



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2023 – 06:53 PM EDT

PDB ID : 2IHU  
Title : Carboxyethylarginine synthase from *Streptomyces clavuligerus*: putative reaction intermediate complex  
Authors : Caines, M.E.; Schofield, C.J.  
Deposited on : 2006-09-27  
Resolution : 2.05 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>.

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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 : **FAILED**  
Xtriage (Phenix) : 1.13  
EDS : 2.35  
buster-report : **FAILED**  
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

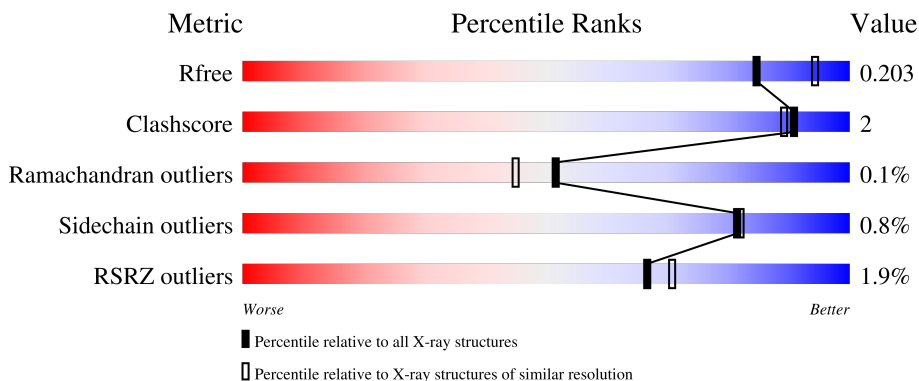
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	573	 2% 93%
1	B	573	 2% 92%
1	C	573	 2% 94%
1	D	573	 2% 92%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	TP8	C	600[A]	X	-	-	-
5	TAR	A	603	X	-	-	-
5	TAR	D	603	X	-	-	-

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 18287 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 Carboxyethylarginine synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	562	Total 4223	C 2679	N 728	O 802	S 14	39	1	0
1	B	552	Total 4168	C 2642	N 720	O 792	S 14	37	3	0
1	C	551	Total 4158	C 2636	N 719	O 790	S 13	32	3	0
1	D	551	Total 4162	C 2639	N 722	O 787	S 14	53	3	0

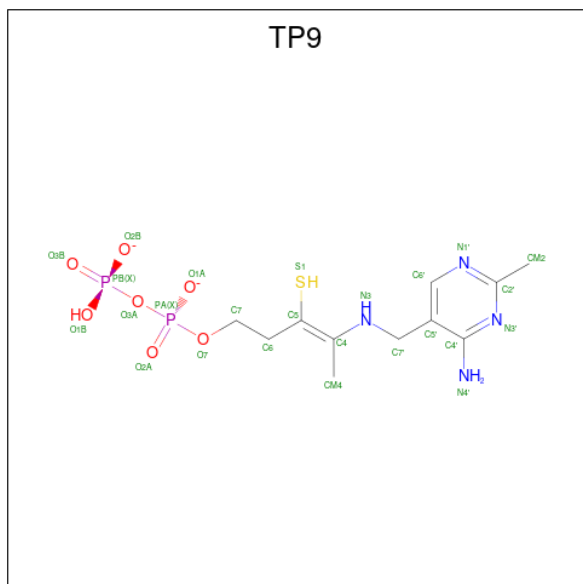
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

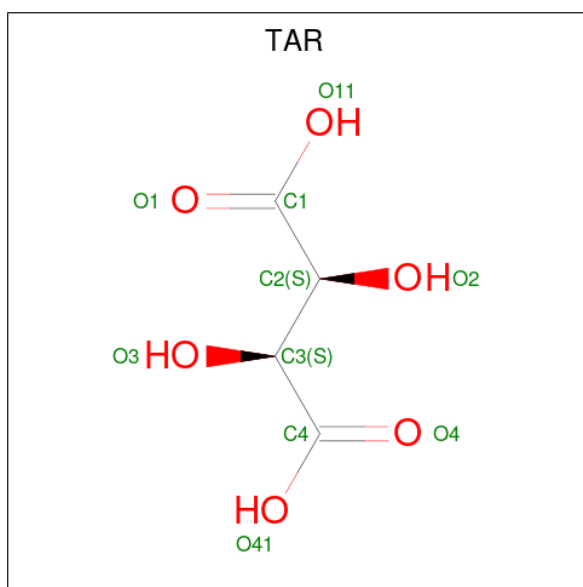
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total 2	K 2	0	0
3	B	1	Total 1	K 1	0	0
3	C	2	Total 2	K 2	0	0
3	D	1	Total 1	K 1	0	0

