WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:47 AM GMT

PDB ID	:	3PV3
Title	:	Structure of Legionella fallonii DegQ (S193A variant)
Authors	:	Wrase, R.; Scott, H.; Hilgenfeld, R.; Hansen, G.
Deposited on	:	2010-12-06
Resolution	:	3.10 Å(reported)

The following versions of software and data (see references ⓘ) 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 3.10 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	Percentile Ranks	Value
Rfree		0.288
Clashscore		15
Ramachandran outliers		1.6%
Sidechain outliers		14.7%
RSRZ outliers		0.6%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
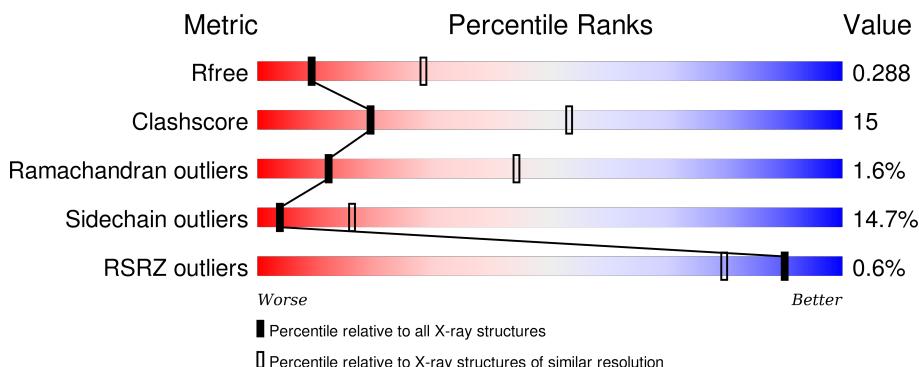
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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	55% 27% 5% 13%
1	B	451	54% 28% 5% 13%
1	C	451	% 52% 29% • 15%
1	D	451	56% 25% • 14%
2	E	20	25% 5% 70%

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Mol	Chain	Length	Quality of chain
2	F	20	35% 65%
2	G	20	30% 70%
2	H	20	40% 60%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 11766 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
			2927	1852	512	556	7			
1	B	392	Total	C	N	O	S	0	0	0
			2924	1853	508	556	7			
1	C	384	Total	C	N	O	S	0	0	0
			2871	1821	501	542	7			
1	D	390	Total	C	N	O	S	0	0	0
			2909	1845	507	550	7			

- Molecule 2 is a protein called Substrate peptide (Poly-Ala).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	6	Total	C	N	O	0	0	0
			30	18	6	6			
2	F	7	Total	C	N	O	0	0	0
			35	21	7	7			
2	G	6	Total	C	N	O	0	0	0
			30	18	6	6			
2	H	8	Total	C	N	O	0	0	0
			40	24	8	8			

3 Residue-property plots ⓘ

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
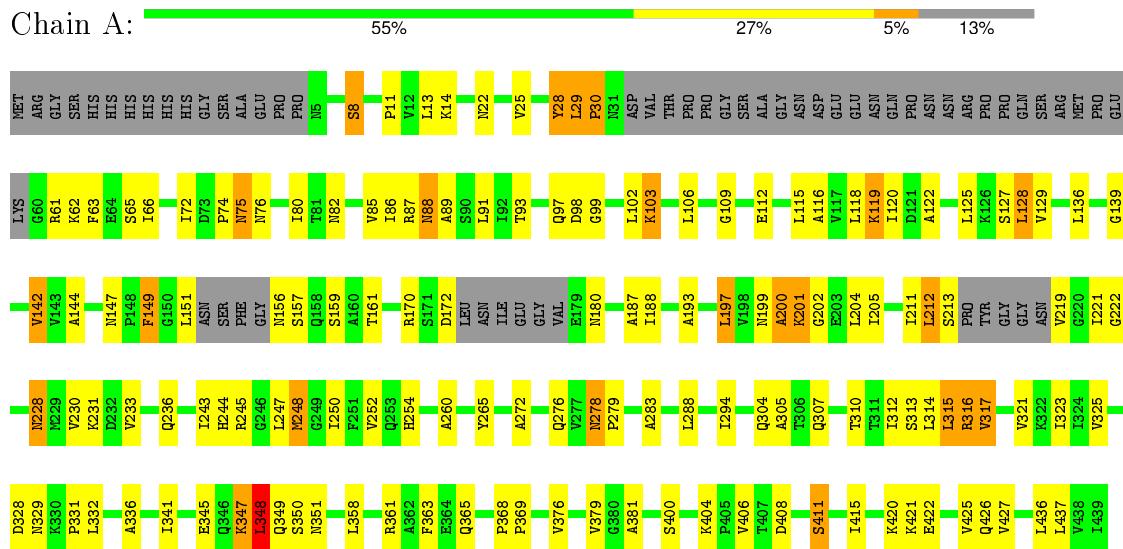
- Molecule 1: DegQ
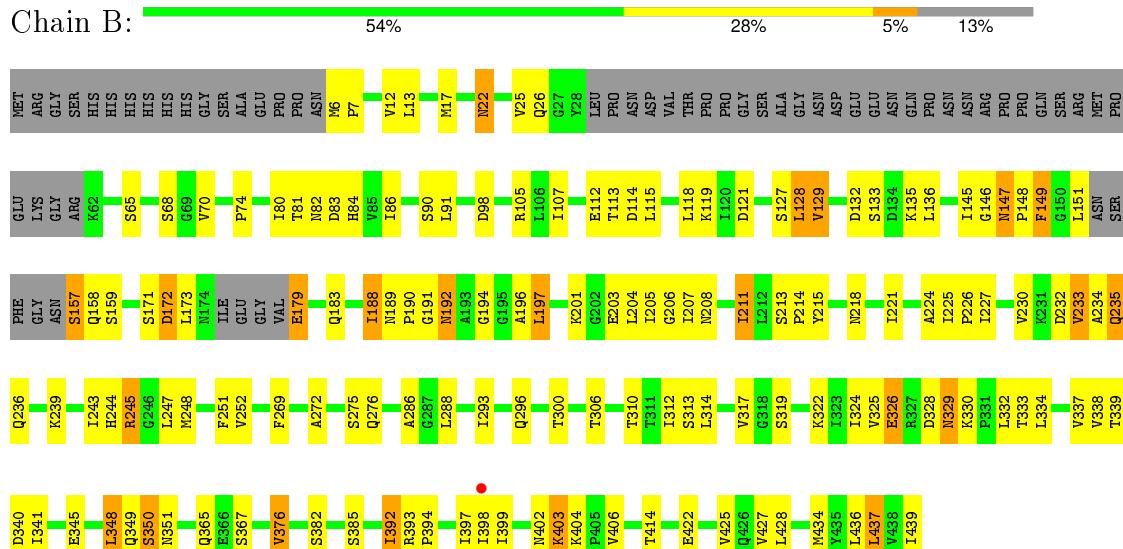
- Molecule 1: DegQ
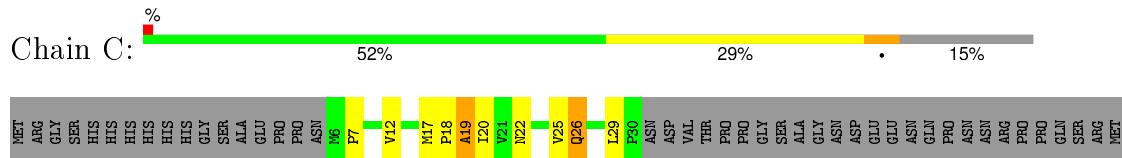
Chain C:

52% 29% 15%

- Molecule 1: DegQ

Chain D:

56% 25% 14%

- Molecule 2: Substrate peptide (Poly-Ala)

Chain E:

25% 5% 70%

- Molecule 2: Substrate peptide (Poly-Ala)

Chain F:

35% 65%

X12 X18 UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK

• Molecule 2: Substrate peptide (Poly-Ala)

Chain G:

30% 70%

X13 X18 UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK

• Molecule 2: Substrate peptide (Poly-Ala)

Chain H:

40% 60%

X11 X18 UNK UNK UNK UNK UNK UNK UNK UNK UNK

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	155.03Å 155.03Å 260.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	59.61 – 3.10 58.61 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.7 (59.61-3.10) 98.6 (58.61-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	1.92 (at 3.13Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.224 , 0.292 0.219 , 0.288	Depositor DCC
R_{free} test set	2109 reflections (5.31%)	DCC
Wilson B-factor (Å^2)	89.9	Xtriage
Anisotropy	0.007	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 54.9	EDS
Estimated twinning fraction	0.180 for h,-h-k,-l	Xtriage
L-test for twinning[2]	$< |L| > = 0.41, < L^2 > = 0.23$	Xtriage
Outliers	0 of 41800 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11766	wwPDB-VP
Average B, all atoms (Å^2)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.31% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (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	0.56	0/2963	0.73	1/4011 (0.0%)
1	B	0.55	0/2962	0.70	0/4012
1	C	0.51	0/2907	0.67	0/3934
1	D	0.54	0/2946	0.69	0/3989
All	All	0.54	0/11778	0.70	1/15946 (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	348	LEU	CA-CB-CG	5.33	127.56	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	2927	0	3044	105	0
1	B	2924	0	3038	88	0
1	C	2871	0	2993	89	0
1	D	2909	0	3028	86	0
2	E	30	0	9	2	0
2	F	35	0	10	0	0
2	G	30	0	8	0	0
2	H	40	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	11766	0	12140	361	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 15.

