Full wwPDB X-ray Structure Validation Report (i)

Aug 16, 2023 – 01:51 AM EDT

PDB ID	:	1YPO
Title	:	Human Oxidized Low Density Lipoprotein Receptor LOX-1 P3 1 21 Space Group
Authors	:	Park, H.; Adsit, F.G.; Boyington, J.C.
Deposited on	:	2005-01-31
Resolution	:	3.00 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:

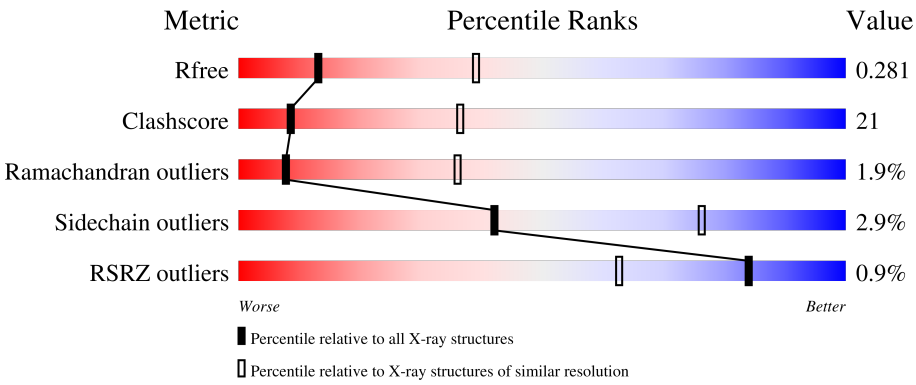
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	132	58% 35% 5% • •
1	B	132	60% 38% •
1	C	132	64% 33% •
1	D	132	.% 55% 41% • •
1	E	132	2% 55% 37% 5% • •

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Mol	Chain	Length	Quality of chain
1	F	132	% 71% 27%
1	G	132	4% 58% 39%
1	H	132	63% 34%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 8358 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 oxidised low density lipoprotein (lectin-like) receptor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	130	1044	672	177	187	8	0	0	0
			Total	C	N	O	S			
1	B	132	1058	680	179	190	9	0	0	0
			Total	C	N	O	S			
1	C	132	1058	680	179	190	9	0	0	0
			Total	C	N	O	S			
1	D	129	1033	666	173	186	8	0	0	0
			Total	C	N	O	S			
1	E	129	1033	666	173	186	8	0	0	0
			Total	C	N	O	S			
1	F	130	1041	671	174	187	9	0	0	0
			Total	C	N	O	S			
1	G	132	1058	680	179	190	9	0	0	0
			Total	C	N	O	S			
1	H	129	1033	666	173	186	8	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	141	MET	-	initiating methionine	UNP P78380
B	141	MET	-	initiating methionine	UNP P78380
C	141	MET	-	initiating methionine	UNP P78380
D	141	MET	-	initiating methionine	UNP P78380
E	141	MET	-	initiating methionine	UNP P78380
F	141	MET	-	initiating methionine	UNP P78380
G	141	MET	-	initiating methionine	UNP P78380
H	141	MET	-	initiating methionine	UNP P78380

3 Residue-property plots (i)

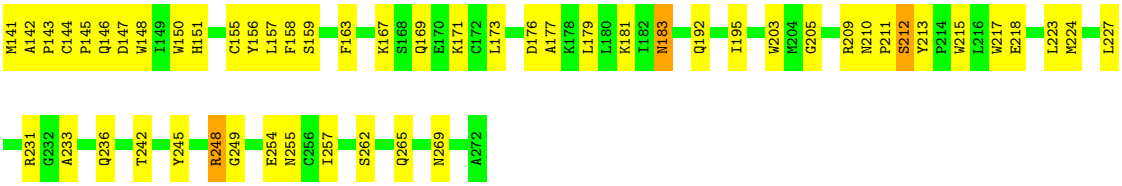
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: oxidised low density lipoprotein (lectin-like) receptor 1

Chain A:

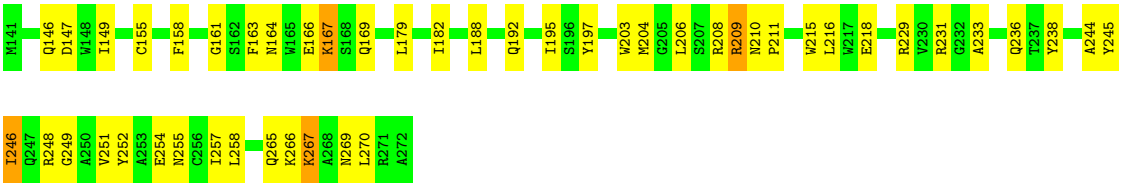
• Molecule 1: oxidised low density lipoprotein (lectin-like) receptor 1

Chain B:



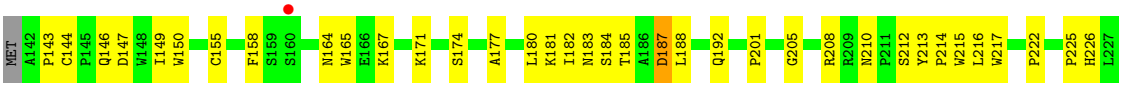
• Molecule 1: oxidised low density lipoprotein (lectin-like) receptor 1

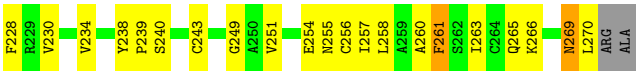
Chain C:



• Molecule 1: oxidised low density lipoprotein (lectin-like) receptor 1

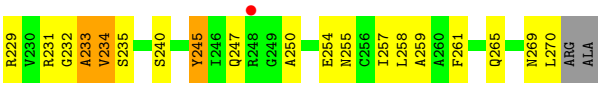
Chain D:





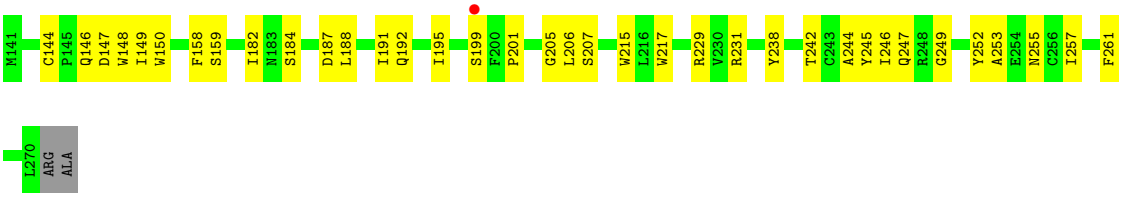
• Molecule 1: oxidised low density lipoprotein (lectin-like) receptor 1

Chain E:



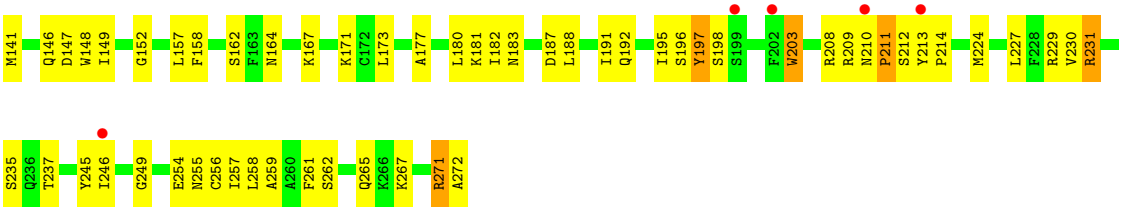
• Molecule 1: oxidised low density lipoprotein (lectin-like) receptor 1

Chain F:



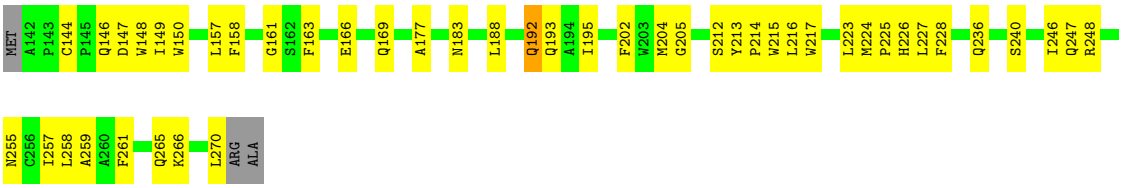
• Molecule 1: oxidised low density lipoprotein (lectin-like) receptor 1

Chain G:



• Molecule 1: oxidised low density lipoprotein (lectin-like) receptor 1

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	97.70Å 97.70Å 215.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 3.00 48.85 – 3.00	Depositor EDS
% Data completeness (in resolution range)	93.1 (10.00-3.00) 93.1 (48.85-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	4.16 (at 3.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.228 , 0.285 0.227 , 0.281	Depositor DCC
R_{free} test set	1119 reflections (4.65%)	wwPDB-VP
Wilson B-factor (Å^2)	53.8	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 34.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	8358	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.44% 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	0.35	0/1078	0.62	1/1465 (0.1%)
1	B	0.32	0/1092	0.58	0/1482
1	C	0.31	0/1092	0.57	0/1482
1	D	0.31	0/1067	0.55	0/1451
1	E	0.36	0/1067	0.58	0/1451
1	F	0.31	0/1075	0.54	0/1461
1	G	0.31	0/1092	0.52	0/1482
1	H	0.30	0/1067	0.55	0/1451
All	All	0.32	0/8630	0.56	1/11725 (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})
1	A	270	LEU	CA-CB-CG	6.56	130.39	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	1044	0	994	46	0
1	B	1058	0	1008	51	0
1	C	1058	0	1008	44	0
1	D	1033	0	981	48	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1033	0	981	51	0
1	F	1041	0	990	30	0
1	G	1058	0	1008	49	0
1	H	1033	0	981	38	0
All	All	8358	0	7951	338	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 21.

