



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 11:25 PM GMT

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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

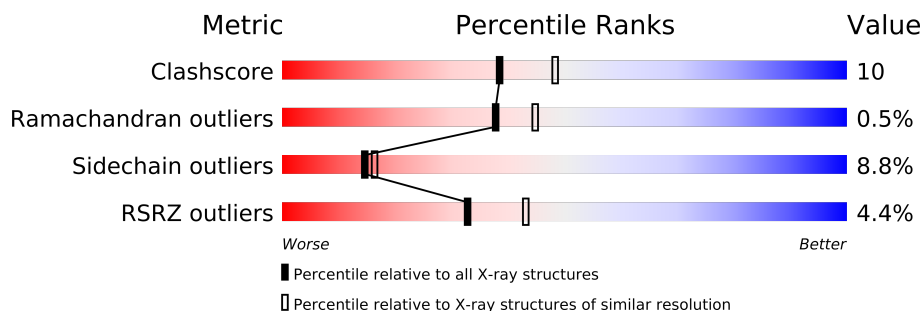
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	326	
1	B	326	
1	C	326	
1	D	326	
1	E	326	
1	F	326	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14499 atoms, of which 0 are hydrogen and 0 are deuterium.

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

There are 6 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is water.

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

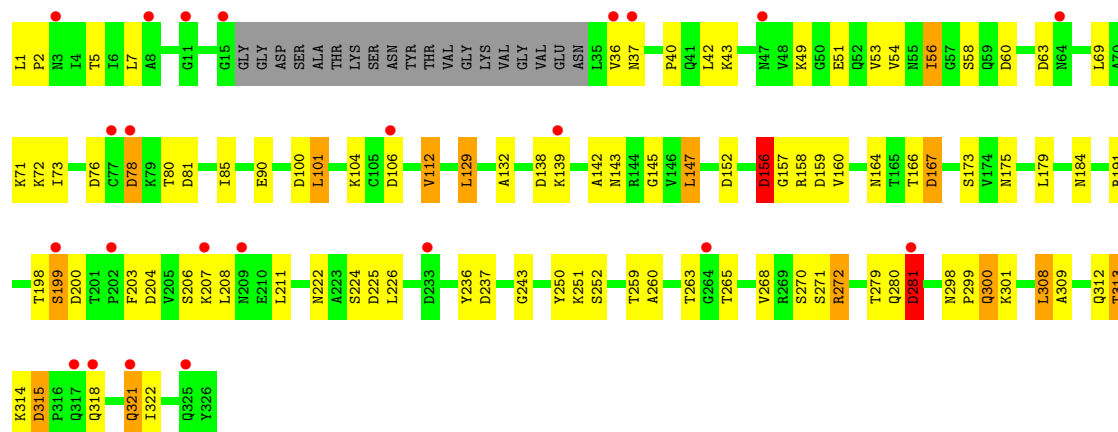
Continued on next page...

Continued from previous page...

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

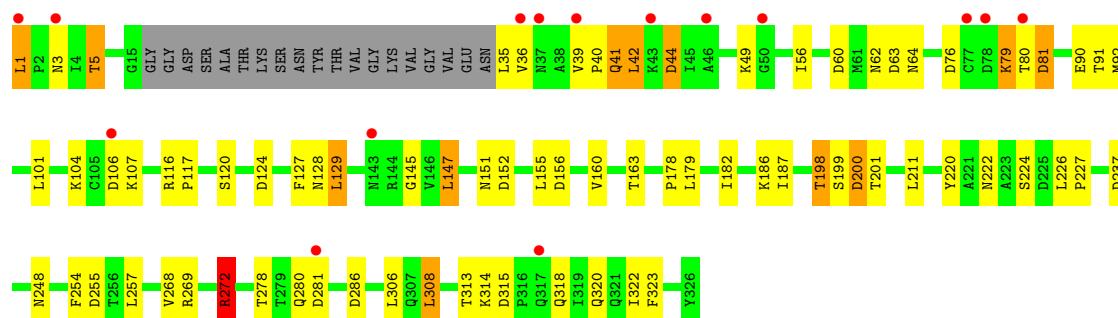
- Molecule 1: L-ASPARAGINASE II

Chain D:



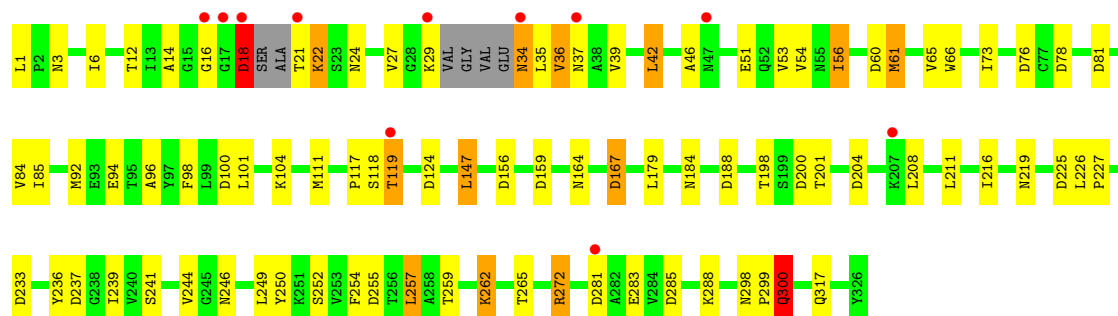
- Molecule 1: L-ASPARAGINASE II

Chain E:



- Molecule 1: L-ASPARAGINASE II

Chain F:



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 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
$\langle I/\sigma(I) \rangle$ 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.	DCC
Wilson B-factor (Å ²)	35.4	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 42.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 74882 reflections	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.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	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(°)	Ideal(°)
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	63	0	0	0	0
2	C	89	0	0	4	0
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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 10.