All (361) 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:A:29:LEU:HB3	1:A:30:PRO:HD2	1.36	1.07
1:A:188:ILE:O	1:A:211:ILE:HD11	1.55	1.04
1:D:197:LEU:HD22	1:D:205:ILE:HD11	1.40	1.01
1:A:102:LEU:HD21	1:A:122:ALA:HB2	1.48	0.94
1:A:29:LEU:HB3	1:A:30:PRO:CD	2.00	0.92
1:A:316:ARG:HH11	1:A:316:ARG:HG3	1.36	0.90
1:A:188:ILE:O	1:A:211:ILE:CD1	2.21	0.88
1:B:136:LEU:HD11	1:B:205:ILE:HD13	1.55	0.87
1:C:296:GLN:HE21	1:C:324:ILE:HD12	1.38	0.86
1:D:115:LEU:HD12	1:D:233:VAL:HG21	1.55	0.86
1:B:183:GLN:HE22	1:C:159:SER:HB2	1.39	0.86
1:B:25:VAL:HG21	1:B:86:ILE:HA	1.57	0.86
1:A:115:LEU:HD11	1:A:230:VAL:HG22	1.57	0.85
1:A:142:VAL:HG13	1:A:197:LEU:HD21	1.60	0.84
1:B:399:ILE:HD13	1:B:428:LEU:HD13	1.60	0.84
1:D:112:GLU:CB	1:D:245:ARG:HH22	1.93	0.82
1:B:403:LYS:HE2	1:B:403:LYS:HA	1.62	0.82
1:A:74:PRO:HG3	1:A:127:SER:HB3	1.64	0.79
1:C:261:GLN:HG3	1:C:267:GLU:HB3	1.63	0.79
1:C:113:THR:HA	1:C:178:VAL:HB	1.63	0.79
1:A:193:ALA:HB2	2:E:15:UNK:O	1.82	0.78
1:A:151:LEU:HB2	1:A:157:SER:OG	1.85	0.77
1:A:136:LEU:HD11	1:A:205:ILE:HD13	1.65	0.77
1:A:142:VAL:HG13	1:A:197:LEU:CD2	2.15	0.75
1:D:102:LEU:HD21	1:D:122:ALA:HB2	1.69	0.75
1:B:115:LEU:HD21	1:B:225:ILE:HD12	1.67	0.75
1:D:80:ILE:HD12	1:D:230:VAL:HG13	1.69	0.74
1:B:348:LEU:C	1:B:350:SER:H	1.91	0.73
1:D:112:GLU:HB2	1:D:245:ARG:HH22	1.53	0.73
1:A:25:VAL:HB	1:A:65:SER:HB3	1.69	0.73
1:C:102:LEU:HD12	1:C:120:ILE:HD12	1.71	0.72
1:B:399:ILE:HD13	1:B:428:LEU:CD1	2.20	0.72
1:B:247:LEU:HD13	1:B:341:ILE:HD11	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:THR:HG21	1:B:233:VAL:HG11	1.70	0.71
1:D:312:ILE:HA	1:D:315:LEU:HD12	1.73	0.70
1:A:347:LYS:HA	1:A:350:SER:OG	1.91	0.70
1:A:316:ARG:CG	1:A:316:ARG:HH11	2.05	0.69
1:A:72:ILE:HG21	1:A:80:ILE:HD11	1.74	0.69
1:C:148:PRO:HA	1:C:191:GLY:HA3	1.75	0.69
1:C:136:LEU:HD11	1:C:205:ILE:HD13	1.75	0.69
1:B:382:SER:HB3	1:B:385:SER:HB3	1.75	0.69
1:C:288:LEU:HD12	1:C:292:ASP:OD2	1.93	0.69
1:C:279:PRO:HA	1:C:284:GLU:CD	2.13	0.68
1:C:382:SER:HB3	1:C:385:SER:HB3	1.73	0.68
1:B:422:GLU:HB2	1:B:437:LEU:HD21	1.75	0.68
1:A:102:LEU:CD2	1:A:122:ALA:HB2	2.23	0.67
1:C:254:HIS:HA	1:C:305:ALA:HB2	1.75	0.67
1:B:235:GLN:O	1:B:239:LYS:HD3	1.95	0.67
1:B:183:GLN:NE2	1:C:159:SER:HB2	2.09	0.66
1:D:251:PHE:HB2	1:D:276:GLN:HG2	1.77	0.66
1:D:112:GLU:HB3	1:D:245:ARG:HH22	1.60	0.65
1:C:417:GLN:HA	1:C:417:GLN:HE21	1.61	0.65
1:B:84:HIS:HD1	1:B:114:ASP:CG	2.00	0.65
1:B:197:LEU:HD23	1:B:208:ASN:HD21	1.62	0.65
1:B:189:ASN:O	1:B:192:ASN:HB2	1.97	0.64
1:A:142:VAL:CG1	1:A:197:LEU:HD21	2.27	0.64
1:A:348:LEU:HA	1:A:351:ASN:HB3	1.79	0.64
1:C:19:ALA:HB1	1:C:128:LEU:HD22	1.80	0.64
1:D:246:GLY:HA3	1:D:338:VAL:HG13	1.80	0.64
1:A:151:LEU:HB2	1:A:157:SER:CB	2.27	0.63
1:A:25:VAL:HG13	1:A:89:ALA:HB2	1.81	0.63
1:D:127:SER:OG	1:D:128:LEU:N	2.32	0.63
1:D:189:ASN:H	1:D:192:ASN:HD22	1.47	0.62
1:C:20:ILE:HG13	1:C:145:ILE:HG21	1.82	0.62
1:B:365:GLN:HE21	1:B:367:SER:HB3	1.64	0.62
1:B:208:ASN:HD22	1:B:224:ALA:HB2	1.64	0.62
1:C:358:LEU:HA	1:C:380:GLY:O	2.00	0.62
1:D:317:VAL:HA	1:D:338:VAL:HG12	1.81	0.62
1:A:252:VAL:HG21	1:A:272:ALA:HB1	1.81	0.62
1:C:170:ARG:HD2	1:C:179:GLU:HG3	1.81	0.62
1:C:179:GLU:HB2	1:C:310:THR:CG2	2.30	0.61
1:A:22:ASN:HD21	1:A:147:ASN:ND2	1.98	0.61
1:A:248:MET:HG2	1:A:250:ILE:HD11	1.83	0.61
1:A:331:PRO:O	1:A:332:LEU:HD23	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:13:LEU:HD21	1:D:143:VAL:HG11	1.83	0.61
1:A:127:SER:OG	1:A:128:LEU:N	2.34	0.60
1:D:73:ASP:HB3	1:D:78:VAL:HB	1.83	0.60
1:D:107:ILE:HD11	1:D:119:LYS:HB2	1.82	0.60
1:D:197:LEU:HD22	1:D:205:ILE:CD1	2.23	0.60
1:A:86:ILE:HG21	1:A:118:LEU:HD11	1.83	0.60
1:D:414:THR:O	1:D:417:GLN:HB2	2.01	0.60
1:D:312:ILE:HA	1:D:315:LEU:CD1	2.31	0.60
1:C:417:GLN:HA	1:C:417:GLN:NE2	2.16	0.59
1:B:251:PHE:HB2	1:B:276:GLN:HG2	1.83	0.59
1:B:269:PHE:HE1	1:B:293:ILE:HG21	1.67	0.59
1:C:151:LEU:HD12	1:C:157:SER:C	2.21	0.59
1:D:360:LEU:HD13	1:D:376:VAL:HG21	1.85	0.59
1:B:392:ILE:O	1:B:393:ARG:NH1	2.34	0.59
1:A:180:ASN:HB2	1:A:310:THR:HG21	1.85	0.59
