Full wwPDB X-ray Structure Validation Report (i)

Jun 18, 2024 – 03:01 PM EDT

PDB ID	:	4ABY
Title	:	Crystal structure of Deinococcus radiodurans RecN head domain
Authors	:	Pellegrino, S.; Radzimanowski, J.; de Sanctis, D.; McSweeney, S.; Timmins, J.
Deposited on	:	2011-12-12
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 (i)) were used in the production of this report:

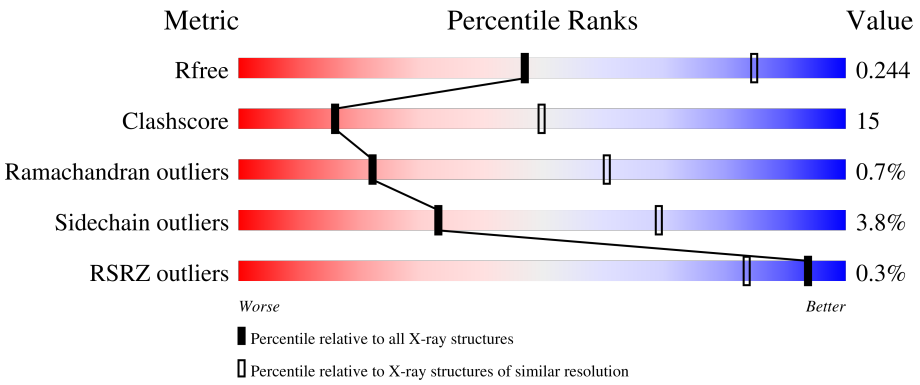
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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	415	66% 19% • 14%
1	B	415	65% 20% • 13%
1	C	415	56% 25% • 15%
1	D	415	% 50% 23% • 25%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 10447 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 DNA REPAIR PROTEIN RECN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	358	2694	1674	504	511	1	4	0	0	0
1	B	361	2715	1686	508	516	1	4	0	0	0
1	C	351	2619	1628	485	501	1	4	0	0	0
1	D	311	2317	1442	428	442	1	4	0	0	0

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP Q9WXF2
A	-4	ILE	-	expression tag	UNP Q9WXF2
A	-3	ASP	-	expression tag	UNP Q9WXF2
A	-2	PRO	-	expression tag	UNP Q9WXF2
A	-1	PHE	-	expression tag	UNP Q9WXF2
A	0	THR	-	expression tag	UNP Q9WXF2
A	352	GLU	-	linker	UNP Q9WXF2
A	353	SER	-	linker	UNP Q9WXF2
A	354	SER	-	linker	UNP Q9WXF2
A	355	LYS	-	linker	UNP Q9WXF2
A	356	HIS	-	linker	UNP Q9WXF2
A	357	PRO	-	linker	UNP Q9WXF2
A	358	THR	-	linker	UNP Q9WXF2
A	359	SER	-	linker	UNP Q9WXF2
A	360	LEU	-	linker	UNP Q9WXF2
A	361	VAL	-	linker	UNP Q9WXF2
A	362	PRO	-	linker	UNP Q9WXF2
A	363	ARG	-	linker	UNP Q9WXF2
A	364	GLY	-	linker	UNP Q9WXF2
A	365	SER	-	linker	UNP Q9WXF2
B	-5	GLY	-	expression tag	UNP Q9WXF2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	ILE	-	expression tag	UNP Q9WXF2
B	-3	ASP	-	expression tag	UNP Q9WXF2
B	-2	PRO	-	expression tag	UNP Q9WXF2
B	-1	PHE	-	expression tag	UNP Q9WXF2
B	0	THR	-	expression tag	UNP Q9WXF2
B	352	GLU	-	linker	UNP Q9WXF2
B	353	SER	-	linker	UNP Q9WXF2
B	354	SER	-	linker	UNP Q9WXF2
B	355	LYS	-	linker	UNP Q9WXF2
B	356	HIS	-	linker	UNP Q9WXF2
B	357	PRO	-	linker	UNP Q9WXF2
B	358	THR	-	linker	UNP Q9WXF2
B	359	SER	-	linker	UNP Q9WXF2
B	360	LEU	-	linker	UNP Q9WXF2
B	361	VAL	-	linker	UNP Q9WXF2
B	362	PRO	-	linker	UNP Q9WXF2
B	363	ARG	-	linker	UNP Q9WXF2
B	364	GLY	-	linker	UNP Q9WXF2
B	365	SER	-	linker	UNP Q9WXF2
C	-5	GLY	-	expression tag	UNP Q9WXF2
C	-4	ILE	-	expression tag	UNP Q9WXF2
C	-3	ASP	-	expression tag	UNP Q9WXF2
C	-2	PRO	-	expression tag	UNP Q9WXF2
C	-1	PHE	-	expression tag	UNP Q9WXF2
C	0	THR	-	expression tag	UNP Q9WXF2
C	352	GLU	-	linker	UNP Q9WXF2
C	353	SER	-	linker	UNP Q9WXF2
C	354	SER	-	linker	UNP Q9WXF2
C	355	LYS	-	linker	UNP Q9WXF2
C	356	HIS	-	linker	UNP Q9WXF2
C	357	PRO	-	linker	UNP Q9WXF2
C	358	THR	-	linker	UNP Q9WXF2
C	359	SER	-	linker	UNP Q9WXF2
C	360	LEU	-	linker	UNP Q9WXF2
C	361	VAL	-	linker	UNP Q9WXF2
C	362	PRO	-	linker	UNP Q9WXF2
C	363	ARG	-	linker	UNP Q9WXF2
C	364	GLY	-	linker	UNP Q9WXF2
C	365	SER	-	linker	UNP Q9WXF2
D	-5	GLY	-	expression tag	UNP Q9WXF2
D	-4	ILE	-	expression tag	UNP Q9WXF2
D	-3	ASP	-	expression tag	UNP Q9WXF2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	PRO	-	expression tag	UNP Q9WXF2
D	-1	PHE	-	expression tag	UNP Q9WXF2
D	0	THR	-	expression tag	UNP Q9WXF2
D	352	GLU	-	linker	UNP Q9WXF2
D	353	SER	-	linker	UNP Q9WXF2
D	354	SER	-	linker	UNP Q9WXF2
D	355	LYS	-	linker	UNP Q9WXF2
D	356	HIS	-	linker	UNP Q9WXF2
D	357	PRO	-	linker	UNP Q9WXF2
D	358	THR	-	linker	UNP Q9WXF2
D	359	SER	-	linker	UNP Q9WXF2
D	360	LEU	-	linker	UNP Q9WXF2
D	361	VAL	-	linker	UNP Q9WXF2
D	362	PRO	-	linker	UNP Q9WXF2
D	363	ARG	-	linker	UNP Q9WXF2
D	364	GLY	-	linker	UNP Q9WXF2
D	365	SER	-	linker	UNP Q9WXF2

