



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 06:51 am BST

PDB ID : 2V8V  
Title : Crystal structure of mutant R322A of beta-alanine synthase from *Saccharomyces kluyveri*  
Authors : Lundgren, S.; Andersen, B.; Piskur, J.; Dobritsch, D.  
Deposited on : 2007-08-15  
Resolution : 2.90 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.

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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 : 2.11  
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) : 2.11

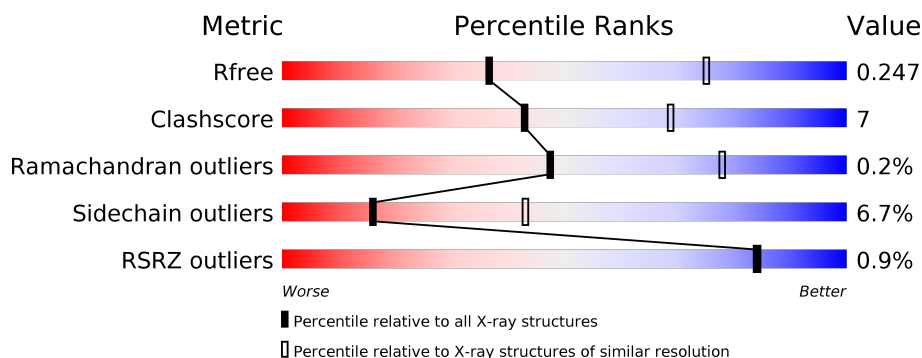
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	474	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 16%, orange 16%, yellow 16%, green 74%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>74%</span> <span>16%</span> <span>• 8%</span> </div> </div>
1	B	474	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 15%, green 74%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>74%</span> <span>15%</span> <span>• 9%</span> </div> </div>
1	C	474	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 2%, yellow 14%, green 76%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>76%</span> <span>14%</span> <span>• 9%</span> </div> </div>
1	D	474	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, orange 0%, yellow 13%, green 77%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>77%</span> <span>13%</span> <span>• 8%</span> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13410 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 BETA-ALANINE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	435	Total	C	N	O	S	0	1	0
			3360	2120	575	649	16			
1	B	431	Total	C	N	O	S	0	0	0
			3324	2097	567	644	16			
1	C	431	Total	C	N	O	S	0	0	0
			3324	2097	567	644	16			
1	D	435	Total	C	N	O	S	0	0	0
			3355	2117	572	650	16			

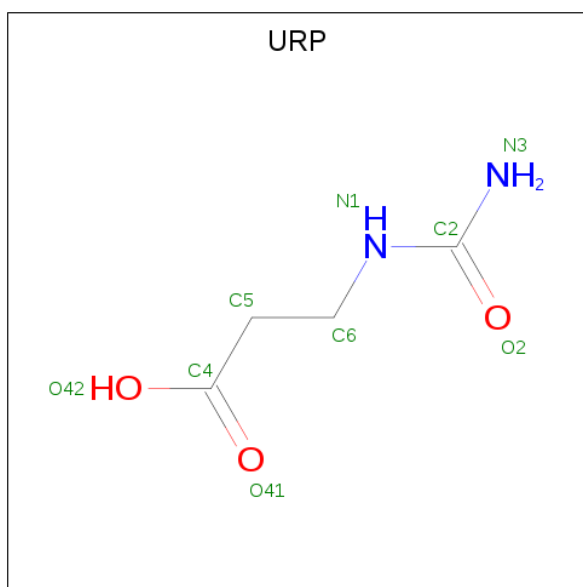
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	322	ALA	ARG	engineered mutation	UNP Q96W94
B	322	ALA	ARG	engineered mutation	UNP Q96W94
C	322	ALA	ARG	engineered mutation	UNP Q96W94
D	322	ALA	ARG	engineered mutation	UNP Q96W94

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

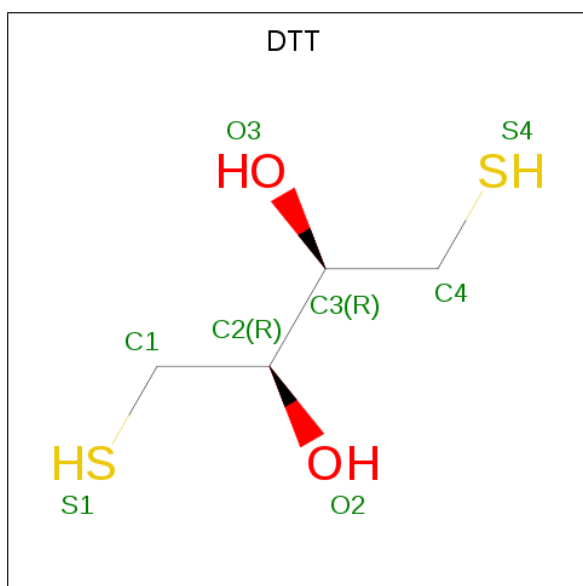
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Zn	0	0
			2	2		
2	A	2	Total	Zn	0	0
			2	2		
2	D	2	Total	Zn	0	0
			2	2		
2	C	2	Total	Zn	0	0
			2	2		

