



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 02:00 PM EDT

PDB ID : 4J1Y / pdb_00004j1y
Title : The X-ray crystal structure of human complement protease C1s zymogen
Authors : Perry, A.J.; Wijeyewickrema, L.C.; Wilmann, P.G.; Gunzburg, M.J.;
D'Andrea, L.; Irving, J.A.; Pang, S.S.; Duncan, R.C.; Wilce, J.A.; Whisstock,
J.C.; Pike, R.N.
Deposited on : 2013-02-03
Resolution : 2.66 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

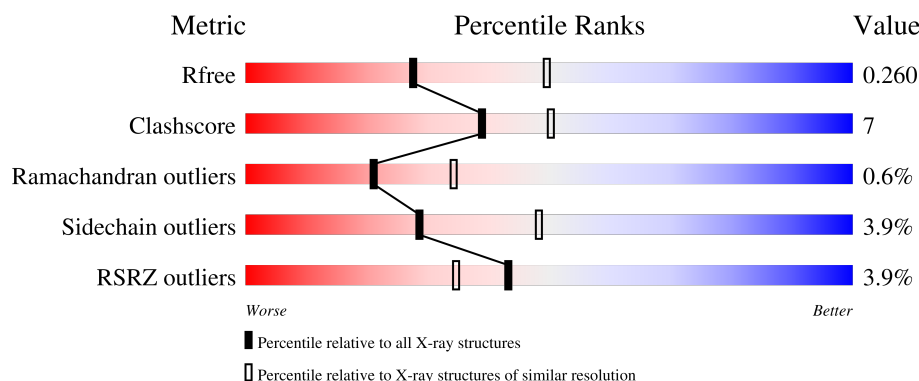
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.66 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	397	2% 77% 17% • 5%
1	B	397	5% 73% 17% • 9%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5661 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 Complement C1s subcomponent.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	378	Total	C	N	O	S	9	2	0
			2882	1828	485	544	25			
1	B	363	Total	C	N	O	S	15	4	1
			2738	1734	454	526	24			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	436	ALA	GLN	engineered mutation	UNP P09871
A	438	ALA	ILE	engineered mutation	UNP P09871
B	436	ALA	GLN	engineered mutation	UNP P09871
B	438	ALA	ILE	engineered mutation	UNP P09871

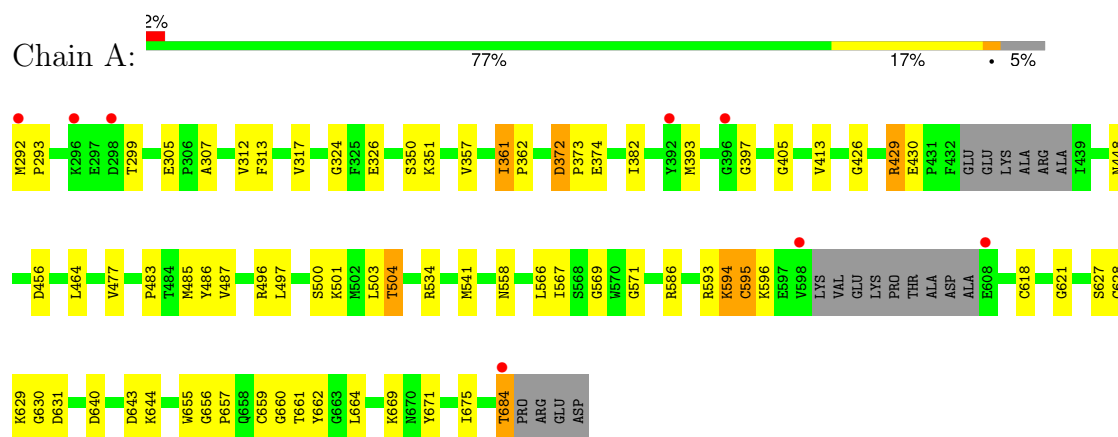
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	33	Total	O	0	0
			33	33		
2	B	8	Total	O	0	0
			8	8		

