Full wwPDB X-ray Structure Validation Report (i)

Apr 21, 2016 – 04:14 PM EDT

PDB ID	:	4ZEZ
Title	:	Crystal structure of HCV 1406 TCR/HCV NS3: 1406-1415/HLA-A2 complex
Authors	:	Wang, Y.; Piepenbrink, K.H.; Baker, B.M.
Deposited on	:	2015-04-20
Resolution	:	2.40 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:

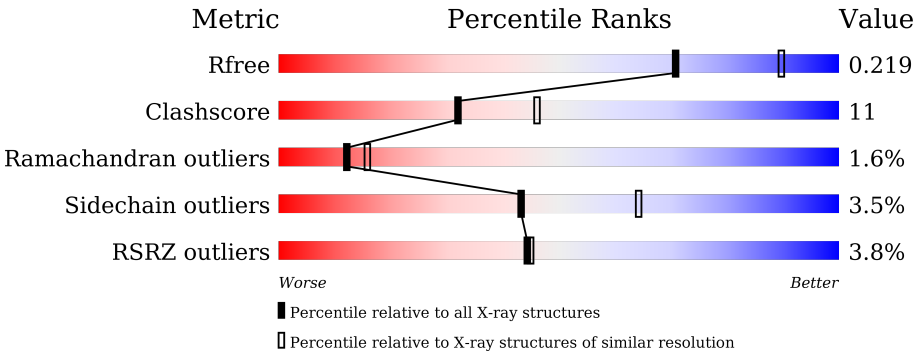
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027257
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027257

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 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	275	8% 65% 27% • 5%
1	D	275	6% 69% 25% • 5%
2	B	100	4% 67% 30% ••
2	E	100	11% 62% 33% • •
3	C	10	80% 20%
3	F	10	80% 20%

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Mol	Chain	Length	Quality of chain
4	G	211	76% 20%
4	I	211	72% 22%
5	H	245	72% 23%
5	J	245	72% 23%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13445 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 HLA class I histocompatibility antigen, A-2 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	261	Total	C	N	O	S	0	0	0
			2138	1339	387	403	9			
1	D	262	Total	C	N	O	S	0	0	0
			2159	1349	396	406	8			

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	0	0	0
			825	524	140	157	4			
2	E	98	Total	C	N	O	S	0	0	0
			819	521	139	155	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769
E	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called HCV NS3 peptide residues1406-1415.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	10	Total	C	N	O	0	0	0
			70	46	12	12			
3	F	10	Total	C	N	O	0	0	0
			70	46	12	12			

- Molecule 4 is a protein called HCV TCR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	I	207	Total	C	N	O	S	3	0	0
			1645	1032	268	334	11			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	207	Total	C	N	O	S	0	0	0
			1647	1033	268	334	12			

- Molecule 5 is a protein called HCV TCR beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	J	240	Total	C	N	O	S	0	0	0
			1931	1215	336	371	9			
5	H	241	Total	C	N	O	S	0	0	0
			1939	1219	337	374	9			

- Molecule 6 is water.

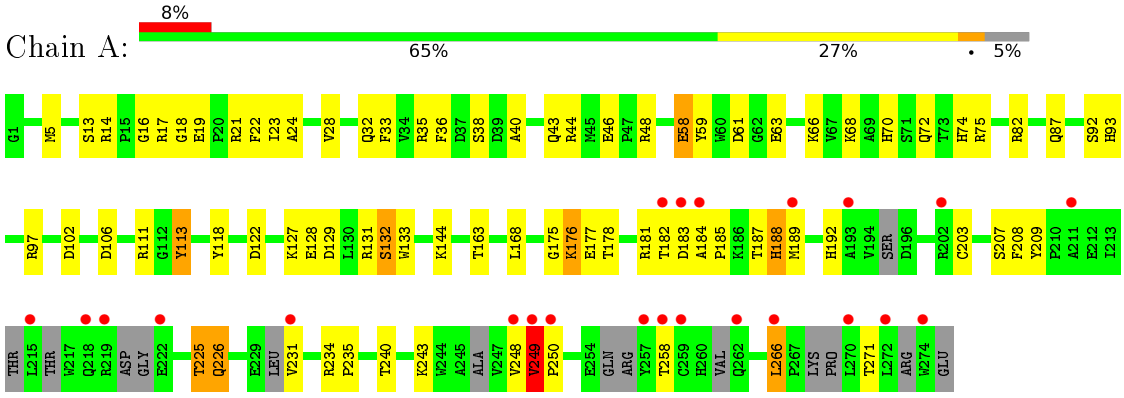
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	40	Total	O	0	0
			40	40		
6	B	11	Total	O	0	0
			11	11		
6	D	26	Total	O	0	0
			26	26		
6	E	7	Total	O	0	0
			7	7		
6	F	1	Total	O	0	0
			1	1		
6	I	35	Total	O	0	0
			35	35		
6	J	31	Total	O	0	0
			31	31		
6	G	19	Total	O	0	0
			19	19		
6	H	32	Total	O	0	0
			32	32		

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.

