Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 11:47 AM GMT

PDB ID	:	3PV5
Title	:	Structure of Legionella fallonii DegQ (N189G/P190G variant)
Authors	:	Wrase, R.; Scott, H.; Hilgenfeld, R.; Hansen, G.
Deposited on	:	2010-12-06
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:

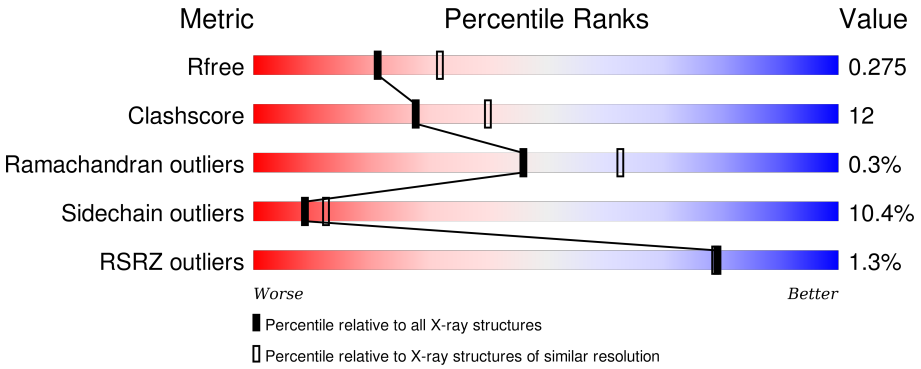
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (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	451	68% 16% • 13%
1	B	451	67% 16% • 15%
1	C	451	63% 18% • 15%
1	D	451	62% 18% • 16%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11611 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 DegQ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	392	Total	C	N	O	S	0	0	0
			2924	1852	511	554	7			
1	B	383	Total	C	N	O	S	0	0	0
			2846	1807	494	539	6			
1	C	384	Total	C	N	O	S	0	0	0
			2859	1813	499	540	7			
1	D	379	Total	C	N	O	S	0	0	0
			2819	1790	489	534	6			

- Molecule 2 is water.

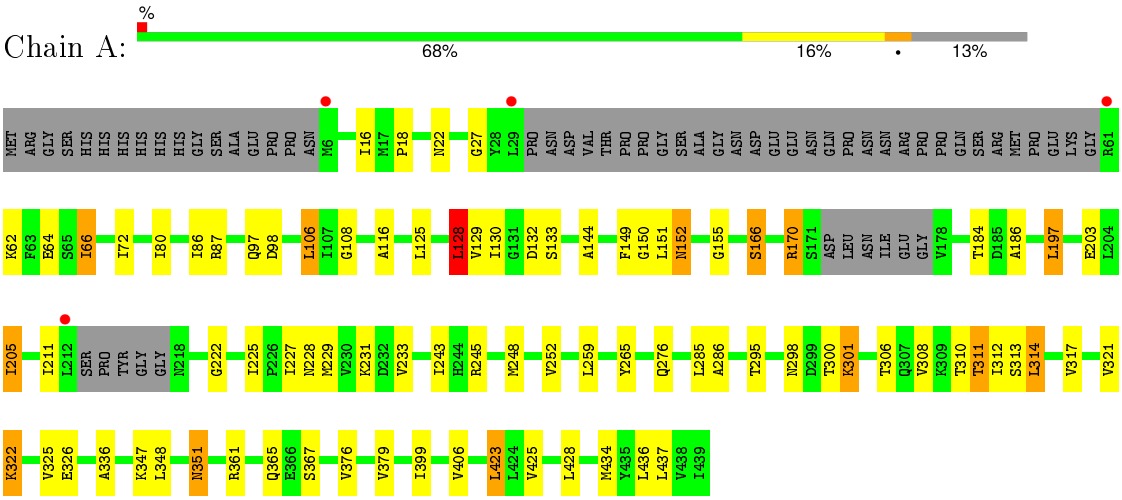
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	50	Total	O	0	0
			50	50		
2	B	40	Total	O	0	0
			40	40		
2	C	32	Total	O	0	0
			32	32		
2	D	41	Total	O	0	0
			41	41		

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.

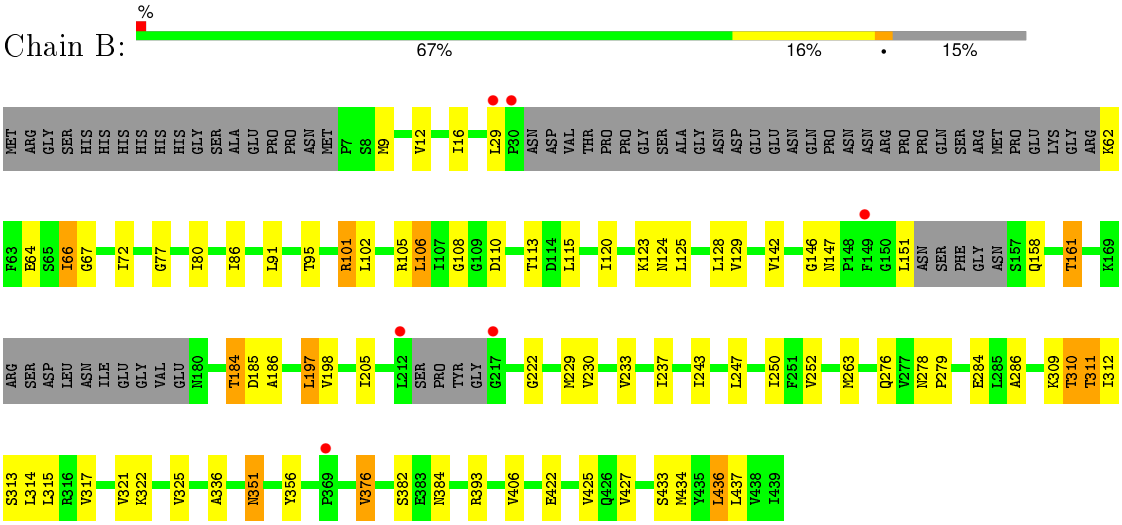
- Molecule 1: DegQ

Chain A:



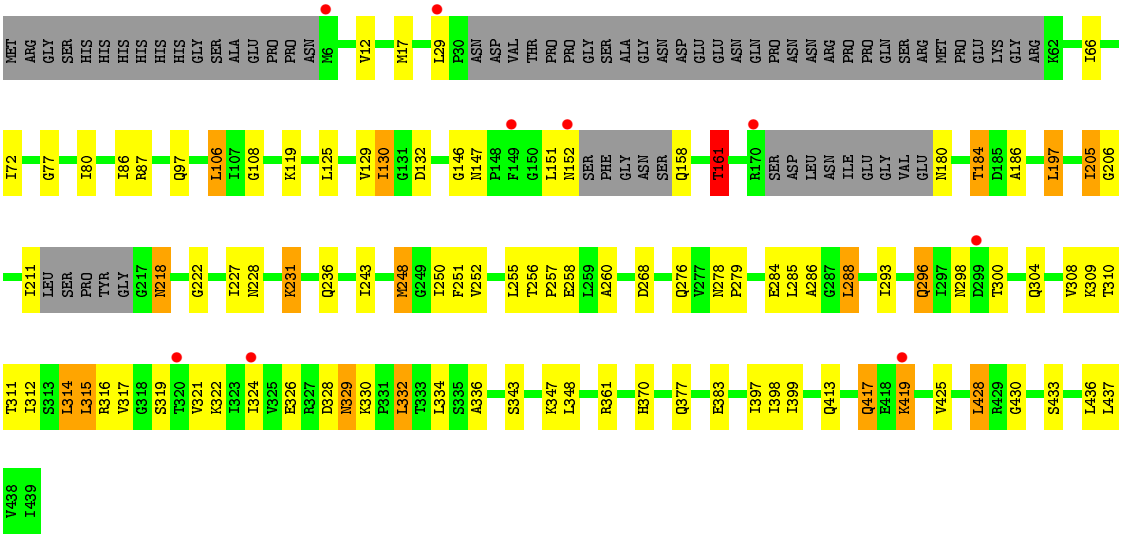
- Molecule 1: DegQ

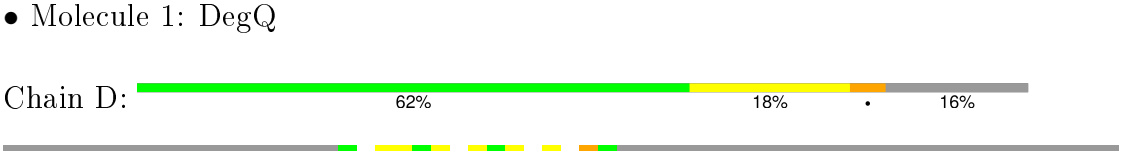
Chain B:

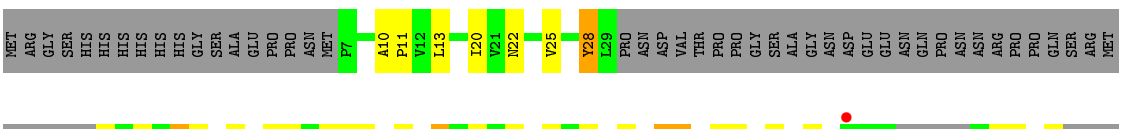


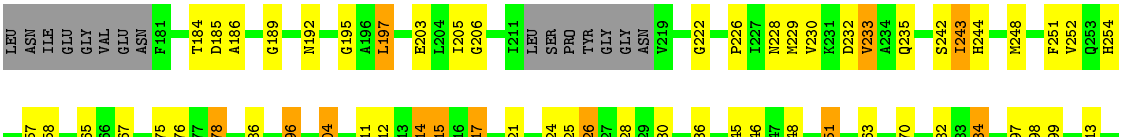
- Molecule 1: DegQ

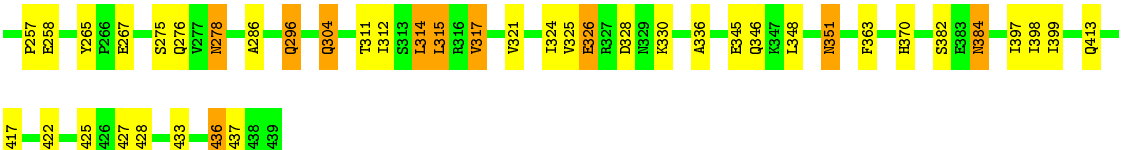
Chain C:











- Molecule 1: DegQ

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	137.11Å 137.11Å 326.91Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.46 – 2.40 43.95 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (44.46-2.40) 99.9 (43.95-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.40 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.231 , 0.285 0.224 , 0.275	Depositor DCC
R_{free} test set	4493 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	50.1	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 38.6	EDS
Estimated twinning fraction	0.000 for -h,1/3*h-1/3*k-1/3*l,-4/3*h-8/3*k+1/3*l 0.000 for -1/3*h+1/3*k+1/3*l,-k,8/3*h+4/3*k+1/3*l 0.003 for -2/3*h-1/3*k-1/3*l,-1/3*h-2/3*k+1/3*l,-4/3*h+4/3*k+1/3*l 0.000 for 1/3*h+2/3*k-1/3*l,-k,-8/3*h-4/3*k-1/3*l 0.000 for -1/3*h-2/3*k+1/3*l,-2/3*h-1/3*k-1/3*l,4/3*h-4/3*k-1/3*l 0.000 for -h,2/3*h+1/3*k+1/3*l,4/3*h+8/3*k-1/3*l 0.018 for h,-h-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 89540 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11611	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% 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	1.02	2/2960 (0.1%)	0.94	3/4005 (0.1%)
1	B	1.00	0/2881	0.97	4/3899 (0.1%)
1	C	0.91	0/2894	0.89	3/3916 (0.1%)
1	D	0.96	0/2853	0.91	1/3860 (0.0%)
All	All	0.97	2/11588 (0.0%)	0.93	11/15680 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	116	ALA	CA-CB	-6.55	1.38	1.52
1	A	144	ALA	CA-CB	5.35	1.63	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	101	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	D	101	ARG	NE-CZ-NH1	6.55	123.57	120.30
1	A	245	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	B	393	ARG	NE-CZ-NH2	-5.97	117.31	120.30
1	C	161	THR	CB-CA-C	-5.86	95.79	111.60
1	B	263	MET	CG-SD-CE	-5.43	91.51	100.20
1	C	361	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	A	166	SER	CB-CA-C	-5.14	100.33	110.10
1	C	130	ILE	CB-CA-C	-5.13	101.34	111.60
1	A	128	LEU	CA-CB-CG	5.06	126.93	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	436	LEU	CB-CG-CD1	5.05	119.58	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	150	GLY	Peptide

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	2924	0	3045	79	0
1	B	2846	0	2971	50	0
1	C	2859	0	2982	80	0
1	D	2819	0	2944	73	0
2	A	50	0	0	0	0
2	B	40	0	0	0	0
2	C	32	0	0	0	0
2	D	41	0	0	2	0
All	All	11611	0	11942	276	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 12.

