Full wwPDB X-ray Structure Validation Report (i)

Oct 25, 2023 – 04:19 PM EDT

PDB ID	:	2Z2R
Title	:	Nucleosome assembly proteins I (NAP-1, 74-365)
Authors	:	Park, Y.J.; Luger, K.
Deposited on	:	2007-05-25
Resolution	:	3.20 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

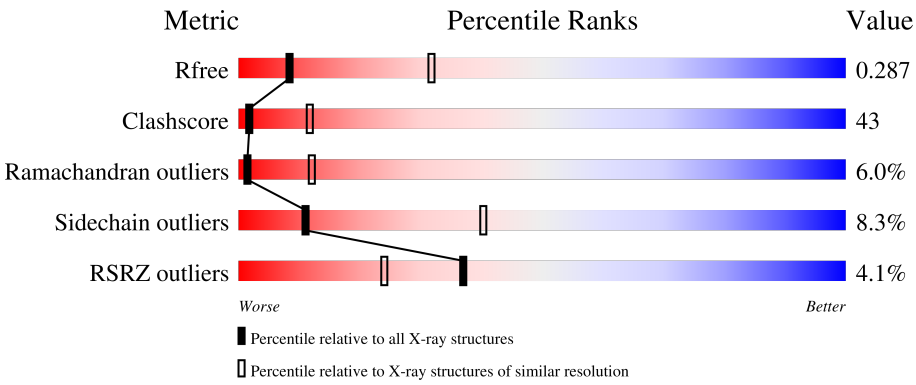
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.20 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}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	292	5% 33% 51% 10% 6%
1	B	292	2% 39% 46% 5% • 8%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 4468 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 Nucleosome assembly protein.

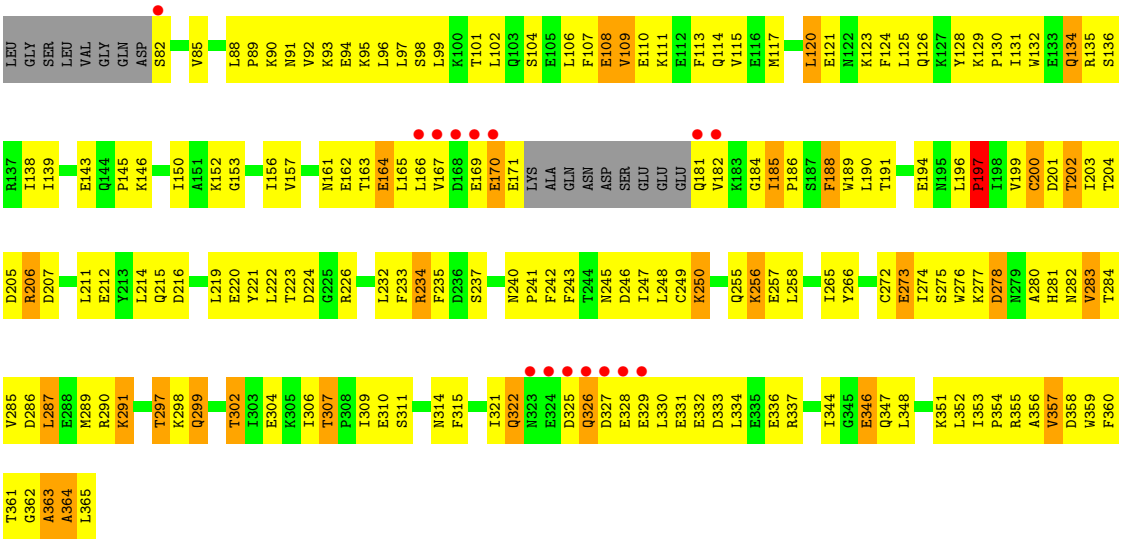
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	275	2263	1447	362	449	5	0	0	0
			Total	C	N	O	S			
1	B	268	2205	1416	354	430	5	0	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

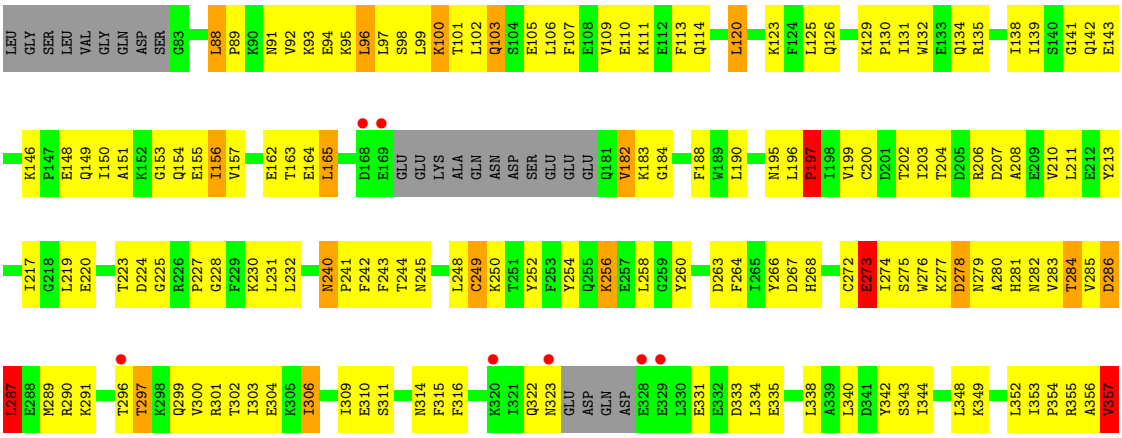
• Molecule 1: Nucleosome assembly protein

