



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 10, 2024 – 01:46 am GMT

PDB ID : 6TNL  
Title : GSTF1 from Alopecurus myosuroides  
Authors : Pohl, E.; Eno, R.F.M.; Freitag-Pohl, S.; Edwards, R.  
Deposited on : 2019-12-09  
Resolution : 1.95 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 : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.003 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

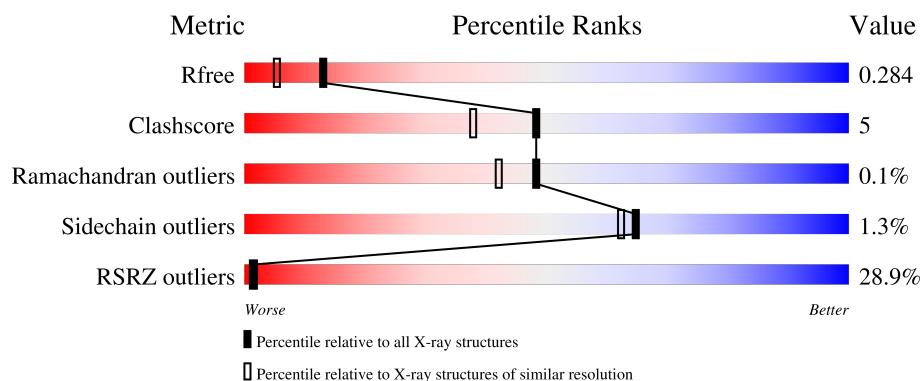
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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))
$R_{free}$	164625	3187 (1.96-1.96)
Clashscore	180529	3412 (1.96-1.96)
Ramachandran outliers	177936	3390 (1.96-1.96)
Sidechain outliers	177891	3390 (1.96-1.96)
RSRZ outliers	164620	3186 (1.96-1.96)

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	AAA	219	<div> <div>67%</div> <div> <div>74%</div> <div>11%</div> <div>•</div> <div>13%</div> </div> </div>
1	BBB	219	<div> <div>5%</div> <div> <div>78%</div> <div>8%</div> <div>•</div> <div>13%</div> </div> </div>
1	CCC	219	<div> <div>53%</div> <div> <div>78%</div> <div>8%</div> <div>•</div> <div>13%</div> </div> </div>
1	DDD	219	<div> <div>7%</div> <div> <div>78%</div> <div>8%</div> <div>•</div> <div>14%</div> </div> </div>
1	EEE	219	<div> <div>7%</div> <div> <div>76%</div> <div>9%</div> <div>•</div> <div>14%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	FFF	219	

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
2	SO4	CCC	301	-	-	X	-

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 18467 atoms, of which 8828 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.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	190	Total	C	H	N	O	S	55	0	0
			2946	975	1453	241	269	8			
1	BBB	190	Total	C	H	N	O	S	60	1	0
			2983	985	1475	243	272	8			
1	CCC	191	Total	C	H	N	O	S	57	0	0
			2982	984	1475	244	271	8			
1	DDD	189	Total	C	H	N	O	S	59	1	0
			2971	981	1467	244	271	8			
1	EEE	189	Total	C	H	N	O	S	58	2	0
			3000	988	1485	246	273	8			
1	FFF	192	Total	C	H	N	O	S	57	0	0
			2983	986	1473	244	272	8			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	CCC	1	Total O S 5 4 1	0	0
2	EEE	1	Total O S 5 4 1	0	0
2	FFF	1	Total O S 5 4 1	0	0

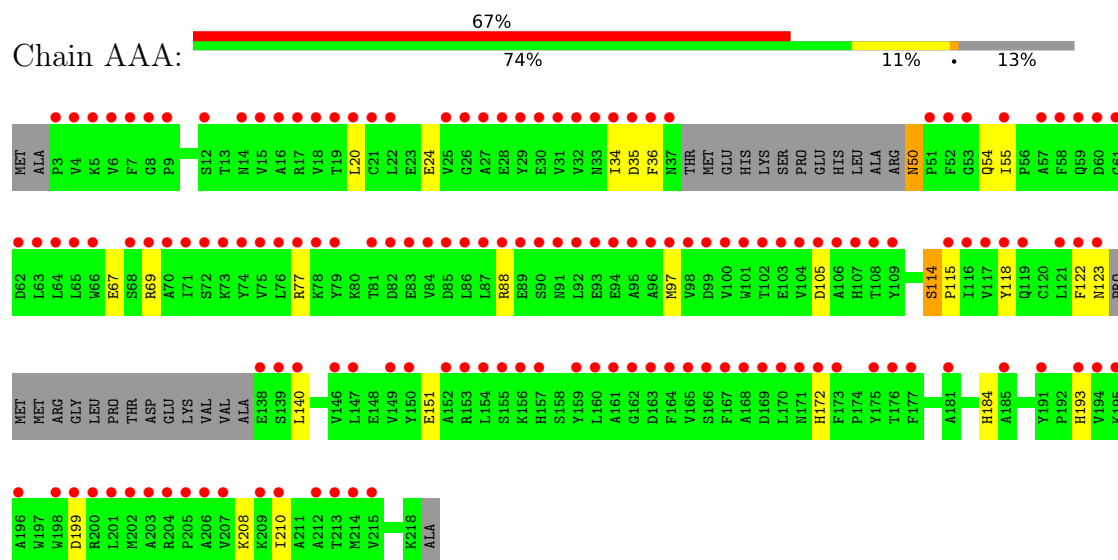
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	57	Total O 57 57	0	0
3	BBB	117	Total O 117 117	0	0
3	CCC	76	Total O 76 76	0	0
3	DDD	105	Total O 105 105	0	0
3	EEE	113	Total O 113 113	0	0
3	FFF	119	Total O 119 119	0	0

