



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 28, 2026 – 12:45 AM UTC

PDB ID : 6TNL / pdb_00006tnl
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	FAILED
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

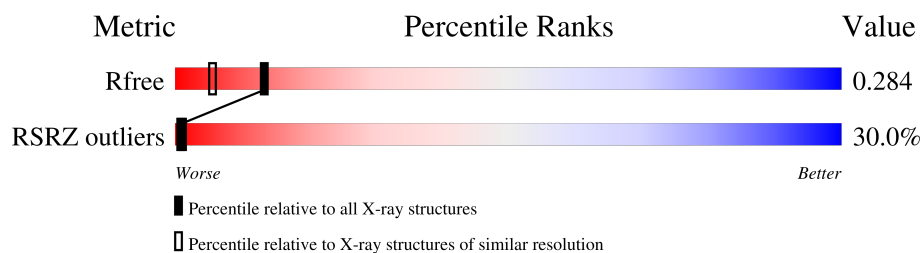
1 Overall quality at a glance

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}	180053	3494 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition [i](#)

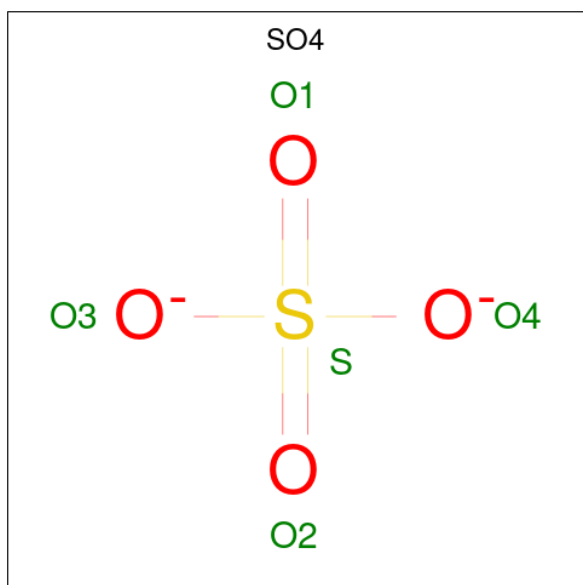
There are 3 unique types of molecules in this entry. The entry contains 18467 atoms, of which 8828 are hydrogens and 0 are deuteriums.

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 (CCD ID: SO4) (formula: O₄S).



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

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3 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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 (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	30.2	Xtrriage
Anisotropy	0.124	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 39.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.38$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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4.2 Too-close contacts [i](#)

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4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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4.3.2 Protein sidechains [i](#)

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4.3.3 RNA [i](#)

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

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	0.55	0	2,6,8	0.71	0
1	CSS	DDD	120	1	4,6,7	0.46	0	2,6,8	0.73	0
1	CSS	BBB	120	1	4,6,7	0.56	0	2,6,8	0.74	0
1	CSS	AAA	120	1	4,6,7	0.57	0	2,6,8	1.01	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CSS	CCC	120	1	4,6,7	0.52	0	2,6,8	0.73	0
1	CSS	FFF	120	1	4,6,7	0.67	0	2,6,8	0.77	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	DDD	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	CCC	120	1	-	0/1/5/7	-
1	CSS	FFF	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.

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 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	0.39	0	6,6,6	0.18	0
2	SO4	FFF	301	-	4,4,4	0.33	0	6,6,6	0.20	0
2	SO4	EEE	301	-	4,4,4	0.38	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.

No monomer is involved in short contacts.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 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, 95th 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 ²)	Q<0.9
1	AAA	189/219 (86%)	3.11	150 (79%) 0 0	35, 47, 67, 88	0
1	BBB	189/219 (86%)	0.35	13 (6%) 23 26	19, 28, 54, 75	1 (0%)
1	CCC	190/219 (86%)	2.57	118 (62%) 0 0	29, 46, 67, 100	0
1	DDD	188/219 (85%)	0.48	18 (9%) 13 15	18, 30, 55, 92	1 (0%)
1	EEE	188/219 (85%)	0.36	19 (10%) 12 14	13, 28, 51, 75	2 (1%)
1	FFF	191/219 (87%)	0.46	22 (11%) 9 11	19, 28, 55, 91	0
All	All	1135/1314 (86%)	1.22	340 (29%) 1 1	13, 36, 63, 100	4 (0%)

