



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:41 PM GMT

PDB ID : 1GSF  
Title : GLUTATHIONE TRANSFERASE A1-1 COMPLEXED WITH  
ETHACRYNIC ACID  
Authors : L'Hermite, G.; Sinning, I.; Cameron, A.D.; Jones, T.A.  
Deposited on : 1995-06-09  
Resolution : 2.70 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

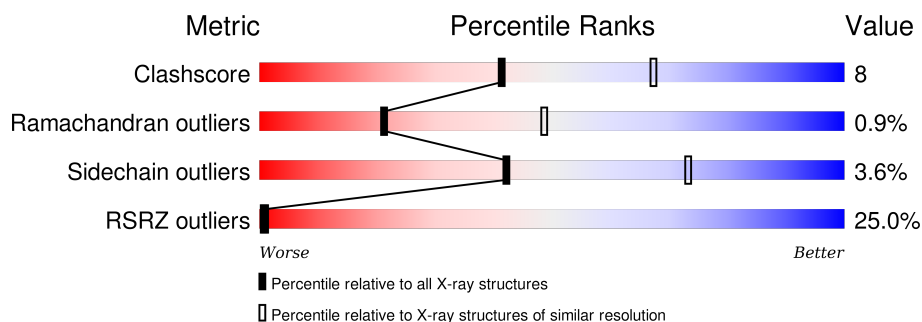
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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. 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	221	
1	B	221	
1	C	221	
1	D	221	

## 2 Entry composition [i](#)

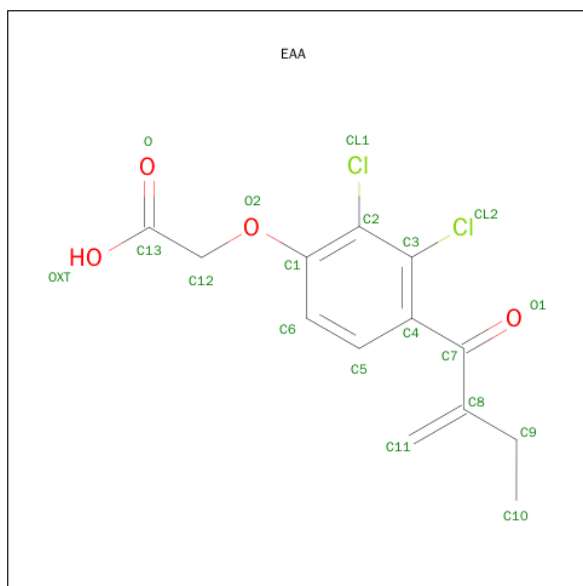
There are 3 unique types of molecules in this entry. The entry contains 7454 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 GLUTATHIONE TRANSFERASE A1-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	221	Total	C	N	O	S	0	1	0
			1807	1170	304	325	8			
1	B	221	Total	C	N	O	S	0	1	0
			1807	1170	304	325	8			
1	C	221	Total	C	N	O	S	0	1	0
			1807	1170	304	325	8			
1	D	221	Total	C	N	O	S	0	1	0
			1807	1170	304	325	8			

- Molecule 2 is ETHACRYNIC ACID (three-letter code: EAA) (formula: C<sub>13</sub>H<sub>12</sub>Cl<sub>2</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Cl	O	0	0
			19	13	2	4		
2	B	1	Total	C	Cl	O	0	0
			19	13	2	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	Cl	O	0	0
			19	13	2	4		
2	D	1	Total	C	Cl	O	0	0
			19	13	2	4		

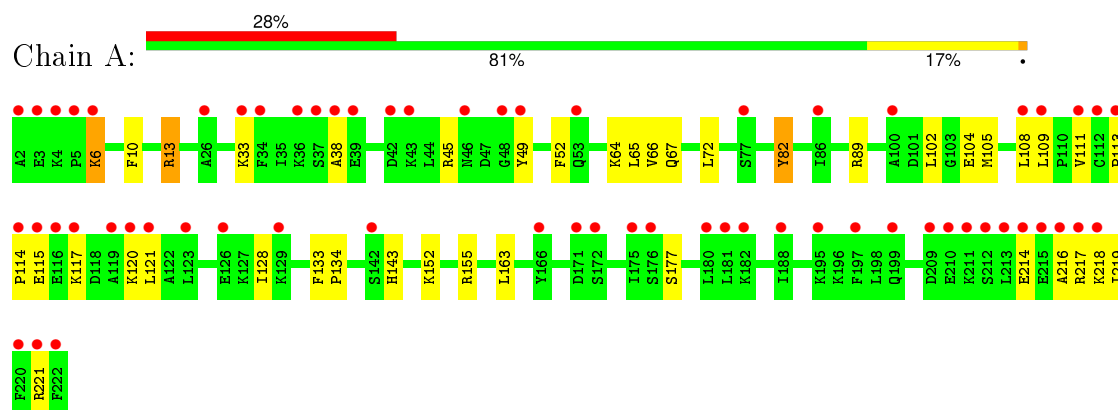
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	74	Total	O	0	0
			74	74		
3	B	76	Total	O	0	0
			76	76		

