Full wwPDB X-ray Structure Validation Report ⓘ

Sep 12, 2023 – 01:57 AM EDT

PDB ID	:	4MTK
Title	:	Crystal structure of PA0091 VgrG1, the central spike of the Type VI Secretion System
Authors	:	Sycheva, L.V.; Shneider, M.M.; Leiman, P.G.
Deposited on	:	2013-09-19
Resolution	:	3.32 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:

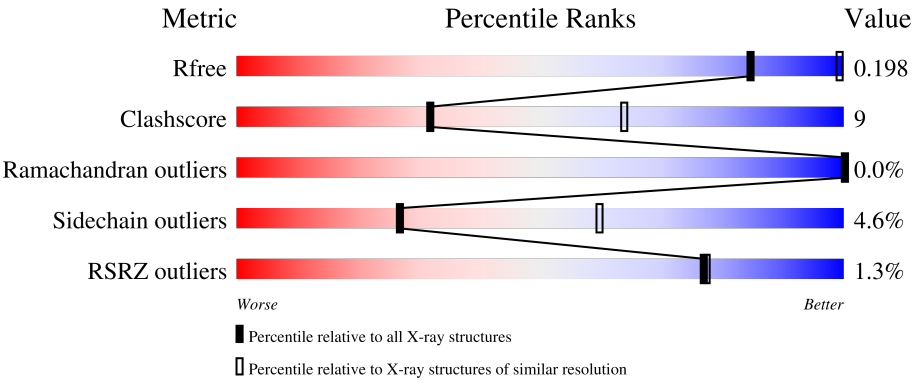
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.32 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	1089 (3.36-3.28)
Clashscore	141614	1137 (3.36-3.28)
Ramachandran outliers	138981	1115 (3.36-3.28)
Sidechain outliers	138945	1114 (3.36-3.28)
RSRZ outliers	127900	1059 (3.36-3.28)

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	A	643	67% 27%
1	B	643	74% 21%
1	C	643	76% 21%
1	D	643	78% 19%
1	E	643	76% 20%

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Mol	Chain	Length	Quality of chain
1	F	643	

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	A	714	-	-	-	X
2	SO4	A	722	-	-	-	X
2	SO4	A	727	-	-	-	X
2	SO4	A	728	-	-	-	X
2	SO4	A	734	-	-	-	X
2	SO4	A	739	-	-	-	X
2	SO4	A	741	-	-	-	X
2	SO4	A	746	-	-	-	X
2	SO4	A	748	-	-	-	X
2	SO4	B	719	-	-	X	-
2	SO4	B	721	-	-	-	X
2	SO4	B	732	-	-	X	-
2	SO4	B	735	-	-	X	-
2	SO4	B	739	-	-	X	X
2	SO4	B	746	-	-	-	X
2	SO4	B	749	-	-	-	X
2	SO4	C	714	-	-	-	X
2	SO4	C	722	-	-	-	X
2	SO4	C	726	-	-	-	X
2	SO4	C	727	-	-	-	X
2	SO4	C	731	-	-	X	-
2	SO4	C	732	-	-	-	X
2	SO4	C	733	-	-	-	X
2	SO4	C	734	-	-	-	X
2	SO4	C	739	-	-	X	-
2	SO4	C	741	-	-	-	X
2	SO4	C	743	-	-	-	X
2	SO4	D	726	-	-	-	X
2	SO4	D	728	-	-	-	X
2	SO4	E	729	-	-	-	X
2	SO4	E	730	-	-	-	X
2	SO4	F	719	-	-	-	X
2	SO4	F	725	-	-	-	X
2	SO4	F	731	-	-	-	X
2	SO4	F	733	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	F	741	-	-	-	X
2	SO4	F	742	-	-	-	X
3	TAM	D	735	-	-	-	X

2 Entry composition

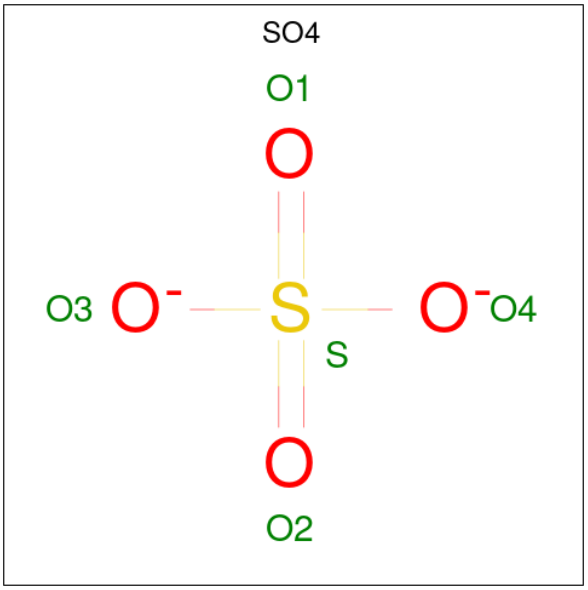
There are 4 unique types of molecules in this entry. The entry contains 31170 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 VgrG1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	627	Total	C	N	O	S	0	0	0
			4977	3113	910	939	15			
1	B	627	Total	C	N	O	S	0	0	0
			4977	3113	910	939	15			
1	C	627	Total	C	N	O	S	0	0	0
			4977	3113	910	939	15			
1	D	627	Total	C	N	O	S	0	0	0
			4977	3113	910	939	15			
1	E	627	Total	C	N	O	S	0	0	0
			4977	3113	910	939	15			
1	F	627	Total	C	N	O	S	0	0	0
			4977	3113	910	939	15			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
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2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
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2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
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2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
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2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
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2	B	1	Total O S 5 4 1	0	0
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2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
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2	B	1	Total O S 5 4 1	0	0
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2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
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2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
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2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
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2	D	1	Total O S 5 4 1	0	0
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2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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2	E	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
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2	E	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
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2	E	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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2	F	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
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2	F	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	F	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
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2	F	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0

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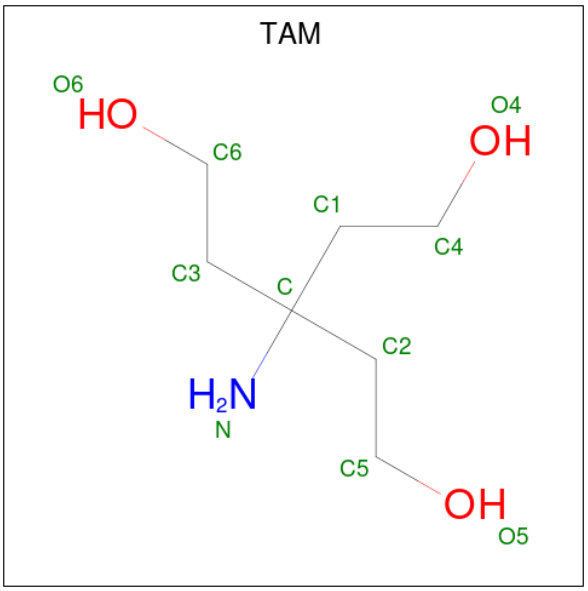
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	F	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0

- Molecule 3 is TRIS(HYDROXYETHYL)AMINOMETHANE (three-letter code: TAM) (formula: $C_7H_{17}NO_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 11 7 1 3	0	0
3	D	1	Total C N O 11 7 1 3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O 1 1	0	0
4	B	1	Total O 1 1	0	0
4	C	1	Total O 1 1	0	0
4	D	1	Total O 1 1	0	0