- Molecule 2 is water.

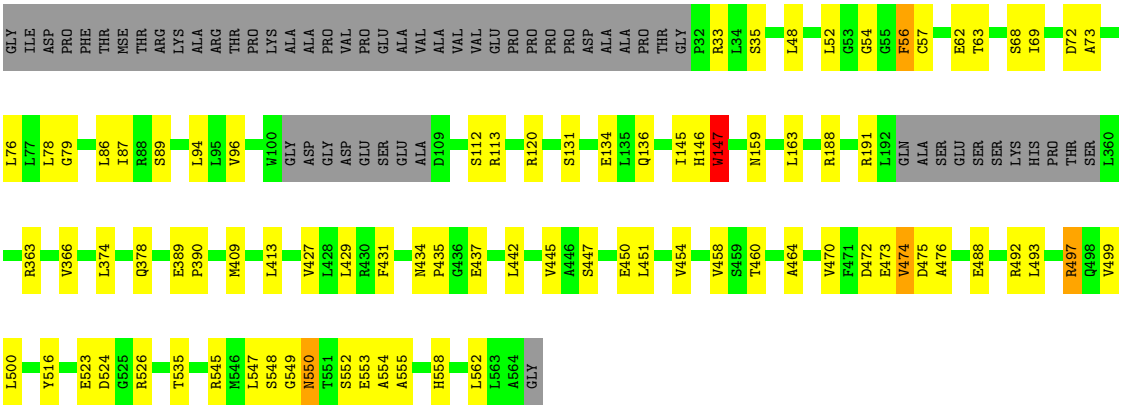
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	26	26	26	0	0
			Total	O		
2	B	46	46	46	0	0
			Total	O		
2	C	18	18	18	0	0
			Total	O		
2	D	12	12	12	0	0

3 Residue-property plots (i)

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

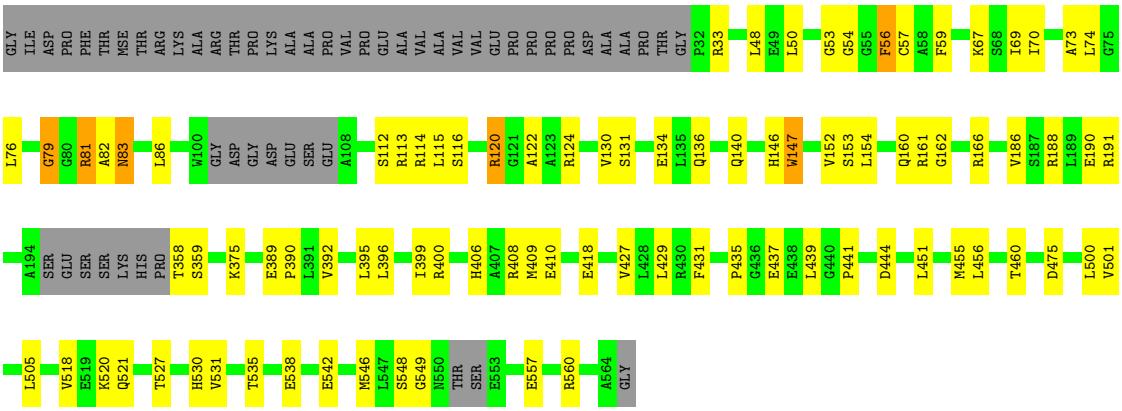
• Molecule 1: DNA REPAIR PROTEIN RECN

Chain A:



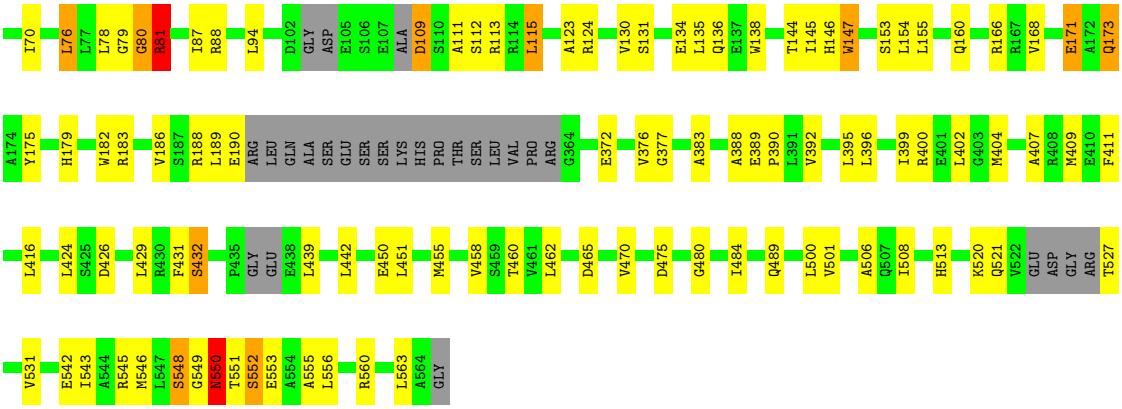
• Molecule 1: DNA REPAIR PROTEIN RECN

Chain B:



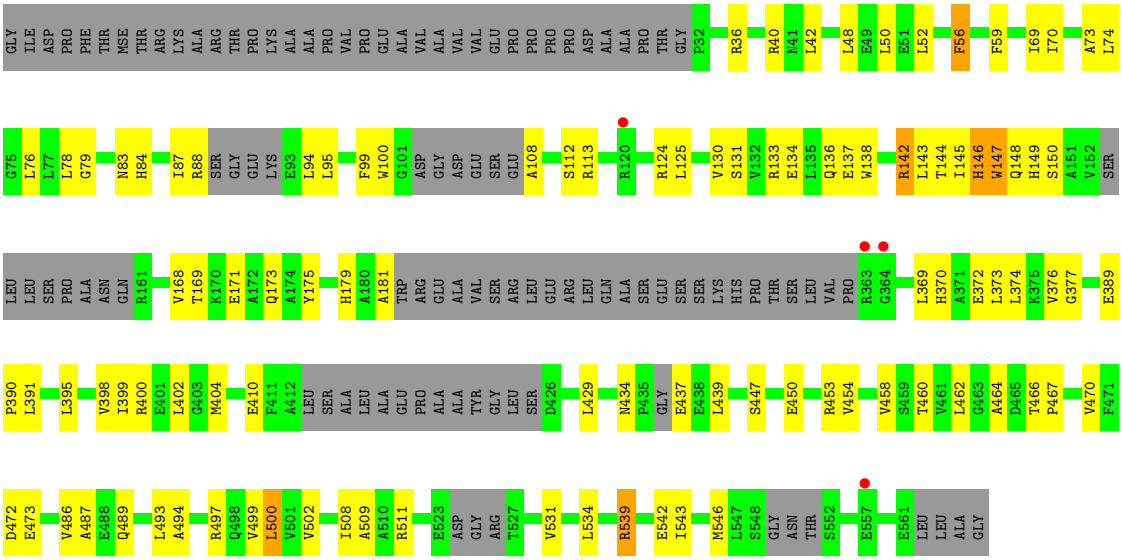
• Molecule 1: DNA REPAIR PROTEIN RECN

Chain C:



• Molecule 1: DNA REPAIR PROTEIN RECN

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	129.86Å 61.99Å 133.82Å 90.00° 102.74° 90.00°	Depositor
Resolution (Å)	49.51 – 3.00 49.51 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.51-3.00) 99.4 (49.51-3.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.79 (at 3.01Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.209 , 0.249 0.209 , 0.244	Depositor DCC
R_{free} test set	2117 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	46.9	Xtriage
Anisotropy	0.432	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 37.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.027 for l,-k,h	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	10447	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% 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	0.44	0/2725	0.56	1/3679 (0.0%)
1	B	0.45	0/2745	0.52	1/3705 (0.0%)
1	C	0.46	0/2646	0.58	4/3570 (0.1%)
1	D	0.36	0/2336	0.52	2/3145 (0.1%)
All	All	0.43	0/10452	0.55	8/14099 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	474	VAL	N-CA-CB	-14.17	80.33	111.50
1	D	146	HIS	N-CA-C	8.60	134.23	111.00
1	B	79	GLY	N-CA-C	-6.39	97.12	113.10
1	C	81	ARG	N-CA-C	-6.36	93.83	111.00
1	C	80	GLY	N-CA-C	6.34	128.95	113.10
1	D	146	HIS	C-N-CA	-6.29	105.97	121.70
1	C	109	ASP	N-CA-CB	-5.22	101.21	110.60
1	C	550	ASN	N-CA-C	5.14	124.89	111.00

