



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 05:21 am GMT

PDB ID : 1EAY  
Title : CHEY-BINDING (P2) DOMAIN OF CHEA IN COMPLEX WITH CHEY FROM ESCHERICHIA COLI  
Authors : Mcevoy, M.M.; Hausrath, A.C.; Randolph, G.B.; Remington, S.J.; Dahlquist, F.W.  
Deposited on : 1998-04-23  
Resolution : 2.00 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
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

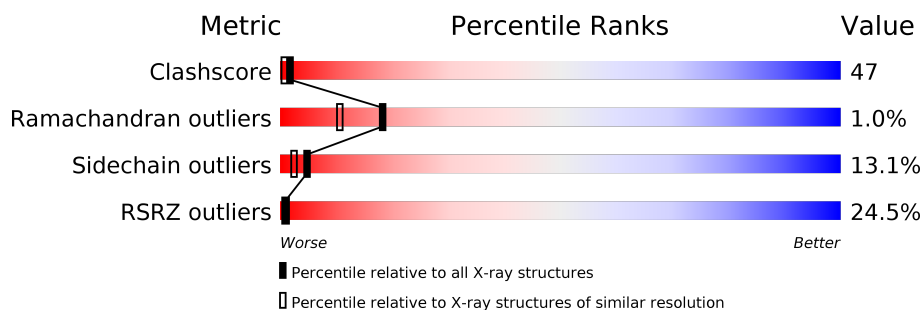
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

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>20%</div> <div>30%</div> <div>52%</div> <div>16%</div> <div>.</div> </div>
1	B	128	<div> <div>26%</div> <div>24%</div> <div>63%</div> <div>10%</div> <div>.</div> </div>
2	C	74	<div> <div>23%</div> <div>24%</div> <div>46%</div> <div>19%</div> <div>.</div> <div>9%</div> </div>
2	D	74	<div> <div>27%</div> <div>32%</div> <div>41%</div> <div>19%</div> <div>.</div> <div>7%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3058 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 CHEY.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	128	Total	C	N	O	S	0	0	0
			953	612	154	181	6			
1	B	128	Total	C	N	O	S	0	0	0
			966	617	158	185	6			

- Molecule 2 is a protein called CHEA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	67	Total	C	N	O	S	0	0	0
			501	317	80	103	1			
2	D	69	Total	C	N	O	S	0	0	0
			514	325	82	106	1			

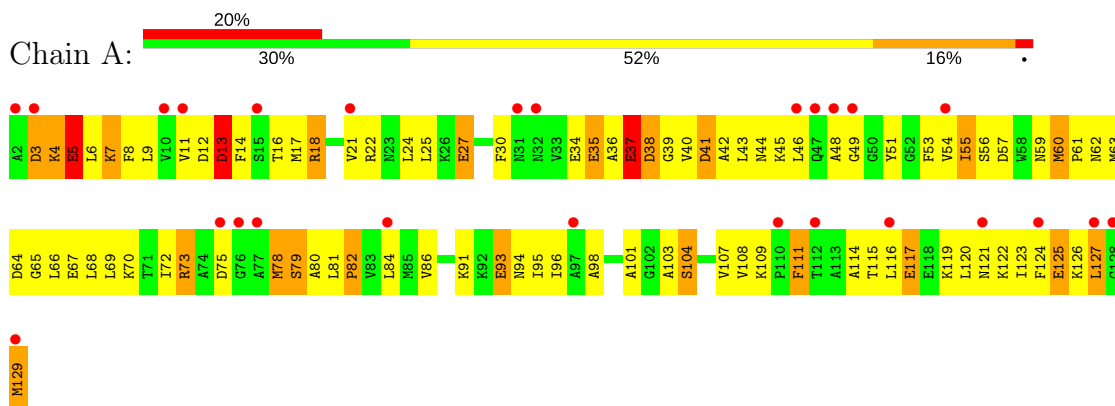
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	54	Total	O	0	0
			54	54		
3	B	32	Total	O	0	0
			32	32		
3	C	27	Total	O	0	0
			27	27		
3	D	11	Total	O	0	0
			11	11		

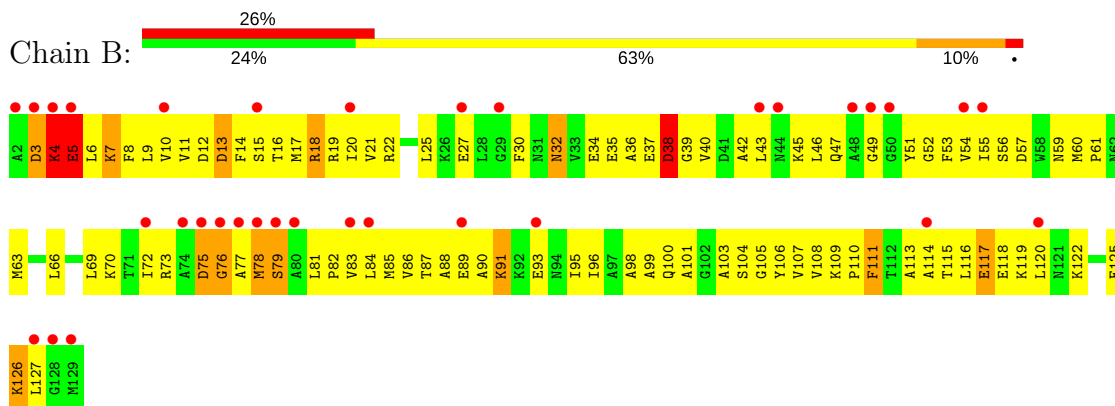
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