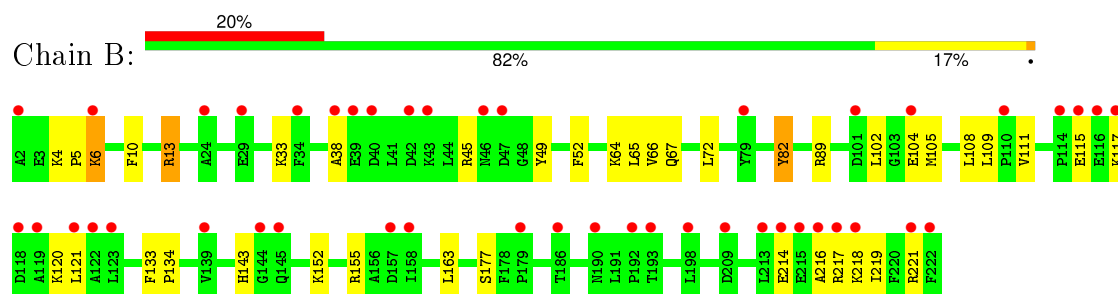
### 3 Residue-property plots [i](#)

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

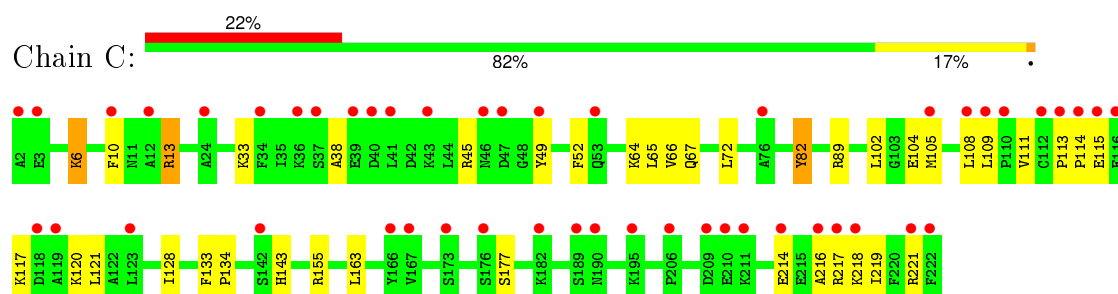
#### • Molecule 1: GLUTATHIONE TRANSFERASE A1-1



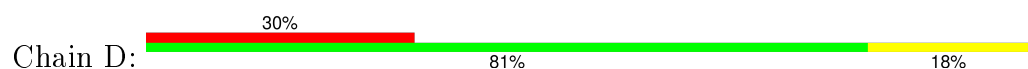
#### • Molecule 1: GLUTATHIONE TRANSFERASE A1-1