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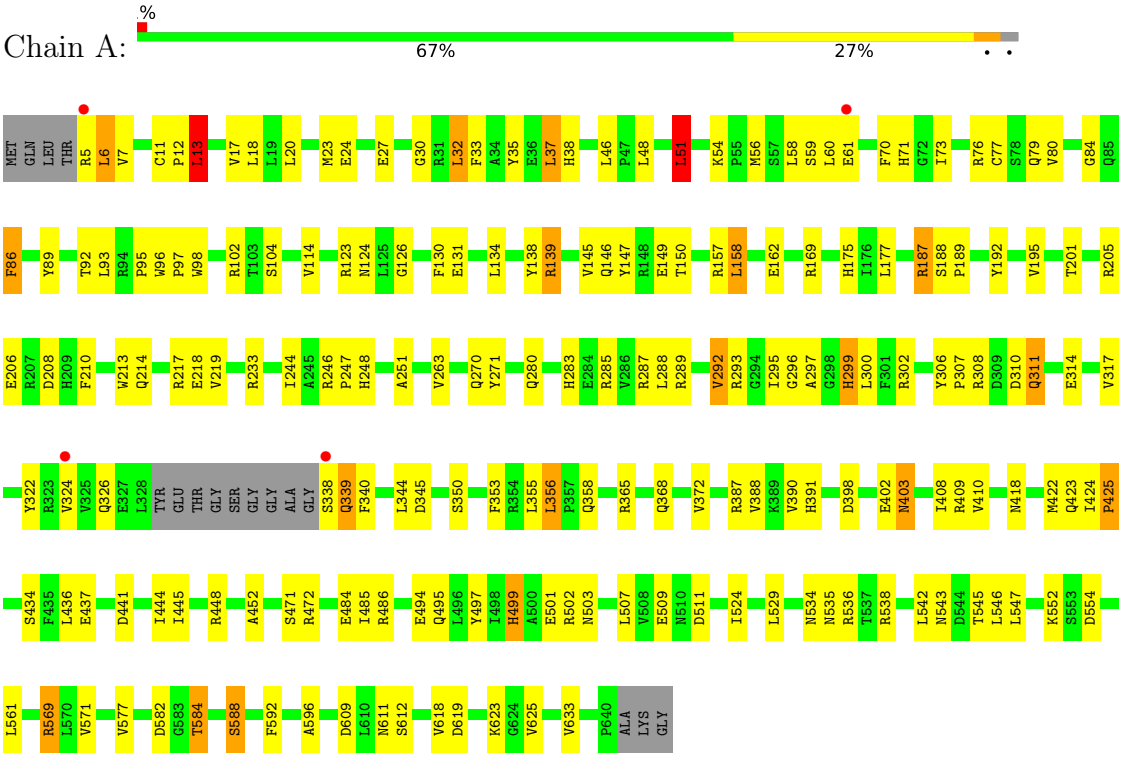
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total O 1 1	0	0
4	F	1	Total O 1 1	0	0

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.

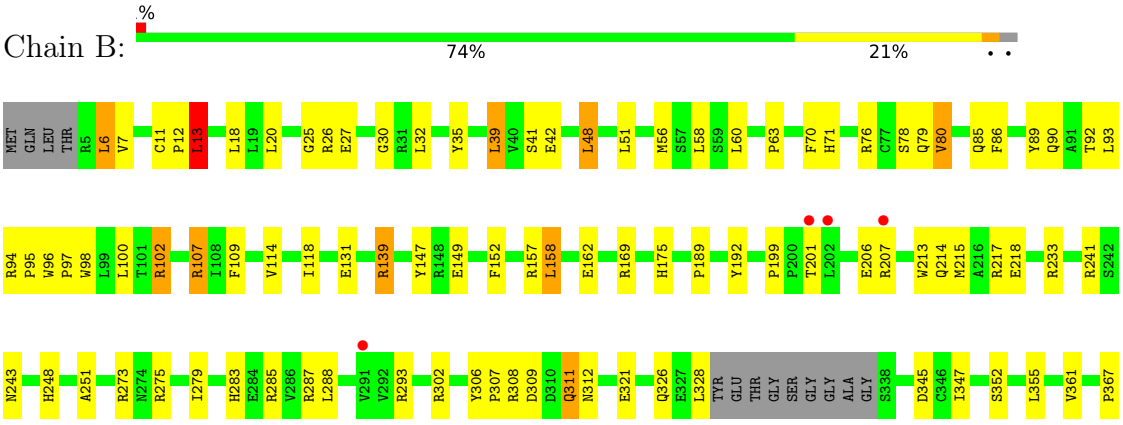
• Molecule 1: VgrG1

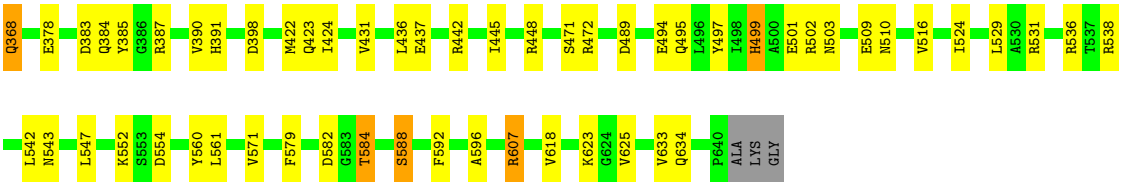
Chain A:

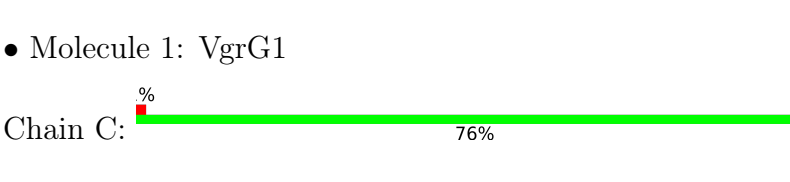


• Molecule 1: VgrG1

Chain B:

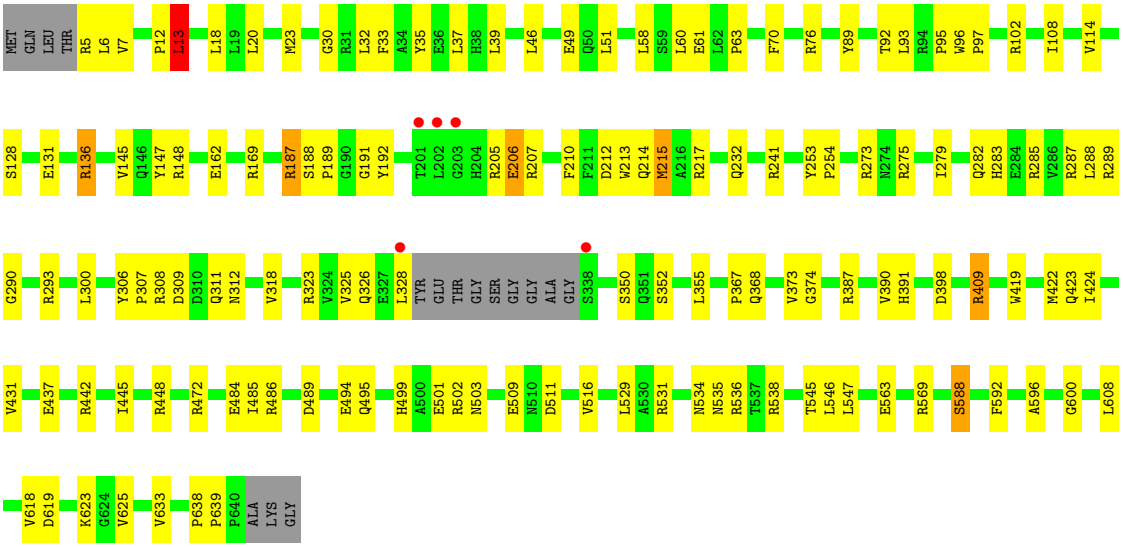






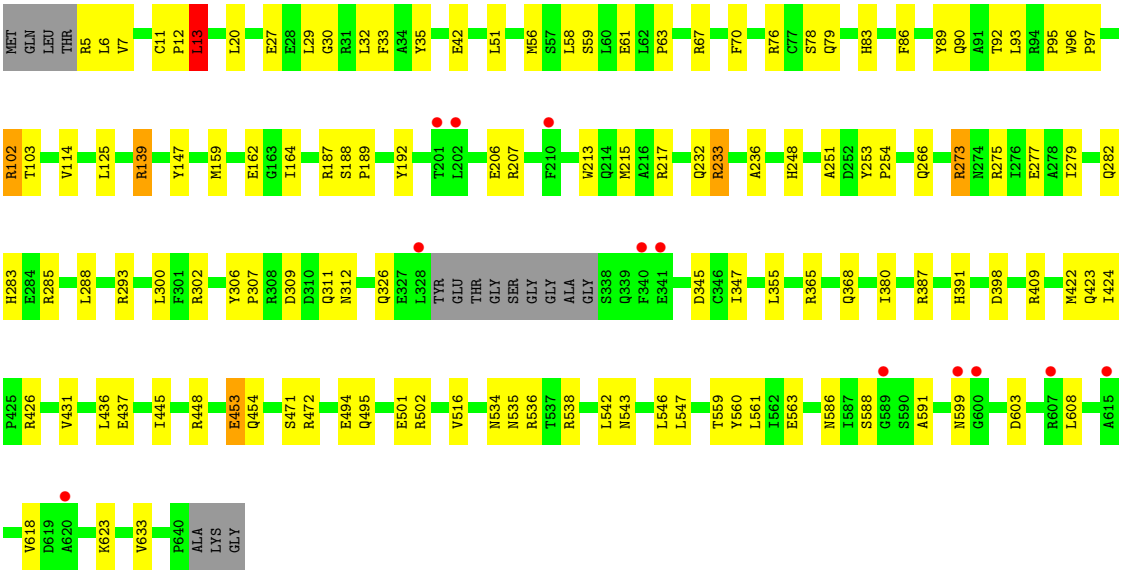
• Molecule 1: VgrG1

Chain C:



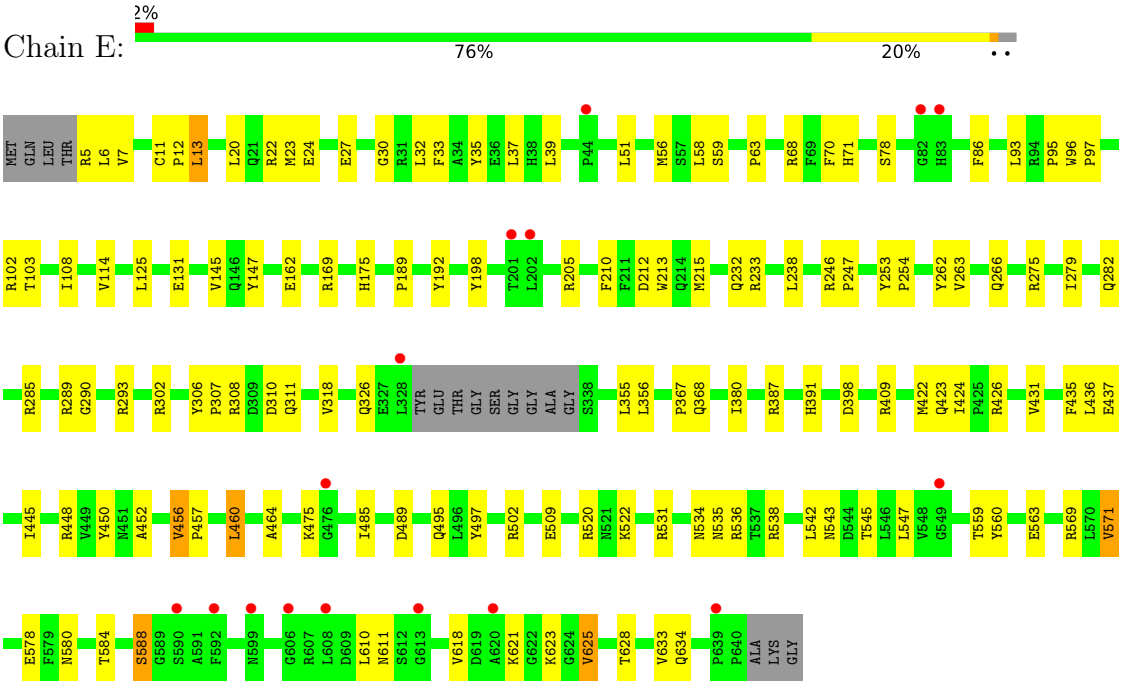
• Molecule 1: VgrG1

Chain D:



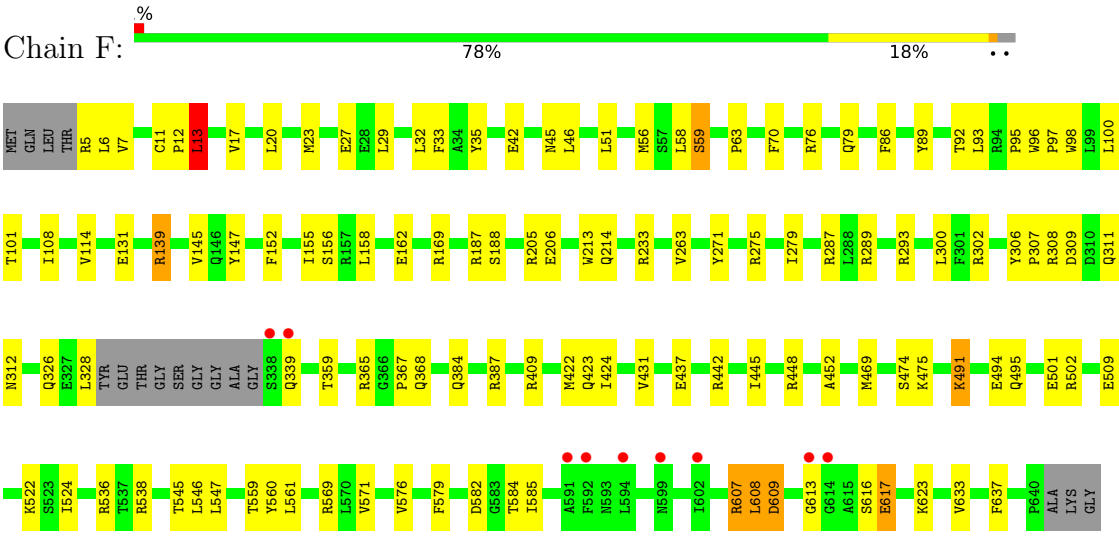
• Molecule 1: VgrG1

Chain E:



- Molecule 1: VgrG1

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	168.28Å 168.28Å 652.85Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.14 – 3.32 49.14 – 3.32	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.14-3.32) 99.8 (49.14-3.32)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.04 (at 3.33Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.170 , 0.195 0.174 , 0.198	Depositor DCC
R_{free} test set	3053 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å^2)	70.2	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 70.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.049 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	31170	wwPDB-VP
Average B, all atoms (Å^2)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.14% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: TAM, SO4

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	0.28	0/5095	0.70	4/6905 (0.1%)
1	B	0.23	0/5095	0.48	1/6905 (0.0%)
1	C	0.23	0/5095	0.49	1/6905 (0.0%)
1	D	0.22	0/5095	0.46	1/6905 (0.0%)
1	E	0.22	0/5095	0.44	0/6905
1	F	0.22	0/5095	0.46	1/6905 (0.0%)
All	All	0.24	0/30570	0.51	8/41430 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	84	GLY	N-CA-C	8.04	133.21	113.10
1	A	13	LEU	CA-CB-CG	6.46	130.15	115.30
1	A	51	LEU	CA-CB-CG	5.97	129.03	115.30
1	F	13	LEU	CA-CB-CG	5.63	128.26	115.30
1	D	13	LEU	CA-CB-CG	5.39	127.70	115.30
1	C	13	LEU	CA-CB-CG	5.21	127.29	115.30
1	B	13	LEU	CA-CB-CG	5.14	127.13	115.30
1	A	37	LEU	CA-CB-CG	5.04	126.90	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	339	GLN	Peptide

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	4977	0	4794	144	1
1	B	4977	0	4794	117	0
1	C	4977	0	4794	100	0
1	D	4977	0	4794	79	0
1	E	4977	0	4794	86	0
1	F	4977	0	4794	79	0
2	A	245	0	0	6	0
2	B	250	0	0	16	0
2	C	220	0	0	13	0
2	D	175	0	0	10	0
2	E	170	0	0	1	0
2	F	220	0	0	5	0
3	A	11	0	17	2	0
3	D	11	0	17	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
All	All	31170	0	28798	535	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 9.