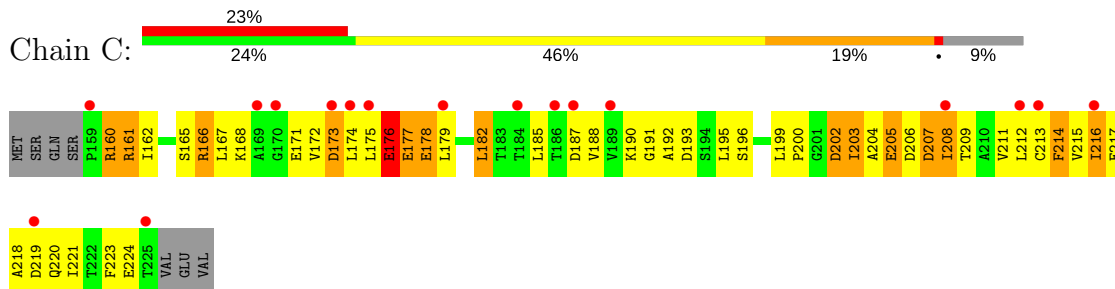
#### • Molecule 1: CHEY



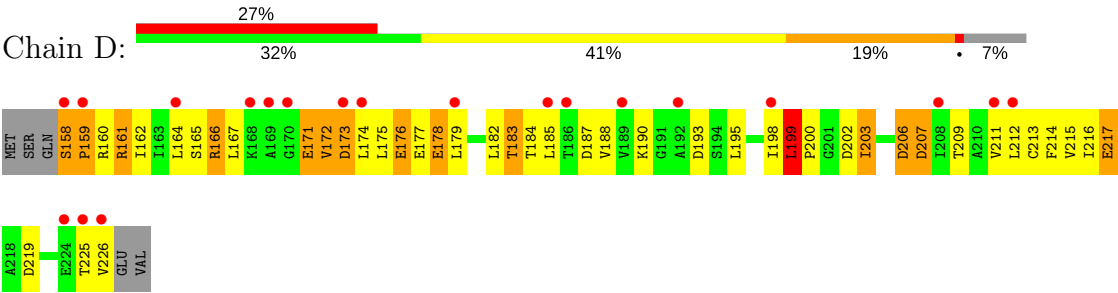
#### • Molecule 1: CHEY



#### • Molecule 2: CHEA



#### • Molecule 2: CHEA



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.50Å 64.20Å 158.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 21.21 – 1.95	Depositor EDS
% Data completeness (in resolution range)	78.0 (20.00-2.00) 74.3 (21.21-1.95)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	10.71 (at 1.95Å)	Xtriage
Refinement program	TNT V. 5-F	Depositor
R, $R_{free}$	0.217 , (Not available) 0.225 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	8.3	Xtriage
Anisotropy	1.127	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 343.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.30$ , $\langle L^2 \rangle = 0.13$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	3058	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% 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, 0.333 respectively for untwinned datasets, and 0.375, 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	1.37	8/965 (0.8%)	1.58	15/1302 (1.2%)
1	B	1.32	7/978 (0.7%)	1.57	11/1318 (0.8%)
2	C	1.41	5/505 (1.0%)	1.72	17/687 (2.5%)
2	D	1.41	5/518 (1.0%)	1.79	20/706 (2.8%)
All	All	1.37	25/2966 (0.8%)	1.64	63/4013 (1.6%)

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	27	GLU	CD-OE2	6.55	1.32	1.25
1	A	67	GLU	CD-OE1	6.47	1.32	1.25
2	C	178	GLU	CD-OE1	6.44	1.32	1.25
2	D	178	GLU	CD-OE1	6.43	1.32	1.25
2	D	217	GLU	CD-OE1	6.38	1.32	1.25
1	B	5	GLU	CD-OE1	6.21	1.32	1.25
1	B	125	GLU	CD-OE2	6.17	1.32	1.25
1	A	5	GLU	CD-OE2	6.13	1.32	1.25
2	C	217	GLU	CD-OE1	6.13	1.32	1.25
1	A	125	GLU	CD-OE1	6.00	1.32	1.25
2	C	176	GLU	CD-OE2	5.98	1.32	1.25
1	A	37	GLU	CD-OE1	5.96	1.32	1.25
1	B	37	GLU	CD-OE2	5.88	1.32	1.25
1	B	89	GLU	CD-OE1	5.81	1.32	1.25
2	D	176	GLU	CD-OE2	5.79	1.32	1.25
2	D	177	GLU	CD-OE1	5.76	1.31	1.25
1	A	117	GLU	CD-OE1	5.71	1.31	1.25
1	A	35	GLU	CD-OE1	5.63	1.31	1.25
2	C	205	GLU	CD-OE2	5.57	1.31	1.25
1	A	27	GLU	CD-OE1	5.57	1.31	1.25
1	A	93	GLU	CD-OE1	5.57	1.31	1.25
1	B	117	GLU	CD-OE2	5.45	1.31	1.25
1	B	34	GLU	CD-OE2	5.37	1.31	1.25
2	C	177	GLU	CD-OE1	5.31	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	171	GLU	CD-OE2	5.25	1.31	1.25