All (276) 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:72:ILE:HD13	1:B:80:ILE:HD11	1.24	1.09
1:C:197:LEU:HD13	1:C:205:ILE:HD11	1.37	1.05
1:A:399:ILE:HD13	1:A:428:LEU:HD11	1.07	1.03
1:D:184:THR:HG21	2:D:459:HOH:O	1.59	1.01
1:C:184:THR:HG23	1:C:186:ALA:H	1.24	0.99
1:C:276:GLN:HE21	1:C:278:ASN:HD21	1.09	0.96
1:A:72:ILE:HD13	1:A:80:ILE:HD11	1.44	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:ILE:HD13	1:A:428:LEU:CD1	1.95	0.95
1:C:197:LEU:CD1	1:C:205:ILE:HD11	1.98	0.94
1:C:72:ILE:HD13	1:C:80:ILE:HD13	1.46	0.94
1:B:184:THR:HG23	1:B:186:ALA:H	1.32	0.92
1:D:243:ILE:N	1:D:243:ILE:HD12	1.84	0.92
1:A:197:LEU:HD13	1:A:205:ILE:HD11	1.53	0.91
1:C:276:GLN:HE21	1:C:278:ASN:ND2	1.67	0.91
1:B:146:GLY:HA2	1:B:158:GLN:HE21	1.35	0.90
1:A:72:ILE:HD13	1:A:80:ILE:CD1	2.01	0.89
1:C:66:ILE:HD13	1:C:152:ASN:HD22	1.36	0.89
1:A:72:ILE:CD1	1:A:80:ILE:HD11	2.02	0.89
1:D:197:LEU:HD13	1:D:205:ILE:HD11	1.54	0.88
1:A:86:ILE:HD12	1:A:86:ILE:C	1.95	0.86
1:B:72:ILE:HD13	1:B:80:ILE:CD1	2.07	0.84
1:A:225:ILE:CG2	1:A:229:MET:CE	2.56	0.84
1:B:197:LEU:HD13	1:B:205:ILE:CD1	2.09	0.83
1:C:211:ILE:O	1:C:211:ILE:HG22	1.79	0.83
1:C:72:ILE:CD1	1:C:80:ILE:HD13	2.09	0.81
1:A:225:ILE:CG2	1:A:229:MET:HE2	2.11	0.81
1:C:257:PRO:O	1:C:260:ALA:HB3	1.82	0.80
1:C:72:ILE:CD1	1:C:80:ILE:CD1	2.62	0.78
1:A:86:ILE:HD12	1:A:87:ARG:N	1.99	0.78
1:C:205:ILE:HD12	1:C:206:GLY:N	1.99	0.77
1:B:72:ILE:CD1	1:B:80:ILE:HD11	2.11	0.76
1:B:184:THR:HG22	1:B:222:GLY:CA	2.15	0.75
1:C:276:GLN:NE2	1:C:278:ASN:HD21	1.84	0.75
1:A:399:ILE:CD1	1:A:428:LEU:HD11	2.03	0.74
1:D:398:ILE:HG23	1:D:425:VAL:HG13	1.69	0.74
1:C:66:ILE:HD12	1:C:66:ILE:O	1.86	0.74
1:A:399:ILE:CG2	1:A:428:LEU:HD13	2.18	0.74
1:A:184:THR:HG23	1:A:186:ALA:H	1.52	0.74
1:C:205:ILE:HD12	1:C:205:ILE:C	2.06	0.73
1:A:295:THR:O	1:A:301:LYS:HD2	1.88	0.73
1:C:86:ILE:C	1:C:86:ILE:HD12	2.09	0.73
1:B:72:ILE:HG21	1:B:80:ILE:HD12	1.72	0.70
1:D:197:LEU:HD13	1:D:205:ILE:CD1	2.20	0.70
1:C:72:ILE:HD13	1:C:80:ILE:CD1	2.23	0.69
1:C:205:ILE:CD1	1:C:205:ILE:C	2.61	0.69
1:D:243:ILE:CD1	1:D:243:ILE:N	2.56	0.69
1:C:250:ILE:CG2	1:C:252:VAL:HG23	2.23	0.68
1:C:147:ASN:H	1:C:158:GLN:HE21	1.39	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:GLY:HA2	1:B:158:GLN:NE2	2.09	0.68
1:B:351:ASN:C	1:B:351:ASN:OD1	2.31	0.68
1:C:180:ASN:O	1:C:180:ASN:CG	2.32	0.68
1:A:197:LEU:HD13	1:A:205:ILE:CD1	2.24	0.67
1:A:184:THR:HG22	1:A:222:GLY:CA	2.25	0.67
1:A:86:ILE:C	1:A:86:ILE:CD1	2.63	0.66
1:A:225:ILE:HG23	1:A:229:MET:CE	2.25	0.66
1:C:428:LEU:HD12	1:C:433:SER:OG	1.95	0.66
1:D:66:ILE:HD12	1:D:67:GLY:N	2.10	0.66
1:C:250:ILE:CG2	1:C:251:PHE:N	2.59	0.66
1:D:184:THR:HG23	1:D:186:ALA:H	1.60	0.66
1:A:22:ASN:HD21	1:A:66:ILE:HD13	1.59	0.66
1:B:197:LEU:HD13	1:B:205:ILE:HD11	1.77	0.65
1:A:72:ILE:HG21	1:A:80:ILE:HD12	1.78	0.65
1:B:161:THR:HG22	1:D:185:ASP:OD2	1.96	0.65
1:C:250:ILE:HG22	1:C:251:PHE:N	2.12	0.65
1:B:113:THR:HB	1:B:229:MET:HE3	1.79	0.65
1:D:278:ASN:N	1:D:278:ASN:HD22	1.93	0.64
1:A:351:ASN:C	1:A:351:ASN:OD1	2.35	0.64
1:A:399:ILE:HG23	1:A:428:LEU:HD13	1.79	0.64
1:C:184:THR:HG23	1:C:186:ALA:N	2.06	0.64