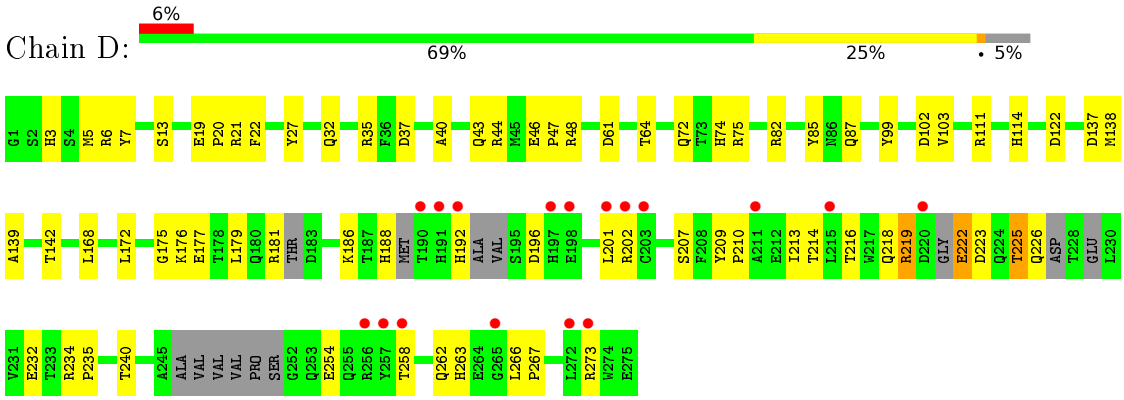
• Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain

Chain A:



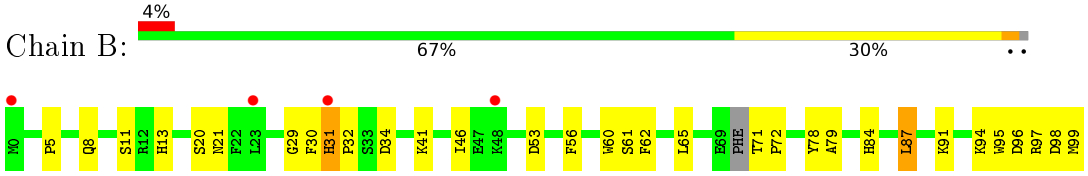
• Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain

Chain D:



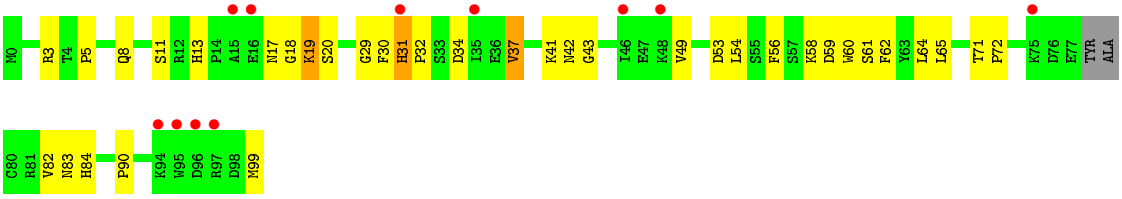
• Molecule 2: Beta-2-microglobulin

Chain B:

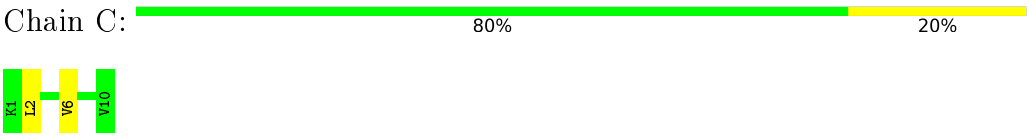


• Molecule 2: Beta-2-microglobulin

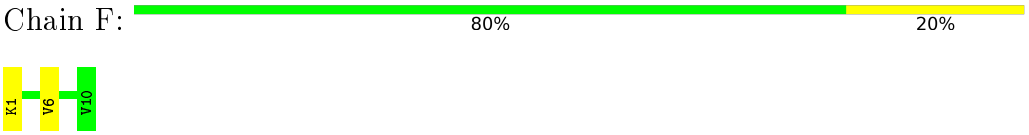
Chain E:



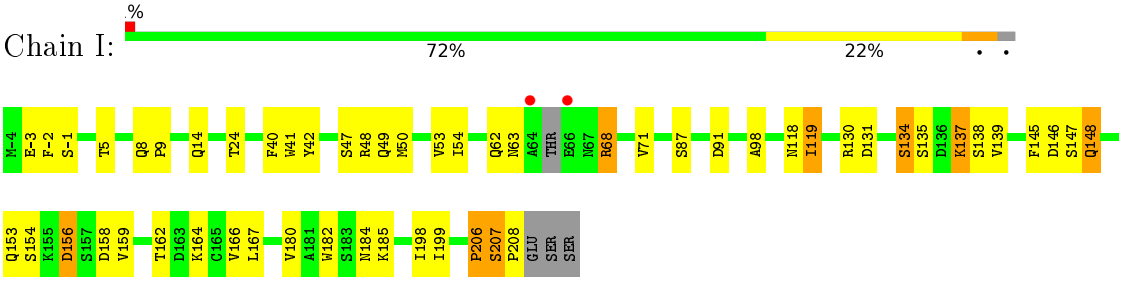
• Molecule 3: HCV NS3 peptide residues1406-1415



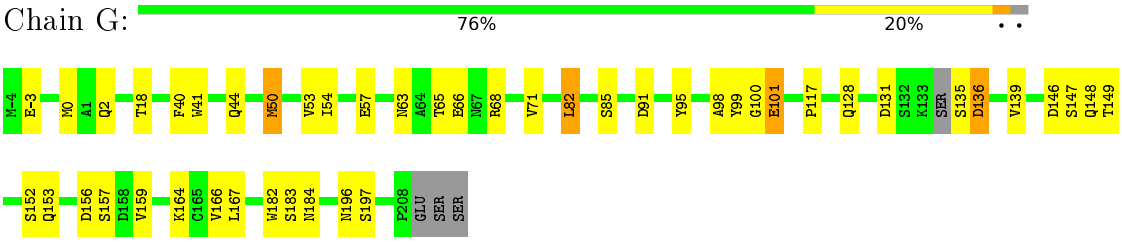
• Molecule 3: HCV NS3 peptide residues1406-1415



