Full wwPDB X-ray Structure Validation Report (i)

Jan 25, 2017 – 02:28 PM EST

PDB ID	:	1IC8
Title	:	HEPATOCYTE NUCLEAR FACTOR 1A BOUND TO DNA : MODY3 GENE PRODUCT
Authors	:	Chi, Y-.I.; Frantz, J.D.; Oh, B-.C.; Hansen, L.; Dhe-Paganon, S.; Shoelson, S.E.
Deposited on	:	2001-03-30
Resolution	:	2.60 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:

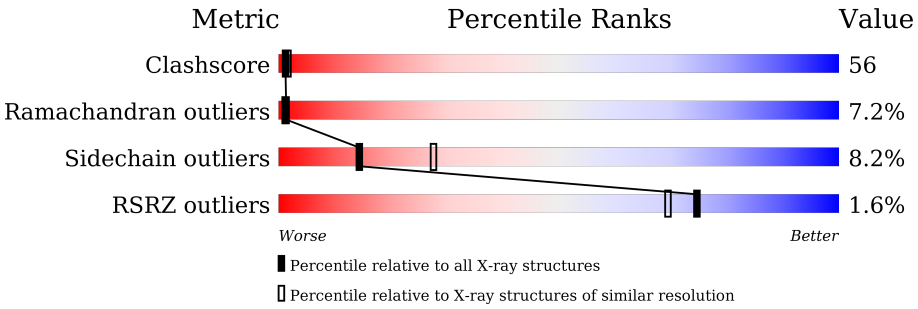
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

1 Overall quality at a glance

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

The reported resolution of this entry is 2.60 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	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	E	21	19% 81%
2	F	21	19% 81%
3	A	194	2% 20% 57% 9% • 12%
3	B	194	27% 56% 6% • 11%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3826 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 DNA chain called 5'-D(*CP*TP*TP*GP*GP*TP*TP*AP*AP*TP*AP*AP*TP*TP*CP*AP*CP*CP*AP*GP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	21	Total	C	N	O	P	0	0	0
			426	206	76	124	20			

- Molecule 2 is a DNA chain called 5'-D(*TP*CP*TP*GP*GP*TP*GP*AP*AP*TP*TP*AP*TP*TP*AP*AP*CP*CP*AP*AP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	21	Total	C	N	O	P	0	0	0
			429	207	78	124	20			

- Molecule 3 is a protein called HEPATOCYTE NUCLEAR FACTOR 1-ALPHA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	170	Total	C	N	O	S	0	0	0
			1399	868	266	261	4			
3	B	173	Total	C	N	O	S	0	0	0
			1433	892	272	265	4			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	45	Total	O	0	0
			45	45		
4	B	60	Total	O	0	0
			60	60		
4	E	18	Total	O	0	0
			18	18		
4	F	16	Total	O	0	0
			16	16		

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: 5'-D(*CP*TP*TP*GP*GP*TP*TP*AP*AP*TP*AP*AP*TP*TP*CP*AP*CP*CP*AP*GP*A)-3'

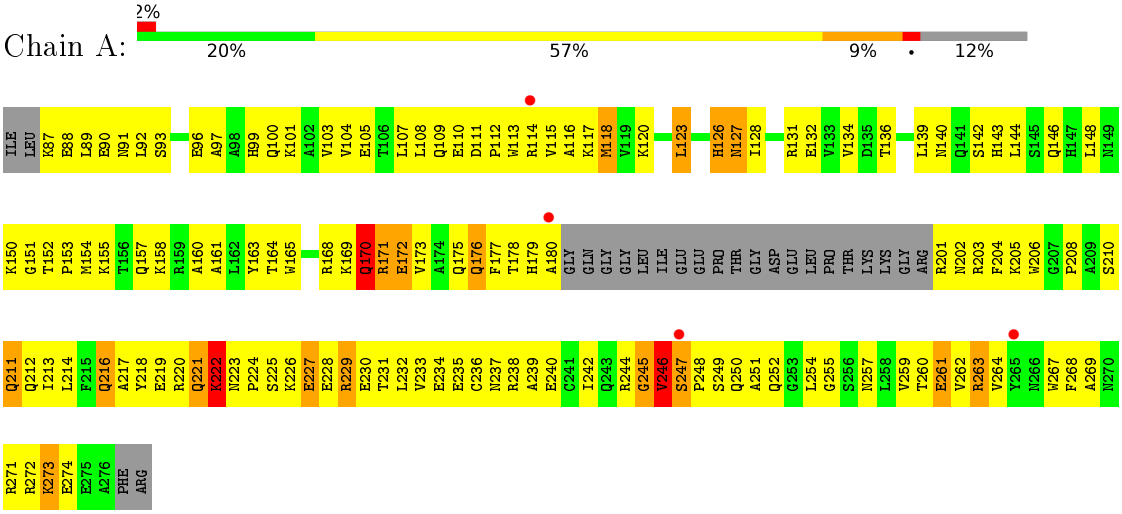
Chain E:

• Molecule 2: 5'-D(*TP*CP*TP*GP*GP*TP*GP*AP*AP*TP*TP*AP*TP*TP*AP*AP*CP*CP*AP*AP*G)-3'

Chain F:

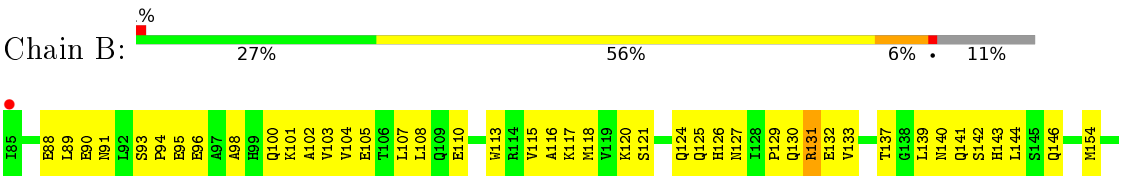
• Molecule 3: HEPATOCYTE NUCLEAR FACTOR 1-ALPHA

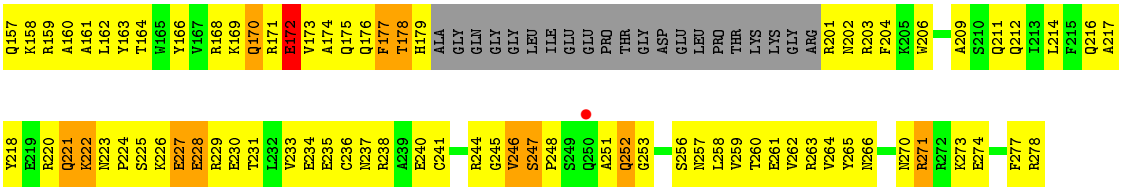
Chain A:



• Molecule 3: HEPATOCYTE NUCLEAR FACTOR 1-ALPHA

Chain B:




Q157 K158 R159 A160 A161 L162 Y163 T164 W165 Y166 V167 R168 K169 Q170 R171 E172 V173 A174 Q175 Q176 F177 T178 H179 ALA GLY GLN GLY GLY LEU ILE GLU GLU PRO THR GLY ASP GLU LEU PRO THR LYS LYS GLY ARG R201 N202 R203 F204 K205 W206 A209 S210 Q211 Q212 I213 L214 F215 Q216 A217
Y218 E219 R220 Q221 K222 N223 P224 S225 K226 E227 E228 R229 E230 T231 L232 V233 E234 E235 C236 N237 R238 A239 E240 C241 R244 G245 V246 S247 P248 S249 Q250 A251 Q252 G253 S256 N257 L258 V259 T260 E261 V262 R263 V264 Y265 N266 N270 R271 R272 K273 E274 F277 R278

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α, β, γ	50.39Å 50.39Å 207.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.40 – 2.60 29.36 – 2.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) (29.40-2.60) 93.5 (29.36-2.60)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.82 (at 2.61Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.254 , 0.312 0.267 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	60.5	Xtriage
Anisotropy	0.497	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 48.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.477 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	3826	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.89% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	E	0.58	0/477	0.78	0/734
2	F	0.54	0/481	0.77	0/741
3	A	0.48	0/1426	0.75	3/1923 (0.2%)
3	B	0.47	0/1461	0.67	1/1968 (0.1%)
All	All	0.50	0/3845	0.73	4/5366 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	171	ARG	NE-CZ-NH2	7.21	123.91	120.30
3	B	220	ARG	NE-CZ-NH2	6.69	123.64	120.30
3	A	263	ARG	NE-CZ-NH2	6.42	123.51	120.30
3	A	118	MET	CG-SD-CE	5.47	108.95	100.20

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	E	426	0	240	44	0
2	F	429	0	240	48	0
3	A	1399	0	1378	162	0
3	B	1433	0	1417	148	0
4	A	45	0	0	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	60	0	0	4	0
4	E	18	0	0	0	0
4	F	16	0	0	2	0
All	All	3826	0	3275	385	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 56.