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	2694	0	2722	56	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2715	0	2744	67	0
1	C	2619	0	2625	96	0
1	D	2317	0	2315	84	0
2	A	26	0	0	0	0
2	B	46	0	0	0	0
2	C	18	0	0	0	0
2	D	12	0	0	0	0
All	All	10447	0	10406	303	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 (303) 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:C:80:GLY:O	1:C:81:ARG:HB2	1.57	1.03
1:B:152:VAL:HG22	1:B:152:VAL:O	1.58	1.03
1:C:168:VAL:HG12	1:C:168:VAL:O	1.54	1.01
1:D:148:GLN:NE2	1:D:472:ASP:OD2	1.99	0.95
1:C:432:SER:HB2	1:C:439:LEU:HD12	1.48	0.94
1:A:472:ASP:O	1:A:473:GLU:HB2	1.69	0.92
1:B:116:SER:HB3	1:B:120:ARG:HG3	1.54	0.90
1:B:535:THR:HG22	1:B:538:GLU:HG2	1.55	0.89
1:B:160:GLN:HE21	1:B:429:LEU:H	1.23	0.83
1:D:169:THR:HG22	1:D:173:GLN:HE21	1.42	0.83
1:C:154:LEU:HB2	1:C:455:MSE:HE1	1.61	0.83
1:C:521:GLN:O	1:C:527:THR:HA	1.81	0.80
1:D:447:SER:HB2	1:D:450:GLU:HB2	1.62	0.79
1:B:112:SER:HB2	1:B:124:ARG:HB2	1.67	0.76
1:B:152:VAL:O	1:B:152:VAL:CG2	2.30	0.76
1:C:146:HIS:CE1	1:C:455:MSE:HE2	2.22	0.74
1:D:147:TRP:HE3	1:D:147:TRP:O	1.71	0.74
1:A:549:GLY:O	1:A:550:ASN:CB	2.36	0.73
1:A:552:SER:O	1:A:555:ALA:N	2.19	0.73
1:D:147:TRP:CE3	1:D:147:TRP:C	2.62	0.72
1:D:144:THR:OG1	1:D:466:THR:OG1	1.88	0.72
1:D:48:LEU:HD11	1:D:531:VAL:HG23	1.71	0.72
1:A:549:GLY:O	1:A:550:ASN:HB2	1.90	0.72
1:C:56:PHE:HB3	1:C:513:HIS:HD2	1.55	0.71
1:C:131:SER:HB3	1:C:134:GLU:HG3	1.72	0.71
1:A:472:ASP:O	1:A:473:GLU:CB	2.37	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:404:MSE:SE	1:D:450:GLU:HG2	2.42	0.70
1:A:68:SER:HA	1:A:72:ASP:HB2	1.73	0.69
1:C:171:GLU:OE2	1:C:383:ALA:HB1	1.93	0.69
1:C:130:VAL:HG13	1:C:134:GLU:HB2	1.75	0.69
1:C:549:GLY:C	1:C:550:ASN:OD1	2.30	0.69
1:D:74:LEU:HB3	1:D:143:LEU:HD21	1.74	0.69
1:A:188:ARG:HA	1:A:191:ARG:HG3	1.75	0.69
1:A:545:ARG:HA	1:A:550:ASN:H	1.58	0.68
1:A:434:ASN:HB2	1:A:437:GLU:HG3	1.77	0.67
1:C:87:ILE:HG12	1:C:94:LEU:HD23	1.77	0.67
1:C:56:PHE:H	1:C:513:HIS:CD2	2.11	0.67
1:D:147:TRP:O	1:D:147:TRP:CE3	2.47	0.67
1:A:146:HIS:O	1:A:147:TRP:HB3	1.94	0.67
1:C:182:TRP:O	1:C:186:VAL:HG23	1.96	0.66
1:D:79:GLY:HA3	1:D:136:GLN:HG3	1.78	0.66
1:D:168:VAL:HG12	1:D:168:VAL:O	1.94	0.66
1:B:114:ARG:HG2	1:B:120:ARG:HH12	1.61	0.66
1:A:147:TRP:CE3	1:A:147:TRP:C	2.69	0.66
1:C:46:THR:HG23	1:C:47:GLN:N	2.10	0.66
1:B:131:SER:OG	1:B:134:GLU:HG3	1.95	0.66
1:D:181:ALA:HB1	1:D:369:LEU:HD13	1.77	0.66
1:D:395:LEU:O	1:D:399:ILE:HG12	1.95	0.66
1:A:434:ASN:HB3	1:A:435:PRO:HD2	1.78	0.66
1:C:41:ASN:HD22	1:C:88:ARG:HD3	1.62	0.65
1:B:57:CYS:HB2	1:B:500:LEU:HD23	1.79	0.65
1:D:79:GLY:HA3	1:D:136:GLN:CG	2.27	0.65
1:C:123:ALA:HB1	1:C:135:LEU:HD22	1.79	0.64
1:D:447:SER:CB	1:D:450:GLU:HB2	2.27	0.64
1:D:131:SER:OG	1:D:134:GLU:HG3	1.98	0.64
1:C:168:VAL:O	1:C:168:VAL:CG1	2.30	0.64
1:A:147:TRP:C	1:A:147:TRP:HE3	2.01	0.63
1:C:46:THR:HG23	1:C:47:GLN:H	1.63	0.63
1:C:548:SER:C	1:C:550:ASN:H	1.97	0.63
1:D:434:ASN:HB2	1:D:437:GLU:HG3	1.81	0.63
1:C:166:ARG:HD2	1:C:462:LEU:HD22	1.82	0.62
1:C:416:LEU:HB2	1:C:424:LEU:O	1.99	0.62
1:C:372:GLU:O	1:C:376:VAL:HG23	1.99	0.62
1:C:56:PHE:HE1	1:C:501:VAL:HG22	1.63	0.62
1:D:169:THR:CG2	1:D:173:GLN:HE21	2.12	0.62
1:C:171:GLU:OE2	1:C:383:ALA:CB	2.47	0.61
1:B:79:GLY:HA3	1:B:136:GLN:HG2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:70:ILE:HG22	1:D:470:VAL:CG1	2.30	0.61
1:C:396:LEU:O	1:C:400:ARG:HG3	2.00	0.61
1:B:160:GLN:NE2	1:B:429:LEU:H	1.95	0.61