All (340) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	123	ASN	11.6
1	CCC	123	ASN	8.8
1	FFF	124	PRO	8.3
1	DDD	37	ASN	7.3
1	AAA	59	GLN	7.2
1	CCC	37	ASN	6.8
1	CCC	137	ALA	6.8
1	AAA	58	PHE	6.7
1	FFF	123	ASN	6.7
1	AAA	37	ASN	6.5
1	BBB	123	ASN	6.2
1	CCC	95	ALA	6.1
1	FFF	37	ASN	6.1
1	AAA	100	VAL	6.0
1	AAA	122	PHE	5.7
1	CCC	162	GLY	5.5
1	AAA	86	LEU	5.4
1	AAA	162	GLY	5.4
1	CCC	91	ASN	5.4

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Mol	Chain	Res	Type	RSRZ
1	CCC	118	TYR	5.4
1	AAA	91	ASN	5.4
1	AAA	95	ALA	5.4
1	AAA	66	TRP	5.3
1	AAA	75	VAL	5.3
1	CCC	92	LEU	5.2
1	CCC	25	VAL	5.2
1	AAA	118	TYR	5.1
1	CCC	79	TYR	5.1
1	AAA	79	TYR	5.0
1	DDD	138	GLU	5.0
1	CCC	66	TRP	4.9
1	AAA	25	VAL	4.9
1	CCC	26	GLY	4.9
1	CCC	165	VAL	4.9
1	CCC	55	ILE	4.9
1	CCC	164	PHE	4.8
1	AAA	98	VAL	4.8
1	AAA	72	SER	4.8
1	CCC	75	VAL	4.8
1	CCC	100	VAL	4.8
1	CCC	96	ALA	4.7
1	FFF	137	ALA	4.7
1	AAA	21	CYS	4.7
1	CCC	86	LEU	4.7
1	AAA	90	SER	4.7
1	EEE	118	TYR	4.6
1	AAA	168	ALA	4.6
1	CCC	74	TYR	4.6
1	AAA	165	VAL	4.6
1	CCC	98	VAL	4.6
1	AAA	64	LEU	4.5
1	CCC	63	LEU	4.5
1	CCC	64	LEU	4.5
1	AAA	57	ALA	4.5
1	AAA	70	ALA	4.5
1	CCC	58	PHE	4.5
1	AAA	76	LEU	4.5
1	AAA	92	LEU	4.5
1	AAA	77	ARG	4.5
1	CCC	51	PRO	4.5
1	AAA	164	PHE	4.5

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Mol	Chain	Res	Type	RSRZ
1	CCC	90	SER	4.4
1	AAA	4	VAL	4.4
1	CCC	159	TYR	4.4
1	AAA	96	ALA	4.4
1	AAA	74	TYR	4.4
1	AAA	27	ALA	4.4
1	FFF	118	TYR	4.3
1	EEE	51	PRO	4.3
1	AAA	65	LEU	4.3
1	CCC	4	VAL	4.3
1	DDD	118	TYR	4.3
1	DDD	51	PRO	4.3
1	CCC	76	LEU	4.3
1	AAA	26	GLY	4.3
1	AAA	139	SER	4.3
1	AAA	201	LEU	4.2
1	AAA	31	VAL	4.2
1	AAA	175	TYR	4.2
1	AAA	99	ASP	4.2
1	AAA	63	LEU	4.2
1	AAA	119	GLN	4.1
1	CCC	70	ALA	4.1
1	AAA	138	GLU	4.1
1	CCC	72	SER	4.1
1	FFF	122	PHE	4.1
1	CCC	27	ALA	4.1
1	BBB	118	TYR	4.1
1	DDD	34	ILE	4.1
1	DDD	55	ILE	4.0
1	EEE	55	ILE	4.0
1	AAA	101	TRP	4.0
1	AAA	102	THR	4.0
1	AAA	18	VAL	4.0
1	AAA	20	LEU	3.9
1	AAA	22	LEU	3.9
1	CCC	65	LEU	3.9
1	CCC	168	ALA	3.9
1	BBB	138	GLU	3.9
1	CCC	218	LYS	3.9
1	CCC	18	VAL	3.9
1	CCC	163	ASP	3.9
1	DDD	123	ASN	3.8