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	207	ASP	CB-CG-OD1	9.63	126.97	118.30
1	B	38	ASP	CB-CG-OD1	8.45	125.91	118.30
1	B	38	ASP	CB-CG-OD2	-8.08	111.03	118.30
1	A	18	ARG	NE-CZ-NH1	7.84	124.22	120.30
1	A	38	ASP	CB-CG-OD1	7.65	125.19	118.30
1	A	3	ASP	CB-CG-OD1	-7.46	111.59	118.30
2	D	207	ASP	CB-CG-OD2	-7.37	111.67	118.30
1	B	18	ARG	NE-CZ-NH1	7.14	123.87	120.30
1	B	3	ASP	CB-CG-OD2	-7.12	111.89	118.30
2	D	206	ASP	CB-CG-OD2	-6.99	112.01	118.30
2	D	173	ASP	CB-CG-OD1	6.95	124.55	118.30
2	D	206	ASP	CB-CG-OD1	6.74	124.36	118.30
2	D	193	ASP	CB-CG-OD1	-6.69	112.28	118.30
2	C	206	ASP	CB-CG-OD2	6.64	124.28	118.30
2	C	219	ASP	CB-CG-OD2	-6.62	112.34	118.30
1	A	13	ASP	CB-CG-OD2	-6.59	112.37	118.30
2	D	187	ASP	CB-CG-OD1	-6.59	112.37	118.30
2	C	202	ASP	CB-CG-OD2	-6.56	112.39	118.30
1	A	57	ASP	CB-CG-OD2	-6.54	112.42	118.30
1	B	3	ASP	CB-CG-OD1	6.47	124.12	118.30
1	A	55	ILE	N-CA-C	-6.46	93.55	111.00
2	D	219	ASP	CB-CG-OD2	-6.41	112.54	118.30
2	D	173	ASP	CB-CG-OD2	-6.38	112.56	118.30
2	C	214	PHE	CB-CA-C	-6.35	97.69	110.40
2	C	207	ASP	CB-CG-OD2	-6.31	112.62	118.30
2	C	193	ASP	CB-CG-OD1	6.29	123.96	118.30
1	B	57	ASP	CB-CG-OD1	6.24	123.91	118.30
2	D	202	ASP	CB-CG-OD1	6.21	123.89	118.30
1	A	75	ASP	CB-CG-OD2	-6.16	112.75	118.30
2	C	202	ASP	CB-CG-OD1	6.15	123.84	118.30
1	B	57	ASP	CB-CG-OD2	-6.15	112.77	118.30
2	C	193	ASP	CB-CG-OD2	-6.14	112.77	118.30
1	A	13	ASP	CB-CG-OD1	6.10	123.79	118.30
2	C	207	ASP	CB-CG-OD1	6.08	123.77	118.30
1	A	3	ASP	CB-CG-OD2	6.02	123.72	118.30
1	A	38	ASP	CB-CG-OD2	-6.02	112.88	118.30
2	C	206	ASP	CB-CG-OD1	-6.01	112.89	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	75	ASP	CB-CG-OD1	-5.99	112.91	118.30
1	B	75	ASP	CB-CG-OD2	5.94	123.64	118.30
2	D	219	ASP	CB-CG-OD1	5.91	123.62	118.30
2	D	193	ASP	CB-CG-OD2	5.90	123.61	118.30
2	C	173	ASP	CB-CG-OD2	5.86	123.58	118.30
2	C	173	ASP	CB-CG-OD1	-5.86	113.03	118.30
2	D	187	ASP	CB-CG-OD2	5.80	123.52	118.30
2	C	187	ASP	CB-CG-OD2	-5.79	113.09	118.30
1	B	12	ASP	CB-CG-OD2	5.77	123.49	118.30
2	D	199	LEU	CB-CA-C	-5.74	99.29	110.20
1	A	82	PRO	N-CA-CB	5.73	110.18	103.30
2	C	187	ASP	CB-CG-OD1	5.69	123.42	118.30
2	D	202	ASP	CB-CG-OD2	-5.62	113.24	118.30
2	D	158	SER	N-CA-CB	5.55	118.83	110.50
2	D	160	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	B	13	ASP	CB-CG-OD2	-5.46	113.39	118.30
2	C	219	ASP	CB-CG-OD1	5.46	123.21	118.30
1	A	12	ASP	CB-CG-OD2	-5.35	113.49	118.30
1	A	73	ARG	NE-CZ-NH1	5.32	122.96	120.30
2	C	182	LEU	CB-CA-C	-5.28	100.17	110.20
1	A	7	LYS	N-CA-CB	5.23	120.02	110.60
2	D	166	ARG	NE-CZ-NH1	5.22	122.91	120.30
2	D	161	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	A	41	ASP	CB-CG-OD1	5.17	122.95	118.30
2	C	196	SER	N-CA-CB	5.06	118.09	110.50
2	D	159	PRO	N-CA-CB	5.03	109.33	103.30

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	953	0	957	96	0
1	B	966	0	977	109	0
2	C	501	0	505	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	514	0	518	36	0
3	A	54	0	0	6	0
3	B	32	0	0	4	0
3	C	27	0	0	0	0
3	D	11	0	0	0	0
All	All	3058	0	2957	277	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 47.