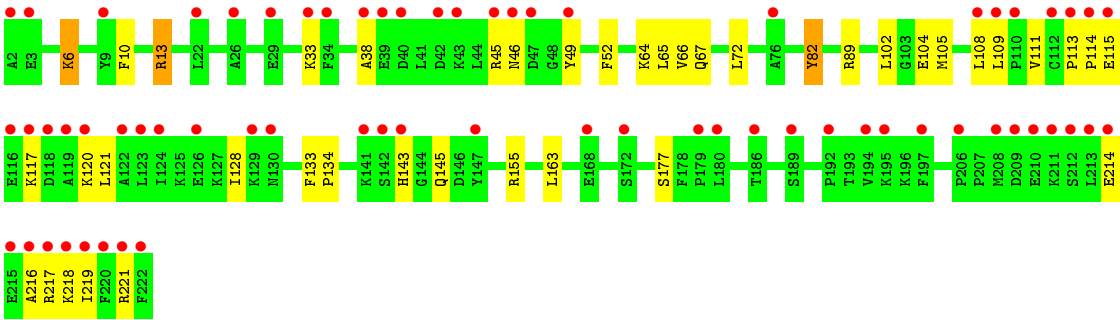


#### • Molecule 1: GLUTATHIONE TRANSFERASE A1-1



#### • Molecule 1: GLUTATHIONE TRANSFERASE A1-1





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.80Å 95.60Å 105.30Å 90.00° 92.20° 90.00°	Depositor
Resolution (Å)	7.50 – 2.70 10.02 – 2.70	Depositor EDS
% Data completeness (in resolution range)	94.9 (7.50-2.70) 94.2 (10.02-2.70)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.99 (at 2.71Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.229 , 0.261 0.318 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	44.0	Xtriage
Anisotropy	0.356	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 64.7	EDS
Estimated twinning fraction	0.012 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 25690 reflections (0.004%)	Xtriage
$F_o, F_c$ correlation	0.83	EDS
Total number of atoms	7454	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 34.76 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 6.4903e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 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: EAA

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	0.50	0/1843	0.67	0/2475
1	B	0.50	0/1843	0.67	0/2475
1	C	0.50	0/1843	0.67	0/2475
1	D	0.50	0/1843	0.67	0/2475
All	All	0.50	0/7372	0.67	0/9900

There are no bond length outliers.

There are no bond angle outliers.

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	1807	0	1875	40	0
1	B	1807	0	1875	40	0
1	C	1807	0	1875	40	0
1	D	1807	0	1875	39	1
2	A	19	0	11	0	0
2	B	19	0	11	0	0
2	C	19	0	11	0	0
2	D	19	0	11	0	0
3	A	74	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	76	0	0	1	0
All	All	7454	0	7544	126	1

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 8.