1:A:464:ALA:HB3	1:A:497:ARG:HD3	1.83	0.61
1:A:87:ILE:HA	1:A:94:LEU:HD23	1.83	0.60
1:A:147:TRP:HE3	1:A:147:TRP:O	1.84	0.60
1:A:389:GLU:HB2	1:A:390:PRO:HD3	1.84	0.60
1:C:527:THR:O	1:C:527:THR:HG23	2.01	0.60
1:B:358:THR:HG22	1:B:359:SER:H	1.65	0.59
1:D:543:ILE:HA	1:D:546:MSE:HE2	1.85	0.59
1:A:552:SER:O	1:A:554:ALA:N	2.35	0.59
1:D:138:TRP:CH2	1:D:142:ARG:HD2	2.38	0.59
1:C:551:THR:O	1:C:553:GLU:N	2.36	0.59
1:D:78:LEU:HD11	1:D:145:ILE:HG13	1.85	0.58
1:C:146:HIS:CE1	1:C:455:MSE:CE	2.87	0.58
1:D:70:ILE:HG22	1:D:470:VAL:HG11	1.84	0.58
1:A:474:VAL:CG1	1:A:475:ASP:N	2.67	0.58
1:C:404:MSE:HE1	1:C:450:GLU:HB3	1.85	0.58
1:B:408:ARG:NH2	1:B:437:GLU:O	2.37	0.58
1:D:487:ALA:HB2	1:D:508:ILE:HA	1.86	0.57
1:B:160:GLN:HE21	1:B:429:LEU:N	2.00	0.57
1:D:69:ILE:HG22	1:D:70:ILE:HD13	1.87	0.57
1:A:460:THR:HG22	1:A:493:LEU:HB2	1.86	0.57
1:B:389:GLU:HB3	1:B:390:PRO:HD3	1.86	0.57
1:C:168:VAL:CG1	1:C:171:GLU:HB2	2.35	0.57
1:A:552:SER:H	1:A:555:ALA:HB3	1.68	0.56
1:B:456:LEU:O	1:B:460:THR:HG23	2.03	0.56
1:C:189:LEU:O	1:C:190:GLU:HG3	2.04	0.56
1:B:33:ARG:NE	1:B:53:GLY:HA2	2.20	0.56
1:C:542:GLU:O	1:C:546:MSE:HG3	2.06	0.56
1:A:57:CYS:HB2	1:A:500:LEU:HD23	1.88	0.56
1:B:535:THR:CG2	1:B:538:GLU:HG2	2.31	0.56
1:C:78:LEU:CD1	1:C:145:ILE:HD12	2.35	0.56
1:D:370:HIS:CE1	1:D:374:LEU:HD11	2.40	0.56
1:B:535:THR:HG22	1:B:538:GLU:CG	2.31	0.56
1:D:70:ILE:CG2	1:D:470:VAL:HG13	2.36	0.55
1:D:94:LEU:HD23	1:D:95:LEU:N	2.21	0.55
1:A:131:SER:OG	1:A:134:GLU:HG3	2.07	0.55
1:B:146:HIS:O	1:B:147:TRP:HB3	2.05	0.55
1:A:549:GLY:O	1:A:550:ASN:CG	2.45	0.55
1:D:464:ALA:HB3	1:D:497:ARG:HD2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:TRP:CE3	1:C:147:TRP:C	2.80	0.54
1:D:78:LEU:CD1	1:D:145:ILE:HG13	2.37	0.54
1:D:400:ARG:HA	1:D:404:MSE:O	2.06	0.54
1:B:147:TRP:CE3	1:B:147:TRP:C	2.81	0.54
1:A:145:ILE:HG13	1:A:470:VAL:HB	1.90	0.54
1:C:42:LEU:O	1:C:43:ALA:C	2.45	0.54
1:C:144:THR:HG23	1:C:153:SER:HB3	1.89	0.54
1:C:548:SER:OG	1:C:555:ALA:HB2	2.08	0.54
1:C:432:SER:CB	1:C:439:LEU:HD12	2.29	0.54
1:A:447:SER:HB3	1:A:450:GLU:HG3	1.89	0.54
1:D:534:LEU:CD2	1:D:542:GLU:HG2	2.38	0.53
1:D:146:HIS:ND1	1:D:150:SER:HB3	2.23	0.53
1:C:551:THR:O	1:C:553:GLU:OE1	2.25	0.53
1:D:543:ILE:HD13	1:D:546:MSE:CE	2.37	0.53
1:D:398:VAL:O	1:D:402:LEU:HG	2.08	0.53
1:A:159:ASN:O	1:A:163:LEU:HD13	2.08	0.53
1:B:76:LEU:HB3	1:B:113:ARG:HG2	1.90	0.53
1:A:552:SER:O	1:A:553:GLU:C	2.45	0.53
1:D:460:THR:HG21	1:D:489:GLN:HG3	1.89	0.53
1:C:160:GLN:NE2	1:C:429:LEU:H	2.07	0.52
1:B:67:LYS:O	1:B:67:LYS:CG	2.54	0.52
1:C:506:ALA:HB1	1:C:543:ILE:HG23	1.91	0.52
1:B:81:ARG:HH11	1:B:81:ARG:HG3	1.74	0.52
1:B:153:SER:OG	1:B:154:LEU:N	2.43	0.52
1:D:450:GLU:HG3	1:D:453:ARG:HH21	1.75	0.52
1:B:548:SER:OG	1:B:549:GLY:N	2.41	0.52
1:A:454:VAL:O	1:A:458:VAL:HG23	2.10	0.52
1:B:520:LYS:HD3	1:B:527:THR:HG21	1.91	0.52
1:B:130:VAL:HG13	1:B:134:GLU:HB2	1.91	0.51
1:D:50:LEU:HD22	1:D:531:VAL:HG11	1.92	0.51
1:A:470:VAL:HG22	1:A:500:LEU:HB2	1.91	0.51
1:B:188:ARG:HG2	1:B:191:ARG:NH2	2.26	0.51
1:B:406:HIS:CB	1:B:435:PRO:HG3	2.40	0.51
1:B:409:MSE:HE3	1:B:431:PHE:CD1	2.46	0.51
1:C:79:GLY:HA2	1:C:113:ARG:NH1	2.25	0.51
1:D:146:HIS:O	1:D:147:TRP:C	2.43	0.51
1:C:548:SER:C	1:C:550:ASN:N	2.63	0.51
1:C:154:LEU:HB2	1:C:455:MSE:CE	2.39	0.50
1:C:45:ILE:HD12	1:C:45:ILE:H	1.76	0.50
1:C:78:LEU:O	1:C:136:GLN:HG2	2.11	0.50
1:C:179:HIS:O	1:C:183:ARG:HG2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:56:PHE:CB	1:C:513:HIS:HD2	2.24	0.50