1:A:314:LEU:N	1:A:314:LEU:HD13	2.14	0.63
1:D:265:TYR:HE2	1:D:326:GLU:HG2	1.63	0.63
1:C:255:LEU:CD1	1:C:293:ILE:HD11	2.29	0.63
1:C:399:ILE:HG21	1:C:428:LEU:HD22	1.80	0.62
1:D:436:LEU:HD22	1:D:436:LEU:N	2.14	0.62
1:A:399:ILE:HG21	1:A:428:LEU:HD13	1.81	0.62
1:D:184:THR:HG22	1:D:222:GLY:CA	2.30	0.62
1:C:286:ALA:HB2	1:C:336:ALA:HA	1.81	0.62
1:D:86:ILE:C	1:D:86:ILE:HD12	2.20	0.62
1:D:258:GLU:HG3	2:D:473:HOH:O	1.99	0.61
1:D:229:MET:O	1:D:233:VAL:HG13	2.00	0.61
1:A:225:ILE:HG22	1:A:229:MET:HE2	1.83	0.61
1:A:133:SER:HB3	1:A:227:ILE:HG22	1.84	0.60
1:B:184:THR:HG22	1:B:222:GLY:HA3	1.83	0.60
1:B:185:ASP:OD2	1:C:161:THR:HG22	2.01	0.60
1:C:328:ASP:O	1:C:329:ASN:HB2	2.01	0.59
1:A:286:ALA:HB2	1:A:336:ALA:HB2	1.84	0.59
1:D:146:GLY:HA2	1:D:158:GLN:HE21	1.67	0.59
1:C:255:LEU:HD13	1:C:293:ILE:HD11	1.83	0.59
1:D:192:ASN:HD21	1:D:195:GLY:H	1.50	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:VAL:HG13	1:A:406:VAL:HG11	1.85	0.59
1:D:13:LEU:HD21	1:D:143:VAL:HG11	1.85	0.59
1:A:225:ILE:HG23	1:A:229:MET:HE2	1.80	0.58
1:C:211:ILE:O	1:C:211:ILE:CG2	2.50	0.58
1:D:10:ALA:HB3	1:D:11:PRO:HD3	1.84	0.58
1:C:250:ILE:HG21	1:C:252:VAL:HG23	1.86	0.58
1:D:257:PRO:HB3	1:D:267:GLU:HG2	1.85	0.58
1:A:184:THR:HG22	1:A:222:GLY:O	2.04	0.58
1:D:382:SER:OG	1:D:384:ASN:ND2	2.37	0.58
1:C:311:THR:O	1:C:315:LEU:HD23	2.04	0.57
1:C:72:ILE:HD11	1:C:80:ILE:CD1	2.34	0.56
1:A:428:LEU:N	1:A:428:LEU:HD12	2.20	0.56
1:B:376:VAL:HG13	1:B:406:VAL:CG1	2.36	0.56
1:A:129:VAL:HG22	1:A:203:GLU:HG2	1.87	0.56
1:C:308:VAL:HG13	1:C:312:ILE:HD11	1.89	0.55
1:B:142:VAL:HB	1:B:197:LEU:CD2	2.36	0.55
1:C:286:ALA:O	1:C:334:LEU:HD22	2.07	0.55
1:D:22:ASN:HD21	1:D:66:ILE:HD13	1.72	0.55
1:C:398:ILE:HG23	1:C:425:VAL:CG2	2.36	0.55
1:D:351:ASN:O	1:D:351:ASN:ND2	2.38	0.54
1:A:106:LEU:HD22	1:A:108:GLY:N	2.22	0.54
1:B:142:VAL:HB	1:B:197:LEU:HD21	1.90	0.54
1:D:370:HIS:CD2	1:D:428:LEU:HD21	2.43	0.54
1:B:184:THR:HG23	1:B:186:ALA:N	2.12	0.54
1:C:86:ILE:CD1	1:C:86:ILE:C	2.76	0.54
1:A:399:ILE:HG21	1:A:428:LEU:CD1	2.38	0.53
1:D:192:ASN:ND2	1:D:195:GLY:H	2.06	0.53
1:B:276:GLN:NE2	1:B:278:ASN:HD21	2.07	0.53
1:D:205:ILE:C	1:D:205:ILE:HD12	2.27	0.53
1:D:184:THR:HG22	1:D:222:GLY:HA3	1.89	0.53
1:A:184:THR:HG23	1:A:186:ALA:N	2.23	0.53
1:B:86:ILE:HD12	1:B:86:ILE:C	2.29	0.53
1:A:72:ILE:CD1	1:A:80:ILE:CD1	2.72	0.53
1:C:184:THR:HG22	1:C:222:GLY:CA	2.39	0.53
1:B:106:LEU:HD22	1:B:108:GLY:N	2.23	0.52
1:C:66:ILE:HD13	1:C:152:ASN:ND2	2.16	0.52
1:A:265:TYR:HE2	1:A:326:GLU:HG2	1.75	0.52
1:D:384:ASN:HD22	1:D:384:ASN:H	1.58	0.52
1:D:128:LEU:HD12	1:D:128:LEU:N	2.25	0.52
1:A:106:LEU:HD22	1:A:108:GLY:H	1.75	0.52
1:D:25:VAL:HG13	1:D:89:ALA:CB	2.39	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:130:ILE:HG21	1:C:231:LYS:HD2	1.91	0.52
1:B:422:GLU:HB2	1:B:437:LEU:HD22	1.91	0.52
1:C:197:LEU:CD1	1:C:205:ILE:CD1	2.82	0.52
1:C:86:ILE:HD12	1:C:87:ARG:N	2.24	0.51
1:A:225:ILE:CG2	1:A:229:MET:HE1	2.39	0.51
1:A:72:ILE:CG2	1:A:80:ILE:HD12	2.40	0.51
1:A:170:ARG:HA	1:A:306:THR:HG21	1.93	0.51
1:B:80:ILE:HD13	1:B:230:VAL:CG1	2.41	0.51