All (126) 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:89[B]:ARG:CZ	1:B:89[B]:ARG:HH22	1.07	1.65
1:C:89[B]:ARG:HH22	1:D:89[B]:ARG:CZ	1.05	1.59
1:C:89[B]:ARG:CZ	1:D:89[B]:ARG:HH22	1.16	1.57
1:A:89[B]:ARG:HH22	1:B:89[B]:ARG:CZ	1.19	1.51
1:C:89[B]:ARG:HH12	1:D:89[B]:ARG:NH1	1.29	1.31
1:C:89[B]:ARG:NH1	1:D:89[B]:ARG:HH12	1.26	1.29
1:A:89[B]:ARG:HH12	1:B:89[B]:ARG:NH1	1.28	1.29
1:A:89[B]:ARG:NH1	1:B:89[B]:ARG:HH12	1.32	1.26
1:C:89[B]:ARG:CZ	1:D:89[B]:ARG:NH2	1.96	0.88
1:C:89[B]:ARG:NH1	1:D:89[B]:ARG:NH1	2.02	0.85
1:A:89[B]:ARG:HH21	1:B:89[B]:ARG:NH2	1.33	0.82
1:A:89[B]:ARG:NH1	1:B:89[B]:ARG:NH1	2.05	0.81
1:C:89[B]:ARG:NH2	1:D:89[B]:ARG:CZ	1.87	0.80
1:A:89[B]:ARG:NH2	1:B:89[B]:ARG:CZ	1.99	0.80
1:C:89[B]:ARG:NH2	1:D:89[B]:ARG:HH21	1.31	0.79
1:A:89[B]:ARG:CZ	1:B:89[B]:ARG:NH2	1.90	0.73
1:A:89[B]:ARG:NH2	1:B:89[B]:ARG:HH21	1.21	0.71
1:B:45:ARG:HH12	1:B:221:ARG:HH22	1.41	0.69
1:C:89[B]:ARG:NH2	1:D:89[B]:ARG:NH2	0.73	0.68
1:A:89[B]:ARG:NH2	1:B:89[B]:ARG:HH22	0.35	0.67
1:D:45:ARG:HH12	1:D:221:ARG:HH22	1.41	0.67
1:A:45:ARG:HH12	1:A:221:ARG:HH22	1.41	0.67
1:C:89[B]:ARG:HH21	1:D:89[B]:ARG:NH2	1.19	0.67
1:C:45:ARG:HH12	1:C:221:ARG:HH22	1.41	0.67
1:A:89[B]:ARG:NH2	1:B:89[B]:ARG:NH2	0.76	0.66
1:C:89[B]:ARG:HH22	1:D:89[B]:ARG:NH2	0.35	0.65
1:C:89[B]:ARG:CZ	1:D:89[B]:ARG:HH12	2.07	0.64
1:C:89[B]:ARG:CZ	1:D:89[B]:ARG:NH1	2.60	0.63
1:C:109:LEU:HD21	1:C:121:LEU:HD13	1.80	0.63
1:A:109:LEU:HD21	1:A:121:LEU:HD13	1.80	0.63
1:D:109:LEU:HD21	1:D:121:LEU:HD13	1.80	0.63
1:B:109:LEU:HD21	1:B:121:LEU:HD13	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89[B]:ARG:HH12	1:D:89[B]:ARG:HH12	0.66	0.60
1:A:89[B]:ARG:HH12	1:B:89[B]:ARG:HH12	0.67	0.59
1:A:89[B]:ARG:HH22	1:B:89[B]:ARG:NH2	0.19	0.59
1:A:89[B]:ARG:NH1	1:B:89[B]:ARG:CZ	2.63	0.59
1:C:89[B]:ARG:CZ	1:D:89[B]:ARG:CZ	2.63	0.57
1:C:89[B]:ARG:NH2	1:D:89[B]:ARG:HH22	0.20	0.55
1:A:89[B]:ARG:HH22	1:B:89[B]:ARG:HH21	0.98	0.55
1:D:214:GLU:OE2	1:D:217:ARG:HD3	2.07	0.55
1:B:214:GLU:OE2	1:B:217:ARG:HD3	2.07	0.55
1:B:82:TYR:CD1	1:B:89[A]:ARG:HG2	2.42	0.55
1:A:214:GLU:OE2	1:A:217:ARG:HD3	2.07	0.55
1:A:82:TYR:CD1	1:A:89[A]:ARG:HG2	2.42	0.54
1:C:82:TYR:CD1	1:C:89[A]:ARG:HG2	2.42	0.54
1:D:82:TYR:CD1	1:D:89[A]:ARG:HG2	2.42	0.54
1:C:214:GLU:OE2	1:C:217:ARG:HD3	2.07	0.54
1:C:217:ARG:O	1:C:221:ARG:HA	2.08	0.54
1:A:89[B]:ARG:HH12	1:B:89[B]:ARG:CZ	2.09	0.53
1:A:217:ARG:O	1:A:221:ARG:HA	2.08	0.53
1:D:217:ARG:O	1:D:221:ARG:HA	2.08	0.53
1:B:217:ARG:O	1:B:221:ARG:HA	2.08	0.53
1:C:111:VAL:O	1:C:111:VAL:HG12	2.09	0.53
1:D:111:VAL:O	1:D:111:VAL:HG12	2.09	0.52
1:B:111:VAL:HG12	1:B:111:VAL:O	2.09	0.52
1:A:111:VAL:HG12	1:A:111:VAL:O	2.09	0.51
1:B:66:VAL:O	1:B:67:GLN:HB2	2.11	0.51
1:B:152:LYS:HE2	3:B:284:HOH:O	2.11	0.50
1:A:66:VAL:O	1:A:67:GLN:HB2	2.11	0.50
1:A:152:LYS:HE2	3:A:279:HOH:O	2.11	0.50
1:D:66:VAL:O	1:D:67:GLN:HB2	2.11	0.50
1:C:66:VAL:O	1:C:67:GLN:HB2	2.11	0.49