Chain A:



• Molecule 1: Nucleosome assembly protein

Chain B:



F360
L365

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α, β, γ	125.00Å 125.00Å 146.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.20 29.69 – 3.18	Depositor EDS
% Data completeness (in resolution range)	86.4 (50.00-3.20) 94.3 (29.69-3.18)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.24 (at 3.18Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.260 , 0.300 0.243 , 0.287	Depositor DCC
R_{free} test set	1930 reflections (9.73%)	wwPDB-VP
Wilson B-factor (Å^2)	86.2	Xtriage
Anisotropy	0.439	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 79.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	4468	wwPDB-VP
Average B, all atoms (Å^2)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% 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 (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	A	0.43	0/2309	0.69	1/3116 (0.0%)
1	B	0.45	0/2250	0.73	2/3035 (0.1%)
All	All	0.44	0/4559	0.71	3/6151 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	273	GLU	N-CA-C	6.29	127.98	111.00
1	B	287	LEU	CA-CB-CG	5.82	128.69	115.30
1	B	165	LEU	CA-CB-CG	5.53	128.01	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2263	0	2203	218	0
1	B	2205	0	2163	192	0
All	All	4468	0	4366	383	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 43.

All (383) 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:B:245:ASN:ND2	1:B:275:SER:H	1.55	1.04
1:A:291:LYS:HA	1:A:302:THR:HA	1.43	1.00
1:A:285:VAL:HG21	1:A:306:ILE:HG23	1.43	1.00
1:B:88:LEU:HB3	1:B:89:PRO:CD	1.98	0.94
1:B:297:THR:HB	1:B:299:GLN:HG2	1.53	0.91
1:B:309:ILE:HG22	1:B:310:GLU:N	1.87	0.89
1:A:353:ILE:HB	1:A:354:PRO:HD3	1.53	0.88
1:A:190:LEU:HD23	1:A:211:LEU:HB2	1.55	0.88
1:B:203:ILE:O	1:B:203:ILE:HD12	1.75	0.87
1:A:256:LYS:HD2	1:A:257:GLU:H	1.39	0.87
1:B:285:VAL:HG11	1:B:306:ILE:HG12	1.57	0.86
1:A:291:LYS:HB3	1:A:302:THR:HB	1.58	0.85
1:B:291:LYS:HG2	1:B:302:THR:HG22	1.57	0.84
1:B:331:GLU:O	1:B:335:GLU:HB2	1.80	0.82
1:A:311:SER:H	1:A:314:ASN:ND2	1.78	0.82
1:A:199:VAL:O	1:A:202:THR:HB	1.82	0.80
1:B:309:ILE:HG22	1:B:310:GLU:H	1.44	0.79
1:A:243:PHE:HB2	1:A:245:ASN:HD22	1.47	0.79
1:A:285:VAL:HG21	1:A:306:ILE:CG2	2.13	0.78
1:A:364:ALA:HA	1:B:260:TYR:HE1	1.47	0.78
1:B:183:LYS:HG3	1:B:184:GLY:H	1.48	0.78
1:B:153:GLY:O	1:B:157:VAL:HG23	1.84	0.77
1:A:165:LEU:HD21	1:B:96:LEU:HD23	1.66	0.77
1:A:129:LYS:HB2	1:A:130:PRO:HD3	1.66	0.77
1:B:249:CYS:C	1:B:272:CYS:SG	2.64	0.76
1:A:282:ASN:HD21	1:A:284:THR:HG22	1.50	0.76
1:B:245:ASN:HD22	1:B:275:SER:H	1.32	0.76
1:A:256:LYS:HE3	1:A:256:LYS:H	1.51	0.75
1:B:195:ASN:O	1:B:197:PRO:HD3	1.86	0.75
1:A:196:LEU:HD22	1:A:352:LEU:HB2	1.69	0.75
1:B:89:PRO:HG2	1:B:92:VAL:HB	1.68	0.75
1:B:219:LEU:HD11	1:B:349:LYS:HG3	1.69	0.75
1:A:98:SER:O	1:A:101:THR:HB	1.88	0.74
1:B:245:ASN:ND2	1:B:275:SER:N	2.35	0.73
1:B:248:LEU:O	1:B:249:CYS:HB3	1.88	0.73
1:B:98:SER:O	1:B:102:LEU:HD13	1.88	0.73
1:A:282:ASN:ND2	1:A:284:THR:HG22	2.03	0.73