1:C:197:LEU:HB3	1:C:205:ILE:CD1	2.40	0.51
1:B:250:ILE:HD12	1:B:312:ILE:HD11	1.91	0.51
1:D:192:ASN:HD21	1:D:195:GLY:N	2.08	0.51
1:C:197:LEU:HB3	1:C:205:ILE:HD11	1.93	0.50
1:C:180:ASN:O	1:C:180:ASN:OD1	2.29	0.50
1:D:80:ILE:CD1	1:D:117:VAL:HG22	2.41	0.50
1:D:110:ASP:HB2	1:D:243:ILE:HD13	1.92	0.50
1:D:205:ILE:HD12	1:D:206:GLY:N	2.26	0.50
1:A:184:THR:HG22	1:A:222:GLY:H	1.77	0.50
1:A:184:THR:HG22	1:A:222:GLY:N	2.27	0.50
1:B:161:THR:HG23	1:D:185:ASP:HB3	1.93	0.50
1:D:265:TYR:CE2	1:D:326:GLU:HG2	2.47	0.49
1:A:365:GLN:HG2	1:A:367:SER:OG	2.11	0.49
1:D:20:ILE:HD12	1:D:20:ILE:N	2.27	0.49
1:B:250:ILE:HD12	1:B:312:ILE:CD1	2.42	0.49
1:C:296:GLN:CD	1:C:324:ILE:HD12	2.33	0.49
1:D:115:LEU:HD11	1:D:230:VAL:HG22	1.95	0.49
1:C:298:ASN:HA	1:C:322:LYS:HB3	1.95	0.49
1:C:417:GLN:O	1:C:419:LYS:HD3	2.12	0.49
1:D:86:ILE:C	1:D:86:ILE:CD1	2.81	0.49
1:D:66:ILE:HD12	1:D:67:GLY:H	1.75	0.49
1:C:197:LEU:HD13	1:C:205:ILE:CD1	2.27	0.48
1:C:184:THR:HG22	1:C:222:GLY:HA3	1.95	0.48
1:C:147:ASN:ND2	1:C:152:ASN:OD1	2.46	0.48
1:C:377:GLN:HG3	1:C:397:ILE:HD13	1.95	0.48
1:C:326:GLU:HG2	1:C:329:ASN:HA	1.96	0.48
1:B:66:ILE:HD12	1:B:67:GLY:N	2.28	0.48
1:B:279:PRO:HA	1:B:284:GLU:OE1	2.12	0.48
1:A:286:ALA:CB	1:A:336:ALA:HB2	2.42	0.48
1:D:312:ILE:HA	1:D:315:LEU:HD22	1.96	0.48
1:A:265:TYR:CE2	1:A:326:GLU:HG2	2.49	0.48
1:D:398:ILE:HG12	1:D:425:VAL:HG11	1.96	0.48
1:B:184:THR:CG2	1:B:222:GLY:HA3	2.43	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:ASP:OD1	1:A:98:ASP:C	2.53	0.48
1:A:184:THR:CG2	1:A:222:GLY:CA	2.92	0.47
1:A:225:ILE:HG23	1:A:229:MET:HE1	1.95	0.47
1:B:321:VAL:HG12	1:B:336:ALA:O	2.14	0.47
1:D:363:PHE:CD2	1:D:397:ILE:HD12	2.49	0.47
1:A:184:THR:CG2	1:A:222:GLY:HA3	2.44	0.47
1:C:72:ILE:HD11	1:C:80:ILE:HD11	1.95	0.47
1:C:66:ILE:HD12	1:C:66:ILE:C	2.35	0.47
1:A:243:ILE:N	1:A:243:ILE:HD12	2.29	0.47
1:A:310:THR:O	1:A:311:THR:C	2.52	0.47
1:B:310:THR:O	1:B:311:THR:C	2.53	0.47
1:B:113:THR:HG22	1:B:229:MET:HE1	1.96	0.47
1:B:376:VAL:HG13	1:B:406:VAL:HG11	1.97	0.47
1:D:86:ILE:HD12	1:D:87:ARG:N	2.31	0.46
1:C:377:GLN:HG3	1:C:397:ILE:CD1	2.45	0.46
1:D:427:VAL:HG22	1:D:436:LEU:HD21	1.98	0.46
1:A:184:THR:HG22	1:A:222:GLY:C	2.36	0.46
1:A:314:LEU:N	1:A:314:LEU:CD1	2.79	0.46
1:A:376:VAL:HG13	1:A:406:VAL:CG1	2.44	0.46
1:A:399:ILE:CG2	1:A:428:LEU:CD1	2.92	0.46
1:A:132:ASP:HA	1:A:228:ASN:HD21	1.80	0.46
1:C:310:THR:O	1:C:314:LEU:HD22	2.16	0.46
1:A:437:LEU:HD13	1:C:258:GLU:HB3	1.97	0.46
1:C:106:LEU:HD22	1:C:108:GLY:N	2.31	0.46
1:C:132:ASP:HA	1:C:228:ASN:HD21	1.81	0.46
1:D:132:ASP:HA	1:D:228:ASN:HD21	1.81	0.45
1:A:205:ILE:HD12	1:A:205:ILE:C	2.37	0.45
1:D:244:HIS:HD2	1:D:317:VAL:HG13	1.82	0.45
1:D:314:LEU:HD13	1:D:314:LEU:N	2.31	0.45
1:B:110:ASP:HB2	1:B:243:ILE:HD12	1.97	0.45
1:D:129:VAL:HG22	1:D:203:GLU:HG2	1.98	0.45
1:C:279:PRO:HA	1:C:284:GLU:OE1	2.17	0.45
1:A:228:ASN:HD22	1:A:228:ASN:N	2.14	0.45
1:D:10:ALA:HB3	1:D:11:PRO:CD	2.45	0.45
1:D:106:LEU:HD22	1:D:108:GLY:H	1.81	0.45
1:A:22:ASN:ND2	1:A:66:ILE:HD13	2.31	0.44
1:B:102:LEU:HD12	1:B:120:ILE:HD12	1.99	0.44
1:D:242:SER:C	1:D:243:ILE:HD12	2.36	0.44
