



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:57 PM UTC

PDB ID : 2V8I / pdb_00002v8i
Title : Structure of a Family 2 Pectate Lyase in a Native Form
Authors : Abbott, D.W.; Boraston, A.B.
Deposited on : 2007-08-08
Resolution : 1.50 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

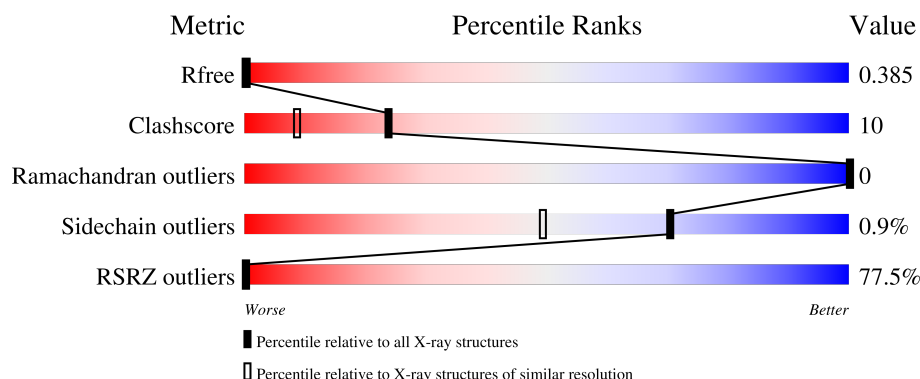
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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}	180053	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

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 $\leq 5\%$. 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	543	78% 90% 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	IOD	A	1547	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	IOD	A	1549	-	-	X	-
2	IOD	A	1552	-	-	X	-
2	IOD	A	1554	-	-	X	-
2	IOD	A	1555	-	-	X	-
2	IOD	A	1560	-	-	X	-
2	IOD	A	1563	-	-	X	-
2	IOD	A	1564	-	-	X	-
2	IOD	A	1567	-	-	X	-
2	IOD	A	1568	-	-	X	-
2	IOD	A	1569	-	-	X	-
2	IOD	A	1572	-	-	X	-
2	IOD	A	1573	-	-	X	-
2	IOD	A	1576	-	-	X	-
2	IOD	A	1588	-	-	X	-
2	IOD	A	1589	-	-	X	-
2	IOD	A	1592	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5172 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 PECTATE LYASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	543	Total	C	N	O	S	0	5	0
			4362	2766	756	827	13			

- Molecule 2 is IODIDE ION (CCD ID: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	51	Total	I	0	0
			51	51		

