Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:10 PM 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)

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

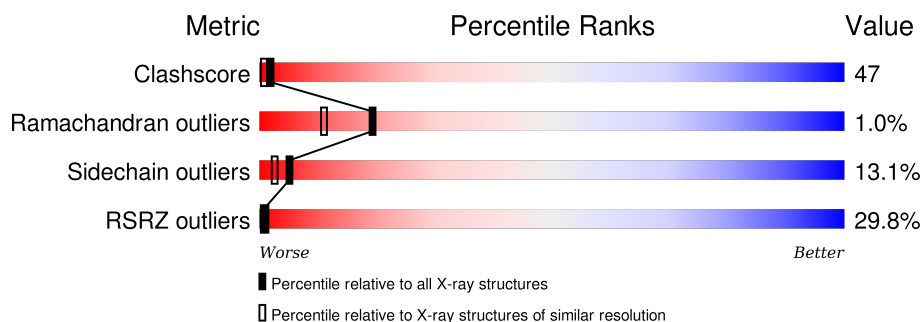|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.00 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	Percentile Ranks	Value
Clashscore		47
Ramachandran outliers		1.0%
Sidechain outliers		13.1%
RSRZ outliers		29.8%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (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 >=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 <=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	27% / 30% 52% 16% •
1	B	128	30% / 24% 63% 10% •
2	C	74	28% / 24% 46% 19% • 9%
2	D	74	31% / 32% 41% 19% • 7%

2 Entry composition (i)

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.

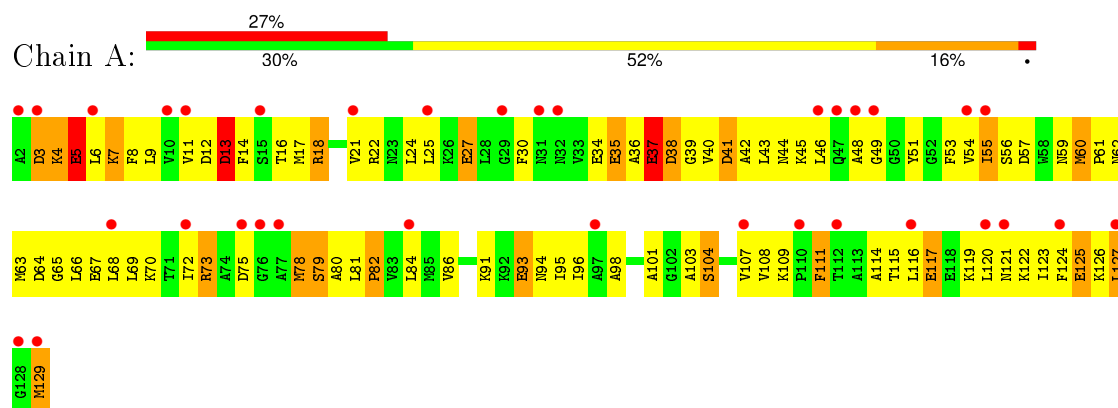| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	67	Total	C	N	O	S	0	0	0
			501	317	80	103	1			
2	D	69	Total	C	N	O	S	0	0	0
			514	325	82	106	1			

- Molecule 3 is water.

