



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 16, 2023 – 04:03 AM EDT

PDB ID : 1ZG8  
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](mailto: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 : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35

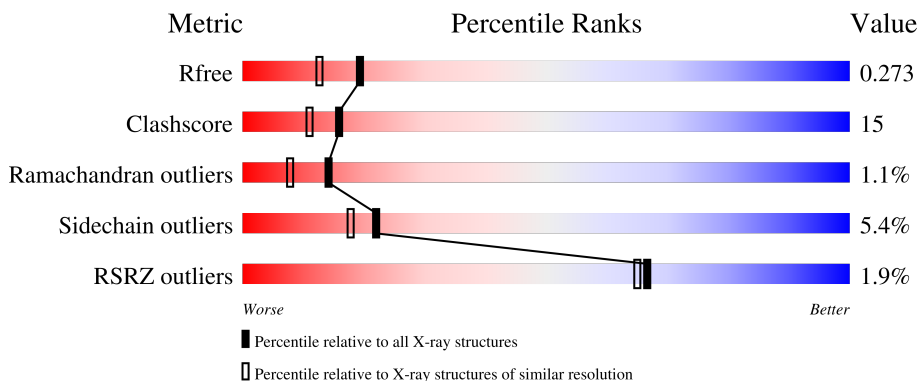
# 1 Overall quality at a glance

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))
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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  $\geq 3$ , 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	 76% 21%
1	B	306	 71% 26%
1	C	306	 57% 37% 5%

## 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.

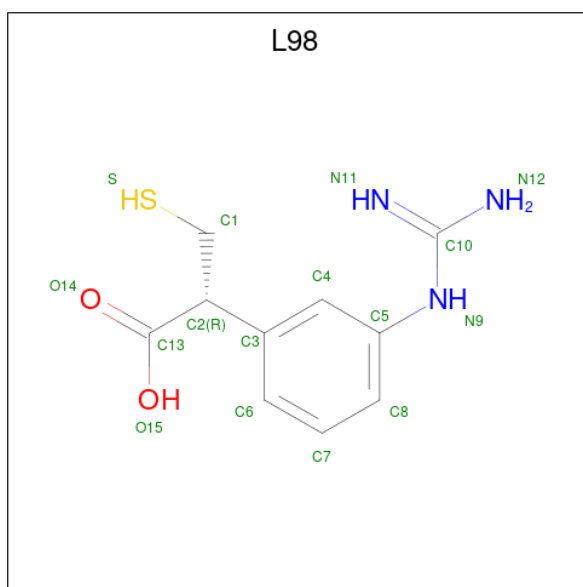
- Molecule 1 is a protein called procarboxypeptidase B.

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

- Molecule 2 is ZINC ION (three-letter code: 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-SULFANYLPROPANOIC ACID (three-letter code: L98) (formula: C<sub>10</sub>H<sub>13</sub>N<sub>3</sub>O<sub>2</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
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		

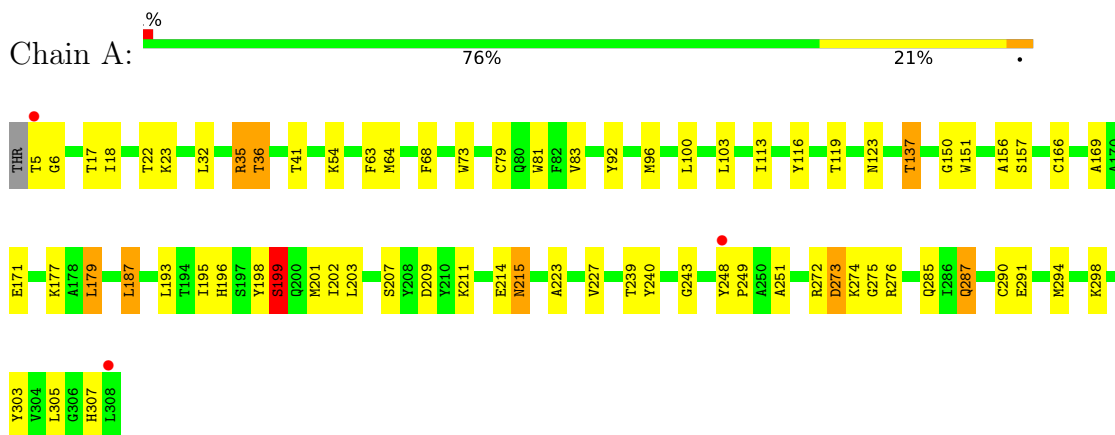
- Molecule 4 is water.