All (385) 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:F:404:DG:H2"	2:F:405:DG:H5"	1.12	1.08
3:A:127:ASN:HB3	3:A:257:ASN:ND2	1.72	1.03
3:A:176:GLN:HG2	3:A:246:VAL:HG11	1.36	1.03
3:A:222:LYS:H	3:A:222:LYS:HD3	1.20	1.03
1:E:304:DG:H2"	1:E:305:DG:H5"	1.41	1.00
2:F:404:DG:C2'	2:F:405:DG:H5"	1.94	0.97
1:E:304:DG:H2"	1:E:305:DG:C5'	1.95	0.97
2:F:405:DG:H2"	2:F:406:DT:H5'	1.46	0.95
3:A:237:ASN:HD21	3:A:259:VAL:H	1.11	0.94
2:F:401:DT:H1'	2:F:402:DC:O5'	1.68	0.94
3:B:225:SER:OG	3:B:228:GLU:HB2	1.71	0.91
2:F:404:DG:H2"	2:F:405:DG:C5'	2.00	0.90
3:A:248:PRO:HG2	3:A:251:ALA:HB2	1.51	0.90
3:A:247:SER:H	3:A:248:PRO:CD	1.87	0.87
3:B:93:SER:HB3	3:B:96:GLU:HB3	1.56	0.87
3:A:260:THR:OG1	3:A:262:VAL:HG22	1.75	0.86
3:B:171:ARG:HG3	3:B:172:GLU:N	1.90	0.85
3:A:232:LEU:HA	3:A:235:GLU:HB3	1.61	0.81
3:A:216:GLN:HB3	3:A:220:ARG:HH12	1.47	0.80
3:A:252:GLN:HA	4:A:1104:HOH:O	1.82	0.79
3:B:140:ASN:ND2	3:B:143:HIS:H	1.80	0.79
3:A:93:SER:HB3	3:A:96:GLU:HB3	1.65	0.79
3:A:223:ASN:HA	4:A:1082:HOH:O	1.82	0.78
3:B:154:MET:HE2	3:B:159:ARG:N	1.98	0.78
3:B:127:ASN:HB3	3:B:257:ASN:OD1	1.84	0.78
3:A:127:ASN:HB3	3:A:257:ASN:HD21	1.46	0.78
3:A:87:LYS:HE2	3:A:87:LYS:HA	1.65	0.77
3:A:223:ASN:HD21	3:A:225:SER:HB3	1.50	0.77
1:E:304:DG:C2'	1:E:305:DG:H5"	2.15	0.77
2:F:401:DT:H2"	2:F:402:DC:OP2	1.83	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:121:SER:O	3:B:125:GLN:HG2	1.84	0.76
3:B:172:GLU:O	3:B:172:GLU:HG2	1.86	0.75
3:A:127:ASN:HB3	3:A:257:ASN:HD22	1.52	0.74
3:A:140:ASN:ND2	3:A:143:HIS:H	1.84	0.74
3:A:221:GLN:OE1	3:A:223:ASN:HB3	1.87	0.74
3:B:237:ASN:ND2	3:B:259:VAL:HB	2.02	0.74
1:E:312:DA:H2"	1:E:313:DT:H5'	1.69	0.73
1:E:320:DG:H2"	1:E:321:DA:C8	2.24	0.73
3:A:134:VAL:HG13	3:A:139:LEU:O	1.89	0.73
3:A:217:ALA:HB2	3:A:232:LEU:HD11	1.69	0.73
2:F:417:DC:OP1	2:F:417:DC:H4'	1.86	0.73
3:B:140:ASN:HD22	3:B:143:HIS:HB2	1.52	0.73
3:A:151:GLY:HA3	3:B:277:PHE:HB2	1.71	0.72
3:B:251:ALA:O	3:B:253:GLY:N	2.22	0.72
3:B:271:ARG:O	3:B:274:GLU:HB3	1.89	0.72
3:B:240:GLU:O	3:B:244:ARG:HG2	1.89	0.72
2:F:401:DT:H1'	2:F:402:DC:P	2.31	0.71
3:A:260:THR:O	3:A:264:VAL:HG23	1.91	0.71
3:A:272:ARG:HG3	3:A:272:ARG:HH11	1.55	0.70
3:B:93:SER:HB3	3:B:96:GLU:CB	2.20	0.70
3:B:169:LYS:C	3:B:171:ARG:H	1.95	0.70
3:A:222:LYS:N	3:A:222:LYS:HD3	2.00	0.70
3:B:225:SER:O	3:B:228:GLU:N	2.22	0.69
3:B:107:LEU:HD22	3:B:115:VAL:HG13	1.73	0.69
3:A:247:SER:H	3:A:248:PRO:HD3	1.57	0.69
2:F:418:DC:H2"	2:F:419:DA:C8	2.27	0.69
3:A:238:ARG:O	3:A:242:ILE:HG13	1.93	0.69
3:B:216:GLN:C	3:B:218:TYR:H	1.96	0.69
3:B:247:SER:N	3:B:248:PRO:CD	2.56	0.68
3:A:178:THR:C	3:A:180:ALA:H	1.97	0.68
3:A:236:CYS:HB3	3:A:259:VAL:HG21	1.75	0.68
3:B:101:LYS:O	3:B:105:GLU:HB2	1.94	0.68
3:B:246:VAL:O	3:B:246:VAL:HG23	1.94	0.68
3:B:140:ASN:HD21	3:B:142:SER:HB3	1.58	0.67
3:B:216:GLN:O	3:B:218:TYR:N	2.28	0.67
3:A:269:ALA:O	3:A:272:ARG:HB2	1.94	0.67
3:B:248:PRO:HB2	3:B:251:ALA:HB2	1.77	0.67
3:A:169:LYS:C	3:A:171:ARG:H	1.97	0.67
3:B:240:GLU:OE1	3:B:244:ARG:NH2	2.28	0.66
2:F:408:DA:H2"	2:F:409:DA:H5'	1.75	0.66
3:B:172:GLU:HA	3:B:175:GLN:HG3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:127:ASN:HD21	3:A:205:LYS:HD2	1.61	0.66
1:E:304:DG:H2"	1:E:305:DG:H5'	1.75	0.66
1:E:320:DG:H2"	1:E:321:DA:N7	2.11	0.66
3:A:113:TRP:O	3:A:117:LYS:HG2	1.96	0.66
3:A:229:ARG:O	3:A:233:VAL:HG23	1.97	0.65
