Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:44 PM GMT

PDB ID	:	4MKR
Title	:	Structure of the apo form of a Zingiber officinale double bond reductase
Authors	:	Buratto, J.; Langlois d'Estaintot, B.; Granier, T.; Gallois, B.; Willis, M.A.; Sang, Y.; Flores-Sanchez, I.J.; Gang, D.R.
Deposited on	:	2013-09-05
Resolution	:	2.58 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.58 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.
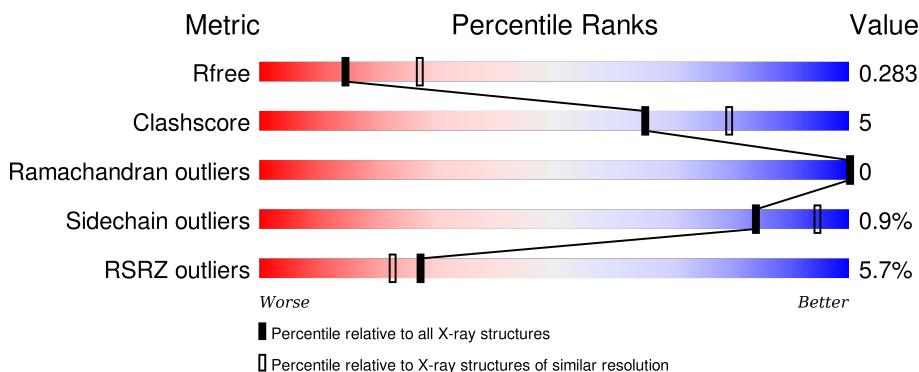
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2636 (2.60-2.56)
Clashscore	102246	3003 (2.60-2.56)
Ramachandran outliers	100387	2956 (2.60-2.56)
Sidechain outliers	100360	2956 (2.60-2.56)
RSRZ outliers	91569	2642 (2.60-2.56)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	358	
1	B	358	
1	C	358	
1	D	358	
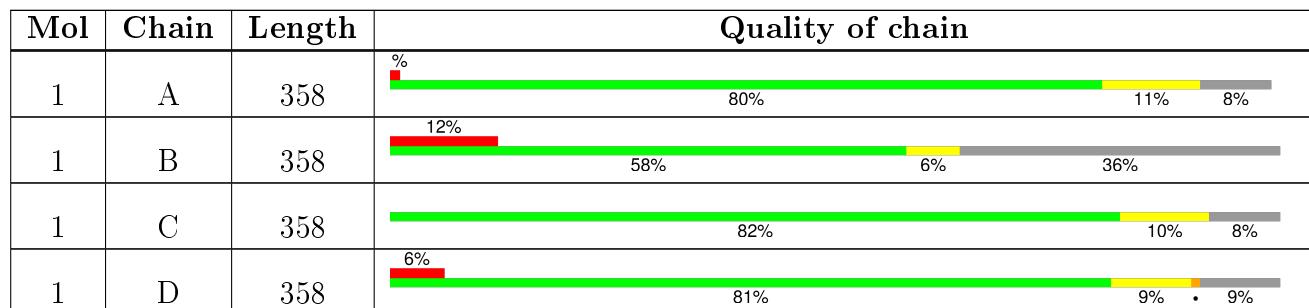
2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9244 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 Zingiber officinale double bond reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	328	Total 2518	C 1643	N 406	O 457	S 12	0	0	0
1	B	228	Total 1644	C 1069	N 271	O 297	S 7	0	0	0
1	C	330	Total 2521	C 1644	N 409	O 456	S 12	0	1	0
1	D	327	Total 2442	C 1591	N 396	O 444	S 11	0	0	0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	44	Total 44	O 44	0	0
2	B	12	Total 12	O 12	0	0
2	C	43	Total 43	O 43	0	0
2	D	20	Total 20	O 20	0	0