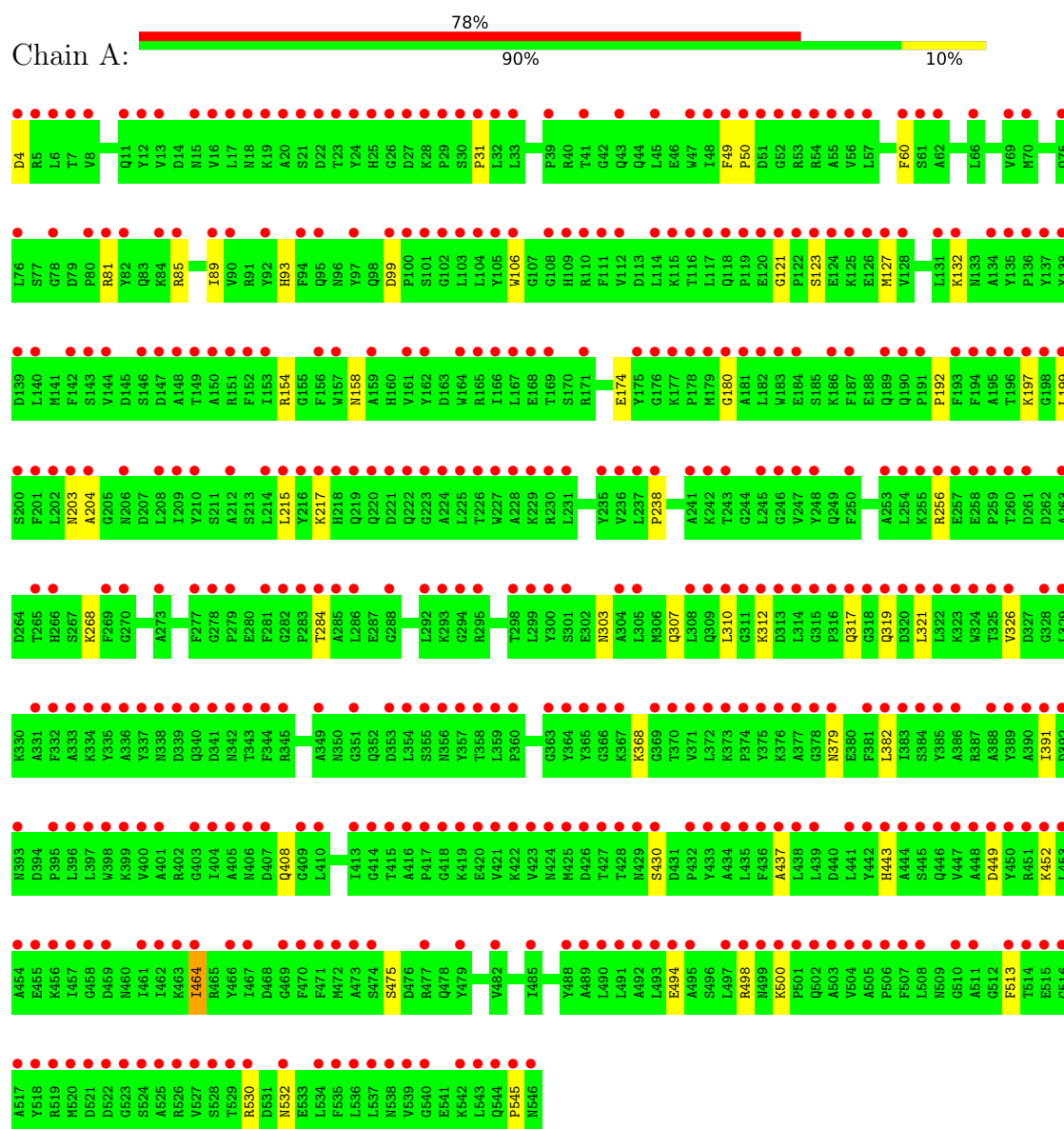
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	759	Total	O	0	0
			759	759		

3 Residue-property plots

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: PECTATE LYASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.49Å 95.64Å 126.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.59 – 1.50 19.59 – 1.50	Depositor EDS
% Data completeness (in resolution range)	97.4 (19.59-1.50) 97.4 (19.59-1.50)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.222 , 0.243 0.381 , 0.385	Depositor DCC
R_{free} test set	5574 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	21.2	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 51.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	5172	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.10% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: IOD

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	0.55	0/4477	0.74	2/6061 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	121	GLY	CA-C-N	6.81	126.44	119.56
1	A	121	GLY	C-N-CA	6.81	126.44	119.56