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Mol	Chain	Res	Type	RSRZ
1	FFF	138	GLU	3.8
1	AAA	196	ALA	3.8
1	DDD	139	SER	3.8
1	CCC	77	ARG	3.8
1	AAA	84	VAL	3.7
1	AAA	207	VAL	3.7
1	AAA	87	LEU	3.7
1	AAA	140	LEU	3.7
1	AAA	60	ASP	3.7
1	DDD	122	PHE	3.7
1	AAA	206	ALA	3.7
1	CCC	138	GLU	3.7
1	CCC	61	GLY	3.7
1	AAA	68	SER	3.6
1	CCC	21	CYS	3.6
1	CCC	32	VAL	3.6
1	AAA	36	PHE	3.6
1	CCC	87	LEU	3.6
1	CCC	62	ASP	3.6
1	AAA	159	TYR	3.6
1	AAA	30	GLU	3.6
1	AAA	161	ALA	3.6
1	AAA	51	PRO	3.6
1	AAA	104	VAL	3.6
1	CCC	122	PHE	3.6
1	AAA	3	PRO	3.5
1	AAA	81	THR	3.5
1	AAA	73	LYS	3.5
1	EEE	123	ASN	3.5
1	CCC	60	ASP	3.5
1	CCC	88	ARG	3.5
1	CCC	78	LYS	3.5
1	AAA	71	ILE	3.5
1	AAA	7	PHE	3.5
1	EEE	122	PHE	3.5
1	AAA	203	ALA	3.5
1	CCC	20	LEU	3.5
1	EEE	218	LYS	3.5
1	AAA	19	THR	3.5
1	CCC	84	VAL	3.5
1	BBB	122	PHE	3.5
1	AAA	107	HIS	3.5