- Molecule 3 is N-(AMINOCARBONYL)-BETA-ALANINE (three-letter code: URP) (formula: C<sub>4</sub>H<sub>8</sub>N<sub>2</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			9	4	2	3		
3	C	1	Total	C	N	O	0	0
			9	4	2	3		
3	D	1	Total	C	N	O	0	0
			9	4	2	3		

- Molecule 4 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (three-letter code: DTT) (formula:  $C_4H_{10}O_2S_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	O	S	0	0
			8	4	2	2		

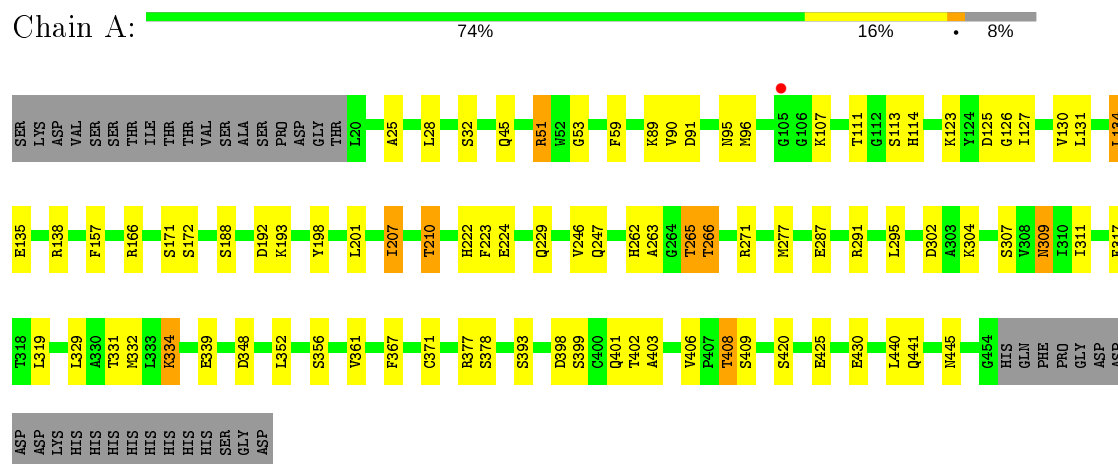
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O	0	0
			1	1		
5	B	1	Total	O	0	0
			1	1		
5	C	1	Total	O	0	0
			1	1		
5	D	1	Total	O	0	0
			1	1		

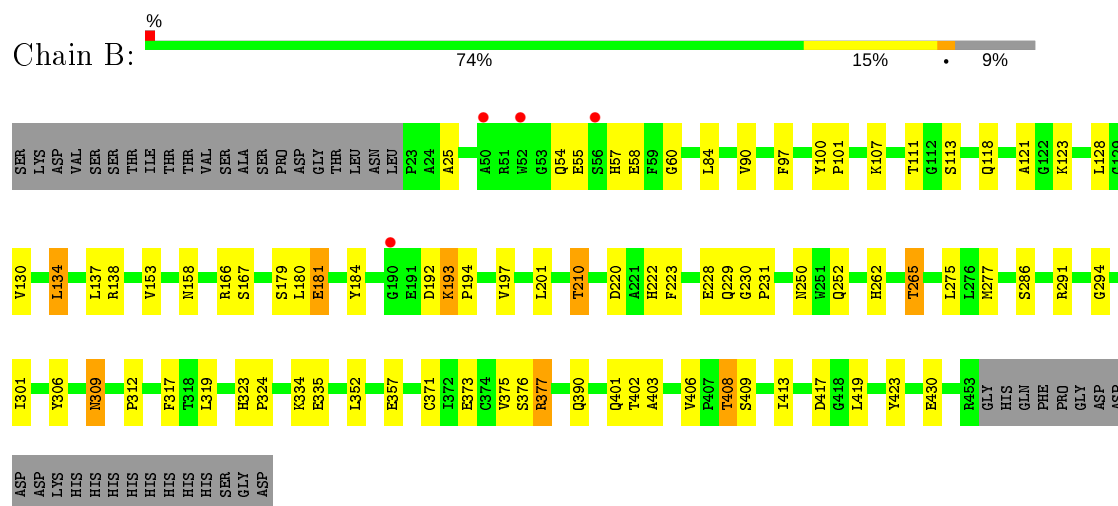
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