1:D:244:HIS:HB3	1:D:317:VAL:HG12	1.83	0.59
1:D:133:SER:H	1:D:228:ASN:ND2	2.01	0.58
1:C:115:LEU:HD11	1:C:230:VAL:HG22	1.85	0.58
1:B:399:ILE:CD1	1:B:428:LEU:HD13	2.33	0.58
1:B:226:PRO:O	1:B:230:VAL:HG23	2.03	0.58
1:A:120:ILE:HD11	1:A:125:LEU:HD21	1.86	0.58
1:A:252:VAL:CG2	1:A:272:ALA:HB1	2.35	0.57
1:C:170:ARG:O	1:C:170:ARG:HG3	2.05	0.57
1:B:348:LEU:O	1:B:350:SER:N	2.38	0.57
1:B:148:PRO:HA	1:B:191:GLY:HA3	1.85	0.57
1:D:83:ASP:OD1	1:D:87:ARG:NH1	2.36	0.56
1:D:22:ASN:HD21	1:D:147:ASN:ND2	2.04	0.56
1:A:278:ASN:HD22	1:A:279:PRO:HD2	1.69	0.56
1:D:292:ASP:HB3	1:D:325:VAL:CG2	2.36	0.56
1:C:296:GLN:HE21	1:C:324:ILE:CD1	2.12	0.56
1:B:348:LEU:C	1:B:350:SER:N	2.60	0.55
1:A:400:SER:HA	1:A:406:VAL:HG23	1.88	0.55
1:D:426:GLN:HB2	1:D:435:TYR:CE1	2.41	0.55
1:A:28:TYR:HA	1:A:62:LYS:HA	1.88	0.55
1:B:132:ASP:HB3	1:B:135:LYS:HG2	1.89	0.55
1:A:233:VAL:HB	1:A:243:ILE:CD1	2.37	0.55
1:A:115:LEU:CD1	1:A:230:VAL:HG22	2.32	0.55
1:C:183:GLN:HE21	1:C:221:ILE:HG23	1.70	0.55
1:A:347:LYS:O	1:A:349:GLN:N	2.39	0.55
1:C:151:LEU:HD23	1:C:151:LEU:O	2.07	0.55
1:D:17:MET:HE3	1:D:160:ALA:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:296:GLN:HB3	1:B:324:ILE:HB	1.90	0.54
1:A:345:GLU:O	1:A:347:LYS:O	2.25	0.54
1:D:239:LYS:HD2	1:D:240:PHE:CE2	2.42	0.54
1:B:288:LEU:HD11	1:B:325:VAL:HG21	1.89	0.54
1:C:18:PRO:C	1:C:20:ILE:H	2.11	0.54
1:B:328:ASP:C	1:B:329:ASN:HD22	2.11	0.54
1:C:432:GLY:HA2	1:D:276:GLN:HE22	1.73	0.54
1:D:132:ASP:HA	1:D:228:ASN:HD21	1.73	0.53
1:C:17:MET:N	1:C:18:PRO:CD	2.71	0.53
1:B:399:ILE:O	1:B:406:VAL:HB	2.08	0.53
1:D:349:GLN:HG2	1:D:356:TYR:CD2	2.44	0.53
1:D:435:TYR:C	1:D:436:LEU:HD12	2.29	0.53
1:C:279:PRO:HA	1:C:284:GLU:OE1	2.09	0.53
1:D:78:VAL:HG11	1:D:238:ILE:HD11	1.91	0.53
1:D:238:ILE:HG22	1:D:239:LYS:N	2.23	0.53
1:B:179:GLU:HG2	1:B:310:THR:HG22	1.91	0.53
1:C:304:GLN:HB2	1:C:307:GLN:HG3	1.91	0.53
1:A:29:LEU:CB	1:A:30:PRO:CD	2.83	0.53
1:A:248:MET:HE1	1:A:336:ALA:HB3	1.90	0.53
1:B:393:ARG:HB3	1:B:394:PRO:HD2	1.90	0.53
1:D:296:GLN:HB3	1:D:324:ILE:HB	1.89	0.53
1:C:102:LEU:CD1	1:C:120:ILE:HD12	2.39	0.53
1:C:269:PHE:HD1	1:C:270:GLN:N	2.07	0.53
1:A:425:VAL:CG1	1:A:427:VAL:HG13	2.39	0.53
1:A:161:THR:HG21	1:A:187:ALA:O	2.09	0.53
1:C:312:ILE:HA	1:C:315:LEU:HD22	1.90	0.52
1:B:211:ILE:HG22	1:B:221:ILE:O	2.08	0.52
1:A:200:ALA:HB3	1:B:6:MET:SD	2.50	0.52
1:A:361:ARG:HD3	1:A:379:VAL:HG21	1.90	0.52
1:A:221:ILE:HG22	1:A:221:ILE:O	2.09	0.52
1:D:247:LEU:HB2	1:D:341:ILE:HG13	1.91	0.52
1:A:248:MET:HE3	1:A:323:ILE:HD11	1.91	0.52
1:B:189:ASN:HB3	1:B:190:PRO:HD2	1.91	0.51
1:D:325:VAL:O	1:D:325:VAL:HG13	2.09	0.51
1:A:199:ASN:O	1:A:202:GLY:N	2.43	0.51
1:A:247:LEU:HD23	1:A:341:ILE:HA	1.92	0.51
1:C:108:GLY:HA3	1:C:237:ILE:HG21	1.92	0.51
1:B:84:HIS:ND1	1:B:114:ASP:OD2	2.44	0.51
1:A:254:HIS:HA	1:A:305:ALA:HB2	1.92	0.51
1:C:97:GLN:HE21	1:C:98:ASP:N	2.08	0.51
1:D:325:VAL:CG1	1:D:325:VAL:O	2.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:402:ASN:O	1:B:404:LYS:HG3	2.11	0.51
1:B:245:ARG:HH21	1:B:313:SER:HB3	1.76	0.51
1:C:170:ARG:HD2	1:C:179:GLU:CG	2.42	0.50
1:A:420:LYS:C	1:A:422:GLU:H	2.14	0.50
1:A:193:ALA:CB	2:E:15:UNK:O	2.56	0.50
1:C:205:ILE:HA	1:C:227:ILE:HB	1.94	0.50
1:C:344:HIS:O	1:C:347:LYS:N	2.45	0.50
1:B:206:GLY:HA2	1:B:225:ILE:O	2.12	0.50
1:A:76:ASN:O	1:A:119:LYS:HD3	2.11	0.50
1:A:72:ILE:HG21	1:A:80:ILE:CD1	2.40	0.50
1:C:131:GLY:O	1:C:227:ILE:HG21	2.12	0.50
1:D:22:ASN:HD21	1:D:147:ASN:HD22	1.60	0.50
1:C:143:VAL:HG13	1:C:161:THR:O	2.12	0.50
1:D:147:ASN:HB2	1:D:158:GLN:HE21	1.76	0.50
1:A:248:MET:HB3	1:A:250:ILE:HG13	1.92	0.50
1:D:73:ASP:CB	1:D:78:VAL:HB	2.42	0.49
1:D:421:LYS:HG3	1:D:422:GLU:HG3	1.94	0.49
1:A:272:ALA:HB3	1:A:294:ILE:HB	1.94	0.49
1:C:390:ALA:HB2	1:C:438:VAL:HA	1.94	0.49
1:A:197:LEU:HD13	1:A:205:ILE:HD11	1.94	0.49
1:B:399:ILE:CD1	1:B:428:LEU:CD1	2.91	0.49
1:A:28:TYR:N	1:A:28:TYR:CD1	2.81	0.49
1:C:180:ASN:HB2	1:C:229:MET:HE1	1.93	0.49
1:A:363:PHE:CE2	1:A:365:GLN:HB3	2.47	0.49
1:C:384:ASN:CG	1:C:384:ASN:O	2.51	0.49
1:A:328:ASP:O	1:A:329:ASN:HB2	2.13	0.49
