Full wwPDB X-ray Structure Validation Report ⓘ

Jun 21, 2021 – 12:12 PM BST

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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

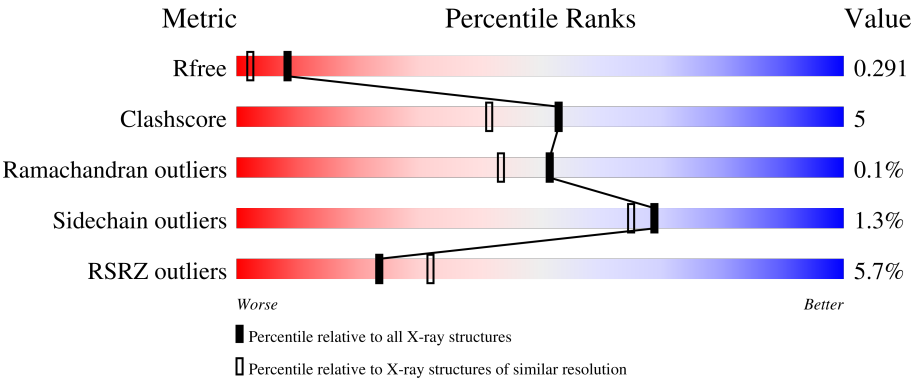
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.20
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.20

1 Overall quality at a glance (i)

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.



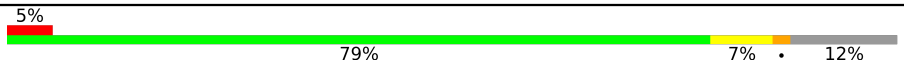
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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 >=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 <=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	9% 74% 11% • 13%
1	BBB	219	3% 78% 8% • 13%
1	CCC	219	7% 78% 8% • 13%
1	DDD	219	2% 78% 8% 14%
1	EEE	219	4% 76% 9% • 14%

Continued on next page...

Continued from previous page...

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

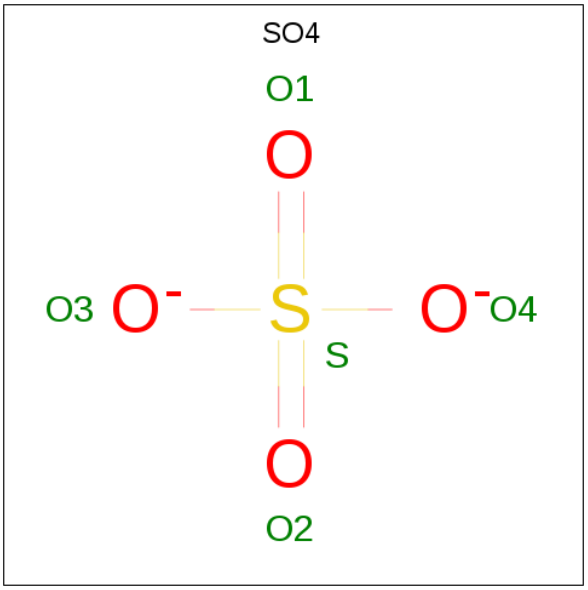
There are 3 unique types of molecules in this entry. The entry contains 18467 atoms, of which 8828 are hydrogens and 0 are deuteriums.

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_4S).



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.

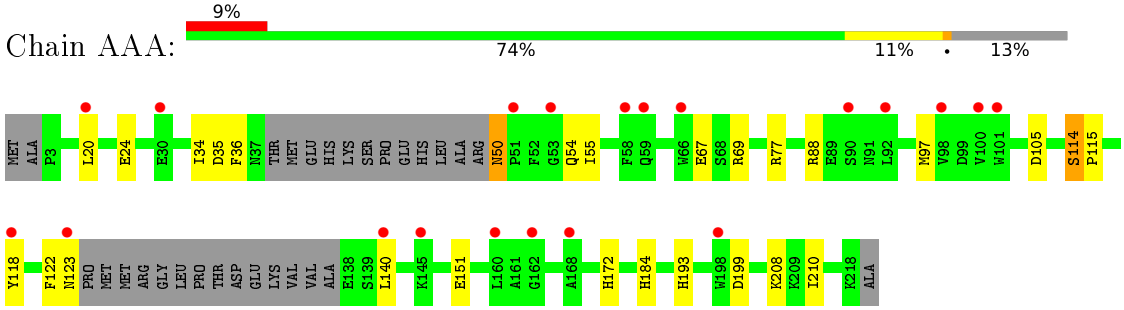
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	57	Total O 57 57	0	0
3	BBB	117	Total O 117 117	0	0
3	CCC	76	Total O 76 76	0	0
3	DDD	105	Total O 105 105	0	0
3	EEE	113	Total O 113 113	0	0
3	FFF	119	Total O 119 119	0	0

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.