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		

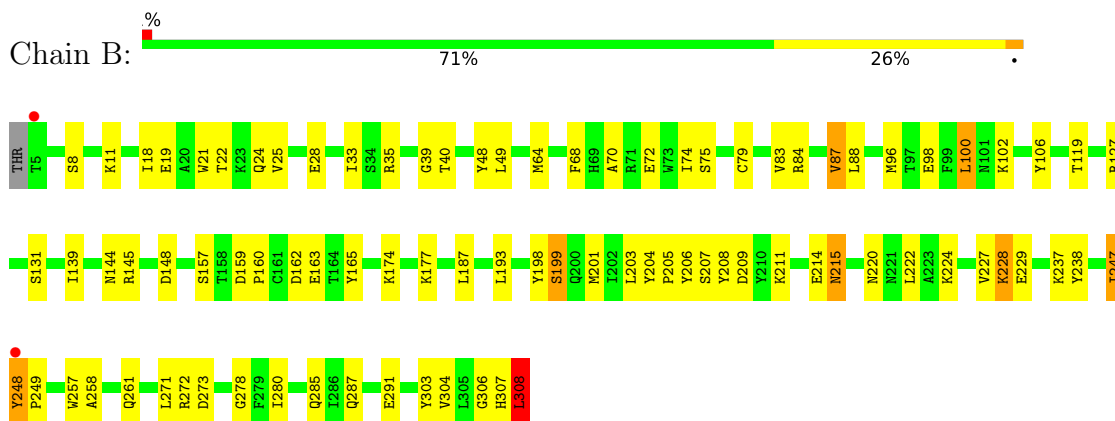
### 3 Residue-property plots [i](#)

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.