1:B:105:ARG:O	1:B:118:LEU:HA	2.13	0.49
1:D:148:PRO:HA	1:D:190:PRO:O	2.13	0.49
1:D:422:GLU:HB3	1:D:439:ILE:HG22	1.95	0.49
1:C:102:LEU:HD13	1:C:120:ILE:HB	1.95	0.49
1:B:402:ASN:C	1:B:404:LYS:H	2.16	0.49
1:C:246:GLY:HA3	1:C:338:VAL:CG1	2.42	0.49
1:A:312:ILE:HA	1:A:315:LEU:HD22	1.94	0.49
1:B:70:VAL:HG21	1:B:196:ALA:HB2	1.93	0.48
1:A:82:ASN:HB2	1:A:85:VAL:HG23	1.95	0.48
1:A:316:ARG:CG	1:A:316:ARG:NH1	2.69	0.48
1:A:425:VAL:HG12	1:A:427:VAL:HG13	1.96	0.48
1:C:243:ILE:HG21	1:C:245:ARG:NH2	2.28	0.48
1:C:18:PRO:HB2	1:C:126:LYS:HB2	1.94	0.48
1:D:408:ASP:OD1	1:D:411:SER:HB3	2.13	0.48
1:C:198:VAL:HG23	1:C:199:ASN:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:215:TYR:N	1:D:215:TYR:CD1	2.81	0.48
1:B:26:GLN:O	1:B:90:SER:N	2.46	0.48
1:C:83:ASP:HB2	1:C:115:LEU:O	2.12	0.48
1:A:80:ILE:HD13	1:A:230:VAL:CG1	2.43	0.48
1:C:343:SER:O	1:C:346:GLN:HB2	2.14	0.48
1:D:150:GLY:O	1:D:151:LEU:HB2	2.13	0.48
1:B:82:ASN:O	1:B:83:ASP:C	2.51	0.48
1:D:312:ILE:C	1:D:314:LEU:H	2.16	0.48
1:A:25:VAL:HG13	1:A:89:ALA:CB	2.43	0.48
1:C:197:LEU:HD23	1:C:205:ILE:CD1	2.43	0.48
1:A:63:PHE:HE1	1:A:65:SER:HB2	1.79	0.47
1:D:375:GLY:HA2	1:D:406:VAL:O	2.14	0.47
1:A:212:LEU:HD12	1:A:212:LEU:C	2.34	0.47
1:A:8:SER:O	1:A:11:PRO:HD2	2.14	0.47
1:B:74:PRO:HG3	1:B:127:SER:HB3	1.96	0.47
1:C:298:ASN:O	1:C:322:LYS:NZ	2.45	0.47
1:D:402:ASN:O	1:D:403:LYS:HG2	2.14	0.47
1:B:251:PHE:HB3	1:B:275:SER:HB3	1.96	0.47
1:D:17:MET:CE	1:D:160:ALA:HB2	2.45	0.47
1:D:188:ILE:O	1:D:211:ILE:HG21	2.13	0.47
1:D:292:ASP:HB3	1:D:325:VAL:HG22	1.96	0.47
1:D:237:ILE:O	1:D:241:GLY:HA2	2.14	0.47
1:D:257:PRO:HB3	1:D:267:GLU:O	2.15	0.47
1:C:124:ASN:C	1:C:124:ASN:HD22	2.18	0.47
1:C:199:ASN:C	1:C:199:ASN:OD1	2.53	0.46
1:B:107:ILE:HD11	1:B:119:LYS:HB2	1.96	0.46
1:B:145:ILE:HG22	1:B:146:GLY:H	1.80	0.46
1:D:197:LEU:O	1:D:205:ILE:HG13	2.15	0.46
1:D:115:LEU:HD12	1:D:233:VAL:CG2	2.38	0.46
1:B:127:SER:OG	1:B:128:LEU:N	2.42	0.46
1:A:112:GLU:OE2	1:A:245:ARG:HD2	2.16	0.46
1:D:218:ASN:C	1:D:220:GLY:H	2.19	0.46
1:C:425:VAL:HG12	1:C:427:VAL:HG13	1.98	0.46
1:D:131:GLY:N	1:D:204:LEU:O	2.42	0.46
1:D:112:GLU:HB3	1:D:245:ARG:NH2	2.26	0.46
1:A:128:LEU:HD21	1:A:204:LEU:HB2	1.97	0.46
1:A:347:LYS:HB3	1:A:348:LEU:HD23	1.98	0.46
1:C:197:LEU:HD13	1:C:208:ASN:HD21	1.81	0.45
1:B:382:SER:HB3	1:B:385:SER:CB	2.44	0.45
1:C:324:ILE:HG12	1:C:333:THR:HG23	1.98	0.45
1:A:233:VAL:HB	1:A:243:ILE:HD11	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:246:GLY:HA3	1:C:338:VAL:HG12	1.99	0.45
1:C:62:LYS:HE3	1:C:63:PHE:N	2.31	0.45
1:A:236:GLN:CD	1:A:243:ILE:HG12	2.36	0.45
1:C:296:GLN:CB	1:C:301:LYS:HA	2.46	0.45
1:B:208:ASN:ND2	1:B:224:ALA:HB2	2.30	0.45
1:A:211:ILE:CG2	1:A:212:LEU:N	2.79	0.45
1:B:393:ARG:HB3	1:B:394:PRO:CD	2.47	0.45
1:C:197:LEU:HD23	1:C:205:ILE:HD12	1.99	0.45
1:B:248:MET:HA	1:B:248:MET:CE	2.47	0.45
1:B:376:VAL:HG13	1:B:398:ILE:HB	1.97	0.45
1:C:312:ILE:O	1:C:315:LEU:HB2	2.17	0.45
1:B:22:ASN:ND2	1:B:147:ASN:HD22	2.15	0.45
1:D:197:LEU:CD2	1:D:205:ILE:HD11	2.30	0.44
1:D:292:ASP:HB3	1:D:325:VAL:HG21	1.99	0.44
1:A:283:ALA:HB1	1:A:288:LEU:HD23	1.99	0.44
1:D:331:PRO:C	1:D:332:LEU:HD23	2.38	0.44
1:B:172:ASP:OD1	1:B:172:ASP:N	2.50	0.44
1:C:281:SER:O	1:C:285:LEU:HG	2.16	0.44
1:B:252:VAL:CG1	1:B:272:ALA:HB1	2.47	0.44
1:D:17:MET:N	1:D:18:PRO:CD	2.81	0.44
1:A:228:ASN:HA	1:A:231:LYS:HD3	2.00	0.44
1:A:188:ILE:HD12	1:A:222:GLY:HA3	1.98	0.44
1:B:204:LEU:HD21	1:B:207:ILE:HD11	1.99	0.44
1:B:213:SER:HA	1:B:214:PRO:HD2	1.90	0.44
1:C:237:ILE:HG13	1:C:243:ILE:CD1	2.48	0.44
1:D:218:ASN:O	1:D:220:GLY:N	2.51	0.44
1:D:141:PHE:CD2	1:D:164:ILE:HG22	2.52	0.44
1:D:248:MET:HB3	1:D:250:ILE:HG12	2.00	0.44
1:B:329:ASN:N	1:B:329:ASN:HD22	2.16	0.43
1:D:237:ILE:O	1:D:241:GLY:CA	2.65	0.43
1:A:139:GLY:HA3	1:B:13:LEU:HD12	1.99	0.43
1:D:282:PRO:HG3	1:D:339:THR:HG23	1.99	0.43
1:C:181:PHE:HB3	1:C:223:PHE:HB3	2.00	0.43
1:B:286:ALA:O	1:B:334:LEU:HD22	2.18	0.43
1:A:142:VAL:HG13	1:A:197:LEU:HD22	1.97	0.43
1:D:83:ASP:O	1:D:87:ARG:HG3	2.18	0.43
1:B:129:VAL:HG22	1:B:203:GLU:HG2	2.00	0.43