1:B:297:THR:HB	1:B:299:GLN:CG	2.17	0.73
1:A:219:LEU:HD23	1:A:220:GLU:N	2.04	0.73
1:A:114:GLN:HG3	1:A:258:LEU:HD11	1.71	0.72
1:A:237:SER:HB2	1:A:246:ASP:OD2	1.89	0.72
1:A:297:THR:HB	1:A:299:GLN:HG2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:LEU:O	1:B:344:ILE:HG13	1.89	0.71
1:A:90:LYS:HG3	1:A:91:ASN:H	1.55	0.71
1:B:129:LYS:HB2	1:B:130:PRO:HD3	1.71	0.71
1:B:240:ASN:ND2	1:B:242:PHE:H	1.87	0.71
1:A:282:ASN:OD1	1:A:284:THR:HG22	1.92	0.70
1:B:219:LEU:HD23	1:B:220:GLU:N	2.06	0.70
1:B:105:GLU:O	1:B:109:VAL:HG23	1.92	0.70
1:B:240:ASN:HD21	1:B:242:PHE:HB2	1.57	0.70
1:A:204:THR:OG1	1:A:207:ASP:OD1	2.10	0.69
1:B:245:ASN:HD21	1:B:275:SER:H	1.41	0.69
1:A:128:TYR:HE1	1:B:110:GLU:HG2	1.57	0.69
1:A:203:ILE:HD12	1:A:203:ILE:O	1.92	0.69
1:B:88:LEU:HB3	1:B:89:PRO:HD3	1.73	0.69
1:A:282:ASN:O	1:A:283:VAL:HB	1.93	0.69
1:A:125:LEU:HA	1:A:128:TYR:HD2	1.57	0.68
1:A:311:SER:H	1:A:314:ASN:HD21	1.41	0.68
1:A:289:MET:HG2	1:A:304:GLU:HA	1.76	0.68
1:A:92:VAL:HG12	1:A:96:LEU:HD11	1.76	0.68
1:A:243:PHE:CD2	1:A:245:ASN:HB2	2.29	0.68
1:A:351:LYS:O	1:A:354:PRO:HD2	1.94	0.68
1:A:190:LEU:HD23	1:A:211:LEU:CB	2.22	0.67
1:A:165:LEU:CD2	1:B:96:LEU:HD23	2.24	0.67
1:A:135:ARG:NH1	1:A:356:ALA:HB3	2.10	0.67
1:A:245:ASN:HD21	1:A:275:SER:H	1.43	0.66
1:B:103:GLN:O	1:B:106:LEU:HB2	1.94	0.66
1:B:199:VAL:HG22	1:B:344:ILE:HG23	1.77	0.66
1:A:255:GLN:HG2	1:A:265:ILE:O	1.94	0.66
1:A:242:PHE:O	1:A:276:TRP:HA	1.97	0.65
1:B:111:LYS:HD2	1:B:258:LEU:HD13	1.78	0.65
1:A:332:GLU:O	1:A:336:GLU:HG3	1.97	0.65
1:A:282:ASN:HD21	1:A:284:THR:CG2	2.09	0.64
1:B:232:LEU:N	1:B:232:LEU:HD12	2.13	0.64
1:A:114:GLN:O	1:A:117:MET:HB3	1.98	0.64
1:A:145:PRO:HB2	1:A:150:ILE:HD11	1.80	0.63
1:A:337:ARG:HB2	1:A:337:ARG:NH1	2.13	0.63
1:B:88:LEU:CB	1:B:89:PRO:CD	2.75	0.63
1:B:282:ASN:OD1	1:B:284:THR:HG23	1.99	0.63
1:B:273:GLU:CD	1:B:274:ILE:N	2.52	0.63
1:B:309:ILE:CG2	1:B:310:GLU:H	2.12	0.63
1:B:309:ILE:CG2	1:B:310:GLU:N	2.58	0.63
1:A:233:PHE:O	1:A:247:ILE:HA	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:LYS:CG	1:B:184:GLY:H	2.10	0.63
1:A:98:SER:O	1:A:102:LEU:HD12	2.00	0.62
1:B:93:LYS:O	1:B:97:LEU:HD23	1.98	0.62
1:A:256:LYS:HD2	1:A:257:GLU:N	2.11	0.62
1:B:126:GLN:HE22	1:B:129:LYS:NZ	1.97	0.62
1:A:99:LEU:HD22	1:B:135:ARG:HG3	1.82	0.62
1:A:132:TRP:HA	1:A:135:ARG:HG2	1.82	0.61
1:A:165:LEU:O	1:B:97:LEU:HD21	2.00	0.61
1:A:245:ASN:ND2	1:A:275:SER:H	1.98	0.61
1:A:90:LYS:O	1:A:94:GLU:HG3	2.00	0.61
1:A:196:LEU:HD12	1:A:197:PRO:HD2	1.83	0.61
1:A:245:ASN:HD21	1:A:275:SER:N	1.99	0.61
1:A:249:CYS:O	1:A:272:CYS:HB2	2.00	0.61
1:A:139:ILE:HD13	1:A:188:PHE:CE2	2.36	0.61
1:A:181:GLN:HG3	1:B:91:ASN:ND2	2.15	0.60
1:A:364:ALA:HA	1:B:260:TYR:CE1	2.34	0.60
1:A:282:ASN:CG	1:A:284:THR:HG22	2.22	0.60
1:A:106:LEU:O	1:A:109:VAL:HG23	2.00	0.60
1:A:90:LYS:CG	1:A:91:ASN:H	2.15	0.60
1:B:353:ILE:HB	1:B:354:PRO:HD3	1.83	0.59
1:B:135:ARG:NH1	1:B:356:ALA:HB3	2.17	0.59
1:A:204:THR:O	1:A:207:ASP:N	2.34	0.59
1:B:322:GLN:O	1:B:323:ASN:HB2	2.00	0.59
1:A:91:ASN:O	1:A:95:LYS:HG2	2.03	0.59