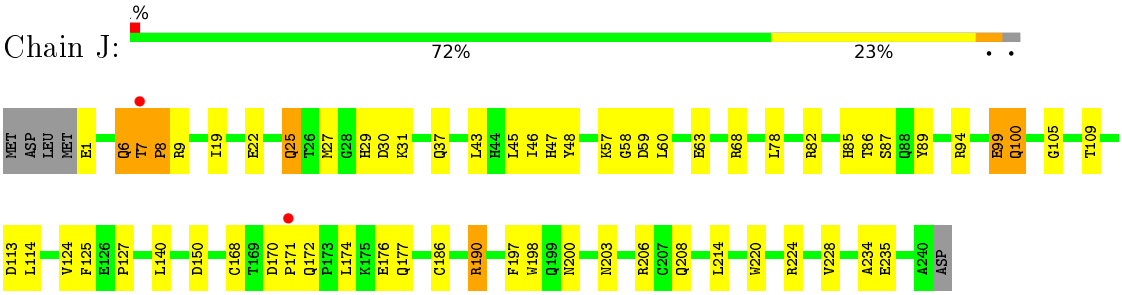
• Molecule 4: HCV TCR alpha chain



• Molecule 4: HCV TCR alpha chain

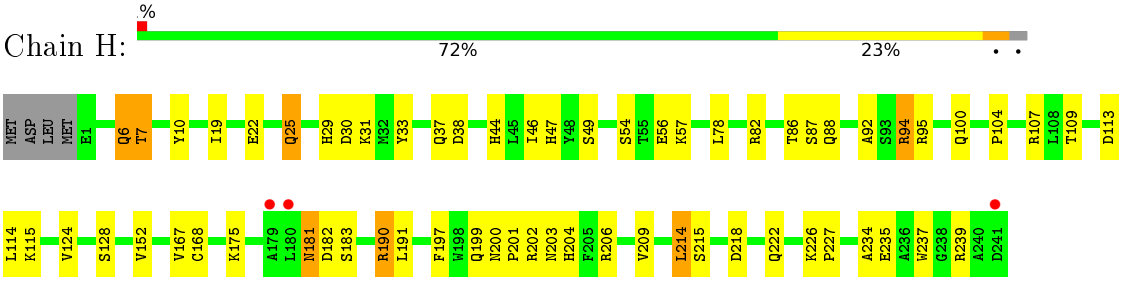


• Molecule 5: HCV TCR beta chain



• Molecule 5: HCV TCR beta chain

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	128.76Å 128.76Å 223.59Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.65 – 2.40 48.72 – 2.07	Depositor EDS
% Data completeness (in resolution range)	98.5 (44.65-2.40) 73.3 (48.72-2.07)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.13 (at 2.08Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.180 , 0.216 0.184 , 0.219	Depositor DCC
R_{free} test set	1452 reflections (1.86%)	DCC
Wilson B-factor (Å^2)	26.8	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 34.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.36$, $< L^2 > = 0.19$	Xtriage
Estimated twinning fraction	0.467 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	13445	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.13% 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	0.23	0/2192	0.39	0/2960
1	D	0.22	0/2216	0.38	0/2994
2	B	0.24	0/846	0.43	0/1143
2	E	0.23	0/840	0.43	0/1134
3	C	0.31	0/69	0.50	0/91
3	F	0.24	0/69	0.57	0/91
4	G	0.24	0/1682	0.43	1/2275 (0.0%)
4	I	0.25	0/1680	0.43	0/2272
5	H	0.23	0/1994	0.40	0/2715
5	J	0.23	0/1986	0.42	0/2704
All	All	0.23	0/13574	0.41	1/18379 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	82	LEU	CA-CB-CG	5.96	129.01	115.30

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	2138	0	1975	54	0
1	D	2159	0	2002	48	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	825	0	793	22	0
2	E	819	0	788	29	0
3	C	70	0	83	1	0
3	F	70	0	83	1	0
4	G	1647	0	1557	28	0
4	I	1645	0	1553	38	0
5	H	1939	0	1837	39	0
5	J	1931	0	1833	42	0
6	A	40	0	0	4	0
6	B	11	0	0	0	0
6	D	26	0	0	0	0
6	E	7	0	0	0	0
6	F	1	0	0	0	0
6	G	19	0	0	0	0
6	H	32	0	0	2	0
6	I	35	0	0	2	0
6	J	31	0	0	1	0
All	All	13445	0	12504	272	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 11.