All (535) 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:588:SER:HB3	1:A:618:VAL:HG12	1.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:TYR:HB2	1:A:93:LEU:HB2	1.56	0.86
1:C:588:SER:HB2	1:C:618:VAL:HG12	1.61	0.83
1:A:208:ASP:HB3	1:A:292:VAL:HA	1.60	0.83
1:B:588:SER:HB2	1:B:618:VAL:HG12	1.61	0.82
1:D:368:GLN:NE2	1:F:437:GLU:OE1	2.14	0.80
1:A:285:ARG:NH1	1:A:345:ASP:OD2	2.17	0.77
1:C:35:TYR:HB2	1:C:93:LEU:HB2	1.66	0.77
1:F:5:ARG:HG3	1:F:6:LEU:HD12	1.65	0.77
1:C:273:ARG:NH1	2:C:731:SO4:S	2.60	0.75
1:A:295:ILE:HG21	1:A:344:LEU:HD21	1.68	0.75
1:F:131:GLU:OE1	1:F:169:ARG:NH2	2.19	0.74
1:A:60:LEU:HD21	1:A:293:ARG:HD2	1.68	0.74
1:E:569:ARG:HG2	1:E:578:GLU:HG2	1.69	0.73
1:A:95:PRO:HB2	1:A:97:PRO:HD2	1.69	0.73
1:F:35:TYR:HB2	1:F:93:LEU:HB2	1.70	0.73
1:A:356:LEU:HB3	1:A:358:GLN:HG3	1.71	0.73
1:D:561:LEU:HD12	1:F:569:ARG:HH21	1.53	0.72
1:A:147:TYR:OH	1:C:437:GLU:OE1	2.07	0.72
1:A:437:GLU:OE2	1:B:147:TYR:OH	2.08	0.72
1:F:7:VAL:HG21	1:F:20:LEU:HD23	1.70	0.72
1:A:214:GLN:HG2	1:B:80:VAL:HA	1.72	0.71
1:E:423:GLN:O	1:E:448:ARG:NH2	2.23	0.71
1:E:22:ARG:NH2	1:E:24:GLU:OE2	2.23	0.71
1:D:35:TYR:HB2	1:D:93:LEU:HB2	1.73	0.70
1:D:285:ARG:NH1	1:D:345:ASP:OD2	2.24	0.70
1:B:437:GLU:OE1	1:C:147:TYR:OH	2.10	0.70
1:A:7:VAL:HG21	1:A:20:LEU:HD23	1.73	0.69
1:D:147:TYR:OH	1:F:437:GLU:OE1	2.11	0.69
1:F:98:TRP:O	1:F:101:THR:OG1	2.09	0.69
1:A:423:GLN:O	1:A:448:ARG:NH2	2.25	0.69
1:F:423:GLN:O	1:F:448:ARG:NH2	2.26	0.68
1:B:241:ARG:NH2	2:B:739:SO4:O1	2.26	0.68
1:D:437:GLU:OE2	1:E:147:TYR:OH	2.11	0.68
1:B:149:GLU:OE2	1:B:157:ARG:NH2	2.27	0.68
1:C:423:GLN:O	1:C:448:ARG:NH2	2.25	0.68
1:E:437:GLU:OE1	1:F:147:TYR:OH	2.12	0.68
1:A:11:CYS:HB2	1:A:12:PRO:HD2	1.76	0.68
1:E:588:SER:HB2	1:E:618:VAL:HG12	1.74	0.68
1:F:95:PRO:HB2	1:F:97:PRO:HD2	1.77	0.67
1:A:296:GLY:O	1:A:299:HIS:HB2	1.95	0.67
1:E:456:VAL:HG21	1:E:460:LEU:HD22	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:ARG:NH1	1:A:206:GLU:OE1	2.28	0.67
1:D:423:GLN:O	1:D:448:ARG:NH2	2.28	0.67
1:C:531:ARG:NH2	2:C:705:SO4:O2	2.28	0.66
1:D:233:ARG:HG2	1:D:236:ALA:HB2	1.77	0.66
1:A:218:GLU:HG3	1:B:76:ARG:HB3	1.77	0.66
1:E:35:TYR:HB2	1:E:93:LEU:HB2	1.77	0.66
1:B:423:GLN:O	1:B:448:ARG:NH2	2.29	0.65
1:E:58:LEU:HB2	1:E:70:PHE:HB2	1.78	0.65
1:A:486:ARG:NH2	2:A:739:SO4:O1	2.30	0.65
1:B:60:LEU:HD21	1:B:293:ARG:HD2	1.79	0.64
1:A:23:MET:HG3	1:A:37:LEU:HD12	1.79	0.64
1:A:189:PRO:HG2	1:A:192:TYR:HB2	1.79	0.64
1:A:365:ARG:NH2	2:A:715:SO4:O1	2.31	0.64
1:C:95:PRO:HB2	1:C:97:PRO:HD2	1.79	0.64
1:A:471:SER:OG	1:A:472:ARG:N	2.30	0.64
1:A:437:GLU:OE2	1:B:368:GLN:NE2	2.30	0.64
1:B:206:GLU:HG2	1:B:207:ARG:HG3	1.79	0.64
1:A:35:TYR:CZ	1:A:70:PHE:HD2	2.16	0.64
1:C:282:GLN:HA	1:C:285:ARG:HH11	1.63	0.64
1:D:502:ARG:NH1	2:D:710:SO4:O3	2.32	0.63
1:E:103:THR:HG21	1:E:125:LEU:HD21	1.81	0.63
1:F:609:ASP:N	1:F:609:ASP:OD1	2.31	0.63
1:B:471:SER:OG	1:B:472:ARG:N	2.30	0.63
1:A:391:HIS:ND1	1:A:398:ASP:OD2	2.32	0.63
1:C:387:ARG:HG2	1:C:409:ARG:HA	1.80	0.63
1:E:95:PRO:HB2	1:E:97:PRO:HD2	1.79	0.63
1:E:387:ARG:HG2	1:E:409:ARG:HA	1.81	0.62
1:B:35:TYR:HB2	1:B:93:LEU:HB2	1.80	0.62
1:A:388:VAL:HG11	1:A:425:PRO:HB2	1.81	0.62
2:A:708:SO4:O3	1:C:308:ARG:NH2	2.30	0.62
1:A:422:MET:HE2	1:A:424:ILE:HG12	1.82	0.62
1:A:502:ARG:HB3	1:B:494:GLU:O	1.99	0.62
1:D:5:ARG:N	1:D:61:GLU:OE1	2.32	0.62
1:A:494:GLU:O	1:C:502:ARG:HB3	2.00	0.62
1:B:502:ARG:HB3	1:C:494:GLU:O	2.00	0.62
1:C:486:ARG:NH2	2:C:712:SO4:O4	2.31	0.62
1:A:538:ARG:HH21	1:B:536:ARG:HD2	1.66	0.61
1:B:95:PRO:HB2	1:B:97:PRO:HD2	1.83	0.61
1:F:20:LEU:HD21	1:F:23:MET:HB2	1.82	0.61
1:E:20:LEU:HD11	1:E:23:MET:HB2	1.83	0.60
1:C:187:ARG:NH2	2:C:717:SO4:O2	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:323:ARG:NH2	2:C:739:SO4:S	2.74	0.60
1:B:20:LEU:O	1:B:326:GLN:NE2	2.35	0.60
1:C:422:MET:HE2	1:C:424:ILE:HG12	1.84	0.60
1:E:282:GLN:HA	1:E:285:ARG:HH11	1.66	0.60
1:B:422:MET:HE2	1:B:424:ILE:HG12	1.83	0.60
1:D:471:SER:OG	1:D:472:ARG:N	2.33	0.59
1:A:145:VAL:N	1:A:441:ASP:OD1	2.33	0.59
1:D:623:LYS:NZ	2:D:723:SO4:O1	2.33	0.59
1:A:561:LEU:HD11	1:C:623:LYS:HG3	1.84	0.59
1:D:58:LEU:HB2	1:D:70:PHE:HB2	1.85	0.59
1:C:131:GLU:OE1	1:C:169:ARG:NH1	2.36	0.59
1:B:502:ARG:HG2	1:B:503:ASN:H	1.67	0.59
1:A:71:HIS:HB3	1:A:175:HIS:HB3	1.85	0.58
1:A:30:GLY:HA3	1:A:355:LEU:HD11	1.85	0.58
1:F:387:ARG:HG2	1:F:409:ARG:HA	1.85	0.58
1:A:79:GLN:HG2	1:A:89:TYR:CE1	2.39	0.58
1:D:95:PRO:HB2	1:D:97:PRO:HD2	1.86	0.58
1:F:205:ARG:NH1	1:F:206:GLU:OE1	2.37	0.58
1:C:232:GLN:NE2	2:C:719:SO4:O1	2.37	0.58
1:A:293:ARG:HG2	1:A:340:PHE:CD1	2.39	0.58
1:C:241:ARG:NH2	2:C:710:SO4:O3	2.37	0.58
1:A:547:LEU:HB3	1:A:633:VAL:HG22	1.86	0.57
1:C:5:ARG:N	1:C:61:GLU:OE1	2.37	0.57