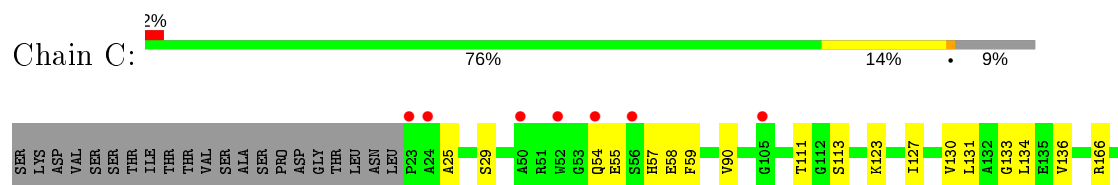
#### • Molecule 1: BETA-ALANINE SYNTHASE

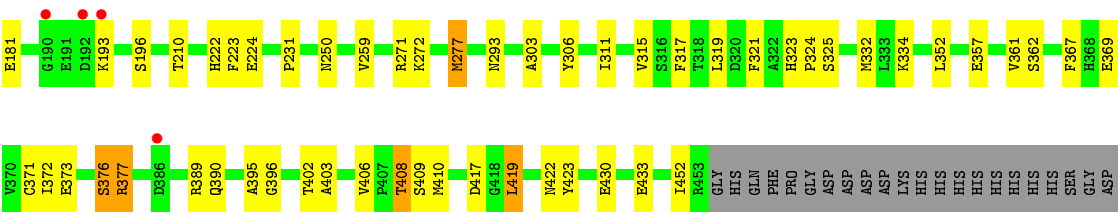


#### • Molecule 1: BETA-ALANINE SYNTHASE

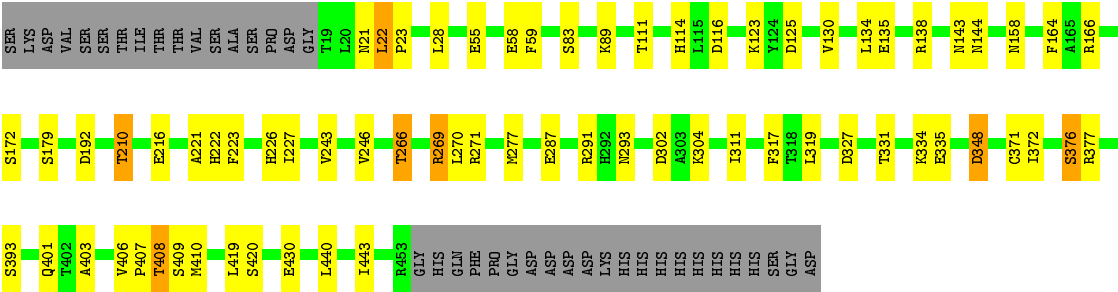


#### • Molecule 1: BETA-ALANINE SYNTHASE





● Molecule 1: BETA-ALANINE SYNTHASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.48Å 84.90Å 104.85Å 67.45° 67.81° 62.75°	Depositor
Resolution (Å)	45.00 – 2.90 43.80 – 2.90	Depositor EDS
% Data completeness (in resolution range)	93.5 (45.00-2.90) 84.6 (43.80-2.90)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.25 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.194 , 0.246 0.198 , 0.247	Depositor DCC
$R_{free}$ test set	2012 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.8	Xtriage
Anisotropy	0.390	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 27.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.430 for h,h-k,h-l	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	13410	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.54% 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: ZN, URP, DTT

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	0.59	0/3440	0.69	1/4666 (0.0%)
1	B	0.53	0/3401	0.64	0/4613
1	C	0.54	0/3401	0.66	0/4613
1	D	0.59	0/3432	0.67	1/4657 (0.0%)
All	All	0.56	0/13674	0.67	2/18549 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	125	ASP	CB-CG-OD1	6.58	124.22	118.30
1	D	125	ASP	CB-CG-OD1	5.87	123.58	118.30

