Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:30 AM GMT

PDB ID	:	3M4D
Title	:	Crystal structure of the M113N mutant of alpha-hemolysin
Authors	:	Montoya, M.; Gouaux, E.
Deposited on	:	2010-03-10
Resolution	:	1.90 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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

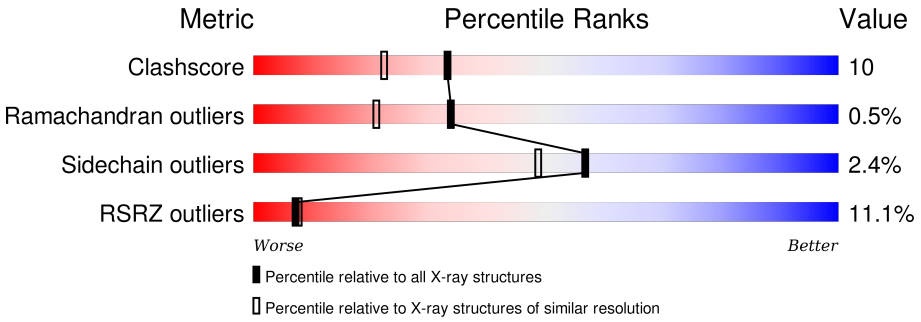
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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	293	11% 81% 18%
1	B	293	13% 81% 18%
1	C	293	11% 80% 18%
1	D	293	14% 77% 22%
1	E	293	10% 83% 16%
1	F	293	9% 83% 15%
1	G	293	10% 77% 20%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 16762 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 Alpha-hemolysin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	293	Total	C	N	O	S	41	0	0
			2338	1465	402	465	6			
1	B	293	Total	C	N	O	S	45	0	0
			2345	1471	402	466	6			
1	C	293	Total	C	N	O	S	59	0	0
			2345	1471	402	466	6			
1	D	293	Total	C	N	O	S	66	0	0
			2345	1471	402	466	6			
1	E	293	Total	C	N	O	S	49	0	0
			2341	1467	402	466	6			
1	F	293	Total	C	N	O	S	62	0	0
			2345	1471	402	466	6			
1	G	293	Total	C	N	O	S	52	0	0
			2345	1471	402	466	6			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	113	ASN	MET	ENGINEERED	UNP P09616
B	113	ASN	MET	ENGINEERED	UNP P09616
C	113	ASN	MET	ENGINEERED	UNP P09616
D	113	ASN	MET	ENGINEERED	UNP P09616
E	113	ASN	MET	ENGINEERED	UNP P09616
F	113	ASN	MET	ENGINEERED	UNP P09616
G	113	ASN	MET	ENGINEERED	UNP P09616

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	45	Total	O	0	0
			45	45		
2	B	52	Total	O	0	0
			52	52		

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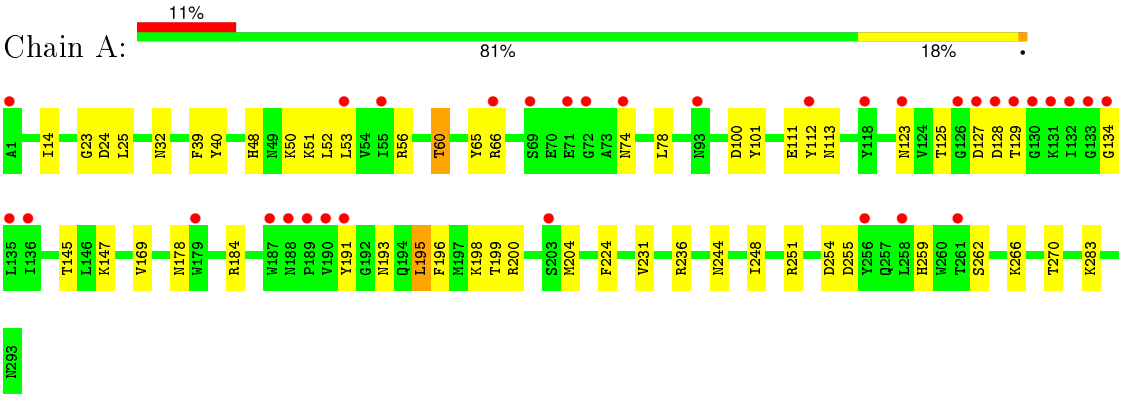
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	52	Total O 52 52	0	0
2	D	48	Total O 48 48	0	0
2	E	46	Total O 46 46	0	0
2	F	54	Total O 54 54	0	0
2	G	61	Total O 61 61	0	0

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 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.

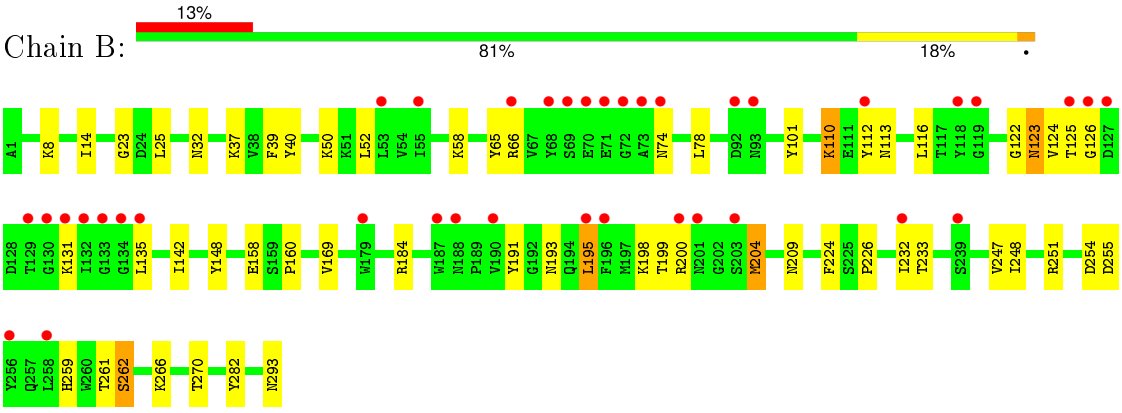
- Molecule 1: Alpha-hemolysin

Chain A:



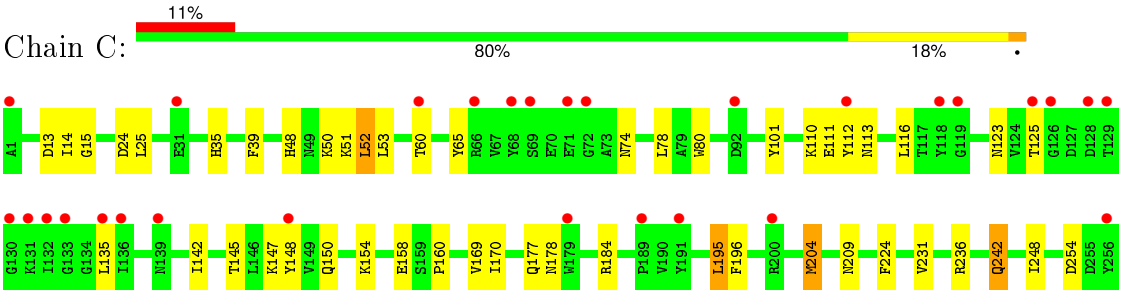
- Molecule 1: Alpha-hemolysin

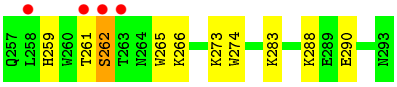
Chain B:



- Molecule 1: Alpha-hemolysin

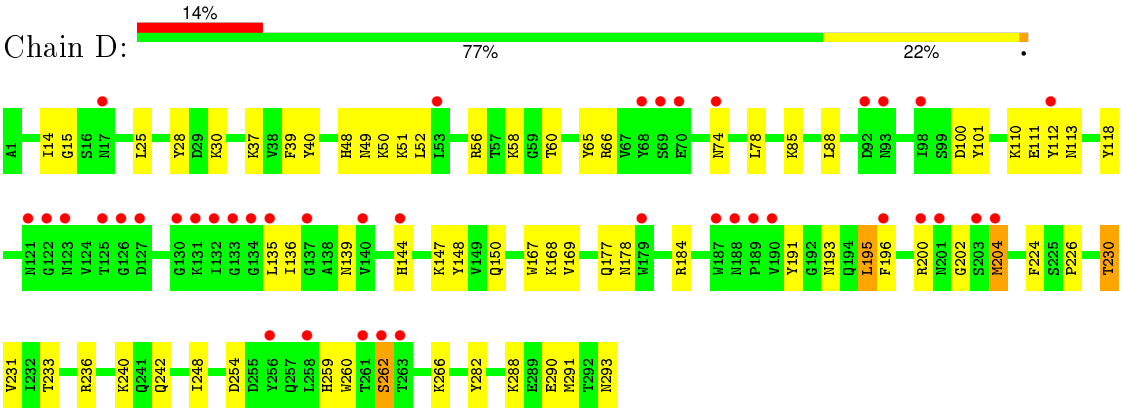
Chain C:





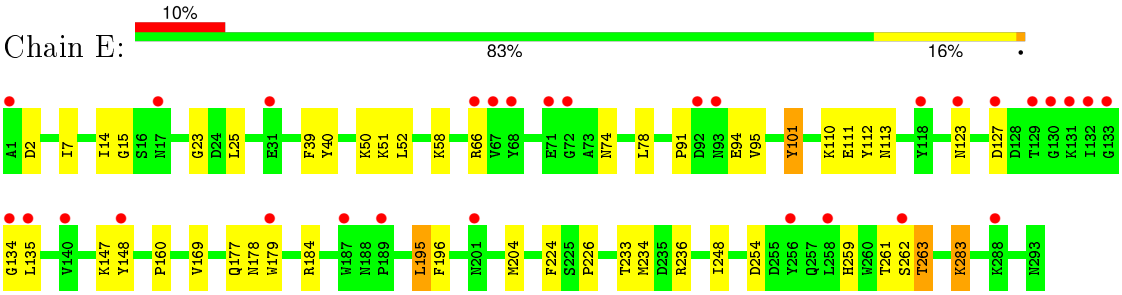
• Molecule 1: Alpha-hemolysin

Chain D:



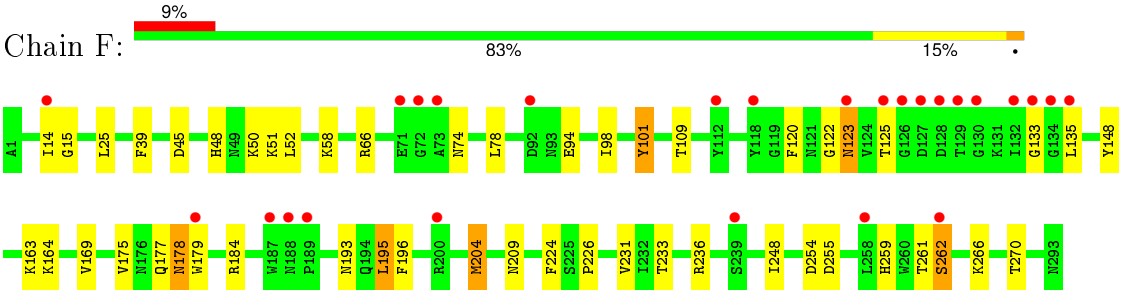
• Molecule 1: Alpha-hemolysin

Chain E:



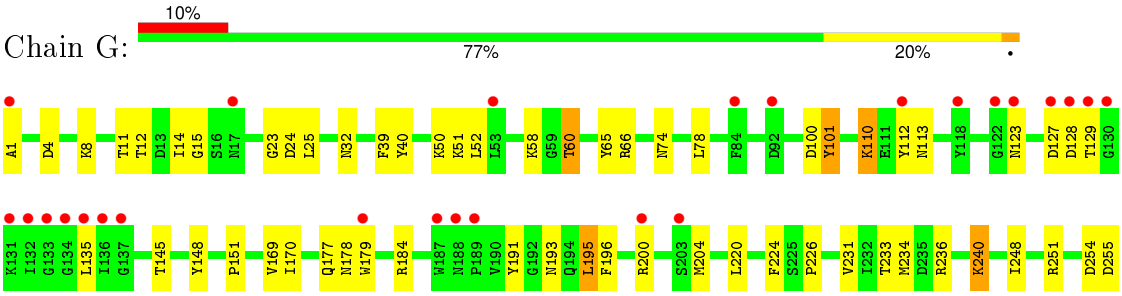
• Molecule 1: Alpha-hemolysin

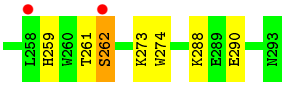
Chain F:



• Molecule 1: Alpha-hemolysin

Chain G:




L258
H259
W260
T261
S262
K273
W274
K288
E289
E290
N293

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	151.15Å 134.59Å 132.90Å 90.00° 90.78° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 19.88 – 1.87	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-1.90) 98.7 (19.88-1.87)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.32 (at 1.87Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.240 , 0.265 0.236 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	21.8	Xtriage
Anisotropy	0.218	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 50.6	EDS
Estimated twinning fraction	0.007 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 215562 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	16762	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.41% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

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	0.32	0/2389	0.61	0/3233
1	B	0.32	0/2397	0.63	0/3244
1	C	0.32	0/2397	0.64	0/3244
1	D	0.33	0/2397	0.63	0/3244
1	E	0.32	0/2393	0.61	0/3238
1	F	0.32	0/2397	0.61	0/3244
1	G	0.33	0/2397	0.64	0/3244
All	All	0.32	0/16767	0.62	0/22691

There are no bond length outliers.