1:B:288:LEU:CD1	1:B:325:VAL:HG21	2.49	0.43
1:A:363:PHE:CZ	1:A:365:GLN:HB3	2.54	0.43
1:C:236:GLN:O	1:C:240:PHE:HD2	2.02	0.43
1:B:201:LYS:HE3	1:B:203:GLU:OE2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:ILE:HD13	1:A:80:ILE:HD11	2.00	0.43
1:A:109:GLY:HA2	1:A:116:ALA:HA	2.00	0.43
1:D:400:SER:HB3	1:D:426:GLN:HB3	2.00	0.43
1:B:248:MET:HA	1:B:248:MET:HE2	2.01	0.43
1:B:22:ASN:HD21	1:B:147:ASN:ND2	2.15	0.43
1:A:86:ILE:HD11	1:A:116:ALA:HB1	2.01	0.43
1:B:171:SER:HA	1:B:179:GLU:N	2.33	0.43
1:C:286:ALA:O	1:C:334:LEU:HD22	2.19	0.43
1:D:132:ASP:OD1	1:D:132:ASP:C	2.57	0.43
1:A:400:SER:OG	1:A:426:GLN:CB	2.66	0.43
1:A:199:ASN:O	1:A:201:LYS:N	2.52	0.42
1:A:75:ASN:O	1:A:76:ASN:CG	2.56	0.42
1:A:149:PHE:HE2	1:C:221:ILE:HD13	1.84	0.42
1:D:247:LEU:HB2	1:D:341:ILE:CG1	2.49	0.42
1:A:404:LYS:HD2	1:A:415:ILE:HG12	2.00	0.42
1:C:147:ASN:ND2	1:C:151:LEU:HB3	2.35	0.42
1:C:245:ARG:HD3	1:C:313:SER:HB3	2.01	0.42
1:C:235:GLN:HA	1:C:238:ILE:HD12	2.00	0.42
1:B:188:ILE:HA	1:B:192:ASN:ND2	2.35	0.42
1:B:325:VAL:CG1	1:B:326:GLU:N	2.83	0.42
1:A:188:ILE:O	1:A:211:ILE:HD12	2.15	0.42
1:B:133:SER:OG	1:B:227:ILE:N	2.51	0.42
1:D:439:ILE:HD12	1:D:439:ILE:OXT	2.20	0.42
1:A:260:ALA:O	1:A:265:TYR:HB2	2.19	0.42
1:C:282:PRO:HG3	1:C:339:THR:HG22	2.02	0.42
1:C:296:GLN:HB2	1:C:301:LYS:HA	2.02	0.42
1:D:112:GLU:CB	1:D:245:ARG:NH2	2.73	0.42
1:D:22:ASN:ND2	1:D:147:ASN:HD22	2.18	0.42
1:C:413:GLN:O	1:C:414:THR:C	2.58	0.42
1:B:68:SER:O	1:B:194:GLY:HA3	2.19	0.42
1:D:286:ALA:O	1:D:334:LEU:HD22	2.19	0.42
1:B:427:VAL:HG22	1:B:434:MET:O	2.19	0.42
1:B:376:VAL:HG12	1:B:406:VAL:CG1	2.50	0.41
1:A:25:VAL:CG1	1:A:89:ALA:HB2	2.48	0.41
1:C:83:ASP:HA	1:C:116:ALA:HB2	2.01	0.41
1:B:22:ASN:HD21	1:B:147:ASN:HD22	1.68	0.41
1:D:419:LYS:C	1:D:420:LYS:HG3	2.40	0.41
1:C:252:VAL:HG12	1:C:253:GLN:N	2.36	0.41
1:A:144:ALA:HB3	1:A:161:THR:OG1	2.19	0.41
1:C:26:GLN:HG3	1:C:64:GLU:HG3	2.01	0.41
1:C:376:VAL:HG11	1:C:409:VAL:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:197:LEU:HB2	1:C:208:ASN:HD21	1.84	0.41
1:A:379:VAL:CG1	1:A:379:VAL:O	2.67	0.41
1:B:107:ILE:HD11	1:B:119:LYS:CB	2.50	0.41
1:A:358:LEU:HD23	1:A:381:ALA:CB	2.50	0.41
1:D:312:ILE:CA	1:D:315:LEU:HD12	2.48	0.41
1:A:244:HIS:H	1:A:316:ARG:NH1	2.19	0.41
1:C:108:GLY:HA3	1:C:237:ILE:CG2	2.51	0.41
1:C:251:PHE:HB3	1:C:276:GLN:HB3	2.02	0.41
1:A:156:ASN:CG	1:A:156:ASN:O	2.59	0.41
1:B:232:ASP:C	1:B:234:ALA:N	2.74	0.41
1:A:244:HIS:CD2	1:A:317:VAL:HG13	2.54	0.41
1:A:244:HIS:H	1:A:316:ARG:HH12	1.69	0.41
1:D:437:LEU:HD13	1:D:439:ILE:HG23	2.03	0.41
1:C:390:ALA:CB	1:C:438:VAL:HA	2.50	0.41
1:C:259:LEU:O	1:C:260:ALA:C	2.58	0.41
1:A:408:ASP:OD1	1:A:411:SER:HB3	2.20	0.41
1:A:87:ARG:HB3	1:A:88:ASN:ND2	2.36	0.41
1:C:81:THR:OG1	1:C:82:ASN:N	2.54	0.41
1:A:304:GLN:HB3	1:A:307:GLN:HG3	2.02	0.41
1:D:261:GLN:HA	1:D:265:TYR:O	2.20	0.41
1:B:317:VAL:HG21	1:B:340:ASP:HB2	2.03	0.41
1:B:6:MET:HE2	1:B:7:PRO:O	2.21	0.40
1:D:150:GLY:O	1:D:151:LEU:CB	2.68	0.40
1:B:227:ILE:HA	1:B:227:ILE:HD12	1.83	0.40
1:B:151:LEU:O	1:B:157:SER:O	2.39	0.40
1:D:277:VAL:HG12	1:D:284:GLU:HB2	2.04	0.40
1:A:93:THR:HA	1:A:103:LYS:HA	2.03	0.40
1:D:136:LEU:HD11	1:D:205:ILE:HD13	2.02	0.40
1:C:147:ASN:HD21	1:C:151:LEU:N	2.18	0.40
1:B:252:VAL:HG11	1:B:272:ALA:HB1	2.02	0.40
1:C:25:VAL:C	1:C:26:GLN:HE21	2.24	0.40
1:C:418:GLU:O	1:C:420:LYS:N	2.54	0.40
1:C:86:ILE:HG13	1:C:86:ILE:H	1.75	0.40
1:B:422:GLU:HB2	1:B:437:LEU:CD2	2.48	0.40
1:D:327:ARG:O	1:D:328:ASP:C	2.60	0.40
1:A:180:ASN:O	1:A:180:ASN:ND2	2.55	0.40
1:A:368:PRO:HA	1:A:369:PRO:HA	1.89	0.40
1:B:337:VAL:O	1:B:338:VAL:C	2.58	0.40
1:B:236:GLN:OE1	1:B:243:ILE:HG23	2.21	0.40
1:C:435:TYR:N	1:D:253:GLN:OE1	2.52	0.40
1:A:97:GLN:C	1:A:99:GLY:N	2.74	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	382/451 (85%)	338 (88%)	37 (10%)	7 (2%)	11	42
1	B	384/451 (85%)	335 (87%)	45 (12%)	4 (1%)	19	58
1	C	374/451 (83%)	336 (90%)	31 (8%)	7 (2%)	10	40
1	D	380/451 (84%)	341 (90%)	33 (9%)	6 (2%)	12	44
All	All	1520/1804 (84%)	1350 (89%)	146 (10%)	24 (2%)	12	44