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	3360	0	3252	57	0
1	B	3324	0	3209	50	0
1	C	3324	0	3208	38	0
1	D	3355	0	3243	45	0
2	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	B	9	0	7	0	0
3	C	9	0	7	2	0
3	D	9	0	7	0	0
4	C	8	0	9	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
All	All	13410	0	12942	178	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 (178) 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:D:403:ALA:HA	1:D:408:THR:CG2	2.04	0.86
1:A:265:THR:HG21	1:B:229:GLN:O	1.77	0.84
1:A:403:ALA:HA	1:A:408:THR:HG23	1.59	0.83
1:C:57:HIS:O	1:C:123:LYS:NZ	2.12	0.82
1:D:22:LEU:HB2	1:D:23:PRO:HD2	1.64	0.77
1:B:57:HIS:O	1:B:123:LYS:NZ	2.17	0.77
1:D:22:LEU:HD23	1:D:22:LEU:H	1.48	0.76
1:C:403:ALA:HA	1:C:408:THR:CG2	2.16	0.75
1:B:403:ALA:HA	1:B:408:THR:HG23	1.69	0.75
1:D:406:VAL:O	1:D:408:THR:HG22	1.87	0.74
1:A:406:VAL:O	1:A:408:THR:HG22	1.87	0.74
1:C:403:ALA:HA	1:C:408:THR:HG23	1.68	0.74
1:A:309:ASN:HD22	1:A:309:ASN:C	1.91	0.74
1:D:291:ARG:NH2	1:D:335:GLU:OE1	2.19	0.74
1:A:266:THR:HG23	1:B:231:PRO:HG3	1.70	0.74
1:A:403:ALA:HA	1:A:408:THR:CG2	2.17	0.73
1:A:59:PHE:O	1:A:123:LYS:HE2	1.89	0.73
1:D:22:LEU:N	1:D:22:LEU:CD2	2.55	0.70
1:D:22:LEU:H	1:D:22:LEU:CD2	2.03	0.70
1:B:403:ALA:HA	1:B:408:THR:CG2	2.22	0.69
1:B:84:LEU:HD21	1:B:138:ARG:HG3	1.73	0.69
1:C:59:PHE:O	1:C:123:LYS:HE2	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:403:ALA:HA	1:D:408:THR:HG21	1.76	0.68
1:A:28:LEU:HD12	1:A:440:LEU:HD11	1.76	0.67
1:B:309:ASN:HD22	1:B:309:ASN:H	1.42	0.67
1:C:317:PHE:HE1	1:C:319:LEU:HD21	1.59	0.67
1:D:55:GLU:HB2	1:D:58:GLU:HG3	1.77	0.66
1:B:262:HIS:HB3	1:B:265:THR:HG22	1.78	0.66
1:A:277:MET:HG3	1:A:352:LEU:HD22	1.77	0.66
1:C:395:ALA:HA	3:C:1457:URP:H51	1.79	0.64
1:C:231:PRO:HG3	1:D:266:THR:HG23	1.79	0.64
1:B:317:PHE:HE1	1:B:319:LEU:HD21	1.63	0.64
1:D:403:ALA:HA	1:D:408:THR:HG23	1.80	0.64
1:A:222:HIS:HB3	1:A:408:THR:HB	1.82	0.61
1:A:302:ASP:OD2	1:B:306:TYR:OH	2.19	0.60
1:A:135:GLU:OE1	1:A:135:GLU:HA	2.00	0.60
1:C:317:PHE:CE1	1:C:319:LEU:HD21	2.37	0.59
1:D:172:SER:HA	1:D:401:GLN:HE21	1.68	0.59
1:A:229:GLN:O	1:B:265:THR:HG21	2.03	0.59
1:A:171:SER:OG	1:A:398:ASP:OD1	2.19	0.58
1:A:371:CYS:HB2	1:A:409:SER:HB2	1.84	0.58
1:A:25:ALA:HB2	1:A:445:ASN:HD21	1.69	0.57
1:C:306:TYR:OH	1:D:302:ASP:OD2	2.21	0.57
1:C:389:ARG:HG2	1:C:390:GLN:O	2.05	0.57
1:D:28:LEU:HD12	1:D:440:LEU:HD11	1.88	0.56
1:C:406:VAL:O	1:C:408:THR:HG22	2.06	0.56
1:A:246:VAL:HG22	1:A:393:SER:HB3	1.88	0.55
1:B:371:CYS:HB3	1:B:409:SER:HB3	1.88	0.55
1:A:271:ARG:HG2	1:A:311:ILE:HD13	1.89	0.55
1:A:371:CYS:CB	1:A:409:SER:HB2	2.37	0.55
1:C:259:VAL:HG23	1:C:272:LYS:HD2	1.89	0.55
1:A:262:HIS:HB3	1:A:265:THR:HG22	1.89	0.54
1:B:252:GLN:HB2	1:B:319:LEU:HB2	1.89	0.53
1:C:373:GLU:O	1:C:377:ARG:HB2	2.08	0.53
1:B:317:PHE:CE1	1:B:319:LEU:HD21	2.43	0.53
1:C:271:ARG:HG2	1:C:311:ILE:HD13	1.91	0.53