3:A:210:SER:O	3:A:213:ILE:HG22	1.96	0.65
3:B:164:THR:HG22	3:B:168:ARG:HD2	1.78	0.65
1:E:308:DA:H2"	1:E:309:DA:C5'	2.27	0.65
3:B:140:ASN:HD22	3:B:143:HIS:H	1.43	0.65
2:F:416:DA:H2'	2:F:417:DC:C6	2.32	0.65
3:A:131:ARG:HG2	4:A:1079:HOH:O	1.96	0.65
3:A:206:TRP:CE3	3:A:214:LEU:HD11	2.31	0.65
3:A:247:SER:N	3:A:248:PRO:CD	2.59	0.64
1:E:315:DC:C2'	1:E:316:DA:H5"	2.28	0.64
1:E:315:DC:H42	2:F:407:DG:H1	1.45	0.64
3:A:237:ASN:HD21	3:A:259:VAL:N	1.89	0.64
2:F:408:DA:H3'	4:F:1030:HOH:O	1.96	0.64
2:F:405:DG:H2"	2:F:406:DT:C5'	2.22	0.64
3:A:140:ASN:HD22	3:A:143:HIS:H	1.46	0.64
3:A:211:GLN:HA	3:A:214:LEU:HD12	1.79	0.63
3:A:90:GLU:O	3:A:92:LEU:N	2.28	0.63
3:A:97:ALA:O	3:A:101:LYS:HG2	1.99	0.63
3:A:170:GLN:NE2	3:A:170:GLN:N	2.46	0.63
3:B:247:SER:N	3:B:248:PRO:HD3	2.14	0.63
3:A:127:ASN:ND2	3:A:205:LYS:HB3	2.14	0.63
1:E:315:DC:N3	2:F:407:DG:N2	2.40	0.63
3:A:240:GLU:OE1	3:A:244:ARG:NH2	2.32	0.62
1:E:308:DA:H1'	1:E:309:DA:H5"	1.80	0.62
3:A:229:ARG:HG2	3:A:229:ARG:HH11	1.64	0.62
3:A:261:GLU:N	3:A:261:GLU:CD	2.52	0.62
3:B:157:GLN:O	3:B:160:ALA:HB3	2.00	0.62
2:F:403:DT:H2"	2:F:404:DG:C8	2.34	0.62
3:B:238:ARG:HG2	3:B:238:ARG:HH11	1.64	0.62
1:E:315:DC:H2"	1:E:316:DA:H5"	1.80	0.62
1:E:304:DG:N7	3:A:273:LYS:NZ	2.37	0.61
3:A:140:ASN:HD22	3:A:143:HIS:HB2	1.65	0.61
2:F:414:DT:H6	2:F:414:DT:H5'	1.65	0.61
3:B:172:GLU:HB2	3:B:175:GLN:OE1	2.01	0.60
2:F:418:DC:H2"	2:F:419:DA:N7	2.16	0.60
3:B:129:PRO:CD	3:B:202:ASN:HD21	2.14	0.60
2:F:421:DG:H5'	4:F:1131:HOH:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:260:THR:OG1	3:B:263:ARG:HG2	2.01	0.60
3:B:154:MET:HE2	3:B:159:ARG:CA	2.32	0.60
3:A:261:GLU:C	3:A:263:ARG:H	2.02	0.60
1:E:305:DG:O6	3:A:273:LYS:HE3	2.02	0.60
3:B:131:ARG:HH21	3:B:132:GLU:HA	1.66	0.60
3:B:171:ARG:CG	3:B:172:GLU:N	2.65	0.59
3:B:248:PRO:HB2	3:B:251:ALA:CB	2.32	0.59
3:B:216:GLN:C	3:B:218:TYR:N	2.56	0.59
3:A:263:ARG:HG2	3:A:263:ARG:HH11	1.66	0.59
3:A:272:ARG:HG3	3:A:272:ARG:NH1	2.15	0.59
2:F:406:DT:OP1	3:A:155:LYS:HB2	2.02	0.59
2:F:401:DT:C1'	2:F:402:DC:O5'	2.48	0.59
3:A:146:GLN:O	3:A:150:LYS:O	2.21	0.59
3:A:234:GLU:O	3:A:238:ARG:HG3	2.03	0.59
2:F:401:DT:C2'	2:F:402:DC:OP2	2.51	0.59
3:A:225:SER:C	3:A:227:GLU:H	2.06	0.58
3:A:225:SER:OG	3:A:228:GLU:HB2	2.02	0.58
3:B:169:LYS:O	3:B:171:ARG:N	2.36	0.58
3:B:204:PHE:HD1	3:B:257:ASN:HA	1.68	0.58
3:B:274:GLU:HB2	4:B:1101:HOH:O	2.01	0.58
1:E:308:DA:H2"	1:E:309:DA:H5"	1.85	0.58
3:A:178:THR:O	3:A:180:ALA:N	2.36	0.58
3:A:169:LYS:O	3:A:171:ARG:N	2.37	0.58
1:E:302:DT:H2"	1:E:303:DT:C6	2.39	0.58
3:A:224:PRO:HD3	3:A:272:ARG:NH2	2.19	0.58
3:A:170:GLN:C	3:A:172:GLU:H	2.05	0.58
3:B:233:VAL:HG13	3:B:234:GLU:N	2.18	0.58
2:F:408:DA:H1'	2:F:409:DA:H5"	1.86	0.58
3:B:234:GLU:O	3:B:238:ARG:HG3	2.03	0.57
3:B:171:ARG:HG3	3:B:172:GLU:H	1.66	0.57
3:B:223:ASN:HD21	3:B:225:SER:CB	2.16	0.57
3:B:261:GLU:HG3	3:B:262:VAL:N	2.19	0.57
3:B:113:TRP:CH2	3:B:117:LYS:HD2	2.40	0.57
1:E:301:DC:H2'	1:E:302:DT:C6	2.39	0.57
3:A:163:TYR:N	3:A:163:TYR:CD1	2.72	0.57
3:A:247:SER:H	3:A:248:PRO:HD2	1.67	0.57
3:A:176:GLN:HG2	3:A:246:VAL:CG1	2.25	0.57
3:A:144:LEU:HD12	3:A:148:LEU:HD13	1.85	0.57
3:B:88:GLU:CG	3:B:91:ASN:HB2	2.35	0.57
1:E:315:DC:H1'	1:E:316:DA:H5"	1.86	0.57
3:A:260:THR:HG1	3:A:262:VAL:HG22	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:88:GLU:O	3:B:91:ASN:HB2	2.05	0.56