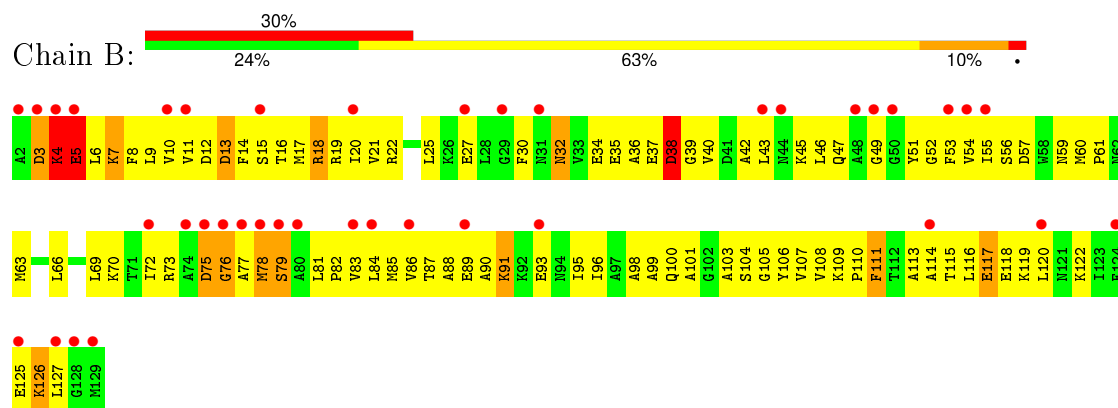| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	54	Total	O	0	0
			54	54		
3	B	32	Total	O	0	0
			32	32		
3	C	27	Total	O	0	0
			27	27		
3	D	11	Total	O	0	0
			11	11		

3 Residue-property plots ⓘ

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.
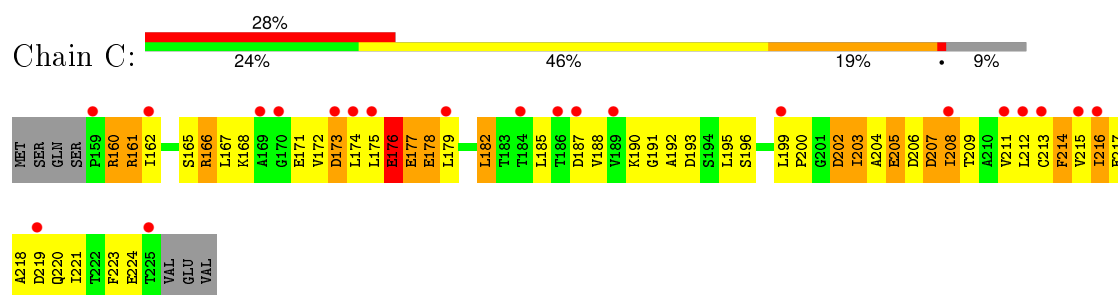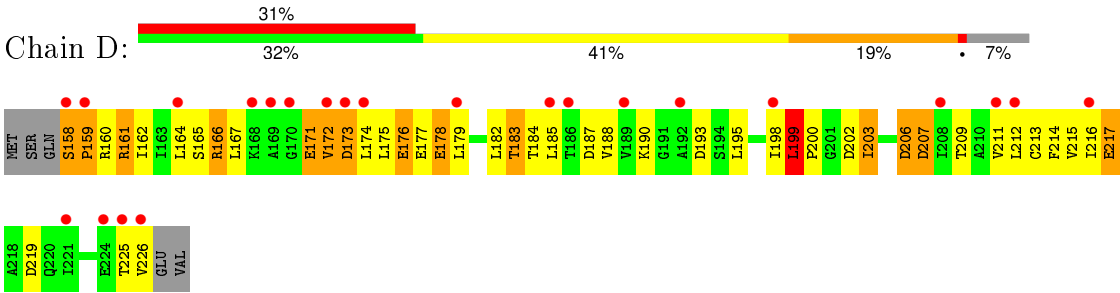
• Molecule 1: CHEY

Chain A:

• Molecule 1: CHEY

Chain B:

• Molecule 2: CHEA

Chain C:

• Molecule 2: CHEA

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	10.71 (at 1.95Å)	Xtriage
Refinement program	TNT V. 5-F	Depositor
R, R_{free}	0.217 , (Not available) 0.226 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	8.3	Xtriage
Anisotropy	1.127	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 348.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.30, < L^2 > = 0.13$	Xtriage
Outliers	0 of 30701 reflections	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	3058	wwPDB-VP
Average B, all atoms (Å^2)	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.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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 (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	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
2:D:161:ARG:HB2	2:D:226:VAL:HG22	1.70	0.73
1:A:25:LEU:HB3	1:A:30:PHE:HB2	1.71	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:B:17:MET:HE2	1:B:21:VAL:HG23	1.72	0.71
1:A:72:ILE:HG23	1:A:78:MET:HB3	1.73	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:198:ILE:N	2:D:198:ILE:HD12	2.10	0.66
2:D:173:ASP:O	2:D:176:GLU:HB3	1.94	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:B:69:LEU:O	1:B:72:ILE:HB	1.96	0.65
1:A:101:ALA:HB2	3:A:151:HOH:O	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
2:C:168:LYS:O	2:C:171:GLU:HB2	1.98	0.63
1:B:96:ILE:O	1:B:99:ALA:N	2.31	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
2:D:162:ILE:HB	2:D:199:LEU:HD22	1.86	0.58
1:B:75:ASP:HB3	1:B:78:MET:CE	2.32	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
1:A:9:LEU:HD11	1:A:36:ALA:HB2	1.86	0.56
2:C:182:LEU:HD11	2:C:211:VAL:HB	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
2:C:218:ALA:HA	2:C:221:ILE:HD12	1.89	0.54
1:A:37:GLU:HB2	3:A:178:HOH:O	2.07	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:B:16:THR:O	1:B:19:ARG:HB3	2.10	0.52
1:A:124:PHE:HD1	1:A:129:MET:CE	2.21	0.52
2:C:166:ARG:CZ	2:C:220:GLN:HG3	2.39	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: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:B:84:LEU:HD12	1:B:105:GLY:C	2.30	0.51
1:A:55:ILE:HG23	1:A:86:VAL:CG2	2.39	0.51
1:B:106:TYR:O	1:B:119:LYS:NZ	2.30	0.51
1:A:95:ILE:HG23	2:C:214:PHE:HE2	1.76	0.51
1:B:40:VAL:N	1:B:63:MET:HB3	2.26	0.51
2:C:182:LEU:HD11	2:C:211:VAL:CG1	2.41	0.51
1:B:93:GLU:CD	1:B:93:GLU:H	2.14	0.51
1:B:13:ASP:N	1:B:13:ASP:OD1	2.34	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:42:ALA:O	1:A:46:LEU:HG	2.11	0.49
1:A:124:PHE:CD1	1:A:129:MET:HE2	2.40	0.49
1:B:90:ALA:HB2	1:B:108:VAL:HG21	1.94	0.49
1:B:43:LEU:HD12	1:B:63:MET:SD	2.51	0.49
1:B:52:GLY:O	1:B:82:PRO:HG2	2.13	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:107:VAL:CG2	1:B:108:VAL:N	2.77	0.48
1:B:101:ALA:HB2	3:B:154:HOH:O	2.13	0.48
1:B:122:LYS:CE	2:D:215:VAL:HG13	2.34	0.48
1:A:6:LEU:HD21	1:A:53:PHE:CD2	2.48	0.48
1:A:109:LYS:HA	1:A:111:PHE:HD2	1.73	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:9:LEU:HD13	1:A:51:TYR:CE1	2.50	0.47
1:A:66:LEU:O	1:A:70:LYS:N	2.45	0.47
2:D:174:LEU:O	2:D:174:LEU:HD12	2.14	0.47
1:A:38:ASP:HB2	1:A:61:PRO:O	2.15	0.47
1:A:24:LEU:O	1:A:25:LEU:C	2.52	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
2:C:215:VAL:HG12	2:C:216:ILE:CD1	2.41	0.47
1:B:84:LEU:HD12	1:B:106:TYR:CA	2.44	0.47
1:A:14:PHE:CD2	1:A:17:MET:HB2	2.50	0.47
1:B:88:ALA:CA	1:B:109:LYS:HE2	2.45	0.47
1:B:7:LYS:HD3	1:B:51:TYR:CE1	2.51	0.46
1:B:6:LEU:HD21	1:B:53:PHE:CD2	2.43	0.46
1:B:109:LYS:HA	1:B:111:PHE:HD1	1.78	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
2:D:161:ARG:HB2	2:D:226:VAL:CG2	2.42	0.46
1:A:43:LEU:HD13	1:A:68:LEU:HD12	1.97	0.46
1:A:13:ASP:OD1	1:A:13:ASP:N	2.32	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:34:GLU:CG	1:A:35:GLU:N	2.78	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
2:D:212:LEU:O	2:D:215:VAL:N	2.37	0.45
1:B:18:ARG:HD2	1:B:35:GLU:CD	2.36	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: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:B:17:MET:HE1	1:B:20:ILE:CG2	2.48	0.44
1:A:124:PHE:CD1	1:A:129:MET:CE	2.99	0.44
1:B:3:ASP:O	1:B:6:LEU:N	2.40	0.44
1:B:7:LYS:O	1:B:7:LYS:HG2	2.17	0.44
1:B:117:GLU:O	1:B:118:GLU:C	2.56	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
2:D:167:LEU:HD11	2:D:195:LEU:HB3	1.99	0.43
1:B:86:VAL:HG12	1:B:87:THR:N	2.33	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
2:C:203:ILE:HG13	2:C:207:ASP:HB2	2.00	0.43
1:B:83:VAL:HG12	1:B:85:MET:SD	2.59	0.43
1:B:115:THR:O	1:B:116:LEU:C	2.56	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:167:LEU:CD1	2:C:195:LEU:HB2	2.49	0.42
2:C:160:ARG:HA	2:C:224:GLU:O	2.19	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:188:VAL:O	2:C:188:VAL:HG12	2.19	0.42
2:C:179:LEU:HG	2:C:212:LEU:HD21	2.00	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
2:D:167:LEU:CD1	2:D:195:LEU:HB3	2.50	0.41
1:A:98:ALA:HB1	1:A:103:ALA:CB	2.48	0.41
2:D:164:LEU:HD22	2:D:216:ILE:HD11	2.02	0.41
1:B:32:ASN:HD22	1:B:32:ASN:C	2.23	0.41
2:D:212:LEU:C	2:D:214:PHE:N	2.73	0.41
1:B:9:LEU:HG	1:B:11:VAL:CG2	2.51	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
2:D:211:VAL:O	2:D:214:PHE:HB2	2.21	0.41
1:B:84:LEU:CD1	1:B:106:TYR:CA	2.99	0.41
1:A:17:MET:CE	1:A:21:VAL:CG2	2.98	0.41
2:C:160:ARG:NE	2:C:223:PHE:HB3	2.34	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
2:D:161:ARG:NH1	2:D:198:ILE:HD11	2.36	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:C:209:THR:O	2:C:213:CYS:SG	2.79	0.40
1:B:75:ASP:CB	1:B:78:MET:CE	2.99	0.40
1:A:17:MET:CE	1:A:21:VAL:HG23	2.51	0.40
2:C:182:LEU:HD11	2:C:211:VAL:CB	2.49	0.40
2:D:162:ILE:HG23	2:D:162:ILE:O	2.21	0.40
1:A:60:MET:HA	1:A:61:PRO:HD3	1.90	0.40
2:D:161:ARG:HG2	2:D:162:ILE:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:ALA:O	1:B:114:ALA:C	2.60	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%)	24	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%)	19	11