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	LEU
1	B	349	GLN
1	D	219	VAL
1	A	98	ASP
1	C	419	LYS
1	D	151	LEU
1	D	239	LYS
1	A	61	ARG
1	A	149	PHE
1	A	200	ALA
1	B	98	ASP
1	B	149	PHE
1	D	353	PRO
1	A	30	PRO
1	B	403	LYS
1	C	19	ALA
1	C	402	ASN
1	C	169	LYS
1	C	190	PRO
1	D	329	ASN

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Mol	Chain	Res	Type
1	A	348	LEU
1	D	434	MET
1	C	74	PRO
1	C	308	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	322/371 (87%)	282 (88%)	40 (12%)	6	23
1	B	321/371 (86%)	268 (84%)	53 (16%)	3	12
1	C	315/371 (85%)	268 (85%)	47 (15%)	4	15
1	D	319/371 (86%)	271 (85%)	48 (15%)	3	15
All	All	1277/1484 (86%)	1089 (85%)	188 (15%)	4	16

All (188) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	SER
1	A	13	LEU
1	A	14	LYS
1	A	28	TYR
1	A	66	ILE
1	A	75	ASN
1	A	88	ASN
1	A	91	LEU
1	A	103	LYS
1	A	106	LEU
1	A	119	LYS
1	A	128	LEU
1	A	129	VAL
1	A	142	VAL
1	A	159	SER
1	A	170	ARG
1	A	172	ASP