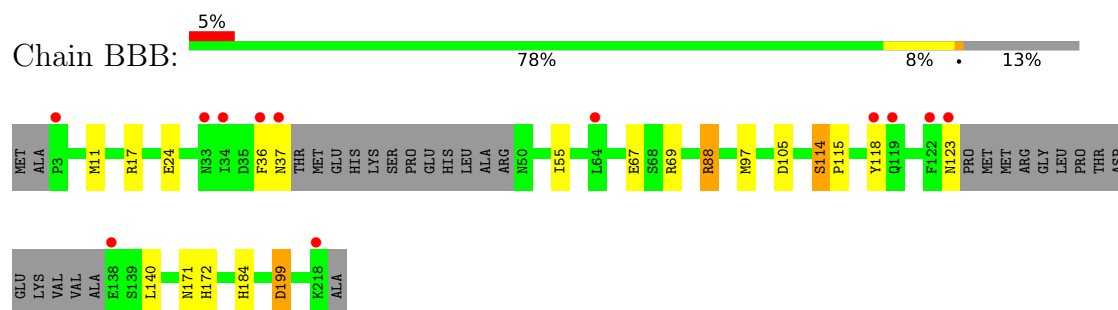
### 3 Residue-property plots [i](#)

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.

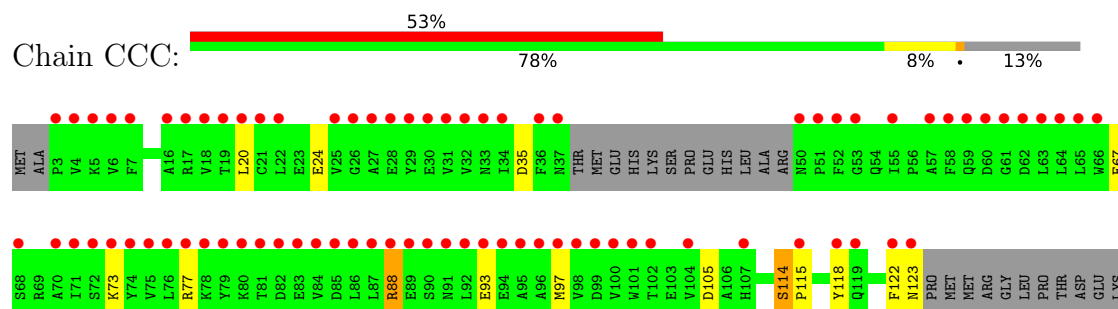
- Molecule 1: Glutathione transferase

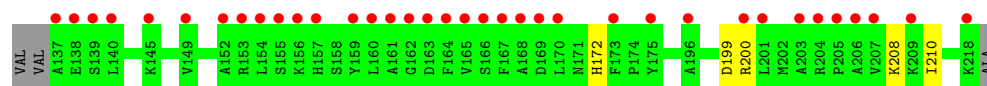


- Molecule 1: Glutathione transferase

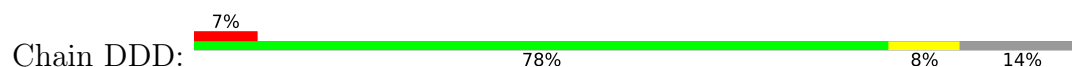


- Molecule 1: Glutathione transferase

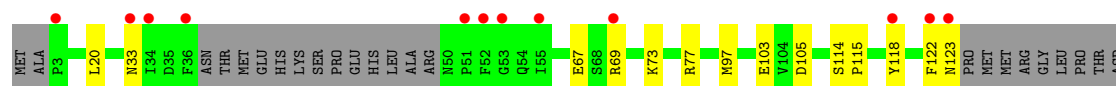
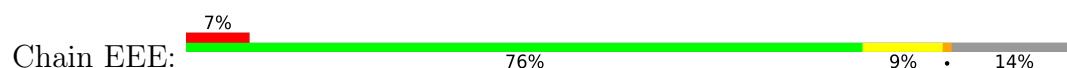




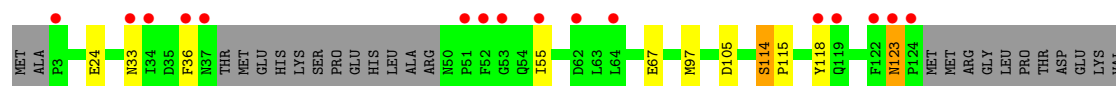
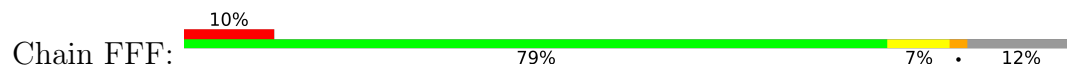
- Molecule 1: Glutathione transferase



