



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:32 AM UTC

PDB ID : 1ZG8 / pdb_00001zg8
Title : Crystal Structure of (R)-2-(3-{[amino(imino)methyl]amino}phenyl)-3-sulfany
lpropanoic acid Bound to Activated Porcine Pancreatic Carboxypeptidase B
Authors : Adler, M.; Bryant, J.; Buckman, B.; Islam, I.; Larsen, B.; Finster, S.; Kent,
L.; May, K.; Mohan, R.; Yuan, S.; Whitlow, M.
Deposited on : 2005-04-20
Resolution : 2.00 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

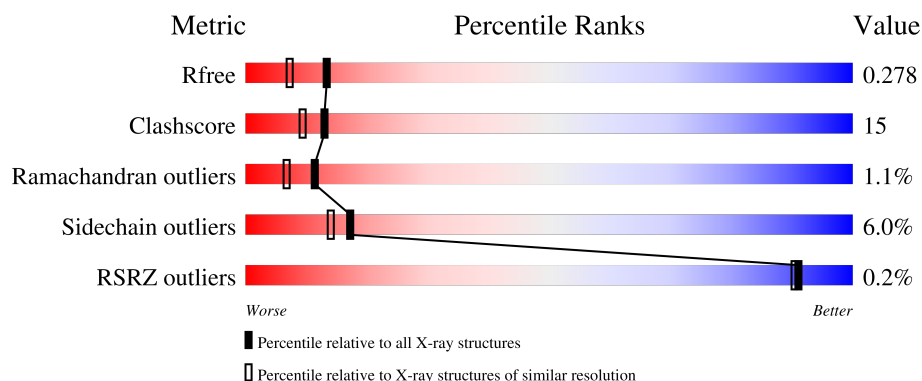
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	306	 71% 25% .
1	B	306	 68% 27% 5%
1	C	306	 55% 35% 9% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7800 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.

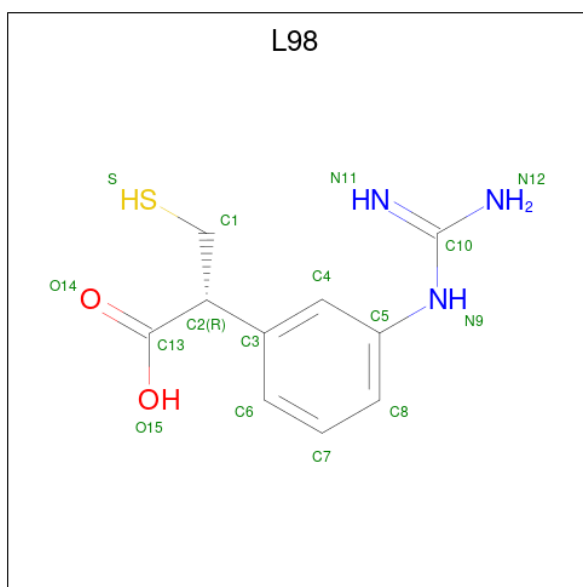
- Molecule 1 is a protein called procarboxypeptidase B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	305	Total	C	N	O	S	0	0	0
			2443	1564	398	469	12			
1	B	305	Total	C	N	O	S	0	0	0
			2443	1564	398	469	12			
1	C	304	Total	C	N	O	S	0	0	0
			2436	1560	397	467	12			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		

- Molecule 3 is (2R)-2-(3-([AMINO(IMINO)METHYL]AMINO)PHENYL)-3-SULFANYLPROPYNOIC ACID (CCD ID: L98) (formula: C₁₀H₁₃N₃O₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			16	10	3	2	1		
3	B	1	Total	C	N	O	S	0	0
			16	10	3	2	1		
3	C	1	Total	C	N	O	S	0	0
			16	10	3	2	1		

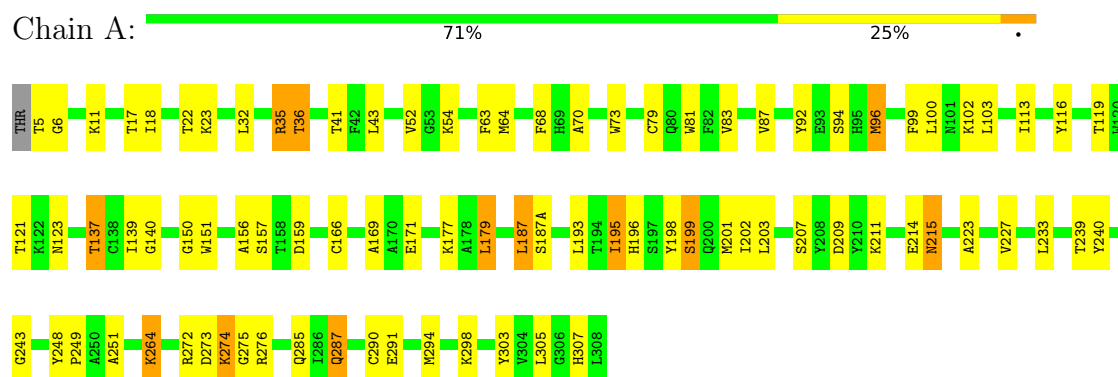
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	167	Total	O	0	0
			167	167		
4	B	179	Total	O	0	0
			179	179		
4	C	81	Total	O	0	0
			81	81		

