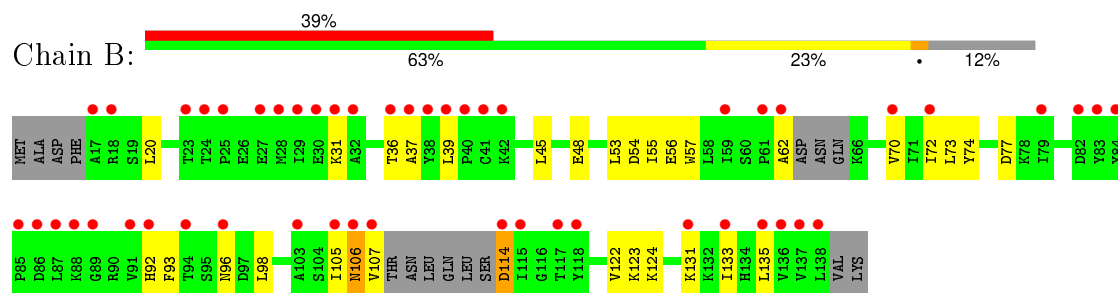
### 3 Residue-property plots

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.

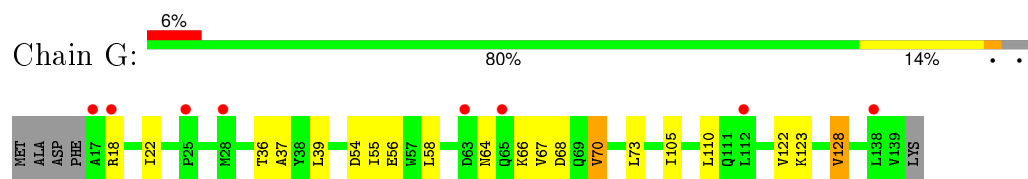
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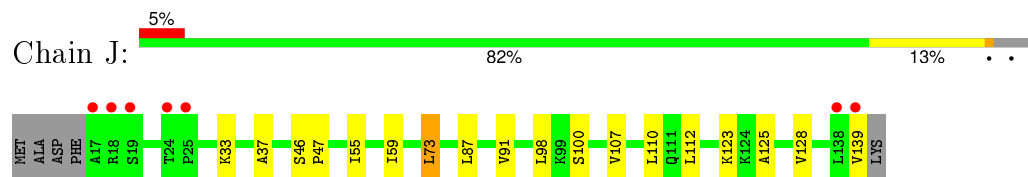
#### • Molecule 1: COXSACKIEVIRUS AND ADENOVIRUS RECEPTOR



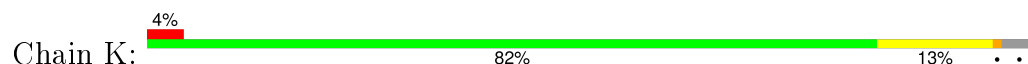
#### • Molecule 1: COXSACKIEVIRUS AND ADENOVIRUS RECEPTOR



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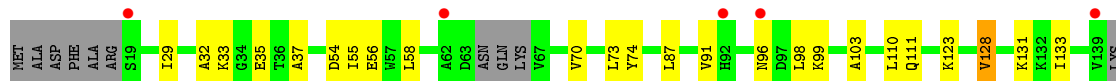
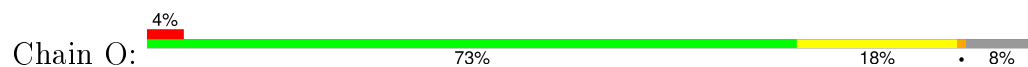


#### • Molecule 1: COXSACKIEVIRUS AND ADENOVIRUS RECEPTOR

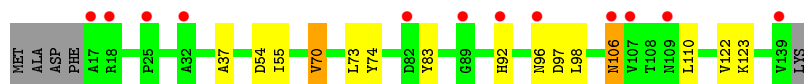
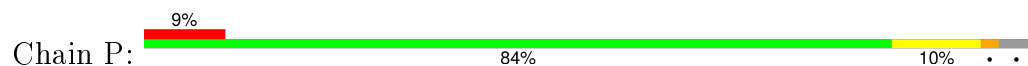




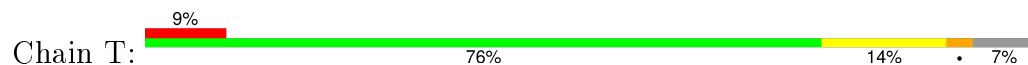
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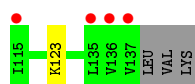
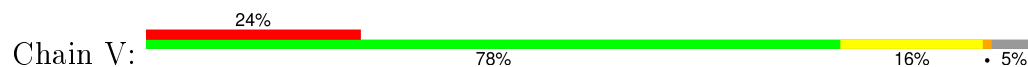
- Molecule 1: COXSACKIEVIRUS AND ADENOVIRUS RECEPTOR



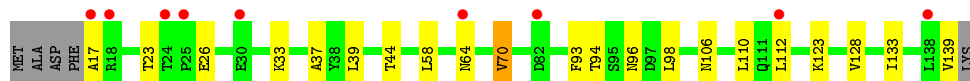
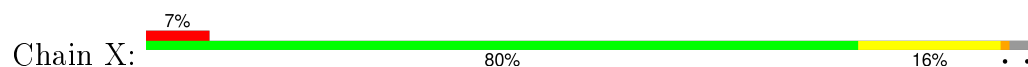
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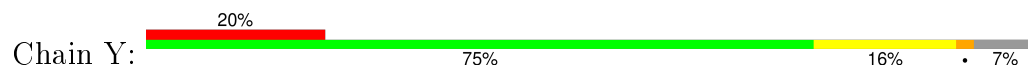
- Molecule 1: COXSACKIEVIRUS AND ADENOVIRUS RECEPTOR



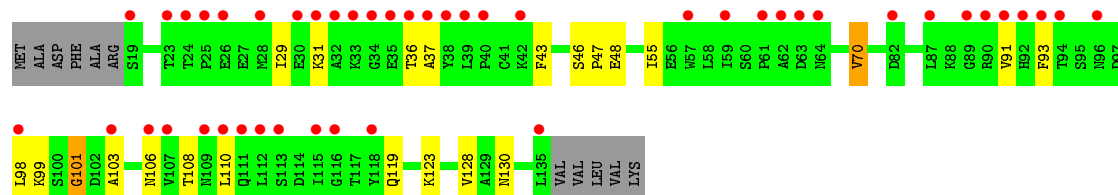
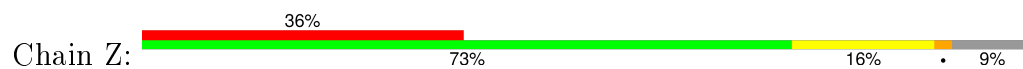
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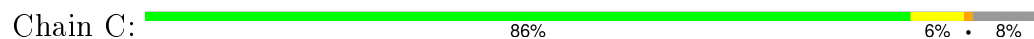
- Molecule 1: COXSACKIEVIRUS AND ADENOVIRUS RECEPTOR