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	4362	0	4224	57	0
2	A	51	0	0	60	0
3	A	759	0	0	31	0
All	All	5172	0	4224	87	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 (87) 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)
2:A:1555:IOD:I	3:A:2357:HOH:O	2.21	1.25
2:A:1576:IOD:I	3:A:2726:HOH:O	2.28	1.19
2:A:1565:IOD:I	2:A:1591:IOD:I	3.06	1.13
2:A:1588:IOD:I	3:A:2713:HOH:O	2.40	1.06
1:A:199:LEU:HB2	2:A:1555:IOD:I	2.33	0.99
1:A:199:LEU:N	2:A:1555:IOD:I	2.67	0.97
2:A:1549:IOD:I	2:A:1552:IOD:I	3.23	0.97
2:A:1552:IOD:I	3:A:2726:HOH:O	2.52	0.96
2:A:1587:IOD:I	3:A:2537:HOH:O	2.56	0.94
2:A:1558:IOD:I	3:A:2627:HOH:O	2.56	0.92
2:A:1572:IOD:I	3:A:2323:HOH:O	2.56	0.92
2:A:1552:IOD:I	2:A:1576:IOD:I	3.27	0.92
2:A:1563:IOD:I	3:A:2486:HOH:O	2.58	0.91
1:A:312:LYS:HE2	2:A:1563:IOD:I	2.41	0.90
2:A:1572:IOD:I	3:A:2107:HOH:O	2.61	0.88
2:A:1556:IOD:I	3:A:2652:HOH:O	2.61	0.88
1:A:81[B]:ARG:NH2	2:A:1569:IOD:I	2.75	0.88
2:A:1560:IOD:I	3:A:2041:HOH:O	2.61	0.87
2:A:1554:IOD:I	3:A:2290:HOH:O	2.62	0.86
1:A:317:GLN:HA	2:A:1568:IOD:I	2.46	0.85
2:A:1560:IOD:I	3:A:2333:HOH:O	2.62	0.85
1:A:49:PHE:HB3	1:A:50:PRO:HD2	1.59	0.84
2:A:1593:IOD:I	3:A:2556:HOH:O	2.65	0.84
1:A:197:LYS:HB2	1:A:256:ARG:HH22	1.45	0.81
2:A:1592:IOD:I	3:A:2494:HOH:O	2.68	0.81
2:A:1557:IOD:I	3:A:2519:HOH:O	2.69	0.80
1:A:199:LEU:CB	2:A:1555:IOD:I	3.01	0.79
2:A:1554:IOD:I	3:A:2315:HOH:O	2.72	0.78
2:A:1570:IOD:I	3:A:2247:HOH:O	2.74	0.75
2:A:1567:IOD:I	3:A:2742:HOH:O	2.73	0.75
1:A:4:ASP:N	2:A:1561:IOD:I	2.91	0.74
1:A:317:GLN:C	2:A:1568:IOD:I	3.02	0.73
1:A:326:VAL:HG21	1:A:391:ILE:HD11	1.71	0.72
1:A:530:ARG:HD3	2:A:1567:IOD:I	2.60	0.72
1:A:174:GLU:OE2	2:A:1564:IOD:I	2.78	0.71
1:A:284:THR:HG21	3:A:2205:HOH:O	1.91	0.71
1:A:530:ARG:CD	2:A:1567:IOD:I	3.09	0.70
2:A:1560:IOD:I	3:A:2133:HOH:O	2.78	0.70
2:A:1574:IOD:I	3:A:2640:HOH:O	2.78	0.70
2:A:1564:IOD:I	3:A:2221:HOH:O	2.79	0.69
1:A:379:ASN:HD21	1:A:408:GLN:HG3	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:LEU:HD21	2:A:1589:IOD:I	2.68	0.63
1:A:317:GLN:CA	2:A:1568:IOD:I	3.17	0.62
1:A:530:ARG:NH1	2:A:1567:IOD:I	2.95	0.61
1:A:530:ARG:HD2	2:A:1567:IOD:I	2.70	0.61
2:A:1589:IOD:I	3:A:2092:HOH:O	2.86	0.61
2:A:1592:IOD:I	3:A:2242:HOH:O	2.87	0.60
1:A:449:ASP:HA	1:A:452:LYS:HE3	1.85	0.58
1:A:500:LYS:HE3	2:A:1588:IOD:I	2.74	0.58
1:A:268:LYS:HB3	2:A:1580:IOD:I	2.74	0.58
1:A:430:SER:OG	1:A:464:ILE:HD11	2.04	0.58
1:A:192:PRO:HB3	1:A:238:PRO:HB3	1.86	0.57
1:A:49:PHE:CB	1:A:50:PRO:HD2	2.32	0.56
1:A:132:LYS:HG3	1:A:203:ASN:HB2	1.88	0.56
1:A:545:PRO:HA	2:A:1548:IOD:I	2.76	0.56
1:A:443:HIS:HD2	2:A:1547:IOD:I	2.58	0.55
1:A:123:SER:HA	3:A:2726:HOH:O	2.07	0.54
1:A:31:PRO:HG3	2:A:1573:IOD:I	2.78	0.54
1:A:89:ILE:O	1:A:93:HIS:HD2	1.91	0.54
2:A:1569:IOD:I	3:A:2136:HOH:O	2.89	0.53
1:A:530:ARG:HD2	2:A:1572:IOD:I	2.78	0.53
1:A:494:GLU:OE2	1:A:498:ARG:NE	2.41	0.53
1:A:199:LEU:CA	2:A:1555:IOD:I	3.26	0.52
1:A:532:ASN:CG	2:A:1567:IOD:I	3.22	0.52
2:A:1573:IOD:I	3:A:2018:HOH:O	2.89	0.52
1:A:197:LYS:HG3	1:A:256:ARG:HH12	1.75	0.52
1:A:379:ASN:ND2	1:A:408:GLN:HG3	2.25	0.52
1:A:310:LEU:HD23	1:A:321:LEU:HD21	1.93	0.50
1:A:154:ARG:HD3	2:A:1589:IOD:I	2.83	0.49
1:A:123:SER:OG	2:A:1549:IOD:I	2.98	0.48
1:A:158:ASN:ND2	1:A:180:GLY:H	2.12	0.48
1:A:60:PHE:HB2	1:A:93:HIS:CE1	2.48	0.48
1:A:532:ASN:OD1	2:A:1567:IOD:I	3.02	0.47
1:A:49:PHE:HB3	1:A:50:PRO:CD	2.38	0.47
1:A:382:LEU:HG	1:A:437:ALA:HB1	1.96	0.46
1:A:85:ARG:NH1	2:A:1569:IOD:I	3.14	0.46
1:A:217:LYS:HB2	1:A:217:LYS:HE2	1.81	0.46
1:A:204:ALA:HB2	3:A:2228:HOH:O	2.16	0.45
1:A:317:GLN:O	2:A:1568:IOD:I	3.05	0.45
2:A:1551:IOD:I	3:A:2599:HOH:O	2.92	0.45
1:A:303:ASN:HD21	1:A:307:GLN:NE2	2.15	0.44
1:A:132:LYS:HE3	1:A:513:PHE:CE2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:LYS:NZ	2:A:1553:IOD:I	3.18	0.42
1:A:197:LYS:CB	1:A:256:ARG:HH22	2.23	0.42
1:A:106:TRP:CD1	1:A:106:TRP:C	2.98	0.41
1:A:319:GLN:NE2	3:A:2497:HOH:O	2.53	0.40
1:A:443:HIS:CD2	2:A:1547:IOD:I	3.42	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	546/543 (101%)	537 (98%)	9 (2%)	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	454/449 (101%)	449 (99%)	5 (1%)	65	41