All (274) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:HA	1:B:150:MET:HE3	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:HA	1:A:139:LYS:HE3	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:C:73:ILE:HD11	1:C:85:ILE:HD11	1.77	0.66
1:A:259:THR:O	1:A:263:THR:HG23	1.95	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(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:D:260:ALA:O	1:D:265:THR:HB	2.01	0.59
1:C:205:VAL:HG22	2:C:396:HOH:O	2.01	0.59
1:E:5:THR:OG1	1:E:80:THR:HG21	2.03	0.59
1:D:142:ALA:O	1:D:143:ASN:HB2	2.02	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
1:D:318:GLN:O	1:D:321:GLN:HG3	2.05	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:E:186:LYS:HG2	1:E:187:ILE:N	2.22	0.55
1:D:157:GLY:O	1:D:301:LYS:NZ	2.40	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:NE2	1:C:300:GLN:H	2.04	0.54
1:D:73:ILE:HD11	1:D:85:ILE:HD11	1.88	0.54
1:E:268:VAL:CG2	1:E:306:LEU:HD22	2.37	0.54
1:A:197:HIS:ND1	1:A:198:THR:OG1	2.34	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:D:318:GLN:O	1:D:322:ILE:HG13	2.09	0.53
1:C:117:PRO:O	1:C:120:SER:HB3	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:203:PHE:CD1	1:D:308:LEU:HB3	2.44	0.52
1:D:145:GLY:O	1:D:147:LEU:HD13	2.09	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:E:220:TYR:CG	1:F:216:ILE:HD12	2.45	0.52
1:B:190:GLN:O	1:B:191:ARG:HG2	2.10	0.52
1:E:79:LYS:HZ2	1:E:79:LYS:CB	2.21	0.52
1:C:185:GLY:O	1:C:186:LYS:HD2	2.09	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:CE	1:A:65:VAL:HB	2.40	0.52
1:A:61:MET:HE1	1:A:65:VAL:HB	1.92	0.52
1:F:241:SER:OG	1:F:249:LEU:HD21	2.09	0.52
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:E:182:ILE:HG12	1:E:187:ILE:HG12	1.92	0.50
1:A:292:VAL:HG13	1:A:320:GLN:HA	1.93	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:280:GLN:O	1:D:281:ASP:C	2.49	0.50
1:D:71:LYS:NZ	1:D:208:LEU:O	2.44	0.50
1:F:104:LYS:NZ	1:F:201:THR:O	2.45	0.49
1:B:78:ASP:OD1	1:B:78:ASP:N	2.30	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:61:MET:HE2	1:C:66:TRP:CD1	2.48	0.48
1:C:24:ASN:OD1	1:C:26:THR:HB	2.13	0.48
1:E:79:LYS:HZ2	1:E:79:LYS:HB3	1.71	0.47
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: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:172:LYS:NZ	2:C:384:HOH:O	2.47	0.47
1:D:225:ASP:HB3	1:D:252:SER:HB3	1.97	0.47
1:C:58:SER:OG	1:C:90:GLU:HB2	2.14	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
1:F:73:ILE:HD11	1:F:85:ILE:HD11	1.96	0.47
1:E:224:SER:HB2	1:F:236:TYR:OH	2.14	0.47
1:B:298:ASN:HB2	1:B:299:PRO:CD	2.45	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:13:ILE:O	1:B:125:GLY:HA3	2.14	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:E:35:LEU:HD23	1:E:129:LEU:HD11	1.96	0.46
1:D:270:SER:OG	1:D:271:SER:N	2.48	0.46
1:F:35:LEU:HD12	1:F:35:LEU:HA	1.41	0.46
1:A:142:ALA:O	1:A:143:ASN:HB2	2.15	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: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:E:40:PRO:HD2	1:E:41:GLN:OE1	2.15	0.46
1:B:224:SER:HB2	1:D:236:TYR:OH	2.16	0.46
1:E:36:VAL:O	1:E:36:VAL:HG22	2.15	0.46
1:E:90:GLU:HB3	1:F:244:VAL:HB	1.98	0.46
1:C:6:ILE:HA	1:C:84:VAL:O	2.16	0.46
1:F:117:PRO:C	1:F:119:THR:H	2.19	0.46
1:E:62:ASN:OD1	1:E:64:ASN:N	2.49	0.46
1:A:112:VAL:HG23	1:A:149:VAL:O	2.16	0.46
1:E:3:ASN:O	1:E:81:ASP:HB2	2.16	0.46
1:A:183[A]:HIS:CD2	1:D:279:THR:HG21	2.51	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:F:239:ILE:HD12	1:F:265:THR:HG21	1.98	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: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:D:37:ASN:O	1:D:40:PRO:HD3	2.16	0.45
1:C:116:ARG:NH1	2:C:394:HOH:O	2.29	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
1:A:227:PRO:HB3	1:C:227:PRO:HB3	1.99	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:B:62:ASN:OD1	1:B:64:ASN:HB2	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:257:LEU:HD12	1:F:257:LEU:HA	1.71	0.44
1:E:308:LEU:HD12	1:E:308:LEU:HA	1.84	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: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:A:226:LEU:HB2	1:A:227:PRO:HD3	1.99	0.44
1:E:79:LYS:O	1:E:80:THR:HB	2.17	0.44
1:D:318:GLN:HA	1:D:321:GLN:CG	2.47	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:F:198:THR:O	1:F:200:ASP:N	2.50	0.43
1:D:101:LEU:HD12	1:D:101:LEU:HA	1.77	0.43
1:C:61:MET:HE1	1:C:65:VAL:CB	2.47	0.43
1:B:272:ARG:HD2	2:D:329:HOH:O	2.18	0.43
1:F:1:LEU:HB3	1:F:46:ALA:HA	1.99	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:308:LEU:HA	1:A:308:LEU:HD12	1.67	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:F:39:VAL:O	1:F:42:LEU:HB2	2.19	0.43
1:C:56:ILE:N	1:C:56:ILE:HD13	2.34	0.43
1:C:315:ASP:OD2	1:C:317:GLN:HG3	2.18	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:HB2	1:B:314:LYS:HE3	1.73	0.42
1:B:314:LYS:NZ	1:F:24:ASN:ND2	2.65	0.42
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:226:LEU:N	1:A:227:PRO:CD	2.83	0.41
1:C:56:ILE:H	1:C:56:ILE:HD13	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:220:TYR:CD1	1:F:216:ILE:HD12	2.55	0.41
1:E:1:LEU:HA	1:E:1:LEU:HD23	1.67	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:N	1:A:76:ASP:OD1	2.53	0.41
1:C:128:ASN:HD22	1:C:128:ASN:HA	1.65	0.41
1:D:315:ASP:O	1:D:318:GLN:N	2.49	0.41
1:B:220:TYR:N	1:B:220:TYR:CD1	2.89	0.41
1:D:1:LEU:HA	1:D:2:PRO:HD3	1.85	0.41
1:E:198:THR:O	1:E:200:ASP:N	2.54	0.41
1:D:80:THR:OG1	1:D:81:ASP:N	2.54	0.41
1:D:309:ALA:HB1	1:D:322:ILE:HD12	2.03	0.41
1:A:53:VAL:O	1:A:54:VAL:CG1	2.69	0.41
1:A:1:LEU:HB3	1:A:46:ALA:HA	2.03	0.41
1:A:193:PRO:HA	1:D:191:ARG:NH1	2.35	0.41
1:A:226:LEU:HA	1:A:226:LEU:HD12	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: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:7:LEU:O	1:A:85:ILE:HA	2.20	0.40
1:A:243:GLY:O	1:A:272:ARG:HG2	2.20	0.40
1:D:250:TYR:O	1:D:251:LYS:C	2.59	0.40
1:C:76:ASP:O	1:C:77:CYS:C	2.59	0.40
1:A:59:GLN:N	1:A:59:GLN:OE1	2.43	0.40
1:A:2:PRO:HG2	1:A:137:ALA:HB1	2.04	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