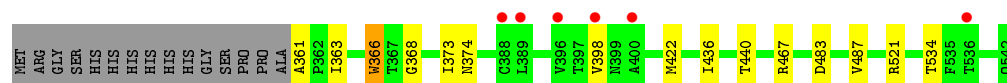
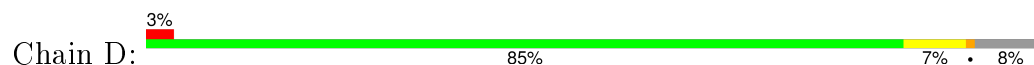
- Molecule 1: COXSACKIEVIRUS AND ADENOVIRUS RECEPTOR



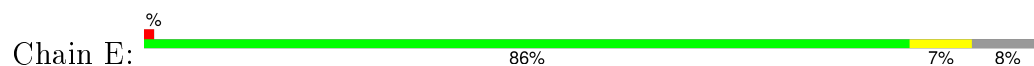
- Molecule 2: FIBER PROTEIN



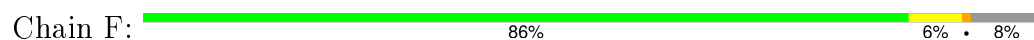
- Molecule 2: FIBER PROTEIN



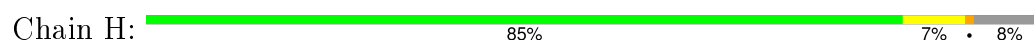
- Molecule 2: FIBER PROTEIN




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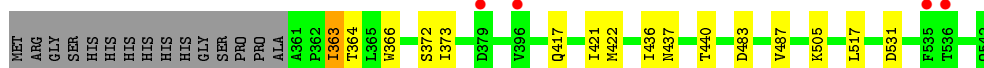
- Molecule 2: FIBER PROTEIN




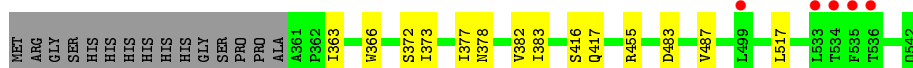
## ● Molecule 2: FIBER PROTEIN

Chain I:  87% 6% 8%


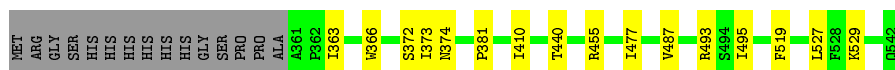
## ● Molecule 2: FIBER PROTEIN

Chain L:  2% 84% 8% 8%


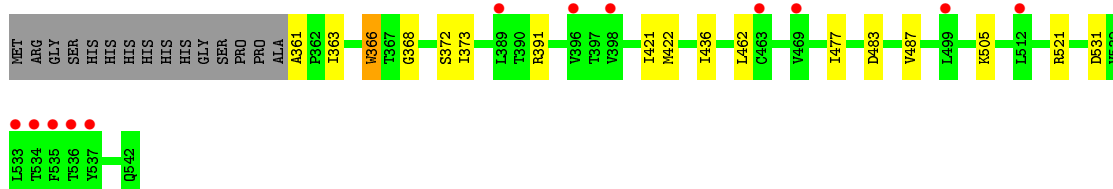
## ● Molecule 2: FIBER PROTEIN

Chain M:  3% 85% 7% 8%


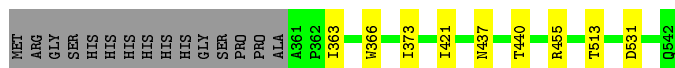
## ● Molecule 2: FIBER PROTEIN

Chain N:  84% 8% 8%


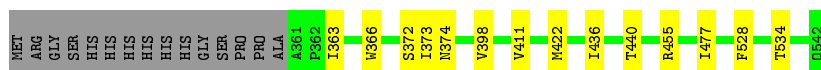
## ● Molecule 2: FIBER PROTEIN

Chain Q:  6% 84% 8% 8%

## ● Molecule 2: FIBER PROTEIN

Chain R:  88% 5% 8%

## ● Molecule 2: FIBER PROTEIN

Chain S:  85% 7% 8%

## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	219.94Å 219.94Å 387.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	192.45 – 2.30 47.67 – 2.30	Depositor EDS
% Data completeness (in resolution range)	92.0 (192.45-2.30) 92.0 (47.67-2.30)	Depositor EDS
$R_{merge}$	0.01	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.39 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.172 , 0.220 0.172 , 0.219	Depositor DCC
$R_{free}$ test set	1890 reflections (1.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	31.8	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 45.9	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 190487 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	29978	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.34% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.37	0/932	0.57	0/1264
1	B	0.78	3/897 (0.3%)	0.63	1/1213 (0.1%)
1	G	0.43	0/977	0.64	0/1326
1	J	0.44	0/977	0.61	0/1326
1	K	0.43	0/982	0.61	0/1332
1	O	0.44	0/934	0.60	0/1268
1	P	0.40	0/977	0.61	0/1326
1	T	0.41	0/946	0.60	0/1284
1	V	0.38	0/962	0.55	0/1305
1	X	0.42	0/977	0.59	0/1326
1	Y	0.38	0/946	0.56	0/1284
1	Z	0.36	0/932	0.52	0/1264
2	C	0.50	0/1441	0.68	0/1964
2	D	0.51	0/1441	0.68	0/1964
2	E	0.51	0/1441	0.66	0/1964
2	F	0.52	0/1441	0.67	0/1964
2	H	0.53	0/1441	0.65	0/1964
2	I	0.50	0/1441	0.65	0/1964
2	L	0.48	0/1441	0.64	0/1964
2	M	0.51	0/1441	0.63	0/1964
2	N	0.47	0/1441	0.63	0/1964
2	Q	0.46	0/1441	0.63	0/1964
2	R	0.45	0/1441	0.65	0/1964
2	S	0.46	0/1441	0.62	0/1964
All	All	0.48	3/28731 (0.0%)	0.63	1/39086 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	62	ALA	C-O	16.91	1.55	1.23
1	B	114	ASP	CG-OD1	7.06	1.41	1.25
1	B	114	ASP	CG-OD2	6.25	1.39	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	114	ASP	CB-CG-OD2	-6.11	112.81	118.30

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	914	0	910	13	0
1	B	881	0	889	22	0
1	G	959	0	966	15	0
1	J	959	0	966	10	0
1	K	963	0	966	13	0
1	O	917	0	920	21	0
1	P	959	0	966	14	0
1	T	928	0	928	16	0
1	V	944	0	946	14	0
1	X	959	0	966	13	0
1	Y	928	0	928	17	0
1	Z	914	0	910	13	0
2	C	1406	0	1382	9	0
2	D	1406	0	1382	10	0
2	E	1406	0	1382	9	0
2	F	1406	0	1382	8	0
2	H	1406	0	1382	8	0
2	I	1406	0	1382	6	0
2	L	1406	0	1382	10	0
2	M	1406	0	1382	6	0
2	N	1406	0	1382	10	0
2	Q	1406	0	1382	10	0
2	R	1406	0	1382	6	0
2	S	1406	0	1382	10	0
3	A	24	0	0	0	0
3	B	15	0	0	0	0
3	C	140	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	127	0	0	2	0
3	E	121	0	0	0	0
3	F	129	0	0	1	0
3	G	53	0	0	0	0
3	H	135	0	0	2	0
3	I	148	0	0	1	0
3	J	45	0	0	0	0
3	K	45	0	0	1	0
3	L	116	0	0	0	0
3	M	134	0	0	0	0
3	N	118	0	0	1	0
3	O	31	0	0	1	0
3	P	54	0	0	2	0
3	Q	101	0	0	1	0
3	R	111	0	0	0	0
3	S	93	0	0	2	0
3	T	32	0	0	0	0
3	V	23	0	0	0	0
3	X	50	0	0	0	0
3	Y	23	0	0	0	0
3	Z	13	0	0	0	0
All	All	29978	0	27845	251	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 4.