- Molecule 1: Glutathione transferase



- Molecule 1: Glutathione transferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	180.78Å 180.78Å 237.89Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.95 – 1.95 41.95 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.1 (41.95-1.95) 99.1 (41.95-1.95)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.74 (at 1.95Å)	Xtrriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.260 , 0.284 0.260 , 0.284	Depositor DCC
$R_{free}$ test set	5352 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.2	Xtrriage
Anisotropy	0.124	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.42 , 39.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.53$ , $\langle L^2 \rangle = 0.38$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	18467	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 95.25 % 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 1.5831e-09. 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, 0.333 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: SO4, CSS

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	AAA	0.82	2/1528 (0.1%)	0.91	2/2085 (0.1%)
1	BBB	0.95	3/1546 (0.2%)	0.99	1/2109 (0.0%)
1	CCC	0.86	3/1541 (0.2%)	0.92	3/2100 (0.1%)
1	DDD	0.96	2/1539 (0.1%)	0.99	2/2098 (0.1%)
1	EEE	0.99	3/1552 (0.2%)	1.00	1/2113 (0.0%)
1	FFF	1.01	5/1545 (0.3%)	1.00	1/2108 (0.0%)
All	All	0.93	18/9251 (0.2%)	0.97	10/12613 (0.1%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	CCC	93	GLU	CD-OE1	10.77	1.37	1.25
1	BBB	67	GLU	CD-OE2	-10.28	1.14	1.25
1	DDD	67	GLU	CD-OE2	-9.09	1.15	1.25
1	FFF	67	GLU	CD-OE2	-8.26	1.16	1.25
1	FFF	199	ASP	CG-OD2	8.22	1.44	1.25
1	EEE	67	GLU	CD-OE2	-7.86	1.17	1.25
1	DDD	199	ASP	CG-OD2	-7.06	1.09	1.25
1	FFF	24	GLU	CD-OE1	-6.55	1.18	1.25
1	BBB	24	GLU	CD-OE1	-6.40	1.18	1.25
1	EEE	199	ASP	CG-OD2	6.34	1.40	1.25
1	EEE	151	GLU	CD-OE2	-6.17	1.18	1.25
1	CCC	24	GLU	CD-OE1	-5.98	1.19	1.25
1	FFF	67	GLU	CD-OE1	-5.93	1.19	1.25
1	FFF	151	GLU	CD-OE1	-5.80	1.19	1.25
1	AAA	24	GLU	CD-OE1	-5.66	1.19	1.25
1	BBB	199	ASP	CG-OD2	-5.31	1.13	1.25
1	AAA	67	GLU	CD-OE2	-5.29	1.19	1.25
1	CCC	67	GLU	CD-OE1	-5.20	1.20	1.25

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	77	ARG	NE-CZ-NH2	-6.49	117.05	120.30
1	CCC	93	GLU	OE1-CD-OE2	6.13	130.66	123.30
1	BBB	88	ARG	NE-CZ-NH2	-5.71	117.45	120.30
1	CCC	88	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	AAA	88	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	DDD	77	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	DDD	163	ASP	CB-CG-OD1	5.21	122.99	118.30
1	EEE	77	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	FFF	199	ASP	CB-CG-OD1	-5.18	113.64	118.30
1	CCC	77	ARG	NE-CZ-NH2	-5.01	117.80	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	1493	1453	1421	22	0
1	BBB	1508	1475	1453	22	1
1	CCC	1507	1475	1447	11	0
1	DDD	1504	1467	1442	12	0
1	EEE	1515	1485	1461	15	2
1	FFF	1510	1473	1443	23	0
2	CCC	5	0	0	2	0
2	EEE	5	0	0	1	0
2	FFF	5	0	0	1	0
3	AAA	57	0	0	7	0
3	BBB	117	0	0	5	0
3	CCC	76	0	0	3	0
3	DDD	105	0	0	4	0
3	EEE	113	0	0	6	0
3	FFF	119	0	0	5	0
All	All	9639	8828	8667	96	2

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 5.