All (338) 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:F:255:ASN:OD1	1:F:257:ILE:HG13	1.77	0.84
1:G:255:ASN:OD1	1:G:257:ILE:HG12	1.76	0.84
1:G:181:LYS:HE2	1:G:183:ASN:HD21	1.46	0.81
1:C:255:ASN:OD1	1:C:257:ILE:HG13	1.79	0.81
1:E:255:ASN:OD1	1:E:257:ILE:HG12	1.81	0.80
1:C:209:ARG:HH11	1:C:209:ARG:HB2	1.47	0.79
1:D:269:ASN:C	1:D:269:ASN:HD22	1.88	0.76
1:A:211:PRO:HD3	1:A:237:THR:HG22	1.68	0.76
1:H:158:PHE:HE2	1:H:195:ILE:HG22	1.51	0.75
1:G:271:ARG:HD3	1:G:272:ALA:N	2.03	0.74
1:D:255:ASN:OD1	1:D:257:ILE:HG13	1.88	0.73
1:E:161:GLY:HA3	1:E:163:PHE:HE1	1.53	0.72
1:G:271:ARG:NE	1:G:272:ALA:HB3	2.04	0.71
1:C:197:TYR:HB3	1:D:261:PHE:CE2	2.26	0.70
1:E:146:GLN:O	1:E:147:ASP:HB2	1.90	0.70
1:C:146:GLN:O	1:C:147:ASP:HB2	1.91	0.69
1:D:181:LYS:HE2	1:D:183:ASN:HD21	1.56	0.69
1:D:182:ILE:HG23	1:D:187:ASP:HB3	1.73	0.68
1:B:169:GLN:HE21	1:B:218:GLU:HG2	1.58	0.68
1:E:269:ASN:O	1:E:270:LEU:HG	1.93	0.68
1:G:192:GLN:NE2	1:G:249:GLY:HA2	2.08	0.68
1:C:257:ILE:HD12	1:C:258:LEU:N	2.08	0.68
1:G:271:ARG:CZ	1:G:272:ALA:HB3	2.23	0.68
1:A:210:ASN:OD1	1:A:212:SER:HB3	1.94	0.67
1:E:183:ASN:O	1:E:184:SER:HB3	1.95	0.67
1:E:208:ARG:HD2	1:E:213:TYR:O	1.95	0.67
1:E:254:GLU:HG3	1:E:258:LEU:HD12	1.76	0.66
1:G:158:PHE:CE2	1:G:195:ILE:HG22	2.31	0.66
1:D:146:GLN:O	1:D:147:ASP:HB2	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:LYS:HE3	1:A:167:LYS:HA	1.77	0.65
1:A:169:GLN:HG3	1:A:218:GLU:OE2	1.96	0.65
1:D:210:ASN:HD21	1:D:212:SER:HB2	1.62	0.65
1:E:216:LEU:HD23	1:E:222:PRO:HA	1.77	0.65
1:H:161:GLY:HA3	1:H:163:PHE:CE1	2.31	0.65
1:C:206:LEU:HD11	1:C:215:TRP:HB3	1.78	0.65
1:E:205:GLY:O	1:E:217:TRP:HA	1.97	0.65
1:H:177:ALA:HB2	1:H:266:LYS:HD3	1.79	0.65
1:D:210:ASN:HB3	1:D:213:TYR:CD1	2.32	0.64
1:G:162:SER:HB2	1:G:261:PHE:CE1	2.32	0.64
1:G:181:LYS:HE2	1:G:183:ASN:ND2	2.12	0.64
1:A:269:ASN:O	1:A:270:LEU:HB3	1.97	0.64
1:A:181:LYS:HE2	1:A:183:ASN:HD21	1.63	0.64
1:H:255:ASN:OD1	1:H:257:ILE:HG13	1.97	0.63
1:E:210:ASN:HB2	1:E:211:PRO:HD2	1.79	0.63
1:H:240:SER:OG	1:H:257:ILE:HG23	1.99	0.63
1:A:158:PHE:HE2	1:A:195:ILE:HG22	1.63	0.63
1:B:203:TRP:HB2	1:B:262:SER:HB3	1.81	0.63
1:B:192:GLN:OE1	1:B:249:GLY:HA2	1.99	0.63
1:A:268:ALA:O	1:A:269:ASN:HB2	1.98	0.62
1:D:143:PRO:HA	1:D:269:ASN:O	2.00	0.62
1:G:271:ARG:HD3	1:G:272:ALA:H	1.65	0.61
1:A:155:CYS:SG	1:A:268:ALA:HA	2.40	0.61
1:G:210:ASN:O	1:G:212:SER:N	2.33	0.61
1:B:143:PRO:HA	1:B:269:ASN:O	2.00	0.61
1:A:202:PHE:HA	1:A:261:PHE:O	2.00	0.61
1:G:203:TRP:HB2	1:G:262:SER:HB3	1.82	0.61
1:D:269:ASN:HD22	1:D:270:LEU:N	1.98	0.61
1:G:195:ILE:O	1:G:198:SER:HB3	2.01	0.61
1:H:161:GLY:HA3	1:H:163:PHE:HE1	1.66	0.61
1:C:266:LYS:HB2	1:C:267:LYS:HZ3	1.64	0.60
1:B:181:LYS:HE2	1:B:183:ASN:HD21	1.66	0.60
1:C:182:ILE:HG21	1:C:188:LEU:HB2	1.84	0.60
1:D:208:ARG:HB2	1:D:213:TYR:CB	2.31	0.60
1:A:146:GLN:O	1:A:147:ASP:HB2	2.02	0.59
1:A:254:GLU:HG3	1:A:258:LEU:HD12	1.85	0.59
1:E:197:TYR:HB3	1:F:261:PHE:CE2	2.37	0.59
1:A:159:SER:CB	1:A:262:SER:H	2.16	0.59
1:D:181:LYS:HE2	1:D:183:ASN:ND2	2.17	0.59
1:G:210:ASN:OD1	1:G:212:SER:HB3	2.02	0.59