There are no bond angle outliers.

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	2338	0	2260	49	0
1	B	2345	0	2267	56	0
1	C	2345	0	2267	63	0
1	D	2345	0	2267	63	0
1	E	2341	0	2257	36	0
1	F	2345	0	2267	45	0
1	G	2345	0	2267	69	0
2	A	45	0	0	4	0
2	B	52	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	52	0	0	1	0
2	D	48	0	0	2	0
2	E	46	0	0	1	0
2	F	54	0	0	1	0
2	G	61	0	0	1	0
All	All	16762	0	15852	324	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (324) 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:G:123:ASN:HB3	1:G:135:LEU:HB3	1.39	1.01
1:F:123:ASN:HB3	1:F:135:LEU:HB3	1.45	0.96
1:C:160:PRO:HD2	1:D:60:THR:HG21	1.51	0.93
1:B:123:ASN:HB3	1:B:135:LEU:HB3	1.52	0.90
1:A:56:ARG:NH2	1:G:12:THR:HG21	1.87	0.88
1:C:242:GLN:HB2	1:C:283:LYS:HE3	1.56	0.88
1:B:8:LYS:HD2	1:C:13:ASP:HB2	1.59	0.85
1:C:14:ILE:HD11	1:D:39:PHE:HE1	1.41	0.85
1:B:160:PRO:HD2	1:C:60:THR:HG21	1.58	0.84
1:B:160:PRO:CG	1:C:60:THR:HG21	2.07	0.84
1:A:56:ARG:HH22	1:G:12:THR:HG21	1.41	0.84
1:B:160:PRO:HG2	1:C:60:THR:HG21	1.60	0.83
1:A:14:ILE:HD11	1:B:39:PHE:HE1	1.41	0.83
1:C:160:PRO:CD	1:D:60:THR:HG21	2.08	0.82
1:B:199:THR:H	1:B:209:ASN:HD21	1.24	0.82
1:E:14:ILE:HD11	1:F:39:PHE:HE1	1.44	0.82
1:B:160:PRO:CD	1:C:60:THR:HG21	2.11	0.81
1:G:24:ASP:C	1:G:25:LEU:HD12	2.02	0.80
1:C:160:PRO:CG	1:D:60:THR:HG21	2.13	0.79
1:C:123:ASN:HB3	1:C:135:LEU:HB3	1.65	0.79
1:C:125:THR:HG22	1:D:135:LEU:HD13	1.63	0.79
1:A:39:PHE:HE1	1:G:14:ILE:HD11	1.46	0.78
1:D:14:ILE:HD11	1:E:39:PHE:HE1	1.48	0.77
1:E:52:LEU:CD2	1:E:233:THR:HG22	2.16	0.76
1:B:255:ASP:HB3	1:B:270:THR:OG1	1.84	0.76
1:F:125:THR:HG22	1:G:135:LEU:HD13	1.67	0.75
2:B:307:HOH:O	1:C:24:ASP:HB3	1.89	0.73
1:D:100:ASP:HB3	1:D:231:VAL:CG1	2.20	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:ASP:HB3	1:A:231:VAL:HG11	1.70	0.71
1:D:100:ASP:HB3	1:D:231:VAL:HG11	1.71	0.71
1:A:100:ASP:HB3	1:A:231:VAL:CG1	2.21	0.70
1:G:51:LYS:HE3	1:G:236:ARG:HG2	1.74	0.70
1:C:242:GLN:CB	1:C:283:LYS:HE3	2.22	0.69
1:A:24:ASP:HB3	2:A:310:HOH:O	1.92	0.69
1:B:160:PRO:HG2	1:C:60:THR:CG2	2.23	0.69
1:D:52:LEU:CD2	1:D:233:THR:HG22	2.23	0.69
1:G:240:LYS:HB2	1:G:240:LYS:NZ	2.07	0.69
1:B:199:THR:H	1:B:209:ASN:ND2	1.91	0.68
1:E:123:ASN:HB3	1:E:135:LEU:HB3	1.74	0.68
1:F:123:ASN:HD21	1:G:135:LEU:HD11	1.58	0.68
1:F:204:MET:HE1	1:F:209:ASN:HA	1.77	0.67
1:F:14:ILE:HD11	1:G:39:PHE:HE1	1.60	0.67
1:F:123:ASN:ND2	1:G:135:LEU:HD11	2.10	0.66
1:B:52:LEU:CD2	1:B:233:THR:HG22	2.26	0.66
1:C:160:PRO:HG2	1:D:60:THR:HG21	1.77	0.65
1:B:52:LEU:HD23	1:B:233:THR:HG22	1.77	0.65
1:G:25:LEU:HD11	1:G:40:TYR:HE1	1.62	0.65
1:D:52:LEU:HD23	1:D:233:THR:HG22	1.79	0.65
1:E:52:LEU:HD23	1:E:233:THR:HG22	1.78	0.64
1:D:148:TYR:OH	1:E:178:ASN:ND2	2.30	0.64
1:F:178:ASN:HD22	1:F:178:ASN:N	1.95	0.64
1:B:14:ILE:HD11	1:C:39:PHE:HE1	1.63	0.63
1:B:199:THR:N	1:B:209:ASN:HD21	1.97	0.62
1:B:191:TYR:CE2	1:B:200:ARG:HB3	2.34	0.62
1:B:112:TYR:C	1:B:113:ASN:HD22	2.03	0.62
1:D:167:TRP:HH2	1:D:230:THR:HG22	1.63	0.62
1:D:112:TYR:C	1:D:113:ASN:HD22	2.03	0.61
1:F:184:ARG:HD2	1:F:254:ASP:OD2	2.00	0.61
1:B:184:ARG:HD2	1:B:254:ASP:OD2	2.01	0.61
1:B:122:GLY:O	1:B:123:ASN:HB2	2.00	0.61
1:F:123:ASN:OD1	1:G:135:LEU:HD11	2.00	0.61
1:F:14:ILE:HD11	1:F:48:HIS:CE1	2.36	0.60
1:C:50:LYS:NZ	2:C:311:HOH:O	2.34	0.60
1:B:125:THR:HG22	1:B:126:GLY:N	2.16	0.60
1:G:52:LEU:HD23	1:G:233:THR:HG22	1.83	0.60
1:C:170:ILE:HD12	1:C:170:ILE:O	2.01	0.59
1:A:178:ASN:HD22	1:A:178:ASN:N	2.01	0.59
1:A:50:LYS:NZ	2:A:313:HOH:O	2.35	0.59
1:G:52:LEU:CD2	1:G:233:THR:HG22	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:288:LYS:HE2	1:C:290:GLU:OE1	2.02	0.59
1:A:184:ARG:HD2	1:A:254:ASP:OD2	2.03	0.59
1:F:148:TYR:OH	1:G:178:ASN:ND2	2.36	0.58
1:D:184:ARG:HD2	1:D:254:ASP:OD2	2.02	0.58