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%)		7	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 (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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^2)	Q<0.9
1	A	128/128 (100%)	1.68	34 (26%)	1	1	17, 33, 65, 83	0
1	B	128/128 (100%)	1.82	39 (30%)	1	1	20, 32, 70, 85	0
2	C	67/74 (90%)	1.68	21 (31%)	1	1	21, 36, 55, 75	0
2	D	69/74 (93%)	1.82	23 (33%)	0	1	23, 37, 64, 78	0
All	All	392/404 (97%)	1.75	117 (29%)	1	1	17, 35, 67, 85	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	169	ALA	7.0
1	B	3	ASP	6.5
1	A	128	GLY	6.3
1	B	49	GLY	6.1
2	D	226	VAL	5.5
1	A	48	ALA	5.3
1	B	128	GLY	5.3
2	D	170	GLY	5.0
1	A	127	LEU	4.8
1	B	48	ALA	4.7
1	B	77	ALA	4.4
2	C	225	THR	4.4
1	B	75	ASP	4.3
2	D	158	SER	4.3
1	B	29	GLY	4.1
1	A	2	ALA	4.0
1	A	47	GLN	4.0
1	B	76	GLY	3.8
1	B	2	ALA	3.7
1	B	5	GLU	3.7
1	B	129	MET	3.4