3:A:158:LYS:O	3:A:161:ALA:N	2.38	0.56
3:B:115:VAL:O	3:B:118:MET:HB2	2.06	0.56
3:A:93:SER:CB	3:A:96:GLU:HB3	2.35	0.56
3:A:230:GLU:HA	3:A:233:VAL:HG23	1.87	0.56
3:B:223:ASN:HD21	3:B:225:SER:HB3	1.70	0.56
1:E:308:DA:C2'	1:E:309:DA:H5"	2.35	0.56
3:B:261:GLU:O	3:B:264:VAL:HG22	2.06	0.55
3:B:246:VAL:C	3:B:248:PRO:HD2	2.26	0.55
3:B:241:CYS:HB3	3:B:247:SER:HA	1.89	0.55
3:A:163:TYR:HD1	3:A:163:TYR:N	2.04	0.55
3:A:230:GLU:HA	3:A:233:VAL:CG2	2.36	0.55
3:B:164:THR:HG22	3:B:168:ARG:CD	2.36	0.55
2:F:415:DA:H2"	2:F:416:DA:O5'	2.06	0.54
3:A:272:ARG:C	3:A:274:GLU:H	2.10	0.54
3:B:100:GLN:O	3:B:103:VAL:HG22	2.07	0.54
1:E:321:DA:C2	2:F:401:DT:C7	2.91	0.54
3:A:204:PHE:CG	3:A:263:ARG:HD3	2.42	0.54
3:B:177:PHE:C	3:B:179:HIS:H	2.11	0.54
3:B:88:GLU:HG3	3:B:91:ASN:HB2	1.90	0.54
1:E:302:DT:H2"	1:E:303:DT:H71	1.90	0.54
3:B:176:GLN:HB2	3:B:246:VAL:HG11	1.90	0.54
3:A:267:TRP:O	3:A:271:ARG:HG2	2.09	0.53
3:B:246:VAL:C	3:B:248:PRO:CD	2.77	0.53
3:B:154:MET:HE2	3:B:159:ARG:HA	1.90	0.53
3:B:176:GLN:NE2	3:B:246:VAL:HG21	2.23	0.53
3:B:172:GLU:HB2	3:B:175:GLN:CD	2.30	0.53
2:F:414:DT:H73	3:B:146:GLN:HE22	1.73	0.53
3:B:163:TYR:N	3:B:163:TYR:CD1	2.76	0.53
3:B:229:ARG:HH11	3:B:265:TYR:HB2	1.74	0.52
3:B:245:GLY:O	3:B:246:VAL:C	2.48	0.52
3:B:278:ARG:HE	3:B:278:ARG:HA	1.73	0.52
1:E:319:DA:H2"	1:E:320:DG:C8	2.43	0.52
3:A:93:SER:HB3	3:A:96:GLU:CB	2.38	0.52
3:B:206:TRP:HB3	3:B:211:GLN:CG	2.39	0.52
3:A:260:THR:OG1	3:A:263:ARG:HG3	2.10	0.52
2:F:416:DA:C2'	2:F:417:DC:C6	2.93	0.52
3:A:208:PRO:O	3:A:212:GLN:HG3	2.10	0.52
3:A:248:PRO:C	3:A:250:GLN:N	2.61	0.52
2:F:402:DC:H2'	2:F:403:DT:H72	1.92	0.52
3:A:210:SER:O	3:A:214:LEU:HG	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:206:TRP:O	3:B:211:GLN:NE2	2.43	0.52
3:A:206:TRP:CZ3	3:A:214:LEU:HD11	2.45	0.51
2:F:420:DA:H2"	2:F:421:DG:C8	2.45	0.51
3:A:107:LEU:HD22	3:A:115:VAL:HG13	1.91	0.51
3:B:221:GLN:O	3:B:223:ASN:N	2.44	0.51
3:B:252:GLN:HG3	3:B:258:LEU:HD11	1.91	0.51
3:B:96:GLU:O	3:B:100:GLN:HG3	2.11	0.51
1:E:301:DC:H2'	1:E:302:DT:H71	1.93	0.51
3:A:248:PRO:C	3:A:250:GLN:H	2.14	0.51
3:A:213:ILE:O	3:A:216:GLN:HB2	2.11	0.51
3:B:238:ARG:NH1	3:B:238:ARG:HG2	2.26	0.51
3:B:230:GLU:HA	3:B:233:VAL:HG12	1.93	0.50
3:A:100:GLN:O	3:A:103:VAL:HB	2.11	0.50
3:A:221:GLN:O	3:A:223:ASN:N	2.44	0.50
3:A:248:PRO:O	3:A:250:GLN:N	2.44	0.50
3:A:154:MET:HG2	3:A:158:LYS:HB2	1.93	0.50
3:B:102:ALA:O	3:B:105:GLU:HB3	2.12	0.50
3:B:90:GLU:HA	3:B:90:GLU:OE1	2.11	0.50
1:E:316:DA:H62	3:B:270:ASN:HD21	1.60	0.50
3:B:120:LYS:O	3:B:124:GLN:HG3	2.11	0.50
3:B:229:ARG:NH1	3:B:265:TYR:HB2	2.27	0.50
3:A:111:ASP:HB3	3:A:114:ARG:HD2	1.94	0.50
2:F:401:DT:C1'	2:F:402:DC:P	2.95	0.50
3:A:203:ARG:HD3	4:A:1010:HOH:O	2.12	0.50
2:F:416:DA:H2"	2:F:417:DC:O4'	2.11	0.50
3:A:271:ARG:O	3:A:274:GLU:HB2	2.12	0.50
3:A:169:LYS:C	3:A:171:ARG:N	2.66	0.49
3:A:178:THR:C	3:A:180:ALA:N	2.64	0.49
3:A:236:CYS:CB	3:A:259:VAL:HG21	2.42	0.49
3:A:214:LEU:HB3	3:A:267:TRP:CE3	2.47	0.49
3:A:204:PHE:CD2	3:A:263:ARG:HD3	2.46	0.49
3:A:126:HIS:CE1	3:A:244:ARG:HD3	2.48	0.49
3:A:233:VAL:CG2	3:A:261:GLU:OE2	2.61	0.49
3:B:169:LYS:C	3:B:171:ARG:N	2.64	0.49
1:E:303:DT:H2"	1:E:304:DG:C8	2.48	0.49
1:E:318:DC:H2"	1:E:319:DA:C8	2.48	0.49
3:A:99:HIS:O	3:A:103:VAL:HG23	2.13	0.49
3:B:209:ALA:HA	3:B:212:GLN:CD	2.32	0.49
3:A:272:ARG:O	3:A:274:GLU:N	2.46	0.49