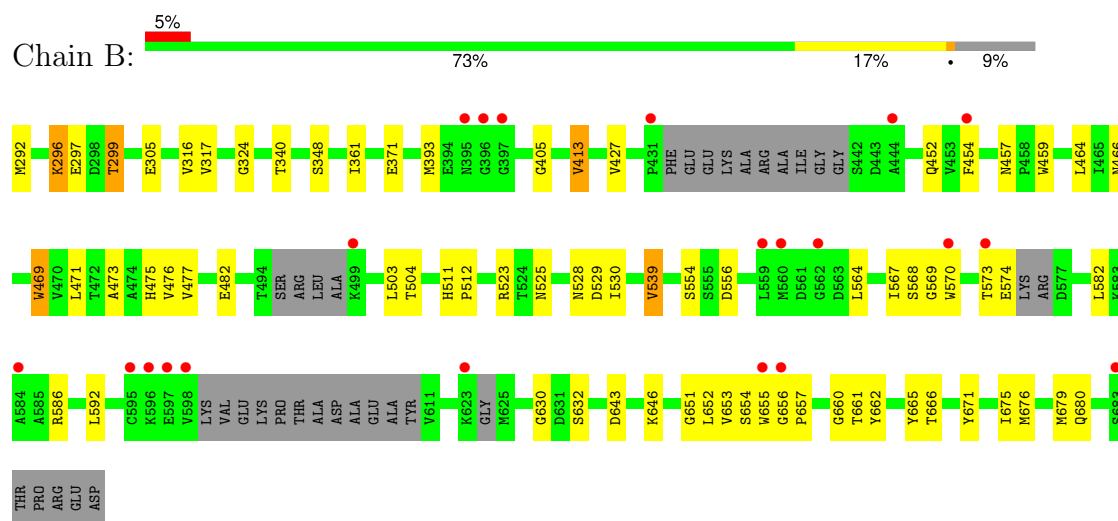
3 Residue-property plots [i](#)

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

• Molecule 1: Complement C1s subcomponent



• Molecule 1: Complement C1s subcomponent



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	149.89Å 158.90Å 78.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	54.27 – 2.66 54.27 – 2.66	Depositor EDS
% Data completeness (in resolution range)	99.3 (54.27-2.66) 92.8 (54.27-2.66)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 2.65Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1048)	Depositor
R, R_{free}	0.201 , 0.259 0.207 , 0.260	Depositor DCC
R_{free} test set	1363 reflections (4.15%)	wwPDB-VP
Wilson B-factor (Å ²)	56.6	Xtriage
Anisotropy	0.617	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 62.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5661	wwPDB-VP
Average B, all atoms (Å ²)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% 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	0.72	0/2966	1.12	16/4039 (0.4%)
1	B	0.66	0/2820	1.06	12/3849 (0.3%)
All	All	0.69	0/5786	1.09	28/7888 (0.4%)

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	629	LYS	N-CA-C	13.03	128.44	112.54
1	A	299	THR	CA-C-N	-9.41	110.71	120.03
1	A	299	THR	C-N-CA	-9.41	110.71	120.03
1	B	299	THR	CA-C-N	-8.91	111.21	120.03
1	B	299	THR	C-N-CA	-8.91	111.21	120.03
1	B	427	VAL	N-CA-C	7.93	115.40	107.55
1	A	456	ASP	CA-C-N	-7.24	114.26	123.16
1	A	456	ASP	C-N-CA	-7.24	114.26	123.16
1	A	350	SER	N-CA-C	-7.23	101.52	110.41
1	A	372	ASP	CA-C-N	6.42	126.33	119.85
1	A	372	ASP	C-N-CA	6.42	126.33	119.85
1	A	571	GLY	N-CA-C	6.30	117.94	111.95
1	B	482	GLU	CA-C-N	6.00	125.91	119.85
1	B	482	GLU	C-N-CA	6.00	125.91	119.85
1	B	569	GLY	N-CA-C	5.96	119.46	110.75
1	B	573	THR	N-CA-C	5.86	120.05	113.02
1	A	504	THR	CA-C-N	5.81	126.70	120.13
1	A	504	THR	C-N-CA	5.81	126.70	120.13
1	B	469	TRP	N-CA-C	5.69	118.76	108.69
1	A	397	GLY	N-CA-C	-5.64	106.47	115.66
1	B	348	SER	N-CA-C	5.48	118.01	111.71
1	B	413	VAL	N-CA-C	5.37	116.43	111.81
1	A	426	GLY	N-CA-C	5.21	122.28	115.40
1	A	374	GLU	N-CA-C	5.16	118.04	111.69
1	A	361	ILE	CA-C-N	5.06	124.97	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	361	ILE	C-N-CA	5.06	124.97	119.76
1	B	292	MET	CA-C-N	5.01	126.12	120.66
1	B	292	MET	C-N-CA	5.01	126.12	120.66

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	2882	0	2732	37	0
1	B	2738	0	2513	37	0
2	A	33	0	0	4	0
2	B	8	0	0	1	0
All	All	5661	0	5245	73	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 7.