1:F:14:ILE:HG22	1:F:15:GLY:N	2.19	0.58
1:G:74:ASN:O	1:G:259:HIS:HA	2.04	0.58
1:D:135:LEU:HD12	1:D:136:ILE:H	1.68	0.58
1:A:178:ASN:ND2	1:G:148:TYR:OH	2.37	0.58
1:B:259:HIS:CE1	1:B:266:LYS:HB3	2.39	0.58
1:G:191:TYR:CE2	1:G:200:ARG:HB3	2.39	0.58
1:F:122:GLY:O	1:F:123:ASN:HB2	2.02	0.57
1:D:191:TYR:CE2	1:D:200:ARG:HB3	2.39	0.57
1:E:148:TYR:OH	1:F:178:ASN:ND2	2.37	0.57
1:D:259:HIS:CE1	1:D:266:LYS:HB3	2.39	0.57
1:G:100:ASP:HB3	1:G:231:VAL:CG1	2.35	0.57
1:A:244:ASN:OD1	1:A:283:LYS:HE2	2.04	0.57
1:D:88:LEU:HD13	1:D:230:THR:HG21	1.87	0.56
1:B:148:TYR:OH	1:C:178:ASN:ND2	2.37	0.56
1:F:74:ASN:O	1:F:259:HIS:HA	2.06	0.56
1:G:24:ASP:O	1:G:25:LEU:HD12	2.06	0.56
1:E:177:GLN:O	1:E:179:TRP:HD1	1.88	0.56
1:C:184:ARG:HD2	1:C:254:ASP:OD2	2.05	0.56
1:F:259:HIS:CE1	1:F:266:LYS:HB3	2.40	0.56
1:G:184:ARG:HD2	1:G:254:ASP:OD2	2.05	0.56
1:C:14:ILE:HD11	1:D:39:PHE:CE1	2.31	0.55
1:E:248:ILE:N	1:E:248:ILE:HD12	2.22	0.55
1:C:52:LEU:HD13	1:C:53:LEU:N	2.22	0.55
1:E:184:ARG:HD2	1:E:254:ASP:OD2	2.05	0.55
1:A:111:GLU:HB3	1:A:147:LYS:HB2	1.88	0.55
1:B:204:MET:HE2	1:B:204:MET:H	1.71	0.55
1:C:261:THR:O	1:C:262:SER:HB3	2.06	0.55
1:F:169:VAL:HG21	1:F:224:PHE:CZ	2.41	0.55
1:F:261:THR:O	1:F:262:SER:CB	2.55	0.55
1:G:100:ASP:HB3	1:G:231:VAL:HG11	1.89	0.54
1:E:14:ILE:HD11	1:F:39:PHE:CE1	2.34	0.54
1:A:113:ASN:HB2	1:A:145:THR:HB	1.88	0.54
1:D:195:LEU:HD13	1:D:196:PHE:CE2	2.42	0.54
1:D:135:LEU:HD12	1:D:136:ILE:N	2.22	0.54
1:A:100:ASP:N	1:A:231:VAL:HG13	2.23	0.54
1:A:100:ASP:H	1:A:231:VAL:HG13	1.73	0.54
1:C:273:LYS:HD2	1:C:274:TRP:CE2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:PRO:HG2	1:D:60:THR:CG2	2.37	0.54
1:F:178:ASN:ND2	1:F:178:ASN:N	2.55	0.53
1:B:74:ASN:O	1:B:259:HIS:HA	2.08	0.53
1:F:51:LYS:HG3	1:F:236:ARG:HG2	1.89	0.53
1:D:248:ILE:N	1:D:248:ILE:HD12	2.23	0.53
1:A:32:ASN:O	1:A:251:ARG:NH1	2.39	0.53
1:A:65:TYR:CE1	1:A:78:LEU:HD21	2.44	0.53
1:G:273:LYS:HD3	1:G:274:TRP:CH2	2.44	0.53
1:C:51:LYS:HE3	1:C:236:ARG:HG2	1.91	0.53
1:G:110:LYS:N	1:G:110:LYS:HD3	2.24	0.53
1:B:8:LYS:HD2	1:C:13:ASP:CB	2.36	0.52
1:B:125:THR:HG22	1:B:126:GLY:H	1.74	0.52
1:F:204:MET:HE1	1:F:209:ASN:CA	2.39	0.52
1:C:169:VAL:HG21	1:C:224:PHE:CZ	2.44	0.52
1:C:195:LEU:HD13	1:C:196:PHE:CE2	2.45	0.52
1:D:28:TYR:CE1	1:D:30:LYS:HG2	2.44	0.52
1:C:51:LYS:HG3	1:C:236:ARG:HG3	1.90	0.52
1:F:123:ASN:CG	1:G:135:LEU:HD11	2.30	0.52
1:G:261:THR:O	1:G:262:SER:HB2	2.09	0.52
1:F:248:ILE:N	1:F:248:ILE:HD12	2.24	0.52
1:B:169:VAL:HG21	1:B:224:PHE:CZ	2.44	0.52
1:B:248:ILE:N	1:B:248:ILE:HD12	2.25	0.52
1:D:100:ASP:N	1:D:231:VAL:HG13	2.25	0.52
1:F:14:ILE:HG23	1:F:45:ASP:OD1	2.10	0.52
1:B:261:THR:O	1:B:262:SER:HB3	2.10	0.52
1:C:125:THR:CG2	1:D:135:LEU:HD13	2.35	0.51
1:D:74:ASN:O	1:D:259:HIS:HA	2.10	0.51
1:D:193:ASN:OD1	1:D:195:LEU:HB2	2.10	0.51
1:B:65:TYR:CE2	1:B:78:LEU:HD21	2.45	0.51
1:A:125:THR:HG22	1:B:135:LEU:HD13	1.92	0.51
1:F:52:LEU:HD22	1:F:231:VAL:HG13	1.92	0.51
1:B:232:ILE:N	1:B:232:ILE:HD12	2.25	0.51
1:C:112:TYR:C	1:C:113:ASN:HD22	2.14	0.51
1:E:50:LYS:NZ	2:E:300:HOH:O	2.44	0.51
1:D:14:ILE:HD11	1:D:48:HIS:CE1	2.46	0.51
1:A:123:ASN:OD1	1:B:135:LEU:HD11	2.11	0.51
1:C:14:ILE:HD11	1:C:48:HIS:CE1	2.46	0.51
1:B:255:ASP:HB3	1:B:270:THR:HG1	1.76	0.51
1:A:100:ASP:CB	1:A:231:VAL:CG1	2.88	0.50
1:D:260:TRP:NE1	1:D:262:SER:HA	2.26	0.50
1:C:204:MET:HE3	1:C:209:ASN:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:204:MET:HE1	1:C:265:TRP:NE1	2.25	0.50
1:F:50:LYS:NZ	2:F:332:HOH:O	2.41	0.50
1:D:240:LYS:CE	1:D:242:GLN:HE21	2.24	0.50
1:A:51:LYS:HG3	1:A:236:ARG:HG2	1.93	0.50
1:C:116:LEU:HB3	1:D:144:HIS:CE1	2.46	0.50
1:D:100:ASP:H	1:D:231:VAL:HG13	1.77	0.50
1:D:240:LYS:HD2	1:D:242:GLN:NE2	2.26	0.50
1:G:112:TYR:C	1:G:113:ASN:HD22	2.15	0.50
1:C:204:MET:HE1	1:C:265:TRP:HE1	1.75	0.50