1:E:158:PHE:HE2	1:E:195:ILE:HG23	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:224:MET:HB3	1:E:227:LEU:HD11	1.83	0.59
1:G:192:GLN:OE1	1:G:246:ILE:HD11	2.03	0.59
1:G:209:ARG:HG2	1:G:209:ARG:HH11	1.68	0.58
1:B:224:MET:CE	1:B:227:LEU:HD21	2.33	0.58
1:E:162:SER:O	1:E:259:ALA:HB1	2.03	0.58
1:G:173:LEU:HA	1:G:177:ALA:O	2.03	0.58
1:D:192:GLN:NE2	1:D:249:GLY:HA3	2.18	0.58
1:B:159:SER:HB3	1:B:262:SER:H	1.68	0.58
1:A:213:TYR:OH	1:D:188:LEU:HD23	2.04	0.58
1:B:224:MET:HB3	1:B:227:LEU:HD11	1.84	0.58
1:F:207:SER:HA	1:F:215:TRP:HZ3	1.68	0.57
1:D:177:ALA:HB2	1:D:266:LYS:HD3	1.87	0.57
1:F:215:TRP:HH2	1:F:242:THR:HG22	1.70	0.57
1:E:161:GLY:HA3	1:E:163:PHE:CE1	2.37	0.57
1:D:155:CYS:O	1:D:265:GLN:HA	2.05	0.57
1:E:254:GLU:CG	1:E:258:LEU:HD12	2.35	0.57
1:G:208:ARG:HB2	1:G:213:TYR:HB2	1.87	0.57
1:D:210:ASN:O	1:D:213:TYR:HB2	2.05	0.56
1:E:197:TYR:HB3	1:F:261:PHE:CZ	2.40	0.56
1:B:224:MET:HE2	1:B:227:LEU:HD21	1.88	0.56
1:F:144:CYS:SG	1:F:150:TRP:HB2	2.45	0.56
1:G:254:GLU:HG3	1:G:255:ASN:N	2.21	0.56
1:G:203:TRP:CE3	1:G:245:TYR:HB3	2.41	0.56
1:A:158:PHE:CE2	1:A:195:ILE:HG22	2.39	0.56
1:C:149:ILE:HD12	1:C:158:PHE:HE1	1.70	0.56
1:C:182:ILE:HD12	1:C:182:ILE:N	2.21	0.56
1:D:210:ASN:ND2	1:D:212:SER:HB2	2.21	0.56
1:G:210:ASN:HB3	1:G:237:THR:CG2	2.35	0.56
1:A:216:LEU:HD23	1:A:222:PRO:HA	1.86	0.56
1:H:223:LEU:HD11	1:H:228:PHE:CZ	2.41	0.55
1:C:238:TYR:CD2	1:C:255:ASN:ND2	2.74	0.55
1:A:192:GLN:HG2	1:E:213:TYR:CE1	2.41	0.55
1:A:192:GLN:HG2	1:E:213:TYR:CD1	2.42	0.55
1:H:270:LEU:HD12	1:H:270:LEU:N	2.21	0.55
1:G:208:ARG:HD2	1:G:213:TYR:O	2.07	0.55
1:F:247:GLN:C	1:F:249:GLY:H	2.10	0.55
1:E:155:CYS:O	1:E:265:GLN:HA	2.06	0.55
1:F:191:ILE:O	1:F:195:ILE:HG12	2.07	0.55
1:D:257:ILE:C	1:D:257:ILE:HD12	2.28	0.55
1:C:203:TRP:CE3	1:C:245:TYR:HB3	2.42	0.54
1:C:245:TYR:HE2	1:C:254:GLU:HB2	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:211:PRO:HG2	1:G:235:SER:O	2.07	0.54
1:G:271:ARG:NH1	1:G:272:ALA:OXT	2.40	0.54
1:C:155:CYS:O	1:C:265:GLN:HA	2.07	0.54
1:G:203:TRP:CE3	1:G:203:TRP:HA	2.43	0.54
1:A:142:ALA:N	1:B:141:MET:N	2.55	0.54
1:B:158:PHE:HE1	1:B:195:ILE:HG22	1.73	0.54
1:C:269:ASN:O	1:C:270:LEU:HG	2.07	0.54
1:E:210:ASN:O	1:E:212:SER:N	2.41	0.54
1:E:233:ALA:C	1:E:235:SER:H	2.10	0.54
1:A:271:ARG:HH11	1:A:271:ARG:HG2	1.72	0.54
1:A:254:GLU:CG	1:A:258:LEU:HD12	2.37	0.54
1:B:169:GLN:HG3	1:B:218:GLU:OE2	2.08	0.54
1:D:269:ASN:C	1:D:269:ASN:ND2	2.61	0.54
1:G:188:LEU:O	1:G:192:GLN:HB2	2.09	0.53
1:G:158:PHE:HE2	1:G:195:ILE:HG22	1.74	0.53
1:C:169:GLN:HG3	1:C:218:GLU:OE2	2.09	0.53
1:A:211:PRO:CD	1:A:237:THR:HG22	2.38	0.53
1:B:203:TRP:CE3	1:B:245:TYR:HB3	2.43	0.53
1:H:240:SER:CB	1:H:257:ILE:HG23	2.39	0.53
1:C:209:ARG:HB2	1:C:209:ARG:NH1	2.22	0.52
1:H:158:PHE:CE2	1:H:195:ILE:HG22	2.39	0.52
1:A:269:ASN:O	1:A:270:LEU:CB	2.57	0.52
1:G:210:ASN:C	1:G:212:SER:H	2.12	0.52
1:H:247:GLN:HG2	1:H:248:ARG:HG2	1.91	0.52
1:A:193:GLN:HA	1:A:196:SER:OG	2.09	0.52
1:E:146:GLN:HG2	1:F:150:TRP:CE3	2.45	0.52
1:B:163:PHE:CE1	1:B:171:LYS:HE3	2.45	0.52
1:B:173:LEU:O	1:B:176:ASP:N	2.36	0.52