All (96) 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:FFF:36:PHE:CZ	1:FFF:55:ILE:HD12	2.02	0.93
1:AAA:199:ASP:OD2	1:CCC:199:ASP:OD2	1.89	0.88
1:DDD:199:ASP:OD2	1:FFF:199:ASP:OD2	1.92	0.85
1:DDD:122:PHE:O	1:DDD:123:ASN:HB2	1.79	0.81
1:BBB:36:PHE:CZ	1:BBB:55:ILE:HD12	2.22	0.74
1:AAA:97:MET:CE	3:AAA:327:HOH:O	2.38	0.72
1:AAA:118:TYR:CD2	3:AAA:355:HOH:O	2.43	0.71
1:CCC:200:ARG:NH1	2:CCC:301:SO4:O3	2.23	0.70
1:AAA:36:PHE:CZ	1:AAA:55:ILE:CD1	2.76	0.68
1:AAA:151:GLU:OE2	1:AAA:193:HIS:HD2	1.76	0.68
1:DDD:151:GLU:OE2	1:DDD:193:HIS:HD2	1.76	0.67
1:EEE:73:LYS:NZ	3:EEE:401:HOH:O	2.21	0.67
1:EEE:151:GLU:OE2	1:EEE:193:HIS:HD2	1.75	0.67
1:FFF:151:GLU:OE2	1:FFF:193:HIS:HD2	1.78	0.66
1:FFF:123:ASN:HA	3:FFF:437:HOH:O	1.96	0.65
1:BBB:97:MET:CE	3:BBB:386:HOH:O	2.45	0.64
1:DDD:97:MET:CE	3:DDD:365:HOH:O	2.46	0.64
1:FFF:118:TYR:CD2	3:FFF:401:HOH:O	2.50	0.64
1:AAA:50:ASN:HD21	1:AAA:54:GLN:H	1.46	0.63
1:BBB:36:PHE:CZ	1:BBB:55:ILE:CD1	2.82	0.62
1:BBB:36:PHE:CE1	1:BBB:55:ILE:CD1	2.83	0.62
1:EEE:69[B]:ARG:NH2	1:EEE:103:GLU:OE2	2.29	0.61
1:AAA:36:PHE:CZ	1:AAA:55:ILE:HD12	2.35	0.61
1:BBB:36:PHE:CE1	1:BBB:55:ILE:HD12	2.36	0.61
1:AAA:118:TYR:CE2	3:AAA:355:HOH:O	2.53	0.61
1:FFF:137:ALA:HB1	3:FFF:452:HOH:O	2.00	0.61
1:FFF:140:LEU:HD11	1:FFF:184:HIS:CE1	2.36	0.60
1:AAA:34:ILE:HD11	1:AAA:55:ILE:HG12	1.84	0.60
1:EEE:97:MET:CE	3:EEE:483:HOH:O	2.49	0.60
1:FFF:36:PHE:CE1	1:FFF:55:ILE:CD1	2.86	0.59
1:AAA:140:LEU:HD11	1:AAA:184:HIS:CE1	2.37	0.59
1:BBB:140:LEU:HD11	1:BBB:184:HIS:CE1	2.37	0.59
1:FFF:36:PHE:CZ	1:FFF:55:ILE:CD1	2.81	0.58
1:AAA:36:PHE:CE1	1:AAA:55:ILE:CD1	2.87	0.58
1:BBB:37:ASN:HB3	1:FFF:186:ALA:HB3	1.85	0.57
1:EEE:123:ASN:C	3:EEE:413:HOH:O	2.43	0.57
1:CCC:118:TYR:CD2	3:CCC:473:HOH:O	2.53	0.57
1:AAA:50:ASN:ND2	3:AAA:303:HOH:O	2.36	0.56
1:EEE:122:PHE:O	1:EEE:123:ASN:C	2.42	0.56
1:CCC:122:PHE:O	1:CCC:123:ASN:C	2.43	0.55
1:BBB:123:ASN:HB3	3:BBB:304:HOH:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:17:ARG:HE	1:BBB:171:ASN:HD22	1.53	0.55
1:FFF:105:ASP:HB2	1:FFF:172:HIS:CE1	2.43	0.54
1:BBB:11:MET:HE3	3:BBB:301:HOH:O	2.07	0.54
1:BBB:36:PHE:HD2	1:FFF:184:HIS:CE1	2.26	0.54
1:CCC:73:LYS:NZ	3:CCC:403:HOH:O	2.41	0.54
1:EEE:200:ARG:NH1	2:EEE:301:SO4:O4	2.39	0.53
1:BBB:184:HIS:CE1	1:FFF:36:PHE:HD2	2.26	0.53
1:FFF:97:MET:CE	3:FFF:492:HOH:O	2.57	0.53
1:DDD:193:HIS:HE1	3:DDD:400:HOH:O	1.91	0.53
1:AAA:193:HIS:HE1	3:AAA:352:HOH:O	1.90	0.53
1:BBB:36:PHE:CD2	1:FFF:184:HIS:CE1	2.97	0.52
1:CCC:105:ASP:HB2	1:CCC:172:HIS:CE1	2.45	0.52
1:AAA:105:ASP:HB2	1:AAA:172:HIS:CE1	2.45	0.52
1:DDD:105:ASP:HB2	1:DDD:172:HIS:CE1	2.45	0.52
1:DDD:118:TYR:CD2	3:DDD:402:HOH:O	2.53	0.52
1:BBB:17:ARG:HE	1:BBB:171:ASN:ND2	2.08	0.51
1:BBB:105:ASP:HB2	1:BBB:172:HIS:CE1	2.46	0.51
1:EEE:193:HIS:HE1	3:EEE:508:HOH:O	1.94	0.51
1:EEE:105:ASP:HB2	1:EEE:172:HIS:CE1	2.45	0.50
1:BBB:184:HIS:CE1	1:FFF:36:PHE:CD2	2.99	0.50
1:FFF:36:PHE:CE1	1:FFF:55:ILE:HD11	2.49	0.48
1:AAA:36:PHE:CE1	1:AAA:55:ILE:HD11	2.49	0.47
1:AAA:122:PHE:O	1:AAA:123:ASN:CB	2.61	0.47
1:FFF:114:SER:N	1:FFF:115:PRO:HD2	2.30	0.47
1:AAA:69:ARG:NH1	3:AAA:307:HOH:O	2.49	0.46
1:BBB:118:TYR:CE1	1:FFF:118:TYR:HB2	2.51	0.46
1:CCC:97:MET:CE	3:CCC:459:HOH:O	2.64	0.46
1:EEE:114:SER:N	1:EEE:115:PRO:HD2	2.31	0.46
1:EEE:138:GLU:HG3	1:EEE:140:LEU:HB2	1.98	0.45
1:BBB:114:SER:N	1:BBB:115:PRO:HD2	2.31	0.45
1:FFF:137:ALA:HB3	1:FFF:140:LEU:HG	1.98	0.45
1:AAA:97:MET:HE1	3:AAA:327:HOH:O	2.13	0.45
1:FFF:200:ARG:NH1	2:FFF:301:SO4:O1	2.42	0.44
1:AAA:114:SER:N	1:AAA:115:PRO:HD2	2.32	0.44
1:BBB:97:MET:HE1	3:BBB:386:HOH:O	2.11	0.44
1:DDD:114:SER:N	1:DDD:115:PRO:HD2	2.33	0.44
1:CCC:114:SER:N	1:CCC:115:PRO:HD2	2.32	0.44
1:AAA:34:ILE:O	1:AAA:34:ILE:HD12	2.18	0.43
1:EEE:151:GLU:OE2	1:EEE:193:HIS:CD2	2.65	0.43
1:EEE:69[A]:ARG:NH2	3:EEE:410:HOH:O	2.52	0.42
1:BBB:88:ARG:HA	1:BBB:88:ARG:HD3	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EEE:97:MET:HE2	3:EEE:483:HOH:O	2.18	0.42
1:CCC:88:ARG:HA	1:CCC:88:ARG:HD3	1.87	0.42
1:CCC:200:ARG:NH2	2:CCC:301:SO4:O3	2.53	0.42
1:DDD:138:GLU:N	3:DDD:307:HOH:O	2.52	0.42
1:BBB:37:ASN:HB3	1:FFF:186:ALA:CB	2.48	0.41
1:BBB:69:ARG:CD	3:BBB:378:HOH:O	2.68	0.41
1:DDD:88:ARG:HA	1:DDD:88:ARG:HD3	1.87	0.41
1:DDD:151:GLU:OE2	1:DDD:193:HIS:CD2	2.65	0.41
1:AAA:151:GLU:OE2	1:AAA:193:HIS:CD2	2.66	0.41
1:DDD:20:LEU:HA	1:DDD:210:ILE:HG13	2.03	0.41
1:EEE:20:LEU:HA	1:EEE:210:ILE:HG13	2.03	0.41
1:CCC:20:LEU:HA	1:CCC:210:ILE:HG13	2.02	0.41
1:FFF:118:TYR:CE2	3:FFF:401:HOH:O	2.74	0.40
1:AAA:20:LEU:HA	1:AAA:210:ILE:HG13	2.04	0.40