1:D:317:PHE:CE1	1:D:319:LEU:HD21	2.44	0.53
1:D:222:HIS:HB3	1:D:408:THR:HB	1.90	0.53
1:B:371:CYS:O	1:B:375:VAL:HG23	2.09	0.52
1:B:90:VAL:O	1:B:210:THR:HG23	2.10	0.52
1:D:403:ALA:CA	1:D:408:THR:HG21	2.39	0.52
1:B:406:VAL:O	1:B:408:THR:HG22	2.10	0.52
1:B:323:HIS:ND1	1:B:324:PRO:HD2	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:373:GLU:O	1:B:377:ARG:HB2	2.10	0.52
1:D:22:LEU:HD23	1:D:22:LEU:N	2.16	0.52
1:B:222:HIS:HB3	1:B:408:THR:HB	1.92	0.52
1:A:309:ASN:C	1:A:309:ASN:ND2	2.61	0.51
1:D:403:ALA:N	1:D:408:THR:HG21	2.25	0.51
1:A:51[B]:ARG:NH1	1:A:53:GLY:O	2.35	0.51
1:D:158:ASN:HD21	1:D:164:PHE:HB2	1.75	0.51
1:D:372:ILE:O	1:D:376:SER:HB2	2.10	0.51
1:C:181:GLU:H	1:C:181:GLU:CD	2.14	0.51
1:B:402:THR:OG1	1:B:408:THR:HG21	2.12	0.50
1:A:207:ILE:O	1:A:207:ILE:HG22	2.12	0.49
1:B:277:MET:HG3	1:B:352:LEU:HD22	1.93	0.49
1:B:181:GLU:H	1:B:181:GLU:CD	2.15	0.49
1:C:111:THR:HA	1:C:223:PHE:O	2.13	0.49
1:D:158:ASN:ND2	1:D:164:PHE:HB2	2.27	0.49
1:A:378:SER:OG	1:A:441:GLN:HB3	2.12	0.49
1:D:22:LEU:HB2	1:D:23:PRO:CD	2.37	0.49
1:A:90:VAL:O	1:A:210:THR:HG23	2.13	0.49
1:C:422:ASN:OD1	1:C:423:TYR:N	2.46	0.49
1:A:157:PHE:CE1	1:A:201:LEU:HD21	2.48	0.48
1:D:59:PHE:O	1:D:123:LYS:HE2	2.14	0.48
1:A:247:GLN:HE22	1:A:295:LEU:HD12	1.79	0.47
1:A:329:LEU:O	1:A:332:MET:HB2	2.14	0.47
1:A:193:LYS:HE2	1:D:327:ASP:OD2	2.14	0.47
1:C:222:HIS:HB3	1:C:408:THR:HB	1.96	0.47
1:D:371:CYS:HB3	1:D:409:SER:HB3	1.96	0.47
1:D:111:THR:HA	1:D:223:PHE:O	2.14	0.47
1:A:111:THR:HA	1:A:223:PHE:O	2.15	0.47
1:B:262:HIS:HB3	1:B:265:THR:CG2	2.43	0.47
1:C:127:ILE:CG2	1:C:131:LEU:HD12	2.44	0.46
1:B:107:LYS:HE3	1:B:220:ASP:OD1	2.14	0.46
1:D:348:ASP:N	1:D:348:ASP:OD2	2.49	0.46
1:A:224:GLU:OE2	1:A:399:SER:OG	2.30	0.46
1:C:323:HIS:ND1	1:C:324:PRO:HD2	2.30	0.46
1:A:265:THR:HG23	1:B:230:GLY:HA2	1.97	0.46
1:A:263:ALA:O	1:A:271:ARG:NH2	2.48	0.46
1:C:55:GLU:HB2	1:C:58:GLU:HG3	1.96	0.46
1:C:419:LEU:HD11	1:C:422:ASN:HD22	1.81	0.46
1:D:226:HIS:HD1	1:D:227:ILE:N	2.13	0.46
1:D:269:ARG:HG2	1:D:270:LEU:HG	1.97	0.46
1:B:60:GLY:HA3	1:B:423:TYR:CD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:396:GLY:H	3:C:1457:URP:C4	2.29	0.46
1:C:303:ALA:HA	1:C:315:VAL:HG22	1.97	0.46
1:C:371:CYS:HB3	1:C:409:SER:HB3	1.98	0.45
1:D:221:ALA:HB1	1:D:407:PRO:O	2.17	0.45
1:B:111:THR:HA	1:B:223:PHE:O	2.17	0.45
1:B:60:GLY:HA3	1:B:423:TYR:HD2	1.81	0.45
1:A:25:ALA:HB2	1:A:445:ASN:ND2	2.32	0.45
1:B:291:ARG:NH2	1:B:335:GLU:OE1	2.49	0.45
1:A:291:ARG:HG3	1:A:291:ARG:HH11	1.81	0.45
1:D:143:ASN:O	1:D:144:ASN:HB2	2.17	0.45
1:A:91:ASP:OD1	1:A:95:ASN:HB2	2.16	0.45
1:B:100:TYR:HA	1:B:101:PRO:HD3	1.89	0.45
1:C:259:VAL:N	1:C:272:LYS:HB2	2.31	0.44
1:C:367:PHE:HB3	1:C:408:THR:O	2.18	0.44
1:B:401:GLN:NE2	1:B:401:GLN:HA	2.31	0.44
1:D:271:ARG:HG2	1:D:311:ILE:HD13	1.99	0.44
1:D:243:VAL:HB	1:D:410:MET:HB2	2.00	0.44