3 Residue-property plots ⓘ

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

• Molecule 1: Zingiber officinale double bond reductase
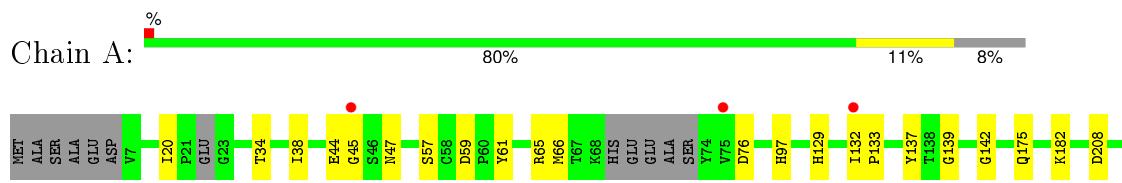
• Molecule 1: Zingiber officinale double bond reductase

• Molecule 1: Zingiber officinale double bond reductase

• Molecule 1: Zingiber officinale double bond reductase

Chain D:
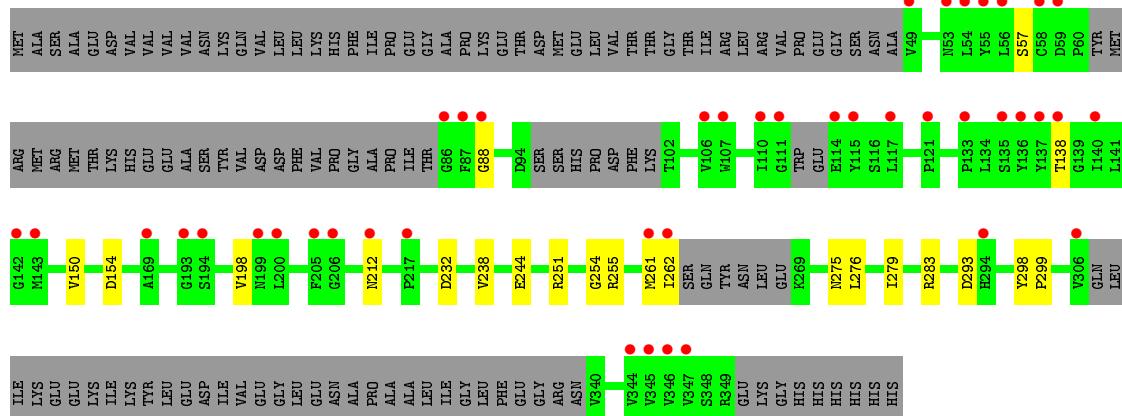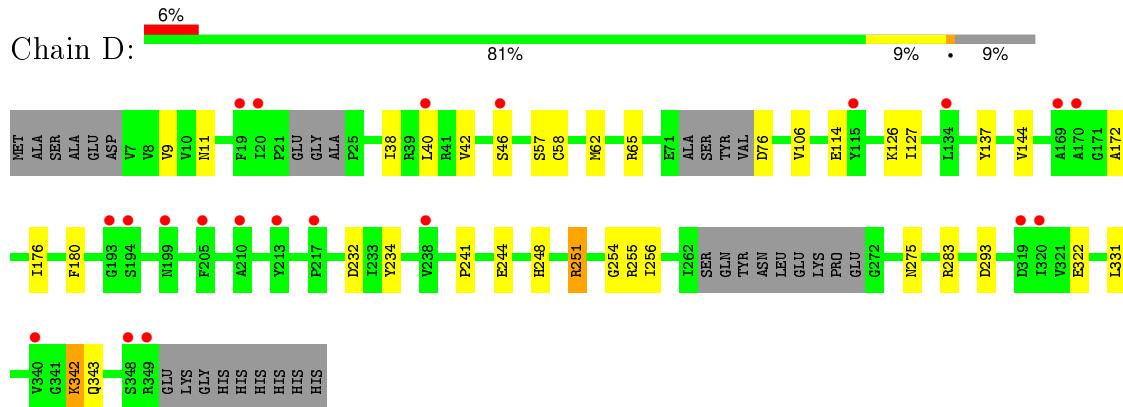
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	50.93Å 76.34Å 93.45Å 80.15° 89.97° 85.66°	Depositor
Resolution (Å)	46.03 – 2.58 46.03 – 2.58	Depositor EDS
% Data completeness (in resolution range)	97.6 (46.03-2.58) 92.5 (46.03-2.58)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.10 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.228 , 0.282 0.230 , 0.283	Depositor DCC
R_{free} test set	2130 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	45.6	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 45.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|> = 0.49$, $<L^2> = 0.32$	Xtriage
Outliers	0 of 42572 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	9244	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.04% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