- Molecule 4 is (3Z)-4-[[[(4-AMINO-2-METHYLPYRIMIDIN-5-YL)METHYL]AMINO}-3-MERCAPTOPENT-3-EN-1-YL TRIHYDROGEN DIPHOSPHATE (three-letter code: TP9) (formula: C<sub>11</sub>H<sub>18</sub>N<sub>4</sub>O<sub>7</sub>P<sub>2</sub>S).



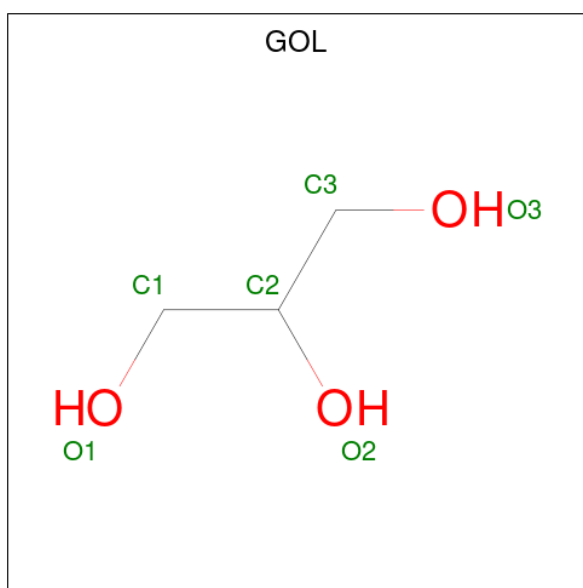
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	P			S
4	A	1	Total	C	N	O	P	S	0	0
			25	11	4	7	2	1		
4	B	1	Total	C	N	O	P	S	0	0
			25	11	4	7	2	1		
4	C	1	Total	C	N	O	P	S	0	1
			25	11	4	7	2	1		
4	D	1	Total	C	N	O	P	S	0	0
			25	11	4	7	2	1		

- Molecule 5 is D(-)-TARTARIC ACID (three-letter code: TAR) (formula: C<sub>4</sub>H<sub>6</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			10	4	6		
5	D	1	Total	C	O	0	0
			10	4	6		

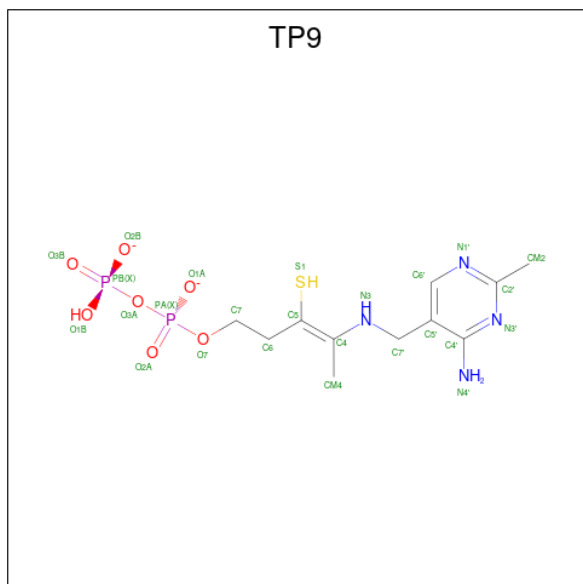
- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is 5-(2-{{[HYDROXY(PHOSPHONOOXY)PHOSPHORYL]OXY}}ETHYL)-2-

[(1Z)-1-HYDROXY-3-(PHOSPHONOXY)PROP-1-EN-1-YL]-3-[[[(4Z)-4-IMINO-2-METHYL-4,5-DIHYDROPYRIMIDIN-5-YL]METHYL]-4-METHYL-1,3-THIAZOL-3-IUM (three-letter code: TP9) (formula: C<sub>11</sub>H<sub>18</sub>N<sub>4</sub>O<sub>7</sub>P<sub>2</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	P			S
7	C	1	35	15	4	12	3	1	0	1

