Full wwPDB X-ray Structure Validation Report (i)

Aug 6, 2023 – 12:18 PM EDT

PDB ID	:	1JJA
Title	:	CRYSTAL STRUCTURE OF ORTHORHOMBIC FORM OF D90E MUTANT OF ESCHERICHIA COLI L-ASPARAGINASE II
Authors	:	Borek, D.; Kozak, M.; Jaskolski, M.
Deposited on	:	2001-07-04
Resolution	:	2.30 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:

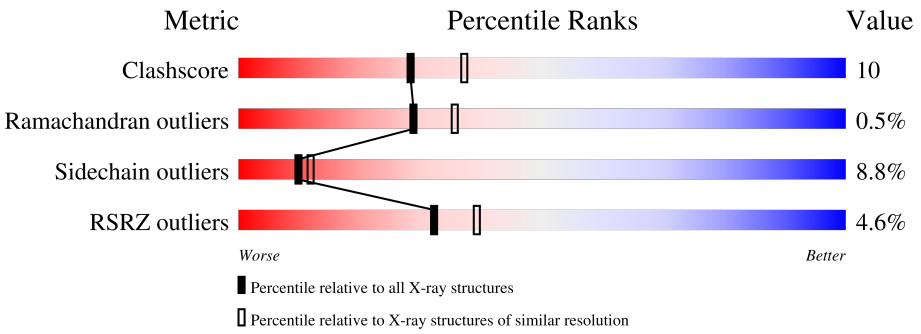
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.30 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))
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	326	6% 67% 24% • 5%
1	B	326	4% 71% 19% • 7%
1	C	326	2% 82% 16% ••
1	D	326	6% 64% 25% • • 6%
1	E	326	5% 70% 20% • 6%
1	F	326	4% 71% 23% • ••

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 14499 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 L-ASPARAGINASE II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	309	2319	1450	397	464	8	0	1	0
1	B	304	2284	1428	390	458	8	0	2	0
1	C	326	2438	1522	417	491	8	0	1	0
1	D	307	2307	1444	394	461	8	0	1	0
1	E	307	2307	1443	394	462	8	0	2	0
1	F	320	2400	1499	411	482	8	0	1	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	90	GLU	ASP	engineered mutation	UNP P00805
B	90	GLU	ASP	engineered mutation	UNP P00805
C	90	GLU	ASP	engineered mutation	UNP P00805
D	90	GLU	ASP	engineered mutation	UNP P00805
E	90	GLU	ASP	engineered mutation	UNP P00805
F	90	GLU	ASP	engineered mutation	UNP P00805

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	57	57	57	0	0
2	B	63	63	63	0	0
2	C	89	89	89	0	0

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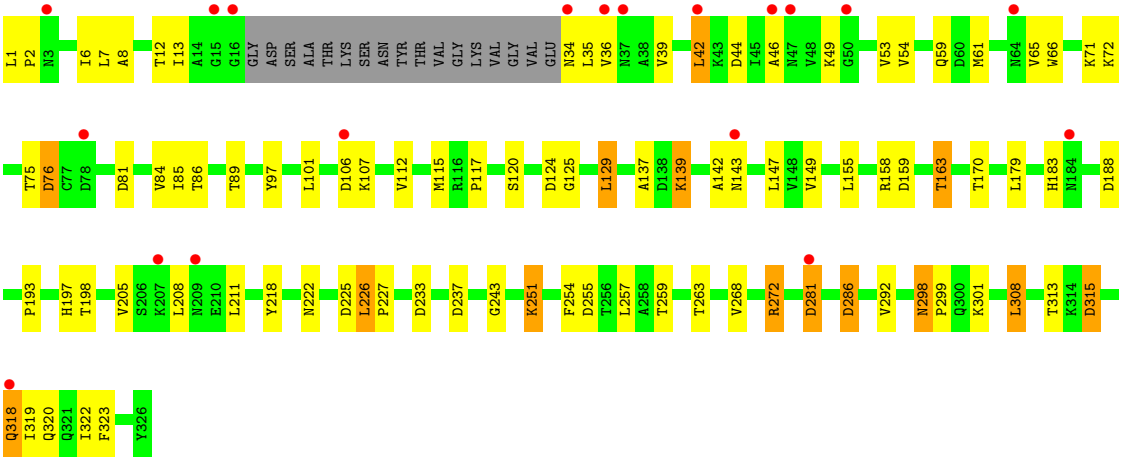
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	D	53	53	53	0	0
			Total	O		
2	E	65	65	65	0	0
			Total	O		
2	F	117	117	117	0	0

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.

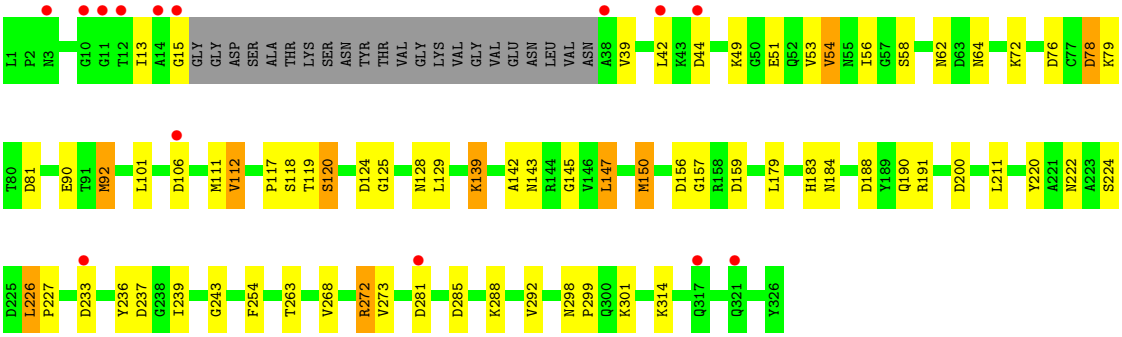
• Molecule 1: L-ASPARAGINASE II

Chain A:



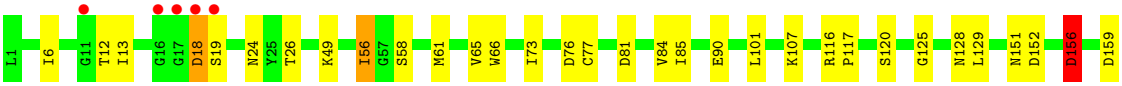
• Molecule 1: L-ASPARAGINASE II

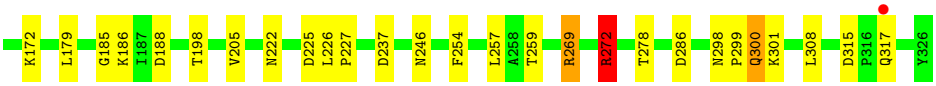
Chain B:



• Molecule 1: L-ASPARAGINASE II

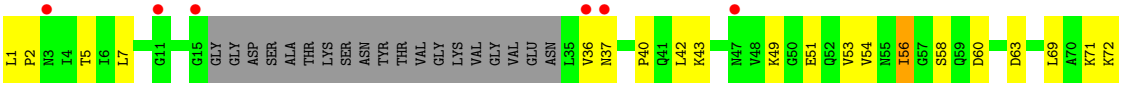
Chain C:

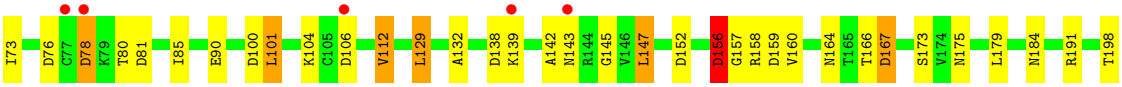


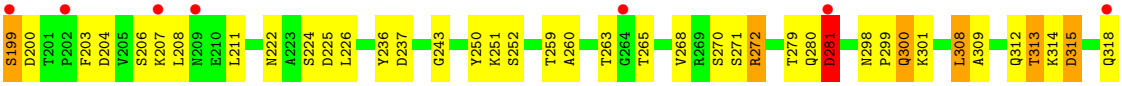


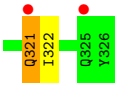
- Molecule 1: L-ASPARAGINASE II

Chain D:



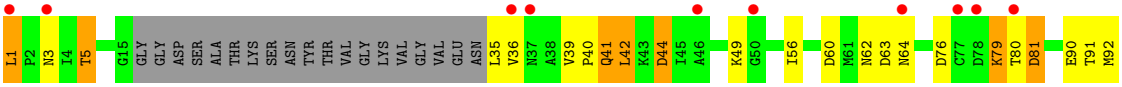


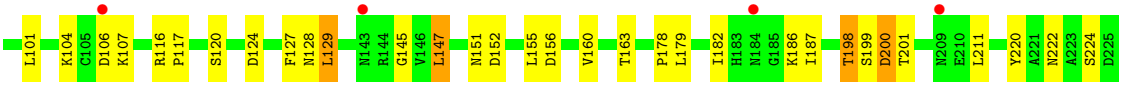


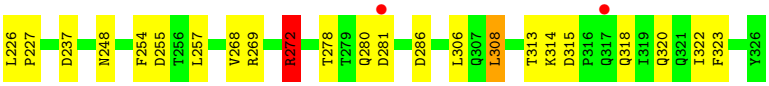


- Molecule 1: L-ASPARAGINASE II

Chain E:

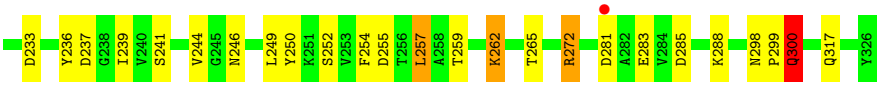






- Molecule 1: L-ASPARAGINASE II

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	225.42Å 128.05Å 62.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.30 10.00 – 2.33	Depositor EDS
% Data completeness (in resolution range)	96.9 (10.00-2.30) 96.9 (10.00-2.33)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.63 (at 2.33Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.186 , 0.204 0.186 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	35.4	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 57.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	14499	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.16% 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	0.62	0/2359	0.95	14/3212 (0.4%)
1	B	0.61	0/2330	0.97	14/3172 (0.4%)
1	C	0.65	0/2480	0.99	12/3377 (0.4%)
1	D	0.60	0/2347	0.92	10/3196 (0.3%)
1	E	0.76	0/2353	1.04	14/3204 (0.4%)
1	F	0.74	0/2440	1.07	19/3319 (0.6%)
All	All	0.67	0/14309	0.99	83/19480 (0.4%)

There are no bond length outliers.