1:D:240:LYS:HE3	1:D:242:GLN:HB2	1.94	0.50
1:D:56:ARG:NH2	2:D:305:HOH:O	2.44	0.50
1:D:111:GLU:HB3	1:D:147:LYS:HB2	1.94	0.49
1:E:91:PRO:HD2	1:E:94:GLU:HG3	1.93	0.49
1:A:248:ILE:HD12	1:A:248:ILE:N	2.27	0.49
1:F:193:ASN:OD1	1:F:195:LEU:HB2	2.11	0.49
1:G:248:ILE:HD12	1:G:248:ILE:N	2.27	0.49
1:C:158:GLU:O	1:C:160:PRO:HD3	2.11	0.49
1:E:177:GLN:O	1:E:178:ASN:HB2	2.11	0.49
1:D:167:TRP:CH2	1:D:230:THR:HG22	2.44	0.49
1:D:51:LYS:HG3	1:D:236:ARG:HG2	1.93	0.49
1:A:169:VAL:HG21	1:A:224:PHE:CZ	2.48	0.49
1:C:74:ASN:O	1:C:259:HIS:HA	2.11	0.49
1:E:95:VAL:HG13	1:E:234:MET:SD	2.52	0.49
1:E:112:TYR:C	1:E:113:ASN:HD22	2.16	0.49
1:D:85:LYS:HE2	1:D:168:LYS:HB3	1.94	0.49
1:A:14:ILE:HD11	1:B:39:PHE:CE1	2.32	0.49
1:A:259:HIS:CE1	1:A:266:LYS:HB3	2.48	0.49
1:F:125:THR:CG2	1:G:135:LEU:HD13	2.41	0.48
1:G:50:LYS:HD3	1:G:233:THR:HB	1.95	0.48
1:D:282:TYR:CD1	1:D:293:ASN:HB3	2.48	0.48
1:D:202:GLY:HA3	1:D:204:MET:CE	2.43	0.48
1:D:169:VAL:HG21	1:D:224:PHE:CZ	2.48	0.48
1:E:261:THR:O	1:E:262:SER:HB2	2.13	0.48
1:E:261:THR:OG1	1:E:263:THR:HG23	2.14	0.48
1:D:65:TYR:CE2	1:D:78:LEU:HD21	2.49	0.48
1:G:240:LYS:HB2	1:G:240:LYS:HZ2	1.77	0.48
1:E:52:LEU:HD21	1:E:233:THR:HG22	1.95	0.48
1:B:158:GLU:O	1:B:160:PRO:HD3	2.14	0.47
1:A:178:ASN:ND2	1:A:178:ASN:N	2.62	0.47
1:F:195:LEU:HD13	1:F:196:PHE:CE2	2.49	0.47
1:F:58:LYS:HA	1:F:226:PRO:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:ASN:CG	1:C:135:LEU:HD11	2.34	0.47
1:A:195:LEU:HD13	1:A:196:PHE:CE2	2.49	0.47
1:D:50:LYS:NZ	2:D:302:HOH:O	2.47	0.47
1:C:177:GLN:O	1:C:178:ASN:HB2	2.15	0.47
1:E:74:ASN:O	1:E:259:HIS:HA	2.14	0.47
1:C:160:PRO:HD2	1:D:60:THR:CG2	2.36	0.47
1:C:35:HIS:HB3	1:C:60:THR:HG22	1.96	0.47
1:C:52:LEU:HD11	1:C:231:VAL:HG13	1.96	0.47
1:C:259:HIS:CE1	1:C:266:LYS:HB3	2.50	0.47
1:F:101:TYR:OH	1:G:60:THR:CG2	2.63	0.47
1:A:14:ILE:HD11	1:A:48:HIS:CE1	2.50	0.47
1:G:240:LYS:CB	1:G:240:LYS:NZ	2.78	0.47
1:D:100:ASP:CB	1:D:231:VAL:CG1	2.92	0.47
1:A:100:ASP:CB	1:A:231:VAL:HG11	2.41	0.47
1:G:261:THR:O	1:G:262:SER:CB	2.63	0.47
1:C:48:HIS:O	1:C:236:ARG:NH2	2.36	0.46
1:C:116:LEU:HD13	1:C:142:ILE:HG12	1.96	0.46
1:C:248:ILE:HD12	1:C:248:ILE:N	2.30	0.46
1:A:193:ASN:OD1	1:A:195:LEU:HB2	2.16	0.46
1:G:58:LYS:HA	1:G:226:PRO:O	2.16	0.46
1:A:39:PHE:CE1	1:G:14:ILE:HD11	2.38	0.46
1:B:124:VAL:O	1:C:135:LEU:HD12	2.16	0.46
1:G:231:VAL:O	1:G:231:VAL:HG13	2.15	0.46
1:D:66:ARG:C	1:D:78:LEU:HD12	2.36	0.46
1:D:14:ILE:HD11	1:E:39:PHE:CE1	2.38	0.46
1:G:100:ASP:N	1:G:231:VAL:CG1	2.79	0.46
1:C:116:LEU:HD23	1:D:144:HIS:HE1	1.81	0.46
1:F:14:ILE:CG2	1:F:15:GLY:N	2.79	0.46
1:B:50:LYS:NZ	2:B:324:HOH:O	2.49	0.46
1:A:74:ASN:O	1:A:259:HIS:HA	2.16	0.46
1:F:101:TYR:OH	1:G:60:THR:HG23	2.16	0.46
1:A:127:ASP:C	1:A:129:THR:H	2.19	0.46
1:G:32:ASN:O	1:G:251:ARG:NH1	2.42	0.46
1:G:1:ALA:HB3	1:G:4:ASP:OD1	2.15	0.46
1:A:60:THR:CG2	1:G:101:TYR:OH	2.64	0.46
1:B:282:TYR:CD1	1:B:293:ASN:HB3	2.51	0.46
1:E:14:ILE:HG22	1:E:15:GLY:N	2.30	0.46
1:B:126:GLY:HA2	1:B:131:LYS:O	2.16	0.45
1:E:195:LEU:HD13	1:E:196:PHE:CE2	2.52	0.45
1:A:125:THR:CG2	1:B:135:LEU:HD13	2.46	0.45
1:B:14:ILE:HD11	1:C:39:PHE:CE1	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:204:MET:CE	1:C:265:TRP:HE1	2.28	0.45
1:E:101:TYR:CZ	1:E:160:PRO:HG3	2.51	0.45
1:C:204:MET:CE	1:C:265:TRP:NE1	2.80	0.45
1:A:191:TYR:CE2	1:A:200:ARG:HB3	2.51	0.45
1:G:177:GLN:O	1:G:178:ASN:HB2	2.17	0.45
1:G:273:LYS:HD3	1:G:274:TRP:CZ2	2.51	0.45
1:E:127:ASP:HA	1:F:133:GLY:HA2	1.99	0.45
1:C:65:TYR:CE2	1:C:78:LEU:HD21	2.52	0.45
1:G:12:THR:CG2	1:G:12:THR:O	2.65	0.44
1:E:110:LYS:HD3	1:F:175:VAL:HG23	1.99	0.44
1:D:118:TYR:HA	1:D:139:ASN:O	2.18	0.44
1:E:195:LEU:HD22	1:E:196:PHE:CE1	2.53	0.44
1:F:52:LEU:CD2	1:F:233:THR:HG22	2.47	0.44
1:F:109:THR:HG22	1:G:151:PRO:HA	2.00	0.44