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	0.80	0/2575	0.87	3/3483 (0.1%)
1	B	0.63	0/1680	0.81	0/2278
1	C	0.78	0/2583	0.88	1/3500 (0.0%)
1	D	0.66	0/2498	0.78	1/3393 (0.0%)
All	All	0.73	0/9336	0.84	5/12654 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	45	GLY	N-CA-C	5.65	127.22	113.10
1	A	255	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	D	251	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	A	65	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	C	63	ARG	NE-CZ-NH1	-5.09	117.76	120.30

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	2518	0	2491	26	0
1	B	1644	0	1480	15	0
1	C	2521	0	2478	27	0
1	D	2442	0	2322	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	44	0	0	1	0
2	B	12	0	0	0	0
2	C	43	0	0	1	0
2	D	20	0	0	4	0
All	All	9244	0	8771	89	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 5.

All (89) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:GLU:CB	1:A:275:ASN:HD22	2.15	0.59
1:D:65:ARG:NH1	1:D:76:ASP:O	2.35	0.59
1:A:132:ILE:HG22	1:A:133:PRO:HD2	1.84	0.58
1:D:144:VAL:HG23	2:D:407:HOH:O	2.05	0.57
1:B:254:GLY:C	1:B:255:ARG:HG3	2.25	0.56
1:B:244:GLU:O	1:B:275:ASN:ND2	2.37	0.56
1:A:254:GLY:C	1:A:255:ARG:HG3	2.25	0.56
1:C:62:MET:CE	1:C:331:LEU:HD13	2.36	0.55
1:A:244:GLU:HB3	1:A:275:ASN:HD22	1.71	0.55
1:A:139:GLY:O	1:A:142:GLY:N	2.31	0.55
1:D:62:MET:CE	1:D:331:LEU:HD13	2.37	0.55
1:C:63:ARG:NH1	1:C:67:THR:OG1	2.40	0.54
1:D:42:VAL:CG1	1:D:46:SER:OG	2.56	0.54
1:C:254:GLY:C	1:C:255:ARG:HG3	2.27	0.54
1:A:244:GLU:CA	1:A:275:ASN:HD22	2.22	0.53
1:D:241:PRO:HD2	2:D:415:HOH:O	2.07	0.53
1:D:57:SER:OG	1:D:342:LYS:NZ	2.32	0.53
1:D:244:GLU:O	1:D:275:ASN:ND2	2.42	0.52
1:C:244:GLU:HA	1:C:275:ASN:HD22	1.74	0.52
1:C:107:TRP:CZ2	1:C:125:PHE:CD2	2.97	0.52
1:A:276:LEU:HD22	1:A:279:ILE:HD12	1.92	0.51
1:D:62:MET:HE2	1:D:331:LEU:CD1	2.41	0.51
1:C:34:THR:HG22	1:C:34:THR:O	2.11	0.50
1:A:132:ILE:O	1:A:133:PRO:C	2.49	0.50
1:C:232:ASP:OD1	1:C:251:ARG:HD3	2.11	0.50
1:C:57:SER:OG	1:C:59:ASP:OD1	2.31	0.49
1:D:244:GLU:CA	1:D:275:ASN:HD22	2.25	0.49
1:C:139:GLY:O	1:C:144:VAL:HB	2.12	0.49
1:C:293:ASP:OD2	1:D:283:ARG:HD3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:SER:OG	1:A:59:ASP:OD1	2.30	0.49
1:C:59:ASP:OD1	1:C:342:LYS:NZ	2.45	0.49
1:C:57:SER:HB2	1:C:138:THR:HB	1.95	0.48
1:B:244:GLU:CA	1:B:275:ASN:HD22	2.27	0.48
1:C:276:LEU:O	1:C:279:ILE:HB	2.14	0.48
1:D:244:GLU:HA	1:D:275:ASN:HD22	1.78	0.48
1:D:62:MET:HE2	1:D:331:LEU:HD13	1.95	0.47
1:D:254:GLY:C	1:D:255:ARG:HG3	2.33	0.47
1:A:283:ARG:HD3	1:B:293:ASP:OD2	2.13	0.47
1:C:283:ARG:HD3	1:D:293:ASP:OD2	2.13	0.47
1:A:293:ASP:OD2	1:B:283:ARG:HD3	2.14	0.47