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	272	ARG	NE-CZ-NH2	-9.25	115.67	120.30
1	E	272	ARG	NE-CZ-NH1	9.22	124.91	120.30
1	C	269	ARG	NE-CZ-NH2	-8.74	115.93	120.30
1	E	156	ASP	CB-CG-OD2	8.52	125.97	118.30
1	C	272	ARG	NE-CZ-NH1	8.07	124.33	120.30
1	E	237	ASP	CB-CG-OD2	7.84	125.36	118.30
1	F	167	ASP	CB-CG-OD2	7.47	125.02	118.30
1	F	272	ARG	NE-CZ-NH1	7.47	124.03	120.30
1	D	237	ASP	CB-CG-OD2	7.37	124.94	118.30
1	B	281	ASP	CB-CG-OD2	7.37	124.93	118.30
1	E	76	ASP	CB-CG-OD2	7.34	124.91	118.30
1	C	188	ASP	CB-CG-OD2	7.31	124.88	118.30
1	B	156	ASP	CB-CG-OD2	7.31	124.88	118.30
1	F	61	MET	CG-SD-CE	-7.18	88.71	100.20
1	F	76	ASP	CB-CG-OD2	7.14	124.72	118.30
1	C	159	ASP	CB-CG-OD2	7.09	124.68	118.30
1	B	159	ASP	CB-CG-OD2	7.07	124.66	118.30
1	E	200	ASP	CB-CG-OD2	6.86	124.48	118.30
1	A	281	ASP	CB-CG-OD2	6.80	124.42	118.30
1	A	237	ASP	CB-CG-OD2	6.80	124.42	118.30
1	B	112	VAL	CB-CA-C	-6.64	98.78	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	237	ASP	CB-CG-OD2	6.62	124.26	118.30
1	A	255	ASP	CB-CG-OD2	6.54	124.19	118.30
1	C	237	ASP	CB-CG-OD2	6.40	124.06	118.30
1	C	156	ASP	CB-CG-OD2	6.38	124.04	118.30
1	D	156	ASP	CB-CG-OD2	6.34	124.00	118.30
1	A	233	ASP	CB-CG-OD2	6.33	124.00	118.30
1	D	78	ASP	CB-CG-OD2	6.32	123.99	118.30
1	A	159	ASP	CB-CG-OD2	6.32	123.99	118.30
1	E	315	ASP	CB-CG-OD2	6.22	123.90	118.30
1	C	225	ASP	CB-CG-OD2	6.21	123.89	118.30
1	C	81	ASP	CB-CG-OD2	6.18	123.86	118.30
1	B	124	ASP	CB-CG-OD2	6.16	123.84	118.30
1	F	78	ASP	CB-CG-OD2	6.16	123.84	118.30
1	E	106	ASP	CB-CG-OD2	6.14	123.82	118.30
1	E	81	ASP	CB-CG-OD2	6.02	123.72	118.30
1	C	152	ASP	CB-CG-OD2	6.02	123.72	118.30
1	D	138	ASP	CB-CG-OD2	5.95	123.65	118.30
1	E	60	ASP	CB-CG-OD2	5.93	123.64	118.30
1	B	233	ASP	CB-CG-OD2	5.90	123.61	118.30
1	C	18	ASP	CB-CG-OD2	5.90	123.61	118.30
1	D	315	ASP	CB-CG-OD2	5.89	123.60	118.30
1	F	285	ASP	CB-CG-OD2	5.87	123.58	118.30
1	F	124	ASP	CB-CG-OD2	5.83	123.55	118.30
1	F	233	ASP	CB-CG-OD2	5.81	123.53	118.30
1	A	315	ASP	CB-CG-OD2	5.81	123.53	118.30
1	B	188	ASP	CB-CG-OD2	5.81	123.53	118.30
1	F	255	ASP	CB-CG-OD2	5.80	123.52	118.30
1	A	124	ASP	CB-CG-OD2	5.73	123.46	118.30
1	E	63	ASP	CB-CG-OD2	5.72	123.45	118.30
1	F	156	ASP	CB-CG-OD2	5.70	123.43	118.30
1	D	60	ASP	CB-CG-OD2	5.69	123.42	118.30
1	B	76	ASP	CB-CG-OD2	5.67	123.40	118.30
1	A	188	ASP	CB-CG-OD2	5.62	123.36	118.30
1	F	300	GLN	CB-CA-C	-5.62	99.15	110.40
1	E	124	ASP	CB-CG-OD2	5.44	123.20	118.30
1	A	106	ASP	CB-CG-OD2	5.42	123.18	118.30
1	E	255	ASP	CB-CG-OD2	5.41	123.17	118.30
1	F	204	ASP	CB-CG-OD2	5.40	123.16	118.30
1	C	269	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	F	188	ASP	CB-CG-OD2	5.38	123.14	118.30
1	E	44	ASP	CB-CG-OD2	5.37	123.13	118.30
1	D	167	ASP	CB-CG-OD1	5.36	123.12	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	76	ASP	CB-CG-OD2	5.34	123.11	118.30
1	A	81	ASP	CB-CG-OD2	5.33	123.10	118.30
1	B	285	ASP	CB-CG-OD2	5.33	123.09	118.30
1	F	147	LEU	CA-CB-CG	5.32	127.53	115.30
1	B	106	ASP	CB-CG-OD2	5.32	123.08	118.30
1	D	281	ASP	CB-CG-OD2	5.32	123.08	118.30
1	B	200	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	225	ASP	CB-CG-OD2	5.25	123.02	118.30
1	C	272	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	F	18	ASP	CB-CG-OD2	5.19	122.97	118.30
1	D	63	ASP	CB-CG-OD2	5.18	122.97	118.30
1	D	100	ASP	CB-CG-OD2	5.13	122.92	118.30
1	B	81	ASP	CB-CG-OD2	5.12	122.91	118.30
1	F	60	ASP	CB-CG-OD2	5.10	122.89	118.30
1	F	159	ASP	CB-CG-OD2	5.10	122.89	118.30
1	B	44	ASP	CB-CG-OD2	5.05	122.85	118.30
1	A	44	ASP	CB-CG-OD2	5.04	122.84	118.30
1	F	237	ASP	CB-CG-OD2	5.03	122.83	118.30
1	A	286	ASP	CB-CG-OD2	5.02	122.82	118.30
1	E	286	ASP	CB-CG-OD2	5.01	122.81	118.30

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	2319	0	2312	65	0
1	B	2284	0	2278	46	0
1	C	2438	0	2429	40	0
1	D	2307	0	2303	60	0
1	E	2307	0	2304	41	0
1	F	2400	0	2390	45	0
2	A	57	0	0	1	0
2	B	63	0	0	0	0
2	C	89	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	53	0	0	1	0
2	E	65	0	0	0	0
2	F	117	0	0	1	0
All	All	14499	0	14016	274	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 10.