1:C:14:ILE:HG22	1:C:15:GLY:N	2.33	0.44
1:D:40:TYR:CE1	1:D:291:MET:HB3	2.53	0.44
1:A:23:GLY:HA3	1:A:40:TYR:CE1	2.53	0.44
1:D:58:LYS:HA	1:D:226:PRO:O	2.18	0.44
1:G:100:ASP:CB	1:G:231:VAL:CG1	2.95	0.44
1:B:32:ASN:O	1:B:251:ARG:NH1	2.40	0.44
1:B:37:LYS:HD2	1:B:37:LYS:C	2.38	0.43
1:F:94:GLU:O	1:F:163:LYS:NZ	2.46	0.43
1:F:98:ILE:HD12	1:F:164:LYS:N	2.34	0.43
1:E:51:LYS:HG3	1:E:236:ARG:HG2	2.00	0.43
1:A:198:LYS:HD2	1:A:199:THR:HG23	1.99	0.43
1:G:251:ARG:NH1	2:G:299:HOH:O	2.52	0.43
1:A:23:GLY:HA3	1:A:40:TYR:CZ	2.52	0.43
1:A:56:ARG:NH2	2:A:303:HOH:O	2.51	0.43
1:D:60:THR:O	1:D:60:THR:HG23	2.18	0.43
1:G:51:LYS:HG3	1:G:236:ARG:CG	2.49	0.43
1:B:204:MET:CE	1:B:204:MET:H	2.32	0.43
1:G:288:LYS:HE2	1:G:290:GLU:CD	2.39	0.43
1:E:111:GLU:HB3	1:E:147:LYS:HB2	2.01	0.43
1:D:37:LYS:C	1:D:37:LYS:HD2	2.39	0.43
1:A:24:ASP:CB	2:A:310:HOH:O	2.61	0.42
1:A:112:TYR:C	1:A:113:ASN:HD22	2.22	0.42
1:B:110:LYS:HD3	1:C:150:GLN:O	2.18	0.42
1:E:2:ASP:HB3	1:E:7:ILE:HB	2.01	0.42
1:G:14:ILE:HG22	1:G:15:GLY:N	2.34	0.42
1:B:125:THR:CG2	1:B:126:GLY:N	2.82	0.42
1:G:193:ASN:OD1	1:G:195:LEU:HB2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:195:LEU:HD22	1:G:196:PHE:CE1	2.54	0.42
1:C:52:LEU:HD21	1:C:231:VAL:CG1	2.49	0.42
1:E:283:LYS:HE3	1:E:283:LYS:HA	2.01	0.42
1:G:170:ILE:HD12	1:G:170:ILE:O	2.19	0.42
1:B:116:LEU:HD13	1:B:142:ILE:HG12	2.01	0.42
1:C:111:GLU:HB3	1:C:147:LYS:HB2	2.00	0.42
1:G:25:LEU:N	1:G:25:LEU:HD12	2.33	0.42
1:A:66:ARG:C	1:A:78:LEU:HD12	2.40	0.42
1:D:49:ASN:O	1:D:50:LYS:HG3	2.19	0.42
1:E:169:VAL:HG21	1:E:224:PHE:CZ	2.54	0.42
1:G:65:TYR:CE2	1:G:78:LEU:HD21	2.54	0.42
1:F:177:GLN:O	1:F:179:TRP:HD1	2.02	0.42
1:D:177:GLN:O	1:D:178:ASN:HB2	2.19	0.42
1:G:240:LYS:HB2	1:G:240:LYS:HZ3	1.84	0.42
1:C:154:LYS:HB2	1:C:170:ILE:HD11	2.01	0.42
1:G:51:LYS:HG3	1:G:236:ARG:HG2	2.01	0.42
1:A:60:THR:HG23	1:G:101:TYR:OH	2.20	0.42
1:G:66:ARG:C	1:G:78:LEU:HD12	2.40	0.42
1:G:113:ASN:HB2	1:G:145:THR:HB	2.02	0.42
1:B:193:ASN:OD1	1:B:195:LEU:HB2	2.19	0.42
1:G:65:TYR:HB2	1:G:220:LEU:O	2.19	0.41
1:A:123:ASN:O	1:A:134:GLY:HA2	2.21	0.41
1:D:14:ILE:HG22	1:D:15:GLY:N	2.34	0.41
1:B:23:GLY:HA3	1:B:40:TYR:CZ	2.55	0.41
1:E:58:LYS:HA	1:E:226:PRO:O	2.20	0.41
1:G:169:VAL:HG21	1:G:224:PHE:CZ	2.56	0.41
1:A:255:ASP:HB3	1:A:270:THR:HB	2.01	0.41
1:G:127:ASP:C	1:G:129:THR:H	2.24	0.41
1:E:23:GLY:HA3	1:E:40:TYR:CE1	2.55	0.41
1:C:80:TRP:CE2	1:C:254:ASP:HB2	2.56	0.41
1:C:113:ASN:HB2	1:C:145:THR:HB	2.02	0.41
1:F:255:ASP:HB3	1:F:270:THR:HB	2.01	0.41
1:B:58:LYS:HA	1:B:226:PRO:O	2.20	0.41
1:B:66:ARG:HH11	1:B:66:ARG:HG3	1.86	0.41
1:D:28:TYR:HE1	1:D:30:LYS:HG2	1.86	0.41
1:D:202:GLY:HA3	1:D:204:MET:HE2	2.01	0.41
1:G:8:LYS:HB2	1:G:11:THR:OG1	2.21	0.41
1:A:52:LEU:HD13	1:A:53:LEU:N	2.35	0.41
1:F:66:ARG:C	1:F:78:LEU:HD12	2.40	0.41
1:G:255:ASP:HB2	1:G:273:LYS:HD2	2.03	0.41
1:E:66:ARG:C	1:E:78:LEU:HD12	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:100:ASP:CB	1:G:231:VAL:HG11	2.50	0.40
1:A:123:ASN:HD21	1:B:135:LEU:CD1	2.34	0.40
1:B:198:LYS:HB3	1:B:209:ASN:ND2	2.37	0.40
1:D:148:TYR:HE2	1:D:150:GLN:OE1	2.03	0.40
1:D:288:LYS:HB2	1:D:290:GLU:HG2	2.03	0.40
1:G:23:GLY:HA3	1:G:40:TYR:CZ	2.56	0.40
1:E:123:ASN:O	1:E:134:GLY:HA2	2.22	0.40
1:F:45:ASP:O	1:F:236:ARG:NH1	2.55	0.40
1:B:247:VAL:C	1:B:248:ILE:HD12	2.41	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	291/293 (99%)	280 (96%)	9 (3%)	2 (1%)	26	14
1	B	291/293 (99%)	276 (95%)	13 (4%)	2 (1%)	26	14
1	C	291/293 (99%)	281 (97%)	9 (3%)	1 (0%)	46	35
1	D	291/293 (99%)	279 (96%)	11 (4%)	1 (0%)	46	35
1	E	291/293 (99%)	280 (96%)	11 (4%)	0	100	100
1	F	291/293 (99%)	278 (96%)	11 (4%)	2 (1%)	26	14
1	G	291/293 (99%)	277 (95%)	12 (4%)	2 (1%)	26	14
All	All	2037/2051 (99%)	1951 (96%)	76 (4%)	10 (0%)	34	21