All (73) 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:B:475[A]:HIS:HE2	1:B:632:SER:HG	1.11	0.89
1:A:628:CYS:HG	1:A:659:CYS:HG	0.79	0.77
1:B:475[A]:HIS:NE2	1:B:632:SER:OG	2.15	0.74
1:A:307:ALA:O	2:A:728:HOH:O	2.11	0.68
1:A:558:ASN:OD1	1:A:669:LYS:NZ	2.29	0.66
1:B:675:ILE:HG22	1:B:679:MET:HE2	1.82	0.62
1:B:466:ASN:HD21	1:B:469:TRP:CD1	2.18	0.61
1:A:486:TYR:CZ	1:A:497:LEU:HD13	2.36	0.60
1:A:594:LYS:O	1:A:596:LYS:N	2.34	0.60
1:B:651:GLY:HA2	1:B:666:THR:O	2.03	0.59
1:B:660:GLY:O	1:B:662:TYR:N	2.37	0.58
1:A:628:CYS:O	2:A:703:HOH:O	2.17	0.58
1:A:631:ASP:HB2	2:A:731:HOH:O	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:660:GLY:O	1:A:662:TYR:N	2.40	0.54
1:A:621:GLY:HA2	1:A:662:TYR:CZ	2.43	0.54
1:A:373:PRO:HB3	1:A:382:ILE:HG22	1.90	0.52
1:B:296:LYS:HD3	1:B:299:THR:HB	1.91	0.52
1:B:464:LEU:HD11	1:B:539:VAL:HG11	1.91	0.52
1:A:324:GLY:HA2	1:A:405:GLY:HA2	1.92	0.52
1:B:466:ASN:HD21	1:B:469:TRP:HD1	1.59	0.51
1:A:671:TYR:O	1:A:675:ILE:HG13	2.12	0.49
1:A:464:LEU:HD21	1:A:541:MET:HE1	1.95	0.49
1:B:570:TRP:CZ2	1:B:582:LEU:HD13	2.49	0.48
1:B:471:LEU:HG	1:B:652:LEU:HD11	1.95	0.48
1:A:594:LYS:C	1:A:596:LYS:H	2.21	0.48
1:B:454:PHE:HB2	1:B:570:TRP:CZ3	2.49	0.48
1:B:324:GLY:HA2	1:B:405:GLY:HA2	1.96	0.47
1:A:595[B]:CYS:SG	1:A:664:LEU:HD13	2.54	0.47
1:A:594:LYS:C	1:A:596:LYS:N	2.72	0.47
1:B:529:ASP:OD2	1:B:654:SER:OG	2.23	0.47
1:B:653:VAL:HG22	1:B:665:TYR:HE1	1.80	0.47
1:B:530:ILE:HG13	1:B:652:LEU:HD12	1.97	0.47
1:B:452:GLN:OE1	1:B:568:SER:OG	2.25	0.47
1:B:459:TRP:CD2	1:B:574:GLU:HG2	2.50	0.47
1:B:564:LEU:HD22	1:B:586:ARG:HG2	1.98	0.46
1:A:429:ARG:CZ	1:A:429:ARG:HA	2.46	0.46
1:A:372:ASP:HA	1:A:373:PRO:HD3	1.77	0.45
1:A:593:ARG:NH2	1:B:361:ILE:HG21	2.31	0.45
1:B:296:LYS:HD2	1:B:297:GLU:O	2.17	0.45
1:B:630:GLY:O	1:B:653:VAL:HG11	2.17	0.45
1:B:567:ILE:HD12	1:B:630:GLY:N	2.31	0.45
1:B:671:TYR:O	1:B:675:ILE:HG13	2.17	0.45
1:B:469:TRP:CE2	1:B:679:MET:HG2	2.52	0.45
1:A:656:GLY:HA3	1:A:657:PRO:HD3	1.79	0.45
1:B:457:ASN:OD1	1:B:457:ASN:N	2.51	0.44
1:A:483:PRO:HG2	1:A:485:MET:HE2	1.99	0.44
1:B:676:MET:O	1:B:680:GLN:HG3	2.17	0.44
1:A:393:MET:HE3	1:A:393:MET:HB2	1.88	0.44
1:B:643:ASP:HB3	1:B:646:LYS:HG2	1.99	0.44
1:A:292:MET:HB3	1:A:293:PRO:HD3	2.00	0.44
1:B:299:THR:HG23	1:B:299:THR:O	2.17	0.44
1:B:473:ALA:O	1:B:476:VAL:HG22	2.16	0.44
1:A:292:MET:HE3	1:A:292:MET:HB2	1.68	0.44
1:A:500:SER:O	1:A:501:LYS:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:595[B]:CYS:HB2	1:A:618:CYS:SG	2.57	0.43
1:A:627:SER:O	1:A:630:GLY:HA3	2.18	0.43
1:B:393:MET:HE3	1:B:393:MET:HB2	1.94	0.43
1:A:534:ARG:HH22	1:A:684:THR:C	2.26	0.43
1:A:640:ASP:HB3	1:A:643:ASP:O	2.19	0.43
1:B:316:VAL:HG22	1:B:340:THR:HG22	2.00	0.43
1:A:326:GLU:CD	1:A:357:VAL:HG12	2.44	0.42
1:A:312:VAL:HG22	1:A:313:PHE:H	1.84	0.42
1:B:528:ASN:N	2:B:702:HOH:O	2.43	0.42
1:A:361:ILE:HA	1:A:362:PRO:HD3	1.83	0.41
1:A:569:GLY:HA3	1:A:631:ASP:CG	2.46	0.41
1:A:566:LEU:HD21	1:A:586:ARG:CZ	2.50	0.41
1:B:523:ARG:HD3	1:B:525:ASN:O	2.20	0.41
1:B:554:SER:OG	1:B:556:ASP:OD1	2.31	0.41
1:A:567:ILE:HD12	1:A:630:GLY:HA2	2.03	0.41
1:A:487:VAL:HA	2:A:726:HOH:O	2.20	0.40
1:B:511:HIS:CG	1:B:512:PRO:HD2	2.57	0.40
1:B:656:GLY:HA3	1:B:657:PRO:HD3	1.93	0.40
1:A:430:GLU:O	1:A:448:ASN:HA	2.22	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	374/397 (94%)	352 (94%)	18 (5%)	4 (1%)	11	19
1	B	355/397 (89%)	330 (93%)	24 (7%)	1 (0%)	36	52
All	All	729/794 (92%)	682 (94%)	42 (6%)	5 (1%)	21	30