All (251) 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)
2:L:373:ILE:HD11	1:V:70:VAL:HG21	1.30	1.07
2:C:374:ASN:HB3	2:C:440:THR:HG21	1.45	0.98
2:D:440:THR:HG23	3:D:2056:HOH:O	1.64	0.95
1:B:70:VAL:HG21	2:D:373:ILE:HD11	1.46	0.95
2:F:462:LEU:HD21	2:F:542:GLN:HG2	1.47	0.94
2:N:374:ASN:HB3	2:N:440:THR:HG21	1.47	0.94
2:F:440:THR:HG23	3:F:2053:HOH:O	1.67	0.93
1:G:55:ILE:CD1	1:G:122:VAL:HG13	2.07	0.85
1:K:55:ILE:CD1	1:K:122:VAL:HG13	2.08	0.84
1:V:37:ALA:HB2	1:V:110:LEU:HD11	1.60	0.83
2:L:373:ILE:CD1	1:V:70:VAL:HG21	2.09	0.83
2:L:373:ILE:HD11	1:V:70:VAL:CG2	2.09	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:373:ILE:HD11	1:X:70:VAL:HG21	1.59	0.82
1:A:92:HIS:CE1	1:A:106:ASN:HD21	1.97	0.82
1:G:70:VAL:HG21	2:R:373:ILE:HD11	1.60	0.81
1:G:55:ILE:HD12	1:G:122:VAL:HG13	1.64	0.80
1:X:37:ALA:HB2	1:X:110:LEU:HD11	1.65	0.79
1:T:55:ILE:HD12	1:T:98:LEU:HD21	1.65	0.78
1:Y:37:ALA:HB2	1:Y:110:LEU:HD11	1.67	0.76
1:Y:39:LEU:HD22	1:Y:133:ILE:HG21	1.68	0.75
1:O:55:ILE:HD12	1:O:98:LEU:HD21	1.68	0.75
1:K:55:ILE:HD12	1:K:122:VAL:HG13	1.68	0.74
1:J:37:ALA:HB2	1:J:110:LEU:HD11	1.71	0.73
1:Y:55:ILE:HD12	1:Y:98:LEU:HD21	1.69	0.72
1:O:29:ILE:HD12	1:O:133:ILE:HG21	1.73	0.71
1:X:17:ALA:HB2	1:X:44:THR:HG21	1.76	0.68
1:B:74:TYR:CD1	1:B:98:LEU:HD13	2.29	0.67
1:X:112:LEU:HD21	1:X:139:VAL:HG23	1.77	0.67
2:F:410:ILE:HD13	2:F:527:LEU:HD12	1.76	0.67
1:G:70:VAL:HG21	2:R:373:ILE:CD1	2.25	0.67
1:G:70:VAL:CG2	2:R:373:ILE:HD11	2.25	0.66
1:Y:87:LEU:HD22	1:Y:91:VAL:HG13	1.77	0.66
2:H:527:LEU:HD23	2:H:529:LYS:HE2	1.77	0.66
2:N:440:THR:HG22	3:N:2051:HOH:O	1.94	0.66
1:O:70:VAL:HG11	1:O:73:LEU:HD21	1.78	0.66
1:Y:123:LYS:HG2	1:Y:128:VAL:HG13	1.77	0.65
2:Q:421:ILE:HD13	2:Q:505:LYS:HE2	1.78	0.64
2:M:377:ILE:HD12	2:M:382:VAL:HG21	1.80	0.63
1:B:93:PHE:CE1	1:B:98:LEU:HD11	2.34	0.63
1:J:87:LEU:HD13	1:J:91:VAL:HG21	1.80	0.63
1:V:17:ALA:HB2	1:V:44:THR:HG21	1.81	0.63
1:K:55:ILE:HD11	1:K:122:VAL:HG13	1.78	0.62
2:Q:361:ALA:N	3:Q:2012:HOH:O	2.32	0.61
1:X:33:LYS:HE2	1:X:139:VAL:HG13	1.81	0.61
1:J:91:VAL:HG22	1:J:107:VAL:HG22	1.82	0.61
1:O:58:LEU:HD23	1:O:70:VAL:HA	1.83	0.61
1:Z:37:ALA:HB2	1:Z:110:LEU:HD11	1.82	0.60
1:G:123:LYS:HG2	1:G:128:VAL:HG13	1.82	0.60
1:B:55:ILE:HD13	1:B:122:VAL:HG13	1.83	0.59
1:K:36:THR:HG22	3:K:2003:HOH:O	2.02	0.59
2:H:483:ASP:O	2:H:487:VAL:HG22	2.03	0.59
1:Y:87:LEU:HD13	1:Y:91:VAL:HG11	1.85	0.59
1:T:36:THR:HG22	1:T:108:THR:HA	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:55:ILE:HD12	1:J:98:LEU:HD21	1.84	0.59
1:B:70:VAL:HG21	2:D:373:ILE:CD1	2.26	0.58
1:P:55:ILE:HD12	1:P:122:VAL:HG22	1.85	0.58
1:T:37:ALA:HB2	1:T:110:LEU:HD11	1.86	0.58
2:M:382:VAL:HG23	2:M:383:ILE:HG12	1.85	0.57
2:S:373:ILE:CD1	1:Z:70:VAL:HG11	2.34	0.57
1:B:39:LEU:HD12	1:B:105:ILE:HD11	1.86	0.57
1:G:58:LEU:HD23	1:G:70:VAL:HA	1.86	0.57
1:Z:29:ILE:HG21	1:Z:31:LYS:HZ1	1.69	0.57
1:J:123:LYS:HG2	1:J:128:VAL:HG13	1.85	0.57
2:C:374:ASN:CB	2:C:440:THR:HG21	2.29	0.56
1:V:55:ILE:O	1:V:73:LEU:HD12	2.05	0.56
1:A:37:ALA:HB2	1:A:110:LEU:HD11	1.86	0.56
2:E:410:ILE:HD13	2:E:527:LEU:HD12	1.87	0.55
1:X:112:LEU:HD11	1:X:139:VAL:CG2	2.37	0.55
1:O:37:ALA:HB2	1:O:110:LEU:HD11	1.89	0.55
1:A:123:LYS:HG2	1:A:128:VAL:HG13	1.88	0.55
2:D:467:ARG:CZ	2:D:467:ARG:HB3	2.38	0.54
1:X:58:LEU:HD23	1:X:70:VAL:HA	1.89	0.54
2:S:373:ILE:HD12	1:Z:70:VAL:HG11	1.89	0.54
1:T:55:ILE:CD1	1:T:98:LEU:HD21	2.36	0.54
1:O:87:LEU:HB3	1:O:91:VAL:HG23	1.90	0.53
1:P:106:ASN:HD22	1:P:106:ASN:C	2.13	0.53
1:B:54:ASP:HB3	1:B:123:LYS:HB2	1.90	0.53
2:H:503:LYS:NZ	3:H:2105:HOH:O	2.31	0.52
1:Z:36:THR:HG23	1:Z:108:THR:HG22	1.92	0.52
1:B:36:THR:HG23	1:B:107:VAL:O	2.10	0.52
2:R:437:ASN:O	2:R:440:THR:HG22	2.10	0.52
2:C:373:ILE:HD11	1:T:70:VAL:HG21	1.91	0.52
2:C:483:ASP:O	2:C:487:VAL:HG22	2.09	0.52
1:V:87:LEU:HD23	1:V:90:ARG:NH2	2.24	0.52
1:T:59:ILE:HG23	1:T:61:PRO:HD3	1.92	0.52
2:S:374:ASN:CB	2:S:440:THR:HG21	2.39	0.52
1:Y:55:ILE:CD1	1:Y:98:LEU:HD21	2.38	0.52
1:B:55:ILE:CD1	1:B:122:VAL:HG13	2.40	0.52
1:G:55:ILE:HD11	1:G:122:VAL:HG13	1.90	0.51
1:B:20:LEU:HD13	1:B:45:LEU:HD23	1.91	0.51
1:O:29:ILE:HD12	1:O:133:ILE:CG2	2.41	0.51
1:O:55:ILE:HD13	1:O:103:ALA:HB2	1.93	0.51
2:L:483:ASP:O	2:L:487:VAL:HG22	2.11	0.51
1:Z:93:PHE:CD1	1:Z:98:LEU:HD21	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:410:ILE:CD1	2:F:527:LEU:HD12	2.41	0.51
2:N:374:ASN:CB	2:N:440:THR:HG21	2.30	0.51
2:E:373:ILE:HD11	1:O:70:VAL:HG21	1.92	0.51
1:X:93:PHE:CG	1:X:98:LEU:HD21	2.46	0.51
2:D:483:ASP:O	2:D:487:VAL:HG22	2.11	0.51
1:O:123:LYS:HG2	1:O:128:VAL:HG13	1.93	0.50
2:D:422:MET:HG2	2:D:436:ILE:HB	1.92	0.50
2:I:395:LEU:HD23	2:I:538:VAL:HA	1.94	0.50
2:L:437:ASN:O	2:L:440:THR:HG22	2.12	0.50
1:P:96:ASN:OD1	1:P:97:ASP:N	2.45	0.49
2:N:373:ILE:HD11	1:Y:70:VAL:HG21	1.94	0.49
1:G:22:ILE:HD11	1:G:122:VAL:HG23	1.95	0.49
1:Y:98:LEU:HD23	1:Y:98:LEU:C	2.33	0.49
2:I:373:ILE:HD12	1:P:70:VAL:HG11	1.95	0.49
1:X:112:LEU:HD11	1:X:139:VAL:HG21	1.95	0.49
1:G:64:ASN:HD21	1:G:66:LYS:NZ	2.10	0.49
1:K:53:LEU:HD11	1:K:55:ILE:HD11	1.96	0.48
2:M:483:ASP:O	2:M:487:VAL:HG22	2.13	0.48
2:C:477:ILE:HG22	2:H:531:ASP:OD2	2.13	0.48
2:C:417:GLN:NE2	3:C:2050:HOH:O	2.40	0.48
1:O:54:ASP:HB3	1:O:123:LYS:HB2	1.94	0.48
1:G:54:ASP:HB3	1:G:123:LYS:HB2	1.95	0.48
1:A:55:ILE:CD1	1:A:122:VAL:HG13	2.43	0.48
1:Y:54:ASP:HB3	1:Y:123:LYS:HB2	1.96	0.48
2:I:373:ILE:HB	1:P:73:LEU:HD11	1.95	0.48
1:K:123:LYS:HG2	1:K:128:VAL:HG13	1.95	0.48
2:E:395:LEU:HD23	2:E:538:VAL:HA	1.96	0.48
2:S:440:THR:HG23	3:S:2007:HOH:O	2.14	0.48
1:Z:55:ILE:HD13	1:Z:103:ALA:HB2	1.96	0.48
1:A:70:VAL:HG21	2:Q:373:ILE:HD11	1.94	0.48
1:B:72:ILE:HG21	1:B:105:ILE:HG21	1.96	0.47
1:K:123:LYS:HG2	1:K:128:VAL:CG1	2.45	0.47
1:A:84:TYR:CD2	1:A:87:LEU:HD12	2.50	0.47
2:S:398:VAL:O	2:S:534:THR:HA	2.15	0.47
2:H:422:MET:HG2	2:H:436:ILE:HB	1.97	0.47
1:X:94:THR:HG22	1:X:106:ASN:ND2	2.30	0.47
1:V:33:LYS:NZ	1:V:111:GLN:OE1	2.48	0.47
2:C:440:THR:HB	3:C:2066:HOH:O	2.15	0.47
1:B:55:ILE:HD12	1:B:122:VAL:HG22	1.96	0.46
1:X:123:LYS:HG2	1:X:128:VAL:HG13	1.97	0.46
1:G:37:ALA:HB2	1:G:110:LEU:HD11	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:43:PHE:CZ	1:Z:101:GLY:HA2	2.51	0.46
1:T:74:TYR:CZ	1:T:77:ASP:HA	2.49	0.46
1:T:28:MET:HG2	1:T:134:HIS:HB2	1.97	0.46