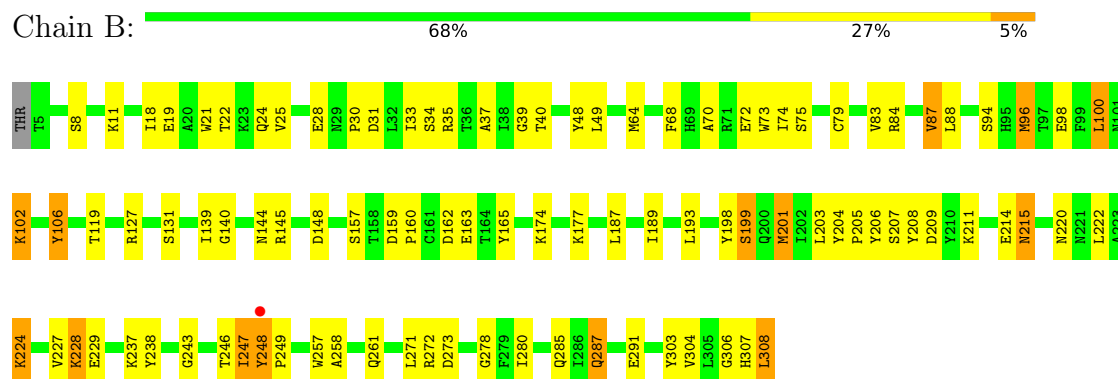
3 Residue-property plots [i](#)

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.

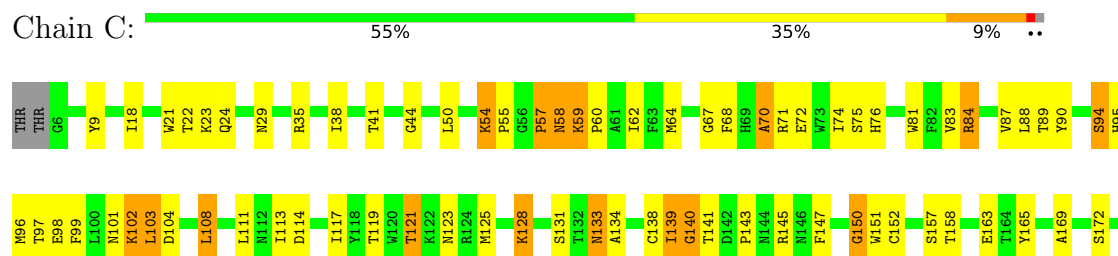
• Molecule 1: procarboxypeptidase B

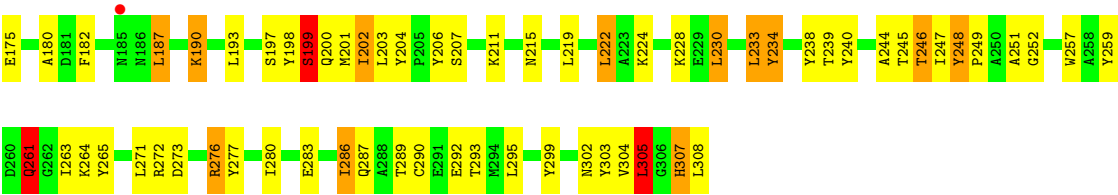


• Molecule 1: procarboxypeptidase B



• Molecule 1: procarboxypeptidase B





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.90Å 99.51Å 136.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.00 8.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.3 (8.00-2.00) 95.3 (8.00-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.62 (at 2.00Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.214 , 0.294 0.208 , 0.278	Depositor DCC
R_{free} test set	2464 reflections (4.09%)	wwPDB-VP
Wilson B-factor (Å ²)	31.3	Xtriage
Anisotropy	0.481	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 87.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7800	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% 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 ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, L98

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	0.75	2/2512 (0.1%)	1.12	14/3418 (0.4%)
1	B	0.73	2/2512 (0.1%)	1.09	13/3418 (0.4%)
1	C	0.65	0/2505	1.15	24/3408 (0.7%)
All	All	0.71	4/7529 (0.1%)	1.12	51/10244 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
All	All	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	96	MET	SD-CE	-8.80	1.57	1.79
1	A	52	VAL	CA-CB	7.18	1.62	1.54
1	B	96	MET	SD-CE	-6.88	1.62	1.79
1	B	201	MET	SD-CE	-6.28	1.63	1.79