1:A:313:SER:CB	1:A:314:LEU:HD13	2.48	0.44
1:D:286:ALA:HB2	1:D:336:ALA:HB2	2.00	0.44
1:B:95:THR:OG1	1:B:101:ARG:HD2	2.16	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:133:SER:H	1:D:228:ASN:ND2	2.16	0.44
1:B:382:SER:OG	1:B:384:ASN:OD1	2.32	0.44
1:A:72:ILE:HD11	1:A:80:ILE:HD11	1.96	0.44
1:D:370:HIS:NE2	1:D:428:LEU:HD21	2.32	0.44
1:B:184:THR:HG22	1:B:222:GLY:C	2.38	0.43
1:B:161:THR:HG23	1:D:185:ASP:CB	2.49	0.43
1:D:311:THR:O	1:D:311:THR:HG22	2.16	0.43
1:C:330:LYS:O	1:C:332:LEU:HD12	2.18	0.43
1:C:146:GLY:HA2	1:C:158:GLN:HG3	2.01	0.43
1:B:286:ALA:HB2	1:B:336:ALA:HB2	2.00	0.43
1:C:370:HIS:NE2	1:C:430:GLY:O	2.37	0.43
1:D:169:LYS:HG3	1:D:304:GLN:HE22	1.83	0.43
1:D:398:ILE:HG23	1:D:425:VAL:CG1	2.44	0.43
1:B:16:ILE:HD12	1:B:198:VAL:HG11	2.01	0.43
1:D:128:LEU:H	1:D:128:LEU:HD12	1.82	0.43
1:C:255:LEU:HD13	1:C:293:ILE:CD1	2.46	0.43
1:A:376:VAL:CG1	1:A:406:VAL:CG1	2.97	0.43
1:D:399:ILE:HD13	1:D:428:LEU:HD12	2.01	0.43
1:C:218:ASN:HB2	1:D:189:GLY:HA2	1.99	0.43
1:A:72:ILE:HD13	1:A:80:ILE:HD12	1.95	0.42
1:B:233:VAL:HG23	1:B:237:ILE:HD12	2.01	0.42
1:A:27:GLY:O	1:A:62:LYS:HA	2.19	0.42
1:B:184:THR:HG22	1:B:222:GLY:N	2.33	0.42
1:C:317:VAL:HG23	1:C:317:VAL:O	2.19	0.42
1:A:152:ASN:HD21	1:A:155:GLY:HA3	1.84	0.42
1:C:227:ILE:HA	1:C:227:ILE:HD12	1.75	0.42
1:D:422:GLU:HB2	1:D:437:LEU:HD22	2.02	0.42
1:A:423:LEU:HD13	1:A:425:VAL:HG23	2.02	0.42
1:C:413:GLN:O	1:C:417:GLN:HG2	2.19	0.42
1:D:328:ASP:O	1:D:330:LYS:CD	2.68	0.42
1:D:413:GLN:O	1:D:417:GLN:HG3	2.19	0.42
1:C:147:ASN:H	1:C:158:GLN:NE2	2.13	0.42
1:C:255:LEU:HD11	1:C:293:ILE:HD11	1.99	0.42
1:A:428:LEU:N	1:A:428:LEU:CD1	2.82	0.42
1:A:298:ASN:O	1:A:322:LYS:NZ	2.53	0.42
1:B:77:GLY:HA2	1:B:125:LEU:HD23	2.02	0.41
1:B:309:LYS:O	1:B:313:SER:HB2	2.20	0.41
1:A:184:THR:CG2	1:A:186:ALA:H	2.27	0.41
1:D:286:ALA:CB	1:D:336:ALA:HB2	2.50	0.41
1:C:248:MET:HE3	1:C:321:VAL:HG11	2.01	0.41
1:C:256:THR:HB	1:C:257:PRO:HD2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:VAL:HG13	1:A:312:ILE:HD12	2.01	0.41
1:C:77:GLY:O	1:C:119:LYS:HA	2.20	0.41
1:D:296:GLN:HB3	1:D:324:ILE:HB	2.02	0.41
1:D:184:THR:CG2	1:D:222:GLY:HA3	2.51	0.41
1:C:286:ALA:HB2	1:C:336:ALA:CA	2.50	0.41
1:D:251:PHE:HB2	1:D:276:GLN:HG2	2.02	0.41
1:A:361:ARG:HG2	1:A:379:VAL:CG2	2.50	0.41
1:B:147:ASN:H	1:B:158:GLN:NE2	2.18	0.41
1:A:128:LEU:HD12	1:A:128:LEU:N	2.36	0.41
1:B:425:VAL:HG12	1:B:427:VAL:HG13	2.02	0.41
1:B:115:LEU:HD11	1:B:230:VAL:HG22	2.03	0.41
1:A:347:LYS:O	1:A:351:ASN:HB3	2.21	0.41
1:A:313:SER:HB2	1:A:314:LEU:HD13	2.03	0.41
1:C:236:GLN:HG2	1:C:243:ILE:HD13	2.03	0.41
1:A:130:ILE:HG21	1:A:231:LYS:HE3	2.03	0.41
1:D:28:TYR:CE2	1:D:62:LYS:HD3	2.56	0.41
1:D:80:ILE:HD11	1:D:117:VAL:HG22	2.02	0.40
1:B:427:VAL:O	1:B:433:SER:HA	2.21	0.40
1:C:288:LEU:HD12	1:C:334:LEU:HD12	2.03	0.40
1:C:296:GLN:NE2	1:C:324:ILE:HD12	2.36	0.40
1:A:308:VAL:CG1	1:A:312:ILE:HD12	2.51	0.40
1:A:18:PRO:HG3	1:A:97:GLN:HE22	1.87	0.40
1:D:321:VAL:HG13	1:D:321:VAL:O	2.21	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	384/451 (85%)	368 (96%)	14 (4%)	2 (0%)	34 48
1	B	373/451 (83%)	354 (95%)	18 (5%)	1 (0%)	46 63