1:A:56:GLU:CB	1:A:73:LEU:HD23	2.45	0.46
1:P:55:ILE:HB	1:P:74:TYR:HB3	1.97	0.46
2:H:369:PRO:HA	3:H:2023:HOH:O	2.16	0.46
1:K:37:ALA:HB2	1:K:110:LEU:HD11	1.96	0.46
2:Q:531:ASP:OD2	2:S:477:ILE:HG22	2.15	0.46
1:B:92:HIS:HB2	1:B:106:ASN:HD21	1.81	0.46
2:E:423:GLU:HB3	2:E:508:ALA:HB2	1.98	0.45
1:A:70:VAL:HG21	2:Q:373:ILE:CD1	2.46	0.45
2:Q:483:ASP:O	2:Q:487:VAL:HG22	2.17	0.45
1:O:87:LEU:HD13	1:O:91:VAL:HG21	1.98	0.45
1:P:73:LEU:CD2	3:P:2014:HOH:O	2.65	0.45
2:Q:477:ILE:HG22	2:R:531:ASP:OD2	2.15	0.45
1:X:17:ALA:HB2	1:X:44:THR:CG2	2.45	0.45
1:K:31:LYS:NZ	1:K:36:THR:O	2.49	0.45
2:S:411:VAL:HG13	2:S:528:PHE:HB2	1.99	0.45
1:P:98:LEU:HD23	1:P:98:LEU:C	2.37	0.45
1:J:73:LEU:C	1:J:73:LEU:HD12	2.37	0.45
2:D:361:ALA:N	3:D:2011:HOH:O	2.49	0.45
1:K:59:ILE:HD13	1:K:118:TYR:CE2	2.52	0.45
1:B:131:LYS:HE2	1:B:133:ILE:HD11	1.99	0.45
2:E:384:ARG:NH2	1:O:70:VAL:HG23	2.31	0.45
1:G:39:LEU:HD12	1:G:105:ILE:HD11	1.99	0.45
2:D:374:ASN:HB3	2:D:440:THR:HG21	1.99	0.44
1:P:73:LEU:HD22	3:P:2014:HOH:O	2.17	0.44
2:D:366:TRP:CE2	2:D:368:GLY:HA2	2.52	0.44
1:G:58:LEU:HD13	1:G:68:ASP:HB3	1.99	0.44
1:V:55:ILE:HB	1:V:74:TYR:HB3	1.99	0.44
1:B:56:GLU:HB2	1:B:73:LEU:HD23	1.99	0.44
1:Y:39:LEU:HD21	1:Y:135:LEU:HD13	2.00	0.44
1:T:87:LEU:HB3	1:T:91:VAL:HG23	2.00	0.44
1:B:20:LEU:HD21	1:B:122:VAL:HG12	2.00	0.44
2:E:373:ILE:HD12	1:O:73:LEU:HD11	2.00	0.44
1:V:55:ILE:HD13	1:V:103:ALA:HB2	2.00	0.44
1:Z:46:SER:OG	1:Z:47:PRO:HD2	2.17	0.44
1:V:38:TYR:CE1	1:V:94:THR:HG21	2.53	0.44
1:Y:20:LEU:HD23	1:Y:21:SER:N	2.33	0.44
1:B:98:LEU:O	1:B:98:LEU:HD23	2.18	0.43
2:E:384:ARG:NH2	1:O:70:VAL:CG2	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:410:ILE:CD1	2:E:527:LEU:HD12	2.48	0.43
2:R:421:ILE:HG12	2:R:513:THR:HG23	2.00	0.43
1:V:54:ASP:HB3	1:V:123:LYS:HB2	2.01	0.43
2:Q:422:MET:HG2	2:Q:436:ILE:HB	2.00	0.43
1:J:46:SER:HB2	1:J:47:PRO:HD2	2.00	0.43
1:Z:119:GLN:HE21	1:Z:130:ASN:ND2	2.17	0.43
2:H:441:THR:HG23	1:J:125:ALA:HB2	2.01	0.43
1:T:29:ILE:HD13	1:T:133:ILE:HG21	2.01	0.43
1:O:55:ILE:CD1	1:O:98:LEU:HD21	2.42	0.43
1:P:54:ASP:HB3	1:P:123:LYS:HB2	2.00	0.43
2:F:386:PHE:O	2:F:400:ALA:HA	2.19	0.43
2:Q:366:TRP:CE2	2:Q:368:GLY:HA2	2.54	0.42
2:M:417:GLN:CD	2:M:517:LEU:HD23	2.40	0.42
2:I:373:ILE:CD1	1:P:70:VAL:HG21	2.49	0.42
2:I:423:GLU:OE2	2:I:505:LYS:HG2	2.19	0.42
1:K:73:LEU:C	1:K:73:LEU:HD12	2.40	0.42
1:O:56:GLU:OE1	3:O:2009:HOH:O	2.21	0.42
1:B:57:TRP:HB2	1:B:72:ILE:HG22	2.02	0.42
2:L:422:MET:HG2	2:L:436:ILE:HB	2.01	0.42
1:P:37:ALA:HB2	1:P:110:LEU:HD11	2.00	0.42
1:A:73:LEU:HD12	1:A:83:TYR:OH	2.20	0.42
1:P:73:LEU:HD12	1:P:83:TYR:OH	2.19	0.42
3:I:2018:HOH:O	1:P:73:LEU:HD21	2.19	0.42
1:O:32:ALA:HB3	1:O:35:GLU:HG3	2.02	0.42
1:K:119:GLN:HA	1:K:131:LYS:O	2.19	0.42
1:O:131:LYS:HE2	1:O:133:ILE:HD11	2.00	0.42
1:J:55:ILE:HD12	1:J:98:LEU:CD2	2.48	0.42
1:A:58:LEU:HD23	1:A:70:VAL:HA	2.01	0.42
1:Z:123:LYS:HG2	1:Z:128:VAL:HG13	2.01	0.42
1:A:92:HIS:CE1	1:A:106:ASN:ND2	2.77	0.42
1:A:55:ILE:HD12	1:A:122:VAL:HG22	2.01	0.42
1:Y:53:LEU:CD2	1:Y:99:LYS:HA	2.50	0.42
2:L:421:ILE:HD13	2:L:505:LYS:HD3	2.02	0.42
1:K:70:VAL:HG13	1:K:83:TYR:HB3	2.01	0.41
1:Y:121:LYS:HG2	1:Y:130:ASN:HB3	2.02	0.41
2:F:542:GLN:HA	2:F:542:GLN:HE21	1.85	0.41
1:O:70:VAL:CG1	1:O:73:LEU:HD21	2.49	0.41
1:B:53:LEU:HD11	1:B:55:ILE:HD11	2.02	0.41
2:E:404:GLY:HA3	2:E:408:TYR:O	2.19	0.41
2:C:373:ILE:HD12	1:T:70:VAL:HG11	2.01	0.41
2:D:398:VAL:O	2:D:534:THR:HA	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:121:LYS:HG2	1:T:130:ASN:HB3	2.03	0.41
1:Y:87:LEU:HD13	1:Y:91:VAL:CG1	2.51	0.41
2:L:531:ASP:OD2	2:N:477:ILE:HG22	2.21	0.41
2:F:413:PRO:HB2	2:M:378:ASN:O	2.20	0.41
1:X:39:LEU:HB3	1:X:133:ILE:HD12	2.02	0.41
2:S:440:THR:CG2	3:S:2007:HOH:O	2.69	0.41
2:N:487:VAL:HG11	2:N:493:ARG:HD2	2.03	0.41
2:S:422:MET:HG2	2:S:436:ILE:HB	2.02	0.41
1:Z:31:LYS:HZ3	1:Z:37:ALA:HB1	1.85	0.41
1:Y:131:LYS:HE2	1:Y:133:ILE:HD11	2.01	0.41
1:V:17:ALA:HB2	1:V:44:THR:CG2	2.51	0.41
2:I:483:ASP:O	2:I:487:VAL:HG22	2.21	0.41
1:J:112:LEU:HD11	1:J:139:VAL:CG2	2.50	0.41
2:F:361:ALA:HB1	2:F:362:PRO:HD2	2.03	0.41
1:T:54:ASP:HB3	1:T:123:LYS:HB2	2.03	0.41
1:T:87:LEU:HD23	1:T:90:ARG:NH2	2.35	0.41
2:N:410:ILE:HD13	2:N:527:LEU:HA	2.02	0.41
2:N:373:ILE:HG22	2:N:381:PRO:HB2	2.04	0.40
1:G:56:GLU:HB2	1:G:73:LEU:HD23	2.01	0.40
2:L:417:GLN:HG2	2:L:517:LEU:HA	2.02	0.40
1:B:96:ASN:N	1:B:96:ASN:OD1	2.44	0.40
2:L:363:ILE:HG12	2:L:364:THR:N	2.36	0.40
1:A:26:GLU:HA	1:A:132:LYS:O	2.21	0.40
2:S:373:ILE:HD11	1:Z:70:VAL:HG11	2.01	0.40
1:B:31:LYS:HG3	1:B:37:ALA:HB2	2.04	0.40
2:C:373:ILE:CD1	1:T:70:VAL:HG21	2.51	0.40
2:N:373:ILE:CD1	1:Y:70:VAL:HG21	2.50	0.40
2:N:495:ILE:HG22	2:N:519:PHE:HA	2.04	0.40
1:O:55:ILE:HB	1:O:74:TYR:HB3	2.04	0.40
1:B:45:LEU:HD13	1:B:124:LYS:HD3	2.02	0.40
1:T:29:ILE:HD13	1:T:133:ILE:CG2	2.52	0.40
2:H:366:TRP:CE2	2:H:368:GLY:HA2	2.56	0.40
1:V:20:LEU:C	1:V:20:LEU:HD23	2.42	0.40
2:Q:391:ARG:HG2	2:Q:462:LEU:HB3	2.03	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	115/128 (90%)	107 (93%)	7 (6%)	1 (1%)	21	24
1	B	107/128 (84%)	96 (90%)	11 (10%)	0	100	100
1	G	121/128 (94%)	115 (95%)	6 (5%)	0	100	100
1	J	121/128 (94%)	119 (98%)	2 (2%)	0	100	100
1	K	121/128 (94%)	116 (96%)	5 (4%)	0	100	100
1	O	114/128 (89%)	107 (94%)	7 (6%)	0	100	100
1	P	121/128 (94%)	115 (95%)	6 (5%)	0	100	100
1	T	117/128 (91%)	109 (93%)	8 (7%)	0	100	100
1	V	119/128 (93%)	114 (96%)	5 (4%)	0	100	100
1	X	121/128 (94%)	117 (97%)	4 (3%)	0	100	100
1	Y	117/128 (91%)	109 (93%)	8 (7%)	0	100	100
1	Z	115/128 (90%)	106 (92%)	8 (7%)	1 (1%)	21	24
2	C	180/197 (91%)	174 (97%)	6 (3%)	0	100	100
2	D	180/197 (91%)	172 (96%)	8 (4%)	0	100	100
2	E	180/197 (91%)	172 (96%)	8 (4%)	0	100	100
2	F	180/197 (91%)	174 (97%)	6 (3%)	0	100	100
2	H	180/197 (91%)	174 (97%)	6 (3%)	0	100	100
2	I	180/197 (91%)	174 (97%)	6 (3%)	0	100	100
2	L	180/197 (91%)	174 (97%)	6 (3%)	0	100	100
2	M	180/197 (91%)	173 (96%)	7 (4%)	0	100	100
2	N	180/197 (91%)	173 (96%)	7 (4%)	0	100	100
2	Q	180/197 (91%)	174 (97%)	6 (3%)	0	100	100
2	R	180/197 (91%)	173 (96%)	7 (4%)	0	100	100
2	S	180/197 (91%)	171 (95%)	9 (5%)	0	100	100
All	All	3569/3900 (92%)	3408 (96%)	159 (4%)	2 (0%)	56	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Z	101	GLY
1	A	24	THR