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	ASP

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Mol	Chain	Res	Type
1	A	127[A]	MET
1	A	127[B]	MET
1	A	464	ILE
1	A	475	SER

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

Mol	Chain	Res	Type
1	A	18	ASN
1	A	43	GLN
1	A	65	ASN
1	A	93	HIS
1	A	95	GLN
1	A	96	ASN
1	A	158	ASN
1	A	189	GLN
1	A	234	GLN
1	A	249	GLN
1	A	303	ASN
1	A	379	ASN
1	A	443	HIS
1	A	499	ASN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 51 ligands modelled in this entry, 51 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	543/543 (100%)	3.05	421 (77%) 0 0	8, 17, 29, 35	5 (0%)

All (421) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	316	PRO	13.8
1	A	284	THR	10.0
1	A	51	ASP	9.5
1	A	199	LEU	9.3
1	A	50	PRO	8.7
1	A	420	GLU	8.7
1	A	527	VAL	8.7
1	A	310	LEU	8.3
1	A	339[A]	ASP	8.1
1	A	391	ILE	7.8
1	A	545	PRO	7.8
1	A	27	ASP	7.3
1	A	28	LYS	7.3
1	A	122	PRO	7.0
1	A	257	GLU	7.0
1	A	49	PHE	6.8
1	A	256	ARG	6.7
1	A	125	LYS	6.6
1	A	498	ARG	6.6
1	A	536	LEU	6.3
1	A	528	SER	6.3
1	A	254	LEU	6.3
1	A	314	LEU	6.2
1	A	312	LYS	6.2
1	A	320	ASP	6.1
1	A	525	ALA	6.1
1	A	19	LYS	5.9