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	374/451 (83%)	352 (94%)	20 (5%)	2 (0%)	34 48
1	D	369/451 (82%)	359 (97%)	10 (3%)	0	100 100
All	All	1500/1804 (83%)	1433 (96%)	62 (4%)	5 (0%)	46 63

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	152	ASN
1	C	329	ASN
1	C	419	LYS
1	A	311	THR
1	B	311	THR

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	321/370 (87%)	290 (90%)	31 (10%)	10 15
1	B	312/370 (84%)	282 (90%)	30 (10%)	10 15
1	C	313/370 (85%)	278 (89%)	35 (11%)	7 10
1	D	309/370 (84%)	274 (89%)	35 (11%)	7 10
All	All	1255/1480 (85%)	1124 (90%)	131 (10%)	9 12

All (131) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ILE
1	A	64	GLU
1	A	66	ILE
1	A	106	LEU
1	A	125	LEU
1	A	128	LEU
1	A	149	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	151	LEU
1	A	166	SER
1	A	170	ARG
1	A	197	LEU
1	A	205	ILE
1	A	211	ILE
1	A	233	VAL
1	A	248	MET
1	A	252	VAL
1	A	259	LEU
1	A	276	GLN
1	A	285	LEU
1	A	300	THR
1	A	301	LYS
1	A	314	LEU
1	A	317	VAL
1	A	321	VAL
1	A	322	LYS
1	A	325	VAL
1	A	348	LEU
1	A	351	ASN
1	A	423	LEU
1	A	434	MET
1	A	436	LEU
1	B	9	MET
1	B	12	VAL
1	B	29	LEU
1	B	62	LYS
1	B	64	GLU
1	B	66	ILE
1	B	91	LEU
1	B	105	ARG
1	B	106	LEU
1	B	123	LYS
1	B	124	ASN
1	B	128	LEU
1	B	129	VAL
1	B	151	LEU
1	B	161	THR
1	B	184	THR
1	B	197	LEU
1	B	247	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	252	VAL
1	B	310	THR
1	B	314	LEU
1	B	315	LEU
1	B	317	VAL
1	B	322	LYS
1	B	325	VAL
1	B	351	ASN
1	B	356	TYR
1	B	376	VAL
1	B	434	MET
1	B	436	LEU
1	C	12	VAL
1	C	17	MET
1	C	29	LEU
1	C	97	GLN
1	C	106	LEU
1	C	125	LEU
1	C	129	VAL
1	C	151	LEU
1	C	161	THR
1	C	184	THR
1	C	197	LEU
1	C	205	ILE
1	C	218	ASN
1	C	231	LYS
1	C	248	MET
1	C	268	ASP
1	C	285	LEU
1	C	288	LEU
1	C	296	GLN
1	C	300	THR
1	C	304	GLN
1	C	309	LYS
1	C	314	LEU
1	C	315	LEU
1	C	316	ARG
1	C	319	SER
1	C	332	LEU
1	C	343	SER
1	C	347	LYS
1	C	348	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	383	GLU
1	C	417	GLN
1	C	428	LEU
1	C	436	LEU
1	C	437	LEU
1	D	28	TYR
1	D	64	GLU
1	D	66	ILE
1	D	90	SER
1	D	91	LEU
1	D	106	LEU
1	D	125	LEU
1	D	128	LEU
1	D	129	VAL
1	D	157	SER
1	D	197	LEU
1	D	226	PRO
1	D	232	ASP
1	D	233	VAL
1	D	235	GLN
1	D	243	ILE
1	D	248	MET
1	D	252	VAL
1	D	254	HIS
1	D	275	SER
1	D	278	ASN
1	D	296	GLN
1	D	304	GLN
1	D	314	LEU
1	D	315	LEU
1	D	317	VAL
1	D	325	VAL
1	D	326	GLU
1	D	345	GLU
1	D	346	GLN
1	D	348	LEU
1	D	351	ASN
1	D	384	ASN
1	D	433	SER
1	D	436	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	22	ASN
1	A	97	GLN
1	A	158	GLN
1	A	228	ASN
1	A	278	ASN
1	A	296	GLN
1	A	346	GLN
1	A	384	ASN
1	B	26	GLN
1	B	76	ASN
1	B	158	GLN
1	B	192	ASN
1	B	208	ASN
1	B	228	ASN
1	B	276	GLN
1	C	15	ASN
1	C	76	ASN
1	C	97	GLN
1	C	158	GLN
1	C	192	ASN
1	C	208	ASN
1	C	228	ASN
1	C	278	ASN
1	C	296	GLN
1	C	329	ASN
1	C	384	ASN
1	C	417	GLN
1	D	22	ASN
1	D	97	GLN
1	D	156	ASN
1	D	158	GLN
1	D	192	ASN
1	D	208	ASN
1	D	228	ASN
1	D	244	HIS
1	D	278	ASN
1	D	296	GLN
1	D	329	ASN
1	D	384	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	A	392/451 (86%)	-0.16	4 (1%)	84	83	21, 42, 63, 83	0
1	B	383/451 (84%)	-0.13	6 (1%)	74	74	22, 41, 60, 78	0
1	C	384/451 (85%)	-0.07	9 (2%)	64	63	25, 45, 81, 93	0
1	D	379/451 (84%)	-0.20	1 (0%)	94	94	26, 43, 60, 71	0
All	All	1538/1804 (85%)	-0.14	20 (1%)	79	79	21, 43, 70, 93	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	30	PRO	4.8
1	A	61	ARG	4.7
1	C	29	LEU	4.4
1	C	299	ASP	4.1
1	B	217	GLY	3.4
1	B	149	PHE	3.3
1	C	152	ASN	3.3
1	C	419	LYS	3.0
1	C	149	PHE	3.0
1	A	29	LEU	2.5
1	C	6	MET	2.5
1	B	29	LEU	2.2
1	A	212	LEU	2.2
1	B	369	PRO	2.2
1	C	324	ILE	2.2
1	C	170	ARG	2.2
1	A	6	MET	2.1
1	B	212	LEU	2.1
1	D	149	PHE	2.1
1	C	320	THR	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 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.