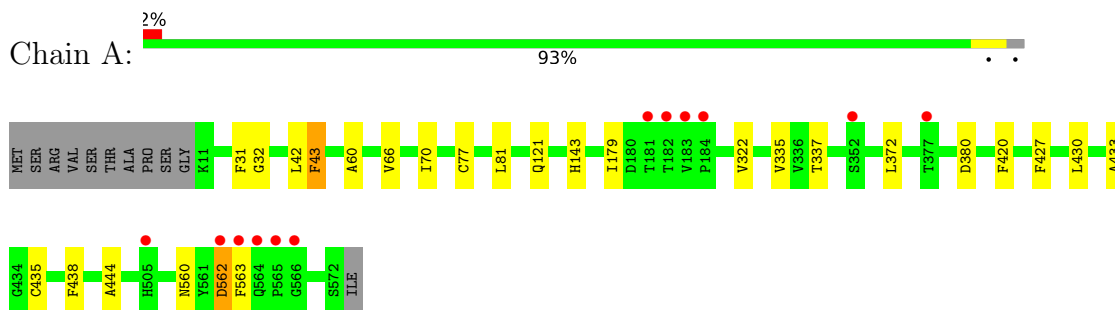
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	358	Total	O	0	0
			358	358		
8	B	377	Total	O	0	0
			377	377		
8	C	344	Total	O	0	0
			344	344		
8	D	326	Total	O	0	0
			326	326		

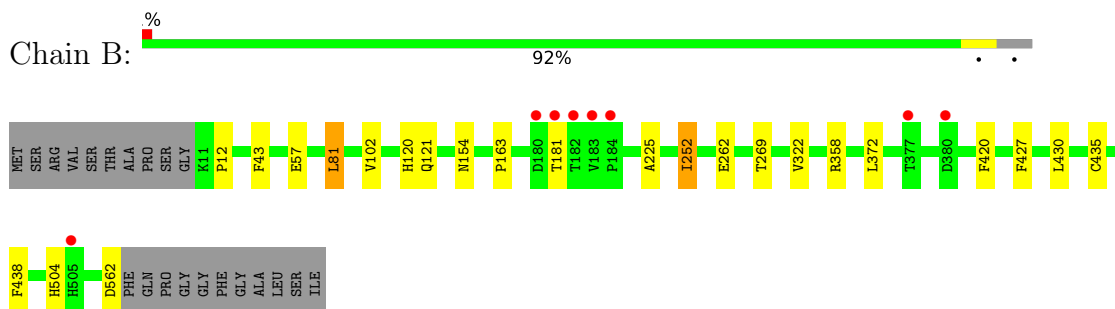
### 3 Residue-property plots

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

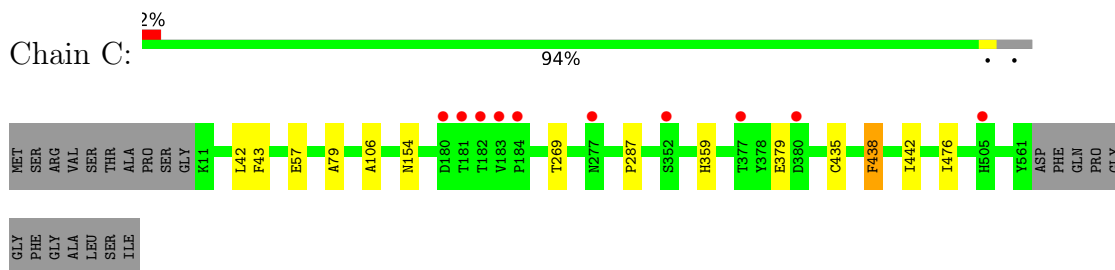
- Molecule 1: Carboxyethylarginine synthase