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Mol	Chain	Res	Type	RSRZ
1	A	6	LEU	5.9
1	A	197	LYS	5.9
1	A	373	LYS	5.9
1	A	523	GLY	5.7
1	A	220	GLN	5.7
1	A	521	ASP	5.7
1	A	324	TRP	5.7
1	A	121	GLY	5.7
1	A	340	GLN	5.7
1	A	11	GLN	5.6
1	A	171	ARG	5.6
1	A	504	VAL	5.6
1	A	519	ARG	5.5
1	A	194	PHE	5.4
1	A	367	LYS	5.4
1	A	55	ALA	5.4
1	A	319	GLN	5.3
1	A	294	GLY	5.3
1	A	546	ASN	5.2
1	A	242	LYS	5.2
1	A	473	ALA	5.2
1	A	497	LEU	5.1
1	A	444	ALA	5.1
1	A	336	ALA	5.1
1	A	265	THR	5.0
1	A	127[A]	MET	5.0
1	A	241	ALA	5.0
1	A	317	GLN	5.0
1	A	48	ILE	5.0
1	A	186	LYS	5.0
1	A	4	ASP	4.9
1	A	123	SER	4.9
1	A	124	GLU	4.9
1	A	253	ALA	4.9
1	A	470	PHE	4.9
1	A	126	GLU	4.7
1	A	23	THR	4.7
1	A	54	ARG	4.7
1	A	464	ILE	4.7
1	A	335	TYR	4.6
1	A	539	VAL	4.5
1	A	520	MET	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	193	PHE	4.5
1	A	399	LYS	4.4
1	A	543	LEU	4.4
1	A	479	TYR	4.4
1	A	321	LEU	4.3
1	A	441	LEU	4.3
1	A	522	ASP	4.3
1	A	413	ILE	4.3
1	A	502	GLN	4.3
1	A	322	LEU	4.2
1	A	326	VAL	4.2
1	A	216	TYR	4.2
1	A	422	LYS	4.2
1	A	24	TYR	4.1
1	A	157	TRP	4.1
1	A	397	LEU	4.1
1	A	435	LEU	4.1
1	A	315	GLY	4.1
1	A	134	ALA	4.1
1	A	162	TYR	4.1
1	A	540	GLY	4.1
1	A	426	ASP	4.1
1	A	382	LEU	4.1
1	A	76	LEU	4.0
1	A	164	TRP	4.0
1	A	152	PHE	4.0
1	A	381	PHE	4.0
1	A	544	GLN	4.0
1	A	421	VAL	4.0
1	A	331	ALA	4.0
1	A	183	TRP	4.0
1	A	212	ALA	4.0
1	A	260	THR	4.0
1	A	161	VAL	3.9
1	A	217	LYS	3.9
1	A	259	PRO	3.9
1	A	499	ASN	3.9
1	A	60	PHE	3.8
1	A	416	ALA	3.8
1	A	449	ASP	3.8
1	A	229	LYS	3.8
1	A	332	PHE	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	144	VAL	3.8
1	A	5	ARG	3.8
1	A	313	ASP	3.8
1	A	500	LYS	3.8
1	A	513	PHE	3.7
1	A	438	LEU	3.7
1	A	132	LYS	3.7
1	A	419	LYS	3.7
1	A	75	GLN	3.7
1	A	214	LEU	3.7
1	A	95	GLN	3.7
1	A	237	LEU	3.7
1	A	467	ILE	3.7
1	A	423	VAL	3.7
1	A	118	GLN	3.7
1	A	433	TYR	3.7
1	A	450	TYR	3.7
1	A	128	VAL	3.6
1	A	222	GLN	3.6
1	A	286	LEU	3.6
1	A	258	GLU	3.6
1	A	105	TYR	3.6
1	A	389	TYR	3.6
1	A	395	PRO	3.6
1	A	32	LEU	3.6
1	A	250	PHE	3.6
1	A	196	THR	3.5
1	A	459	ASP	3.5
1	A	398	TRP	3.5
1	A	334	LYS	3.5
1	A	404	ILE	3.5
1	A	247	VAL	3.5
1	A	29	PRO	3.5
1	A	442	TYR	3.5
1	A	215	LEU	3.5
1	A	396	LEU	3.5
1	A	112	VAL	3.5
1	A	447	VAL	3.5
1	A	417	PRO	3.5
1	A	295	ARG	3.5
1	A	418	GLY	3.5
1	A	18	ASN	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	281	PHE	3.4
1	A	471	PHE	3.4