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	140	GLY	N-CA-C	9.95	124.53	112.48
1	A	140	GLY	N-CA-C	9.65	124.36	111.72
1	A	159	ASP	CA-C-N	8.36	128.09	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	159	ASP	C-N-CA	8.36	128.09	119.56
1	A	274	LYS	N-CA-C	-8.32	102.90	113.72
1	C	307	HIS	N-CA-C	-7.66	101.99	112.03
1	C	70	ALA	N-CA-C	7.52	120.13	111.11
1	C	286	ILE	N-CA-C	7.33	117.41	110.30
1	C	140	GLY	N-CA-C	7.31	122.16	112.65
1	C	133	ASN	N-CA-C	7.28	121.23	110.46
1	C	108	LEU	CA-C-N	7.00	126.52	119.24
1	C	108	LEU	C-N-CA	7.00	126.52	119.24
1	C	145	ARG	N-CA-C	-6.96	104.29	114.39
1	C	261	GLN	N-CA-C	-6.64	104.80	113.17
1	C	246	THR	N-CA-C	6.64	119.50	111.40
1	B	287	GLN	N-CA-C	6.45	117.97	111.07
1	A	70	ALA	N-CA-C	6.36	119.03	111.33
1	C	150	GLY	N-CA-C	-6.30	104.58	114.10
1	A	264	LYS	N-CA-C	6.27	119.10	111.82
1	B	94	SER	N-CA-C	6.13	118.47	111.11
1	B	30	PRO	CA-C-N	6.07	128.42	120.28
1	B	30	PRO	C-N-CA	6.07	128.42	120.28
1	B	34	SER	N-CA-C	-5.99	100.03	109.50
1	A	102	LYS	N-CA-C	5.93	118.99	111.69
1	A	195	ILE	N-CA-C	5.90	117.26	108.23
1	C	44	GLY	N-CA-C	5.85	123.14	115.36
1	C	29	ASN	CA-C-N	5.80	125.47	119.56
1	C	29	ASN	C-N-CA	5.80	125.47	119.56
1	B	31	ASP	N-CA-CB	-5.70	101.74	110.12
1	B	243	GLY	N-CA-C	5.68	119.52	112.64
1	C	139	ILE	N-CA-C	5.63	117.70	108.97
1	C	187	LEU	N-CA-C	5.56	117.34	111.28
1	B	37	ALA	N-CA-C	-5.51	99.91	108.90
1	C	202	ILE	N-CA-C	-5.51	100.19	108.12
1	B	106	TYR	N-CA-C	-5.50	99.77	108.73
1	C	102	LYS	N-CA-C	5.50	118.45	111.69
1	C	62	ILE	N-CA-C	-5.42	100.43	108.45
1	A	139	ILE	N-CA-C	5.42	115.75	108.17
1	A	43	LEU	N-CA-C	5.41	119.58	112.92
1	B	73	TRP	N-CA-C	5.40	117.86	111.33
1	A	233	LEU	N-CA-C	5.39	116.84	110.97
1	A	94	SER	N-CA-C	5.33	117.09	111.28
1	C	128	LYS	N-CA-C	5.29	117.70	109.60
1	A	121	THR	N-CA-C	5.28	119.85	113.41
1	A	87	VAL	N-CA-C	5.25	117.66	111.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	121	THR	N-CA-C	5.24	119.76	112.90
1	C	24	GLN	N-CA-C	5.16	116.75	111.03
1	B	102	LYS	N-CA-C	5.08	119.56	112.90
1	C	228	LYS	N-CA-C	-5.08	105.82	111.36
1	C	134	ALA	N-CA-C	5.07	116.45	109.15
1	B	189	ILE	N-CA-C	5.01	115.45	108.84

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	92	TYR	Sidechain
1	B	208	TYR	Sidechain
1	C	234	TYR	Sidechain

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	2443	0	2324	50	0
1	B	2443	0	2324	61	0
1	C	2436	0	2317	106	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	16	0	10	3	0
3	B	16	0	10	1	0
3	C	16	0	10	3	0
4	A	167	0	0	2	0
4	B	179	0	0	5	0
4	C	81	0	0	1	0
All	All	7800	0	6995	216	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 15.