### 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	104/113 (92%)	98 (94%)	6 (6%)	25	33
1	B	99/113 (88%)	94 (95%)	5 (5%)	29	39
1	G	109/113 (96%)	104 (95%)	5 (5%)	33	44
1	J	109/113 (96%)	105 (96%)	4 (4%)	41	55
1	K	109/113 (96%)	106 (97%)	3 (3%)	51	68
1	O	105/113 (93%)	100 (95%)	5 (5%)	31	42
1	P	109/113 (96%)	106 (97%)	3 (3%)	51	68
1	T	106/113 (94%)	102 (96%)	4 (4%)	40	54
1	V	107/113 (95%)	103 (96%)	4 (4%)	41	55
1	X	109/113 (96%)	104 (95%)	5 (5%)	33	44
1	Y	106/113 (94%)	100 (94%)	6 (6%)	25	34
1	Z	104/113 (92%)	99 (95%)	5 (5%)	31	42
2	C	159/171 (93%)	153 (96%)	6 (4%)	40	54
2	D	159/171 (93%)	156 (98%)	3 (2%)	65	81
2	E	159/171 (93%)	156 (98%)	3 (2%)	65	81
2	F	159/171 (93%)	154 (97%)	5 (3%)	47	64
2	H	159/171 (93%)	156 (98%)	3 (2%)	65	81
2	I	159/171 (93%)	155 (98%)	4 (2%)	55	73
2	L	159/171 (93%)	156 (98%)	3 (2%)	65	81
2	M	159/171 (93%)	154 (97%)	5 (3%)	47	64
2	N	159/171 (93%)	154 (97%)	5 (3%)	47	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Q	159/171 (93%)	155 (98%)	4 (2%)	55	73
2	R	159/171 (93%)	156 (98%)	3 (2%)	65	81
2	S	159/171 (93%)	155 (98%)	4 (2%)	55	73
All	All	3184/3408 (93%)	3081 (97%)	103 (3%)	46	62