All (2) 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:BBB:199:ASP:OD2	1:EEE:199:ASP:OD2[11_445]	1.92	0.28
1:EEE:114:SER:OG	1:EEE:118:TYR:OH[16_545]	2.16	0.04

## 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	AAA	183/219 (84%)	177 (97%)	6 (3%)	0	100	100
1	BBB	184/219 (84%)	179 (97%)	5 (3%)	0	100	100
1	CCC	184/219 (84%)	178 (97%)	6 (3%)	0	100	100
1	DDD	183/219 (84%)	177 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	EEE	184/219 (84%)	178 (97%)	6 (3%)	0	100	100
1	FFF	185/219 (84%)	177 (96%)	7 (4%)	1 (0%)	25	16
All	All	1103/1314 (84%)	1066 (97%)	36 (3%)	1 (0%)	48	42

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	FFF	123	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	AAA	152/188 (81%)	148 (97%)	4 (3%)	41	33
1	BBB	157/188 (84%)	156 (99%)	1 (1%)	84	83
1	CCC	154/188 (82%)	151 (98%)	3 (2%)	52	47
1	DDD	155/188 (82%)	154 (99%)	1 (1%)	84	83
1	EEE	157/188 (84%)	156 (99%)	1 (1%)	84	83
1	FFF	154/188 (82%)	152 (99%)	2 (1%)	65	62
All	All	929/1128 (82%)	917 (99%)	12 (1%)	65	62

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	35	ASP
1	AAA	50	ASN
1	AAA	114	SER
1	AAA	208	LYS
1	BBB	114	SER
1	CCC	35	ASP
1	CCC	114	SER
1	CCC	208	LYS
1	DDD	35	ASP

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Mol	Chain	Res	Type
1	EEE	33	ASN
1	FFF	33	ASN
1	FFF	114	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	CSS	EEE	120	1	4,6,7	0.57	0	1,6,8	0.37	0
1	CSS	BBB	120	1	4,6,7	0.57	0	1,6,8	0.41	0
1	CSS	AAA	120	1	4,6,7	0.56	0	1,6,8	0.01	0
1	CSS	DDD	120	1	4,6,7	0.46	0	1,6,8	0.32	0
1	CSS	FFF	120	1	4,6,7	0.71	0	1,6,8	0.59	0
1	CSS	CCC	120	1	4,6,7	0.54	0	1,6,8	0.34	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
1	CSS	EEE	120	1	-	0/1/5/7	-
1	CSS	BBB	120	1	-	0/1/5/7	-
1	CSS	AAA	120	1	-	0/1/5/7	-
1	CSS	DDD	120	1	-	0/1/5/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSS	FFF	120	1	-	0/1/5/7	-
1	CSS	CCC	120	1	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

3 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	SO4	CCC	301	-	4,4,4	0.37	0	6,6,6	0.17	0
2	SO4	FFF	301	-	4,4,4	0.40	0	6,6,6	0.20	0
2	SO4	EEE	301	-	4,4,4	0.39	0	6,6,6	0.13	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.