5.3.1 Protein backbone ⓘ

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%)	50	60
1	B	302/326 (93%)	290 (96%)	12 (4%)	0	100	100
1	C	325/326 (100%)	318 (98%)	6 (2%)	1 (0%)	50	60
1	D	304/326 (93%)	290 (95%)	12 (4%)	2 (1%)	30	34
1	E	305/326 (94%)	289 (95%)	14 (5%)	2 (1%)	30	34
1	F	315/326 (97%)	302 (96%)	10 (3%)	3 (1%)	22	23
All	All	1857/1956 (95%)	1777 (96%)	71 (4%)	9 (0%)	38	45

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 ⓘ

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%)	15	17
1	B	251/266 (94%)	228 (91%)	23 (9%)	13	15

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	267/266 (100%)	253 (95%)	14 (5%)	32	42
1	D	253/266 (95%)	226 (89%)	27 (11%)	10	10
1	E	254/266 (96%)	229 (90%)	25 (10%)	12	13
1	F	263/266 (99%)	239 (91%)	24 (9%)	14	15
All	All	1542/1596 (97%)	1407 (91%)	135 (9%)	14	16

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
1	B	119	THR
1	B	120	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
1	D	179	LEU
1	D	184	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
1	F	36	VAL
1	F	42	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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

Some 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
1	D	312	GLN
1	E	64	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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 ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.02	17 (5%)	24 33	22, 43, 69, 86	0
1	B	304/326 (93%)	-0.12	10 (3%)	44 54	24, 43, 59, 67	0
1	C	326/326 (100%)	-0.35	6 (1%)	65 74	21, 33, 52, 74	0
1	D	307/326 (94%)	0.13	23 (7%)	14 21	25, 46, 63, 73	0
1	E	307/326 (94%)	-0.07	15 (4%)	28 39	17, 34, 57, 71	0
1	F	320/326 (98%)	-0.26	11 (3%)	43 53	15, 29, 59, 75	0
All	All	1873/1956 (95%)	-0.11	82 (4%)	33 43	15, 38, 61, 86	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	19	SER	6.0
1	A	16	GLY	5.7
1	A	37	ASN	5.2
1	F	47	ASN	5.1
1	F	17	GLY	4.5
1	C	18	ASP	4.5
1	F	34	ASN	4.3
1	E	77	CYS	4.3
1	D	37	ASN	4.1
1	D	11	GLY	4.0
1	B	12	THR	3.9
1	F	16	GLY	3.8
1	F	18	ASP	3.8
1	B	317	GLN	3.8
1	D	207	LYS	3.7
1	B	106	ASP	3.6
1	E	37	ASN	3.6
1	A	106	ASP	3.3
1	A	34	ASN	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	281	ASP	3.3
1	D	209	ASN	3.2
1	A	3	ASN	3.1
1	F	21	THR	3.1
1	F	37	ASN	3.1
1	D	15	GLY	3.1
1	F	29	LYS	3.0
1	E	281	ASP	3.0
1	B	321	GLN	3.0
1	E	46	ALA	2.9
1	D	321	GLN	2.9
1	E	1	LEU	2.9
1	E	106	ASP	2.9
1	D	77	CYS	2.9
1	F	281	ASP	2.9
1	A	50	GLY	2.8
1	B	281	ASP	2.8
1	D	106	ASP	2.8
1	A	281	ASP	2.8
1	A	209	ASN	2.8
1	B	233	ASP	2.8
1	D	3	ASN	2.8
1	E	36	VAL	2.8
1	B	15	GLY	2.7
1	D	202	PRO	2.6
1	B	38	ALA	2.6
1	A	47	ASN	2.5
1	A	46	ALA	2.5
1	E	80	THR	2.5
1	D	318	GLN	2.4
1	C	17	GLY	2.4
1	E	50	GLY	2.4
1	F	207	LYS	2.4
1	C	11	GLY	2.3
1	E	3	ASN	2.3
1	A	15	GLY	2.3
1	A	207	LYS	2.3
1	A	36	VAL	2.3
1	B	3	ASN	2.3
1	D	199	SER	2.3
1	A	64	ASN	2.3
1	D	325	GLN	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	139	LYS	2.2
1	A	77	CYS	2.2
1	C	317	GLN	2.2
1	F	119	THR	2.2
1	A	42	LEU	2.2
1	D	36	VAL	2.2
1	D	317	GLN	2.1
1	E	317	GLN	2.1
1	D	264	GLY	2.1
1	D	233	ASP	2.1
1	D	8	ALA	2.1
1	D	47	ASN	2.1
1	E	43	LYS	2.1
1	E	78	ASP	2.1
1	A	78	ASP	2.1
1	C	184	ASN	2.1
1	D	64	ASN	2.1
1	E	39	VAL	2.0
1	E	143	ASN	2.0
1	B	14	ALA	2.0
1	D	78	ASP	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.