1:F:139:ARG:NH2	1:F:271:TYR:OH	2.37	0.57
1:A:302:ARG:NH1	1:A:314:GLU:HB2	2.19	0.57
1:C:20:LEU:HD21	1:C:23:MET:HB2	1.86	0.57
1:C:569:ARG:NH2	1:C:619:ASP:O	2.36	0.57
1:E:131:GLU:OE1	1:E:169:ARG:NH1	2.37	0.57
1:A:471:SER:OG	1:B:489:ASP:OD1	2.21	0.57
1:A:536:ARG:HD2	1:C:538:ARG:HH21	1.69	0.57
1:A:502:ARG:HG2	1:A:503:ASN:H	1.70	0.57
1:E:27:GLU:OE2	1:E:35:TYR:OH	2.23	0.57
1:A:233:ARG:NH2	1:A:263:VAL:O	2.38	0.57
1:B:552:LYS:NZ	1:B:554:ASP:OD1	2.37	0.57
1:E:502:ARG:HB3	1:F:494:GLU:O	2.05	0.57
1:B:385:TYR:HB2	1:B:387:ARG:HD2	1.87	0.57
1:F:365:ARG:NH2	2:F:727:SO4:S	2.78	0.56
1:A:27:GLU:OE2	1:A:35:TYR:OH	2.22	0.56
1:C:285:ARG:NH2	1:C:318:VAL:HG11	2.20	0.56
1:A:96:TRP:HD1	1:A:175:HIS:CE1	2.24	0.56
1:D:79:GLN:HG2	1:D:89:TYR:CE1	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:273:ARG:NH2	2:B:735:SO4:S	2.78	0.56
1:A:76:ARG:HG2	1:A:92:THR:HB	1.87	0.56
1:C:32:LEU:HD22	1:C:95:PRO:HG2	1.88	0.56
1:E:308:ARG:HH11	1:E:311:GLN:NE2	2.03	0.56
1:B:114:VAL:O	1:B:118:ILE:HG12	2.06	0.55
1:F:58:LEU:HB2	1:F:70:PHE:HB2	1.87	0.55
1:C:547:LEU:HB3	1:C:633:VAL:HG22	1.88	0.55
1:A:497:TYR:HH	1:A:499:HIS:CE1	2.23	0.55
1:E:625:VAL:HG22	1:E:628:THR:H	1.72	0.55
1:F:32:LEU:HD22	1:F:95:PRO:HG2	1.87	0.55
1:C:502:ARG:HG2	1:C:503:ASN:H	1.71	0.55
1:D:30:GLY:HA3	1:D:355:LEU:HD11	1.88	0.55
1:D:187:ARG:NH2	2:D:705:SO4:O4	2.37	0.55
1:E:531:ARG:HB3	1:F:637:PHE:HE1	1.71	0.55
1:F:42:GLU:HG2	1:F:86:PHE:HE1	1.72	0.55
1:B:391:HIS:ND1	1:B:398:ASP:OD2	2.35	0.55
1:B:42:GLU:HG2	1:B:86:PHE:HE1	1.72	0.55
1:E:285:ARG:NH2	1:E:318:VAL:HG11	2.22	0.54
1:A:157:ARG:HG3	1:A:158:LEU:HD13	1.89	0.54
1:A:205:ARG:NH2	1:A:206:GLU:OE2	2.39	0.54
1:A:195:VAL:HG21	1:A:210:PHE:CE2	2.42	0.54
1:D:102:ARG:HD2	1:D:102:ARG:N	2.22	0.54
1:F:502:ARG:NH1	2:F:703:SO4:O2	2.32	0.54
1:E:547:LEU:HB3	1:E:633:VAL:HG22	1.89	0.54
1:B:189:PRO:HG2	1:B:192:TYR:HB2	1.90	0.54
1:A:324:VAL:HG22	1:A:340:PHE:HD2	1.73	0.54
1:A:131:GLU:OE1	1:A:169:ARG:NH2	2.39	0.54
1:C:323:ARG:NH2	2:C:739:SO4:O3	2.30	0.54
1:F:571:VAL:HG13	1:F:576:VAL:HG22	1.90	0.54
1:A:214:GLN:CD	1:A:287:ARG:HH21	2.11	0.54
1:A:310:ASP:OD1	1:A:311:GLN:N	2.40	0.54
1:A:596:ALA:HB2	1:B:592:PHE:HD2	1.73	0.54
1:B:63:PRO:HD3	1:B:293:ARG:HH21	1.73	0.54
1:F:214:GLN:OE1	1:F:287:ARG:NH2	2.38	0.54
1:A:104:SER:HB3	1:A:150:THR:HG22	1.89	0.53
1:B:78:SER:HB2	1:B:90:GLN:HG3	1.90	0.53
1:B:596:ALA:HB2	1:C:592:PHE:HD1	1.74	0.53
1:B:39:LEU:HD12	1:B:89:TYR:HB2	1.90	0.53
1:D:78:SER:OG	1:D:90:GLN:HG3	2.08	0.53
1:D:536:ARG:HD2	1:F:538:ARG:HH21	1.74	0.53
1:E:7:VAL:HG22	1:E:326:GLN:OE1	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:509:GLU:HB2	1:C:501:GLU:O	2.08	0.53
1:C:273:ARG:NH1	2:C:731:SO4:O3	2.41	0.53
1:B:11:CYS:HB3	1:B:56:MET:HG3	1.91	0.53
1:D:547:LEU:HB3	1:D:633:VAL:HG22	1.91	0.53
1:B:497:TYR:OH	1:B:499:HIS:ND1	2.41	0.53
1:C:502:ARG:NH2	2:C:701:SO4:O2	2.42	0.53
1:D:391:HIS:ND1	1:D:398:ASP:OD2	2.37	0.53
1:F:63:PRO:HD3	1:F:293:ARG:HH21	1.72	0.53
1:F:114:VAL:HG21	1:F:162:GLU:HG3	1.91	0.53
1:B:79:GLN:HG2	1:B:89:TYR:CE1	2.44	0.53
1:C:212:ASP:HB3	1:C:289:ARG:HG3	1.89	0.53
1:D:273:ARG:NH2	2:D:722:SO4:O1	2.41	0.53
1:B:302:ARG:NH2	2:B:732:SO4:S	2.81	0.53
1:A:114:VAL:HG21	1:A:162:GLU:HG3	1.91	0.52
1:A:7:VAL:HG22	1:A:326:GLN:OE1	2.09	0.52
1:F:547:LEU:HB3	1:F:633:VAL:HG22	1.90	0.52
1:E:302:ARG:NH1	2:E:716:SO4:O4	2.31	0.52
1:F:7:VAL:HG22	1:F:326:GLN:OE1	2.09	0.52
1:B:32:LEU:HD22	1:B:95:PRO:HG2	1.91	0.52
1:E:422:MET:HE2	1:E:424:ILE:HG12	1.91	0.52
1:F:302:ARG:NH1	2:F:714:SO4:O4	2.42	0.52
1:C:60:LEU:HD21	1:C:293:ARG:HD2	1.92	0.52
1:D:453:GLU:HG3	1:D:454:GLN:H	1.75	0.52
1:A:7:VAL:HG22	1:A:326:GLN:CD	2.30	0.52
1:A:80:VAL:HA	1:C:214:GLN:HG3	1.91	0.52
1:A:509:GLU:HB2	1:B:501:GLU:O	2.10	0.52
1:B:547:LEU:HB3	1:B:633:VAL:HG22	1.91	0.52
1:A:192:TYR:CE2	1:A:292:VAL:HG23	2.46	0.51
1:C:63:PRO:HD3	1:C:293:ARG:HH21	1.75	0.51
1:C:188:SER:OG	1:C:300:LEU:O	2.20	0.51
1:B:384:GLN:N	2:B:740:SO4:O4	2.43	0.51
1:B:102:ARG:HD2	1:B:102:ARG:N	2.25	0.51
1:A:213:TRP:NE1	1:A:311:GLN:HG2	2.25	0.51
1:A:623:LYS:HG3	1:B:561:LEU:HD11	1.92	0.51
1:B:241:ARG:NH2	2:B:739:SO4:S	2.83	0.51
1:D:586:ASN:HB3	1:D:618:VAL:HG21	1.91	0.51
1:A:48:LEU:HB3	1:A:77:CYS:SG	2.50	0.51
1:D:437:GLU:OE2	1:E:368:GLN:NE2	2.44	0.51
1:B:114:VAL:HG13	1:B:158:LEU:HB3	1.93	0.51
1:B:131:GLU:OE1	1:B:169:ARG:NH1	2.43	0.51
1:E:308:ARG:HH11	1:E:311:GLN:HE22	1.57	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:387:ARG:HG2	1:D:409:ARG:HA	1.93	0.51
1:F:27:GLU:OE2	1:F:35:TYR:OH	2.29	0.51
1:E:63:PRO:HD3	1:E:293:ARG:HH21	1.76	0.51
1:A:5:ARG:HB2	1:A:6:LEU:HG	1.92	0.50
1:C:37:LEU:HB3	1:C:39:LEU:HD11	1.91	0.50
1:D:538:ARG:HH21	1:E:536:ARG:HD2	1.75	0.50
1:E:210:PHE:HD1	1:E:290:GLY:HA3	1.76	0.50
