



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 07:58 pm GMT

PDB ID : 5FIQ
Title : Exonuclease domain-containing 1 (Exd1) in the native conformation
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Deposited on : 2015-10-01
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

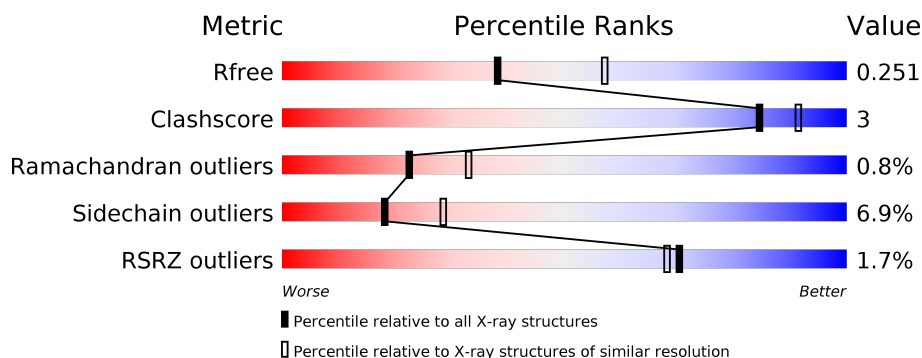
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	3166 (2.40-2.40)
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	243	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>13%</div> <div>•</div> </div> </div>
1	C	243	<div> <div>%</div> <div> <div></div> <div>85%</div> <div>12%</div> <div>••</div> </div> </div>
1	E	243	<div> <div>%</div> <div> <div></div> <div>84%</div> <div>12%</div> <div>••</div> </div> </div>
1	G	243	<div> <div>%</div> <div> <div></div> <div>84%</div> <div>14%</div> <div>••</div> </div> </div>
1	I	243	<div> <div>3%</div> <div> <div></div> <div>85%</div> <div>12%</div> <div>••</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9738 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 EXD1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	242	Total	C	N	O	S	0	0	0
			1950	1242	332	366	10			
1	C	240	Total	C	N	O	S	0	0	0
			1933	1230	329	364	10			
1	E	240	Total	C	N	O	S	0	0	0
			1933	1230	329	364	10			
1	G	240	Total	C	N	O	S	0	0	0
			1936	1233	329	364	10			
1	I	240	Total	C	N	O	S	0	0	0
			1933	1230	329	364	10			

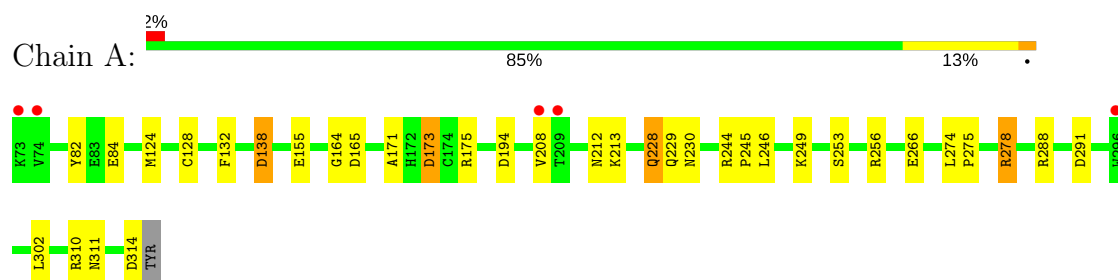
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	21	Total	O	0	0
			21	21		
2	C	13	Total	O	0	0
			13	13		
2	E	12	Total	O	0	0
			12	12		
2	G	6	Total	O	0	0
			6	6		
2	I	1	Total	O	0	0
			1	1		

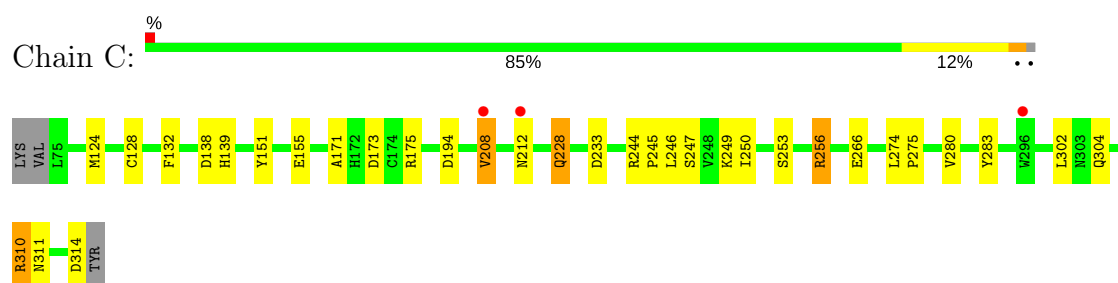
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