All (277) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:VAL:HG12	1:A:56:SER:HB2	1.48	0.94
1:B:122:LYS:HE3	2:D:215:VAL:HG13	1.53	0.90
2:C:175:LEU:HD11	2:C:216:ILE:HD13	1.53	0.89
2:C:166:ARG:NH2	2:C:220:GLN:HA	1.88	0.87
2:D:179:LEU:HB2	2:D:185:LEU:HD11	1.57	0.87
1:A:84:LEU:HD13	1:A:123:ILE:HD11	1.59	0.85
2:D:179:LEU:CB	2:D:185:LEU:HD11	2.07	0.84
1:B:14:PHE:CZ	1:B:16:THR:HB	2.14	0.82
2:C:215:VAL:HG12	2:C:216:ILE:HD12	1.62	0.81
1:A:59:ASN:O	1:A:60:MET:HG3	1.81	0.80
1:A:54:VAL:CG1	1:A:56:SER:HB2	2.12	0.79
2:C:162:ILE:HB	2:C:199:LEU:HD22	1.65	0.79
1:A:109:LYS:HA	1:A:111:PHE:CD2	2.18	0.78
1:A:72:ILE:HA	1:A:78:MET:HE3	1.67	0.77
2:C:166:ARG:NH1	2:C:220:GLN:HG3	2.01	0.76
1:B:59:ASN:O	1:B:60:MET:HG3	1.84	0.76
1:A:124:PHE:HD1	1:A:129:MET:HE2	1.50	0.76
1:B:17:MET:CE	1:B:21:VAL:HG23	2.18	0.74
1:B:66:LEU:HD12	1:B:69:LEU:HD23	1.68	0.74
1:B:6:LEU:HD21	1:B:53:PHE:HD2	1.53	0.74
1:B:18:ARG:HD2	1:B:35:GLU:OE1	1.88	0.73
1:B:10:VAL:O	1:B:35:GLU:HA	1.89	0.73
1:B:46:LEU:HD23	1:B:51:TYR:CD2	2.24	0.73
1:A:25:LEU:HB3	1:A:30:PHE:HB2	1.71	0.73
2:D:161:ARG:HB2	2:D:226:VAL:HG22	1.70	0.73
1:B:11:VAL:HG12	1:B:60:MET:SD	2.28	0.72
1:A:73:ARG:HD3	1:A:79:SER:O	1.88	0.72
1:B:59:ASN:C	1:B:60:MET:HG3	2.11	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:PHE:CZ	1:A:16:THR:HB	2.25	0.71
1:A:72:ILE:HG23	1:A:78:MET:HB3	1.73	0.71
1:B:17:MET:HE2	1:B:21:VAL:HG23	1.72	0.71
1:A:91:LYS:O	1:A:95:ILE:HG13	1.92	0.69
1:B:73:ARG:HD3	1:B:79:SER:O	1.92	0.69
1:B:4:LYS:HA	1:B:30:PHE:CD2	2.27	0.69
1:B:75:ASP:HB3	1:B:78:MET:HE2	1.75	0.69
1:A:91:LYS:HG2	3:A:149:HOH:O	1.92	0.68
1:A:53:PHE:CE1	1:A:84:LEU:HB2	2.29	0.68
1:A:9:LEU:HB2	1:A:51:TYR:CD1	2.28	0.67
1:A:126:LYS:HG3	1:A:126:LYS:O	1.92	0.67
1:A:55:ILE:HG23	1:A:86:VAL:HG23	1.77	0.67
2:D:173:ASP:O	2:D:176:GLU:HB3	1.94	0.66
2:D:198:ILE:N	2:D:198:ILE:HD12	2.10	0.66
1:B:11:VAL:HG13	1:B:36:ALA:HB3	1.77	0.66
1:B:51:TYR:O	1:B:81:LEU:HD21	1.96	0.66
2:D:172:VAL:O	2:D:176:GLU:HB2	1.96	0.65
1:A:101:ALA:HB2	3:A:151:HOH:O	1.96	0.65
1:B:69:LEU:O	1:B:72:ILE:HB	1.96	0.65
1:B:70:LYS:HD2	3:B:152:HOH:O	1.96	0.65
1:B:75:ASP:O	1:B:77:ALA:N	2.30	0.64
1:B:4:LYS:HA	1:B:30:PHE:CE2	2.32	0.64
1:A:53:PHE:HE1	1:A:84:LEU:HB2	1.63	0.64
1:B:46:LEU:HD23	1:B:51:TYR:HD2	1.63	0.64
1:B:38:ASP:HB2	1:B:61:PRO:O	1.97	0.64
1:B:96:ILE:O	1:B:99:ALA:N	2.31	0.63
2:C:168:LYS:O	2:C:171:GLU:HB2	1.98	0.63
1:B:107:VAL:HG22	1:B:108:VAL:N	2.13	0.63
1:A:42:ALA:O	1:A:46:LEU:N	2.31	0.63
1:A:114:ALA:O	1:A:117:GLU:HB3	1.99	0.63
1:A:9:LEU:HG	1:A:11:VAL:HG22	1.81	0.62
1:A:18:ARG:NE	1:A:35:GLU:HB3	2.15	0.62
2:D:173:ASP:OD1	2:D:190:LYS:HE2	2.00	0.62
1:B:17:MET:HE2	1:B:21:VAL:CG2	2.29	0.61
1:A:11:VAL:HG12	1:A:60:MET:SD	2.40	0.61
1:A:59:ASN:C	1:A:60:MET:HG3	2.19	0.61
1:A:45:LYS:O	1:A:48:ALA:HB3	2.00	0.61
2:C:173:ASP:OD1	2:C:190:LYS:NZ	2.29	0.61
1:A:126:LYS:NZ	2:C:213:CYS:O	2.34	0.61
1:A:14:PHE:O	1:A:18:ARG:HG3	2.00	0.60
1:B:9:LEU:HG	1:B:11:VAL:HG22	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:LYS:HA	1:B:111:PHE:CD1	2.37	0.60