1:A:189:TRP:CE2	1:A:216:ASP:HA	2.38	0.59
1:B:142:GLN:O	1:B:142:GLN:HG2	2.02	0.58
1:A:96:LEU:HD12	1:A:96:LEU:H	1.68	0.58
1:B:245:ASN:HD21	1:B:275:SER:N	1.98	0.58
1:B:248:LEU:O	1:B:249:CYS:CB	2.51	0.58
1:B:306:ILE:HG22	1:B:306:ILE:O	2.02	0.58
1:A:90:LYS:HG3	1:A:91:ASN:N	2.18	0.58
1:B:88:LEU:HB3	1:B:89:PRO:HD2	1.79	0.58
1:A:243:PHE:HD2	1:A:245:ASN:HB2	1.68	0.58
1:B:227:PRO:HD2	1:B:254:TYR:O	2.04	0.58
1:A:189:TRP:NE1	1:A:215:GLN:O	2.35	0.57
1:A:153:GLY:O	1:A:157:VAL:HG23	2.04	0.57
1:A:344:ILE:O	1:A:348:LEU:HD22	2.05	0.57
1:A:120:LEU:HD22	1:B:113:PHE:HE1	1.69	0.57
1:A:285:VAL:HG22	1:A:286:ASP:N	2.20	0.57
1:A:189:TRP:NE1	1:A:216:ASP:HA	2.20	0.57
1:B:243:PHE:CD2	1:B:245:ASN:HB2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:LEU:HD12	1:A:96:LEU:N	2.20	0.56
1:A:145:PRO:HB3	1:B:98:SER:HB3	1.87	0.56
1:A:219:LEU:HD23	1:A:219:LEU:C	2.26	0.56
1:A:245:ASN:HD21	1:A:275:SER:HB2	1.70	0.56
1:A:289:MET:CE	1:A:304:GLU:HB2	2.35	0.56
1:A:358:ASP:HB3	1:A:363:ALA:HB3	1.87	0.56
1:B:231:LEU:O	1:B:249:CYS:HB2	2.05	0.56
1:B:278:ASP:OD1	1:B:280:ALA:N	2.38	0.56
1:A:196:LEU:CD2	1:A:352:LEU:HB2	2.36	0.56
1:A:286:ASP:HB2	1:A:309:ILE:HG21	1.87	0.56
1:B:258:LEU:HD12	1:B:258:LEU:N	2.21	0.56
1:B:286:ASP:N	1:B:309:ILE:HG13	2.20	0.56
1:A:134:GLN:NE2	1:A:143:GLU:OE1	2.37	0.56
1:A:96:LEU:O	1:A:99:LEU:N	2.39	0.56
1:B:146:LYS:O	1:B:150:ILE:HG13	2.06	0.56
1:B:266:TYR:HD2	1:B:342:TYR:CD1	2.24	0.56
1:A:92:VAL:HG12	1:A:96:LEU:CD1	2.36	0.55
1:A:363:ALA:O	1:A:365:LEU:N	2.39	0.55
1:B:196:LEU:HD22	1:B:352:LEU:HB2	1.89	0.55
1:A:181:GLN:HG3	1:B:91:ASN:HD22	1.71	0.55
1:A:214:LEU:HD12	1:A:234:ARG:O	2.07	0.55
1:A:355:ARG:HD2	1:B:260:TYR:HE2	1.72	0.55
1:A:364:ALA:HB2	1:B:260:TYR:OH	2.06	0.55
1:A:125:LEU:HA	1:A:128:TYR:CD2	2.40	0.55
1:B:333:ASP:C	1:B:335:GLU:H	2.10	0.55
1:B:338:LEU:O	1:B:338:LEU:HD23	2.07	0.55
1:B:278:ASP:HB3	1:B:281:HIS:HB2	1.88	0.55
1:B:248:LEU:HD22	1:B:274:ILE:HG12	1.89	0.55
1:B:276:TRP:CE3	1:B:282:ASN:HA	2.42	0.55
1:B:219:LEU:HD23	1:B:220:GLU:H	1.71	0.54
1:B:249:CYS:O	1:B:272:CYS:SG	2.64	0.54
1:B:157:VAL:HG12	1:B:162:GLU:O	2.07	0.54
1:A:120:LEU:C	1:A:120:LEU:HD23	2.28	0.54
1:A:162:GLU:O	1:A:164:GLU:HG3	2.07	0.54
1:B:272:CYS:O	1:B:273:GLU:HG3	2.08	0.54
1:A:92:VAL:O	1:A:95:LYS:N	2.40	0.54
1:B:96:LEU:O	1:B:99:LEU:N	2.39	0.54
1:B:183:LYS:HG3	1:B:184:GLY:N	2.18	0.54
1:A:191:THR:O	1:A:194:GLU:HB2	2.08	0.53
1:A:139:ILE:O	1:A:184:GLY:O	2.27	0.53
1:A:108:GLU:O	1:A:111:LYS:HB3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:LEU:O	1:A:97:LEU:C	2.47	0.53
1:A:190:LEU:HD13	1:A:194:GLU:HG3	1.90	0.53
1:B:182:VAL:HG12	1:B:183:LYS:N	2.22	0.53
1:B:114:GLN:HE21	1:B:263:ASP:HA	1.74	0.53
1:A:291:LYS:H	1:A:291:LYS:HD3	1.74	0.53
1:B:98:SER:O	1:B:102:LEU:CD1	2.57	0.53
1:A:325:ASP:O	1:A:326:GLN:HB2	2.09	0.52
1:A:328:GLU:C	1:A:330:LEU:H	2.11	0.52
1:B:131:ILE:O	1:B:134:GLN:HB2	2.09	0.52
1:B:132:TRP:O	1:B:135:ARG:HB3	2.09	0.52
1:B:230:LYS:HA	1:B:250:LYS:O	2.09	0.52
1:B:204:THR:N	1:B:207:ASP:OD1	2.42	0.52