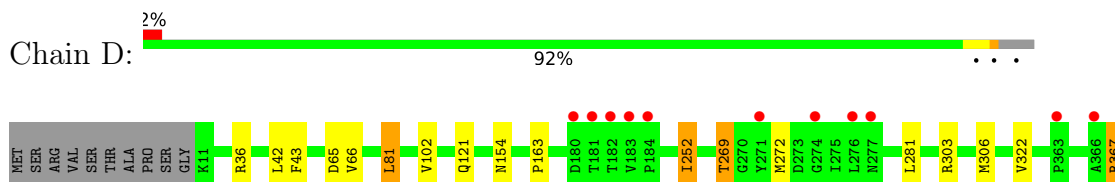
- Molecule 1: Carboxyethylarginine synthase



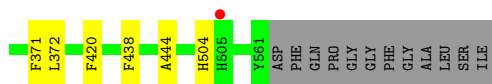
- Molecule 1: Carboxyethylarginine synthase



- Molecule 1: Carboxyethylarginine synthase







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	119.69Å 127.86Å 197.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.13 – 2.05 27.95 – 2.05	Depositor EDS
% Data completeness (in resolution range)	97.0 (28.13-2.05) 97.0 (27.95-2.05)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.89 (at 2.04Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.171 , 0.201 0.175 , 0.203	Depositor DCC
$R_{free}$ test set	8830 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.2	Xtrriage
Anisotropy	0.581	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 51.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	18287	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% 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: K, TAR, MG, GOL, TP9, TP8

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	0.45	0/4322	0.56	0/5902
1	B	0.56	1/4270 (0.0%)	0.62	3/5832 (0.1%)
1	C	0.46	1/4260 (0.0%)	0.55	0/5819
1	D	0.48	1/4264 (0.0%)	0.57	0/5823
All	All	0.49	3/17116 (0.0%)	0.58	3/23376 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	562	ASP	CB-CG	22.08	1.98	1.51
1	D	367	ARG	CB-CG	-9.12	1.27	1.52
1	C	379	GLU	CB-CG	6.07	1.63	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	562	ASP	CA-CB-CG	-13.03	84.72	113.40
1	B	562	ASP	CB-CG-OD2	-10.70	108.67	118.30
1	B	562	ASP	CB-CG-OD1	10.06	127.36	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	4223	0	4177	17	0
1	B	4168	0	4133	18	0
1	C	4158	0	4125	9	0
1	D	4162	0	4136	18	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
3	C	2	0	0	0	0
3	D	1	0	0	0	0
4	A	25	0	17	1	0
4	B	25	0	17	0	0
4	C	25	0	34	4	0
4	D	25	0	17	1	0
5	A	10	0	4	0	0
5	D	10	0	4	0	0
6	B	6	0	8	0	0
7	C	35	0	0	0	0
8	A	358	0	0	0	0
8	B	377	0	0	0	0
8	C	344	0	0	0	0
8	D	326	0	0	1	0
All	All	18287	0	16672	55	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 2.