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

Mol	Chain	Res	Type
1	A	28	MET
1	A	42	LYS
1	A	70	VAL
1	A	99	LYS
1	A	106	ASN
1	A	128	VAL
1	B	48	GLU
1	B	77	ASP
1	B	106	ASN
1	B	114	ASP
1	B	135	LEU
2	C	363	ILE
2	C	366	TRP
2	C	372	SER
2	C	426	GLN
2	C	440	THR
2	C	455	ARG
2	D	363	ILE
2	D	366	TRP
2	D	521	ARG
2	E	366	TRP
2	E	372	SER
2	E	417	GLN
2	F	363	ILE
2	F	366	TRP
2	F	440	THR
2	F	507	VAL
2	F	542	GLN
1	G	18	ARG
1	G	36	THR
1	G	67	VAL
1	G	70	VAL
1	G	128	VAL

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Mol	Chain	Res	Type
2	H	363	ILE
2	H	366	TRP
2	H	417	GLN
2	I	363	ILE
2	I	366	TRP
2	I	379	ASP
2	I	503	LYS
1	J	33	LYS
1	J	59	ILE
1	J	73	LEU
1	J	100	SER
1	K	113	SER
1	K	128	VAL
1	K	130	ASN
2	L	363	ILE
2	L	366	TRP
2	L	372	SER
2	M	363	ILE
2	M	366	TRP
2	M	372	SER
2	M	416	SER
2	M	455	ARG
2	N	363	ILE
2	N	366	TRP
2	N	372	SER
2	N	455	ARG
2	N	529	LYS
1	O	33	LYS
1	O	96	ASN
1	O	99	LYS
1	O	111	GLN
1	O	128	VAL
1	P	70	VAL
1	P	92	HIS
1	P	106	ASN
2	Q	363	ILE
2	Q	366	TRP
2	Q	372	SER
2	Q	521	ARG
2	R	363	ILE
2	R	366	TRP
2	R	455	ARG