1:B:126:LYS:NZ	2:D:213:CYS:O	2.29	0.60
1:A:40:VAL:O	1:A:44:ASN:N	2.28	0.60
1:B:7:LYS:HD3	1:B:51:TYR:CD1	2.37	0.60
2:C:172:VAL:CG1	2:C:190:LYS:HG2	2.33	0.59
1:A:120:LEU:HB3	1:A:124:PHE:CE2	2.38	0.59
1:B:39:GLY:HA3	1:B:63:MET:HB3	1.83	0.59
1:A:107:VAL:HG22	1:A:108:VAL:N	2.17	0.59
1:B:39:GLY:N	1:B:63:MET:O	2.34	0.58
1:A:111:PHE:CD1	1:A:116:LEU:HB2	2.38	0.58
1:A:25:LEU:O	1:A:30:PHE:N	2.33	0.58
1:B:75:ASP:HB3	1:B:78:MET:CE	2.32	0.58
2:D:162:ILE:HB	2:D:199:LEU:HD22	1.86	0.58
1:A:82:PRO:HA	1:A:104:SER:OG	2.03	0.58
1:B:100:GLN:NE2	2:D:207:ASP:OD1	2.32	0.58
1:B:14:PHE:CE2	1:B:16:THR:HB	2.39	0.58
1:B:43:LEU:HD12	1:B:63:MET:CE	2.33	0.57
1:A:53:PHE:HE1	1:A:84:LEU:CB	2.17	0.57
1:A:38:ASP:O	1:A:42:ALA:N	2.30	0.57
2:C:213:CYS:HA	2:C:216:ILE:O	2.04	0.57
2:C:172:VAL:O	2:C:176:GLU:HB3	2.05	0.57
1:A:39:GLY:O	1:A:43:LEU:HB2	2.05	0.56
1:B:42:ALA:O	1:B:46:LEU:N	2.36	0.56
1:B:110:PRO:HA	3:B:135:HOH:O	2.04	0.56
2:C:182:LEU:HD11	2:C:211:VAL:HB	1.86	0.56
1:A:9:LEU:HD11	1:A:36:ALA:HB2	1.86	0.56
2:D:188:VAL:HG13	2:D:195:LEU:HD11	1.87	0.56
1:A:98:ALA:HB1	1:A:103:ALA:HB3	1.87	0.56
1:A:4:LYS:HA	1:A:30:PHE:CD2	2.41	0.56
1:B:42:ALA:HA	1:B:45:LYS:HB2	1.88	0.55
1:A:64:ASP:O	1:A:68:LEU:HB2	2.07	0.55
1:A:93:GLU:H	1:A:93:GLU:CD	2.09	0.55
1:A:49:GLY:HA2	3:A:145:HOH:O	2.07	0.54
1:B:39:GLY:O	1:B:43:LEU:N	2.34	0.54
1:A:65:GLY:O	1:A:68:LEU:HB3	2.08	0.54
1:A:37:GLU:HB2	3:A:178:HOH:O	2.07	0.54
2:C:218:ALA:HA	2:C:221:ILE:HD12	1.89	0.54
2:D:162:ILE:HD11	2:D:212:LEU:HD12	1.89	0.53
1:A:73:ARG:NH1	1:A:80:ALA:HA	2.23	0.53
2:C:188:VAL:HG13	2:C:195:LEU:HD11	1.89	0.53
1:A:7:LYS:HD3	1:A:51:TYR:CE1	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:165:SER:C	2:C:166:ARG:HG3	2.29	0.53
2:D:179:LEU:HB3	2:D:185:LEU:HD11	1.89	0.53
1:B:91:LYS:O	1:B:95:ILE:HG13	2.08	0.53
1:B:4:LYS:HE3	1:B:30:PHE:CZ	2.45	0.52
1:A:124:PHE:HD1	1:A:129:MET:CE	2.21	0.52
1:B:16:THR:O	1:B:19:ARG:HB3	2.10	0.52
1:B:39:GLY:CA	1:B:63:MET:HB3	2.40	0.52
1:B:8:PHE:HD2	1:B:55:ILE:HG13	1.75	0.52
2:C:166:ARG:CZ	2:C:220:GLN:HG3	2.39	0.52
2:C:202:ASP:OD1	2:C:203:ILE:HG22	2.10	0.52
1:B:17:MET:O	1:B:18:ARG:C	2.45	0.52
1:A:109:LYS:HA	1:A:111:PHE:CE2	2.45	0.51
1:A:55:ILE:HG23	1:A:86:VAL:CG2	2.39	0.51
1:B:84:LEU:HD12	1:B:105:GLY:C	2.30	0.51
1:B:106:TYR:O	1:B:119:LYS:NZ	2.30	0.51
1:B:40:VAL:N	1:B:63:MET:HB3	2.26	0.51
1:A:95:ILE:HG23	2:C:214:PHE:HE2	1.76	0.51
1:B:13:ASP:N	1:B:13:ASP:OD1	2.34	0.51
1:B:93:GLU:CD	1:B:93:GLU:H	2.14	0.51
2:C:182:LEU:HD11	2:C:211:VAL:CG1	2.41	0.51
1:A:27:GLU:O	1:A:27:GLU:HG3	2.09	0.51
1:B:55:ILE:CG2	1:B:86:VAL:HG23	2.41	0.51
1:B:75:ASP:O	1:B:76:GLY:C	2.47	0.51
2:C:174:LEU:O	2:C:178:GLU:N	2.44	0.51
1:B:84:LEU:HD12	1:B:106:TYR:HA	1.92	0.51
1:A:41:ASP:O	1:A:45:LYS:HB2	2.11	0.50
2:C:179:LEU:CB	2:C:185:LEU:HD11	2.41	0.50
2:D:174:LEU:HG	2:D:175:LEU:N	2.24	0.50
1:B:53:PHE:HE1	1:B:84:LEU:HB3	1.76	0.50
1:A:70:LYS:HE3	3:A:182:HOH:O	2.10	0.50
1:A:66:LEU:HA	1:A:69:LEU:HB3	1.93	0.50
1:B:55:ILE:HG23	1:B:86:VAL:HG23	1.93	0.49