All (216) 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:203:LEU:HD13	3:A:401:L98:H7	1.25	1.09
1:B:203:LEU:HD13	3:B:501:L98:H7	1.32	1.07
1:C:233:LEU:HD13	1:C:295:LEU:HD11	1.48	0.95
1:C:201:MET:HE1	1:C:247:ILE:HD13	1.49	0.93
1:C:81:TRP:CH2	1:C:287:GLN:HG3	2.05	0.91
1:A:203:LEU:CD1	3:A:401:L98:H7	2.03	0.88
1:C:203:LEU:HD13	3:C:601:L98:H7	1.65	0.78
1:A:273:ASP:HB3	1:A:275:GLY:H	1.48	0.78
1:C:303:TYR:O	1:C:307:HIS:HD2	1.66	0.77
1:A:5:THR:HG22	1:A:6:GLY:H	1.50	0.77
1:C:276:ARG:HG3	1:C:276:ARG:HH11	1.51	0.76
1:A:96:MET:HE2	1:A:100:LEU:HG	1.68	0.76
1:C:60:PRO:HG2	1:C:103:LEU:HB3	1.67	0.75
1:C:81:TRP:HH2	1:C:287:GLN:HG3	1.53	0.73
1:A:137:THR:HG21	1:B:39:GLY:HA2	1.71	0.73
1:C:54:LYS:HD3	1:C:90:TYR:OH	1.88	0.72
1:C:302:ASN:O	1:C:305:LEU:HB2	1.89	0.72
1:C:198:TYR:O	1:C:199:SER:HB2	1.87	0.72
1:C:233:LEU:HD23	1:C:234:TYR:CE2	2.25	0.71
1:B:24:GLN:O	1:B:28:GLU:HG3	1.91	0.70
1:A:215:ASN:H	1:A:215:ASN:HD22	1.39	0.70
1:A:196:HIS:ND1	3:A:401:L98:H12	2.10	0.66
1:C:201:MET:HG2	1:C:239:THR:OG1	1.96	0.65
1:C:35:ARG:HB2	1:C:50:LEU:HD23	1.78	0.65
1:B:303:TYR:O	1:B:307:HIS:HD2	1.80	0.65
1:C:22:THR:HB	1:C:35:ARG:HD2	1.79	0.64
1:A:119:THR:HA	1:A:123:ASN:O	1.97	0.64
1:C:215:ASN:HD21	1:C:264:LYS:HB3	1.62	0.64
1:B:272:ARG:HH11	1:B:285:GLN:HE21	1.46	0.64
1:A:18:ILE:O	1:A:22:THR:HG23	1.98	0.63
1:C:180:ALA:HA	1:C:257:TRP:CH2	2.34	0.63
1:C:94:SER:O	1:C:95:HIS:HB2	1.98	0.63
1:A:5:THR:HA	1:A:17:THR:OG1	1.99	0.62
1:B:40:THR:O	1:B:174:LYS:HE2	1.99	0.62
1:C:131:SER:HB2	4:C:1227:HOH:O	1.98	0.62
1:C:303:TYR:O	1:C:307:HIS:CD2	2.50	0.62
1:C:265:TYR:CE1	1:C:303:TYR:HE2	2.17	0.61
1:B:201:MET:HE2	1:B:203:LEU:HD21	1.82	0.61
1:C:206:TYR:CD2	1:C:211:LYS:HG3	2.35	0.61
1:C:276:ARG:HG3	1:C:276:ARG:NH1	2.15	0.61
1:C:190:LYS:HD2	1:C:308:LEU:HD23	1.81	0.61
1:C:133:ASN:HB2	1:C:138:CYS:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:ASN:H	1:B:215:ASN:HD22	1.50	0.60
1:C:224:LYS:HG3	1:C:240:TYR:OH	2.02	0.60
1:C:71:ARG:HD3	1:C:125:MET:O	2.02	0.59
1:A:150:GLY:O	1:A:251:ALA:HB1	2.03	0.59
1:C:125:MET:HE2	1:C:280:ILE:HD11	1.84	0.58
1:A:63:PHE:CZ	1:A:179:LEU:HD21	2.39	0.58
1:B:257:TRP:O	1:B:261:GLN:HG2	2.03	0.58
1:C:206:TYR:HD2	1:C:211:LYS:O	1.86	0.58
1:B:224:LYS:O	1:B:227:VAL:HG22	2.04	0.57
1:A:276:ARG:HG3	1:A:276:ARG:HH11	1.70	0.57
1:B:272:ARG:HH11	1:B:285:GLN:NE2	2.03	0.57
1:C:169:ALA:O	1:C:172:SER:OG	2.21	0.57