1:G:149:ILE:HG12	1:H:149:ILE:HG12	1.92	0.52
1:C:164:ASN:OD1	1:C:167:LYS:HE2	2.10	0.52
1:H:163:PHE:O	1:H:259:ALA:HA	2.08	0.52
1:B:231:ARG:HG2	1:B:231:ARG:HH11	1.74	0.52
1:D:171:LYS:HA	1:D:174:SER:HB3	1.92	0.52
1:D:208:ARG:HB2	1:D:213:TYR:HB3	1.92	0.52
1:E:150:TRP:CD2	1:F:146:GLN:HG2	2.44	0.52
1:A:146:GLN:HG2	1:B:150:TRP:CD2	2.45	0.51
1:B:233:ALA:HB1	1:B:236:GLN:NE2	2.25	0.51
1:E:231:ARG:NH1	1:E:250:ALA:HB1	2.25	0.51
1:B:173:LEU:HD23	1:B:177:ALA:O	2.10	0.51
1:E:224:MET:HB3	1:E:227:LEU:CD1	2.40	0.51
1:H:224:MET:HB2	1:H:227:LEU:CD1	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:187:ASP:O	1:G:191:ILE:HG12	2.11	0.51
1:D:254:GLU:CG	1:D:258:LEU:HD12	2.42	0.50
1:F:247:GLN:C	1:F:249:GLY:N	2.63	0.50
1:A:255:ASN:OD1	1:A:257:ILE:HG13	2.12	0.50
1:B:156:TYR:N	1:B:156:TYR:CD1	2.79	0.50
1:C:254:GLU:CG	1:C:258:LEU:HD12	2.41	0.50
1:D:225:PRO:O	1:D:226:HIS:HB2	2.12	0.50
1:H:257:ILE:HD12	1:H:257:ILE:C	2.32	0.50
1:B:143:PRO:O	1:B:144:CYS:SG	2.70	0.50
1:E:209:ARG:HD3	1:E:213:TYR:CZ	2.47	0.50
1:A:229:ARG:NH1	1:E:218:GLU:O	2.45	0.50
1:B:248:ARG:O	1:H:214:PRO:HG3	2.11	0.50
1:C:238:TYR:HD2	1:C:255:ASN:ND2	2.09	0.49
1:C:266:LYS:HB2	1:C:267:LYS:NZ	2.26	0.49
1:D:210:ASN:HB3	1:D:213:TYR:CE1	2.47	0.49
1:A:159:SER:HB2	1:A:262:SER:H	1.77	0.49
1:D:164:ASN:OD1	1:D:167:LYS:HG2	2.12	0.49
1:D:183:ASN:O	1:D:184:SER:HB3	2.12	0.49
1:G:196:SER:C	1:G:198:SER:H	2.16	0.49
1:H:144:CYS:SG	1:H:150:TRP:HB2	2.52	0.49
1:B:145:PRO:HB2	1:B:148:TRP:CD1	2.47	0.49
1:D:205:GLY:O	1:D:217:TRP:HA	2.13	0.49
1:A:155:CYS:O	1:A:265:GLN:HA	2.13	0.49
1:G:152:GLY:H	1:H:146:GLN:NE2	2.11	0.49
1:F:182:ILE:HG23	1:F:187:ASP:HB2	1.94	0.48
1:F:207:SER:HA	1:F:215:TRP:CZ3	2.47	0.48
1:G:182:ILE:HD13	1:G:188:LEU:HB2	1.94	0.48
1:E:201:PRO:HA	1:E:247:GLN:HB2	1.96	0.48
1:E:202:PHE:HA	1:E:261:PHE:O	2.14	0.48
1:B:177:ALA:HB1	1:B:265:GLN:O	2.14	0.48
1:D:144:CYS:SG	1:D:150:TRP:HB2	2.54	0.48
1:D:255:ASN:CG	1:D:257:ILE:HG13	2.34	0.48
1:H:163:PHE:CD1	1:H:163:PHE:N	2.82	0.48
1:A:192:GLN:OE1	1:A:249:GLY:HA2	2.13	0.48
1:B:146:GLN:O	1:B:147:ASP:HB2	2.14	0.48
1:C:229:ARG:O	1:C:231:ARG:HD2	2.14	0.47
1:B:181:LYS:HE2	1:B:183:ASN:ND2	2.29	0.47
1:F:242:THR:HG21	1:F:253:ALA:HB1	1.97	0.47
1:E:231:ARG:HH11	1:E:231:ARG:HG3	1.79	0.47
1:G:258:LEU:HD12	1:G:259:ALA:N	2.29	0.47
1:F:205:GLY:O	1:F:217:TRP:HA	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:158:PHE:HE2	1:E:195:ILE:CG2	2.27	0.47
1:B:155:CYS:O	1:B:265:GLN:HA	2.13	0.47
1:D:165:TRP:HB3	1:D:256:CYS:HB3	1.97	0.47
1:H:202:PHE:HA	1:H:261:PHE:O	2.15	0.47
1:F:188:LEU:HD11	1:F:246:ILE:HD12	1.96	0.47
1:C:248:ARG:HE	1:C:248:ARG:HB2	1.58	0.47
1:B:210:ASN:OD1	1:B:212:SER:HB2	2.15	0.47
1:F:206:LEU:HB3	1:F:244:ALA:HB3	1.96	0.47
1:E:232:GLY:C	1:E:234:VAL:H	2.17	0.46
1:G:164:ASN:HB2	1:G:256:CYS:O	2.15	0.46
1:B:192:GLN:HG2	1:H:213:TYR:CD2	2.50	0.46
1:B:254:GLU:HG3	1:B:255:ASN:N	2.30	0.46
1:C:257:ILE:HD12	1:C:257:ILE:C	2.35	0.46
1:H:204:MET:CE	1:H:246:ILE:HB	2.46	0.46
1:A:143:PRO:O	1:A:269:ASN:HB2	2.15	0.46
1:C:254:GLU:HG3	1:C:255:ASN:N	2.31	0.46