1:A:90:VAL:HG22	1:A:96:MET:HG2	2.00	0.44
1:B:275:LEU:HB2	1:B:312:PRO:HG2	1.99	0.44
1:A:352:LEU:N	1:A:352:LEU:HD12	2.33	0.44
1:D:114:HIS:HB2	1:D:116:ASP:OD1	2.18	0.44
1:C:127:ILE:HG23	1:C:131:LEU:HD12	2.00	0.44
1:D:277:MET:HE2	1:D:277:MET:HB3	1.67	0.44
1:D:419:LEU:HG	1:D:420:SER:N	2.33	0.44
1:C:361:VAL:HG12	1:C:362:SER:N	2.32	0.43
1:B:301:ILE:HG13	1:B:317:PHE:HB3	2.00	0.43
1:B:55:GLU:HB2	1:B:58:GLU:HG3	2.00	0.43
1:A:339:GLU:OE1	1:A:339:GLU:HA	2.17	0.43
1:B:97:PHE:N	1:B:97:PHE:CD1	2.86	0.43
1:C:323:HIS:CG	1:C:324:PRO:HD2	2.53	0.43
1:B:197:VAL:O	1:B:201:LEU:HG	2.19	0.43
1:D:246:VAL:HG22	1:D:393:SER:HB3	2.01	0.43
1:A:198:TYR:CE2	1:D:293:ASN:HB2	2.53	0.42
1:A:262:HIS:HB3	1:A:265:THR:CG2	2.48	0.42
1:A:277:MET:HB3	1:A:277:MET:HE2	1.66	0.42
1:B:134:LEU:HD22	1:B:138:ARG:HD3	2.01	0.42
1:C:259:VAL:H	1:C:272:LYS:HB2	1.84	0.42
1:D:89:LYS:HB3	1:D:210:THR:HG21	2.00	0.42
1:C:403:ALA:N	1:C:408:THR:HG21	2.35	0.42
1:A:317:PHE:CE1	1:A:319:LEU:HD21	2.54	0.42
1:A:51[B]:ARG:HB3	1:A:51[B]:ARG:HH11	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:LYS:HG2	1:B:193:LYS:O	2.19	0.42
1:A:334:LYS:HE2	1:A:334:LYS:HB3	1.79	0.42
1:A:402:THR:OG1	1:A:408:THR:HG21	2.20	0.42
1:A:265:THR:CG2	1:B:229:GLN:O	2.60	0.42
1:A:127:ILE:O	1:A:131:LEU:HB2	2.20	0.41
1:B:371:CYS:HB3	1:B:409:SER:CB	2.49	0.41
1:A:89:LYS:HB3	1:A:210:THR:HG21	2.02	0.41
1:B:180:LEU:HD11	1:B:184:TYR:CE1	2.56	0.41
1:B:193:LYS:O	1:B:193:LYS:CG	2.68	0.41
1:A:367:PHE:HB3	1:A:408:THR:O	2.20	0.41
1:C:133:GLY:O	1:C:136:VAL:HB	2.21	0.41
1:D:172:SER:HA	1:D:401:GLN:NE2	2.33	0.41
1:C:321:PHE:HD2	1:C:332:MET:HE3	1.86	0.41
1:A:420:SER:HA	1:A:425:GLU:HG3	2.02	0.41
1:B:128:LEU:HD22	1:B:413:ILE:HD11	2.02	0.41
1:A:134:LEU:HD22	1:A:138:ARG:HG3	2.03	0.41
1:A:265:THR:HG23	1:B:230:GLY:CA	2.51	0.41
1:D:135:GLU:HA	1:D:138:ARG:HB2	2.03	0.41
1:A:131:LEU:HD23	1:A:131:LEU:HA	1.88	0.41
1:B:118:GLN:HB2	1:B:121:ALA:HB2	2.03	0.41
1:B:137:LEU:HD11	1:B:153:VAL:HG23	2.03	0.41
1:D:22:LEU:N	1:D:22:LEU:HD22	2.32	0.41
1:A:114:HIS:CE1	1:A:126:GLY:HA3	2.56	0.40
1:B:192:ASP:O	1:B:194:PRO:HD3	2.20	0.40
1:C:224:GLU:HB3	1:C:410:MET:HG2	2.02	0.40
1:A:172:SER:HA	1:A:401:GLN:HE21	1.86	0.40
1:C:372:ILE:O	1:C:376:SER:HB3	2.21	0.40
1:D:111:THR:HB	1:D:443:ILE:HD11	2.03	0.40
1:B:294:GLY:CA	1:B:323:HIS:HD2	2.34	0.40
1:C:402:THR:OG1	1:C:408:THR:HG21	2.21	0.40
1:C:277:MET:HG3	1:C:352:LEU:HD22	2.04	0.40
1:A:157:PHE:CD1	1:A:201:LEU:HD21	2.56	0.40
1:B:306:TYR:HE2	1:D:21:ASN:HD21	1.69	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	434/474 (92%)	423 (98%)	11 (2%)	0	100	100
1	B	429/474 (90%)	412 (96%)	15 (4%)	2 (0%)	29	61
1	C	429/474 (90%)	412 (96%)	16 (4%)	1 (0%)	47	78
1	D	433/474 (91%)	420 (97%)	13 (3%)	0	100	100
All	All	1725/1896 (91%)	1667 (97%)	55 (3%)	3 (0%)	47	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	25	ALA
1	C	25	ALA
1	B	158	ASN