2:F:405:DG:C2'	2:F:406:DT:H5'	2.33	0.48
3:A:104:VAL:O	3:A:108:LEU:HG	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:405:DG:H5'	3:A:153:PRO:HB2	1.95	0.48
3:B:103:VAL:HG23	3:B:104:VAL:N	2.28	0.48
3:B:221:GLN:C	3:B:223:ASN:H	2.16	0.48
3:B:104:VAL:HG23	3:B:105:GLU:N	2.28	0.48
3:A:168:ARG:HD3	3:A:171:ARG:NH2	2.29	0.48
3:A:227:GLU:C	3:A:229:ARG:H	2.17	0.48
3:A:205:LYS:HD3	3:A:206:TRP:N	2.28	0.48
3:A:216:GLN:O	3:A:217:ALA:C	2.51	0.48
1:E:312:DA:H1'	1:E:313:DT:H5"	1.95	0.48
3:A:217:ALA:O	3:A:221:GLN:N	2.32	0.48
3:B:176:GLN:CD	3:B:246:VAL:HG21	2.33	0.48
1:E:308:DA:C1'	1:E:309:DA:H5"	2.43	0.47
3:A:230:GLU:C	3:A:232:LEU:N	2.67	0.47
3:A:93:SER:O	3:A:97:ALA:N	2.36	0.47
3:B:176:GLN:CB	3:B:246:VAL:HG11	2.44	0.47
3:A:221:GLN:C	3:A:223:ASN:H	2.16	0.47
1:E:308:DA:H2"	1:E:309:DA:H5'	1.97	0.47
2:F:405:DG:O6	3:B:273:LYS:NZ	2.38	0.47
3:B:158:LYS:O	3:B:161:ALA:N	2.48	0.47
1:E:302:DT:C2'	1:E:303:DT:H71	2.44	0.47
2:F:402:DC:H2'	2:F:403:DT:C7	2.45	0.47
3:B:139:LEU:CD2	3:B:158:LYS:HB3	2.44	0.47
2:F:414:DT:C6	2:F:414:DT:H5'	2.48	0.47
3:A:88:GLU:O	3:A:89:LEU:HD23	2.15	0.47
3:B:129:PRO:CG	3:B:202:ASN:HD21	2.28	0.47
1:E:315:DC:C1'	1:E:316:DA:H5"	2.45	0.46
3:B:230:GLU:C	3:B:233:VAL:HG12	2.36	0.46
3:B:171:ARG:C	3:B:173:VAL:H	2.19	0.46
3:B:140:ASN:HD22	3:B:143:HIS:CB	2.24	0.46
3:B:204:PHE:CD1	3:B:257:ASN:HA	2.49	0.46
3:A:126:HIS:O	3:A:127:ASN:C	2.54	0.46
3:A:146:GLN:C	3:A:152:THR:HG1	2.18	0.46
3:A:230:GLU:C	3:A:232:LEU:H	2.18	0.46
3:A:246:VAL:HG23	3:A:247:SER:N	2.29	0.46
2:F:417:DC:H2'	2:F:418:DC:C6	2.51	0.46
3:B:130:GLN:OE1	3:B:141:GLN:NE2	2.43	0.46
3:B:154:MET:CE	3:B:159:ARG:HA	2.46	0.46
3:B:176:GLN:HB3	3:B:246:VAL:HG21	1.97	0.46
3:B:278:ARG:NE	3:B:278:ARG:HA	2.30	0.46
1:E:307:DT:H2"	1:E:308:DA:N7	2.30	0.46
3:A:268:PHE:O	3:A:272:ARG:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:173:VAL:HG22	4:A:1005:HOH:O	2.16	0.45
3:A:232:LEU:HA	3:A:235:GLU:CB	2.40	0.45
3:B:178:THR:O	3:B:179:HIS:C	2.55	0.45
1:E:316:DA:H8	1:E:316:DA:H5'	1.81	0.45
3:A:247:SER:N	3:A:248:PRO:HD2	2.30	0.45
3:A:236:CYS:O	3:A:239:ALA:HB3	2.15	0.45
3:A:237:ASN:ND2	3:A:259:VAL:HB	2.32	0.45
3:B:233:VAL:HG23	3:B:259:VAL:HG12	1.97	0.45
3:A:216:GLN:O	3:A:218:TYR:N	2.50	0.45
3:B:206:TRP:CH2	3:B:214:LEU:HD11	2.51	0.45
2:F:402:DC:OP1	3:B:224:PRO:HB2	2.17	0.45
3:A:254:LEU:O	3:A:255:GLY:C	2.54	0.44
3:A:171:ARG:O	3:A:175:GLN:HG3	2.18	0.44
3:A:216:GLN:O	3:A:219:GLU:N	2.50	0.44
3:A:204:PHE:CD1	3:A:263:ARG:HD3	2.52	0.44
3:A:228:GLU:HA	3:A:231:THR:OG1	2.17	0.44
3:B:158:LYS:C	3:B:160:ALA:N	2.70	0.44
3:B:226:LYS:HA	3:B:229:ARG:HB2	1.99	0.44
3:B:229:ARG:C	3:B:231:THR:H	2.21	0.44
3:A:271:ARG:NH2	4:A:1071:HOH:O	2.50	0.44
3:A:225:SER:O	3:A:227:GLU:N	2.50	0.44
3:B:266:ASN:N	3:B:266:ASN:HD22	2.16	0.44
3:A:214:LEU:O	3:A:267:TRP:CZ3	2.71	0.44
2:F:414:DT:C7	3:B:146:GLN:HE22	2.31	0.44
3:B:176:GLN:CG	3:B:246:VAL:HG21	2.47	0.44
2:F:402:DC:OP1	3:B:224:PRO:CG	2.66	0.44
3:A:268:PHE:O	3:A:269:ALA:C	2.55	0.43
3:B:225:SER:C	3:B:227:GLU:N	2.68	0.43
3:B:246:VAL:O	3:B:246:VAL:CG2	2.65	0.43
3:A:229:ARG:HG2	3:A:229:ARG:NH1	2.31	0.43
3:B:95:GLU:O	3:B:98:ALA:HB3	2.18	0.43
3:A:104:VAL:HG12	3:A:108:LEU:CD1	2.48	0.43
3:A:272:ARG:C	3:A:274:GLU:N	2.71	0.43
3:B:171:ARG:O	3:B:173:VAL:N	2.51	0.43
3:A:233:VAL:HG22	3:A:261:GLU:OE2	2.19	0.43
3:B:104:VAL:O	3:B:108:LEU:HG	2.19	0.43