2:D:159:PRO:HG2	2:D:226:VAL:HB	1.95	0.49
1:A:6:LEU:HD21	1:A:53:PHE:HB2	1.94	0.49
1:A:124:PHE:CD1	1:A:129:MET:HE2	2.40	0.49
1:A:42:ALA:O	1:A:46:LEU:HG	2.11	0.49
1:B:52:GLY:O	1:B:82:PRO:HG2	2.13	0.49
1:B:43:LEU:HD12	1:B:63:MET:SD	2.51	0.49
1:B:90:ALA:HB2	1:B:108:VAL:HG21	1.94	0.49
1:B:84:LEU:HD12	1:B:106:TYR:N	2.27	0.49
1:A:122:LYS:HA	1:A:125:GLU:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:174:LEU:HA	2:C:177:GLU:HB2	1.94	0.49
1:B:6:LEU:CD2	1:B:53:PHE:HD2	2.22	0.49
1:B:4:LYS:HE3	1:B:30:PHE:CE1	2.47	0.48
1:B:25:LEU:HD22	1:B:30:PHE:HB2	1.95	0.48
1:A:94:ASN:ND2	3:A:149:HOH:O	2.33	0.48
2:C:179:LEU:HB3	2:C:185:LEU:HD11	1.95	0.48
1:B:88:ALA:HA	1:B:109:LYS:HE2	1.95	0.48
1:B:101:ALA:HB2	3:B:154:HOH:O	2.13	0.48
1:B:107:VAL:CG2	1:B:108:VAL:N	2.77	0.48
1:A:109:LYS:HA	1:A:111:PHE:HD2	1.73	0.48
1:A:6:LEU:HD21	1:A:53:PHE:CD2	2.48	0.48
1:B:122:LYS:CE	2:D:215:VAL:HG13	2.34	0.48
2:C:203:ILE:HG12	2:C:208:ILE:HG13	1.96	0.47
1:A:54:VAL:HG12	1:A:56:SER:CB	2.32	0.47
1:B:3:ASP:O	1:B:5:GLU:N	2.48	0.47
1:A:66:LEU:O	1:A:70:LYS:N	2.45	0.47
1:A:9:LEU:HD13	1:A:51:TYR:CE1	2.50	0.47
2:D:174:LEU:O	2:D:174:LEU:HD12	2.14	0.47
1:A:24:LEU:O	1:A:25:LEU:C	2.52	0.47
1:A:38:ASP:HB2	1:A:61:PRO:O	2.15	0.47
1:B:39:GLY:C	1:B:63:MET:HB3	2.35	0.47
1:A:43:LEU:HD22	1:A:63:MET:SD	2.55	0.47
1:A:14:PHE:CD2	1:A:17:MET:HB2	2.50	0.47
1:B:84:LEU:HD12	1:B:106:TYR:CA	2.44	0.47
1:B:88:ALA:CA	1:B:109:LYS:HE2	2.45	0.47
2:C:215:VAL:HG12	2:C:216:ILE:CD1	2.41	0.47
1:B:7:LYS:HD3	1:B:51:TYR:CE1	2.51	0.46
1:B:109:LYS:HA	1:B:111:PHE:HD1	1.78	0.46
1:B:6:LEU:HD21	1:B:53:PHE:CD2	2.43	0.46
2:C:166:ARG:HH22	2:C:220:GLN:HA	1.72	0.46
1:A:6:LEU:HD23	1:A:8:PHE:CZ	2.50	0.46
1:A:96:ILE:HD11	2:C:203:ILE:HD12	1.98	0.46
1:A:13:ASP:OD1	1:A:13:ASP:N	2.32	0.46
1:A:43:LEU:HD13	1:A:68:LEU:HD12	1.97	0.46
2:D:161:ARG:HB2	2:D:226:VAL:CG2	2.42	0.46
1:A:34:GLU:CG	1:A:35:GLU:N	2.78	0.46
1:A:84:LEU:HD13	1:A:123:ILE:CD1	2.40	0.46
1:B:3:ASP:C	1:B:5:GLU:H	2.19	0.46
1:A:108:VAL:O	1:A:111:PHE:HD2	1.99	0.46
1:B:53:PHE:HE1	1:B:84:LEU:CB	2.29	0.46
1:B:85:MET:HE3	1:B:85:MET:HB3	1.60	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:ALA:HA	1:B:109:LYS:HG3	1.98	0.45
1:B:72:ILE:HA	1:B:78:MET:HE3	1.99	0.45
1:B:6:LEU:CD2	1:B:53:PHE:CD2	3.00	0.45
1:A:121:ASN:O	1:A:124:PHE:HB2	2.17	0.45
1:A:40:VAL:CG2	1:A:62:ASN:HB3	2.46	0.45
1:B:18:ARG:HD2	1:B:35:GLU:CD	2.36	0.45
2:D:212:LEU:O	2:D:215:VAL:N	2.37	0.45
1:B:66:LEU:CD1	1:B:69:LEU:HD23	2.41	0.45
2:D:203:ILE:HG22	2:D:207:ASP:HB2	1.99	0.45
1:B:98:ALA:O	1:B:103:ALA:N	2.37	0.45
1:B:78:MET:HB2	1:B:78:MET:HE2	1.70	0.45
2:D:158:SER:N	2:D:225:THR:CG2	2.80	0.45
1:A:107:VAL:CG2	1:A:108:VAL:N	2.80	0.44
1:B:86:VAL:CG1	1:B:87:THR:N	2.80	0.44
1:A:17:MET:O	1:A:18:ARG:C	2.52	0.44
2:D:165:SER:HB3	2:D:166:ARG:HG3	1.99	0.44
1:A:9:LEU:HG	1:A:11:VAL:CG2	2.48	0.44
2:C:195:LEU:HD12	2:C:195:LEU:HA	1.71	0.44
1:A:25:LEU:CD2	1:A:116:LEU:HD21	2.48	0.44
1:B:84:LEU:CD1	1:B:106:TYR:HA	2.48	0.44
1:B:119:LYS:O	1:B:120:LEU:C	2.52	0.44