1:A:215:ASN:H	1:A:215:ASN:ND2	2.02	0.56
1:B:159:ASP:HB3	1:B:162:ASP:OD2	2.06	0.56
1:C:64:MET:HA	1:C:193:LEU:O	2.05	0.56
1:B:8:SER:HB3	1:B:11:LYS:HB2	1.88	0.55
1:B:287:GLN:HG3	4:B:1174:HOH:O	2.08	0.54
1:A:103:LEU:HD23	1:A:305:LEU:HD13	1.89	0.54
1:C:113:ILE:HG22	1:C:117:ILE:HD11	1.88	0.54
1:C:202:ILE:O	1:C:240:TYR:HA	2.07	0.54
1:B:238:TYR:OH	1:B:271:LEU:HA	2.07	0.54
1:A:207:SER:OG	1:A:243:GLY:HA3	2.07	0.54
1:C:203:LEU:HD23	1:C:246:THR:HB	1.91	0.53
1:B:83:VAL:O	1:B:87:VAL:HG13	2.08	0.53
1:C:190:LYS:CD	1:C:308:LEU:HD23	2.38	0.53
1:C:215:ASN:ND2	1:C:264:LYS:HB3	2.23	0.53
1:A:215:ASN:HD22	1:A:215:ASN:N	2.00	0.53
1:C:54:LYS:HZ2	1:C:101:ASN:HA	1.73	0.53
1:C:57:PRO:O	1:C:58:ASN:HB2	2.09	0.52
1:C:200:GLN:HB3	1:C:238:TYR:CD1	2.44	0.52
1:B:303:TYR:O	1:B:307:HIS:CD2	2.62	0.52
1:C:81:TRP:O	1:C:84:ARG:HB3	2.09	0.52
1:B:19:GLU:HG3	1:B:48:TYR:CE2	2.45	0.52
1:B:96:MET:HE2	1:B:100:LEU:CD2	2.40	0.51
1:C:230:LEU:HD13	1:C:292:GLU:HB2	1.92	0.51
1:C:201:MET:HE3	1:C:203:LEU:HD11	1.91	0.51
1:C:247:ILE:HG23	1:C:248:TYR:H	1.75	0.51
1:C:72:GLU:O	1:C:75:SER:HB3	2.10	0.51
1:A:96:MET:HE3	1:A:99:PHE:HB2	1.92	0.50
1:A:287:GLN:HG3	4:A:1323:HOH:O	2.11	0.50
1:C:283:GLU:O	1:C:286:ILE:HG13	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:207:SER:O	1:B:249:PRO:HA	2.12	0.50
1:C:9:TYR:CE1	1:C:84:ARG:HB2	2.46	0.50
1:B:131:SER:O	1:B:139:ILE:HG23	2.12	0.50
1:C:72:GLU:HB3	1:C:197:SER:HB3	1.93	0.50
1:C:147:PHE:O	1:C:252:GLY:HA2	2.11	0.50
1:C:119:THR:HA	1:C:123:ASN:O	2.12	0.49
1:A:79:CYS:O	1:A:83:VAL:HG23	2.13	0.49
1:A:198:TYR:O	1:A:199:SER:CB	2.60	0.49
1:B:79:CYS:O	1:B:83:VAL:HG23	2.12	0.49
1:B:21:TRP:HA	1:B:24:GLN:HG2	1.93	0.49
1:A:64:MET:HA	1:A:193:LEU:O	2.13	0.49
1:A:195:ILE:C	1:A:196:HIS:CD2	2.91	0.49
1:B:72:GLU:O	1:B:75:SER:HB3	2.12	0.48
1:A:223:ALA:O	1:A:227:VAL:HG13	2.14	0.48
1:B:64:MET:HA	1:B:193:LEU:O	2.12	0.48
1:B:215:ASN:HD22	1:B:215:ASN:N	2.11	0.48
1:C:222:LEU:HD23	1:C:299:TYR:HE2	1.78	0.48
1:B:307:HIS:CD2	1:B:307:HIS:N	2.82	0.48
1:A:96:MET:HE2	1:A:100:LEU:CG	2.41	0.48
1:A:41:THR:HG21	1:A:113:ILE:HB	1.95	0.48
1:B:228:LYS:HE2	1:B:229:GLU:N	2.29	0.48
1:A:202:ILE:O	1:A:240:TYR:HA	2.14	0.48
1:B:198:TYR:O	1:B:199:SER:CB	2.61	0.48
1:C:157:SER:O	1:C:165:TYR:HD1	1.97	0.48
1:B:127:ARG:HD3	1:B:163:GLU:HB3	1.96	0.47
1:B:272:ARG:HA	1:B:273:ASP:HA	1.71	0.47
1:A:209:ASP:HB3	1:A:211:LYS:HG2	1.96	0.47
1:C:198:TYR:O	1:C:199:SER:CB	2.59	0.47