1:B:115:GLU:CD	1:B:115:GLU:H	2.16	0.49
1:A:115:GLU:H	1:A:115:GLU:CD	2.16	0.49
1:D:115:GLU:CD	1:D:115:GLU:H	2.17	0.48
1:C:115:GLU:H	1:C:115:GLU:CD	2.16	0.48
1:C:113:PRO:HA	1:C:114:PRO:HD2	1.69	0.47
1:C:82:TYR:CE1	1:C:89[B]:ARG:HG2	2.50	0.47
1:D:10:PHE:CE2	1:D:216:ALA:HB2	2.50	0.47
1:B:82:TYR:CE1	1:B:89[B]:ARG:HG2	2.50	0.47
1:A:10:PHE:CE2	1:A:216:ALA:HB2	2.50	0.46
1:B:10:PHE:CE2	1:B:216:ALA:HB2	2.50	0.46
1:A:82:TYR:CE1	1:A:89[B]:ARG:HG2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:82:TYR:CE1	1:D:89[B]:ARG:HG2	2.50	0.46
1:C:10:PHE:CE2	1:C:216:ALA:HB2	2.50	0.45
1:D:38:ALA:HA	1:D:219:ILE:HG23	1.99	0.44
1:A:102:LEU:HD23	1:A:163:LEU:HD21	1.99	0.44
1:C:102:LEU:HD23	1:C:163:LEU:HD21	1.99	0.44
1:A:38:ALA:HA	1:A:219:ILE:HG23	1.99	0.44
1:A:89[B]:ARG:HH21	1:B:89[B]:ARG:HH21	1.18	0.44
1:C:104:GLU:O	1:C:108:LEU:HG	2.18	0.44
1:C:38:ALA:HA	1:C:219:ILE:HG23	1.99	0.44
1:B:102:LEU:HA	1:B:105:MET:HE2	1.99	0.44
1:D:102:LEU:HD23	1:D:163:LEU:HD21	1.99	0.44
1:B:38:ALA:HA	1:B:219:ILE:HG23	1.99	0.44
1:C:102:LEU:HA	1:C:105:MET:HE2	2.00	0.43
1:B:102:LEU:HD23	1:B:163:LEU:HD21	1.99	0.43
1:B:104:GLU:O	1:B:108:LEU:HG	2.18	0.43
1:A:104:GLU:O	1:A:108:LEU:HG	2.18	0.43
1:A:113:PRO:HA	1:A:114:PRO:HD2	1.69	0.43
1:B:120:LYS:NZ	1:B:120:LYS:HB3	2.33	0.43
1:D:104:GLU:O	1:D:108:LEU:HG	2.18	0.43
1:C:52:PHE:HD2	1:C:67:GLN:HE21	1.66	0.43
1:B:52:PHE:HD2	1:B:67:GLN:HE21	1.67	0.43
1:D:113:PRO:HA	1:D:114:PRO:HD2	1.69	0.43
1:D:102:LEU:HA	1:D:105:MET:HE2	2.01	0.43
1:B:72:LEU:HB3	1:B:155:ARG:NH2	2.34	0.43
1:D:72:LEU:HB3	1:D:155:ARG:NH2	2.34	0.43
1:C:72:LEU:HB3	1:C:155:ARG:NH2	2.34	0.42
1:A:102:LEU:HA	1:A:105:MET:CE	2.49	0.42
1:A:120:LYS:HB3	1:A:120:LYS:NZ	2.34	0.42
1:D:120:LYS:NZ	1:D:120:LYS:HB3	2.33	0.42
1:D:52:PHE:HD2	1:D:67:GLN:HE21	1.67	0.42
1:D:102:LEU:HA	1:D:105:MET:CE	2.49	0.42
1:C:6:LYS:HG2	1:C:33:LYS:HE3	2.02	0.42
1:C:120:LYS:HB3	1:C:120:LYS:NZ	2.34	0.42
1:B:102:LEU:HA	1:B:105:MET:CE	2.50	0.42
1:D:6:LYS:HG2	1:D:33:LYS:HE3	2.02	0.41
1:A:52:PHE:HD2	1:A:67:GLN:HE21	1.67	0.41
1:C:102:LEU:HA	1:C:105:MET:CE	2.49	0.41
1:A:72:LEU:HB3	1:A:155:ARG:NH2	2.34	0.41
1:D:49:TYR:CE1	1:D:64:LYS:HE2	2.56	0.41
1:C:102:LEU:HD21	1:C:128:ILE:HG12	2.03	0.41
1:B:133:PHE:N	1:B:134:PRO:CD	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:LYS:HG2	1:A:33:LYS:HE3	2.02	0.41
1:D:102:LEU:HD21	1:D:128:ILE:HG12	2.03	0.41
1:A:133:PHE:N	1:A:134:PRO:CD	2.84	0.41
1:B:6:LYS:HG2	1:B:33:LYS:HE3	2.02	0.41
1:B:49:TYR:CE1	1:B:64:LYS:HE2	2.56	0.41
1:A:102:LEU:HD21	1:A:128:ILE:HG12	2.03	0.40
1:C:133:PHE:N	1:C:134:PRO:CD	2.84	0.40
1:D:133:PHE:N	1:D:134:PRO:CD	2.84	0.40
1:A:49:TYR:CE1	1:A:64:LYS:HE2	2.56	0.40
1:C:38:ALA:CA	1:C:219:ILE:HG23	2.52	0.40
1:C:49:TYR:CE1	1:C:64:LYS:HE2	2.56	0.40
1:B:4:LYS:HA	1:B:5:PRO:HD3	1.89	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:46:ASN:O	1:D:145:GLN:OE1[4_656]	1.66	0.54