1:B:431:VAL:HG21	1:B:445:ILE:HD13	1.93	0.50
1:B:502:ARG:NH2	2:B:701:SO4:O4	2.44	0.50
1:D:63:PRO:HD3	1:D:293:ARG:NH2	2.26	0.50
1:B:241:ARG:HH11	1:B:243:ASN:HD21	1.60	0.50
1:E:37:LEU:HB3	1:E:39:LEU:HD11	1.93	0.50
1:A:139:ARG:NH1	1:A:271:TYR:OH	2.44	0.50
1:B:214:GLN:OE1	1:B:287:ARG:NH2	2.45	0.50
1:D:266:GLN:OE1	1:D:266:GLN:N	2.38	0.50
2:D:736:SO4:O2	1:F:538:ARG:NH1	2.45	0.50
1:E:32:LEU:HD22	1:E:95:PRO:HG2	1.92	0.50
1:C:373:VAL:HG22	1:C:374:GLY:H	1.76	0.50
1:D:591:ALA:O	1:E:584:THR:HA	2.12	0.50
1:D:285:ARG:HD3	1:D:347:ILE:HG22	1.93	0.50
1:E:308:ARG:HG2	1:E:310:ASP:OD1	2.11	0.50
1:B:18:LEU:HD22	1:B:39:LEU:HD13	1.93	0.49
1:B:302:ARG:NH2	2:B:732:SO4:O2	2.45	0.49
1:B:538:ARG:NH1	2:B:750:SO4:O4	2.45	0.49
1:D:114:VAL:HG21	1:D:162:GLU:HG3	1.92	0.49
1:C:529:LEU:HD21	1:C:531:ARG:HH11	1.78	0.49
1:D:42:GLU:HG2	1:D:86:PHE:HE1	1.77	0.49
1:A:501:GLU:O	1:C:509:GLU:HB2	2.13	0.49
1:A:503:ASN:ND2	1:C:511:ASP:HB2	2.28	0.49
1:B:27:GLU:OE2	1:B:35:TYR:OH	2.31	0.49
1:A:17:VAL:HG12	1:A:46:LEU:HD11	1.93	0.49
1:A:507:LEU:HD23	1:B:499:HIS:CE1	2.48	0.49
1:E:114:VAL:HG21	1:E:162:GLU:HG3	1.94	0.49
1:B:285:ARG:HD3	1:B:347:ILE:HG22	1.95	0.49
1:F:17:VAL:HG12	1:F:46:LEU:HD11	1.95	0.49
1:B:12:PRO:O	1:B:13:LEU:HB3	2.12	0.49
1:C:60:LEU:HD21	1:C:293:ARG:HB3	1.95	0.49
1:B:582:ASP:OD1	1:B:584:THR:OG1	2.24	0.48
1:A:11:CYS:SG	1:A:18:LEU:HD12	2.53	0.48
1:C:419:TRP:NE1	2:C:741:SO4:O2	2.36	0.48
1:A:11:CYS:HB3	1:A:56:MET:HG3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:ARG:NH1	2:A:702:SO4:O2	2.43	0.48
1:E:108:ILE:HG12	1:E:145:VAL:HG22	1.95	0.48
1:F:79:GLN:HG2	1:F:89:TYR:CE1	2.48	0.48
1:F:582:ASP:OD1	1:F:584:THR:OG1	2.26	0.48
1:C:308:ARG:NH1	1:C:311:GLN:OE1	2.40	0.48
1:E:380:ILE:HG12	1:E:426:ARG:HG2	1.96	0.48
1:F:11:CYS:HB3	1:F:56:MET:HG3	1.94	0.48
1:B:233:ARG:NH2	2:B:717:SO4:O1	2.44	0.48
1:C:7:VAL:HG22	1:C:326:GLN:OE1	2.12	0.48
1:D:27:GLU:OE2	1:D:35:TYR:OH	2.30	0.48
1:D:213:TRP:HD1	1:D:288:LEU:HD21	1.78	0.48
1:E:578:GLU:OE2	1:E:621:LYS:NZ	2.46	0.48
1:A:96:TRP:CG	1:A:97:PRO:HD3	2.49	0.48
1:C:484:GLU:HG2	1:C:485:ILE:N	2.29	0.48
1:F:289:ARG:NH2	2:F:707:SO4:O3	2.44	0.48
1:C:58:LEU:HB2	1:C:70:PHE:HB2	1.94	0.48
1:A:248:HIS:CE1	1:A:251:ALA:HB2	2.48	0.47
1:C:7:VAL:HG21	1:C:20:LEU:HD23	1.97	0.47
1:D:365:ARG:NH2	2:D:734:SO4:O2	2.47	0.47
1:E:238:LEU:O	1:E:262:TYR:OH	2.25	0.47
1:F:309:ASP:HA	1:F:312:ASN:HD22	1.79	0.47
1:A:410:VAL:HA	1:A:445:ILE:HB	1.95	0.47
1:A:502:ARG:NH2	2:A:701:SO4:O4	2.27	0.47
1:B:241:ARG:NH1	1:B:243:ASN:HD21	2.12	0.47
2:D:708:SO4:O2	1:F:308:ARG:NH2	2.47	0.47
1:B:18:LEU:HD23	1:B:41:SER:HB2	1.95	0.47
1:D:422:MET:HE2	1:D:424:ILE:HG12	1.95	0.47
1:D:275:ARG:O	1:D:279:ILE:HG13	2.14	0.47
1:E:5:ARG:HB3	1:E:6:LEU:HD12	1.97	0.47
1:E:30:GLY:HA3	1:E:355:LEU:HD11	1.96	0.47
1:C:431:VAL:HG21	1:C:445:ILE:HD13	1.95	0.47
1:A:390:VAL:HG22	1:A:408:ILE:HD12	1.97	0.47
1:A:592:PHE:HD2	1:C:596:ALA:HB2	1.80	0.47
3:A:749:TAM:H21	3:A:749:TAM:H41	1.58	0.47
1:B:42:GLU:HG2	1:B:86:PHE:CE1	2.48	0.47
1:A:484:GLU:HG2	1:A:485:ILE:N	2.30	0.47
1:B:217:ARG:HA	1:B:283:HIS:O	2.14	0.47
1:C:30:GLY:HA3	1:C:355:LEU:HD11	1.97	0.47
1:E:308:ARG:NE	1:F:45:ASN:OD1	2.38	0.47
1:F:233:ARG:NH2	1:F:263:VAL:O	2.48	0.47
1:B:538:ARG:HH21	1:C:536:ARG:HD2	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:273:ARG:NH1	2:C:731:SO4:O2	2.48	0.47
1:D:380:ILE:HG21	1:E:464:ALA:HB1	1.97	0.47
1:A:213:TRP:HD1	1:A:288:LEU:HD21	1.80	0.47
1:C:391:HIS:ND1	1:C:398:ASP:OD2	2.44	0.47
1:D:309:ASP:HA	1:D:312:ASN:HD22	1.80	0.47
1:E:96:TRP:CG	1:E:97:PRO:HD3	2.50	0.47
1:E:198:TYR:CD2	1:E:205:ARG:HG2	2.50	0.47
1:B:94:ARG:NH2	2:B:710:SO4:O1	2.47	0.46
1:B:213:TRP:HD1	1:B:288:LEU:HD21	1.79	0.46
1:B:471:SER:OG	1:C:489:ASP:OD2	2.28	0.46
1:B:623:LYS:HD2	1:C:563:GLU:OE2	2.15	0.46
1:C:12:PRO:O	1:C:13:LEU:HB3	2.14	0.46
1:B:30:GLY:HA3	1:B:355:LEU:HD11	1.96	0.46
1:D:453:GLU:HG3	1:D:454:GLN:N	2.30	0.46
1:C:114:VAL:HG21	1:C:162:GLU:HG3	1.96	0.46
1:F:96:TRP:CG	1:F:97:PRO:HD3	2.51	0.46
1:B:436:LEU:HA	1:C:367:PRO:O	2.16	0.46
1:B:502:ARG:HB2	1:C:494:GLU:HB2	1.97	0.46
1:E:475:LYS:O	1:F:491:LYS:HG3	2.15	0.46
1:A:210:PHE:HD1	1:A:289:ARG:O	1.97	0.46
1:A:353:PHE:HZ	1:A:355:LEU:HD23	1.79	0.46
1:A:511:ASP:HB2	1:B:503:ASN:ND2	2.31	0.46
1:C:217:ARG:HA	1:C:283:HIS:O	2.15	0.46
1:D:309:ASP:N	1:D:309:ASP:OD1	2.49	0.46
1:D:471:SER:OG	1:E:489:ASP:OD1	2.28	0.46
1:A:12:PRO:HG3	1:A:54:LYS:HB3	1.98	0.46
1:A:582:ASP:OD1	1:A:584:THR:OG1	2.30	0.46
1:D:139:ARG:NH2	2:D:724:SO4:S	2.89	0.46
1:F:213:TRP:CE2	1:F:311:GLN:HG2	2.51	0.46
1:F:431:VAL:HG21	1:F:445:ILE:HD13	1.97	0.46
1:A:162:GLU:OE2	1:A:271:TYR:OH	2.32	0.46
1:A:306:TYR:HA	1:A:307:PRO:HD2	1.67	0.46