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Mol	Chain	Res	Type
2	S	363	ILE
2	S	366	TRP
2	S	372	SER
2	S	455	ARG
1	T	28	MET
1	T	59	ILE
1	T	70	VAL
1	T	130	ASN
1	V	28	MET
1	V	42	LYS
1	V	70	VAL
1	V	106	ASN
1	X	23	THR
1	X	26	GLU
1	X	64	ASN
1	X	70	VAL
1	X	96	ASN
1	Y	70	VAL
1	Y	73	LEU
1	Y	77	ASP
1	Y	100	SER
1	Y	128	VAL
1	Y	130	ASN
1	Z	48	GLU
1	Z	70	VAL
1	Z	91	VAL
1	Z	99	LYS
1	Z	106	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	HIS
1	A	134	HIS
1	B	106	ASN
2	F	542	GLN
1	G	64	ASN
1	G	134	HIS
1	P	106	ASN
2	S	378	ASN
2	S	458	HIS
2	S	542	GLN

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Mol	Chain	Res	Type
1	T	130	ASN
1	V	106	ASN
1	X	64	ASN
1	X	134	HIS
1	Y	109	ASN
1	Y	111	GLN
1	Z	130	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	117/128 (91%)	1.48	38 (32%) <span>1</span> <span>1</span>	34, 44, 54, 57	0
1	B	113/128 (88%)	2.05	50 (44%) <span>0</span> <span>0</span>	32, 46, 58, 60	0
1	G	123/128 (96%)	0.13	8 (6%) <span>22</span> <span>30</span>	33, 44, 55, 58	0
1	J	123/128 (96%)	0.24	7 (5%) <span>27</span> <span>36</span>	33, 44, 55, 57	0
1	K	123/128 (96%)	0.33	5 (4%) <span>41</span> <span>50</span>	33, 45, 56, 57	0
1	O	118/128 (92%)	0.27	5 (4%) <span>40</span> <span>49</span>	33, 44, 54, 58	0
1	P	123/128 (96%)	0.53	12 (9%) <span>10</span> <span>14</span>	33, 44, 55, 57	0
1	T	119/128 (92%)	0.71	12 (10%) <span>9</span> <span>13</span>	33, 45, 55, 57	0
1	V	121/128 (94%)	1.24	31 (25%) <span>1</span> <span>1</span>	34, 44, 55, 57	0
1	X	123/128 (96%)	0.31	9 (7%) <span>18</span> <span>25</span>	33, 45, 55, 58	0
1	Y	119/128 (92%)	1.06	25 (21%) <span>1</span> <span>2</span>	34, 44, 54, 57	0
1	Z	117/128 (91%)	1.68	46 (39%) <span>0</span> <span>0</span>	34, 45, 55, 57	0
2	C	182/197 (92%)	0.01	0 <span>100</span> <span>100</span>	19, 24, 30, 36	0
2	D	182/197 (92%)	0.32	6 (3%) <span>50</span> <span>59</span>	20, 25, 33, 36	0
2	E	182/197 (92%)	0.05	1 (0%) <span>91</span> <span>94</span>	20, 25, 32, 36	0
2	F	182/197 (92%)	0.04	0 <span>100</span> <span>100</span>	19, 23, 30, 34	0
2	H	182/197 (92%)	-0.12	0 <span>100</span> <span>100</span>	19, 24, 30, 35	0
2	I	182/197 (92%)	0.15	0 <span>100</span> <span>100</span>	19, 25, 30, 35	0
2	L	182/197 (92%)	0.24	4 (2%) <span>65</span> <span>73</span>	22, 27, 34, 36	0
2	M	182/197 (92%)	0.16	5 (2%) <span>58</span> <span>67</span>	21, 25, 30, 33	0
2	N	182/197 (92%)	0.01	0 <span>100</span> <span>100</span>	21, 26, 32, 37	0
2	Q	182/197 (92%)	0.44	12 (6%) <span>22</span> <span>29</span>	22, 29, 34, 39	0
2	R	182/197 (92%)	0.02	0 <span>100</span> <span>100</span>	22, 27, 34, 39	0
2	S	182/197 (92%)	-0.03	0 <span>100</span> <span>100</span>	24, 31, 39, 41	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	3623/3900 (92%)	0.39	276 (7%) 17 24	19, 30, 52, 60	0