1:D:127:ILE:HG23	1:D:137:TYR:CZ	2.50	0.47
1:D:11:ASN:HB2	1:D:38:ILE:HG13	1.95	0.47
1:D:172:ALA:HB2	1:D:342:LYS:HB2	1.96	0.47
1:A:182:LYS:NZ	1:A:208:ASP:OD2	2.47	0.47
1:B:88:GLY:HA2	1:B:138:THR:HG22	1.95	0.47
1:D:232:ASP:OD1	1:D:251:ARG:HD3	2.15	0.47
1:B:276:LEU:O	1:B:279:ILE:HB	2.15	0.47
1:A:47:ASN:O	1:A:97:HIS:HB2	2.15	0.47
1:A:277:PHE:N	1:B:261:MET:HE1	2.30	0.46
1:A:274:HIS:ND1	1:A:274:HIS:N	2.63	0.46
1:A:276:LEU:O	1:A:279:ILE:HB	2.16	0.46
1:C:65:ARG:NH1	2:C:431:HOH:O	2.34	0.46
1:A:59:ASP:HB2	1:A:61:TYR:CE2	2.51	0.46
1:D:38:ILE:HG22	2:D:413:HOH:O	2.16	0.45
1:D:11:ASN:OD1	1:D:114:GLU:HB2	2.17	0.45
1:C:62:MET:CE	1:C:331:LEU:CD1	2.95	0.45
1:C:241:PRO:HD3	1:C:271:GLU:HB2	1.99	0.45
1:D:58:CYS:HB2	1:D:343:GLN:HG2	1.99	0.45
1:C:244:GLU:O	1:C:275:ASN:ND2	2.49	0.44
1:A:129:HIS:HB2	1:A:137:TYR:OH	2.18	0.44
1:C:9:VAL:HG21	1:C:40:LEU:HD21	2.00	0.44
1:D:248:HIS:CE1	2:D:419:HOH:O	2.71	0.43
1:C:244:GLU:CA	1:C:275:ASN:HD22	2.31	0.43
1:D:106:VAL:HG12	1:D:126:LYS:HA	2.00	0.43
1:A:325:GLU:CD	1:A:325:GLU:H	2.20	0.43
1:A:57:SER:OG	1:A:342:LYS:NZ	2.37	0.43
1:B:198:VAL:HG21	1:B:212:ASN:HB2	2.01	0.43
1:D:9:VAL:HG21	1:D:40:LEU:HD11	2.01	0.43
1:B:298:TYR:O	1:B:299:PRO:C	2.57	0.43
1:A:234:TYR:HB3	1:A:256:ILE:HG12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:336:GLU:OE1	1:C:338:ARG:NH1	2.48	0.42
1:D:234:TYR:HB3	1:D:256:ILE:HG12	2.00	0.42
1:C:327:ALA:N	1:C:328:PRO:CD	2.83	0.42
1:A:34:THR:O	1:A:34:THR:HG22	2.20	0.42
1:C:253:LYS:O	1:C:255:ARG:NH1	2.48	0.42
1:B:57:SER:CB	1:B:138:THR:HB	2.50	0.42
1:B:150:VAL:O	1:B:154:ASP:HB3	2.19	0.42
1:A:313:LYS:NZ	2:A:441:HOH:O	2.53	0.41
1:B:232:ASP:OD1	1:B:251:ARG:HD3	2.20	0.41
1:D:176:ILE:HG22	1:D:180:PHE:CE2	2.55	0.41
1:B:244:GLU:HA	1:B:275:ASN:HD22	1.84	0.41
1:A:20:ILE:HD11	1:A:66:MET:HE2	2.02	0.41
1:C:78:PHE:CZ	1:C:84:ILE:HG23	2.55	0.41
1:C:107:TRP:CH2	1:C:125:PHE:CE2	3.08	0.41
1:C:112:TRP:CZ3	1:C:327:ALA:HB1	2.56	0.41
1:C:283:ARG:CD	1:D:293:ASP:OD2	2.68	0.41
1:A:232:ASP:OD1	1:A:251:ARG:HD3	2.21	0.41
1:B:238:VAL:O	1:B:262:ILE:N	2.53	0.41
1:A:175:GLN:HE22	1:A:341:GLY:HA2	1.87	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	320/358 (89%)	310 (97%)	10 (3%)	0	100	100
1	B	216/358 (60%)	206 (95%)	10 (5%)	0	100	100
1	C	325/358 (91%)	315 (97%)	10 (3%)	0	100	100
1	D	319/358 (89%)	312 (98%)	7 (2%)	0	100	100
All	All	1180/1432 (82%)	1143 (97%)	37 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	261/300 (87%)	257 (98%)	4 (2%)	72	89
1	B	145/300 (48%)	145 (100%)	0	100	100
1	C	259/300 (86%)	257 (99%)	2 (1%)	86	95
1	D	240/300 (80%)	238 (99%)	2 (1%)	86	95
All	All	905/1200 (75%)	897 (99%)	8 (1%)	84	94