All (272) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:84:HIS:HB3	2:B:87:LEU:HD13	1.65	0.77
1:D:122:ASP:OD1	2:E:60:TRP:NE1	2.18	0.77
2:B:29:GLY:HA2	2:B:61:SER:HB2	1.69	0.74
2:E:5:PRO:HB3	2:E:30:PHE:HB3	1.72	0.72
4:I:147:SER:O	4:I:164:LYS:NZ	2.23	0.72
1:A:122:ASP:OD2	2:B:60:TRP:NE1	2.23	0.70
4:G:153:GLN:O	4:G:196:ASN:ND2	2.23	0.69
4:G:147:SER:O	4:G:164:LYS:NZ	2.23	0.69
5:H:31:LYS:HB2	5:H:94:ARG:HG3	1.73	0.69
1:D:225:THR:OG1	1:D:226:GLN:N	2.21	0.69
4:I:206:PRO:O	4:I:207:SER:OG	2.10	0.69
1:A:127:LYS:HD3	1:A:132:SER:HB2	1.75	0.68
5:J:170:ASP:OD1	5:J:190:ARG:NH1	2.24	0.68
1:D:175:GLY:O	1:D:177:GLU:N	2.27	0.68
4:I:68:ARG:NH2	4:I:91:ASP:OD2	2.27	0.67
1:A:187:THR:O	1:A:188:HIS:ND1	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:88:GLN:HG3	5:H:107:ARG:HG2	1.76	0.65
2:E:20:SER:HB2	2:E:71:THR:HG22	1.78	0.64
1:D:219:ARG:NH1	1:D:222:GLU:O	2.30	0.64
1:A:32:GLN:NE2	2:B:53:ASP:OD2	2.27	0.64
2:B:96:ASP:HB3	2:B:99:MET:HB2	1.80	0.62
4:I:-3:GLU:HB3	5:J:60:LEU:HB2	1.81	0.62
4:I:137:LYS:NZ	6:I:306:HOH:O	2.33	0.62
4:I:41:TRP:HB2	4:I:54:ILE:HG22	1.80	0.62
4:I:63:ASN:ND2	4:I:71:VAL:O	2.32	0.62
4:G:131:ASP:O	4:G:135:SER:OG	2.17	0.61
4:G:41:TRP:HB2	4:G:54:ILE:HG22	1.82	0.61
1:A:21:ARG:HE	1:A:23:ILE:HD11	1.64	0.61
2:B:20:SER:HB2	2:B:71:THR:HG22	1.83	0.61
2:E:29:GLY:HA2	2:E:61:SER:HB2	1.82	0.61
2:E:56:PHE:HA	2:E:62:PHE:HA	1.82	0.61
2:E:32:PRO:HD2	2:E:84:HIS:HE2	1.65	0.60
5:H:181:ASN:ND2	5:H:182:ASP:OD2	2.34	0.60
4:I:156:ASP:OD2	4:I:158:ASP:N	2.34	0.60
1:A:44:ARG:NH2	1:A:61:ASP:OD1	2.27	0.60
1:D:5:MET:HB2	1:D:168:LEU:HD13	1.82	0.60
1:A:75:ARG:NH1	6:A:306:HOH:O	2.34	0.59
1:A:68:LYS:O	1:A:72:GLN:NE2	2.35	0.59
1:D:201:LEU:HD11	1:D:254:GLU:HB3	1.84	0.59
5:H:95:ARG:NH1	6:H:304:HOH:O	2.36	0.59
1:D:258:THR:HG22	1:D:273:ARG:HG2	1.84	0.59
1:A:175:GLY:O	1:A:177:GLU:N	2.36	0.59
1:D:44:ARG:NH2	1:D:61:ASP:OD1	2.20	0.59
4:I:42:TYR:OH	5:J:99:GLU:O	2.20	0.59
5:H:38:ASP:OD2	5:H:44:HIS:NE2	2.34	0.59
5:J:206:ARG:HG3	5:J:235:GLU:HG2	1.82	0.59
1:D:102:ASP:OD1	1:D:111:ARG:NH1	2.36	0.59
5:H:167:VAL:HG12	5:H:191:LEU:HD13	1.84	0.58
1:D:19:GLU:OE1	1:D:75:ARG:NH1	2.37	0.58
4:I:5:THR:HB	4:I:24:THR:HG23	1.84	0.58
5:J:46:ILE:HG22	5:J:47:HIS:CD2	2.38	0.58
5:H:175:LYS:HE2	5:H:183:SER:HB3	1.85	0.58
4:I:130:ARG:HD3	4:I:138:SER:HB2	1.86	0.58
5:H:124:VAL:HG23	5:H:234:ALA:HB3	1.85	0.58
2:B:11:SER:OG	2:B:21:ASN:OD1	2.15	0.58
2:E:32:PRO:HD2	2:E:84:HIS:NE2	2.19	0.57
5:J:30:ASP:O	5:J:68:ARG:NH1	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:72:GLN:NE2	5:H:56:GLU:OE2	2.36	0.57
5:H:37:GLN:O	5:H:87:SER:OG	2.22	0.57
4:I:148:GLN:NE2	4:G:196:ASN:O	2.38	0.57
5:J:63:GLU:OE1	5:J:82:ARG:NH1	2.36	0.57
1:A:40:ALA:O	1:A:43:GLN:NE2	2.37	0.56
5:J:25:GLN:OE1	5:J:29:HIS:N	2.37	0.56
5:J:31:LYS:HB2	5:J:94:ARG:HB3	1.88	0.56
4:I:158:ASP:HB3	4:I:185:LYS:HZ2	1.70	0.56
1:A:58:GLU:HG2	5:H:82:ARG:HD2	1.87	0.56
5:J:86:THR:HG23	5:J:109:THR:HA	1.87	0.55
4:G:146:ASP:OD1	4:G:149:THR:OG1	2.20	0.55
1:A:248:VAL:HG13	1:A:249:VAL:H	1.70	0.55
1:D:37:ASP:HB3	1:D:40:ALA:HB2	1.88	0.55
2:E:11:SER:OG	2:E:13:HIS:O	2.24	0.55
2:E:31:HIS:HB3	2:E:32:PRO:HD3	1.89	0.55
1:D:32:GLN:NE2	2:E:53:ASP:OD2	2.38	0.55
5:J:174:LEU:O	5:J:186:CYS:N	2.30	0.54
4:G:156:ASP:OD2	4:G:157:SER:N	2.34	0.54
1:D:22:PHE:HE2	1:D:74:HIS:HD1	1.55	0.54
1:A:185:PRO:HG3	1:A:208:PHE:HB3	1.88	0.54
1:A:48:ARG:NH1	6:A:308:HOH:O	2.40	0.54
1:D:7:TYR:OH	3:F:1:LYS:N	2.28	0.54
5:H:25:GLN:NE2	5:H:29:HIS:O	2.41	0.54
5:J:7:THR:HB	5:J:8:PRO:HD3	1.89	0.54
1:A:14:ARG:NH1	1:A:19:GLU:O	2.41	0.54
4:G:167:LEU:HD21	5:H:190:ARG:HB2	1.88	0.54
1:A:243:LYS:NZ	6:A:309:HOH:O	2.41	0.53
1:A:102:ASP:HB2	1:A:111:ARG:HB3	1.91	0.53
2:B:11:SER:OG	2:B:13:HIS:O	2.27	0.53
1:A:225:THR:OG1	1:A:226:GLN:N	2.32	0.53
5:H:92:ALA:HB1	5:H:100:GLN:HB3	1.90	0.53
1:D:266:LEU:HD12	1:D:267:PRO:HD2	1.91	0.53
5:J:197:PHE:O	5:J:203:ASN:ND2	2.35	0.53
4:I:14:GLN:NE2	4:I:118:ASN:OD1	2.38	0.53
1:D:202:ARG:NH1	2:E:99:MET:O	2.42	0.52
1:A:72:GLN:OE1	1:A:75:ARG:NH2	2.42	0.52
1:D:44:ARG:HG2	1:D:64:THR:HG21	1.91	0.52