1:D:240:SER:HB2	1:D:257:ILE:HG23	1.98	0.46
1:C:210:ASN:HB2	1:C:211:PRO:CD	2.46	0.46
1:D:177:ALA:HB1	1:D:265:GLN:O	2.16	0.46
1:B:151:HIS:HB3	1:B:156:TYR:HE1	1.80	0.45
1:H:188:LEU:O	1:H:192:GLN:HB3	2.16	0.45
1:A:146:GLN:O	1:A:147:ASP:CB	2.64	0.45
1:B:192:GLN:HG2	1:H:213:TYR:CE2	2.51	0.45
1:H:225:PRO:O	1:H:226:HIS:HB2	2.16	0.45
1:A:182:ILE:HG23	1:A:187:ASP:HB2	1.98	0.45
1:E:255:ASN:HB3	1:E:258:LEU:HG	1.98	0.45
1:B:255:ASN:OD1	1:B:257:ILE:HG12	2.17	0.45
1:E:160:SER:O	1:E:261:PHE:CE2	2.70	0.45
1:E:173:LEU:HD22	1:E:173:LEU:HA	1.79	0.45
1:A:144:CYS:SG	1:A:150:TRP:HB2	2.57	0.45
1:E:245:TYR:CD1	1:E:245:TYR:C	2.90	0.45
1:F:146:GLN:O	1:F:147:ASP:HB2	2.15	0.45
1:E:191:ILE:O	1:E:195:ILE:HG12	2.17	0.45
1:E:200:PHE:N	1:E:200:PHE:CD2	2.84	0.45
1:C:206:LEU:HD12	1:C:216:LEU:O	2.17	0.44
1:D:149:ILE:HD12	1:D:158:PHE:CE1	2.52	0.44
1:D:228:PHE:CD1	1:D:251:VAL:HG21	2.53	0.44
1:D:254:GLU:HG3	1:D:258:LEU:HD12	1.98	0.44
1:E:232:GLY:O	1:E:234:VAL:N	2.49	0.44
1:F:201:PRO:HD3	1:F:247:GLN:NE2	2.32	0.44
1:F:252:TYR:CD1	1:F:252:TYR:N	2.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:TRP:CZ2	1:B:157:LEU:HD22	2.53	0.44
1:D:215:TRP:CZ2	1:D:230:VAL:HG11	2.53	0.44
1:C:192:GLN:HE22	1:C:249:GLY:C	2.21	0.44
1:C:267:LYS:HD2	1:C:267:LYS:O	2.18	0.44
1:H:205:GLY:O	1:H:217:TRP:HA	2.17	0.44
1:A:204:MET:HG2	1:A:244:ALA:O	2.17	0.44
1:C:245:TYR:O	1:C:251:VAL:HG13	2.18	0.44
1:D:192:GLN:NE2	1:D:249:GLY:CA	2.80	0.44
1:D:254:GLU:HG3	1:D:255:ASN:N	2.32	0.44
1:G:146:GLN:O	1:G:148:TRP:HD1	2.01	0.44
1:B:158:PHE:HE1	1:B:195:ILE:CG2	2.30	0.44
1:B:203:TRP:HB2	1:B:262:SER:CB	2.48	0.44
1:G:146:GLN:O	1:G:147:ASP:HB2	2.18	0.44
1:E:229:ARG:O	1:E:231:ARG:NH1	2.51	0.43
1:G:211:PRO:HD2	1:G:237:THR:OG1	2.18	0.43
1:H:247:GLN:O	1:H:248:ARG:HB2	2.18	0.43
1:A:143:PRO:HA	1:A:269:ASN:HB3	2.01	0.43
1:A:206:LEU:HD11	1:A:215:TRP:HB3	2.00	0.43
1:B:192:GLN:NE2	1:H:212:SER:O	2.49	0.43
1:C:161:GLY:HA3	1:C:163:PHE:CE1	2.53	0.43
1:E:169:GLN:HG3	1:E:218:GLU:OE2	2.18	0.43
1:F:242:THR:CG2	1:F:253:ALA:HB1	2.48	0.43
1:D:216:LEU:HD23	1:D:222:PRO:HA	2.01	0.43
1:B:169:GLN:NE2	1:B:218:GLU:HG2	2.30	0.43
1:D:164:ASN:ND2	1:D:167:LYS:HG2	2.33	0.43
1:F:149:ILE:HD12	1:F:158:PHE:CE1	2.54	0.43
1:G:210:ASN:HB3	1:G:237:THR:HG23	2.00	0.43
1:A:142:ALA:HA	1:B:143:PRO:HD3	2.00	0.43
1:B:179:LEU:HB2	1:B:218:GLU:OE1	2.19	0.43
1:G:141:MET:O	1:G:141:MET:HG3	2.19	0.43
1:H:166:GLU:O	1:H:169:GLN:HB3	2.19	0.43
1:C:208:ARG:NH1	1:C:211:PRO:HA	2.34	0.43
1:E:216:LEU:CD2	1:E:222:PRO:HA	2.48	0.43
1:H:215:TRP:O	1:H:216:LEU:HD23	2.19	0.43
1:C:179:LEU:HB2	1:C:218:GLU:OE1	2.19	0.42
1:E:206:LEU:HD11	1:E:215:TRP:HB3	2.01	0.42
1:D:146:GLN:O	1:D:147:ASP:CB	2.64	0.42
1:G:209:ARG:HG2	1:G:209:ARG:NH1	2.34	0.42
1:A:182:ILE:HD13	1:A:188:LEU:HD13	2.01	0.42
1:C:233:ALA:HB1	1:C:236:GLN:OE1	2.20	0.42
1:A:143:PRO:HD3	1:B:142:ALA:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:TRP:CD2	1:A:157:LEU:HB2	2.54	0.42
1:B:231:ARG:HG2	1:B:231:ARG:NH1	2.35	0.42
1:B:255:ASN:CG	1:B:257:ILE:HG12	2.40	0.42
1:C:188:LEU:O	1:C:192:GLN:HG2	2.20	0.42