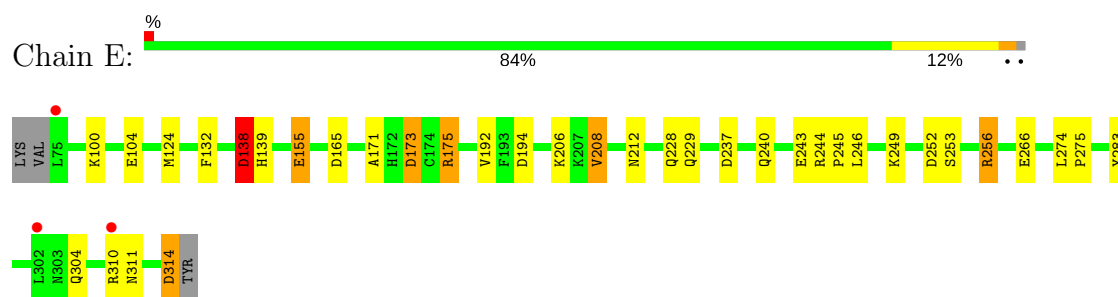
• Molecule 1: EXD1



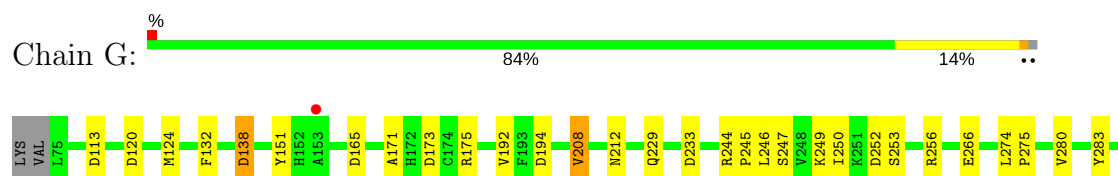
• Molecule 1: EXD1

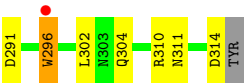


• Molecule 1: EXD1

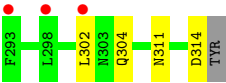
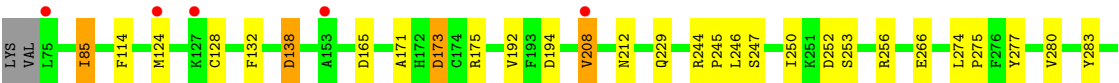
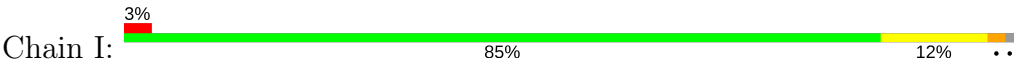


• Molecule 1: EXD1





● Molecule 1: EXD1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	122.54Å 81.58Å 154.75Å 90.00° 111.10° 90.00°	Depositor
Resolution (Å)	50.01 – 2.40 48.12 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.1 (50.01-2.40) 96.1 (48.12-2.40)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, R_{free}	0.221 , 0.247 0.224 , 0.251	Depositor DCC
R_{free} test set	2596 reflections (5.08%)	DCC
Wilson B-factor (Å ²)	41.8	Xtriage
Anisotropy	1.160	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 26.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.013 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9738	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.21% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.13	3/1984 (0.2%)	1.08	6/2669 (0.2%)
1	C	1.02	0/1967	1.02	3/2647 (0.1%)
1	E	1.04	2/1967 (0.1%)	1.03	8/2647 (0.3%)
1	G	0.94	1/1970 (0.1%)	1.04	7/2651 (0.3%)
1	I	0.98	3/1967 (0.2%)	1.03	6/2647 (0.2%)
All	All	1.02	9/9855 (0.1%)	1.04	30/13261 (0.2%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	82	TYR	CZ-OH	7.58	1.50	1.37
1	A	84	GLU	CG-CD	6.90	1.62	1.51
1	I	277	TYR	CG-CD2	6.71	1.47	1.39
1	E	155	GLU	CD-OE2	6.35	1.32	1.25
1	A	138	ASP	CB-CG	-6.05	1.39	1.51
1	G	138	ASP	CB-CG	-5.99	1.39	1.51
1	E	138	ASP	CB-CG	-5.85	1.39	1.51
1	I	277	TYR	CE1-CZ	5.77	1.46	1.38
1	I	114	PHE	CB-CG	-5.12	1.42	1.51