1	A	364	TYR	3.4
1	A	428	THR	3.4
1	A	227	TRP	3.4
1	A	277	PHE	3.4
1	A	385	TYR	3.4
1	A	518	TYR	3.4
1	A	219	GLN	3.4
1	A	376	LYS	3.4
1	A	201	PHE	3.4
1	A	117	LEU	3.4
1	A	89	ILE	3.3
1	A	457	ILE	3.3
1	A	482	VAL	3.3
1	A	187	PHE	3.3
1	A	357	TYR	3.3
1	A	99	ASP	3.3
1	A	349	ALA	3.3
1	A	448	ALA	3.3
1	A	366	GLY	3.3
1	A	463	LYS	3.3
1	A	345	ARG	3.3
1	A	511	ALA	3.3
1	A	542	LYS	3.3
1	A	8	VAL	3.3
1	A	371	VAL	3.3
1	A	269	PHE	3.3
1	A	333	ALA	3.3
1	A	45	LEU	3.2
1	A	410	LEU	3.2
1	A	452	LYS	3.2
1	A	92	TYR	3.2
1	A	300	TYR	3.2
1	A	245	LEU	3.2
1	A	318	GLY	3.2
1	A	393	ASN	3.2
1	A	228	ALA	3.2
1	A	388	ALA	3.2
1	A	503	ALA	3.2
1	A	26	GLY	3.2
1	A	17	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	147	ASP	3.2
1	A	100	PRO	3.2
1	A	530	ARG	3.2
1	A	236	VAL	3.2
1	A	301	SER	3.2
1	A	82	TYR	3.2
1	A	195	ALA	3.2
1	A	365	TYR	3.2
1	A	488	TYR	3.2
1	A	359	LEU	3.1
1	A	178	PRO	3.1
1	A	360	PRO	3.1
1	A	406	ASN	3.1
1	A	13	VAL	3.1
1	A	466	TYR	3.1
1	A	114	LEU	3.1
1	A	142	PHE	3.1
1	A	131	LEU	3.1
1	A	493	LEU	3.1
1	A	537	LEU	3.1
1	A	110	ARG	3.1
1	A	535	PHE	3.1
1	A	461	ILE	3.1
1	A	15	ASN	3.0
1	A	137	TYR	3.0
1	A	369	GLY	3.0
1	A	53	ARG	3.0
1	A	255	LYS	3.0
1	A	119	PRO	3.0
1	A	191	PRO	3.0
1	A	370	THR	3.0
1	A	375	TYR	3.0
1	A	167	LEU	3.0
1	A	323	LYS	3.0
1	A	151[A]	ARG	2.9
1	A	109	HIS	2.9
1	A	69	VAL	2.9
1	A	200	SER	2.9
1	A	115	LYS	2.9
1	A	453	LEU	2.9
1	A	427	THR	2.9
1	A	454	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	166	ILE	2.9
1	A	175	TYR	2.9
1	A	104	LEU	2.9
1	A	299	LEU	2.9
1	A	372	LEU	2.9
1	A	116	THR	2.9
1	A	529	THR	2.9
1	A	458	GLY	2.9
1	A	386	ALA	2.9
1	A	401	ALA	2.9
1	A	31	PRO	2.9
1	A	106	TRP	2.9
1	A	342	ASN	2.9
1	A	532	ASN	2.9
1	A	490	LEU	2.9
1	A	351	GLY	2.9
1	A	524	SER	2.9
1	A	507	PHE	2.8
1	A	169	THR	2.8
1	A	510	GLY	2.8
1	A	80	PRO	2.8
1	A	489	ALA	2.8
1	A	189	GLN	2.8
1	A	266	HIS	2.8
1	A	16	VAL	2.8
1	A	150	ALA	2.8
1	A	390	ALA	2.8
1	A	153	ILE	2.8
1	A	356	ASN	2.8
1	A	182	LEU	2.8
1	A	501	PRO	2.8
1	A	392	ASP	2.7
1	A	190	GLN	2.7
1	A	156	PHE	2.7
1	A	462	ILE	2.7
1	A	39	PRO	2.7
1	A	139	ASP	2.7
1	A	225	LEU	2.7
1	A	263	ALA	2.7
1	A	434	ALA	2.7
1	A	409	GLY	2.7
1	A	344	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	12	TYR	2.7
1	A	439	LEU	2.7
1	A	400	VAL	2.7
1	A	443	HIS	2.7
1	A	176	GLY	2.6
1	A	282	GLY	2.6
1	A	437	ALA	2.6
1	A	7	THR	2.6
1	A	309	GLN	2.6