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ILE
1	A	44	GLU
1	A	76	ASP
1	A	348	SER
1	C	49	VAL
1	C	76	ASP
1	D	322	GLU
1	D	342	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	275	ASN
1	B	275	ASN
1	C	275	ASN
1	D	275	ASN

5.3.3 RNA (i)

There are no RNA molecules 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 (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	328/358 (91%)	0.28	4 (1%)	81	78	23, 39, 58, 78	0
1	B	228/358 (63%)	1.02	43 (18%)	2	1	29, 59, 112, 152	0
1	C	330/358 (92%)	0.23	1 (0%)	94	94	22, 37, 56, 79	0
1	D	327/358 (91%)	0.50	21 (6%)	23	18	31, 52, 76, 88	0
All	All	1213/1432 (84%)	0.46	69 (5%)	27	22	22, 45, 81, 152	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	194	SER	6.7
1	B	193	GLY	6.3
1	B	111	GLY	4.7
1	B	115	TYR	4.7
1	B	169	ALA	4.5
1	B	344	VAL	4.3
1	D	170	ALA	4.3
1	B	135	SER	4.1
1	D	348	SER	4.0
1	B	306	VAL	4.0
1	B	107	TRP	3.8
1	B	54	LEU	3.8
1	D	169	ALA	3.8
1	D	19	PHE	3.7
1	B	49	VAL	3.7
1	B	261	MET	3.7
1	D	205	PHE	3.6
1	D	40	LEU	3.6
1	B	138	THR	3.6
1	D	340	VAL	3.6
1	B	200	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	136	TYR	3.6
1	B	143	MET	3.5
1	B	86	GLY	3.3
1	B	53	ASN	3.3
1	B	199	ASN	3.3
1	B	262	ILE	3.2
1	D	194	SER	3.2
1	B	56	LEU	3.1
1	B	59	ASP	3.1
1	C	214	LYS	3.1
1	D	20	ILE	3.0
1	D	213	TYR	2.9
1	B	346	VAL	2.8
1	B	137	TYR	2.8
1	D	217	PRO	2.8
1	D	199	ASN	2.8
1	A	132	ILE	2.7
1	B	55	TYR	2.7
1	B	87	PHE	2.7
1	D	115	TYR	2.7
1	B	110	ILE	2.6
1	B	205	PHE	2.6
1	A	75	VAL	2.6
1	B	142	GLY	2.6
1	B	121	PRO	2.5
1	B	345	VAL	2.4
1	D	238	VAL	2.4
1	A	45	GLY	2.4
1	B	114	GLU	2.4
1	D	320	ILE	2.4
1	B	88	GLY	2.3
1	D	349	ARG	2.3
1	D	319	ASP	2.3
1	B	140	ILE	2.3
1	B	106	VAL	2.3
1	B	294	HIS	2.2
1	B	212	ASN	2.2
1	B	347	VAL	2.2
1	D	46	SER	2.2
1	D	210	ALA	2.2
1	B	217	PRO	2.1
1	B	206	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	252	ILE	2.0
1	D	193	GLY	2.0
1	B	58	CYS	2.0
1	B	133	PRO	2.0
1	B	117	LEU	2.0
1	D	134	LEU	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.