1:A:297:THR:CB	1:A:299:GLN:HG2	2.38	0.52
1:A:136:SER:O	1:A:139:ILE:HB	2.09	0.52
1:A:282:ASN:O	1:A:283:VAL:CB	2.57	0.52
1:A:113:PHE:CE1	1:A:117:MET:HE2	2.44	0.52
1:B:163:THR:O	1:B:165:LEU:N	2.43	0.52
1:A:232:LEU:HD12	1:A:232:LEU:N	2.25	0.52
1:B:244:THR:HG23	1:B:277:LYS:HE2	1.92	0.52
1:A:329:GLU:O	1:A:333:ASP:HB2	2.10	0.51
1:A:277:LYS:O	1:A:278:ASP:HB2	2.10	0.51
1:B:151:ALA:O	1:B:154:GLN:HB2	2.10	0.51
1:B:196:LEU:CD2	1:B:352:LEU:HB2	2.40	0.51
1:A:89:PRO:HD2	1:A:92:VAL:CG2	2.41	0.51
1:B:289:MET:HG3	1:B:304:GLU:HG2	1.92	0.51
1:A:199:VAL:O	1:A:200:CYS:C	2.48	0.51
1:A:157:VAL:HG12	1:A:163:THR:H	1.76	0.51
1:B:232:LEU:N	1:B:232:LEU:CD1	2.74	0.51
1:B:126:GLN:HE22	1:B:129:LYS:HZ2	1.59	0.51
1:B:322:GLN:O	1:B:323:ASN:CB	2.58	0.51
1:A:131:ILE:O	1:A:134:GLN:HB2	2.11	0.51
1:A:190:LEU:HD13	1:A:190:LEU:C	2.31	0.51
1:A:190:LEU:HD13	1:A:194:GLU:CG	2.40	0.51
1:A:163:THR:HG23	1:A:166:LEU:HD12	1.92	0.51
1:A:282:ASN:OD1	1:A:284:THR:N	2.44	0.51
1:A:170:GLU:O	1:A:171:GLU:C	2.50	0.50
1:B:291:LYS:HG2	1:B:302:THR:CG2	2.36	0.50
1:B:125:LEU:HG	1:B:129:LYS:HE3	1.93	0.50
1:B:282:ASN:HD21	1:B:284:THR:CG2	2.25	0.50
1:A:98:SER:O	1:A:102:LEU:CD1	2.59	0.50
1:A:287:LEU:HD12	1:A:287:LEU:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:LEU:O	1:B:123:LYS:HB3	2.11	0.50
1:A:352:LEU:HD13	1:A:352:LEU:C	2.33	0.50
1:B:249:CYS:O	1:B:316:PHE:HD2	1.94	0.50
1:A:355:ARG:HD2	1:B:260:TYR:CE2	2.47	0.49
1:A:102:LEU:HD12	1:A:102:LEU:H	1.78	0.49
1:A:235:PHE:CE1	1:A:248:LEU:HD12	2.47	0.49
1:B:282:ASN:OD1	1:B:284:THR:CG2	2.60	0.49
1:A:97:LEU:HD12	1:B:154:GLN:N	2.27	0.49
1:A:99:LEU:CD2	1:B:135:ARG:HG3	2.43	0.49
1:A:123:LYS:O	1:A:126:GLN:HB2	2.13	0.49
1:A:289:MET:HE2	1:A:304:GLU:HB2	1.95	0.49
1:A:322:GLN:NE2	1:A:334:LEU:HD22	2.28	0.49
1:A:357:VAL:O	1:A:361:THR:HG23	2.12	0.49
1:B:146:LYS:HB2	1:B:149:GLN:HG3	1.94	0.49
1:B:240:ASN:HD22	1:B:241:PRO:N	2.11	0.49
1:A:92:VAL:O	1:A:93:LYS:C	2.52	0.48
1:A:99:LEU:HA	1:A:102:LEU:HD13	1.94	0.48
1:B:183:LYS:CG	1:B:184:GLY:N	2.75	0.48
1:B:285:VAL:C	1:B:309:ILE:HG13	2.33	0.48
1:A:124:PHE:O	1:A:128:TYR:CD2	2.66	0.48
1:A:245:ASN:ND2	1:A:275:SER:HB2	2.28	0.48
1:A:93:LYS:HA	1:A:96:LEU:HD13	1.94	0.48
1:B:231:LEU:C	1:B:232:LEU:HD12	2.34	0.48
1:B:248:LEU:CD2	1:B:274:ILE:HG12	2.44	0.48
1:B:279:ASN:OD1	1:B:306:ILE:HD11	2.13	0.48
1:A:120:LEU:C	1:A:120:LEU:CD2	2.81	0.48
1:A:185:ILE:HA	1:A:186:PRO:HD3	1.65	0.48
1:B:223:THR:O	1:B:225:GLY:N	2.35	0.48
1:A:92:VAL:CG1	1:A:96:LEU:HD11	2.43	0.48
1:A:131:ILE:O	1:A:134:GLN:CB	2.62	0.48
1:A:285:VAL:HG23	1:A:307:THR:C	2.33	0.48
1:B:134:GLN:O	1:B:138:ILE:HG12	2.13	0.48
1:B:355:ARG:O	1:B:356:ALA:C	2.52	0.48
1:A:138:ILE:HB	1:B:99:LEU:HD21	1.96	0.48
1:B:268:HIS:HA	1:B:342:TYR:OH	2.14	0.48
1:A:206:ARG:NH2	1:A:283:VAL:HA	2.29	0.48
1:B:132:TRP:CD1	1:B:135:ARG:NH2	2.82	0.47
1:A:120:LEU:O	1:A:123:LYS:HB3	2.13	0.47
1:A:222:LEU:O	1:A:224:ASP:N	2.42	0.47
1:B:89:PRO:HG2	1:B:92:VAL:CB	2.41	0.47
1:B:99:LEU:O	1:B:102:LEU:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:THR:O	1:A:166:LEU:N	2.45	0.47