1:C:470:VAL:HG22	1:C:500:LEU:HB2	1.93	0.50
1:C:146:HIS:O	1:C:147:TRP:HB3	2.10	0.50
1:D:179:HIS:HA	1:D:373:LEU:HD13	1.94	0.50
1:A:76:LEU:HB3	1:A:113:ARG:HG2	1.93	0.50
1:D:112:SER:OG	1:D:124:ARG:HB2	2.12	0.50
1:C:392:VAL:HG11	1:C:409:MSE:O	2.12	0.50
1:B:520:LYS:CD	1:B:527:THR:HG21	2.41	0.49
1:B:56:PHE:HE1	1:B:501:VAL:HG22	1.77	0.49
1:B:358:THR:HG22	1:B:359:SER:N	2.28	0.49
1:B:557:GLU:O	1:B:560:ARG:HG2	2.12	0.49
1:D:543:ILE:HA	1:D:546:MSE:CE	2.42	0.49
1:C:46:THR:CG2	1:C:47:GLN:N	2.75	0.49
1:C:57:CYS:HB2	1:C:500:LEU:HD23	1.95	0.49
1:D:410:GLU:HG2	1:D:439:LEU:HD13	1.94	0.49
1:B:56:PHE:CD1	1:B:56:PHE:C	2.86	0.49
1:B:162:GLY:O	1:B:166:ARG:HG3	2.13	0.49
1:B:475:ASP:HB2	1:B:505:LEU:HD12	1.95	0.49
1:D:389:GLU:HB3	1:D:390:PRO:HD3	1.94	0.49
1:B:81:ARG:CZ	1:B:81:ARG:CB	2.90	0.48
1:D:543:ILE:HD13	1:D:546:MSE:HE1	1.95	0.48
1:D:370:HIS:O	1:D:374:LEU:HG	2.13	0.48
1:A:413:LEU:HD22	1:A:427:VAL:HG22	1.96	0.48
1:B:441:PRO:HD2	1:B:444:ASP:OD2	2.13	0.48
1:D:36:ARG:HB3	1:D:99:PHE:HB2	1.95	0.48
1:C:144:THR:HG23	1:C:153:SER:CB	2.44	0.48
1:D:472:ASP:OD1	1:D:473:GLU:HG3	2.12	0.48
1:B:83:ASN:HB3	1:B:86:LEU:HG	1.94	0.48
1:C:173:GLN:OE1	1:C:173:GLN:O	2.30	0.48
1:D:87:ILE:O	1:D:88:ARG:HB2	2.12	0.48
1:B:451:LEU:O	1:B:455:MSE:HG2	2.14	0.48
1:B:521:GLN:CD	1:B:530:HIS:HB2	2.34	0.48
1:D:149:HIS:N	1:D:149:HIS:CD2	2.82	0.48
1:C:80:GLY:O	1:C:81:ARG:CB	2.41	0.48
1:A:545:ARG:O	1:A:549:GLY:HA2	2.13	0.48
1:D:402:LEU:HD22	1:D:486:VAL:HG22	1.94	0.48
1:C:78:LEU:HD11	1:C:145:ILE:HD12	1.95	0.47
1:D:78:LEU:O	1:D:136:GLN:HG2	2.14	0.47
1:B:395:LEU:O	1:B:399:ILE:HG13	2.13	0.47
1:C:112:SER:HB3	1:C:124:ARG:HB2	1.97	0.47
1:C:46:THR:CG2	1:C:47:GLN:H	2.25	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:395:LEU:O	1:C:399:ILE:HG13	2.14	0.47
1:A:94:LEU:HD12	1:A:94:LEU:C	2.35	0.47
1:C:44:THR:O	1:C:44:THR:HG22	2.14	0.47
1:C:50:LEU:HD22	1:C:531:VAL:HG11	1.95	0.47
1:A:545:ARG:O	1:A:549:GLY:N	2.48	0.47
1:A:33:ARG:HD3	1:A:54:GLY:H	1.80	0.47
1:C:458:VAL:HG13	1:C:462:LEU:HD12	1.97	0.47
1:D:142:ARG:HA	1:D:467:PRO:HD2	1.97	0.47
1:D:168:VAL:CG1	1:D:171:GLU:HB2	2.45	0.47
1:D:70:ILE:CG2	1:D:470:VAL:CG1	2.93	0.46
1:A:52:LEU:HA	1:A:516:TYR:OH	2.14	0.46
1:C:407:ALA:HB1	1:C:431:PHE:CZ	2.49	0.46
1:D:52:LEU:HD13	1:D:500:LEU:HD21	1.96	0.46
1:D:138:TRP:CZ2	1:D:142:ARG:HD2	2.49	0.46
1:C:79:GLY:HA2	1:C:113:ARG:HH12	1.81	0.46
1:C:389:GLU:HB3	1:C:390:PRO:HD3	1.98	0.46
1:D:56:PHE:CD1	1:D:56:PHE:C	2.88	0.46
1:B:82:ALA:HB1	1:B:115:LEU:HD21	1.98	0.46
1:B:396:LEU:HD13	1:B:400:ARG:NH2	2.31	0.46
1:D:79:GLY:HA3	1:D:136:GLN:HG2	1.97	0.46
1:C:549:GLY:O	1:C:550:ASN:OD1	2.34	0.45
1:B:79:GLY:HA3	1:B:136:GLN:CG	2.46	0.45
1:B:114:ARG:HB3	1:B:122:ALA:HB3	1.98	0.45
1:C:160:GLN:HE21	1:C:429:LEU:HB3	1.80	0.45
1:D:76:LEU:HB3	1:D:113:ARG:HG2	1.98	0.45
1:D:142:ARG:HH11	1:D:142:ARG:CG	2.30	0.45
1:C:543:ILE:HG13	1:C:563:LEU:HD21	1.97	0.45
1:A:78:LEU:HD23	1:A:78:LEU:HA	1.84	0.45
1:C:59:PHE:CE1	1:C:70:ILE:HD11	2.51	0.45
1:B:542:GLU:O	1:B:546:MSE:HG3	2.17	0.45
1:A:548:SER:O	1:A:549:GLY:C	2.53	0.45
1:C:549:GLY:O	1:C:550:ASN:HB2	2.16	0.45
1:C:402:LEU:HD21	1:C:489:GLN:HG3	1.98	0.45
1:C:409:MSE:HE3	1:C:431:PHE:CD1	2.52	0.45
1:D:454:VAL:O	1:D:458:VAL:HG23	2.17	0.45
1:C:45:ILE:HD12	1:C:45:ILE:N	2.32	0.44
1:C:78:LEU:HD12	1:C:145:ILE:HD12	1.97	0.44
1:C:94:LEU:HD12	1:C:94:LEU:C	2.37	0.44
1:B:140:GLN:NE2	1:B:152:VAL:HG21	2.32	0.44
1:B:408:ARG:HH22	1:B:437:GLU:H	1.64	0.44