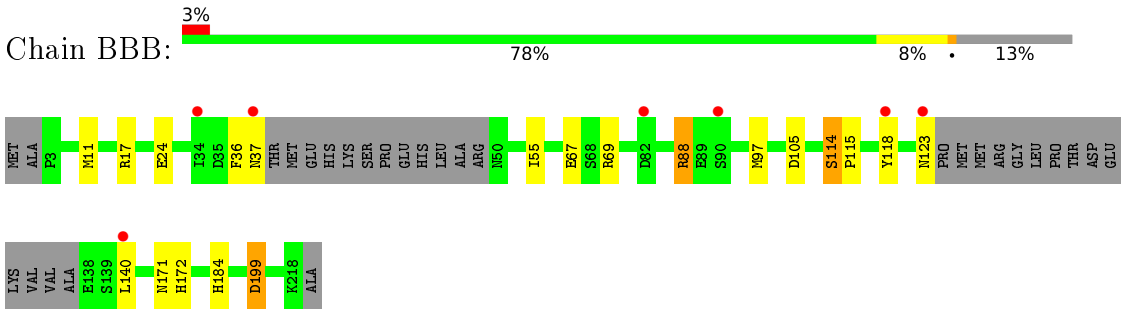
- Molecule 1: Glutathione transferase

Chain AAA:



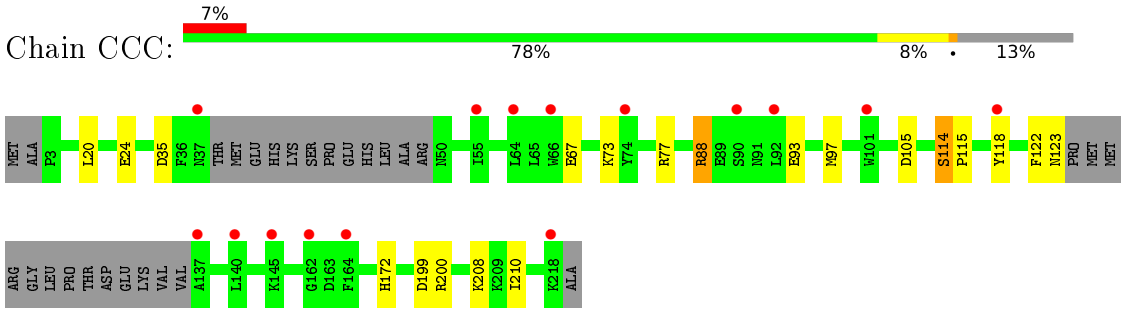
- Molecule 1: Glutathione transferase

Chain BBB:



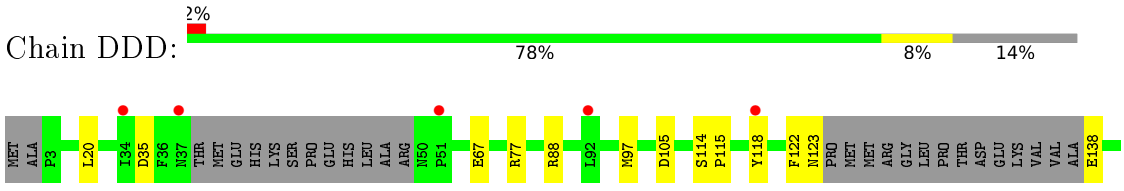
- Molecule 1: Glutathione transferase

Chain CCC:



- Molecule 1: Glutathione transferase

Chain DDD:

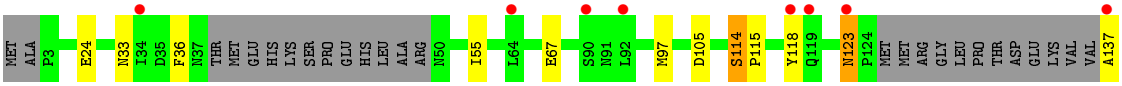


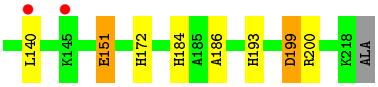
• Molecule 1: Glutathione transferase

Chain EEE:

• Molecule 1: Glutathione transferase

Chain FFF:





4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	3.74 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.260 , 0.284 0.267 , 0.291	Depositor DCC
R_{free} test set	5352 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	30.2	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.42 , 47.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.53$, $< L^2 > = 0.38$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage'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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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(^{o})	Ideal(^{o})
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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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%)	29 17
All	All	1103/1314 (84%)	1066 (97%)	36 (3%)	1 (0%)	51 43

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	FFF	123	ASN

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	AAA	152/188 (81%)	148 (97%)	4 (3%)	46 36
1	BBB	157/188 (84%)	156 (99%)	1 (1%)	86 85
1	CCC	154/188 (82%)	151 (98%)	3 (2%)	57 50
1	DDD	155/188 (82%)	154 (99%)	1 (1%)	86 85
1	EEE	157/188 (84%)	156 (99%)	1 (1%)	86 85
1	FFF	154/188 (82%)	152 (99%)	2 (1%)	69 65
All	All	929/1128 (82%)	917 (99%)	12 (1%)	69 65

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

Continued on next page...

Continued from previous page...

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 (i)

There are no RNA molecules in this entry.