3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	CCC	301	SO4	2	0
2	FFF	301	SO4	1	0
2	EEE	301	SO4	1	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	AAA	189/219 (86%)	2.95	147 (77%) 0 0	35, 47, 67, 88	0
1	BBB	189/219 (86%)	0.24	12 (6%) 27 33	19, 28, 54, 75	1 (0%)
1	CCC	190/219 (86%)	2.42	116 (61%) 0 0	29, 46, 67, 100	0
1	DDD	188/219 (85%)	0.37	16 (8%) 18 22	18, 30, 55, 92	1 (0%)
1	EEE	188/219 (85%)	0.25	16 (8%) 18 22	13, 28, 51, 75	2 (1%)
1	FFF	191/219 (87%)	0.35	21 (10%) 12 15	19, 28, 55, 91	0
All	All	1135/1314 (86%)	1.10	328 (28%) 1 1	13, 36, 63, 100	4 (0%)

All (328) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	123	ASN	11.4
1	CCC	123	ASN	8.6
1	FFF	124	PRO	8.0
1	DDD	37	ASN	7.1
1	AAA	59	GLN	7.0
1	CCC	37	ASN	6.6
1	FFF	123	ASN	6.5
1	AAA	58	PHE	6.5
1	CCC	137	ALA	6.5
1	AAA	37	ASN	6.3
1	BBB	123	ASN	6.0
1	FFF	37	ASN	5.9
1	CCC	95	ALA	5.8
1	AAA	100	VAL	5.7
1	AAA	122	PHE	5.5
1	CCC	91	ASN	5.3
1	AAA	86	LEU	5.2
1	CCC	162	GLY	5.2
1	AAA	91	ASN	5.2

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Mol	Chain	Res	Type	RSRZ
1	CCC	118	TYR	5.2
1	AAA	162	GLY	5.2
1	AAA	95	ALA	5.1
1	AAA	75	VAL	5.1
1	AAA	66	TRP	5.0
1	CCC	92	LEU	5.0
1	CCC	25	VAL	5.0
1	DDD	138	GLU	4.9
1	AAA	118	TYR	4.9
1	CCC	79	TYR	4.9
1	AAA	79	TYR	4.8
1	AAA	25	VAL	4.7
1	CCC	66	TRP	4.7
1	CCC	55	ILE	4.6
1	CCC	165	VAL	4.6
1	CCC	26	GLY	4.6
1	AAA	72	SER	4.6
1	CCC	164	PHE	4.6
1	AAA	98	VAL	4.6
1	AAA	21	CYS	4.6
1	CCC	75	VAL	4.5
1	CCC	100	VAL	4.5
1	CCC	86	LEU	4.5
1	AAA	90	SER	4.5
1	CCC	96	ALA	4.5
1	FFF	137	ALA	4.5
1	EEE	118	TYR	4.4
1	CCC	74	TYR	4.4
1	AAA	77	ARG	4.4
1	AAA	165	VAL	4.4
1	AAA	168	ALA	4.4
1	CCC	98	VAL	4.4
1	AAA	64	LEU	4.3
1	CCC	63	LEU	4.3
1	CCC	64	LEU	4.3
1	CCC	58	PHE	4.3
1	CCC	51	PRO	4.3
1	AAA	76	LEU	4.3
1	AAA	92	LEU	4.3
1	AAA	164	PHE	4.3
1	CCC	90	SER	4.3
1	AAA	57	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
1	AAA	70	ALA	4.3
1	CCC	159	TYR	4.2
1	AAA	4	VAL	4.2
1	AAA	74	TYR	4.2
1	AAA	96	ALA	4.1
1	FFF	118	TYR	4.1
1	EEE	51	PRO	4.1
1	AAA	27	ALA	4.1
1	AAA	65	LEU	4.1
1	AAA	139	SER	4.1
1	DDD	118	TYR	4.1
1	CCC	4	VAL	4.1
1	DDD	51	PRO	4.1
1	CCC	76	LEU	4.1
1	AAA	138	GLU	4.1
1	AAA	99	ASP	4.0
1	AAA	201	LEU	4.0
1	AAA	26	GLY	4.0
1	AAA	119	GLN	4.0
1	AAA	175	TYR	4.0
1	AAA	31	VAL	4.0
1	CCC	72	SER	4.0
1	AAA	63	LEU	4.0
1	FFF	122	PHE	3.9
1	BBB	118	TYR	3.9
1	CCC	70	ALA	3.9
1	DDD	34	ILE	3.9
1	CCC	27	ALA	3.9
1	DDD	55	ILE	3.9
1	EEE	55	ILE	3.9
1	AAA	102	THR	3.8
1	BBB	138	GLU	3.8
1	AAA	101	TRP	3.8
1	AAA	18	VAL	3.8
1	CCC	218	LYS	3.8
1	FFF	138	GLU	3.7
1	AAA	20	LEU	3.7
1	CCC	163	ASP	3.7
1	DDD	123	ASN	3.7
1	AAA	22	LEU	3.7
1	CCC	65	LEU	3.7
1	CCC	77	ARG	3.7