1	A	47	TRP	2.6
1	A	180	GLY	2.6
1	A	223	GLY	2.6
1	A	383	ILE	2.6
1	A	495	ALA	2.6
1	A	97	TYR	2.6
1	A	243	THR	2.6
1	A	238	PRO	2.6
1	A	198	GLY	2.6
1	A	278	GLY	2.6
1	A	288	GLY	2.6
1	A	341	ASP	2.6
1	A	181	ALA	2.6
1	A	81[A]	ARG	2.6
1	A	445	SER	2.6
1	A	210	TYR	2.6
1	A	308	LEU	2.6
1	A	516	GLY	2.6
1	A	325	THR	2.5
1	A	436	PHE	2.5
1	A	218	HIS	2.5
1	A	221	ASP	2.5
1	A	425	MET	2.5
1	A	378	GLY	2.5
1	A	56	VAL	2.5
1	A	506	PRO	2.5
1	A	384	SER	2.5
1	A	415	THR	2.5
1	A	515	GLU	2.5
1	A	177	LYS	2.5
1	A	20	ALA	2.5
1	A	273	ALA	2.5
1	A	338	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	209	ILE	2.5
1	A	329	LEU	2.5
1	A	337	TYR	2.5
1	A	354	LEU	2.5
1	A	246	GLY	2.5
1	A	293	LYS	2.5
1	A	514	THR	2.5
1	A	505	ALA	2.5
1	A	517	ALA	2.5
1	A	363	GLY	2.5
1	A	455	GLU	2.5
1	A	33	LEU	2.5
1	A	534	LEU	2.5
1	A	203	ASN	2.5
1	A	343	THR	2.5
1	A	204	ALA	2.4
1	A	30	SER	2.4
1	A	414	GLY	2.4
1	A	526	ARG	2.4
1	A	235	TYR	2.4
1	A	491	LEU	2.4
1	A	472	MET	2.4
1	A	61	SER	2.4
1	A	285	ALA	2.4
1	A	469	GLY	2.4
1	A	477	ARG	2.4
1	A	261	ASP	2.4
1	A	208	LEU	2.4
1	A	305	LEU	2.4
1	A	149	THR	2.4
1	A	148	ALA	2.4
1	A	328	GLY	2.4
1	A	377	ALA	2.4
1	A	57	LEU	2.4
1	A	140	LEU	2.4
1	A	202	LEU	2.4
1	A	248	TYR	2.4
1	A	52	GLY	2.4
1	A	120	GLU	2.4
1	A	494	GLU	2.4
1	A	90	VAL	2.3
1	A	311	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	492	ALA	2.3
1	A	456	LYS	2.3
1	A	179	MET	2.3
1	A	25	HIS	2.3
1	A	184	GLU	2.3
1	A	94	PHE	2.3
1	A	111	PHE	2.3
1	A	283	PRO	2.3
1	A	374	PRO	2.3
1	A	379	ASN	2.3
1	A	226	THR	2.3
1	A	146	SER	2.3
1	A	84	LYS	2.2
1	A	143	SER	2.2
1	A	446	GLN	2.2
1	A	451	ARG	2.2
1	A	358	THR	2.2
1	A	474	SER	2.2
1	A	424	ASN	2.2
1	A	538	ASN	2.2
1	A	355	SER	2.2
1	A	165	ARG	2.2
1	A	292	LEU	2.1
1	A	508	LEU	2.1
1	A	62	ALA	2.1
1	A	405	ALA	2.1
1	A	78	GLY	2.1
1	A	102	GLY	2.1
1	A	108	GLY	2.1
1	A	485	ILE	2.1
1	A	298	THR	2.1
1	A	230	ARG	2.1
1	A	270	GLY	2.1
1	A	103	LEU	2.1
1	A	224	ALA	2.1
1	A	432	PRO	2.1
1	A	206	ASN	2.1
1	A	135	TYR	2.1
1	A	21	SER	2.1
1	A	70	MET	2.1
1	A	429	ASN	2.1
1	A	159	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	66	LEU	2.1
1	A	403	GLY	2.1
1	A	136	PRO	2.1
1	A	279	PRO	2.1
1	A	41	THR	2.0
1	A	304	ALA	2.0
1	A	43	GLN	2.0
1	A	168	GLU	2.0
1	A	101	SER	2.0
1	A	430	SER	2.0
1	A	407	ASP	2.0
1	A	85	ARG	2.0
1	A	231	LEU	2.0
1	A	22	ASP	2.0
1	A	353	ASP	2.0