1:E:163:PHE:N	1:E:163:PHE:CD1	2.87	0.42
1:F:184:SER:O	1:F:187:ASP:HB2	2.19	0.42
1:F:199:SER:O	1:F:247:GLN:NE2	2.53	0.42
1:A:243:CYS:N	1:A:256:CYS:SG	2.93	0.42
1:C:267:LYS:HZ3	1:C:267:LYS:H	1.68	0.42
1:G:267:LYS:HE3	1:G:267:LYS:HB2	1.78	0.42
1:A:245:TYR:C	1:A:245:TYR:CD1	2.93	0.42
1:C:195:ILE:HD11	1:C:246:ILE:CD1	2.49	0.42
1:F:146:GLN:O	1:F:148:TRP:HD1	2.01	0.42
1:G:210:ASN:C	1:G:212:SER:N	2.73	0.42
1:C:204:MET:HG2	1:C:244:ALA:O	2.20	0.42
1:D:181:LYS:HE2	1:D:183:ASN:OD1	2.20	0.42
1:H:192:GLN:HG3	1:H:193:GLN:N	2.35	0.42
1:H:224:MET:HB2	1:H:227:LEU:HG	2.02	0.42
1:F:245:TYR:C	1:F:245:TYR:CD1	2.94	0.42
1:G:180:LEU:HD12	1:G:265:GLN:OE1	2.19	0.42
1:G:192:GLN:CD	1:G:249:GLY:HA2	2.39	0.42
1:G:229:ARG:O	1:G:231:ARG:HG3	2.20	0.42
1:H:224:MET:HB2	1:H:227:LEU:HD11	2.01	0.42
1:F:229:ARG:O	1:F:231:ARG:HG3	2.20	0.41
1:E:206:LEU:HB2	1:E:217:TRP:CZ3	2.55	0.41
1:C:164:ASN:HD21	1:C:167:LYS:CE	2.33	0.41
1:E:240:SER:CB	1:E:257:ILE:HG23	2.50	0.41
1:F:192:GLN:NE2	1:F:249:GLY:HA3	2.35	0.41
1:A:218:GLU:O	1:A:220:GLY:N	2.53	0.41
1:A:271:ARG:HG2	1:A:271:ARG:NH1	2.35	0.41
1:B:215:TRP:HH2	1:B:242:THR:HG22	1.86	0.41
1:C:238:TYR:HD2	1:C:255:ASN:HD22	1.66	0.41
1:D:180:LEU:N	1:D:263:ILE:O	2.48	0.41
1:E:231:ARG:NH1	1:E:231:ARG:HG3	2.36	0.41
1:B:224:MET:HE1	1:B:227:LEU:HD21	2.00	0.41
1:C:245:TYR:CE2	1:C:254:GLU:HB2	2.53	0.41
1:D:214:PRO:O	1:D:215:TRP:C	2.59	0.41
1:E:177:ALA:HB1	1:E:265:GLN:O	2.20	0.41
1:G:224:MET:HB2	1:G:227:LEU:HD11	2.02	0.41
1:C:163:PHE:CD1	1:C:163:PHE:N	2.88	0.41
1:C:245:TYR:CZ	1:C:252:TYR:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:165:TRP:CG	1:D:243:CYS:SG	3.13	0.41
1:D:238:TYR:HA	1:D:239:PRO:HD3	1.93	0.41
1:E:183:ASN:O	1:E:184:SER:CB	2.67	0.41
1:B:141:MET:N	1:B:141:MET:SD	2.94	0.41
1:B:167:LYS:O	1:B:171:LYS:HG3	2.20	0.41
1:F:184:SER:OG	1:F:187:ASP:OD1	2.38	0.41
1:H:236:GLN:OE1	1:H:236:GLN:N	2.54	0.41
1:B:205:GLY:O	1:B:217:TRP:HA	2.20	0.41
1:B:223:LEU:O	1:B:224:MET:C	2.59	0.41
1:C:166:GLU:O	1:C:169:GLN:HB3	2.21	0.41
1:E:158:PHE:CD1	1:E:158:PHE:N	2.89	0.41
1:H:257:ILE:HD12	1:H:258:LEU:HG	2.03	0.41
1:H:257:ILE:HD12	1:H:258:LEU:N	2.36	0.41
1:B:209:ARG:HD3	1:B:213:TYR:CZ	2.56	0.40
1:B:211:PRO:HD3	1:B:236:GLN:O	2.20	0.40
1:F:238:TYR:HB3	1:F:255:ASN:ND2	2.37	0.40
1:G:167:LYS:O	1:G:171:LYS:HD3	2.21	0.40
1:H:224:MET:CB	1:H:227:LEU:HG	2.51	0.40
1:A:187:ASP:O	1:A:190:PHE:HB3	2.21	0.40
1:D:201:PRO:O	1:D:260:ALA:HB1	2.21	0.40
1:G:148:TRP:CD2	1:G:157:LEU:HB2	2.57	0.40
1:H:148:TRP:CD2	1:H:157:LEU:HB2	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	128/132 (97%)	107 (84%)	15 (12%)	6 (5%)	2 14
1	B	130/132 (98%)	115 (88%)	14 (11%)	1 (1%)	19 57
1	C	130/132 (98%)	116 (89%)	14 (11%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	127/132 (96%)	110 (87%)	15 (12%)	2 (2%)	9	40
1	E	127/132 (96%)	112 (88%)	10 (8%)	5 (4%)	3	17
1	F	128/132 (97%)	115 (90%)	12 (9%)	1 (1%)	19	57
1	G	130/132 (98%)	112 (86%)	13 (10%)	5 (4%)	3	18
1	H	127/132 (96%)	113 (89%)	14 (11%)	0	100	100
All	All	1027/1056 (97%)	900 (88%)	107 (10%)	20 (2%)	8	36