1:A:523:GLU:O	1:A:524:ASP:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:41:ASN:ND2	1:C:88:ARG:HD3	2.32	0.44
1:C:549:GLY:O	1:C:550:ASN:CB	2.65	0.44
1:A:445:VAL:HG21	1:A:451:LEU:HB2	1.99	0.44
1:C:551:THR:O	1:C:552:SER:C	2.56	0.44
1:B:518:VAL:HG22	1:B:531:VAL:HG22	2.00	0.44
1:D:487:ALA:HB1	1:D:511:ARG:HG3	1.99	0.44
1:C:377:GLY:HA3	1:C:424:LEU:HG	1.99	0.43
1:D:175:TYR:CD1	1:D:377:GLY:HA2	2.52	0.43
1:D:391:LEU:CD1	1:D:462:LEU:HD21	2.48	0.43
1:C:76:LEU:HD21	1:C:115:LEU:HD22	2.00	0.43
1:C:175:TYR:HD2	1:C:377:GLY:HA2	1.82	0.43
1:A:363:ARG:O	1:A:366:VAL:HG12	2.17	0.43
1:C:388:ALA:HB1	1:C:411:PHE:HB2	2.01	0.43
1:D:464:ALA:HB3	1:D:497:ARG:NE	2.33	0.43
1:D:147:TRP:C	1:D:147:TRP:CD2	2.91	0.43
1:B:410:GLU:HG2	1:B:439:LEU:HD23	2.00	0.43
1:D:42:LEU:C	1:D:42:LEU:HD23	2.39	0.43
1:A:374:LEU:O	1:A:378:GLN:HG3	2.18	0.43
1:B:130:VAL:CG1	1:B:134:GLU:HB2	2.49	0.43
1:B:389:GLU:HA	1:B:389:GLU:OE1	2.18	0.43
1:C:407:ALA:HA	1:C:432:SER:O	2.19	0.43
1:D:133:ARG:O	1:D:137:GLU:HG3	2.18	0.43
1:A:56:PHE:C	1:A:56:PHE:CD1	2.93	0.43
1:B:69:ILE:O	1:B:73:ALA:HB3	2.19	0.43
1:A:96:VAL:O	1:A:112:SER:HA	2.19	0.42
1:A:409:MSE:HE3	1:A:431:PHE:CD1	2.54	0.42
1:B:186:VAL:O	1:B:190:GLU:HG3	2.19	0.42
1:D:100:TRP:O	1:D:108:ALA:HB3	2.19	0.42
1:B:161:ARG:HG3	1:B:427:VAL:HB	2.00	0.42
1:D:50:LEU:HD21	1:D:59:PHE:HE2	1.84	0.42
1:D:429:LEU:HD23	1:D:429:LEU:C	2.40	0.42
1:D:450:GLU:O	1:D:454:VAL:HG23	2.19	0.42
1:A:79:GLY:HA3	1:A:136:GLN:HG2	2.01	0.42
1:A:429:LEU:HG	1:A:442:LEU:HD11	2.01	0.42
1:B:136:GLN:O	1:B:140:GLN:HG3	2.18	0.42
1:D:464:ALA:HB3	1:D:497:ARG:HE	1.85	0.42
1:A:474:VAL:HG13	1:A:475:ASP:N	2.35	0.42
1:A:475:ASP:N	1:A:475:ASP:OD1	2.51	0.42
1:B:70:ILE:O	1:B:74:LEU:HB2	2.18	0.42
1:A:69:ILE:O	1:A:73:ALA:HB3	2.20	0.42
1:C:480:GLY:O	1:C:484:ILE:HD13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:111:ALA:HB2	1:C:138:TRP:CZ3	2.54	0.42
1:C:475:ASP:HB3	1:C:508:ILE:CD1	2.50	0.42
1:D:464:ALA:HB3	1:D:497:ARG:CD	2.48	0.42
1:A:33:ARG:CD	1:A:54:GLY:H	2.32	0.42
1:A:488:GLU:O	1:A:492:ARG:HG3	2.20	0.42
1:C:396:LEU:HA	1:C:399:ILE:HB	2.02	0.42
1:D:509:ALA:O	1:D:539:ARG:NH2	2.53	0.42
1:A:547:LEU:HD21	1:A:562:LEU:HD11	2.02	0.41
1:A:89:SER:HB3	1:A:526:ARG:HH12	1.85	0.41
1:B:392:VAL:HG11	1:B:409:MSE:O	2.21	0.41
1:B:48:LEU:HD21	1:B:50:LEU:HB2	2.03	0.41
1:B:56:PHE:C	1:B:56:PHE:HD1	2.23	0.41
1:C:63:THR:O	1:C:67:LYS:HG3	2.21	0.41
1:B:406:HIS:CG	1:B:435:PRO:HG3	2.55	0.41
1:C:62:GLU:OE2	1:C:520:LYS:HE3	2.20	0.41
1:D:125:LEU:HG	1:D:130:VAL:HG21	2.02	0.41
1:B:131:SER:HG	1:B:134:GLU:HG3	1.85	0.41
1:C:155:LEU:HD23	1:C:155:LEU:HA	1.91	0.41
1:C:460:THR:HG21	1:C:489:GLN:HE22	1.86	0.41
1:C:182:TRP:CE3	1:C:183:ARG:HD2	2.55	0.41
1:D:56:PHE:HB2	1:D:494:ALA:CB	2.51	0.41
1:D:69:ILE:O	1:D:73:ALA:HB3	2.20	0.41
1:C:451:LEU:O	1:C:455:MSE:HG2	2.21	0.41
1:D:48:LEU:C	1:D:48:LEU:HD23	2.42	0.41
1:C:556:LEU:O	1:C:560:ARG:HB2	2.21	0.40
1:B:81:ARG:HH11	1:B:81:ARG:CG	2.34	0.40
1:D:372:GLU:O	1:D:376:VAL:HG22	2.22	0.40
1:D:460:THR:HG22	1:D:493:LEU:HB2	2.04	0.40
1:A:33:ARG:NH1	1:A:35:SER:HA	2.36	0.40
1:B:59:PHE:CZ	1:B:70:ILE:HD11	2.57	0.40
1:D:56:PHE:HA	1:D:499:VAL:HG22	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	352/415 (85%)	335 (95%)	14 (4%)	3 (1%)	17	55
1	B	353/415 (85%)	339 (96%)	13 (4%)	1 (0%)	41	76
1	C	339/415 (82%)	323 (95%)	11 (3%)	5 (2%)	10	42
1	D	293/415 (71%)	284 (97%)	8 (3%)	1 (0%)	41	76
All	All	1337/1660 (80%)	1281 (96%)	46 (3%)	10 (1%)	22	60