1:E:210:PHE:CD1	1:E:290:GLY:HA3	2.51	0.46
1:F:384:GLN:N	2:F:715:SO4:O4	2.49	0.46
1:A:436:LEU:HA	1:B:367:PRO:O	2.16	0.46
3:A:749:TAM:H61	3:A:749:TAM:H11	1.72	0.46
1:B:273:ARG:NH2	2:B:735:SO4:O1	2.49	0.46
1:C:147:TYR:CE2	1:C:148:ARG:HG3	2.51	0.46
1:D:7:VAL:N	1:D:326:GLN:OE1	2.46	0.46
1:E:520:ARG:HH21	1:E:522:LYS:HD3	1.79	0.46
1:F:63:PRO:HD3	1:F:293:ARG:NH2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:ALA:HB2	1:C:232:GLN:HA	1.97	0.46
1:B:139:ARG:NH1	2:B:719:SO4:S	2.89	0.46
1:B:531:ARG:NH2	2:B:726:SO4:O2	2.45	0.46
1:D:12:PRO:O	1:D:13:LEU:HB3	2.15	0.46
1:F:108:ILE:HG12	1:F:145:VAL:HG22	1.97	0.45
1:B:100:LEU:HB2	1:B:152:PHE:HB2	1.97	0.45
1:B:542:LEU:HB3	1:B:543:ASN:H	1.57	0.45
1:E:12:PRO:O	1:E:13:LEU:HB3	2.15	0.45
1:F:12:PRO:O	1:F:13:LEU:HB3	2.16	0.45
1:F:275:ARG:O	1:F:279:ILE:HG13	2.16	0.45
1:D:96:TRP:CG	1:D:97:PRO:HD3	2.51	0.45
1:D:253:TYR:HA	1:D:254:PRO:HD3	1.87	0.45
1:E:71:HIS:HB3	1:E:175:HIS:HB3	1.99	0.45
1:E:538:ARG:HH21	1:F:536:ARG:HD2	1.82	0.45
1:E:11:CYS:HB3	1:E:56:MET:HG3	1.99	0.45
1:B:218:GLU:HG3	1:C:76:ARG:HB3	1.99	0.45
1:D:67:ARG:N	2:D:731:SO4:O4	2.48	0.45
1:E:275:ARG:O	1:E:279:ILE:HG13	2.16	0.45
1:A:73:ILE:O	1:A:93:LEU:HA	2.17	0.45
1:A:76:ARG:HA	1:C:217:ARG:O	2.17	0.45
1:F:33:PHE:CE2	1:F:95:PRO:HB3	2.51	0.45
1:B:139:ARG:NH1	2:B:719:SO4:O3	2.49	0.45
1:B:309:ASP:HA	1:B:312:ASN:HD22	1.81	0.45
1:A:79:GLN:HG2	1:A:89:TYR:CD1	2.52	0.45
1:B:25:GLY:O	1:B:26:ARG:HD3	2.16	0.45
1:A:145:VAL:HG12	1:A:147:TYR:HB2	1.99	0.45
1:A:217:ARG:HA	1:A:283:HIS:O	2.15	0.45
1:A:219:VAL:HB	1:B:98:TRP:CH2	2.51	0.45
1:C:189:PRO:HG2	1:C:192:TYR:HB2	1.99	0.45
1:F:188:SER:OG	1:F:300:LEU:O	2.21	0.45
1:A:33:PHE:CE2	1:A:95:PRO:HB3	2.52	0.44
1:D:436:LEU:HA	1:E:367:PRO:O	2.17	0.44
1:A:37:LEU:HD21	1:A:58:LEU:HD11	1.98	0.44
1:A:195:VAL:HG21	1:A:210:PHE:HE2	1.83	0.44
1:B:199:PRO:HB2	1:B:201:THR:HG22	1.99	0.44
1:C:136:ARG:H	1:C:136:ARG:HG3	1.49	0.44
1:C:253:TYR:HA	1:C:254:PRO:HD3	1.85	0.44
1:D:11:CYS:HB3	1:D:56:MET:HG3	1.98	0.44
1:D:431:VAL:HG21	1:D:445:ILE:HD13	2.00	0.44
1:A:296:GLY:HA2	1:A:322:TYR:OH	2.18	0.44
1:B:32:LEU:HD21	1:B:97:PRO:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:LEU:HB2	1:B:70:PHE:HB2	1.98	0.44
1:B:96:TRP:CG	1:B:97:PRO:HD3	2.52	0.44
1:F:607:ARG:H	1:F:607:ARG:HD2	1.82	0.44
1:A:104:SER:HA	1:A:150:THR:HA	1.99	0.44
1:A:308:ARG:HH11	1:A:311:GLN:NE2	2.16	0.44
1:B:26:ARG:HD2	1:B:321:GLU:HG2	1.99	0.44
1:D:217:ARG:HA	1:D:283:HIS:O	2.17	0.44
1:D:494:GLU:O	1:F:502:ARG:HB3	2.17	0.44
1:B:76:ARG:HG2	1:B:92:THR:HB	2.00	0.44
1:B:157:ARG:HD3	1:B:361:VAL:HA	1.98	0.44
1:B:308:ARG:NH2	2:B:711:SO4:O1	2.47	0.44
1:D:302:ARG:NH1	2:D:716:SO4:O2	2.50	0.44
1:E:542:LEU:HB3	1:E:543:ASN:H	1.50	0.44
1:E:623:LYS:HG3	1:F:561:LEU:HD11	1.98	0.44
1:A:524:ILE:HG13	1:B:516:VAL:HB	2.00	0.44
1:C:205:ARG:NH1	1:C:206:GLU:OE1	2.51	0.44
1:F:100:LEU:HB2	1:F:152:PHE:HB2	1.99	0.44
1:C:76:ARG:HG2	1:C:92:THR:HB	1.99	0.44
1:C:275:ARG:O	1:C:279:ILE:HG12	2.18	0.44
1:A:502:ARG:HB2	1:B:494:GLU:HB2	2.00	0.44
1:B:107:ARG:HD3	1:B:109:PHE:CZ	2.53	0.44
1:C:96:TRP:CG	1:C:97:PRO:HD3	2.52	0.44
1:D:306:TYR:CD1	1:D:307:PRO:HD2	2.53	0.44
1:E:212:ASP:HB3	1:E:289:ARG:HB2	1.99	0.44
1:F:522:LYS:HE3	1:F:524:ILE:HD13	1.98	0.44
1:A:402:GLU:HG2	1:A:403:ASN:OD1	2.16	0.43
1:B:524:ILE:HG13	1:C:516:VAL:HB	2.00	0.43
1:D:603:ASP:OD1	1:F:613:GLY:N	2.37	0.43
1:C:63:PRO:HD3	1:C:293:ARG:NH2	2.33	0.43
1:C:472:ARG:HA	1:C:472:ARG:HD3	1.85	0.43
3:D:735:TAM:H12	3:D:735:TAM:H61	1.59	0.43
1:F:162:GLU:OE2	1:F:271:TYR:OH	2.33	0.43
1:C:6:LEU:HB3	1:C:326:GLN:OE1	2.18	0.43
1:C:46:LEU:HB2	1:C:89:TYR:CE2	2.53	0.43
1:A:219:VAL:HB	1:B:98:TRP:HH2	1.83	0.43
1:E:189:PRO:HG2	1:E:192:TYR:HB2	2.00	0.43
1:B:285:ARG:NH1	1:B:345:ASP:OD2	2.51	0.43
1:E:233:ARG:NH2	1:E:263:VAL:O	2.52	0.43
1:A:123:ARG:NH2	2:A:730:SO4:O4	2.52	0.43
1:A:134:LEU:HD13	1:A:138:TYR:CE1	2.53	0.43
1:A:326:GLN:HG2	1:A:338:SER:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:609:ASP:HB3	1:A:612:SER:HB3	1.99	0.43
1:E:391:HIS:ND1	1:E:398:ASP:OD2	2.45	0.43
1:E:580:ASN:HB2	1:E:584:THR:HG22	2.00	0.43
1:F:7:VAL:HA	1:F:59:SER:O	2.19	0.43
1:A:577:VAL:HG21	1:B:579:PHE:CZ	2.53	0.43
1:B:306:TYR:CD1	1:B:307:PRO:HD2	2.53	0.43
1:B:510:ASN:ND2	1:C:503:ASN:OD1	2.36	0.43
1:C:213:TRP:HD1	1:C:288:LEU:HD21	1.83	0.43
1:C:309:ASP:HA	1:C:312:ASN:HD22	1.84	0.43
1:C:306:TYR:CD1	1:C:307:PRO:HD2	2.54	0.43
1:D:248:HIS:CE1	1:D:251:ALA:HB2	2.54	0.43
1:D:623:LYS:HD2	1:E:563:GLU:OE2	2.19	0.43
1:A:246:ARG:HA	1:A:247:PRO:HD3	1.86	0.43
1:A:542:LEU:HB3	1:A:543:ASN:H	1.59	0.43
1:B:378:GLU:N	1:B:378:GLU:OE1	2.52	0.43
1:D:380:ILE:HG12	1:D:426:ARG:HD3	2.01	0.43
1:E:266:GLN:OE1	1:E:266:GLN:N	2.39	0.43
1:E:306:TYR:CD1	1:E:307:PRO:HD2	2.54	0.43