## 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	220/221 (100%)	209 (95%)	9 (4%)	2 (1%)	21	49
1	B	220/221 (100%)	209 (95%)	9 (4%)	2 (1%)	21	49
1	C	220/221 (100%)	209 (95%)	9 (4%)	2 (1%)	21	49
1	D	220/221 (100%)	209 (95%)	9 (4%)	2 (1%)	21	49
All	All	880/884 (100%)	836 (95%)	36 (4%)	8 (1%)	21	49

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	117	LYS
1	B	117	LYS
1	C	117	LYS
1	D	117	LYS
1	A	13	ARG
1	B	13	ARG
1	C	13	ARG
1	D	13	ARG

### 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	196/195 (100%)	189 (96%)	7 (4%)	42	73
1	B	196/195 (100%)	189 (96%)	7 (4%)	42	73
1	C	196/195 (100%)	189 (96%)	7 (4%)	42	73
1	D	196/195 (100%)	189 (96%)	7 (4%)	42	73
All	All	784/780 (100%)	756 (96%)	28 (4%)	42	73

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LYS
1	A	13	ARG
1	A	65	LEU
1	A	82	TYR
1	A	143	HIS
1	A	177	SER
1	A	218	LYS
1	B	6	LYS
1	B	13	ARG
1	B	65	LEU
1	B	82	TYR
1	B	143	HIS
1	B	177	SER
1	B	218	LYS

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Mol	Chain	Res	Type
1	C	6	LYS
1	C	13	ARG
1	C	65	LEU
1	C	82	TYR
1	C	143	HIS
1	C	177	SER
1	C	218	LYS
1	D	6	LYS
1	D	13	ARG
1	D	65	LEU
1	D	82	TYR
1	D	143	HIS
1	D	177	SER
1	D	218	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	GLN
1	A	67	GLN
1	A	130	ASN
1	A	145	GLN
1	A	199	GLN
1	B	53	GLN
1	B	67	GLN
1	B	130	ASN
1	B	145	GLN
1	B	199	GLN
1	C	53	GLN
1	C	130	ASN
1	C	199	GLN
1	D	53	GLN
1	D	130	ASN
1	D	199	GLN

### 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 ⓘ

4 ligands are modelled in this entry.

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$
2	EAA	A	223	-	15,19,19	1.66	2 (13%)	18,26,26	1.29	2 (11%)
2	EAA	B	223	-	15,19,19	1.66	2 (13%)	18,26,26	1.29	2 (11%)
2	EAA	C	223	-	15,19,19	1.65	2 (13%)	18,26,26	1.29	2 (11%)
2	EAA	D	223	-	15,19,19	1.65	2 (13%)	18,26,26	1.29	2 (11%)

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
2	EAA	A	223	-	-	0/12/15/15	0/1/1/1
2	EAA	B	223	-	-	0/12/15/15	0/1/1/1
2	EAA	C	223	-	-	0/12/15/15	0/1/1/1
2	EAA	D	223	-	-	0/12/15/15	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	223	EAA	C11-C8	-4.71	1.22	1.32
2	A	223	EAA	C11-C8	-4.69	1.22	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	223	EAA	C11-C8	-4.68	1.22	1.32
2	D	223	EAA	C11-C8	-4.67	1.22	1.32
2	C	223	EAA	C4-C7	-2.81	1.43	1.49
2	B	223	EAA	C4-C7	-2.81	1.43	1.49
2	A	223	EAA	C4-C7	-2.80	1.43	1.49
2	D	223	EAA	C4-C7	-2.79	1.43	1.49

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	223	EAA	O2-C12-C13	2.24	112.36	108.01
2	B	223	EAA	O2-C12-C13	2.24	112.36	108.01
2	A	223	EAA	O2-C12-C13	2.25	112.39	108.01
2	C	223	EAA	O2-C12-C13	2.26	112.39	108.01
2	C	223	EAA	O2-C1-C2	2.92	121.08	115.84
2	D	223	EAA	O2-C1-C2	2.92	121.08	115.84
2	A	223	EAA	O2-C1-C2	2.93	121.09	115.84
2	B	223	EAA	O2-C1-C2	2.94	121.11	115.84