All (55) 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:303[A]:ARG:HB2	1:D:306[A]:MET:HE3	1.66	0.78
1:D:372:LEU:HD21	1:D:420:PHE:HB3	1.70	0.73
1:B:12:PRO:HG2	1:B:181:THR:HG21	1.75	0.69
1:B:262[B]:GLU:CG	1:B:358:ARG:NH1	2.65	0.59
1:A:372:LEU:HD21	1:A:420:PHE:HB3	1.85	0.58
1:B:372:LEU:HD21	1:B:420:PHE:HB3	1.87	0.56
1:D:269:THR:O	1:D:272:MET:HG2	2.05	0.56
1:A:435:CYS:O	1:B:121:GLN:HG2	2.06	0.56
1:D:281:LEU:HD21	1:D:306[B]:MET:SD	2.47	0.55
1:B:81:LEU:H	1:B:81:LEU:HD23	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:81:LEU:HD23	1:D:81:LEU:H	1.72	0.53
1:A:380:ASP:HB2	1:A:560:ASN:ND2	2.23	0.53
4:C:600[A]:TP8:H102	1:D:36:ARG:HB3	1.91	0.53
1:C:287:PRO:HG2	1:C:359:HIS:CD2	2.43	0.53
1:B:225:ALA:HB2	1:B:252:ILE:HG12	1.90	0.52
1:C:438:PHE:CD2	4:C:600[A]:TP8:HM43	2.45	0.51
1:A:427:PHE:HB3	1:A:430:LEU:HD21	1.93	0.50
1:B:262[B]:GLU:HG3	1:B:358:ARG:NH1	2.27	0.50
1:D:367:ARG:O	1:D:371:PHE:HB2	2.13	0.49
1:A:322:VAL:HG11	1:C:154:ASN:HB3	1.94	0.49
1:D:303[A]:ARG:HG3	1:D:306[A]:MET:HE1	1.94	0.49
4:C:600[A]:TP8:O8	4:C:600[A]:TP8:N4,	2.48	0.46
1:A:70:ILE:HD11	1:A:430:LEU:HD11	1.98	0.46
1:D:102:VAL:O	1:D:163:PRO:HA	2.16	0.46
1:A:121:GLN:HG2	1:B:435:CYS:O	2.17	0.45
1:D:303[A]:ARG:HB2	1:D:306[A]:MET:CE	2.41	0.45
1:A:380:ASP:HB2	1:A:560:ASN:HD22	1.81	0.45
1:C:57:GLU:OE2	4:D:600:TP9:N1'	2.50	0.45
1:A:42:LEU:O	1:A:43:PHE:HB2	2.17	0.45
1:D:252:ILE:HA	8:D:897:HOH:O	2.17	0.45
1:C:42:LEU:HG	1:D:504:HIS:CG	2.52	0.44
1:C:435:CYS:O	1:D:121:GLN:HG2	2.18	0.44
1:D:42:LEU:O	1:D:43:PHE:HB2	2.18	0.43
1:A:143:HIS:HA	1:A:179:ILE:HD13	2.01	0.43
4:C:600[A]:TP8:N4,	4:C:600[A]:TP8:C2	2.82	0.43
4:A:600:TP9:N1'	1:B:57:GLU:OE2	2.52	0.43
1:A:433:ALA:O	1:B:120:HIS:ND1	2.52	0.43
1:B:427:PHE:HB3	1:B:430:LEU:HD21	2.01	0.42
1:D:66:VAL:HG21	1:D:444:ALA:HA	2.00	0.42
1:D:303[A]:ARG:CZ	1:D:306[A]:MET:CE	2.98	0.42
1:A:31:PHE:O	1:A:77:CYS:HA	2.18	0.42
1:A:81:LEU:HD23	1:A:81:LEU:H	1.84	0.42
1:C:79:ALA:O	1:C:106:ALA:HA	2.19	0.42
1:B:154:ASN:HB3	1:D:322:VAL:HG11	2.01	0.42
1:B:12:PRO:HG2	1:B:181:THR:CG2	2.48	0.41
1:C:42:LEU:O	1:C:43:PHE:HB2	2.19	0.41
1:B:225:ALA:HB2	1:B:252:ILE:CG1	2.50	0.41
1:B:102:VAL:O	1:B:163:PRO:HA	2.20	0.41
1:A:66:VAL:HG21	1:A:444:ALA:HA	2.02	0.41
1:B:252:ILE:O	1:B:252:ILE:HG13	2.20	0.41
1:A:335:VAL:HG12	1:A:337:THR:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:322:VAL:HG11	1:D:154:ASN:HB3	2.02	0.40
1:A:42:LEU:HG	1:B:504:HIS:CG	2.56	0.40
1:A:32:GLY:HA2	1:A:60:ALA:CB	2.51	0.40
1:C:442:ILE:HG23	1:C:476:ILE:HD11	2.03	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	561/573 (98%)	548 (98%)	11 (2%)	2 (0%)	34	24
1	B	553/573 (96%)	539 (98%)	13 (2%)	1 (0%)	47	39
1	C	552/573 (96%)	538 (98%)	14 (2%)	0	100	100
1	D	552/573 (96%)	540 (98%)	12 (2%)	0	100	100
All	All	2218/2292 (97%)	2165 (98%)	50 (2%)	3 (0%)	51	45

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	PHE
1	A	562	ASP
1	B	43	PHE

### 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	444/452 (98%)	441 (99%)	3 (1%)	84	84
1	B	440/452 (97%)	436 (99%)	4 (1%)	78	79
1	C	439/452 (97%)	437 (100%)	2 (0%)	88	89
1	D	439/452 (97%)	434 (99%)	5 (1%)	73	73
All	All	1762/1808 (98%)	1748 (99%)	14 (1%)	81	82

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	438	PHE
1	A	562	ASP
1	A	563	PHE
1	B	81	LEU
1	B	252	ILE
1	B	269	THR
1	B	438	PHE
1	C	269	THR
1	C	438	PHE
1	D	65	ASP
1	D	81	LEU
1	D	252	ILE
1	D	269	THR
1	D	438	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	308	GLN
1	A	560	ASN
1	C	308	GLN
1	D	308	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

Mogul failed to run properly - this section is therefore empty.