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Mol	Chain	Res	Type	RSRZ
1	CCC	168	ALA	3.7
1	CCC	18	VAL	3.7
1	DDD	139	SER	3.6
1	CCC	138	GLU	3.6
1	AAA	196	ALA	3.6
1	AAA	60	ASP	3.6
1	AAA	84	VAL	3.5
1	AAA	207	VAL	3.5
1	AAA	87	LEU	3.5
1	AAA	140	LEU	3.5
1	AAA	30	GLU	3.5
1	DDD	122	PHE	3.5
1	AAA	68	SER	3.5
1	CCC	21	CYS	3.5
1	CCC	62	ASP	3.5
1	AAA	206	ALA	3.5
1	CCC	61	GLY	3.5
1	AAA	36	PHE	3.4
1	AAA	73	LYS	3.4
1	CCC	32	VAL	3.4
1	CCC	87	LEU	3.4
1	AAA	159	TYR	3.4
1	CCC	78	LYS	3.4
1	CCC	88	ARG	3.4
1	EEE	218	LYS	3.4
1	AAA	51	PRO	3.4
1	EEE	123	ASN	3.4
1	CCC	122	PHE	3.4
1	CCC	60	ASP	3.4
1	AAA	81	THR	3.4
1	AAA	104	VAL	3.4
1	AAA	161	ALA	3.4
1	AAA	3	PRO	3.4
1	AAA	71	ILE	3.3
1	AAA	7	PHE	3.3
1	EEE	122	PHE	3.3
1	AAA	19	THR	3.3
1	AAA	107	HIS	3.3
1	CCC	20	LEU	3.3
1	BBB	122	PHE	3.3
1	CCC	84	VAL	3.3
1	AAA	203	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	AAA	163	ASP	3.3
1	CCC	157	HIS	3.3
1	CCC	68	SER	3.2
1	CCC	139	SER	3.2
1	AAA	89	GLU	3.2
1	AAA	16	ALA	3.2
1	CCC	3	PRO	3.2
1	CCC	166	SER	3.2
1	CCC	152	ALA	3.2
1	AAA	15	VAL	3.2
1	FFF	139	SER	3.2
1	BBB	34	ILE	3.2
1	FFF	55	ILE	3.2
1	AAA	152	ALA	3.2
1	AAA	32	VAL	3.1
1	CCC	22	LEU	3.1
1	AAA	93	GLU	3.1
1	CCC	99	ASP	3.1
1	CCC	156	LYS	3.1
1	CCC	102	THR	3.1
1	AAA	88	ARG	3.1
1	AAA	215	VAL	3.1
1	CCC	93	GLU	3.1
1	CCC	161	ALA	3.1
1	CCC	196	ALA	3.1
1	AAA	173	PHE	3.1
1	EEE	36	PHE	3.1
1	AAA	85	ASP	3.1
1	CCC	101	TRP	3.0
1	AAA	154	LEU	3.0
1	CCC	83	GLU	3.0
1	AAA	78	LYS	3.0
1	AAA	34	ILE	3.0
1	CCC	71	ILE	3.0
1	EEE	53	GLY	3.0
1	BBB	64[A]	LEU	3.0
1	CCC	81	THR	3.0
1	CCC	201	LEU	3.0
1	CCC	200	ARG	3.0
1	AAA	62	ASP	3.0
1	CCC	34	ILE	3.0
1	AAA	157	HIS	3.0