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	221/221 (100%)	1.65	62 (28%) 1 0	7, 35, 85, 118	0
1	B	221/221 (100%)	1.35	45 (20%) 1 1	7, 35, 85, 118	0
1	C	221/221 (100%)	1.21	48 (21%) 1 1	7, 35, 85, 118	0
1	D	221/221 (100%)	1.59	66 (29%) 1 0	7, 35, 85, 118	0
All	All	884/884 (100%)	1.45	221 (25%) 1 1	7, 36, 88, 118	0

All (221) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	216	ALA	7.7
1	D	222	PHE	7.3
1	D	39	GLU	7.2
1	B	218	LYS	7.0
1	C	217	ARG	6.7
1	A	214	GLU	6.6
1	C	2	ALA	6.4
1	D	215	GLU	6.2
1	A	2	ALA	5.8
1	A	115	GLU	5.7
1	D	213	LEU	5.6
1	C	222	PHE	5.5
1	D	211	LYS	5.4
1	A	119	ALA	5.3
1	D	217	ARG	5.1
1	C	114	PRO	5.0
1	B	215	GLU	5.0
1	D	212	SER	4.8
1	D	119	ALA	4.8
1	A	116	GLU	4.7
1	A	215	GLU	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	222	PHE	4.5
1	C	110	PRO	4.5
1	B	190	ASN	4.5
1	A	211	LYS	4.5
1	A	217	ARG	4.4
1	C	210	GLU	4.4
1	D	108	LEU	4.4
1	C	216	ALA	4.4
1	C	40	ASP	4.4
1	D	214	GLU	4.3
1	D	126	GLU	4.3
1	D	218	LYS	4.3
1	A	113	PRO	4.2
1	C	218	LYS	4.2
1	D	38	ALA	4.2
1	D	113	PRO	4.2
1	A	112	CYS	4.2
1	D	123	LEU	4.0
1	C	43	LYS	4.0
1	A	43	LYS	4.0
1	B	217	ARG	4.0
1	A	209	ASP	4.0
1	A	220	PHE	3.9
1	B	216	ALA	3.9
1	C	118	ASP	3.9
1	B	193	THR	3.9
1	D	114	PRO	3.8
1	B	39	GLU	3.8
1	D	40	ASP	3.8
1	B	2	ALA	3.7
1	B	214	GLU	3.7
1	D	172	SER	3.7
1	D	3	GLU	3.7
1	C	49	TYR	3.6
1	D	192	PRO	3.6
1	B	186	THR	3.6
1	D	117	LYS	3.5
1	C	47	ASP	3.5
1	C	115	GLU	3.5
1	D	221	ARG	3.5
1	A	42	ASP	3.5
1	C	173	SER	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	130	ASN	3.5
1	B	158	ILE	3.5
1	A	117	LYS	3.4
1	A	114	PRO	3.4
1	A	212	SER	3.4
1	B	47	ASP	3.4
1	B	114	PRO	3.4
1	C	221	ARG	3.4
1	A	172	SER	3.4
1	A	39	GLU	3.3
1	A	197	PHE	3.3
1	C	113	PRO	3.3
1	D	129	LYS	3.3
1	B	222	PHE	3.3
1	A	38	ALA	3.3
1	A	33	LYS	3.2
1	A	176	SER	3.2
1	A	111	VAL	3.2
1	A	126	GLU	3.2
1	D	216	ALA	3.2
1	D	46	ASN	3.2
1	A	218	LYS	3.2
1	D	219	ILE	3.2
1	B	24	ALA	3.1
1	B	209	ASP	3.1
1	D	180	LEU	3.1
1	A	221	ARG	3.1
1	A	199	GLN	3.1
1	B	192	PRO	3.0
1	C	41	LEU	3.0
1	C	119	ALA	3.0
1	D	142	SER	3.0
1	A	100	ALA	3.0
1	D	210	GLU	3.0
1	B	46	ASN	3.0
1	A	36	LYS	2.9
1	D	42	ASP	2.9
1	D	168	GLU	2.9
1	D	33	LYS	2.9
1	D	2	ALA	2.9
1	B	116	GLU	2.9
1	A	175	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	112	CYS	2.9
1	B	118	ASP	2.8