All (274) 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:D:112:VAL:HG11	1:D:132:ALA:HB2	1.23	1.09
1:F:21:THR:O	1:F:22:LYS:HB2	1.62	0.98
1:D:156:ASP:O	1:D:160:VAL:HG12	1.66	0.96
1:E:79:LYS:NZ	1:E:79:LYS:HB3	1.84	0.92
1:A:205:VAL:HA	1:A:208:LEU:HD13	1.52	0.90
1:A:272:ARG:NH2	1:C:300:GLN:HG2	1.89	0.87
1:D:112:VAL:HG11	1:D:132:ALA:CB	2.08	0.83
1:E:79:LYS:HB3	1:E:79:LYS:HZ3	1.45	0.79
1:C:156:ASP:HB3	1:C:179:LEU:HD11	1.65	0.79
1:E:79:LYS:NZ	1:E:79:LYS:CB	2.48	0.77
1:B:150:MET:HE3	1:B:150:MET:HA	1.66	0.76
1:E:39:VAL:HB	1:E:42:LEU:HD22	1.68	0.76
1:A:298:ASN:C	1:A:298:ASN:HD22	1.87	0.75
1:A:139:LYS:HE3	1:A:139:LYS:HA	1.67	0.75
1:A:39:VAL:CG1	1:A:42:LEU:HD13	2.19	0.73
1:A:163:THR:HB	1:A:170:THR:O	1.87	0.73
1:D:5:THR:HG22	1:D:7:LEU:CD1	2.21	0.71
1:B:117:PRO:HD2	1:B:120:SER:OG	1.90	0.71
1:A:205:VAL:HA	1:A:208:LEU:CD1	2.21	0.71
1:C:61:MET:HE1	1:C:65:VAL:CG1	2.21	0.71
1:F:39:VAL:HB	1:F:42:LEU:HD22	1.72	0.70
1:B:92:MET:HE2	1:B:111:MET:HB3	1.76	0.68
1:B:183[A]:HIS:CE1	1:B:184:ASN:ND2	2.61	0.68
1:E:280:GLN:HG2	1:E:281:ASP:OD2	1.94	0.67
1:A:61:MET:HE1	1:A:65:VAL:CG1	2.25	0.67
1:B:314:LYS:NZ	1:F:24:ASN:HD22	1.92	0.67
1:D:53:VAL:O	1:D:54:VAL:HG13	1.95	0.67
1:D:72:LYS:HE3	1:D:76:ASP:OD2	1.95	0.66
1:A:259:THR:O	1:A:263:THR:HG23	1.95	0.66
1:C:73:ILE:HD11	1:C:85:ILE:HD11	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:MET:CE	1:C:65:VAL:HB	2.26	0.65
1:E:268:VAL:HG23	1:E:306:LEU:HD22	1.79	0.65
1:B:226:LEU:HB2	1:B:227:PRO:HD3	1.77	0.65
1:B:128:ASN:ND2	1:B:150:MET:HE1	2.12	0.64
1:A:75:THR:HG22	1:A:76:ASP:OD1	1.97	0.64
1:B:145:GLY:O	1:B:147:LEU:HD13	1.98	0.64
1:C:298:ASN:OD1	1:C:301:LYS:HG3	1.97	0.64
1:A:71:LYS:NZ	1:A:208:LEU:O	2.27	0.63
1:A:8:ALA:HA	1:A:86:THR:OG1	1.99	0.63
1:F:225:ASP:HB3	1:F:252:SER:HB3	1.82	0.62
1:B:183[A]:HIS:CE1	1:B:184:ASN:HD21	2.18	0.62
1:C:18:ASP:O	1:C:19:SER:OG	2.16	0.62
1:B:272:ARG:NH2	1:D:300:GLN:HG2	2.15	0.61
1:E:227:PRO:HB3	1:F:227:PRO:HB3	1.81	0.61
1:B:92:MET:CE	1:B:111:MET:HB3	2.31	0.61
1:A:272:ARG:CZ	1:C:300:GLN:HG2	2.31	0.60
1:A:272:ARG:NH2	1:C:300:GLN:CG	2.61	0.60
1:B:243:GLY:O	1:B:272:ARG:HG2	2.02	0.60
1:B:268:VAL:HG22	1:B:292:VAL:CG1	2.31	0.60
1:C:61:MET:HE3	1:C:65:VAL:HB	1.83	0.60
1:F:3:ASN:O	1:F:81:ASP:HB2	2.01	0.60
1:A:298:ASN:HB2	1:A:299:PRO:CD	2.32	0.60
1:D:5:THR:HG22	1:D:7:LEU:HD12	1.84	0.60
1:B:150:MET:HA	1:B:150:MET:CE	2.32	0.59
1:C:205:VAL:HG22	2:C:396:HOH:O	2.01	0.59
1:D:260:ALA:O	1:D:265:THR:HB	2.01	0.59
1:D:142:ALA:O	1:D:143:ASN:HB2	2.02	0.59
1:E:5:THR:OG1	1:E:80:THR:HG21	2.03	0.59
1:D:164:ASN:HD22	1:D:166:THR:H	1.49	0.59
1:D:164:ASN:ND2	1:D:166:THR:H	2.01	0.59
1:D:203:PHE:CE1	1:D:308:LEU:HB3	2.38	0.59
1:D:112:VAL:CG1	1:D:132:ALA:HB2	2.15	0.59
1:B:92:MET:HE2	1:B:111:MET:CB	2.33	0.58
1:D:243:GLY:O	1:D:272:ARG:HG2	2.03	0.57
1:A:39:VAL:HG11	1:A:42:LEU:HD13	1.85	0.57
1:C:128:ASN:HD21	1:C:151:ASN:H	1.52	0.57
1:A:117:PRO:O	1:A:120:SER:HB3	2.05	0.57
1:F:56:ILE:CD1	1:F:65:VAL:HG21	2.35	0.56
1:F:246:ASN:HB3	1:F:283:GLU:HG3	1.86	0.56
1:E:104:LYS:NZ	1:E:201:THR:O	2.39	0.56
1:F:12:THR:HG22	1:F:18:ASP:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:318:GLN:O	1:D:321:GLN:HG3	2.05	0.55
1:C:12:THR:HA	2:C:369:HOH:O	2.07	0.55
1:D:53:VAL:HG12	1:D:54:VAL:HG22	1.89	0.55
1:D:157:GLY:O	1:D:301:LYS:NZ	2.40	0.55
1:E:186:LYS:HG2	1:E:187:ILE:N	2.22	0.55
1:C:18:ASP:O	1:C:19:SER:CB	2.55	0.55
1:C:269:ARG:HD3	1:C:286:ASP:OD1	2.07	0.55
1:F:262:LYS:HE2	2:F:415:HOH:O	2.07	0.55
1:C:300:GLN:H	1:C:300:GLN:NE2	2.04	0.54
1:D:73:ILE:HD11	1:D:85:ILE:HD11	1.88	0.54
1:A:197:HIS:ND1	1:A:198:THR:OG1	2.34	0.54
1:E:268:VAL:CG2	1:E:306:LEU:HD22	2.37	0.54
1:D:313:THR:OG1	1:D:314:LYS:N	2.41	0.54
1:B:15:GLY:N	1:B:118[B]:SER:OG	2.41	0.54
1:A:218:TYR:OH	1:C:300:GLN:NE2	2.39	0.54
1:A:53:VAL:HG12	1:A:54:VAL:HG13	1.90	0.54
1:E:41:GLN:N	1:E:41:GLN:OE1	2.39	0.54
1:E:155:LEU:HD23	1:E:178:PRO:HB3	1.90	0.54
1:A:298:ASN:C	1:A:298:ASN:ND2	2.60	0.54
1:C:13:ILE:O	1:C:125:GLY:HA3	2.08	0.54
1:A:298:ASN:ND2	1:A:301:LYS:H	2.05	0.54
1:C:246:ASN:OD1	1:C:278:THR:HA	2.08	0.53