1:A:115:THR:O	1:A:116:LEU:C	2.53	0.44
1:A:127:LEU:HD12	1:A:127:LEU:HA	1.50	0.44
1:A:124:PHE:CD1	1:A:129:MET:CE	2.99	0.44
1:B:17:MET:HE1	1:B:20:ILE:CG2	2.48	0.44
1:B:3:ASP:O	1:B:6:LEU:N	2.40	0.44
1:B:117:GLU:O	1:B:118:GLU:C	2.56	0.44
1:B:7:LYS:O	1:B:7:LYS:HG2	2.17	0.44
2:C:204:ALA:O	2:C:205:GLU:C	2.56	0.44
1:B:43:LEU:CD1	1:B:63:MET:SD	3.06	0.43
1:B:86:VAL:HG12	1:B:87:THR:N	2.33	0.43
2:D:167:LEU:HD11	2:D:195:LEU:HB3	1.99	0.43
2:D:183:THR:OG1	2:D:200:PRO:HG2	2.18	0.43
1:A:55:ILE:CG2	1:A:86:VAL:CG2	2.97	0.43
1:A:39:GLY:HA3	1:A:63:MET:O	2.18	0.43
2:D:183:THR:HG23	2:D:184:THR:N	2.33	0.43
1:B:75:ASP:CB	1:B:78:MET:HE2	2.46	0.43
1:A:68:LEU:O	1:A:72:ILE:HG13	2.19	0.43
1:B:115:THR:O	1:B:116:LEU:C	2.56	0.43
1:B:83:VAL:HG12	1:B:85:MET:SD	2.59	0.43
2:C:203:ILE:HG13	2:C:207:ASP:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:VAL:O	1:B:111:PHE:HD1	2.02	0.43
1:B:54:VAL:HG12	1:B:56:SER:HB2	1.99	0.43
1:B:17:MET:HE3	1:B:21:VAL:HG23	1.98	0.43
2:C:171:GLU:O	2:C:175:LEU:HB2	2.18	0.42
2:C:175:LEU:HA	2:C:175:LEU:HD23	1.62	0.42
2:C:160:ARG:HA	2:C:224:GLU:O	2.19	0.42
2:C:167:LEU:CD1	2:C:195:LEU:HB2	2.49	0.42
1:B:17:MET:CE	1:B:20:ILE:HB	2.50	0.42
1:B:40:VAL:HG23	1:B:63:MET:HB2	2.01	0.42
2:D:165:SER:C	2:D:166:ARG:HG3	2.39	0.42
2:C:191:GLY:O	2:C:192:ALA:C	2.55	0.42
2:C:161:ARG:HG3	2:C:162:ILE:N	2.35	0.42
2:C:179:LEU:HG	2:C:212:LEU:HD21	2.00	0.42
2:C:188:VAL:O	2:C:188:VAL:HG12	2.19	0.42
2:C:182:LEU:HD11	2:C:211:VAL:HG11	2.01	0.42
1:A:81:LEU:HD12	1:A:81:LEU:HA	1.91	0.42
1:A:98:ALA:HB1	1:A:103:ALA:CB	2.48	0.41
1:B:32:ASN:HD22	1:B:32:ASN:C	2.23	0.41
2:D:167:LEU:CD1	2:D:195:LEU:HB3	2.50	0.41
2:D:164:LEU:HD22	2:D:216:ILE:HD11	2.02	0.41
2:D:212:LEU:C	2:D:214:PHE:N	2.73	0.41
1:A:18:ARG:O	1:A:22:ARG:HB2	2.21	0.41
1:A:3:ASP:C	1:A:5:GLU:H	2.23	0.41
1:B:9:LEU:HG	1:B:11:VAL:CG2	2.51	0.41
1:A:17:MET:CE	1:A:21:VAL:CG2	2.98	0.41
1:B:84:LEU:CD1	1:B:106:TYR:CA	2.99	0.41
2:C:160:ARG:NE	2:C:223:PHE:HB3	2.34	0.41
2:D:211:VAL:O	2:D:214:PHE:HB2	2.21	0.41
1:B:49:GLY:HA3	3:B:148:HOH:O	2.20	0.41
2:D:182:LEU:HA	2:D:182:LEU:HD12	1.85	0.41
2:D:209:THR:O	2:D:213:CYS:SG	2.79	0.41
1:A:122:LYS:HE2	2:C:171:GLU:OE2	2.20	0.41
1:B:17:MET:HE3	1:B:21:VAL:N	2.36	0.41
2:D:161:ARG:NH1	2:D:198:ILE:HD11	2.36	0.41
1:A:17:MET:CE	1:A:21:VAL:HG23	2.51	0.40
1:B:75:ASP:CB	1:B:78:MET:CE	2.99	0.40
2:C:182:LEU:HD11	2:C:211:VAL:CB	2.49	0.40
2:C:209:THR:O	2:C:213:CYS:SG	2.79	0.40
1:A:60:MET:HA	1:A:61:PRO:HD3	1.90	0.40
2:D:162:ILE:HG23	2:D:162:ILE:O	2.21	0.40
1:B:113:ALA:O	1:B:114:ALA:C	2.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:161:ARG:HG2	2:D:162:ILE:N	2.36	0.40
1:B:17:MET:C	1:B:19:ARG:N	2.73	0.40
2:C:199:LEU:HA	2:C:200:PRO:HD2	1.92	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	126/128 (98%)	119 (94%)	6 (5%)	1 (1%)	22	15
1	B	126/128 (98%)	112 (89%)	11 (9%)	3 (2%)	7	2
2	C	65/74 (88%)	61 (94%)	4 (6%)	0	100	100
2	D	67/74 (90%)	64 (96%)	3 (4%)	0	100	100
All	All	384/404 (95%)	356 (93%)	24 (6%)	4 (1%)	18	10