### 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	358/392 (91%)	331 (92%)	27 (8%)	13	37
1	B	354/392 (90%)	330 (93%)	24 (7%)	16	42
1	C	354/392 (90%)	329 (93%)	25 (7%)	14	40
1	D	358/392 (91%)	338 (94%)	20 (6%)	21	52
All	All	1424/1568 (91%)	1328 (93%)	96 (7%)	16	43

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	SER
1	A	45	GLN
1	A	51[A]	ARG
1	A	51[B]	ARG
1	A	107	LYS
1	A	113	SER
1	A	130	VAL
1	A	134	LEU
1	A	166	ARG
1	A	188	SER
1	A	192	ASP
1	A	207	ILE
1	A	210	THR
1	A	265	THR
1	A	266	THR
1	A	287	GLU
1	A	304	LYS
1	A	307	SER
1	A	309	ASN
1	A	331	THR
1	A	334	LYS
1	A	348	ASP
1	A	356	SER
1	A	361	VAL
1	A	377	ARG
1	A	408	THR
1	A	430	GLU
1	B	54	GLN
1	B	113	SER
1	B	130	VAL
1	B	134	LEU
1	B	166	ARG
1	B	167	SER
1	B	179	SER
1	B	181	GLU
1	B	193	LYS
1	B	210	THR
1	B	228	GLU
1	B	250	ASN
1	B	265	THR
1	B	286	SER
1	B	309	ASN
1	B	334	LYS