## 5.5 Carbohydrates [i](#)

Mogul failed to run properly - this section is therefore empty.

## 5.6 Ligand geometry [i](#)

Mogul failed to run properly - this section is therefore empty.

## 5.7 Other polymers [i](#)

Mogul failed to run properly - this section is therefore empty.

## 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	562/573 (98%)	-0.47	12 (2%) 63 67	11, 20, 32, 45	14 (2%)
1	B	552/573 (96%)	-0.48	8 (1%) 75 78	11, 19, 30, 45	11 (1%)
1	C	551/573 (96%)	-0.44	10 (1%) 68 71	11, 20, 30, 45	15 (2%)
1	D	551/573 (96%)	-0.40	12 (2%) 62 66	11, 20, 31, 45	19 (3%)
All	All	2216/2292 (96%)	-0.45	42 (1%) 66 71	11, 19, 31, 45	59 (2%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	183	VAL	7.2
1	C	182	THR	5.8
1	C	183	VAL	5.8
1	B	182	THR	5.2
1	D	182	THR	5.1
1	A	182	THR	5.0
1	B	181	THR	4.6
1	A	183	VAL	4.6
1	D	183	VAL	4.1
1	C	184	PRO	3.7
1	A	563	PHE	3.4
1	C	380	ASP	3.3
1	D	277	ASN	3.3
1	D	184	PRO	3.2
1	A	181	THR	3.2
1	C	181	THR	3.1
1	A	565	PRO	3.0
1	B	377	THR	3.0
1	D	505	HIS	3.0
1	D	271	TYR	3.0
1	D	274	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	184	PRO	2.8
1	D	366	ALA	2.7
1	A	564	GLN	2.6
1	D	363	PRO	2.5
1	C	505	HIS	2.5
1	B	180	ASP	2.4
1	D	181	THR	2.4
1	C	277	ASN	2.4
1	B	505	HIS	2.4
1	D	276	LEU	2.4
1	A	566	GLY	2.4
1	C	352	SER	2.3
1	C	377	THR	2.3
1	A	505	HIS	2.3
1	B	380	ASP	2.3
1	A	562	ASP	2.2
1	C	180	ASP	2.2
1	D	180	ASP	2.1
1	A	352	SER	2.0
1	B	184	PRO	2.0
1	A	377	THR	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 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
5	TAR	D	603	10/10	0.81	0.20	65,66,67,67	0
6	GOL	B	603	6/6	0.82	0.17	64,64,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	TAR	A	603	10/10	0.88	0.17	51,53,53,54	0
3	K	C	602	1/1	0.95	0.07	35,35,35,35	0
3	K	A	602	1/1	0.96	0.06	30,30,30,30	0
3	K	D	602	1/1	0.96	0.08	32,32,32,32	0
4	TP8	C	600[A]	35/35	0.96	0.12	13,17,31,31	35
4	TP9	B	600	25/25	0.97	0.08	17,21,27,32	0
4	TP9	C	600[B]	25/25	0.97	0.09	22,24,24,25	25
4	TP9	D	600	25/25	0.97	0.08	15,25,29,33	0
4	TP9	A	600	25/25	0.98	0.08	15,19,25,30	0
3	K	B	602	1/1	0.98	0.08	29,29,29,29	0
3	K	C	1502	1/1	0.99	0.05	23,23,23,23	0
2	MG	D	601	1/1	0.99	0.06	12,12,12,12	0
2	MG	A	601	1/1	0.99	0.09	8,8,8,8	0
2	MG	B	601	1/1	0.99	0.10	11,11,11,11	0
2	MG	C	601	1/1	0.99	0.11	11,11,11,11	0
3	K	A	1501	1/1	1.00	0.05	21,21,21,21	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.