5:J:57:LYS:O	5:J:59:ASP:N	2.36	0.52
1:A:5:MET:HB2	1:A:168:LEU:HD13	1.91	0.52
1:D:207:SER:HA	1:D:240:THR:HB	1.90	0.52
1:A:235:PRO:HG2	2:B:65:LEU:HD22	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:184:ASN:ND2	6:I:311:HOH:O	2.42	0.52
4:I:50:MET:HE3	5:J:43:LEU:HD11	1.92	0.52
2:E:3:ARG:H	2:E:31:HIS:HB2	1.73	0.52
1:D:209:TYR:CD2	1:D:210:PRO:HD3	2.45	0.52
4:G:100:GLY:O	4:G:101:GLU:HB2	2.10	0.52
2:B:56:PHE:HA	2:B:62:PHE:HA	1.90	0.51
4:I:145:PHE:HE1	4:I:164:LYS:HE3	1.75	0.51
5:J:37:GLN:O	5:J:87:SER:OG	2.28	0.51
1:A:181:ARG:HB3	1:A:209:TYR:CZ	2.46	0.51
2:B:20:SER:HA	2:B:71:THR:HA	1.92	0.51
1:D:263:HIS:HB3	1:D:266:LEU:HB3	1.92	0.51
4:G:183:SER:OG	4:G:184:ASN:N	2.43	0.51
5:J:63:GLU:OE2	5:J:85:HIS:NE2	2.35	0.51
1:D:13:SER:HA	1:D:20:PRO:HB3	1.93	0.51
1:D:235:PRO:HG2	2:E:65:LEU:HD12	1.92	0.51
2:B:41:LYS:HD3	2:B:46:ILE:HD11	1.93	0.50
5:H:114:LEU:HD22	5:H:214:LEU:HD11	1.93	0.50
5:J:220:TRP:HZ2	5:J:224:ARG:HG3	1.76	0.50
1:A:189:MET:HG2	1:A:203:CYS:HA	1.94	0.50
1:D:172:LEU:HD23	1:D:179:LEU:HD13	1.92	0.50
5:H:206:ARG:HG3	5:H:235:GLU:HG2	1.94	0.50
2:E:54:LEU:HA	2:E:64:LEU:HD13	1.93	0.50
4:G:136:ASP:OD2	4:G:136:ASP:N	2.45	0.49
5:H:46:ILE:HG22	5:H:47:HIS:CD2	2.47	0.49
1:D:139:ALA:O	1:D:142:THR:OG1	2.30	0.49
1:A:207:SER:HA	1:A:240:THR:HB	1.94	0.49
1:D:225:THR:HG1	1:D:226:GLN:H	1.55	0.49
1:D:35:ARG:HG3	2:E:53:ASP:CG	2.33	0.49
4:G:117:PRO:O	4:G:147:SER:OG	2.20	0.49
4:G:139:VAL:HG12	4:G:182:TRP:HB3	1.94	0.49
4:I:-1:SER:HB2	4:G:-3:GLU:HG2	1.95	0.49
4:G:91:ASP:O	4:G:95:TYR:OH	2.22	0.49
5:J:1:GLU:N	6:J:308:HOH:O	2.45	0.49
4:I:154:SER:OG	4:I:156:ASP:OD1	2.18	0.48
2:E:19:LYS:N	2:E:19:LYS:HD2	2.28	0.48
1:D:218:GLN:HA	1:D:219:ARG:NH1	2.29	0.48
5:J:7:THR:OG1	5:J:22:GLU:N	2.43	0.48
1:A:35:ARG:HG3	1:A:46:GLU:HB2	1.95	0.48
5:H:202:ARG:NH1	6:H:302:HOH:O	2.34	0.48
5:J:124:VAL:HG23	5:J:234:ALA:HB3	1.95	0.48
2:B:20:SER:HA	2:B:72:PRO:HD2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:32:PRO:HB2	2:E:34:ASP:OD1	2.13	0.48
2:E:37:VAL:HB	2:E:82:VAL:HG12	1.96	0.48
5:H:200:ASN:HB3	5:H:203:ASN:ND2	2.28	0.48
1:D:209:TYR:CG	1:D:210:PRO:HD3	2.49	0.48
4:G:99:TYR:OH	4:G:101:GLU:OE2	2.20	0.47
4:I:158:ASP:HB3	4:I:185:LYS:NZ	2.30	0.47
1:D:48:ARG:NH2	2:E:53:ASP:OD1	2.47	0.47
4:G:166:VAL:N	5:H:168:CYS:SG	2.87	0.47
5:J:206:ARG:NH1	5:J:208:GLN:OE1	2.25	0.47
1:A:231:VAL:O	1:A:243:LYS:HE3	2.15	0.47
5:H:113:ASP:OD2	5:H:114:LEU:N	2.48	0.47
5:J:113:ASP:OD1	5:J:114:LEU:N	2.48	0.47
4:G:128:GLN:O	5:H:128:SER:OG	2.32	0.47
1:A:82:ARG:NH2	1:A:87:GLN:O	2.48	0.47
1:D:35:ARG:NH2	1:D:48:ARG:HH21	2.12	0.47
4:I:134:SER:OG	4:I:135:SER:N	2.45	0.47
2:B:78:TYR:O	2:B:95:TRP:N	2.27	0.47
4:I:207:SER:OG	4:I:208:PRO:HD3	2.15	0.47
2:E:56:PHE:HB3	2:E:62:PHE:CD2	2.50	0.46
5:H:86:THR:HG23	5:H:109:THR:HA	1.97	0.46
5:H:152:VAL:HG13	5:H:209:VAL:HG13	1.97	0.46
5:H:197:PHE:O	5:H:203:ASN:ND2	2.32	0.46
1:A:59:TYR:O	1:A:63:GLU:HG2	2.16	0.46
4:I:139:VAL:HG12	4:I:182:TRP:HB3	1.98	0.46
1:A:16:GLY:C	1:A:18:GLY:H	2.18	0.46
1:D:40:ALA:O	1:D:43:GLN:NE2	2.47	0.46
1:D:99:TYR:HB3	1:D:114:HIS:CD2	2.51	0.46
5:H:19:ILE:HB	5:H:78:LEU:HB2	1.97	0.46
4:I:-2:PHE:HE1	5:J:46:ILE:HA	1.81	0.46
2:E:41:LYS:O	2:E:43:GLY:N	2.48	0.46
4:G:18:THR:HG22	4:G:85:SER:HA	1.97	0.46
5:J:85:HIS:O	5:J:89:TYR:OH	2.28	0.46
1:A:102:ASP:OD1	1:A:113:TYR:OH	2.32	0.46
5:H:10:TYR:CE2	5:H:107:ARG:HD3	2.51	0.46
4:I:131:ASP:HB2	5:J:125:PHE:CE2	2.51	0.46
4:I:156:ASP:OD2	4:I:159:VAL:N	2.34	0.46
1:A:133:TRP:HB2	1:A:144:LYS:HG3	1.98	0.45
1:A:16:GLY:O	1:A:18:GLY:N	2.49	0.45
1:A:178:THR:O	1:A:181:ARG:NE	2.49	0.45
4:I:167:LEU:HD21	5:J:190:ARG:HB2	1.98	0.45
4:I:162:THR:HG21	5:J:190:ARG:NH1	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:152:SER:H	4:G:197:SER:HB2	1.81	0.45
5:J:57:LYS:C	5:J:59:ASP:H	2.19	0.45
1:A:14:ARG:HH21	1:A:21:ARG:HG2	1.82	0.45
2:E:17:ASN:HA	2:E:72:PRO:HG2	1.98	0.45
1:D:82:ARG:NE	1:D:87:GLN:O	2.35	0.45
1:A:14:ARG:NH2	1:A:21:ARG:HG2	2.32	0.45
2:B:98:ASP:N	2:B:98:ASP:OD1	2.50	0.45
1:A:258:THR:HB	1:A:271:THR:OG1	2.17	0.45
4:G:0:MET:HG3	4:G:2:GLN:H	1.82	0.45