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	124	MET	CG-SD-CE	7.27	111.83	100.20
1	I	85	ILE	CA-CB-CG1	7.05	124.39	111.00
1	G	165	ASP	CB-CG-OD1	-6.98	112.02	118.30
1	A	288	ARG	NE-CZ-NH2	-6.43	117.08	120.30
1	A	84	GLU	OE1-CD-OE2	-6.38	115.65	123.30
1	I	252	ASP	CB-CG-OD1	6.10	123.79	118.30
1	G	252	ASP	CB-CG-OD1	5.91	123.62	118.30
1	G	233	ASP	CB-CG-OD2	-5.87	113.01	118.30
1	E	256	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	G	124	MET	CG-SD-CE	5.84	109.54	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	278	ARG	CB-CG-CD	5.81	126.72	111.60
1	I	138	ASP	CB-CG-OD1	-5.81	113.07	118.30
1	E	124	MET	CG-SD-CE	5.74	109.38	100.20
1	C	256	ARG	NE-CZ-NH1	5.71	123.15	120.30
1	E	252	ASP	CB-CG-OD1	5.68	123.41	118.30
1	A	291	ASP	CB-CG-OD1	5.62	123.36	118.30
1	A	138	ASP	N-CA-CB	-5.60	100.52	110.60
1	I	165	ASP	CB-CG-OD1	-5.57	113.29	118.30
1	E	138	ASP	N-CA-CB	-5.43	100.82	110.60
1	G	291	ASP	CB-CG-OD1	5.37	123.13	118.30
1	I	85	ILE	CG1-CB-CG2	-5.30	99.75	111.40
1	I	138	ASP	N-CA-CB	-5.23	101.19	110.60
1	A	165	ASP	CB-CG-OD1	-5.21	113.61	118.30
1	E	138	ASP	CB-CG-OD1	-5.15	113.67	118.30
1	E	237	ASP	CB-CG-OD1	5.11	122.89	118.30
1	E	175	ARG	CG-CD-NE	5.10	122.52	111.80
1	E	165	ASP	CB-CG-OD1	-5.08	113.72	118.30
1	G	113	ASP	CB-CG-OD1	5.06	122.86	118.30
1	G	120	ASP	CB-CG-OD2	5.04	122.83	118.30
1	C	233	ASP	CB-CG-OD2	-5.02	113.78	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1950	0	1966	8	0
1	C	1933	0	1942	16	0
1	E	1933	0	1942	16	0
1	G	1936	0	1951	17	0
1	I	1933	0	1942	14	0
2	A	21	0	0	0	0
2	C	13	0	0	0	0
2	E	12	0	0	1	0
2	G	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	1	0	0	0	0
All	All	9738	0	9743	52	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 3.