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Mol	Chain	Res	Type	RSRZ
2	D	173	ASP	3.4
2	C	186	THR	3.4
1	A	124	PHE	3.4
1	A	3	ASP	3.4
1	A	129	MET	3.3
1	B	50	GLY	3.3
2	D	159	PRO	3.2
1	A	121	ASN	3.2
2	D	225	THR	3.2
2	C	219	ASP	3.1
1	B	20	ILE	3.1
2	C	169	ALA	3.0
1	A	75	ASP	3.0
1	A	10	VAL	3.0
2	C	189	VAL	3.0
2	D	189	VAL	3.0
2	C	159	PRO	2.9
2	D	208	ILE	2.9
1	B	84	LEU	2.9
1	B	54	VAL	2.9
1	B	89	GLU	2.9
1	B	120	LEU	2.8
1	B	127	LEU	2.8
1	A	49	GLY	2.8
2	C	179	LEU	2.8
2	D	192	ALA	2.8
1	A	110	PRO	2.8
1	B	44	ASN	2.7
1	B	55	ILE	2.7
1	B	74	ALA	2.7
1	A	21	VAL	2.7
1	A	77	ALA	2.7
2	D	174	LEU	2.7
2	D	211	VAL	2.6
1	B	114	ALA	2.6
2	D	179	LEU	2.5
2	D	168	LYS	2.5
2	D	198	ILE	2.5
2	C	175	LEU	2.5
1	B	79	SER	2.5
2	C	212	LEU	2.5
1	B	78	MET	2.5

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Mol	Chain	Res	Type	RSRZ
2	C	174	LEU	2.5
2	D	186	THR	2.5
2	D	212	LEU	2.4
2	C	184	THR	2.4
2	D	224	GLU	2.4
2	C	213	CYS	2.4
1	B	80	ALA	2.4
1	A	32	ASN	2.4
1	B	4	LYS	2.4
1	B	43	LEU	2.4
1	A	76	GLY	2.3
1	A	84	LEU	2.3
2	D	164	LEU	2.3
1	A	11	VAL	2.3
1	A	112	THR	2.3
1	A	46	LEU	2.3
1	B	72	ILE	2.3
1	B	15	SER	2.3
2	C	208	ILE	2.3
1	A	97	ALA	2.3
1	B	10	VAL	2.2
1	B	83	VAL	2.2
2	C	173	ASP	2.2
1	B	27	GLU	2.2
1	A	116	LEU	2.2
2	C	216	ILE	2.2
1	B	124	PHE	2.2
1	A	54	VAL	2.2
2	C	211	VAL	2.2
1	B	93	GLU	2.1
1	A	55	ILE	2.1
2	C	187	ASP	2.1
1	A	15	SER	2.1
2	C	170	GLY	2.1
1	A	68	LEU	2.1
1	A	120	LEU	2.1
2	D	185	LEU	2.1
1	A	6	LEU	2.1
1	B	11	VAL	2.1
1	A	31	ASN	2.1
2	C	162	ILE	2.1
2	C	199	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	72	ILE	2.1
1	A	25	LEU	2.1
1	A	29	GLY	2.1
1	A	107	VAL	2.1
1	B	86	VAL	2.1
1	B	31	ASN	2.0
1	B	125	GLU	2.0
2	D	172	VAL	2.0
1	B	53	PHE	2.0
2	C	215	VAL	2.0
2	D	216	ILE	2.0
2	D	221	ILE	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.