1:B:314:LYS:HZ1	1:F:24:ASN:HD22	1.55	0.53
1:C:117:PRO:O	1:C:120:SER:HB3	2.09	0.53
1:D:318:GLN:O	1:D:322:ILE:HG13	2.09	0.53
1:F:14:ALA:HA	1:F:118:SER:HB2	1.90	0.53
1:B:272:ARG:HG3	1:B:273:VAL:N	2.24	0.53
1:D:145:GLY:O	1:D:147:LEU:HD13	2.09	0.52
1:D:203:PHE:CD1	1:D:308:LEU:HB3	2.44	0.52
1:A:298:ASN:HB2	1:A:299:PRO:HD3	1.91	0.52
1:B:272:ARG:CZ	1:D:300:GLN:HG2	2.40	0.52
1:B:190:GLN:O	1:B:191:ARG:HG2	2.10	0.52
1:E:220:TYR:CG	1:F:216:ILE:HD12	2.45	0.52
1:C:185:GLY:O	1:C:186:LYS:HD2	2.09	0.52
1:E:79:LYS:CB	1:E:79:LYS:HZ2	2.21	0.52
1:B:268:VAL:HG22	1:B:292:VAL:HG11	1.92	0.52
1:D:164:ASN:HD22	1:D:167:ASP:H	1.57	0.52
1:A:34:ASN:O	1:A:36:VAL:N	2.43	0.52
1:A:61:MET:HE1	1:A:65:VAL:HB	1.92	0.52
1:A:61:MET:CE	1:A:65:VAL:HB	2.40	0.52
1:F:241:SER:OG	1:F:249:LEU:HD21	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:VAL:CG1	1:B:42:LEU:HD13	2.40	0.51
1:F:92:MET:HG3	1:F:111:MET:HE2	1.91	0.51
1:B:128:ASN:ND2	1:B:150:MET:CE	2.73	0.51
1:C:61:MET:HE1	1:C:65:VAL:HG11	1.93	0.51
1:A:13:ILE:O	1:A:125:GLY:HA3	2.10	0.51
1:F:21:THR:O	1:F:22:LYS:CB	2.45	0.51
1:D:69:LEU:O	1:D:73:ILE:HG13	2.11	0.51
1:D:298:ASN:HB2	1:D:299:PRO:HD2	1.92	0.51
1:E:39:VAL:O	1:E:42:LEU:HB2	2.10	0.51
1:A:292:VAL:HG13	1:A:320:GLN:HA	1.93	0.50
1:E:182:ILE:HG12	1:E:187:ILE:HG12	1.92	0.50
1:F:219:ASN:HD22	1:F:250:TYR:H	1.57	0.50
1:A:61:MET:HE2	1:A:66:TRP:CD1	2.46	0.50
1:D:71:LYS:NZ	1:D:208:LEU:O	2.44	0.50
1:D:280:GLN:O	1:D:281:ASP:C	2.49	0.50
1:B:78:ASP:OD1	1:B:78:ASP:N	2.30	0.49
1:F:104:LYS:NZ	1:F:201:THR:O	2.45	0.49
1:D:36:VAL:CG1	1:D:43:LYS:HG3	2.42	0.49
1:B:142:ALA:O	1:B:143:ASN:HB2	2.12	0.49
1:B:190:GLN:C	1:B:191:ARG:HG2	2.33	0.49
1:D:58:SER:OG	1:D:90:GLU:HB2	2.12	0.49
1:E:269:ARG:O	1:E:278:THR:HG21	2.13	0.49
1:D:104:LYS:HD3	1:D:199:SER:HA	1.95	0.48
1:D:204:ASP:OD1	1:D:206:SER:OG	2.30	0.48
1:E:318:GLN:O	1:E:322:ILE:HG13	2.14	0.48
1:B:139:LYS:NZ	1:B:139:LYS:HB3	2.28	0.48
1:F:53:VAL:HG12	1:F:54:VAL:HG13	1.95	0.48
1:F:36:VAL:HG12	1:F:37:ASN:HD22	1.79	0.48
1:F:298:ASN:HB2	1:F:299:PRO:CD	2.44	0.48
1:C:24:ASN:OD1	1:C:26:THR:HB	2.13	0.48
1:C:61:MET:HE2	1:C:66:TRP:CD1	2.48	0.48
1:A:39:VAL:HG12	1:A:42:LEU:HD13	1.93	0.47
1:D:104:LYS:NZ	1:D:203:PHE:O	2.40	0.47
1:E:79:LYS:HB3	1:E:79:LYS:HZ2	1.71	0.47
1:C:172:LYS:NZ	2:C:384:HOH:O	2.47	0.47
1:D:36:VAL:HG12	1:D:43:LYS:HE2	1.97	0.47
1:D:259:THR:O	1:D:263:THR:HG23	2.14	0.47
1:C:58:SER:OG	1:C:90:GLU:HB2	2.14	0.47
1:D:225:ASP:HB3	1:D:252:SER:HB3	1.97	0.47
1:A:268:VAL:HG22	1:A:292:VAL:HB	1.95	0.47
1:B:58:SER:OG	1:B:90:GLU:OE1	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:224:SER:HB2	1:F:236:TYR:OH	2.14	0.47
1:F:73:ILE:HD11	1:F:85:ILE:HD11	1.96	0.47
1:B:13:ILE:O	1:B:125:GLY:HA3	2.14	0.47
1:B:298:ASN:HB2	1:B:299:PRO:CD	2.45	0.47
1:A:318:GLN:O	1:A:322:ILE:HG13	2.14	0.47
1:B:157:GLY:O	1:B:301:LYS:NZ	2.48	0.47
1:A:142:ALA:O	1:A:143:ASN:HB2	2.15	0.46
1:D:270:SER:OG	1:D:271:SER:N	2.48	0.46
1:E:35:LEU:HD23	1:E:129:LEU:HD11	1.96	0.46
1:F:35:LEU:HA	1:F:35:LEU:HD12	1.41	0.46
1:C:61:MET:HE1	1:C:65:VAL:HB	1.96	0.46
1:C:128:ASN:ND2	1:C:151:ASN:H	2.13	0.46
1:D:56:ILE:N	1:D:56:ILE:HD13	2.29	0.46
1:A:298:ASN:ND2	1:A:301:LYS:HG3	2.30	0.46
1:D:36:VAL:HG12	1:D:43:LYS:HG3	1.97	0.46
1:B:224:SER:HB2	1:D:236:TYR:OH	2.16	0.46
1:B:314:LYS:HD2	1:F:16:GLY:O	2.16	0.46
1:B:314:LYS:HZ3	1:F:24:ASN:HD22	1.63	0.46
1:C:6:ILE:HA	1:C:84:VAL:O	2.16	0.46
1:E:36:VAL:O	1:E:36:VAL:HG22	2.15	0.46
1:E:40:PRO:HD2	1:E:41:GLN:OE1	2.15	0.46
1:E:90:GLU:HB3	1:F:244:VAL:HB	1.98	0.46
1:E:62:ASN:OD1	1:E:64:ASN:N	2.49	0.46
1:F:117:PRO:C	1:F:119:THR:H	2.19	0.46
1:A:112:VAL:HG23	1:A:149:VAL:O	2.16	0.46
1:A:183[A]:HIS:CD2	1:D:279:THR:HG21	2.51	0.46
1:E:3:ASN:O	1:E:81:ASP:HB2	2.16	0.46
1:A:39:VAL:O	1:A:42:LEU:HB2	2.15	0.46
1:E:320:GLN:O	1:E:323:PHE:N	2.49	0.46
1:D:159:ASP:OD2	1:D:173:SER:HB3	2.16	0.46
1:F:66:TRP:HB3	1:F:98:PHE:CE2	2.51	0.46
1:F:239:ILE:HD12	1:F:265:THR:HG21	1.98	0.46
1:A:61:MET:HE1	1:A:65:VAL:HG11	1.99	0.45
1:A:320:GLN:O	1:A:323:PHE:N	2.48	0.45
1:A:298:ASN:HD21	1:A:301:LYS:HG3	1.81	0.45