5.4 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	DDD	120	1	4,6,7	0.46	0	1,6,8	0.32	0
1	CSS	CCC	120	1	4,6,7	0.54	0	1,6,8	0.34	0
1	CSS	AAA	120	1	4,6,7	0.56	0	1,6,8	0.01	0
1	CSS	FFF	120	1	4,6,7	0.71	0	1,6,8	0.59	0
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

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	DDD	120	1	-	0/1/5/7	-
1	CSS	CCC	120	1	-	0/1/5/7	-
1	CSS	AAA	120	1	-	0/1/5/7	-
1	CSS	FFF	120	1	-	0/1/5/7	-

Continued on next page...

Continued from previous page...

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	-

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 monosaccharides 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	EEE	301	-	4,4,4	0.39	0	6,6,6	0.13	0
2	SO4	FFF	301	-	4,4,4	0.40	0	6,6,6	0.20	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	EEE	301	SO4	1	0
2	FFF	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^{th} 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%)	1.01	20 (10%) 6 10	38, 48, 68, 87	0
1	BBB	189/219 (86%)	-0.01	7 (3%) 41 51	20, 29, 55, 85	0
1	CCC	190/219 (86%)	0.87	15 (7%) 12 19	31, 47, 66, 100	0
1	DDD	188/219 (85%)	0.01	5 (2%) 54 63	21, 31, 58, 94	0
1	EEE	188/219 (85%)	0.02	8 (4%) 35 45	21, 29, 55, 74	0
1	FFF	191/219 (87%)	0.06	10 (5%) 27 37	20, 28, 55, 92	0
All	All	1135/1314 (86%)	0.33	65 (5%) 23 32	20, 37, 65, 100	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	CCC	137	ALA	5.4
1	CCC	92	LEU	5.2
1	FFF	137	ALA	4.9
1	AAA	92	LEU	4.6
1	DDD	51	PRO	4.0
1	AAA	59	GLN	3.7
1	EEE	140	LEU	3.6
1	CCC	140	LEU	3.6
1	AAA	140	LEU	3.5
1	BBB	37	ASN	3.4
1	FFF	118	TYR	3.4
1	CCC	37	ASN	3.3
1	FFF	90	SER	3.2
1	CCC	118	TYR	3.1
1	AAA	118	TYR	3.1
1	FFF	119	GLN	3.0
1	FFF	64	LEU	3.0
1	EEE	55	ILE	2.9
1	CCC	162	GLY	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	EEE	92	LEU	2.8
1	DDD	118	TYR	2.8
1	FFF	145	LYS	2.7
1	BBB	118	TYR	2.7
1	FFF	123	ASN	2.7
1	BBB	34	ILE	2.6
1	AAA	66	TRP	2.6
1	CCC	64	LEU	2.5
1	FFF	92	LEU	2.5
1	AAA	58	PHE	2.5
1	CCC	218	LYS	2.5
1	EEE	118	TYR	2.5
1	AAA	101	TRP	2.5
1	AAA	100	VAL	2.5
1	EEE	36	PHE	2.5
1	BBB	140	LEU	2.5
1	EEE	138	GLU	2.4
1	DDD	34	ILE	2.4
1	AAA	51	PRO	2.4
1	AAA	198	TRP	2.4
1	CCC	164	PHE	2.4
1	CCC	55	ILE	2.4
1	DDD	37	ASN	2.3
1	CCC	101	TRP	2.3
1	DDD	92[A]	LEU	2.3
1	BBB	90	SER	2.3
1	AAA	145	LYS	2.3
1	CCC	66	TRP	2.3
1	CCC	90	SER	2.3
1	FFF	34	ILE	2.2
1	AAA	53	GLY	2.2
1	CCC	145	LYS	2.2
1	FFF	140	LEU	2.2
1	AAA	98	VAL	2.2
1	AAA	162	GLY	2.1
1	AAA	90	SER	2.1
1	EEE	90[A]	SER	2.1
1	AAA	168	ALA	2.1
1	BBB	123	ASN	2.1
1	AAA	20	LEU	2.1
1	AAA	30	GLU	2.0
1	BBB	82	ASP	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	EEE	145	LYS	2.0
1	CCC	74	TYR	2.0
1	AAA	123	ASN	2.0
1	AAA	160	LEU	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^{th} 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	0.74	0.14	58,60,76,76	1
1	CSS	DDD	120	7/8	0.75	0.12	50,52,69,69	1
1	CSS	CCC	120	7/8	0.84	0.09	46,48,66,66	1
1	CSS	FFF	120	7/8	0.84	0.10	42,44,64,64	1
1	CSS	EEE	120	7/8	0.86	0.11	43,46,67,67	1
1	CSS	BBB	120	7/8	0.86	0.12	41,44,63,63	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^{th} 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
2	SO4	CCC	301	5/5	0.88	0.17	60,77,81,82	0
2	SO4	EEE	301	5/5	0.96	0.09	61,63,65,67	0
2	SO4	FFF	301	5/5	0.96	0.11	54,56,62,72	0

6.5 Other polymers (i)

There are no such residues in this entry.