3:B:248:PRO:O	3:B:251:ALA:HB3	2.18	0.43
3:A:123:LEU:HD12	3:A:128:ILE:HB	2.01	0.43
3:A:217:ALA:HB3	3:A:268:PHE:HZ	1.84	0.43
1:E:302:DT:H2"	1:E:303:DT:C5	2.53	0.43
3:A:157:GLN:O	3:A:160:ALA:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:214:LEU:HD13	3:A:267:TRP:CD1	2.54	0.43
1:E:307:DT:H2"	1:E:308:DA:C8	2.54	0.43
3:A:168:ARG:HD3	3:A:171:ARG:HH21	1.83	0.43
3:A:201:ARG:HB2	3:A:202:ASN:H	1.61	0.43
3:B:133:VAL:HG11	3:B:144:LEU:HD21	2.01	0.43
3:A:92:LEU:HD23	3:A:92:LEU:C	2.39	0.42
1:E:304:DG:C2'	1:E:305:DG:C5'	2.82	0.42
3:A:217:ALA:HB3	3:A:268:PHE:CZ	2.54	0.42
3:B:169:LYS:HA	3:B:171:ARG:NH1	2.35	0.42
3:B:223:ASN:ND2	3:B:225:SER:HB3	2.34	0.42
1:E:301:DC:H2'	1:E:302:DT:C5	2.54	0.42
3:A:213:ILE:HD12	3:A:216:GLN:HG2	2.01	0.42
3:A:214:LEU:HD13	3:A:267:TRP:CG	2.53	0.42
3:B:104:VAL:CG2	3:B:105:GLU:N	2.82	0.42
3:B:137:THR:HB	3:B:139:LEU:HG	2.02	0.42
3:B:162:LEU:HD12	3:B:162:LEU:HA	1.79	0.42
3:B:236:CYS:C	3:B:238:ARG:N	2.73	0.42
3:A:114:ARG:O	3:A:118:MET:HG3	2.20	0.42
3:A:132:GLU:O	3:A:136:THR:HG23	2.19	0.42
3:A:164:THR:O	3:A:165:TRP:C	2.58	0.42
3:A:170:GLN:NE2	3:A:170:GLN:CA	2.83	0.42
3:A:261:GLU:C	3:A:263:ARG:N	2.69	0.42
3:B:142:SER:O	3:B:146:GLN:HG2	2.19	0.42
3:A:216:GLN:HG3	3:A:220:ARG:HH22	1.85	0.42
2:F:405:DG:C2'	2:F:406:DT:C5'	2.95	0.42
3:B:248:PRO:O	3:B:251:ALA:N	2.47	0.42
3:A:225:SER:C	3:A:227:GLU:N	2.69	0.42
3:A:245:GLY:O	3:A:246:VAL:O	2.37	0.42
3:B:233:VAL:HG13	3:B:234:GLU:H	1.85	0.42
3:B:235:GLU:O	3:B:238:ARG:HB2	2.19	0.42
3:B:133:VAL:HG13	3:B:137:THR:HG21	2.02	0.42
3:B:252:GLN:NE2	4:B:1056:HOH:O	2.53	0.42
3:B:177:PHE:O	3:B:179:HIS:N	2.47	0.41
3:A:213:ILE:O	3:A:216:GLN:N	2.53	0.41
3:B:125:GLN:NE2	4:B:1096:HOH:O	2.48	0.41
3:B:233:VAL:CG1	3:B:234:GLU:N	2.83	0.41
1:E:312:DA:C2'	1:E:313:DT:H5'	2.45	0.41
3:B:233:VAL:HG13	3:B:234:GLU:HG3	2.03	0.41
3:B:202:ASN:O	3:B:256:SER:HB2	2.20	0.41
3:A:112:PRO:O	3:A:116:ALA:N	2.47	0.41
3:A:96:GLU:O	3:A:99:HIS:HB3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:312:DA:H1'	1:E:313:DT:C5'	2.50	0.41
2:F:401:DT:O4'	2:F:402:DC:O4'	2.38	0.41
3:B:166:TYR:O	3:B:170:GLN:HG3	2.20	0.41
3:A:212:GLN:O	3:A:216:GLN:OE1	2.39	0.41
3:B:222:LYS:O	3:B:224:PRO:HD3	2.20	0.41
3:B:227:GLU:O	3:B:231:THR:OG1	2.38	0.41
2:F:417:DC:OP1	2:F:417:DC:C4'	2.62	0.41
3:A:224:PRO:HD3	4:A:1082:HOH:O	2.19	0.41
3:A:237:ASN:HD22	3:A:237:ASN:HA	1.63	0.41
3:B:116:ALA:O	3:B:117:LYS:C	2.59	0.41
3:B:126:HIS:HB3	4:B:1050:HOH:O	2.21	0.41
3:A:120:LYS:NZ	4:A:1004:HOH:O	2.54	0.41
3:B:163:TYR:O	3:B:166:TYR:HB3	2.21	0.41
2:F:405:DG:H1'	2:F:406:DT:H5"	2.04	0.41
2:F:414:DT:H73	3:B:146:GLN:NE2	2.36	0.41
3:A:140:ASN:HD22	3:A:143:HIS:N	2.16	0.40
3:A:140:ASN:O	3:A:143:HIS:N	2.53	0.40
3:B:172:GLU:C	3:B:174:ALA:N	2.72	0.40
3:B:223:ASN:ND2	3:B:228:GLU:OE1	2.54	0.40
3:B:251:ALA:C	3:B:253:GLY:N	2.75	0.40
2:F:408:DA:H2"	2:F:409:DA:C5'	2.49	0.40
1:E:316:DA:C2	2:F:406:DT:N3	2.80	0.40
3:B:137:THR:C	3:B:139:LEU:N	2.73	0.40
3:B:171:ARG:CG	3:B:172:GLU:H	2.29	0.40
1:E:305:DG:H2"	1:E:306:DT:O5'	2.21	0.40
1:E:316:DA:H2	2:F:406:DT:O2	2.04	0.40
1:E:319:DA:C2'	1:E:320:DG:C8	3.04	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
3	A	166/194 (86%)	126 (76%)	27 (16%)	13 (8%)	1 1
3	B	169/194 (87%)	124 (73%)	34 (20%)	11 (6%)	1 1
All	All	335/388 (86%)	250 (75%)	61 (18%)	24 (7%)	1 1