1	A	138	TYR	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	IOD	A	1567	1/1	0.91	0.47	26,26,26,26	0
2	IOD	A	1597	1/1	0.92	0.23	13,13,13,13	1
2	IOD	A	1581	1/1	0.93	0.42	25,25,25,25	0
2	IOD	A	1588	1/1	0.93	0.23	23,23,23,23	0
2	IOD	A	1564	1/1	0.93	0.45	18,18,18,18	0
2	IOD	A	1575	1/1	0.94	0.35	27,27,27,27	0
2	IOD	A	1594	1/1	0.94	0.38	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	IOD	A	1587	1/1	0.94	0.33	28,28,28,28	0
2	IOD	A	1568	1/1	0.95	0.39	30,30,30,30	0
2	IOD	A	1553	1/1	0.95	0.37	17,17,17,17	0
2	IOD	A	1555	1/1	0.95	0.34	19,19,19,19	0
2	IOD	A	1585	1/1	0.95	0.32	26,26,26,26	0
2	IOD	A	1586	1/1	0.96	0.30	21,21,21,21	0
2	IOD	A	1570	1/1	0.96	0.36	24,24,24,24	0
2	IOD	A	1561	1/1	0.96	0.38	16,16,16,16	0
2	IOD	A	1548	1/1	0.96	0.13	13,13,13,13	1
2	IOD	A	1569	1/1	0.96	0.39	21,21,21,21	0
2	IOD	A	1572	1/1	0.97	0.38	20,20,20,20	0
2	IOD	A	1573	1/1	0.97	0.43	22,22,22,22	0
2	IOD	A	1556	1/1	0.97	0.33	16,16,16,16	0
2	IOD	A	1589	1/1	0.97	0.31	13,13,13,13	0
2	IOD	A	1566	1/1	0.97	0.38	25,25,25,25	0
2	IOD	A	1550	1/1	0.97	0.23	12,12,12,12	0
2	IOD	A	1562	1/1	0.98	0.37	18,18,18,18	0
2	IOD	A	1582	1/1	0.98	0.17	5,5,5,5	0
2	IOD	A	1554	1/1	0.98	0.33	16,16,16,16	0
2	IOD	A	1557	1/1	0.98	0.24	14,14,14,14	0
2	IOD	A	1559	1/1	0.98	0.32	21,21,21,21	0
2	IOD	A	1552	1/1	0.98	0.32	18,18,18,18	0
2	IOD	A	1576	1/1	0.98	0.40	29,29,29,29	0
2	IOD	A	1590	1/1	0.98	0.34	23,23,23,23	0
2	IOD	A	1593	1/1	0.98	0.40	19,19,19,19	0
2	IOD	A	1577	1/1	0.98	0.30	14,14,14,14	0
2	IOD	A	1595	1/1	0.98	0.21	15,15,15,15	0
2	IOD	A	1596	1/1	0.98	0.24	12,12,12,12	0
2	IOD	A	1578	1/1	0.98	0.34	20,20,20,20	0
2	IOD	A	1583	1/1	0.99	0.21	11,11,11,11	0
2	IOD	A	1584	1/1	0.99	0.25	7,7,7,7	0
2	IOD	A	1558	1/1	0.99	0.31	22,22,22,22	0
2	IOD	A	1565	1/1	0.99	0.33	19,19,19,19	0
2	IOD	A	1574	1/1	0.99	0.18	6,6,6,6	0
2	IOD	A	1549	1/1	0.99	0.24	10,10,10,10	0
2	IOD	A	1560	1/1	0.99	0.37	15,15,15,15	0
2	IOD	A	1547	1/1	0.99	0.18	3,3,3,3	0
2	IOD	A	1591	1/1	0.99	0.21	3,3,3,3	0
2	IOD	A	1592	1/1	0.99	0.26	4,4,4,4	0
2	IOD	A	1551	1/1	0.99	0.31	12,12,12,12	0
2	IOD	A	1579	1/1	0.99	0.36	15,15,15,15	0
2	IOD	A	1580	1/1	0.99	0.36	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	IOD	A	1563	1/1	0.99	0.32	12,12,12,12	0
2	IOD	A	1571	1/1	0.99	0.18	2,2,2,2	0

6.5 Other polymers [i](#)

There are no such residues in this entry.