1:A:146:LYS:HD3	1:A:146:LYS:N	2.30	0.47
1:A:240:ASN:HD21	1:A:242:PHE:HD1	1.62	0.47
1:B:148:GLU:O	1:B:151:ALA:HB3	2.14	0.47
1:B:207:ASP:HB3	1:B:283:VAL:HG11	1.95	0.47
1:B:282:ASN:ND2	1:B:284:THR:CG2	2.77	0.47
1:B:340:LEU:O	1:B:343:SER:HB3	2.13	0.47
1:A:135:ARG:O	1:A:139:ILE:HG13	2.14	0.47
1:A:256:LYS:H	1:A:256:LYS:CE	2.26	0.47
1:B:243:PHE:HD2	1:B:245:ASN:HB2	1.78	0.47
1:A:89:PRO:HD2	1:A:92:VAL:HG21	1.96	0.47
1:A:89:PRO:O	1:A:90:LYS:C	2.53	0.47
1:A:106:LEU:HD13	1:A:110:GLU:HG3	1.97	0.47
1:A:125:LEU:CA	1:A:128:TYR:HD2	2.27	0.47
1:A:163:THR:O	1:A:165:LEU:N	2.47	0.47
1:A:190:LEU:O	1:A:194:GLU:HG2	2.14	0.47
1:B:285:VAL:CG1	1:B:306:ILE:HG12	2.39	0.47
1:A:282:ASN:OD1	1:A:283:VAL:N	2.48	0.47
1:A:362:GLY:O	1:A:365:LEU:HB2	2.14	0.47
1:A:297:THR:O	1:A:298:LYS:HB2	2.15	0.46
1:B:99:LEU:O	1:B:101:THR:N	2.48	0.46
1:B:217:ILE:HG22	1:B:353:ILE:HD11	1.97	0.46
1:B:277:LYS:O	1:B:278:ASP:HB2	2.14	0.46
1:B:344:ILE:HG22	1:B:348:LEU:CD2	2.45	0.46
1:B:199:VAL:O	1:B:202:THR:N	2.41	0.46
1:B:240:ASN:ND2	1:B:242:PHE:HD1	2.14	0.46
1:A:289:MET:HE3	1:A:304:GLU:HB2	1.98	0.46
1:A:138:ILE:HG21	1:B:98:SER:OG	2.16	0.46
1:B:266:TYR:HB3	1:B:342:TYR:CZ	2.50	0.46
1:A:237:SER:CB	1:A:246:ASP:OD2	2.61	0.46
1:A:283:VAL:O	1:A:309:ILE:HD11	2.16	0.46
1:B:141:GLY:C	1:B:143:GLU:H	2.19	0.46
1:B:154:GLN:HA	1:B:154:GLN:HE21	1.80	0.46
1:B:231:LEU:O	1:B:249:CYS:CB	2.64	0.46
1:B:256:LYS:N	1:B:256:LYS:HD2	2.32	0.45
1:A:128:TYR:HD1	1:B:106:LEU:CD2	2.29	0.45
1:B:99:LEU:C	1:B:101:THR:N	2.69	0.45
1:B:135:ARG:NH1	1:B:356:ALA:CB	2.80	0.45
1:B:273:GLU:CD	1:B:273:GLU:C	2.75	0.45
1:A:111:LYS:O	1:A:115:VAL:HG23	2.16	0.45
1:A:129:LYS:HB2	1:A:130:PRO:CD	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:ARG:HB2	1:B:99:LEU:HD22	1.99	0.45
1:B:228:GLY:HA3	1:B:252:TYR:O	2.16	0.45
1:A:337:ARG:HH11	1:A:337:ARG:CB	2.29	0.45
1:B:95:LYS:O	1:B:96:LEU:C	2.54	0.45
1:B:114:GLN:NE2	1:B:263:ASP:HA	2.31	0.45
1:A:96:LEU:HB2	1:B:165:LEU:HD11	1.99	0.45
1:A:120:LEU:HD23	1:A:120:LEU:O	2.17	0.45
1:A:199:VAL:HG22	1:A:344:ILE:HG23	1.99	0.45
1:A:322:GLN:HE21	1:A:334:LEU:HD22	1.82	0.45
1:B:240:ASN:HD21	1:B:242:PHE:CB	2.29	0.44
1:B:153:GLY:O	1:B:154:GLN:C	2.56	0.44
1:A:90:LYS:CG	1:A:91:ASN:N	2.77	0.44
1:A:240:ASN:ND2	1:A:242:PHE:H	2.15	0.44
1:A:240:ASN:ND2	1:A:242:PHE:HD1	2.15	0.44
1:A:291:LYS:HD3	1:A:291:LYS:N	2.32	0.44
1:B:213:TYR:CZ	1:B:241:PRO:HD3	2.53	0.44
1:B:273:GLU:C	1:B:274:ILE:HG13	2.38	0.44
1:B:258:LEU:HD12	1:B:258:LEU:H	1.83	0.44
1:B:296:THR:O	1:B:296:THR:HG22	2.18	0.44
1:A:104:SER:OG	1:B:156:ILE:HD13	2.18	0.44
1:A:106:LEU:O	1:A:107:PHE:C	2.56	0.44
1:B:106:LEU:O	1:B:109:VAL:N	2.45	0.44
1:A:128:TYR:CE1	1:B:110:GLU:HG2	2.45	0.43
1:A:203:ILE:HD12	1:A:203:ILE:C	2.38	0.43
1:A:135:ARG:NH1	1:A:356:ALA:CB	2.78	0.43
1:A:152:LYS:O	1:A:156:ILE:HG13	2.17	0.43
1:A:243:PHE:HB2	1:A:245:ASN:ND2	2.25	0.43
1:A:282:ASN:CG	1:A:285:VAL:HG12	2.39	0.43
1:B:232:LEU:HA	1:B:249:CYS:HB3	1.99	0.43
1:B:267:ASP:O	1:B:268:HIS:HB3	2.18	0.43