All (52) 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:G:296:TRP:O	1:G:296:TRP:HE3	1.57	0.88
1:G:296:TRP:O	1:G:296:TRP:CE3	2.41	0.72
1:C:208:VAL:HG22	1:E:208:VAL:HG22	1.79	0.65
1:A:274:LEU:HD13	1:A:278:ARG:NH1	2.13	0.63
1:G:175:ARG:NH2	1:I:304:GLN:O	2.31	0.62
1:A:228:GLN:NE2	1:A:230:ASN:H	2.02	0.58
1:G:296:TRP:CE3	1:G:296:TRP:C	2.77	0.58
1:C:304:GLN:O	1:E:175:ARG:NH2	2.40	0.55
1:G:283:TYR:CE2	1:I:175:ARG:HD2	2.43	0.54
1:G:175:ARG:HD2	1:I:283:TYR:CE2	2.42	0.54
1:E:314:ASP:C	2:E:2012:HOH:O	2.47	0.53
1:C:138:ASP:OD1	1:C:139:HIS:CD2	2.64	0.51
1:G:304:GLN:O	1:I:175:ARG:NH2	2.44	0.51
1:C:175:ARG:HD2	1:E:283:TYR:CE2	2.47	0.49
1:G:283:TYR:CD2	1:I:175:ARG:HD2	2.48	0.47
1:E:100:LYS:HE3	1:E:104:GLU:OE2	2.14	0.47
1:C:175:ARG:NH2	1:E:304:GLN:O	2.48	0.47
1:I:171:ALA:O	1:I:194:ASP:HA	2.15	0.47
1:A:244:ARG:HA	1:A:245:PRO:C	2.36	0.47
1:C:175:ARG:HD2	1:E:283:TYR:CD2	2.50	0.46
1:C:283:TYR:CE2	1:E:175:ARG:HD2	2.51	0.46
1:I:173:ASP:OD1	1:I:175:ARG:HD3	2.16	0.46
1:E:244:ARG:HA	1:E:245:PRO:C	2.36	0.46
1:E:138:ASP:HB3	1:E:139:HIS:ND1	2.31	0.46
1:G:244:ARG:HA	1:G:245:PRO:C	2.37	0.45
1:E:171:ALA:O	1:E:194:ASP:HA	2.17	0.45
1:E:240:GLN:NE2	1:E:243:GLU:OE1	2.50	0.45
1:E:274:LEU:N	1:E:275:PRO:CD	2.80	0.45
1:I:244:ARG:HA	1:I:245:PRO:C	2.37	0.45
1:C:244:ARG:HA	1:C:245:PRO:C	2.38	0.45
1:C:274:LEU:N	1:C:275:PRO:CD	2.80	0.44
1:G:171:ALA:O	1:G:194:ASP:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:208:VAL:HG22	1:I:208:VAL:HG22	2.00	0.44
1:A:171:ALA:O	1:A:194:ASP:HA	2.18	0.44
1:A:173:ASP:OD1	1:A:175:ARG:HD3	2.18	0.43
1:C:171:ALA:O	1:C:194:ASP:HA	2.18	0.43
1:C:247:SER:OG	1:C:250:ILE:HG12	2.20	0.42
1:G:175:ARG:HD2	1:I:283:TYR:CD2	2.54	0.42
1:I:274:LEU:N	1:I:275:PRO:CD	2.82	0.42
1:G:280:VAL:HG11	1:I:192:VAL:O	2.19	0.42
1:C:151:TYR:CE2	1:C:155:GLU:HG3	2.55	0.42
1:C:283:TYR:CD2	1:E:175:ARG:HD2	2.55	0.42
1:C:310:ARG:HD3	1:G:151:TYR:CE1	2.55	0.42
1:G:192:VAL:O	1:I:280:VAL:HG11	2.20	0.42
1:C:280:VAL:HG11	1:E:192:VAL:O	2.20	0.42
1:A:228:GLN:HE22	1:A:230:ASN:H	1.68	0.41
1:A:164:GLY:HA2	1:C:228:GLN:HG2	2.02	0.41
1:E:173:ASP:OD1	1:E:175:ARG:HD3	2.20	0.41
1:I:247:SER:OG	1:I:250:ILE:HG12	2.21	0.41
1:G:274:LEU:N	1:G:275:PRO:CD	2.84	0.40
1:A:274:LEU:N	1:A:275:PRO:CD	2.84	0.40
1:G:247:SER:OG	1:G:250:ILE:HG12	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	240/243 (99%)	226 (94%)	12 (5%)	2 (1%)	22	33
1	C	238/243 (98%)	225 (94%)	12 (5%)	1 (0%)	38	54
1	E	238/243 (98%)	225 (94%)	11 (5%)	2 (1%)	22	33
1	G	238/243 (98%)	224 (94%)	12 (5%)	2 (1%)	22	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	238/243 (98%)	223 (94%)	13 (6%)	2 (1%)	22	33
All	All	1192/1215 (98%)	1123 (94%)	60 (5%)	9 (1%)	22	33