1:A:315:ASP:O	1:A:319:ILE:HG13	2.17	0.45
1:C:116:ARG:NH1	2:C:394:HOH:O	2.29	0.45
1:D:37:ASN:O	1:D:40:PRO:HD3	2.16	0.45
1:E:272:ARG:NH2	1:F:300:GLN:HG3	2.32	0.45
1:A:34:ASN:C	1:A:36:VAL:H	2.20	0.45
1:A:61:MET:HE1	1:A:65:VAL:CB	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:PRO:HB3	1:C:227:PRO:HB3	1.99	0.45
1:B:62:ASN:OD1	1:B:64:ASN:HB2	2.16	0.45
1:D:158:ARG:O	1:D:301:LYS:NZ	2.49	0.45
1:E:128:ASN:HD21	1:E:151:ASN:H	1.64	0.45
1:E:308:LEU:HD12	1:E:308:LEU:HA	1.84	0.44
1:F:257:LEU:HD12	1:F:257:LEU:HA	1.71	0.44
1:A:53:VAL:O	1:A:54:VAL:HG13	2.16	0.44
1:B:236:TYR:OH	1:D:224:SER:HB2	2.17	0.44
1:A:226:LEU:HB2	1:A:227:PRO:HD3	1.99	0.44
1:C:61:MET:CE	1:C:66:TRP:CD1	3.00	0.44
1:D:53:VAL:O	1:D:54:VAL:CG1	2.65	0.44
1:D:318:GLN:HA	1:D:321:GLN:CG	2.47	0.44
1:E:79:LYS:O	1:E:80:THR:HB	2.17	0.44
1:E:91:THR:O	1:E:92:MET:C	2.56	0.44
1:F:164:ASN:OD1	1:F:167:ASP:HB2	2.18	0.44
1:F:219:ASN:ND2	1:F:250:TYR:H	2.16	0.44
1:D:156:ASP:O	1:D:160:VAL:CG1	2.54	0.44
1:E:145:GLY:O	1:E:147:LEU:HD13	2.18	0.44
1:F:198:THR:C	1:F:200:ASP:H	2.21	0.44
1:B:128:ASN:CG	1:B:150:MET:CE	2.86	0.43
1:D:101:LEU:HD12	1:D:101:LEU:HA	1.77	0.43
1:F:198:THR:O	1:F:200:ASP:N	2.50	0.43
1:B:272:ARG:HD2	2:D:329:HOH:O	2.18	0.43
1:C:61:MET:HE1	1:C:65:VAL:CB	2.47	0.43
1:F:1:LEU:HB3	1:F:46:ALA:HA	1.99	0.43
1:A:308:LEU:HD12	1:A:308:LEU:HA	1.67	0.43
1:B:51:GLU:CD	1:B:72:LYS:NZ	2.71	0.43
1:B:53:VAL:HG12	1:B:54:VAL:HG22	2.01	0.43
1:A:34:ASN:C	1:A:36:VAL:N	2.72	0.43
1:E:160:VAL:HG13	1:E:160:VAL:O	2.19	0.43
1:F:94:GLU:HG2	1:F:300:GLN:HB3	1.99	0.43
1:A:281:ASP:OD1	1:A:286:ASP:N	2.52	0.43
1:C:56:ILE:HD13	1:C:56:ILE:N	2.34	0.43
1:C:315:ASP:OD2	1:C:317:GLN:HG3	2.18	0.43
1:F:39:VAL:O	1:F:42:LEU:HB2	2.19	0.43
1:A:97:TYR:CE1	1:A:158:ARG:HG3	2.54	0.42
1:A:6:ILE:HA	1:A:84:VAL:O	2.19	0.42
1:D:198:THR:O	1:D:200:ASP:N	2.52	0.42
1:F:34:ASN:HD22	1:F:34:ASN:HA	1.53	0.42
1:B:314:LYS:HE3	1:B:314:LYS:HB2	1.73	0.42
1:B:314:LYS:NZ	1:F:24:ASN:ND2	2.65	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:251:LYS:HA	1:D:251:LYS:HD3	1.84	0.42
1:A:72:LYS:O	1:A:75:THR:HB	2.20	0.42
1:A:251:LYS:HB3	1:A:251:LYS:HE2	1.31	0.42
1:F:6:ILE:HA	1:F:84:VAL:O	2.20	0.42
1:D:129:LEU:HD23	1:D:129:LEU:HA	1.90	0.42
1:A:226:LEU:N	1:A:227:PRO:CD	2.83	0.41
1:C:56:ILE:HD13	1:C:56:ILE:H	1.84	0.41
1:A:89:THR:HG21	1:A:115:MET:SD	2.60	0.41
1:B:226:LEU:N	1:B:227:PRO:CD	2.83	0.41
1:E:41:GLN:H	1:E:41:GLN:CD	2.22	0.41
1:E:1:LEU:HD23	1:E:1:LEU:HA	1.67	0.41
1:E:220:TYR:CD1	1:F:216:ILE:HD12	2.55	0.41
1:C:298:ASN:HB2	1:C:299:PRO:CD	2.50	0.41
1:E:313:THR:OG1	1:E:314:LYS:N	2.53	0.41
2:A:345:HOH:O	1:C:272:ARG:HD2	2.21	0.41
1:A:76:ASP:OD1	1:A:76:ASP:N	2.53	0.41
1:B:220:TYR:N	1:B:220:TYR:CD1	2.89	0.41
1:C:128:ASN:HD22	1:C:128:ASN:HA	1.65	0.41
1:D:1:LEU:HA	1:D:2:PRO:HD3	1.85	0.41
1:D:80:THR:OG1	1:D:81:ASP:N	2.54	0.41
1:D:315:ASP:O	1:D:318:GLN:N	2.49	0.41
1:E:198:THR:O	1:E:200:ASP:N	2.54	0.41
1:A:1:LEU:HB3	1:A:46:ALA:HA	2.03	0.41
1:A:53:VAL:O	1:A:54:VAL:CG1	2.69	0.41
1:A:193:PRO:HA	1:D:191:ARG:NH1	2.35	0.41
1:D:309:ALA:HB1	1:D:322:ILE:HD12	2.03	0.41
1:A:226:LEU:HD12	1:A:226:LEU:HA	1.93	0.40
1:A:42:LEU:HD11	1:A:129:LEU:HD13	2.03	0.40
1:B:298:ASN:HB2	1:B:299:PRO:HD2	2.02	0.40
1:A:7:LEU:O	1:A:85:ILE:HA	2.20	0.40
1:B:314:LYS:HZ3	1:F:24:ASN:ND2	2.19	0.40
1:D:159:ASP:OD1	1:D:175:ASN:HB2	2.21	0.40
1:A:243:GLY:O	1:A:272:ARG:HG2	2.20	0.40
1:C:76:ASP:O	1:C:77:CYS:C	2.59	0.40
1:D:250:TYR:O	1:D:251:LYS:C	2.59	0.40
1:A:2:PRO:HG2	1:A:137:ALA:HB1	2.04	0.40
1:A:59:GLN:OE1	1:A:59:GLN:N	2.43	0.40
1:E:116:ARG:HA	1:E:117:PRO:HD3	1.95	0.40
1:F:96:ALA:O	1:F:100:ASP:HB2	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	306/326 (94%)	288 (94%)	17 (6%)	1 (0%)	41	50
1	B	302/326 (93%)	290 (96%)	12 (4%)	0	100	100
1	C	325/326 (100%)	318 (98%)	6 (2%)	1 (0%)	41	50
1	D	304/326 (93%)	290 (95%)	12 (4%)	2 (1%)	22	26
1	E	305/326 (94%)	289 (95%)	14 (5%)	2 (1%)	22	26
1	F	315/326 (97%)	302 (96%)	10 (3%)	3 (1%)	15	17
All	All	1857/1956 (95%)	1777 (96%)	71 (4%)	9 (0%)	29	35