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	268	ALA
1	A	269	ASN
1	A	270	LEU
1	D	261	PHE
1	E	211	PRO
1	E	184	SER
1	E	233	ALA
1	E	234	VAL
1	G	211	PRO
1	B	248	ARG
1	D	234	VAL
1	A	159	SER
1	A	219	ASP
1	E	208	ARG
1	F	159	SER
1	G	197	TYR
1	G	214	PRO
1	G	230	VAL
1	G	231	ARG
1	A	257	ILE

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	112/113 (99%)	107 (96%)	5 (4%)	27	64
1	B	113/113 (100%)	111 (98%)	2 (2%)	59	85
1	C	113/113 (100%)	109 (96%)	4 (4%)	36	71
1	D	111/113 (98%)	108 (97%)	3 (3%)	44	77
1	E	111/113 (98%)	106 (96%)	5 (4%)	27	64
1	F	112/113 (99%)	112 (100%)	0	100	100
1	G	113/113 (100%)	110 (97%)	3 (3%)	44	77
1	H	111/113 (98%)	107 (96%)	4 (4%)	35	70
All	All	896/904 (99%)	870 (97%)	26 (3%)	42	76

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	167	LYS
1	A	229	ARG
1	A	269	ASN
1	A	270	LEU
1	A	271	ARG
1	B	183	ASN
1	B	212	SER
1	C	167	LYS
1	C	209	ARG
1	C	246	ILE
1	C	267	LYS
1	D	185	THR
1	D	187	ASP
1	D	269	ASN
1	E	173	LEU
1	E	176	ASP
1	E	192	GLN
1	E	211	PRO
1	E	245	TYR
1	G	197	TYR
1	G	203	TRP
1	G	271	ARG
1	H	147	ASP
1	H	183	ASN
1	H	192	GLN
1	H	265	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	183	ASN
1	A	236	GLN
1	B	169	GLN
1	B	183	ASN
1	C	169	GLN
1	C	183	ASN
1	C	193	GLN
1	D	183	ASN
1	D	269	ASN
1	F	247	GLN
1	G	183	ASN
1	H	146	GLN
1	H	183	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no 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	130/132 (98%)	-0.28	0	100	100	29, 40, 54, 77	0
1	B	132/132 (100%)	-0.19	0	100	100	28, 45, 59, 74	0
1	C	132/132 (100%)	-0.30	0	100	100	22, 38, 47, 71	0
1	D	129/132 (97%)	-0.14	1 (0%)	86	65	34, 50, 67, 74	0
1	E	129/132 (97%)	-0.19	2 (1%)	72	44	28, 46, 59, 67	0
1	F	130/132 (98%)	-0.23	1 (0%)	86	65	24, 43, 56, 66	0
1	G	132/132 (100%)	0.13	5 (3%)	40	16	45, 59, 78, 84	0
1	H	129/132 (97%)	-0.23	0	100	100	33, 46, 58, 62	0
All	All	1043/1056 (98%)	-0.18	9 (0%)	84	63	22, 46, 66, 84	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	199	SER	3.2
1	G	210	ASN	3.2
1	G	213	TYR	3.0
1	E	248	ARG	2.9
1	D	160	SER	2.6
1	E	199	SER	2.6
1	G	246	ILE	2.4
1	F	199	SER	2.3
1	G	202	PHE	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.