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	262	SER
1	B	262	SER

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Mol	Chain	Res	Type
1	C	262	SER
1	B	123	ASN
1	F	262	SER
1	G	262	SER
1	A	128	ASP
1	D	262	SER
1	F	123	ASN
1	G	128	ASP

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	258/259 (100%)	253 (98%)	5 (2%)	65	59
1	B	259/259 (100%)	254 (98%)	5 (2%)	65	59
1	C	259/259 (100%)	251 (97%)	8 (3%)	47	37
1	D	259/259 (100%)	253 (98%)	6 (2%)	58	51
1	E	258/259 (100%)	252 (98%)	6 (2%)	58	51
1	F	259/259 (100%)	253 (98%)	6 (2%)	58	51
1	G	259/259 (100%)	251 (97%)	8 (3%)	47	37
All	All	1811/1813 (100%)	1767 (98%)	44 (2%)	57	49

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LEU
1	A	60	THR
1	A	101	TYR
1	A	195	LEU
1	A	204	MET
1	B	25	LEU
1	B	101	TYR
1	B	110	LYS
1	B	195	LEU

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Mol	Chain	Res	Type
1	B	204	MET
1	C	25	LEU
1	C	52	LEU
1	C	101	TYR
1	C	110	LYS
1	C	148	TYR
1	C	195	LEU
1	C	204	MET
1	C	242	GLN
1	D	25	LEU
1	D	101	TYR
1	D	110	LYS
1	D	195	LEU
1	D	204	MET
1	D	230	THR
1	E	25	LEU
1	E	101	TYR
1	E	195	LEU
1	E	204	MET
1	E	263	THR
1	E	283	LYS
1	F	25	LEU
1	F	101	TYR
1	F	120	PHE
1	F	178	ASN
1	F	195	LEU
1	F	204	MET
1	G	60	THR
1	G	101	TYR
1	G	110	LYS
1	G	179	TRP
1	G	195	LEU
1	G	204	MET
1	G	234	MET
1	G	240	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	64	GLN
1	A	74	ASN

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Mol	Chain	Res	Type
1	A	113	ASN
1	A	178	ASN
1	A	242	GLN
1	A	259	HIS
1	B	17	ASN
1	B	64	GLN
1	B	74	ASN
1	B	89	GLN
1	B	113	ASN
1	B	178	ASN
1	B	209	ASN
1	B	242	GLN
1	B	259	HIS
1	C	64	GLN
1	C	74	ASN
1	C	89	GLN
1	C	113	ASN
1	C	150	GLN
1	C	178	ASN
1	C	257	GLN
1	C	259	HIS
1	D	17	ASN
1	D	64	GLN
1	D	74	ASN
1	D	89	GLN
1	D	113	ASN
1	D	144	HIS
1	D	178	ASN
1	D	242	GLN
1	D	244	ASN
1	D	259	HIS
1	E	64	GLN
1	E	74	ASN
1	E	89	GLN
1	E	113	ASN
1	E	178	ASN
1	E	259	HIS
1	F	64	GLN
1	F	74	ASN
1	F	89	GLN
1	F	113	ASN
1	F	150	GLN

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Mol	Chain	Res	Type
1	F	178	ASN
1	F	242	GLN
1	F	259	HIS
1	G	17	ASN
1	G	64	GLN
1	G	74	ASN
1	G	89	GLN
1	G	113	ASN
1	G	150	GLN
1	G	178	ASN
1	G	259	HIS

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^{th} 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	293/293 (100%)	0.62	33 (11%) 7 7	14, 24, 52, 69	13 (4%)
1	B	292/293 (99%)	0.59	38 (13%) 5 5	13, 24, 54, 66	12 (4%)
1	C	293/293 (100%)	0.50	33 (11%) 7 7	14, 24, 51, 65	16 (5%)
1	D	292/293 (99%)	0.52	40 (13%) 4 4	13, 24, 50, 60	19 (6%)
1	E	293/293 (100%)	0.48	30 (10%) 9 10	13, 24, 50, 61	17 (5%)
1	F	293/293 (100%)	0.58	26 (8%) 12 13	13, 24, 52, 66	19 (6%)
1	G	292/293 (99%)	0.44	28 (9%) 10 11	14, 23, 46, 65	16 (5%)
All	All	2048/2051 (99%)	0.53	228 (11%) 7 8	13, 24, 52, 69	112 (5%)