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	476	ALA
1	A	550	ASN
1	C	81	ARG
1	C	550	ASN
1	C	552	SER
1	B	54	GLY
1	D	83	ASN
1	C	188	ARG
1	A	147	TRP
1	C	34	LEU

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	273/312 (88%)	262 (96%)	11 (4%)	31	68
1	B	275/312 (88%)	268 (98%)	7 (2%)	47	79
1	C	264/312 (85%)	250 (95%)	14 (5%)	22	58
1	D	232/312 (74%)	224 (97%)	8 (3%)	37	72
All	All	1044/1248 (84%)	1004 (96%)	40 (4%)	33	69

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	LEU
1	A	56	PHE
1	A	62	GLU
1	A	63	THR
1	A	86	LEU
1	A	120	ARG
1	A	147	TRP
1	A	497	ARG
1	A	499	VAL
1	A	535	THR
1	A	558	HIS
1	B	56	PHE
1	B	81	ARG
1	B	83	ASN
1	B	120	ARG
1	B	147	TRP
1	B	375	LYS
1	B	418	GLU
1	C	62	GLU
1	C	76	LEU
1	C	81	ARG
1	C	109	ASP
1	C	115	LEU
1	C	147	TRP
1	C	171	GLU
1	C	173	GLN
1	C	426	ASP
1	C	432	SER
1	C	442	LEU
1	C	465	ASP
1	C	545	ARG
1	C	548	SER
1	D	40	ARG
1	D	56	PHE
1	D	84	HIS
1	D	142	ARG
1	D	147	TRP
1	D	500	LEU
1	D	502	VAL
1	D	539	ARG

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

Mol	Chain	Res	Type
1	A	136	GLN
1	A	179	HIS
1	A	434	ASN
1	B	83	ASN
1	B	136	GLN
1	B	160	GLN
1	B	434	ASN
1	C	41	ASN
1	C	160	GLN
1	C	489	GLN
1	C	513	HIS
1	D	47	GLN
1	D	136	GLN
1	D	149	HIS
1	D	173	GLN
1	D	370	HIS
1	D	504	HIS

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	354/415 (85%)	-0.56	0	100	100	19, 31, 60, 86	0
1	B	357/415 (86%)	-0.66	0	100	100	18, 29, 55, 81	0
1	C	347/415 (83%)	-0.46	0	100	100	24, 53, 75, 93	0
1	D	307/415 (73%)	-0.26	4 (1%)	77	51	26, 56, 75, 108	0
All	All	1365/1660 (82%)	-0.49	4 (0%)	94	84	18, 41, 71, 108	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	363	ARG	2.8
1	D	120	ARG	2.4
1	D	364	GLY	2.1
1	D	557	GLU	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 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.