1:B:157:SER:O	1:B:165:TYR:HA	2.14	0.47
1:C:74:ILE:HG12	1:C:289:THR:HG21	1.96	0.47
1:C:139:ILE:CG2	1:C:140:GLY:N	2.77	0.47
1:A:272:ARG:HH11	1:A:285:GLN:HE21	1.63	0.47
1:B:145:ARG:HG3	1:B:145:ARG:HH11	1.80	0.47
1:C:84:ARG:O	1:C:87:VAL:HG22	2.14	0.47
1:C:90:TYR:CD1	1:C:97:THR:HA	2.50	0.47
1:C:157:SER:O	1:C:165:TYR:HA	2.15	0.47
1:C:265:TYR:CZ	1:C:303:TYR:HE2	2.32	0.47
1:A:156:ALA:HB1	1:A:166:CYS:HB3	1.97	0.47
1:C:139:ILE:HG22	1:C:140:GLY:N	2.30	0.47
1:A:294:MET:O	1:A:298:LYS:HG3	2.15	0.46
1:C:41:THR:HG21	1:C:113:ILE:HB	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:TRP:CG	1:A:290:CYS:HB3	2.49	0.46
1:B:201:MET:HG3	1:B:203:LEU:HD11	1.96	0.46
1:C:94:SER:O	1:C:96:MET:N	2.48	0.46
1:C:117:ILE:O	1:C:121:THR:HG23	2.15	0.46
1:B:215:ASN:H	1:B:215:ASN:ND2	2.11	0.46
1:C:38:ILE:HD11	1:C:108:LEU:HD11	1.98	0.46
1:C:125:MET:CE	1:C:280:ILE:HD11	2.44	0.46
1:C:128:LYS:HB3	1:C:141:THR:O	2.16	0.46
1:A:287:GLN:O	1:A:291:GLU:HG2	2.16	0.46
1:A:198:TYR:O	1:A:199:SER:HB2	2.16	0.46
1:A:73:TRP:CD1	1:A:116:TYR:HE1	2.34	0.46
1:C:84:ARG:O	1:C:88:LEU:HG	2.16	0.46
1:A:5:THR:HG23	1:A:17:THR:HA	1.99	0.45
1:C:247:ILE:HG23	1:C:248:TYR:N	2.30	0.45
1:A:207:SER:O	1:A:249:PRO:HA	2.16	0.45
1:C:302:ASN:HA	1:C:305:LEU:HD23	1.99	0.45
1:C:89:THR:OG1	1:C:96:MET:HG2	2.17	0.45
1:A:171:GLU:OE2	1:A:177:LYS:HD3	2.15	0.45
1:B:177:LYS:HE3	1:B:177:LYS:HB2	1.58	0.45
1:C:35:ARG:HB2	1:C:50:LEU:CD2	2.45	0.45
1:C:99:PHE:CD2	1:C:305:LEU:HD21	2.52	0.45
1:C:244:ALA:O	1:C:249:PRO:HD3	2.17	0.45
1:B:247:ILE:HG22	1:B:248:TYR:CD2	2.52	0.45
1:C:18:ILE:O	1:C:21:TRP:HB3	2.17	0.45
1:B:96:MET:HE2	1:B:100:LEU:HD22	1.99	0.45
1:B:98:GLU:HG3	1:B:102:LYS:HD2	1.98	0.44
1:C:304:VAL:O	1:C:307:HIS:N	2.50	0.44
1:C:150:GLY:O	1:C:251:ALA:HB1	2.18	0.44
1:B:258:ALA:O	1:B:261:GLN:HB2	2.18	0.44
1:C:204:TYR:HB2	1:C:219:LEU:HD13	1.99	0.44
1:B:205:PRO:HA	1:B:206:TYR:HA	1.74	0.43
1:A:201:MET:HA	1:A:239:THR:O	2.17	0.43
1:B:209:ASP:HB3	1:B:211:LYS:HG2	1.99	0.43
1:C:234:TYR:HD2	1:C:292:GLU:OE1	2.02	0.43
1:C:238:TYR:OH	1:C:271:LEU:HA	2.18	0.43
1:B:201:MET:HE1	1:B:246:THR:HG22	2.00	0.43
1:C:247:ILE:HG21	3:C:601:L98:C7	2.49	0.43
1:A:303:TYR:O	1:A:307:HIS:CD2	2.72	0.43
1:A:171:GLU:HB3	1:A:177:LYS:HE2	2.00	0.43
1:C:201:MET:CE	1:C:247:ILE:HD13	2.33	0.43
1:A:195:ILE:C	1:A:196:HIS:HD2	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:207:SER:O	1:C:249:PRO:HA	2.18	0.43