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	173	ASP
1	I	229	GLN
1	A	173	ASP
1	A	229	GLN
1	C	173	ASP
1	E	173	ASP
1	E	229	GLN
1	G	173	ASP
1	G	229	GLN

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	220/224 (98%)	202 (92%)	18 (8%)	13	20
1	C	218/224 (97%)	204 (94%)	14 (6%)	20	32
1	E	218/224 (97%)	203 (93%)	15 (7%)	18	28
1	G	219/224 (98%)	205 (94%)	14 (6%)	20	32
1	I	218/224 (97%)	204 (94%)	14 (6%)	20	32
All	All	1093/1120 (98%)	1018 (93%)	75 (7%)	18	28

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	124	MET
1	A	128	CYS
1	A	132	PHE

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Mol	Chain	Res	Type
1	A	138	ASP
1	A	155	GLU
1	A	208	VAL
1	A	212	ASN
1	A	213	LYS
1	A	228	GLN
1	A	246	LEU
1	A	249	LYS
1	A	253	SER
1	A	256	ARG
1	A	266	GLU
1	A	302	LEU
1	A	310	ARG
1	A	311	ASN
1	A	314	ASP
1	C	128	CYS
1	C	132	PHE
1	C	208	VAL
1	C	212	ASN
1	C	228	GLN
1	C	246	LEU
1	C	249	LYS
1	C	253	SER
1	C	256	ARG
1	C	266	GLU
1	C	302	LEU
1	C	310	ARG
1	C	311	ASN
1	C	314	ASP
1	E	132	PHE
1	E	138	ASP
1	E	155	GLU
1	E	206	LYS
1	E	208	VAL
1	E	212	ASN
1	E	228	GLN
1	E	246	LEU
1	E	249	LYS
1	E	253	SER
1	E	256	ARG
1	E	266	GLU
1	E	310	ARG

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Mol	Chain	Res	Type
1	E	311	ASN
1	E	314	ASP
1	G	132	PHE
1	G	138	ASP
1	G	208	VAL
1	G	212	ASN
1	G	246	LEU
1	G	249	LYS
1	G	253	SER
1	G	256	ARG
1	G	266	GLU
1	G	296	TRP
1	G	302	LEU
1	G	310	ARG
1	G	311	ASN
1	G	314	ASP
1	I	85	ILE
1	I	124	MET
1	I	128	CYS
1	I	132	PHE
1	I	138	ASP
1	I	208	VAL
1	I	212	ASN
1	I	246	LEU
1	I	253	SER
1	I	256	ARG
1	I	266	GLU
1	I	302	LEU
1	I	311	ASN
1	I	314	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	GLN
1	A	110	ASN
1	A	228	GLN
1	A	230	ASN
1	C	97	GLN
1	C	139	HIS
1	E	97	GLN
1	E	183	HIS

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Mol	Chain	Res	Type
1	E	240	GLN
1	G	97	GLN
1	G	110	ASN
1	G	183	HIS
1	G	262	HIS
1	I	97	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	242/243 (99%)	-0.13	5 (2%) 64 61	33, 47, 83, 107	0
1	C	240/243 (98%)	-0.12	3 (1%) 77 75	36, 53, 91, 115	0
1	E	240/243 (98%)	-0.08	3 (1%) 77 75	40, 57, 90, 115	0
1	G	240/243 (98%)	-0.10	2 (0%) 86 84	40, 61, 99, 120	0
1	I	240/243 (98%)	0.10	8 (3%) 47 45	41, 66, 103, 121	0
All	All	1202/1215 (98%)	-0.07	21 (1%) 70 68	33, 56, 96, 121	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	296	TRP	6.0
1	A	208	VAL	3.6
1	A	209	THR	3.5
1	I	75	LEU	3.5
1	C	208	VAL	3.4
1	I	302	LEU	3.3
1	G	296	TRP	3.2
1	A	73	LYS	3.2
1	I	293	PHE	3.1
1	E	302	LEU	2.9
1	I	208	VAL	2.8
1	G	153	ALA	2.7
1	C	212	ASN	2.3
1	I	124	MET	2.3
1	E	310	ARG	2.2
1	A	296	TRP	2.2
1	I	298	LEU	2.2
1	A	74	VAL	2.1
1	I	153	ALA	2.1
1	E	75	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	127	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.