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Mol	Chain	Res	Type	RSRZ
1	AAA	16	ALA	3.4
1	CCC	157	HIS	3.4
1	AAA	163	ASP	3.4
1	CCC	152	ALA	3.4
1	CCC	3	PRO	3.4
1	AAA	15	VAL	3.4
1	AAA	152	ALA	3.4
1	CCC	68	SER	3.4
1	CCC	139	SER	3.4
1	BBB	34	ILE	3.3
1	FFF	55	ILE	3.3
1	CCC	166	SER	3.3
1	AAA	32	VAL	3.3
1	CCC	22	LEU	3.3
1	FFF	139	SER	3.3
1	AAA	89	GLU	3.3
1	AAA	215	VAL	3.3
1	CCC	161	ALA	3.3
1	CCC	196	ALA	3.3
1	CCC	102	THR	3.3
1	CCC	101	TRP	3.3
1	CCC	99	ASP	3.2
1	AAA	173	PHE	3.2
1	EEE	36	PHE	3.2
1	AAA	93	GLU	3.2
1	AAA	154	LEU	3.2
1	CCC	156	LYS	3.2
1	EEE	53	GLY	3.2
1	AAA	88	ARG	3.2
1	AAA	85	ASP	3.2
1	AAA	34	ILE	3.2
1	CCC	71	ILE	3.2
1	BBB	64[A]	LEU	3.2
1	CCC	201	LEU	3.2
1	CCC	93	GLU	3.2
1	CCC	34	ILE	3.1
1	CCC	81	THR	3.1
1	CCC	31	VAL	3.1
1	FFF	34	ILE	3.1
1	AAA	157	HIS	3.1
1	AAA	62	ASP	3.1
1	CCC	83	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	AAA	78	LYS	3.1
1	CCC	200	ARG	3.1
1	AAA	205	PRO	3.1
1	BBB	37	ASN	3.1
1	EEE	69[A]	ARG	3.1
1	AAA	146	VAL	3.0
1	CCC	175	TYR	3.0
1	AAA	167	PHE	3.0
1	CCC	30	GLU	3.0
1	AAA	166	SER	3.0
1	FFF	51	PRO	3.0
1	AAA	108	THR	3.0
1	AAA	191	TYR	3.0
1	AAA	209	LYS	3.0
1	AAA	116	ILE	3.0
1	AAA	170	LEU	2.9
1	CCC	57	ALA	2.9
1	AAA	156	LYS	2.9
1	AAA	109	TYR	2.9
1	CCC	140	LEU	2.9
1	AAA	149	VAL	2.9
1	DDD	36	PHE	2.9
1	AAA	105	ASP	2.9
1	AAA	169	ASP	2.9
1	AAA	53	GLY	2.9
1	CCC	33	ASN	2.8
1	CCC	107	HIS	2.8
1	CCC	82	ASP	2.8
1	DDD	140	LEU	2.8
1	AAA	213	THR	2.8
1	CCC	5	LYS	2.8
1	AAA	212	ALA	2.8
1	BBB	36	PHE	2.8
1	DDD	52	PHE	2.8
1	AAA	171	ASN	2.8
1	CCC	19	THR	2.8
1	CCC	170	LEU	2.8
1	AAA	94	GLU	2.7
1	CCC	155	SER	2.7
1	FFF	119	GLN	2.7
1	DDD	33	ASN	2.7
1	AAA	8	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	FFF	64	LEU	2.7
1	FFF	3	PRO	2.7
1	AAA	155	SER	2.7
1	DDD	90	SER	2.7
1	AAA	195	LYS	2.7
1	AAA	6	VAL	2.7
1	CCC	36	PHE	2.7
1	CCC	154	LEU	2.7
1	CCC	205	PRO	2.7
1	AAA	61	GLY	2.6
1	CCC	206	ALA	2.6
1	AAA	17	ARG	2.6
1	AAA	153	ARG	2.6
1	DDD	92[A]	LEU	2.6
1	AAA	210	ILE	2.6
1	CCC	104	VAL	2.6
1	CCC	89	GLU	2.6
1	CCC	73	LYS	2.6
1	FFF	218	LYS	2.6
1	EEE	140	LEU	2.6
1	AAA	55	ILE	2.6
1	AAA	97	MET	2.6
1	CCC	153	ARG	2.6
1	CCC	53	GLY	2.6
1	CCC	29	TYR	2.6
1	FFF	52	PHE	2.6
1	CCC	28	GLU	2.6
1	AAA	5	LYS	2.6
1	BBB	218	LYS	2.6
1	AAA	28	GLU	2.5
1	AAA	83	GLU	2.5
1	AAA	160	LEU	2.5
1	CCC	209	LYS	2.5
1	CCC	207	VAL	2.5
1	BBB	119	GLN	2.5
1	BBB	3	PRO	2.5
1	DDD	3	PRO	2.5
1	AAA	69	ARG	2.5
1	CCC	169	ASP	2.5
1	CCC	160	LEU	2.5
1	CCC	167	PHE	2.5
1	AAA	204	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	AAA	12	SER	2.5
1	AAA	82	ASP	2.5
1	AAA	115	PRO	2.5
1	EEE	3	PRO	2.5
1	CCC	50	ASN	2.4
1	CCC	203	ALA	2.4
1	AAA	198	TRP	2.4
1	CCC	17	ARG	2.4
1	BBB	33	ASN	2.4
1	EEE	33	ASN	2.4
1	FFF	53	GLY	2.4
1	AAA	172	HIS	2.4
1	AAA	29	TYR	2.4
1	AAA	52	PHE	2.4
1	CCC	7	PHE	2.4
1	FFF	36	PHE	2.4
1	CCC	85	ASP	2.4
1	CCC	16	ALA	2.4
1	CCC	59	GLN	2.4
1	FFF	33	ASN	2.4
1	AAA	193	HIS	2.4
1	AAA	185	ALA	2.4
1	AAA	194	VAL	2.4
1	CCC	6	VAL	2.4
1	AAA	214	MET	2.4
1	AAA	147	LEU	2.3
1	AAA	106	ALA	2.3
1	EEE	34	ILE	2.3
1	EEE	139	SER	2.3
1	EEE	138	GLU	2.3
1	AAA	181	ALA	2.3
1	CCC	94	GLU	2.3
1	AAA	150	TYR	2.3
1	AAA	177	PHE	2.3
1	AAA	9	PRO	2.3
1	CCC	80	LYS	2.3
1	CCC	115	PRO	2.2
1	CCC	145	LYS	2.2
1	AAA	121	LEU	2.2
1	EEE	52	PHE	2.2
1	AAA	176	THR	2.2
1	CCC	119	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	CCC	52	PHE	2.2
1	CCC	173	PHE	2.2
1	AAA	197	TRP	2.2
1	AAA	14	ASN	2.2
1	CCC	97	MET	2.2
1	AAA	117	VAL	2.2
1	CCC	149	VAL	2.2
1	AAA	35	ASP	2.2
1	AAA	200	ARG	2.2
1	CCC	204	ARG	2.2
1	AAA	202	MET	2.1
1	AAA	199	ASP	2.1
1	FFF	62	ASP	2.1
1	FFF	145	LYS	2.1
1	AAA	33	ASN	2.1
1	FFF	32	VAL	2.1
1	AAA	103	GLU	2.1
1	AAA	56	PRO	2.1
1	BBB	51	PRO	2.1
1	CCC	108	THR	2.1
1	DDD	64	LEU	2.1
1	EEE	35	ASP	2.1
1	CCC	69	ARG	2.1
1	EEE	61	GLY	2.0
1	DDD	82	ASP	2.0
1	AAA	23	GLU	2.0
1	EEE	50	ASN	2.0

5.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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, 95th 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 ²)	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

5.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.4 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, 95th 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

5.5 Other polymers [i](#)

There are no such residues in this entry.