1:C:280:ILE:N	1:C:280:ILE:HD13	2.34	0.43
1:A:36:THR:HB	4:A:1071:HOH:O	2.19	0.42
1:A:23:LYS:HB2	1:A:35:ARG:NH2	2.34	0.42
1:C:114:ASP:HA	1:C:117:ILE:HD12	2.01	0.42
1:C:182:PHE:CD2	1:C:182:PHE:C	2.97	0.42
1:C:248:TYR:OH	3:C:601:L98:H2	2.19	0.42
1:B:49:LEU:HD21	1:B:106:TYR:CD2	2.54	0.42
1:A:274:LYS:HD2	1:A:274:LYS:HA	1.76	0.42
1:B:33:ILE:HD11	1:B:87:VAL:HG11	2.02	0.42
1:B:74:ILE:HD12	1:B:74:ILE:HA	1.89	0.42
1:B:18:ILE:O	1:B:22:THR:HG23	2.20	0.42
1:B:237:LYS:HE3	4:B:1220:HOH:O	2.19	0.42
1:C:111:LEU:HD11	1:C:175:GLU:HB3	2.02	0.42
1:B:21:TRP:HA	1:B:24:GLN:HE21	1.85	0.41
1:B:96:MET:HG3	1:B:100:LEU:HD22	2.02	0.41
1:B:160:PRO:HA	1:B:165:TYR:CG	2.55	0.41
1:C:292:GLU:O	1:C:295:LEU:HB2	2.20	0.41
1:B:70:ALA:HB1	1:B:119:THR:HG23	2.02	0.41
1:B:204:TYR:OH	1:B:220:ASN:HB2	2.20	0.41
1:B:306:GLY:HA3	4:B:1306:HOH:O	2.19	0.41
1:C:272:ARG:HH21	1:C:292:GLU:CD	2.27	0.41
1:C:67:GLY:HA2	1:C:76:HIS:CE1	2.54	0.41
1:C:70:ALA:HB1	1:C:119:THR:HG23	2.02	0.41
1:C:90:TYR:HD1	1:C:97:THR:HA	1.85	0.41
1:A:32:LEU:HD23	1:A:54:LYS:HD2	2.03	0.41
1:A:151:TRP:CH2	1:A:169:ALA:HA	2.55	0.41
1:A:187:LEU:HD22	1:A:187:LEU:HA	1.86	0.41
1:B:19:GLU:HG3	1:B:48:TYR:HE2	1.85	0.41
1:C:83:VAL:O	1:C:87:VAL:HG13	2.21	0.41
1:C:81:TRP:CG	1:C:290:CYS:HB3	2.55	0.41
1:C:272:ARG:HA	1:C:273:ASP:HA	1.71	0.41
1:A:81:TRP:CD1	1:A:290:CYS:HB3	2.56	0.41
1:B:198:TYR:CE1	1:B:278:GLY:HA2	2.56	0.41
1:B:304:VAL:O	1:B:308:LEU:HG	2.20	0.41
1:C:128:LYS:HD3	1:C:163:GLU:HA	2.03	0.41
1:C:259:TYR:HA	1:C:263:ILE:O	2.21	0.41
1:C:59:LYS:HE3	1:C:104:ASP:OD1	2.20	0.41
1:B:84:ARG:O	1:B:88:LEU:HB2	2.19	0.41
1:B:187:LEU:HA	1:B:187:LEU:HD23	1.78	0.41
1:C:113:ILE:O	1:C:117:ILE:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:THR:O	1:C:143:PRO:HD3	2.21	0.41
1:C:151:TRP:CH2	1:C:169:ALA:HA	2.56	0.41
1:C:222:LEU:HD23	1:C:299:TYR:CE2	2.56	0.41
1:B:291:GLU:HG2	4:B:1315:HOH:O	2.20	0.40
1:C:98:GLU:O	1:C:102:LYS:HB2	2.21	0.40
1:C:187:LEU:HD11	1:C:261:GLN:O	2.20	0.40
1:B:127:ARG:NH1	4:B:1410:HOH:O	2.53	0.40
1:C:230:LEU:CD2	1:C:293:THR:HA	2.52	0.40
1:C:261:GLN:NE2	1:C:261:GLN:HA	2.35	0.40
1:C:276:ARG:HD2	1:C:277:TYR:CE1	2.57	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	303/306 (99%)	289 (95%)	13 (4%)	1 (0%)	36	35
1	B	303/306 (99%)	292 (96%)	8 (3%)	3 (1%)	12	8
1	C	302/306 (99%)	274 (91%)	22 (7%)	6 (2%)	6	2
All	All	908/918 (99%)	855 (94%)	43 (5%)	10 (1%)	11	7