1	D	110	PRO	2.8
1	B	115	GLU	2.8
1	D	206	PRO	2.8
1	A	123	LEU	2.8
1	A	210	GLU	2.8
1	C	214	GLU	2.8
1	D	109	LEU	2.8
1	D	43	LYS	2.8
1	D	220	PHE	2.8
1	B	40	ASP	2.8
1	D	179	PRO	2.7
1	A	120	LYS	2.7
1	A	195	LYS	2.7
1	D	29	GLU	2.7
1	D	195	LYS	2.7
1	C	116	GLU	2.7
1	A	109	LEU	2.7
1	D	116	GLU	2.7
1	A	171	ASP	2.7
1	B	117	LYS	2.6
1	A	77	SER	2.6
1	A	86	ILE	2.6
1	C	109	LEU	2.6
1	A	5	PRO	2.6
1	A	6	LYS	2.6
1	B	38	ALA	2.5
1	D	141	LYS	2.5
1	A	188	ILE	2.5
1	D	208	MET	2.5
1	C	36	LYS	2.5
1	B	157	ASP	2.5
1	D	9	TYR	2.5
1	D	120	LYS	2.5
1	C	209	ASP	2.5
1	B	221	ARG	2.5
1	A	213	LEU	2.5
1	C	142	SER	2.5
1	D	122	ALA	2.4
1	C	46	ASN	2.4
1	C	34	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	48	GLY	2.4
1	C	211	LYS	2.4
1	D	124	ILE	2.4
1	B	144	GLY	2.4
1	B	6	LYS	2.4
1	C	176	SER	2.4
1	C	39	GLU	2.4
1	B	42	ASP	2.4
1	A	121	LEU	2.4
1	D	34	PHE	2.4
1	C	108	LEU	2.3
1	C	123	LEU	2.3
1	A	142	SER	2.3
1	B	139	VAL	2.3
1	A	166	TYR	2.3
1	B	101	ASP	2.3
1	B	119	ALA	2.3
1	A	46	ASN	2.3
1	A	129	LYS	2.3
1	B	29	GLU	2.3
1	B	123	LEU	2.3
1	A	34	PHE	2.3
1	C	37	SER	2.3
1	D	118	ASP	2.3
1	C	166	TYR	2.3
1	C	190	ASN	2.2
1	C	167	VAL	2.2
1	B	104	GLU	2.2
1	D	76	ALA	2.2
1	D	143	HIS	2.2
1	C	206	PRO	2.2
1	A	4	LYS	2.2
1	A	3	GLU	2.2
1	D	45	ARG	2.2
1	C	10	PHE	2.2
1	A	53	GLN	2.2
1	B	43	LYS	2.2
1	B	198	LEU	2.2
1	D	209	ASP	2.2
1	A	37	SER	2.2
1	C	189	SER	2.2
1	B	34	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	26	ALA	2.2
1	C	76	ALA	2.2
1	B	121	LEU	2.1
1	D	26	ALA	2.1
1	D	49	TYR	2.1
1	D	147	TYR	2.1
1	B	122	ALA	2.1
1	D	47	ASP	2.1
1	C	12	ALA	2.1
1	C	3	GLU	2.1
1	C	53	GLN	2.1
1	B	213	LEU	2.1
1	A	49	TYR	2.1
1	C	182	LYS	2.1
1	A	108	LEU	2.1
1	A	181	LEU	2.1
1	C	105	MET	2.1
1	D	115	GLU	2.1
1	B	79	TYR	2.1
1	A	180	LEU	2.0
1	A	182	LYS	2.0
1	B	110	PRO	2.0
1	C	24	ALA	2.0
1	B	145	GLN	2.0
1	D	22	LEU	2.0
1	D	189	SER	2.0
1	C	195	LYS	2.0
1	D	186	THR	2.0
1	D	194	VAL	2.0
1	B	179	PRO	2.0
1	D	112	CYS	2.0
1	D	197	PHE	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 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	EAA	C	223	19/19	0.71	0.34	0.32	74,74,74,74	0
2	EAA	A	223	19/19	0.65	0.33	0.08	74,74,74,74	0
2	EAA	B	223	19/19	0.77	0.27	-0.10	74,74,74,74	0
2	EAA	D	223	19/19	0.80	0.28	-0.44	74,74,74,74	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.