All (276) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	32	ALA	8.9
1	Y	112	LEU	6.9
1	V	34	GLY	6.6
1	B	91	VAL	6.3
1	B	136	VAL	6.3
1	Z	112	LEU	6.0
1	B	138	LEU	5.7
1	A	107	VAL	5.6
1	Z	25	PRO	5.6
1	Y	115	ILE	5.4
1	Z	107	VAL	5.4
1	B	137	VAL	5.4
1	B	107	VAL	5.1
1	B	39	LEU	5.1
1	Z	31	LYS	5.1
1	B	37	ALA	5.1
1	V	108	THR	5.0
1	Y	137	VAL	4.9
1	T	112	LEU	4.9
1	V	107	VAL	4.9
1	B	25	PRO	4.8
1	V	82	ASP	4.8
1	A	25	PRO	4.7
1	B	115	ILE	4.7
1	B	24	THR	4.6
1	B	105	ILE	4.6
1	Z	113	SER	4.6
1	B	18	ARG	4.6
1	Z	24	THR	4.5
1	V	33	LYS	4.4
1	T	25	PRO	4.4
1	V	109	ASN	4.4
1	V	87	LEU	4.4
1	A	32	ALA	4.4
1	V	37	ALA	4.3
1	P	25	PRO	4.3
1	B	85	PRO	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	83	TYR	4.3
1	Z	98	LEU	4.2
1	X	25	PRO	4.2
1	V	89	GLY	4.2
1	Z	110	LEU	4.1
1	Z	91	VAL	4.1
1	A	39	LEU	4.1
1	B	28	MET	4.1
1	A	91	VAL	4.0
1	V	92	HIS	4.0
1	B	30	GLU	4.0
1	V	110	LEU	4.0
1	T	136	VAL	4.0
1	B	84	TYR	4.0
1	V	85	PRO	4.0
1	A	36	THR	4.0
1	Z	135	LEU	4.0
1	Z	36	THR	3.9
1	A	64	ASN	3.9
1	B	61	PRO	3.9
1	Z	64	ASN	3.9
1	V	137	VAL	3.9
1	Z	23	THR	3.8
1	A	65	GLN	3.8
1	X	82	ASP	3.8
1	A	37	ALA	3.7
1	B	17	ALA	3.7
1	Y	37	ALA	3.7
1	Z	32	ALA	3.7
1	B	133	ILE	3.7
1	B	114	ASP	3.7
1	P	82	ASP	3.7
1	V	112	LEU	3.7
1	B	106	ASN	3.7
1	Y	135	LEU	3.6
1	B	27	GLU	3.6
1	A	85	PRO	3.6
1	V	135	LEU	3.6
1	A	112	LEU	3.5
2	Q	398	VAL	3.5
1	B	41	CYS	3.5
1	T	82	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
1	Y	32	ALA	3.5
1	J	24	THR	3.5
1	Z	37	ALA	3.5
1	V	28	MET	3.5
1	B	117	THR	3.5
1	A	92	HIS	3.5
1	Y	64	ASN	3.5
1	B	62	ALA	3.5
1	B	135	LEU	3.4
1	Z	30	GLU	3.4
1	B	92	HIS	3.4
1	Y	29	ILE	3.4
1	B	86	ASP	3.4
1	Y	28	MET	3.4
1	X	138	LEU	3.3
1	P	96	ASN	3.3
1	Y	113	SER	3.3
1	Z	93	PHE	3.3
1	Z	115	ILE	3.3
1	Z	35	GLU	3.3
1	B	94	THR	3.3
1	V	111	GLN	3.3
1	Y	136	VAL	3.3
1	B	82	ASP	3.3
1	Z	96	ASN	3.3
1	K	16	PHE	3.3
1	A	105	ILE	3.3
1	J	17	ALA	3.3
1	Z	28	MET	3.3
1	V	35	GLU	3.2
1	B	72	ILE	3.2
1	Z	57	TRP	3.2
1	B	96	ASN	3.2
1	P	139	VAL	3.2
1	A	33	LYS	3.2
1	Y	39	LEU	3.2
1	Z	62	ALA	3.2
1	V	96	ASN	3.2
1	Y	30	GLU	3.2
1	Y	110	LEU	3.1
1	X	112	LEU	3.1
1	A	31	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	59	ILE	3.1
1	B	103	ALA	3.0
1	A	84	TYR	3.0
1	K	25	PRO	3.0
1	V	84	TYR	3.0
1	G	18	ARG	3.0
1	Y	25	PRO	3.0
1	K	138	LEU	3.0
1	P	92	HIS	3.0
1	B	38	TYR	3.0
1	V	91	VAL	2.9
1	Z	94	THR	2.9
2	Q	499	LEU	2.9
1	O	139	VAL	2.9
2	D	398	VAL	2.9
1	V	25	PRO	2.9
1	T	113	SER	2.9
1	Z	106	ASN	2.9
1	Y	107	VAL	2.9
1	Z	39	LEU	2.9
1	Z	61	PRO	2.9
1	B	131	LYS	2.8
1	Z	89	GLY	2.8
1	J	138	LEU	2.8
1	B	70	VAL	2.8
1	B	87	LEU	2.8
1	Y	105	ILE	2.8
1	Z	42	LYS	2.8
1	Z	118	TYR	2.8
1	B	89	GLY	2.8
1	O	96	ASN	2.8
1	Y	33	LYS	2.8
1	A	63	ASP	2.8
1	P	107	VAL	2.8
2	Q	389	LEU	2.8
1	K	65	GLN	2.7
1	P	89	GLY	2.7
1	Z	116	GLY	2.7
1	B	118	TYR	2.7
1	Z	82	ASP	2.7
1	Z	38	TYR	2.7
1	A	108	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	96	ASN	2.7
1	B	36	THR	2.7
1	X	64	ASN	2.7
1	T	111	GLN	2.7
1	Y	111	GLN	2.7
1	A	19	SER	2.6
1	X	18	ARG	2.6
1	T	63	ASP	2.6
1	V	136	VAL	2.6
1	T	87	LEU	2.6
2	Q	512	LEU	2.6
1	P	109	ASN	2.6
1	Y	109	ASN	2.6
1	A	116	GLY	2.6
1	G	25	PRO	2.6
1	A	82	ASP	2.6
1	Z	87	LEU	2.6
1	V	88	LYS	2.6
1	Z	40	PRO	2.6
1	A	106	ASN	2.5
1	G	28	MET	2.5
1	G	112	LEU	2.5
2	D	396	VAL	2.5
1	A	133	ILE	2.5
1	Z	59	ILE	2.5
1	A	93	PHE	2.5
1	P	106	ASN	2.5
1	V	32	ALA	2.5
1	Y	87	LEU	2.5
1	Z	33	LYS	2.5
1	A	35	GLU	2.5
1	T	108	THR	2.5
2	D	389	LEU	2.5
1	V	93	PHE	2.4
2	M	535	PHE	2.4
1	A	109	ASN	2.4
1	Z	26	GLU	2.4
1	J	18	ARG	2.4
1	V	90	ARG	2.4
1	O	19	SER	2.4
1	P	32	ALA	2.4
2	D	388	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	65	GLN	2.4
1	Z	109	ASN	2.4
1	P	18	ARG	2.4
1	B	88	LYS	2.3
1	Z	34	GLY	2.3
1	J	19	SER	2.3
1	B	31	LYS	2.3
1	J	139	VAL	2.3
1	Z	111	GLN	2.3
1	V	86	ASP	2.3
2	Q	537	TYR	2.3
2	Q	536	THR	2.3
1	A	89	GLY	2.3
1	Y	34	GLY	2.3
2	M	499	LEU	2.3
1	A	24	THR	2.3
2	D	536	THR	2.3
2	Q	396	VAL	2.3
1	Y	85	PRO	2.3
1	A	118	TYR	2.3
1	O	62	ALA	2.3
1	P	17	ALA	2.3
2	E	400	ALA	2.3
1	G	138	LEU	2.3
1	K	28	MET	2.3
1	B	59	ILE	2.2
1	Z	19	SER	2.2
2	Q	469	VAL	2.2
2	Q	463	CYS	2.2
2	Q	535	PHE	2.2
1	V	65	GLN	2.2
1	A	97	ASP	2.2
1	Z	63	ASP	2.2
1	X	24	THR	2.2
1	T	89	GLY	2.2
2	M	533	LEU	2.2
1	A	48	GLU	2.2
2	L	396	VAL	2.2
1	Y	63	ASP	2.2
2	L	379	ASP	2.2
1	A	117	THR	2.2
1	X	30	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
2	L	536	THR	2.1
2	Q	534	THR	2.1
1	T	97	ASP	2.1
1	B	29	ILE	2.1
1	B	79	ILE	2.1
1	J	25	PRO	2.1
2	Q	533	LEU	2.1
1	Z	92	HIS	2.1
1	A	94	THR	2.1
1	X	17	ALA	2.1
2	D	400	ALA	2.1
1	V	115	ILE	2.1
1	Z	103	ALA	2.1
1	A	111	GLN	2.1
1	G	63	ASP	2.1
1	B	23	THR	2.0
1	A	38	TYR	2.0
1	B	42	LYS	2.0
1	T	92	HIS	2.0
1	Z	90	ARG	2.0
1	Y	36	THR	2.0
2	M	534	THR	2.0
2	M	536	THR	2.0
1	A	110	LEU	2.0
1	V	36	THR	2.0
1	G	17	ALA	2.0
2	L	535	PHE	2.0
1	O	92	HIS	2.0
1	B	40	PRO	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 ⓘ

There are no such residues in this entry.