5:H:115:LYS:HE3	5:H:222:GLN:OE1	2.17	0.45
5:H:49:SER:OG	5:H:54:SER:O	2.18	0.45
1:A:129:ASP:O	1:A:131:ARG:HD2	2.18	0.44
1:D:6:ARG:HH12	2:E:58:LYS:HE3	1.82	0.44
5:J:25:GLN:HB3	5:J:25:GLN:HE21	1.55	0.44
1:A:66:LYS:HE3	3:C:2:LEU:HB2	2.00	0.44
1:D:27:TYR:CE1	1:D:32:GLN:HB2	2.52	0.44
1:A:111:ARG:HG3	1:A:128:GLU:OE2	2.18	0.44
1:A:183:ASP:H	1:A:209:TYR:HE1	1.65	0.44
4:G:40:PHE:HB2	4:G:98:ALA:HB3	1.99	0.44
4:I:198:ILE:HD11	4:G:148:GLN:HB3	2.00	0.44
4:I:40:PHE:HB2	4:I:98:ALA:HB3	2.00	0.44
5:H:113:ASP:OD1	5:H:115:LYS:NZ	2.42	0.43
1:A:176:LYS:HG3	1:A:177:GLU:H	1.83	0.43
1:A:249:VAL:HA	1:A:250:PRO:HD3	1.88	0.43
1:D:232:GLU:HB2	2:E:8:GLN:NE2	2.33	0.43
5:H:226:LYS:HA	5:H:227:PRO:HD3	1.88	0.43
4:I:47:SER:O	4:I:49:GLN:N	2.51	0.43
4:I:8:GLN:HA	4:I:9:PRO:HD3	1.85	0.43
4:I:166:VAL:N	5:J:168:CYS:SG	2.92	0.43
5:J:200:ASN:HB3	5:J:203:ASN:ND2	2.34	0.43
2:B:5:PRO:HD3	2:B:84:HIS:HD1	1.84	0.43
5:H:7:THR:HG1	5:H:22:GLU:H	1.65	0.43
4:I:68:ARG:NH2	4:I:87:SER:HA	2.33	0.43
1:D:46:GLU:HA	1:D:47:PRO:HD3	1.79	0.43
2:B:79:ALA:HA	2:B:94:LYS:HA	2.00	0.43
1:D:186:LYS:HD3	1:D:207:SER:HB2	2.00	0.43
1:D:219:ARG:HH12	1:D:223:ASP:HA	1.83	0.43
1:A:28:VAL:HG23	1:A:33:PHE:CE2	2.54	0.42
1:A:13:SER:HG	1:A:93:HIS:H	1.66	0.42
2:B:5:PRO:HB3	2:B:30:PHE:HB3	2.00	0.42
5:J:150:ASP:OD1	5:J:150:ASP:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:63:ASN:HB3	4:G:71:VAL:HG13	2.02	0.42
5:J:127:PRO:HD2	5:J:198:TRP:CZ2	2.54	0.42
1:D:214:THR:OG1	1:D:262:GLN:HB3	2.19	0.42
4:G:156:ASP:HB3	4:G:159:VAL:HG12	2.01	0.42
5:H:33:TYR:CE2	5:H:94:ARG:HD2	2.53	0.42
1:D:181:ARG:CZ	1:D:209:TYR:HB2	2.49	0.42
2:B:31:HIS:HB3	2:B:32:PRO:HD3	2.01	0.42
5:J:19:ILE:HB	5:J:78:LEU:HB2	2.02	0.42
5:H:199:GLN:HA	5:H:239:ARG:O	2.20	0.42
2:B:32:PRO:O	2:B:34:ASP:N	2.43	0.42
5:J:170:ASP:HA	5:J:171:PRO:HD3	1.94	0.42
5:J:127:PRO:HD3	5:J:140:LEU:HG	2.02	0.41
1:A:13:SER:O	1:A:92:SER:OG	2.21	0.41
1:A:184:ALA:HA	1:A:185:PRO:HD3	1.90	0.41
1:A:22:PHE:HB3	1:A:38:SER:HB3	2.01	0.41
5:H:25:GLN:HE21	5:H:29:HIS:N	2.18	0.41
4:G:68:ARG:HB3	4:G:85:SER:O	2.20	0.41
5:H:6:GLN:HG3	5:H:104:PRO:HD2	2.02	0.41
1:A:24:ALA:HB3	1:A:36:PHE:HB3	2.02	0.41
1:D:85:TYR:OH	1:D:137:ASP:OD2	2.24	0.41
5:J:6:GLN:HG3	5:J:105:GLY:H	1.85	0.41
1:A:106:ASP:N	1:A:106:ASP:OD1	2.54	0.41
1:A:87:GLN:OE1	1:A:118:TYR:OH	2.18	0.41
5:H:204:HIS:HB2	5:H:237:TRP:CH2	2.56	0.41
1:A:234:ARG:HD3	2:B:8:GLN:OE1	2.21	0.41
5:J:174:LEU:N	5:J:186:CYS:O	2.47	0.41
1:A:22:PHE:HE1	1:A:74:HIS:HD1	1.69	0.41
5:H:215:SER:N	5:H:218:ASP:OD2	2.51	0.41
4:I:54:ILE:HG21	4:I:71:VAL:HG21	2.02	0.41
2:E:18:GLY:C	2:E:19:LYS:HD2	2.41	0.41
5:J:214:LEU:O	5:J:228:VAL:HG13	2.21	0.41
1:A:97:ARG:NH1	6:A:311:HOH:O	2.46	0.41
1:D:138:MET:H	1:D:138:MET:HG2	1.59	0.41
1:D:3:HIS:HB2	1:D:103:VAL:HG12	2.03	0.41
2:E:59:ASP:OD1	2:E:59:ASP:N	2.53	0.41
4:G:44:GLN:HB2	4:G:50:MET:HE3	2.02	0.41
4:I:162:THR:HB	4:I:180:VAL:H	1.85	0.41
5:J:45:LEU:HD21	5:J:48:TYR:CD2	2.56	0.41
4:I:47:SER:C	4:I:49:GLN:H	2.24	0.40
1:A:266:LEU:HD22	1:A:266:LEU:HA	1.93	0.40
2:B:87:LEU:HD23	2:B:91:LYS:H	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:172:LEU:HA	1:D:179:LEU:HD12	2.03	0.40
1:D:234:ARG:HE	1:D:234:ARG:HB2	1.71	0.40
2:E:20:SER:HA	2:E:71:THR:HA	2.03	0.40
2:E:58:LYS:H	2:E:58:LYS:HD2	1.86	0.40
4:G:57:GLU:N	4:G:57:GLU:OE1	2.54	0.40
4:I:119:ILE:HD11	4:I:146:ASP:HA	2.03	0.40
5:J:25:GLN:HG2	5:J:27:MET:H	1.86	0.40
5:H:200:ASN:HA	5:H:201:PRO:HD3	1.94	0.40
1:D:213:ILE:HD13	1:D:263:HIS:CD2	2.56	0.40
2:E:83:ASN:HB2	2:E:90:PRO:HB3	2.04	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	241/275 (88%)	228 (95%)	8 (3%)	5 (2%)	9 10
1	D	247/275 (90%)	240 (97%)	5 (2%)	2 (1%)	24 35
2	B	95/100 (95%)	89 (94%)	4 (4%)	2 (2%)	9 10
2	E	94/100 (94%)	88 (94%)	4 (4%)	2 (2%)	9 10
3	C	8/10 (80%)	7 (88%)	0	1 (12%)	0 0
3	F	8/10 (80%)	7 (88%)	0	1 (12%)	0 0
4	G	203/211 (96%)	194 (96%)	8 (4%)	1 (0%)	34 48
4	I	203/211 (96%)	188 (93%)	10 (5%)	5 (2%)	7 7
5	H	239/245 (98%)	230 (96%)	9 (4%)	0	100 100
5	J	238/245 (97%)	222 (93%)	9 (4%)	7 (3%)	6 5
All	All	1576/1682 (94%)	1493 (95%)	57 (4%)	26 (2%)	12 16