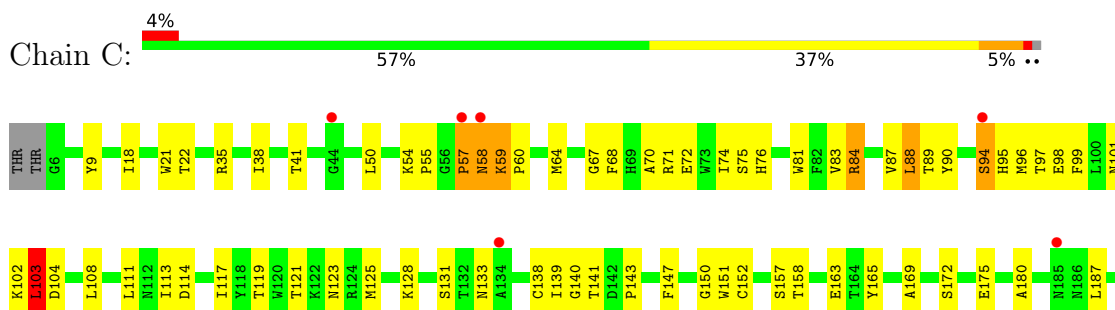
- Molecule 1: procarboxypeptidase B

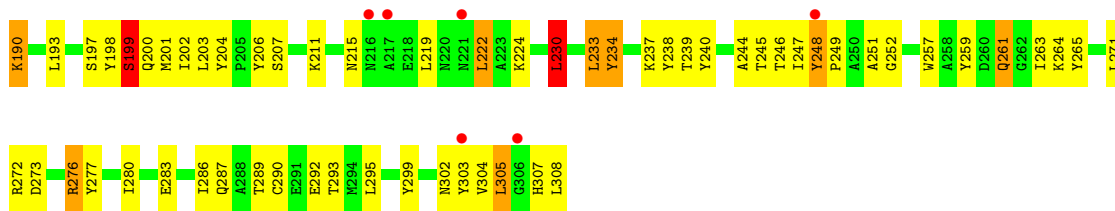


- Molecule 1: procarboxypeptidase B



- Molecule 1: procarboxypeptidase B





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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) 97.0 (8.00-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.62 (at 2.00Å)	Xtrriage
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.214 , 0.294 0.203 , 0.273	Depositor DCC
$R_{free}$ test set	2464 reflections (4.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.3	Xtrriage
Anisotropy	0.481	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 88.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7800	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: L98, ZN

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	0.63	0/2512	0.79	0/3418
1	B	0.61	0/2512	0.78	1/3418 (0.0%)
1	C	0.56	0/2505	0.78	3/3408 (0.1%)
All	All	0.60	0/7529	0.78	4/10244 (0.0%)

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

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	C	88	LEU	CA-CB-CG	5.78	128.59	115.30
1	C	230	LEU	CA-CB-CG	5.65	128.30	115.30
1	C	103	LEU	CA-CB-CG	5.61	128.21	115.30
1	B	308	LEU	CA-CB-CG	5.31	127.51	115.30

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 [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	2443	0	2324	47	0
1	B	2443	0	2324	60	0
1	C	2436	0	2317	104	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	210	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 (210) 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: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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:276:ARG:HG3	1:C:276:ARG:HH11	1.51	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: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
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:B:201:MET:HE2	1:B:203:LEU:HD21	1.83	0.59
1:A:150:GLY:O	1:A:251:ALA:HB1	2.03	0.59
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:201:MET:CE	1:C:247:ILE:HD13	2.33	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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:54:LYS:HZ2	1:C:101:ASN:HA	1.74	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:C:230:LEU:HD13	1:C:292:GLU:HB2	1.92	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:287:GLN:HG3	4:A:1323:HOH:O	2.11	0.50
1:C:201:MET:HE1	1:C:247:ILE:HD13	1.93	0.50
1:C:283:GLU:O	1:C:286:ILE:HG13	2.12	0.50
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:54:LYS:HD3	1:C:90:TYR:HH	1.76	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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:C:201:MET:HB2	1:C:201:MET:HE2	1.75	0.46
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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:201:MET:HE2	1:B:203:LEU:HD11	1.98	0.44
1:A:195:ILE:C	1:A:196:HIS:CD2	2.91	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: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: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: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:96:MET:HE3	1:B:100:LEU:HD22	2.02	0.42
1:A:96:MET:HE2	1:A:100:LEU:HG	2.01	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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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 [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	303/306 (99%)	289 (95%)	13 (4%)	1 (0%)	41	37
1	B	303/306 (99%)	292 (96%)	8 (3%)	3 (1%)	15	9
1	C	302/306 (99%)	274 (91%)	22 (7%)	6 (2%)	7	3
All	All	908/918 (99%)	855 (94%)	43 (5%)	10 (1%)	14	8

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
1	C	55	PRO
1	C	59	LYS
1	B	280	ILE

### 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	258/259 (100%)	245 (95%)	13 (5%)	24	20
1	B	258/259 (100%)	245 (95%)	13 (5%)	24	20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	257/259 (99%)	241 (94%)	16 (6%)	18	13
All	All	773/777 (100%)	731 (95%)	42 (5%)	22	18

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
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	199	SER
1	A	214	GLU
1	A	215	ASN
1	A	248	TYR
1	A	273	ASP
1	A	287	GLN
1	B	25	VAL
1	B	35	ARG
1	B	68	PHE
1	B	87	VAL
1	B	100	LEU
1	B	144	ASN
1	B	148	ASP
1	B	214	GLU
1	B	215	ASN
1	B	222	LEU
1	B	228	LYS
1	B	248	TYR
1	B	308	LEU
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