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Mol	Chain	Res	Type
1	B	357	GLU
1	B	376	SER
1	B	377	ARG
1	B	390	GLN
1	B	408	THR
1	B	417	ASP
1	B	419	LEU
1	B	430	GLU
1	C	29	SER
1	C	54	GLN
1	C	90	VAL
1	C	113	SER
1	C	130	VAL
1	C	134	LEU
1	C	166	ARG
1	C	193	LYS
1	C	196	SER
1	C	210	THR
1	C	250	ASN
1	C	277	MET
1	C	293	ASN
1	C	325	SER
1	C	334	LYS
1	C	357	GLU
1	C	369	GLU
1	C	376	SER
1	C	377	ARG
1	C	408	THR
1	C	417	ASP
1	C	419	LEU
1	C	430	GLU
1	C	433	GLU
1	C	452	ILE
1	D	22	LEU
1	D	83	SER
1	D	130	VAL
1	D	134	LEU
1	D	166	ARG
1	D	179	SER
1	D	192	ASP
1	D	210	THR
1	D	216	GLU

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Mol	Chain	Res	Type
1	D	266	THR
1	D	269	ARG
1	D	287	GLU
1	D	304	LYS
1	D	331	THR
1	D	334	LYS
1	D	348	ASP
1	D	376	SER
1	D	377	ARG
1	D	408	THR
1	D	430	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	54	GLN
1	A	57	HIS
1	A	143	ASN
1	A	158	ASN
1	A	247	GLN
1	A	309	ASN
1	A	390	GLN
1	A	401	GLN
1	A	445	ASN
1	B	54	GLN
1	B	203	ASN
1	B	250	ASN
1	B	309	ASN
1	B	401	GLN
1	C	54	GLN
1	C	203	ASN
1	C	250	ASN
1	C	366	ASN
1	C	405	HIS
1	C	445	ASN
1	D	57	HIS
1	D	158	ASN
1	D	217	ASN
1	D	250	ASN
1	D	397	HIS
1	D	401	GLN

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Mol	Chain	Res	Type
1	D	405	HIS
1	D	445	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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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	$\# Z  > 2$
4	DTT	C	1456	1	7,7,7	0.38	0	4,8,8	1.28	0
3	URP	D	1456	-	5,8,8	0.60	0	6,9,9	1.41	1 (16%)
3	URP	B	1456	-	5,8,8	0.52	0	6,9,9	0.70	0
3	URP	C	1457	-	5,8,8	0.61	0	6,9,9	1.35	0

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
4	DTT	C	1456	1	-	2/8/8/8	-
3	URP	D	1456	-	-	3/4/6/6	-
3	URP	B	1456	-	-	2/4/6/6	-
3	URP	C	1457	-	-	3/4/6/6	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1456	URP	N3-C2-N1	2.04	119.01	116.85

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1457	URP	C4-C5-C6-N1
3	D	1456	URP	C4-C5-C6-N1
4	C	1456	DTT	C2-C3-C4-S4
3	C	1457	URP	O2-C2-N1-C6
3	C	1457	URP	N3-C2-N1-C6
3	D	1456	URP	O2-C2-N1-C6
3	D	1456	URP	N3-C2-N1-C6
3	B	1456	URP	O2-C2-N1-C6
3	B	1456	URP	N3-C2-N1-C6
4	C	1456	DTT	O3-C3-C4-S4

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1457	URP	2	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 ⓘ

### 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, 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	435/474 (91%)	-0.36	1 (0%) 95 95	30, 36, 39, 42	0
1	B	431/474 (90%)	-0.12	4 (0%) 84 84	30, 36, 38, 42	0
1	C	431/474 (90%)	-0.11	11 (2%) 56 52	30, 36, 39, 41	0
1	D	435/474 (91%)	-0.35	0 100 100	30, 36, 39, 43	0
All	All	1732/1896 (91%)	-0.24	16 (0%) 84 84	30, 36, 39, 43	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	105	GLY	4.1
1	B	190	GLY	3.9
1	A	105	GLY	2.9
1	C	192	ASP	2.7
1	B	56	SER	2.5
1	C	24	ALA	2.5
1	C	190	GLY	2.5
1	B	50	ALA	2.4
1	C	50	ALA	2.2
1	C	56	SER	2.2
1	C	52	TRP	2.2
1	B	52	TRP	2.1
1	C	54	GLN	2.1
1	C	386	ASP	2.0
1	C	23	PRO	2.0
1	C	193	LYS	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

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( $\text{\AA}^2$ )	Q<0.9
3	URP	C	1457	9/9	0.90	0.31	52,56,63,64	0
4	DTT	C	1456	8/8	0.92	0.17	54,62,64,67	0
3	URP	D	1456	9/9	0.93	0.28	75,76,77,78	0
3	URP	B	1456	9/9	0.93	0.22	46,49,50,51	0
2	ZN	C	1455	1/1	0.93	0.05	36,36,36,36	0
2	ZN	B	1455	1/1	0.99	0.04	38,38,38,38	0
2	ZN	A	1455	1/1	0.99	0.04	29,29,29,29	0
2	ZN	C	1454	1/1	0.99	0.02	34,34,34,34	0
2	ZN	A	1456	1/1	0.99	0.03	35,35,35,35	0
2	ZN	B	1454	1/1	0.99	0.03	36,36,36,36	0
2	ZN	D	1455	1/1	1.00	0.02	33,33,33,33	0
2	ZN	D	1454	1/1	1.00	0.05	29,29,29,29	0

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

There are no such residues in this entry.