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	176	LYS
2	B	97	ARG
3	C	6	VAL
1	D	176	LYS
3	F	6	VAL
4	I	62	GLN
4	I	207	SER
5	J	8	PRO
5	J	176	GLU
1	A	226	GLN
2	E	42	ASN
4	I	48	ARG
4	I	206	PRO
5	J	9	ARG
5	J	58	GLY
4	G	101	GLU
1	A	17	ARG
1	A	249	VAL
2	B	31	HIS
1	D	196	ASP
4	I	134	SER
5	J	177	GLN
1	A	163	THR
2	E	31	HIS
5	J	100	GLN
5	J	172	GLN

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	219/231 (95%)	209 (95%)	10 (5%)	33 51
1	D	221/231 (96%)	214 (97%)	7 (3%)	46 68
2	B	94/95 (99%)	93 (99%)	1 (1%)	80 92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	E	94/95 (99%)	91 (97%)	3 (3%)	46 68
3	C	7/8 (88%)	7 (100%)	0	100 100
3	F	7/8 (88%)	7 (100%)	0	100 100
4	G	187/192 (97%)	181 (97%)	6 (3%)	46 68
4	I	187/192 (97%)	179 (96%)	8 (4%)	35 55
5	H	214/218 (98%)	205 (96%)	9 (4%)	36 56
5	J	213/218 (98%)	207 (97%)	6 (3%)	51 72
All	All	1443/1488 (97%)	1393 (96%)	50 (4%)	43 64