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Mol	Chain	Res	Type	RSRZ
1	EEE	69[A]	ARG	3.0
1	CCC	31	VAL	3.0
1	CCC	30	GLU	2.9
1	FFF	34	ILE	2.9
1	BBB	37	ASN	2.9
1	AAA	205	PRO	2.9
1	AAA	166	SER	2.9
1	AAA	209	LYS	2.9
1	CCC	175	TYR	2.9
1	AAA	167	PHE	2.9
1	AAA	146	VAL	2.9
1	FFF	51	PRO	2.9
1	AAA	108	THR	2.8
1	AAA	156	LYS	2.8
1	AAA	191	TYR	2.8
1	AAA	116	ILE	2.8
1	AAA	170	LEU	2.8
1	AAA	109	TYR	2.7
1	AAA	105	ASP	2.7
1	AAA	169	ASP	2.7
1	CCC	57	ALA	2.7
1	CCC	5	LYS	2.7
1	CCC	33	ASN	2.7
1	CCC	140	LEU	2.7
1	CCC	82	ASP	2.7
1	CCC	107	HIS	2.7
1	DDD	36	PHE	2.7
1	AAA	149	VAL	2.7
1	AAA	213	THR	2.7
1	AAA	53	GLY	2.7
1	DDD	140	LEU	2.7
1	AAA	94	GLU	2.7
1	BBB	36	PHE	2.6
1	DDD	52	PHE	2.6
1	AAA	171	ASN	2.6
1	CCC	19	THR	2.6
1	AAA	212	ALA	2.6
1	FFF	119	GLN	2.6
1	AAA	195	LYS	2.6
1	CCC	170	LEU	2.6
1	DDD	33	ASN	2.6
1	CCC	155	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	AAA	155	SER	2.6
1	DDD	90	SER	2.6
1	AAA	17	ARG	2.5
1	AAA	153	ARG	2.5
1	FFF	3	PRO	2.5
1	FFF	64	LEU	2.5
1	CCC	89	GLU	2.5
1	AAA	8	GLY	2.5
1	CCC	73	LYS	2.5
1	FFF	218	LYS	2.5
1	AAA	6	VAL	2.5
1	CCC	36	PHE	2.5
1	CCC	205	PRO	2.5
1	CCC	154	LEU	2.5
1	CCC	153	ARG	2.5
1	CCC	28	GLU	2.5
1	AAA	5	LYS	2.5
1	AAA	97	MET	2.5
1	BBB	218	LYS	2.5
1	AAA	61	GLY	2.5
1	AAA	210	ILE	2.5
1	DDD	92[A]	LEU	2.5
1	CCC	206	ALA	2.5
1	AAA	28	GLU	2.5
1	AAA	83	GLU	2.5
1	CCC	104	VAL	2.5
1	CCC	209	LYS	2.4
1	AAA	55	ILE	2.4
1	EEE	140	LEU	2.4
1	FFF	52	PHE	2.4
1	CCC	29	TYR	2.4
1	CCC	53	GLY	2.4
1	BBB	119	GLN	2.4
1	AAA	69	ARG	2.4
1	AAA	160	LEU	2.4
1	AAA	204	ARG	2.4
1	CCC	169	ASP	2.4
1	BBB	3	PRO	2.4
1	DDD	3	PRO	2.4
1	CCC	207	VAL	2.4
1	AAA	12	SER	2.3
1	AAA	82	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	CCC	167	PHE	2.3
1	CCC	17	ARG	2.3
1	CCC	50	ASN	2.3
1	CCC	160	LEU	2.3
1	AAA	115	PRO	2.3
1	EEE	3	PRO	2.3
1	BBB	33	ASN	2.3
1	EEE	33	ASN	2.3
1	AAA	172	HIS	2.3
1	CCC	59	GLN	2.3
1	CCC	85	ASP	2.3
1	FFF	33	ASN	2.3
1	AAA	52	PHE	2.3
1	AAA	193	HIS	2.3
1	CCC	7	PHE	2.3
1	FFF	36	PHE	2.3
1	AAA	29	TYR	2.3
1	CCC	203	ALA	2.2
1	FFF	53	GLY	2.2
1	AAA	214	MET	2.2
1	AAA	198	TRP	2.2
1	EEE	138	GLU	2.2
1	CCC	16	ALA	2.2
1	CCC	94	GLU	2.2
1	AAA	194	VAL	2.2
1	CCC	6	VAL	2.2
1	EEE	139	SER	2.2
1	AAA	147	LEU	2.2
1	AAA	185	ALA	2.2
1	EEE	34	ILE	2.2
1	CCC	80	LYS	2.2
1	AAA	106	ALA	2.2
1	CCC	145	LYS	2.1
1	AAA	177	PHE	2.1
1	AAA	181	ALA	2.1
1	AAA	9	PRO	2.1
1	AAA	150	TYR	2.1
1	CCC	115	PRO	2.1
1	CCC	119	GLN	2.1
1	AAA	121	LEU	2.1
1	EEE	52	PHE	2.1
1	AAA	176	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	CCC	97	MET	2.1
1	AAA	14	ASN	2.1
1	AAA	200	ARG	2.1
1	CCC	204	ARG	2.1
1	AAA	35	ASP	2.0
1	CCC	52	PHE	2.0
1	CCC	173	PHE	2.0
1	FFF	145	LYS	2.0
1	AAA	202	MET	2.0
1	AAA	199	ASP	2.0
1	FFF	62	ASP	2.0
1	AAA	103	GLU	2.0
1	AAA	117	VAL	2.0
1	CCC	149	VAL	2.0
1	AAA	33	ASN	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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
1	CSS	AAA	120	7/8	0.78	0.20	58,60,76,76	1
1	CSS	BBB	120	7/8	0.85	0.14	41,44,63,63	1
1	CSS	DDD	120	7/8	0.85	0.15	50,52,69,69	1
1	CSS	EEE	120	7/8	0.85	0.14	43,46,67,67	1
1	CSS	FFF	120	7/8	0.87	0.14	42,44,64,64	1
1	CSS	CCC	120	7/8	0.88	0.14	46,48,66,66	1

## 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( $\text{\AA}^2$ )	Q<0.9
2	SO4	CCC	301	5/5	0.79	0.14	60,77,81,82	0
2	SO4	EEE	301	5/5	0.89	0.10	61,63,65,67	0
2	SO4	FFF	301	5/5	0.91	0.09	54,56,62,72	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.