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	91	ASN
3	A	179	HIS
3	A	222	LYS
3	A	246	VAL
3	A	247	SER
3	B	246	VAL
3	B	252	GLN
3	A	245	GLY
3	A	273	LYS
3	B	89	LEU
3	B	170	GLN
3	B	172	GLU
3	B	217	ALA
3	B	222	LYS
3	A	170	GLN
3	A	226	LYS
3	A	249	SER
3	B	178	THR
3	A	216	GLN
3	B	110	GLU
3	A	110	GLU
3	A	127	ASN
3	B	247	SER
3	B	94	PRO

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
3	A	150/169 (89%)	134 (89%)	16 (11%)	8 15
3	B	154/169 (91%)	145 (94%)	9 (6%)	25 49
All	All	304/338 (90%)	279 (92%)	25 (8%)	14 27

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	105	GLU
3	A	109	GLN
3	A	123	LEU
3	A	126	HIS
3	A	142	SER
3	A	170	GLN
3	A	172	GLU
3	A	176	GLN
3	A	177	PHE
3	A	211	GLN
3	A	221	GLN
3	A	222	LYS
3	A	227	GLU
3	A	229	ARG
3	A	246	VAL
3	A	261	GLU
3	B	131	ARG
3	B	172	GLU
3	B	177	PHE
3	B	201	ARG
3	B	203	ARG
3	B	221	GLN
3	B	227	GLU
3	B	228	GLU
3	B	271	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	109	GLN
3	A	126	HIS
3	A	127	ASN
3	A	140	ASN
3	A	170	GLN

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Mol	Chain	Res	Type
3	A	212	GLN
3	A	237	ASN
3	A	257	ASN
3	A	266	ASN
3	B	140	ASN
3	B	146	GLN
3	B	157	GLN
3	B	176	GLN
3	B	202	ASN
3	B	216	GLN
3	B	221	GLN
3	B	223	ASN
3	B	243	GLN
3	B	257	ASN
3	B	266	ASN
3	B	270	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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	E	21/21 (100%)	-0.66	0	100	100	30, 46, 78, 92	0
2	F	21/21 (100%)	-0.68	0	100	100	31, 48, 78, 83	0
3	A	170/194 (87%)	-0.07	4 (2%)	62	56	31, 58, 91, 96	0
3	B	173/194 (89%)	-0.09	2 (1%)	81	77	28, 59, 95, 100	0
All	All	385/430 (89%)	-0.14	6 (1%)	74	69	28, 59, 91, 100	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	265	TYR	3.1
3	A	180	ALA	2.9
3	B	250	GLN	2.6
3	B	85	ILE	2.4
3	A	247	SER	2.3
3	A	114	ARG	2.1

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 (i)

There are no such residues in this entry.