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	199	SER
1	A	199	SER
1	B	199	SER
1	C	58	ASN
1	C	94	SER
1	C	305	LEU
1	B	247	ILE

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Mol	Chain	Res	Type
1	C	55	PRO
1	C	59	LYS
1	B	280	ILE

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	258/259 (100%)	244 (95%)	14 (5%)	20	17
1	B	258/259 (100%)	244 (95%)	14 (5%)	20	17
1	C	257/259 (99%)	239 (93%)	18 (7%)	14	10
All	All	773/777 (100%)	727 (94%)	46 (6%)	17	14

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LYS
1	A	35	ARG
1	A	36	THR
1	A	68	PHE
1	A	137	THR
1	A	157	SER
1	A	179	LEU
1	A	187	LEU
1	A	187(A)	SER
1	A	214	GLU
1	A	215	ASN
1	A	248	TYR
1	A	264	LYS
1	A	287	GLN
1	B	25	VAL
1	B	35	ARG
1	B	68	PHE
1	B	87	VAL
1	B	100	LEU

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Mol	Chain	Res	Type
1	B	144	ASN
1	B	148	ASP
1	B	214	GLU
1	B	215	ASN
1	B	222	LEU
1	B	224	LYS
1	B	228	LYS
1	B	248	TYR
1	B	308	LEU
1	C	23	LYS
1	C	54	LYS
1	C	57	PRO
1	C	68	PHE
1	C	84	ARG
1	C	103	LEU
1	C	152	CYS
1	C	158	THR
1	C	190	LYS
1	C	199	SER
1	C	222	LEU
1	C	230	LEU
1	C	233	LEU
1	C	245	THR
1	C	248	TYR
1	C	261	GLN
1	C	276	ARG
1	C	305	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	ASN
1	A	185	ASN
1	A	200	GLN
1	A	215	ASN
1	A	261	GLN
1	A	285	GLN
1	A	287	GLN
1	A	307	HIS
1	B	24	GLN
1	B	29	ASN
1	B	46	ASN

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Mol	Chain	Res	Type
1	B	144	ASN
1	B	215	ASN
1	B	216	ASN
1	B	220	ASN
1	B	285	GLN
1	B	302	ASN
1	B	307	HIS
1	C	24	GLN
1	C	185	ASN
1	C	200	GLN
1	C	307	HIS

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 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	L98	B	501	2	15,16,16	1.64	4 (26%)	20,21,21	1.18	2 (10%)
3	L98	C	601	2	15,16,16	1.67	4 (26%)	20,21,21	1.33	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	L98	A	401	2	15,16,16	1.89	5 (33%)	20,21,21	1.41	2 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	L98	B	501	2	-	2/14/14/14	0/1/1/1
3	L98	C	601	2	-	2/14/14/14	0/1/1/1
3	L98	A	401	2	-	5/14/14/14	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	L98	C5-N9	-3.55	1.34	1.41
3	A	401	L98	C10-N9	-3.37	1.33	1.38
3	B	501	L98	C5-N9	-2.99	1.35	1.41
3	B	501	L98	C10-N9	-2.93	1.34	1.38
3	B	501	L98	C4-C3	2.79	1.43	1.39
3	C	601	L98	C5-N9	-2.77	1.36	1.41
3	A	401	L98	C4-C3	2.33	1.42	1.39
3	A	401	L98	C4-C5	2.28	1.43	1.39
3	C	601	L98	C4-C3	2.27	1.42	1.39
3	C	601	L98	C6-C3	2.27	1.42	1.39
3	C	601	L98	C4-C5	2.13	1.42	1.39
3	B	501	L98	C6-C3	2.09	1.42	1.39
3	A	401	L98	C1-S	-2.01	1.77	1.81

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	L98	C2-C1-S	-4.20	109.62	114.15
3	C	601	L98	O15-C13-O14	-3.38	116.41	124.08
3	B	501	L98	O15-C13-O14	-2.91	117.48	124.08
3	A	401	L98	O15-C13-O14	-2.75	117.84	124.08
3	C	601	L98	C2-C1-S	-2.14	111.84	114.15
3	B	501	L98	O15-C13-C2	2.02	121.55	114.42

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	601	L98	C13-C2-C3-C4
3	A	401	L98	C13-C2-C3-C4
3	A	401	L98	C13-C2-C3-C6
3	C	601	L98	C13-C2-C3-C6
3	A	401	L98	O15-C13-C2-C1
3	B	501	L98	C13-C2-C3-C4
3	B	501	L98	C13-C2-C3-C6
3	A	401	L98	O14-C13-C2-C3
3	A	401	L98	O15-C13-C2-C3

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	501	L98	1	0
3	C	601	L98	3	0
3	A	401	L98	3	0

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 [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	305/306 (99%)	-0.66	0	100 100	19, 28, 41, 59	0
1	B	305/306 (99%)	-0.65	1 (0%)	90 89	17, 28, 43, 63	0
1	C	304/306 (99%)	-0.10	1 (0%)	90 89	25, 41, 60, 75	0
All	All	914/918 (99%)	-0.47	2 (0%)	91 90	17, 31, 54, 75	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	248	TYR	2.5
1	C	185	ASN	2.4

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(Å ²)	Q<0.9
3	L98	C	601	16/16	0.89	0.08	43,61,76,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	L98	B	501	16/16	0.92	0.07	34,38,51,57	0
3	L98	A	401	16/16	0.92	0.07	31,37,44,46	0
2	ZN	B	500	1/1	0.95	0.04	28,28,28,28	0
2	ZN	A	400	1/1	0.96	0.04	28,28,28,28	0
2	ZN	C	600	1/1	0.99	0.03	32,32,32,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.