1:A:82:SER:O	1:A:85:VAL:HG12	2.18	0.43
1:A:129:LYS:NZ	1:A:220:GLU:HG2	2.34	0.43
1:B:285:VAL:HA	1:B:309:ILE:HG13	2.00	0.43
1:A:240:ASN:HD22	1:A:241:PRO:CD	2.31	0.43
1:A:129:LYS:CB	1:A:130:PRO:HD3	2.42	0.43
1:A:287:LEU:O	1:A:287:LEU:CD1	2.67	0.43
1:B:360:PHE:CD1	1:B:360:PHE:C	2.91	0.43
1:B:290:ARG:NH2	1:B:303:ILE:HD12	2.34	0.43
1:A:360:PHE:CE1	1:B:96:LEU:HD11	2.54	0.43
1:A:185:ILE:HD12	1:B:96:LEU:CD1	2.49	0.42
1:B:249:CYS:O	1:B:272:CYS:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:TYR:CD2	1:B:342:TYR:CG	3.08	0.42
1:B:203:ILE:HD12	1:B:203:ILE:C	2.38	0.42
1:A:327:ASP:HB2	1:A:331:GLU:HG3	2.01	0.42
1:B:208:ALA:O	1:B:211:LEU:N	2.53	0.42
1:B:240:ASN:HD22	1:B:242:PHE:H	1.65	0.42
1:A:88:LEU:HD22	1:A:92:VAL:HG11	2.00	0.42
1:B:250:LYS:NZ	1:B:315:PHE:CE1	2.87	0.42
1:A:125:LEU:HD22	1:A:221:TYR:CD1	2.55	0.42
1:B:91:ASN:HA	1:B:94:GLU:CD	2.40	0.42
1:A:169:GLU:O	1:A:170:GLU:HG3	2.20	0.42
1:A:199:VAL:O	1:A:201:ASP:N	2.52	0.42
1:A:250:LYS:HE3	1:A:315:PHE:O	2.19	0.42
1:A:325:ASP:O	1:A:326:GLN:CB	2.67	0.42
1:B:114:GLN:HG3	1:B:258:LEU:CD2	2.50	0.42
1:B:135:ARG:HH11	1:B:356:ALA:HB3	1.84	0.42
1:A:351:LYS:C	1:A:354:PRO:HD2	2.39	0.42
1:A:189:TRP:CZ2	1:A:216:ASP:HA	2.55	0.41
1:A:346:GLU:O	1:A:347:GLN:C	2.58	0.41
1:B:103:GLN:O	1:B:106:LEU:N	2.52	0.41
1:A:240:ASN:HA	1:A:241:PRO:HD3	1.83	0.41
1:A:274:ILE:HG21	1:A:276:TRP:CE2	2.55	0.41
1:A:278:ASP:HB3	1:A:281:HIS:HB2	2.02	0.41
1:B:207:ASP:HA	1:B:210:VAL:HG23	2.02	0.41
1:B:286:ASP:CA	1:B:309:ILE:HD11	2.50	0.41
1:A:245:ASN:HD22	1:A:245:ASN:H	1.67	0.41
1:A:274:ILE:HG22	1:A:275:SER:N	2.35	0.41
1:A:321:ILE:O	1:A:322:GLN:C	2.58	0.41
1:A:356:ALA:O	1:A:359:TRP:N	2.52	0.41
1:B:287:LEU:HD21	1:B:304:GLU:HB3	2.01	0.41
1:B:100:LYS:O	1:B:103:GLN:HB3	2.20	0.41
1:B:211:LEU:HD23	1:B:211:LEU:HA	1.92	0.41
1:A:233:PHE:N	1:A:233:PHE:CD1	2.88	0.41
1:A:256:LYS:CD	1:A:257:GLU:HG3	2.50	0.41
1:A:285:VAL:CG2	1:A:306:ILE:HG23	2.31	0.41
1:B:311:SER:H	1:B:314:ASN:ND2	2.19	0.41
1:A:97:LEU:HD21	1:B:165:LEU:O	2.20	0.41
1:A:129:LYS:O	1:A:130:PRO:C	2.59	0.41
1:B:240:ASN:HD22	1:B:240:ASN:C	2.24	0.41
1:B:242:PHE:O	1:B:277:LYS:HG2	2.21	0.41
1:B:300:VAL:HG22	1:B:301:ARG:N	2.36	0.41
1:B:272:CYS:O	1:B:273:GLU:O	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:LEU:HD13	1:B:157:VAL:HG21	2.03	0.41
1:A:353:ILE:CB	1:A:354:PRO:CD	2.99	0.41
1:A:108:GLU:OE1	1:A:108:GLU:HA	2.21	0.41
1:B:139:ILE:HD13	1:B:188:PHE:CD2	2.57	0.40
1:A:283:VAL:C	1:A:285:VAL:N	2.73	0.40
1:B:266:TYR:CD2	1:B:342:TYR:CD1	3.08	0.40
1:B:357:VAL:O	1:B:360:PHE:N	2.54	0.40
1:A:102:LEU:HD12	1:A:102:LEU:N	2.35	0.40
1:B:88:LEU:HD23	1:B:88:LEU:HA	1.91	0.40
1:B:129:LYS:CB	1:B:130:PRO:HD3	2.48	0.40
1:A:278:ASP:OD1	1:A:280:ALA:HB3	2.21	0.40
1:B:88:LEU:H	1:B:93:LYS:NZ	2.20	0.40
1:B:241:PRO:HD2	1:B:242:PHE:CD1	2.56	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	271/292 (93%)	206 (76%)	47 (17%)	18 (7%)	1 9
1	B	262/292 (90%)	207 (79%)	41 (16%)	14 (5%)	2 15
All	All	533/584 (91%)	413 (78%)	88 (16%)	32 (6%)	1 12