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Mol	Chain	Res	Type
1	A	197	LEU
1	A	201	LYS
1	A	212	LEU
1	A	213	SER
1	A	219	VAL
1	A	228	ASN
1	A	248	MET
1	A	276	GLN
1	A	278	ASN
1	A	313	SER
1	A	314	LEU
1	A	315	LEU
1	A	316	ARG
1	A	317	VAL
1	A	321	VAL
1	A	325	VAL
1	A	347	LYS
1	A	348	LEU
1	A	376	VAL
1	A	411	SER
1	A	421	LYS
1	A	436	LEU
1	A	437	LEU
1	B	12	VAL
1	B	17	MET
1	B	22	ASN
1	B	65	SER
1	B	80	ILE
1	B	81	THR
1	B	91	LEU
1	B	112	GLU
1	B	121	ASP
1	B	128	LEU
1	B	129	VAL
1	B	147	ASN
1	B	149	PHE
1	B	157	SER
1	B	158	GLN
1	B	159	SER
1	B	172	ASP
1	B	173	LEU
1	B	179	GLU

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Mol	Chain	Res	Type
1	B	188	ILE
1	B	192	ASN
1	B	197	LEU
1	B	211	ILE
1	B	215	TYR
1	B	218	ASN
1	B	233	VAL
1	B	235	GLN
1	B	244	HIS
1	B	245	ARG
1	B	300	THR
1	B	306	THR
1	B	312	ILE
1	B	314	LEU
1	B	319	SER
1	B	322	LYS
1	B	326	GLU
1	B	329	ASN
1	B	330	LYS
1	B	332	LEU
1	B	333	THR
1	B	339	THR
1	B	345	GLU
1	B	348	LEU
1	B	350	SER
1	B	351	ASN
1	B	376	VAL
1	B	392	ILE
1	B	397	ILE
1	B	414	THR
1	B	425	VAL
1	B	436	LEU
1	B	437	LEU
1	B	439	ILE
1	C	7	PRO
1	C	12	VAL
1	C	22	ASN
1	C	26	GLN
1	C	29	LEU
1	C	62	LYS
1	C	63	PHE
1	C	75	ASN

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Mol	Chain	Res	Type
1	C	85	VAL
1	C	88	ASN
1	C	91	LEU
1	C	97	GLN
1	C	105	ARG
1	C	124	ASN
1	C	129	VAL
1	C	151	LEU
1	C	159	SER
1	C	168	LEU
1	C	169	LYS
1	C	176	GLU
1	C	197	LEU
1	C	198	VAL
1	C	219	VAL
1	C	242	SER
1	C	244	HIS
1	C	251	PHE
1	C	269	PHE
1	C	301	LYS
1	C	312	ILE
1	C	314	LEU
1	C	315	LEU
1	C	317	VAL
1	C	322	LYS
1	C	325	VAL
1	C	328	ASP
1	C	338	VAL
1	C	340	ASP
1	C	348	LEU
1	C	361	ARG
1	C	376	VAL
1	C	400	SER
1	C	407	THR
1	C	417	GLN
1	C	421	LYS
1	C	429	ARG
1	C	437	LEU
1	C	439	ILE
1	D	9	MET
1	D	17	MET
1	D	22	ASN

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Mol	Chain	Res	Type
1	D	28	TYR
1	D	29	LEU
1	D	31	ASN
1	D	63	PHE
1	D	65	SER
1	D	80	ILE
1	D	90	SER
1	D	91	LEU
1	D	96	LEU
1	D	102	LEU
1	D	106	LEU
1	D	124	ASN
1	D	129	VAL
1	D	142	VAL
1	D	151	LEU
1	D	201	LYS
1	D	212	LEU
1	D	215	TYR
1	D	238	ILE
1	D	244	HIS
1	D	245	ARG
1	D	252	VAL
1	D	256	THR
1	D	258	GLU
1	D	275	SER
1	D	280	ASN
1	D	285	LEU
1	D	314	LEU
1	D	317	VAL
1	D	321	VAL
1	D	322	LYS
1	D	325	VAL
1	D	329	ASN
1	D	332	LEU
1	D	339	THR
1	D	346	GLN
1	D	351	ASN
1	D	376	VAL
1	D	403	LYS
1	D	404	LYS
1	D	417	GLN
1	D	422	GLU

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Mol	Chain	Res	Type
1	D	425	VAL
1	D	434	MET
1	D	438	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	15	ASN
1	A	88	ASN
1	A	97	GLN
1	A	147	ASN
1	A	180	ASN
1	A	192	ASN
1	A	208	ASN
1	A	235	GLN
1	A	244	HIS
1	A	278	ASN
1	A	296	GLN
1	A	346	GLN
1	A	384	ASN
1	A	417	GLN
1	B	22	ASN
1	B	76	ASN
1	B	158	GLN
1	B	183	GLN
1	B	192	ASN
1	B	208	ASN
1	B	228	ASN
1	B	235	GLN
1	B	278	ASN
1	B	329	ASN
1	B	351	ASN
1	B	365	GLN
1	C	26	GLN
1	C	75	ASN
1	C	97	GLN
1	C	124	ASN
1	C	147	ASN
1	C	208	ASN
1	C	228	ASN
1	C	261	GLN

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Mol	Chain	Res	Type
1	C	280	ASN
1	C	296	GLN
1	C	346	GLN
1	C	365	GLN
1	C	370	HIS
1	C	417	GLN
1	D	22	ASN
1	D	97	GLN
1	D	158	GLN
1	D	189	ASN
1	D	192	ASN
1	D	208	ASN
1	D	228	ASN
1	D	276	GLN
1	D	307	GLN
1	D	329	ASN
1	D	351	ASN
1	D	417	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 carbohydrates 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	392/451 (86%)	-0.02	0	100	100	63, 79, 99, 119	0
1	B	392/451 (86%)	0.03	1 (0%)	94	88	63, 90, 104, 108	0
1	C	384/451 (85%)	0.11	6 (1%)	74	55	66, 99, 114, 125	0
1	D	390/451 (86%)	-0.02	2 (0%)	91	83	60, 85, 102, 116	0
2	E	0/20	-	-			-	-
2	F	0/20	-	-			-	-
2	G	0/20	-	-			-	-
2	H	0/20	-	-			-	-
All	All	1558/1884 (82%)	0.02	9 (0%)	90	80	60, 87, 109, 125	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	215	TYR	3.0
1	C	142	VAL	2.6
1	C	102	LEU	2.5
1	C	92	ILE	2.1
1	C	182	ILE	2.1
1	D	392	ILE	2.1
1	C	115	LEU	2.0
1	B	398	ILE	2.0
1	C	117	VAL	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.