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	GLU
1	A	70	HIS
1	A	113	TYR
1	A	132	SER
1	A	182	THR
1	A	188	HIS
1	A	192	HIS
1	A	225	THR
1	A	249	VAL
1	A	266	LEU
2	B	87	LEU
1	D	21	ARG
1	D	188	HIS
1	D	192	HIS
1	D	216	THR
1	D	219	ARG
1	D	222	GLU
1	D	225	THR
2	E	19	LYS
2	E	37	VAL
2	E	49	VAL
4	I	53	VAL
4	I	68	ARG
4	I	119	ILE
4	I	137	LYS
4	I	148	GLN
4	I	153	GLN
4	I	156	ASP

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Mol	Chain	Res	Type
4	I	199	ILE
5	J	6	GLN
5	J	7	THR
5	J	25	GLN
5	J	99	GLU
5	J	100	GLN
5	J	190	ARG
4	G	50	MET
4	G	53	VAL
4	G	65	THR
4	G	66	GLU
4	G	82	LEU
4	G	136	ASP
5	H	6	GLN
5	H	7	THR
5	H	25	GLN
5	H	30	ASP
5	H	57	LYS
5	H	94	ARG
5	H	181	ASN
5	H	190	ARG
5	H	214	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
5	J	199	GLN
5	H	208	GLN

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	261/275 (94%)	-0.14	23 (8%) 12 12	29, 56, 143, 254	0
1	D	262/275 (95%)	-0.20	17 (6%) 22 22	35, 65, 151, 193	0
2	B	99/100 (99%)	-0.28	4 (4%) 42 43	43, 89, 140, 166	0
2	E	98/100 (98%)	0.22	11 (11%) 7 7	51, 101, 166, 203	0
3	C	10/10 (100%)	-0.81	0 100 100	33, 43, 53, 54	0
3	F	10/10 (100%)	-0.74	0 100 100	46, 52, 61, 72	0
4	G	207/211 (98%)	-0.84	0 100 100	29, 54, 94, 118	0
4	I	207/211 (98%)	-0.69	2 (0%) 84 83	26, 60, 106, 153	1 (0%)
5	H	241/245 (98%)	-0.69	3 (1%) 81 81	26, 46, 94, 178	0
5	J	240/245 (97%)	-0.72	2 (0%) 87 87	25, 49, 86, 139	0
All	All	1635/1682 (97%)	-0.47	62 (3%) 44 45	25, 57, 135, 254	1 (0%)

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	211	ALA	13.0
1	D	190	THR	8.6
1	A	274	TRP	7.6
1	D	257	TYR	6.2
1	D	211	ALA	6.0
1	D	220	ASP	5.6
1	A	257	TYR	5.4
5	H	241	ASP	5.2
4	I	64	ALA	5.0
2	E	95	TRP	5.0
2	E	75	LYS	4.8
1	A	189	MET	4.7
2	E	97	ARG	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	248	VAL	4.6
5	H	179	ALA	4.5
2	E	46	ILE	4.4
1	A	249	VAL	4.3
1	A	193	ALA	4.3
2	E	15	ALA	4.2
1	A	258	THR	3.9
1	A	250	PRO	3.8
1	A	262	GLN	3.7
1	D	201	LEU	3.7
2	E	31	HIS	3.7
1	D	258	THR	3.5
5	H	180	LEU	3.5
2	E	96	ASP	3.4
1	A	202	ARG	3.4
1	D	273	ARG	3.4
1	A	184	ALA	3.2
4	I	66	GLU	3.2
1	D	197	HIS	3.2
1	A	272	LEU	3.0
1	D	272	LEU	3.0
2	E	94	LYS	3.0
2	B	23	LEU	3.0
1	A	183	ASP	3.0
1	D	191	HIS	2.9
1	A	270	LEU	2.9
1	A	218	GLN	2.8
2	E	48	LYS	2.8
1	A	215	LEU	2.8
2	B	0	MET	2.7
1	D	256	ARG	2.5
1	D	265	GLY	2.5
1	D	215	LEU	2.5
1	A	259	CYS	2.5
2	E	35	ILE	2.5
2	B	48	LYS	2.5
1	D	203	CYS	2.5
1	D	198	GLU	2.5
1	A	266	LEU	2.4
1	D	202	ARG	2.3
2	E	16	GLU	2.3
1	A	182	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	192	HIS	2.3
5	J	171	PRO	2.2
1	A	222	GLU	2.2
1	A	231	VAL	2.1
2	B	31	HIS	2.0
1	A	219	ARG	2.0
5	J	7	THR	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.