All (228) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	179	TRP	8.4
1	A	132	ILE	7.7
1	G	179	TRP	7.3
1	D	179	TRP	6.9
1	A	179	TRP	6.4
1	F	126	GLY	6.3
1	C	179	TRP	6.1
1	G	130	GLY	6.0
1	E	179	TRP	5.8
1	F	128	ASP	5.6
1	B	258	LEU	5.6
1	G	129	THR	5.6
1	C	132	ILE	5.4
1	F	133	GLY	5.4
1	F	132	ILE	5.3
1	A	133	GLY	5.2
1	F	118	TYR	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	126	GLY	4.9
1	B	118	TYR	4.9
1	A	128	ASP	4.8
1	D	133	GLY	4.8
1	A	118	TYR	4.8
1	C	130	GLY	4.7
1	B	72	GLY	4.6
1	F	135	LEU	4.6
1	G	134	GLY	4.6
1	B	132	ILE	4.5
1	B	73	ALA	4.4
1	F	73	ALA	4.4
1	E	262	SER	4.3
1	G	131	LYS	4.3
1	C	68	TYR	4.3
1	G	133	GLY	4.2
1	A	258	LEU	4.2
1	A	129	THR	4.2
1	B	135	LEU	4.2
1	B	129	THR	4.1
1	D	93	ASN	4.1
1	E	130	GLY	4.1
1	F	125	THR	4.1
1	D	132	ILE	4.0
1	B	133	GLY	4.0
1	C	126	GLY	4.0
1	F	258	LEU	4.0
1	C	133	GLY	4.0
1	D	125	THR	3.9
1	G	137	GLY	3.9
1	B	134	GLY	3.8
1	G	135	LEU	3.8
1	C	131	LYS	3.8
1	D	144	HIS	3.8
1	F	123	ASN	3.8
1	B	179	TRP	3.8
1	G	112	TYR	3.7
1	C	125	THR	3.7
1	E	68	TYR	3.7
1	D	258	LEU	3.6
1	E	72	GLY	3.6
1	C	129	THR	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	135	LEU	3.5
1	D	112	TYR	3.5
1	B	125	THR	3.5
1	A	188	ASN	3.5
1	D	126	GLY	3.5
1	B	203	SER	3.5
1	F	129	THR	3.5
1	C	1	ALA	3.5
1	C	258	LEU	3.5
1	F	200	ARG	3.5
1	A	66	ARG	3.4
1	E	118	TYR	3.4
1	F	127	ASP	3.4
1	B	201	ASN	3.4
1	E	123	ASN	3.4
1	B	93	ASN	3.4
1	B	187	TRP	3.4
1	B	71	GLU	3.4
1	E	132	ILE	3.3
1	G	187	TRP	3.3
1	B	126	GLY	3.2
1	D	131	LYS	3.2
1	G	118	TYR	3.2
1	A	190	VAL	3.2
1	C	263	THR	3.2
1	E	133	GLY	3.2
1	A	189	PRO	3.2
1	B	66	ARG	3.1
1	B	200	ARG	3.1
1	G	127	ASP	3.1
1	E	129	THR	3.1
1	E	135	LEU	3.1
1	A	130	GLY	3.1
1	C	148	TYR	3.1
1	A	127	ASP	3.1
1	B	188	ASN	3.1
1	A	53	LEU	3.0
1	E	189	PRO	3.0
1	D	122	GLY	3.0
1	G	122	GLY	3.0
1	F	188	ASN	3.0
1	G	123	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	17	ASN	3.0
1	B	92	ASP	3.0
1	A	72	GLY	2.9
1	A	112	TYR	2.9
1	B	74	ASN	2.9
1	F	92	ASP	2.9
1	E	17	ASN	2.9
1	E	71	GLU	2.8
1	A	136	ILE	2.8
1	C	136	ILE	2.8
1	B	130	GLY	2.8
1	D	130	GLY	2.8
1	F	134	GLY	2.8
1	E	148	TYR	2.8
1	D	123	ASN	2.8
1	A	191	TYR	2.8
1	B	127	ASP	2.8
1	D	92	ASP	2.8
1	A	135	LEU	2.8
1	A	261	THR	2.8
1	C	128	ASP	2.8
1	B	112	TYR	2.8
1	D	262	SER	2.8
1	G	92	ASP	2.7
1	D	200	ARG	2.7
1	E	258	LEU	2.7
1	D	135	LEU	2.7
1	C	200	ARG	2.7
1	D	201	ASN	2.7
1	E	92	ASP	2.7
1	C	118	TYR	2.7
1	A	131	LYS	2.6
1	D	188	ASN	2.6
1	B	195	LEU	2.6
1	A	123	ASN	2.6
1	F	130	GLY	2.6
1	E	131	LYS	2.6
1	E	1	ALA	2.6
1	G	258	LEU	2.6
1	G	189	PRO	2.6
1	D	134	GLY	2.6
1	A	71	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	232	ILE	2.6
1	B	68	TYR	2.6
1	D	187	TRP	2.5
1	C	112	TYR	2.5
1	C	256	TYR	2.5
1	D	196	PHE	2.5
1	F	239	SER	2.5
1	D	121	ASN	2.5
1	A	134	GLY	2.5
1	D	263	THR	2.5
1	D	69	SER	2.5
1	D	203	SER	2.5
1	G	262	SER	2.5
1	F	112	TYR	2.5
1	C	92	ASP	2.5
1	D	140	VAL	2.4
1	B	70	GLU	2.4
1	B	119	GLY	2.4
1	E	31	GLU	2.4
1	A	203	SER	2.4
1	A	69	SER	2.4
1	A	256	TYR	2.4
1	F	262	SER	2.4
1	D	204	MET	2.4
1	A	55	ILE	2.3
1	F	71	GLU	2.3
1	E	127	ASP	2.3
1	B	53	LEU	2.3
1	C	189	PRO	2.3
1	G	1	ALA	2.3
1	B	239	SER	2.3
1	C	262	SER	2.3
1	D	70	GLU	2.3
1	D	190	VAL	2.3
1	D	127	ASP	2.3
1	D	189	PRO	2.3
1	A	93	ASN	2.3
1	G	53	LEU	2.3
1	C	119	GLY	2.3
1	F	72	GLY	2.3
1	C	66	ARG	2.2
1	C	71	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	187	TRP	2.2
1	E	187	TRP	2.2
1	B	131	LYS	2.2
1	E	134	GLY	2.2
1	C	261	THR	2.2
1	C	139	ASN	2.2
1	G	188	ASN	2.2
1	F	187	TRP	2.2
1	A	74	ASN	2.2
1	E	256	TYR	2.2
1	G	200	ARG	2.2
1	G	203	SER	2.2
1	F	189	PRO	2.2
1	D	53	LEU	2.2
1	B	190	VAL	2.2
1	B	69	SER	2.2
1	B	196	PHE	2.2
1	G	132	ILE	2.2
1	A	1	ALA	2.1
1	G	128	ASP	2.1
1	G	84	PHE	2.1
1	E	93	ASN	2.1
1	E	288	LYS	2.1
1	B	55	ILE	2.1
1	C	60	THR	2.1
1	D	98	ILE	2.1
1	F	14	ILE	2.1
1	G	136	ILE	2.1
1	D	256	TYR	2.1
1	C	31	GLU	2.1
1	C	69	SER	2.1
1	C	72	GLY	2.1
1	D	137	GLY	2.1
1	D	68	TYR	2.1
1	E	140	VAL	2.1
1	E	67	VAL	2.0
1	D	74	ASN	2.0
1	E	66	ARG	2.0
1	E	201	ASN	2.0
1	B	256	TYR	2.0
1	C	191	TYR	2.0
1	D	261	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	G	17	ASN	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.