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	C	233	LEU
1	C	237	LYS
1	C	245	THR
1	C	248	TYR
1	C	261	GLN
1	C	276	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
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	46	ASN
1	B	144	ASN
1	B	215	ASN
1	B	285	GLN
1	B	307	HIS
1	C	24	GLN
1	C	185	ASN
1	C	186	ASN
1	C	200	GLN
1	C	261	GLN
1	C	307	HIS

### 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 monosaccharides 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	1.60	4 (26%)	21,21,21	1.19	1 (4%)
3	L98	C	601	2	15,16,16	1.63	4 (26%)	21,21,21	1.37	3 (14%)
3	L98	A	401	2	15,16,16	1.86	4 (26%)	21,21,21	1.43	3 (14%)

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	-	2/14/14/14	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	L98	C5-N9	-3.54	1.34	1.41
3	A	401	L98	C10-N9	-3.50	1.33	1.37
3	B	501	L98	C10-N9	-3.00	1.34	1.37
3	B	501	L98	C5-N9	-2.98	1.35	1.41
3	C	601	L98	C5-N9	-2.76	1.36	1.41
3	B	501	L98	C4-C3	2.64	1.43	1.39
3	A	401	L98	C4-C5	2.28	1.43	1.39
3	C	601	L98	C6-C3	2.27	1.42	1.39
3	A	401	L98	C4-C3	2.22	1.42	1.39
3	C	601	L98	C4-C3	2.16	1.42	1.39
3	C	601	L98	C4-C5	2.12	1.42	1.39
3	B	501	L98	C6-C3	2.09	1.42	1.39

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	L98	C2-C1-S	-4.17	109.62	114.19
3	C	601	L98	O15-C13-O14	-3.38	116.41	124.09
3	B	501	L98	O15-C13-O14	-2.91	117.48	124.09
3	A	401	L98	O15-C13-O14	-2.75	117.84	124.09
3	C	601	L98	C2-C1-S	-2.14	111.84	114.19
3	A	401	L98	C3-C2-C13	2.11	112.57	109.27
3	C	601	L98	C3-C2-C13	2.02	112.43	109.27

There are no chirality outliers.

All (6) torsion outliers are listed below:

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

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	305/306 (99%)	-0.52	3 (0%) 82 81	19, 28, 41, 59	0
1	B	305/306 (99%)	-0.51	2 (0%) 87 87	17, 28, 43, 63	0
1	C	304/306 (99%)	0.21	12 (3%) 39 38	25, 41, 60, 75	0
All	All	914/918 (99%)	-0.27	17 (1%) 66 65	17, 31, 54, 75	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	217	ALA	4.2
1	C	58	ASN	4.0
1	C	185	ASN	3.9
1	C	57	PRO	3.6
1	C	306	GLY	3.0
1	A	248	TYR	2.9
1	C	94	SER	2.8
1	B	5	THR	2.7
1	C	134	ALA	2.6
1	A	308	LEU	2.3
1	A	5	THR	2.3
1	B	248	TYR	2.3
1	C	44	GLY	2.3
1	C	216	ASN	2.2
1	C	221	ASN	2.2
1	C	248	TYR	2.1
1	C	303	TYR	2.1

### 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 monosaccharides 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	L98	C	601	16/16	0.90	0.14	43,61,76,77	0
3	L98	A	401	16/16	0.94	0.11	31,37,44,46	0
3	L98	B	501	16/16	0.95	0.11	34,38,51,57	0
2	ZN	B	500	1/1	0.97	0.05	28,28,28,28	0
2	ZN	A	400	1/1	0.98	0.05	28,28,28,28	0
2	ZN	C	600	1/1	0.99	0.02	32,32,32,32	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.