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	22	LYS
1	A	35	LEU
1	D	281	ASP
1	E	199	SER
1	D	199	SER
1	F	281	ASP
1	C	198	THR
1	E	198	THR
1	F	27	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	254/266 (96%)	232 (91%)	22 (9%)	10 12
1	B	251/266 (94%)	228 (91%)	23 (9%)	9 11
1	C	267/266 (100%)	253 (95%)	14 (5%)	23 32
1	D	253/266 (95%)	226 (89%)	27 (11%)	6 7
1	E	254/266 (96%)	229 (90%)	25 (10%)	8 9
1	F	263/266 (99%)	239 (91%)	24 (9%)	9 11
All	All	1542/1596 (97%)	1407 (91%)	135 (9%)	10 12

All (135) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	THR
1	A	42	LEU
1	A	49	LYS
1	A	101	LEU
1	A	107	LYS
1	A	129	LEU
1	A	139	LYS
1	A	147	LEU
1	A	155	LEU
1	A	163	THR
1	A	179	LEU
1	A	211	LEU
1	A	222	ASN
1	A	226	LEU
1	A	251	LYS
1	A	254	PHE
1	A	257	LEU
1	A	272	ARG
1	A	298	ASN
1	A	308	LEU
1	A	313	THR
1	A	318	GLN
1	B	49	LYS
1	B	54	VAL
1	B	56	ILE
1	B	78	ASP
1	B	79	LYS
1	B	92	MET
1	B	101	LEU
1	B	112	VAL