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	4	LYS
1	B	79	SER
1	A	79	SER
1	B	76	GLY

### 5.3.2 Protein sidechains [i](#)

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	95/102 (93%)	84 (88%)	11 (12%)	6	3
1	B	99/102 (97%)	85 (86%)	14 (14%)	4	2
2	C	55/64 (86%)	48 (87%)	7 (13%)	5	3
2	D	57/64 (89%)	49 (86%)	8 (14%)	4	2
All	All	306/332 (92%)	266 (87%)	40 (13%)	5	2

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	5	GLU
1	A	13	ASP
1	A	37	GLU
1	A	60	MET
1	A	78	MET
1	A	104	SER
1	A	111	PHE
1	A	119	LYS
1	A	127	LEU
1	A	129	MET
1	B	4	LYS
1	B	5	GLU
1	B	7	LYS
1	B	15	SER
1	B	22	ARG
1	B	32	ASN
1	B	38	ASP
1	B	47	GLN
1	B	78	MET
1	B	91	LYS
1	B	104	SER
1	B	111	PHE
1	B	126	LYS
1	B	127	LEU
2	C	160	ARG
2	C	161	ARG
2	C	166	ARG
2	C	176	GLU
2	C	203	ILE
2	C	208	ILE

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Mol	Chain	Res	Type
2	C	216	ILE
2	D	171	GLU
2	D	172	VAL
2	D	178	GLU
2	D	183	THR
2	D	199	LEU
2	D	203	ILE
2	D	206	ASP
2	D	217	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	B	23	ASN
1	B	32	ASN
1	B	44	ASN
1	B	121	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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	128/128 (100%)	1.57	26 (20%) <b>1</b> <b>1</b>	17, 33, 65, 83	0
1	B	128/128 (100%)	1.71	33 (25%) <b>1</b> <b>1</b>	20, 32, 70, 85	0
2	C	67/74 (90%)	1.57	17 (25%) <b>1</b> <b>1</b>	21, 36, 55, 75	0
2	D	69/74 (93%)	1.71	20 (28%) <b>1</b> <b>1</b>	23, 37, 64, 78	0
All	All	392/404 (97%)	1.64	96 (24%) <b>1</b> <b>1</b>	17, 35, 67, 85	0

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	169	ALA	6.7
1	B	3	ASP	6.3
1	A	128	GLY	6.1
1	B	49	GLY	5.9
2	D	226	VAL	5.2
1	A	48	ALA	5.1
1	B	128	GLY	5.0
2	D	170	GLY	4.8
1	A	127	LEU	4.6
1	B	48	ALA	4.5
2	C	225	THR	4.2
1	B	77	ALA	4.2
1	B	75	ASP	4.1
2	D	158	SER	4.1
1	B	29	GLY	3.9
1	A	47	GLN	3.9
1	A	2	ALA	3.8
1	B	76	GLY	3.7
1	B	5	GLU	3.6
1	B	2	ALA	3.5
1	B	129	MET	3.3

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Mol	Chain	Res	Type	RSRZ
2	D	173	ASP	3.3
2	C	186	THR	3.2
1	A	129	MET	3.2
1	A	3	ASP	3.2
1	A	124	PHE	3.2
1	B	50	GLY	3.1
1	A	121	ASN	3.1
2	D	159	PRO	3.1
2	C	219	ASP	3.0
2	D	225	THR	3.0
1	A	75	ASP	2.9
1	B	20	ILE	2.9
2	C	169	ALA	2.8
2	C	159	PRO	2.8
1	A	10	VAL	2.8
1	B	89	GLU	2.8
2	C	189	VAL	2.8
1	B	84	LEU	2.7
2	D	189	VAL	2.7
2	D	208	ILE	2.7
1	B	120	LEU	2.7
1	B	54	VAL	2.7
1	A	49	GLY	2.7
1	B	127	LEU	2.7
1	A	110	PRO	2.6
1	B	44	ASN	2.6
2	C	179	LEU	2.6
2	D	192	ALA	2.6
1	A	77	ALA	2.5
1	B	55	ILE	2.5
2	D	174	LEU	2.5
1	B	74	ALA	2.5
1	A	21	VAL	2.5
2	D	168	LYS	2.4
1	B	79	SER	2.4
2	D	211	VAL	2.4
1	B	114	ALA	2.4
2	D	179	LEU	2.4
2	C	175	LEU	2.4
1	B	78	MET	2.4
2	D	198	ILE	2.4
2	C	212	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	186	THR	2.3
2	D	224	GLU	2.3
2	C	174	LEU	2.3
2	C	184	THR	2.3
1	B	4	LYS	2.3
1	A	32	ASN	2.3
2	C	213	CYS	2.3
2	D	212	LEU	2.2
1	A	76	GLY	2.2
1	B	80	ALA	2.2
1	B	43	LEU	2.2
1	A	112	THR	2.2
1	A	84	LEU	2.2
2	D	164	LEU	2.2
1	B	15	SER	2.2
1	A	46	LEU	2.1
1	A	11	VAL	2.1
1	B	72	ILE	2.1
1	B	27	GLU	2.1
1	A	97	ALA	2.1
2	C	208	ILE	2.1
2	C	173	ASP	2.1
1	B	10	VAL	2.1
1	B	93	GLU	2.1
1	A	116	LEU	2.0
1	B	83	VAL	2.0
1	A	15	SER	2.0
1	A	31	ASN	2.0
2	C	187	ASP	2.0
2	C	216	ILE	2.0
2	D	185	LEU	2.0
1	A	54	VAL	2.0
2	C	170	GLY	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 [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.