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	185	ILE
1	A	197	PRO
1	A	283	VAL
1	A	322	GLN
1	A	364	ALA

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Mol	Chain	Res	Type
1	B	88	LEU
1	B	164	GLU
1	B	182	VAL
1	A	164	GLU
1	A	170	GLU
1	A	363	ALA
1	B	197	PRO
1	B	224	ASP
1	B	249	CYS
1	B	273	GLU
1	A	188	PHE
1	A	205	ASP
1	A	223	THR
1	A	226	ARG
1	A	278	ASP
1	B	155	GLU
1	B	200	CYS
1	B	278	ASP
1	A	200	CYS
1	B	156	ILE
1	B	334	LEU
1	A	326	GLN
1	A	346	GLU
1	B	100	LYS
1	A	266	TYR
1	A	357	VAL
1	B	357	VAL

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	251/265 (95%)	227 (90%)	24 (10%)	8 32
1	B	244/265 (92%)	227 (93%)	17 (7%)	15 48
All	All	495/530 (93%)	454 (92%)	41 (8%)	11 40

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	GLU
1	A	109	VAL
1	A	120	LEU
1	A	121	GLU
1	A	134	GLN
1	A	161	ASN
1	A	167	VAL
1	A	182	VAL
1	A	197	PRO
1	A	202	THR
1	A	206	ARG
1	A	212	GLU
1	A	234	ARG
1	A	250	LYS
1	A	256	LYS
1	A	273	GLU
1	A	287	LEU
1	A	290	ARG
1	A	291	LYS
1	A	297	THR
1	A	299	GLN
1	A	302	THR
1	A	307	THR
1	A	310	GLU
1	B	96	LEU
1	B	103	GLN
1	B	107	PHE
1	B	120	LEU
1	B	190	LEU
1	B	197	PRO
1	B	206	ARG
1	B	240	ASN
1	B	256	LYS
1	B	264	PHE
1	B	273	GLU
1	B	284	THR
1	B	286	ASP
1	B	287	LEU
1	B	297	THR
1	B	306	ILE
1	B	357	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	161	ASN
1	A	195	ASN
1	A	240	ASN
1	A	245	ASN
1	A	292	GLN
1	A	314	ASN
1	A	322	GLN
1	B	91	ASN
1	B	126	GLN
1	B	142	GLN
1	B	154	GLN
1	B	195	ASN
1	B	240	ASN
1	B	245	ASN
1	B	255	GLN
1	B	314	ASN
1	B	347	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	275/292 (94%)	-0.14	15 (5%)	25	14	27, 69, 164, 198	0
1	B	268/292 (91%)	-0.29	7 (2%)	56	40	25, 66, 157, 202	0
All	All	543/584 (92%)	-0.21	22 (4%)	37	24	25, 68, 159, 202	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	326	GLN	6.1
1	B	323	ASN	5.9
1	A	324	GLU	5.4
1	A	328	GLU	5.2
1	A	325	ASP	5.0
1	A	329	GLU	4.4
1	A	323	ASN	3.3
1	A	169	GLU	3.2
1	B	168	ASP	3.1
1	A	327	ASP	2.8
1	B	296	THR	2.6
1	B	328	GLU	2.6
1	A	168	ASP	2.5
1	B	169	GLU	2.4
1	A	182	VAL	2.3
1	A	181	GLN	2.3
1	A	82	SER	2.2
1	A	167	VAL	2.2
1	B	329	GLU	2.2
1	A	170	GLU	2.1
1	B	320	LYS	2.1
1	A	166	LEU	2.1

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 monosaccharides 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.