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	594	LYS
1	A	595[A]	CYS
1	A	595[B]	CYS
1	A	661	THR
1	B	661	THR

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	307/333 (92%)	295 (96%)	12 (4%)	28	48
1	B	287/333 (86%)	276 (96%)	11 (4%)	29	49
All	All	594/666 (89%)	571 (96%)	23 (4%)	28	48

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	305	GLU
1	A	317	VAL
1	A	351	LYS
1	A	413	VAL
1	A	429	ARG
1	A	477	VAL
1	A	496	ARG
1	A	503	LEU
1	A	504	THR
1	A	644	LYS
1	A	655	TRP
1	A	684	THR
1	B	296	LYS
1	B	305	GLU
1	B	317	VAL
1	B	371	GLU
1	B	413	VAL
1	B	477	VAL
1	B	503	LEU

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Mol	Chain	Res	Type
1	B	504	THR
1	B	539	VAL
1	B	592	LEU
1	B	655	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	395	ASN
1	A	670	ASN
1	B	448	ASN
1	B	507	HIS
1	B	558	ASN

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 oligosaccharides 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	378/397 (95%)	0.26	8 (2%) 63 57	27, 86, 131, 156	5 (1%)
1	B	362/397 (91%)	0.65	21 (5%) 29 22	70, 111, 163, 198	5 (1%)
All	All	740/794 (93%)	0.45	29 (3%) 43 35	27, 97, 153, 198	10 (1%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	559	LEU	5.4
1	A	598	VAL	4.0
1	B	598	VAL	4.0
1	A	684	THR	3.5
1	B	395	ASN	3.4
1	B	397	GLY	3.1
1	B	499	LYS	3.1
1	B	396	GLY	2.9
1	A	396	GLY	2.8
1	A	392	TYR	2.8
1	B	595[A]	CYS	2.7
1	A	298	ASP	2.7
1	B	454	PHE	2.5
1	A	608	GLU	2.4
1	B	573	THR	2.4
1	B	570	TRP	2.4
1	B	431	PRO	2.4
1	B	560	MET	2.3
1	B	584	ALA	2.3
1	B	596	LYS	2.3
1	B	562	GLY	2.3
1	B	656	GLY	2.3
1	B	597	GLU	2.2
1	B	683	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	292	MET	2.1
1	B	444	ALA	2.1
1	B	655	TRP	2.1
1	B	623	LYS	2.1
1	A	296	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 oligosaccharides 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.