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Mol	Chain	Res	Type
1	B	119	THR
1	B	120	SER
1	B	129	LEU
1	B	139	LYS
1	B	147	LEU
1	B	150	MET
1	B	179	LEU
1	B	211	LEU
1	B	222	ASN
1	B	226	LEU
1	B	239	ILE
1	B	254	PHE
1	B	263	THR
1	B	272	ARG
1	B	288	LYS
1	C	49	LYS
1	C	56	ILE
1	C	101	LEU
1	C	107	LYS
1	C	129	LEU
1	C	156	ASP
1	C	222	ASN
1	C	226	LEU
1	C	254	PHE
1	C	257	LEU
1	C	259	THR
1	C	272	ARG
1	C	300	GLN
1	C	308	LEU
1	D	42	LEU
1	D	49	LYS
1	D	51	GLU
1	D	56	ILE
1	D	78	ASP
1	D	101	LEU
1	D	106	ASP
1	D	112	VAL
1	D	129	LEU
1	D	139	LYS
1	D	147	LEU
1	D	152	ASP
1	D	156	ASP

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Mol	Chain	Res	Type
1	D	179	LEU
1	D	184	ASN
1	D	207	LYS
1	D	211	LEU
1	D	222	ASN
1	D	226	LEU
1	D	268	VAL
1	D	272	ARG
1	D	281	ASP
1	D	300	GLN
1	D	308	LEU
1	D	312	GLN
1	D	313	THR
1	D	321	GLN
1	E	1	LEU
1	E	5	THR
1	E	41	GLN
1	E	42	LEU
1	E	44	ASP
1	E	49	LYS
1	E	56	ILE
1	E	79	LYS
1	E	101	LEU
1	E	107	LYS
1	E	120	SER
1	E	127	PHE
1	E	129	LEU
1	E	147	LEU
1	E	152	ASP
1	E	163	THR
1	E	179	LEU
1	E	211	LEU
1	E	222	ASN
1	E	226	LEU
1	E	248	ASN
1	E	254	PHE
1	E	257	LEU
1	E	272	ARG
1	E	308	LEU
1	F	18	ASP
1	F	29	LYS
1	F	34	ASN

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Mol	Chain	Res	Type
1	F	36	VAL
1	F	42	LEU
1	F	51	GLU
1	F	56	ILE
1	F	61	MET
1	F	101	LEU
1	F	119	THR
1	F	147	LEU
1	F	179	LEU
1	F	184	ASN
1	F	208	LEU
1	F	211	LEU
1	F	226	LEU
1	F	254	PHE
1	F	257	LEU
1	F	259	THR
1	F	262	LYS
1	F	272	ARG
1	F	288	LYS
1	F	300	GLN
1	F	317	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	64	ASN
1	A	128	ASN
1	A	184	ASN
1	A	209	ASN
1	A	298	ASN
1	A	321	GLN
1	B	184	ASN
1	B	190	GLN
1	B	321	GLN
1	C	128	ASN
1	C	300	GLN
1	C	324	ASN
1	D	128	ASN
1	D	164	ASN
1	D	184	ASN
1	D	209	ASN

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Mol	Chain	Res	Type
1	D	312	GLN
1	E	64	ASN
1	E	128	ASN
1	E	184	ASN
1	E	209	ASN
1	F	24	ASN
1	F	34	ASN
1	F	37	ASN
1	F	128	ASN
1	F	219	ASN
1	F	300	GLN
1	F	317	GLN
1	F	318	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	309/326 (94%)	-0.00	19 (6%)	21	27	22, 43, 69, 86	0
1	B	304/326 (93%)	-0.14	14 (4%)	32	39	24, 43, 59, 67	0
1	C	326/326 (100%)	-0.38	6 (1%)	68	74	21, 33, 52, 74	0
1	D	307/326 (94%)	0.10	20 (6%)	18	24	25, 46, 63, 73	0
1	E	307/326 (94%)	-0.10	16 (5%)	27	34	17, 34, 57, 71	0
1	F	320/326 (98%)	-0.28	12 (3%)	40	47	15, 29, 59, 75	0
All	All	1873/1956 (95%)	-0.14	87 (4%)	32	39	15, 38, 61, 86	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	16	GLY	6.2
1	C	19	SER	5.6
1	A	37	ASN	5.3
1	F	34	ASN	4.9
1	F	47	ASN	4.6
1	D	37	ASN	4.6
1	F	17	GLY	4.4
1	F	16	GLY	4.3
1	D	207	LYS	4.2
1	E	77	CYS	4.1
1	C	18	ASP	4.1
1	D	11	GLY	3.8
1	F	18	ASP	3.7
1	E	37	ASN	3.7
1	B	12	THR	3.6
1	F	29	LYS	3.6
1	A	34	ASN	3.6
1	D	209	ASN	3.5
1	B	106	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	317	GLN	3.5
1	B	38	ALA	3.3
1	F	37	ASN	3.3
1	A	50	GLY	3.3
1	A	106	ASP	3.3
1	D	281	ASP	3.2
1	F	21	THR	3.2
1	A	209	ASN	3.2
1	E	106	ASP	3.2
1	D	3	ASN	3.1
1	E	36	VAL	3.1
1	F	281	ASP	2.9
1	E	46	ALA	2.9
1	D	321	GLN	2.9
1	B	233	ASP	2.9
1	D	106	ASP	2.9
1	A	3	ASN	2.8
1	D	318	GLN	2.7
1	D	199	SER	2.7
1	E	1	LEU	2.6
1	A	47	ASN	2.6
1	A	281	ASP	2.6
1	A	207	LYS	2.5
1	B	14	ALA	2.5
1	D	77	CYS	2.5
1	B	321	GLN	2.5
1	A	15	GLY	2.5
1	B	15	GLY	2.4
1	E	281	ASP	2.4
1	D	202	PRO	2.4
1	C	17	GLY	2.4
1	D	15	GLY	2.4
1	B	281	ASP	2.4
1	C	317	GLN	2.4
1	A	42	LEU	2.4
1	D	264	GLY	2.3
1	E	80	THR	2.3
1	A	78	ASP	2.3
1	E	317	GLN	2.3
1	B	10	GLY	2.3
1	B	44	ASP	2.3
1	D	139	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	11	GLY	2.2
1	A	184	ASN	2.2
1	E	78	ASP	2.2
1	B	3	ASN	2.2
1	E	3	ASN	2.2
1	E	184	ASN	2.2
1	F	207	LYS	2.2
1	C	16	GLY	2.2
1	A	143	ASN	2.2
1	E	143	ASN	2.2
1	D	47	ASN	2.1
1	D	325	GLN	2.2
1	D	78	ASP	2.1
1	A	36	VAL	2.1
1	A	46	ALA	2.1
1	C	11	GLY	2.1
1	E	50	GLY	2.1
1	D	143	ASN	2.1
1	A	64	ASN	2.1
1	E	64	ASN	2.1
1	E	209	ASN	2.1
1	A	318	GLN	2.0
1	F	26	THR	2.0
1	B	42	LEU	2.0
1	D	36	VAL	2.0
1	F	119	THR	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.