1:E:485:ILE:HA	1:E:497:TYR:O	2.19	0.43
1:A:503:ASN:CG	1:C:511:ASP:HB2	2.38	0.42
1:B:71:HIS:HB3	1:B:175:HIS:HB3	2.01	0.42
1:E:450:TYR:CZ	1:E:457:PRO:HD3	2.54	0.42
1:A:502:ARG:HG2	1:A:503:ASN:N	2.34	0.42
1:B:114:VAL:HG21	1:B:162:GLU:HG3	2.00	0.42
1:D:232:GLN:HA	1:E:452:ALA:HB2	2.01	0.42
1:E:509:GLU:HB2	1:F:501:GLU:O	2.19	0.42
1:D:501:GLU:O	1:F:509:GLU:HB2	2.19	0.42
1:E:431:VAL:HG21	1:E:445:ILE:HD13	2.00	0.42
1:B:63:PRO:HD3	1:B:293:ARG:NH2	2.32	0.42
1:C:33:PHE:CE2	1:C:95:PRO:HB3	2.53	0.42
1:D:189:PRO:HG2	1:D:192:TYR:HB2	2.00	0.42
1:F:306:TYR:CD1	1:F:307:PRO:HD2	2.54	0.42
1:E:308:ARG:NH1	1:E:311:GLN:HE22	2.16	0.42
1:E:571:VAL:HG21	1:E:623:LYS:HB2	2.02	0.42
1:A:356:LEU:HD12	1:A:356:LEU:HA	1.85	0.42
1:A:372:VAL:HA	1:A:390:VAL:HA	2.00	0.42
1:A:569:ARG:NH2	1:A:619:ASP:O	2.51	0.42
1:B:502:ARG:HG2	1:B:503:ASN:N	2.32	0.42
1:C:534:ASN:HB3	1:C:535:ASN:H	1.66	0.42
1:D:542:LEU:HB3	1:D:543:ASN:H	1.60	0.42
1:A:32:LEU:HD22	1:A:98:TRP:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:TRP:NE1	1:B:311:GLN:HG2	2.35	0.42
1:D:188:SER:OG	1:D:300:LEU:O	2.22	0.42
3:D:735:TAM:H22	1:F:469:MET:HE3	2.02	0.42
1:F:213:TRP:NE1	1:F:311:GLN:HG2	2.34	0.42
1:A:23:MET:HG2	1:A:24:GLU:N	2.34	0.42
1:A:51:LEU:O	1:A:54:LYS:HB2	2.19	0.42
1:A:353:PHE:CZ	1:A:355:LEU:HD23	2.55	0.42
1:D:103:THR:HG21	1:D:125:LEU:HD21	2.02	0.42
1:D:534:ASN:HB3	1:D:535:ASN:H	1.66	0.42
1:E:611:ASN:OD1	1:F:608:LEU:HD21	2.19	0.42
1:F:616:SER:OG	1:F:617:GLU:N	2.53	0.42
1:C:210:PHE:HD1	1:C:290:GLY:HA3	1.84	0.42
1:A:86:PHE:HD1	1:A:86:PHE:HA	1.74	0.42
1:A:297:ALA:HA	1:A:317:VAL:HB	2.02	0.42
1:A:324:VAL:HG22	1:A:340:PHE:CD2	2.54	0.42
1:A:408:ILE:HG22	1:A:444:ILE:HA	2.01	0.42
1:B:248:HIS:CE1	1:B:251:ALA:HB2	2.55	0.42
1:E:63:PRO:HD3	1:E:293:ARG:NH2	2.34	0.42
1:A:146:GLN:HG3	1:A:149:GLU:HG3	2.02	0.41
1:B:328:LEU:HD12	1:B:328:LEU:HA	1.88	0.41
1:C:210:PHE:CD1	1:C:290:GLY:HA3	2.55	0.41
1:C:484:GLU:CG	1:C:485:ILE:N	2.83	0.41
1:E:213:TRP:CE2	1:E:311:GLN:HG2	2.56	0.41
1:A:188:SER:OG	1:A:300:LEU:O	2.19	0.41
1:A:410:VAL:HG22	1:A:445:ILE:HD12	2.01	0.41
1:A:511:ASP:HB2	1:B:503:ASN:CG	2.40	0.41
1:E:37:LEU:HD21	1:E:58:LEU:HD11	2.01	0.41
1:E:534:ASN:HB3	1:E:535:ASN:H	1.66	0.41
1:B:383:ASP:OD2	1:B:387:ARG:HD3	2.21	0.41
1:B:217:ARG:NH1	1:C:49:GLU:OE2	2.53	0.41
1:C:287:ARG:NH1	1:C:289:ARG:HE	2.19	0.41
1:D:206:GLU:HG2	1:D:207:ARG:N	2.36	0.41
1:E:33:PHE:CE2	1:E:95:PRO:HB3	2.56	0.41
1:E:253:TYR:HA	1:E:254:PRO:HD3	1.86	0.41
1:E:436:LEU:HA	1:F:367:PRO:O	2.20	0.41
1:A:552:LYS:NZ	1:A:554:ASP:OD1	2.52	0.41
1:C:213:TRP:CZ2	1:C:215:MET:HB2	2.55	0.41
1:E:368:GLN:HG2	1:E:435:PHE:HE1	1.85	0.41
1:C:108:ILE:HG12	1:C:145:VAL:HG22	2.03	0.41
1:F:29:LEU:HD12	1:F:29:LEU:HA	1.91	0.41
1:F:579:PHE:HE1	1:F:585:ILE:HG23	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:ILE:HG13	1:A:280:GLN:HG3	2.02	0.41
1:A:387:ARG:HG2	1:A:409:ARG:HA	2.02	0.41
1:B:6:LEU:HB2	1:B:326:GLN:OE1	2.20	0.41
1:D:563:GLU:OE2	1:F:623:LYS:HD2	2.20	0.41
1:A:96:TRP:CD2	1:A:97:PRO:HD3	2.56	0.41
1:A:147:TYR:OH	1:A:368:GLN:NE2	2.53	0.41
1:B:48:LEU:HD12	1:B:48:LEU:HA	1.84	0.41
1:D:33:PHE:CE2	1:D:95:PRO:HB3	2.56	0.41
1:D:608:LEU:HD23	1:D:608:LEU:HA	1.96	0.41
1:A:124:ASN:C	1:A:126:GLY:H	2.23	0.41
1:A:130:PHE:HA	1:A:177:LEU:O	2.21	0.41
1:A:246:ARG:NH2	1:A:280:GLN:OE1	2.49	0.41
1:A:295:ILE:CG2	1:A:344:LEU:HD21	2.44	0.41
1:B:607:ARG:H	1:B:607:ARG:HG3	1.58	0.41
1:D:273:ARG:NE	1:D:277:GLU:OE2	2.54	0.41
1:D:516:VAL:HB	1:F:524:ILE:HG13	2.03	0.41
1:E:102:ARG:HH11	1:E:102:ARG:HA	1.86	0.41
1:F:422:MET:HE2	1:F:424:ILE:HG12	2.03	0.41
1:E:246:ARG:HA	1:E:247:PRO:HD3	1.91	0.41
1:F:155:ILE:HG13	1:F:156:SER:N	2.36	0.41
1:A:145:VAL:CG1	1:A:147:TYR:HB2	2.52	0.40
1:E:86:PHE:HD1	1:E:86:PHE:HA	1.80	0.40
1:A:20:LEU:HD12	1:A:38:HIS:O	2.22	0.40
1:A:592:PHE:CE2	1:C:600:GLY:HA3	2.55	0.40
1:C:20:LEU:O	1:C:326:GLN:NE2	2.53	0.40
1:C:213:TRP:CE2	1:C:311:GLN:HG2	2.57	0.40
1:D:76:ARG:HG2	1:D:92:THR:HB	2.03	0.40
1:F:76:ARG:HG2	1:F:92:THR:HB	2.03	0.40
1:B:241:ARG:NH2	2:B:739:SO4:O4	2.55	0.40
1:C:285:ARG:HH21	1:C:318:VAL:HG11	1.87	0.40
1:C:638:PRO:HA	1:C:639:PRO:HD3	1.93	0.40
1:D:20:LEU:O	1:D:326:GLN:NE2	2.53	0.40
1:F:474:SER:HA	1:F:475:LYS:HA	1.85	0.40
1:A:7:VAL:HG22	1:A:326:GLN:NE2	2.37	0.40
1:A:534:ASN:HB3	1:A:535:ASN:H	1.67	0.40
1:D:29:LEU:HD12	1:D:29:LEU:HA	1.89	0.40
1:D:561:LEU:CD2	1:D:563:GLU:HG3	2.52	0.40
1:E:232:GLN:HA	1:F:452:ALA:HB2	2.04	0.40
1:E:279:ILE:O	1:E:282:GLN:HG2	2.21	0.40
1:B:275:ARG:O	1:B:279:ILE:HG12	2.21	0.40
1:C:191:GLY:N	2:C:736:SO4:O2	2.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:159:MET:HB3	1:D:164:ILE:O	2.22	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:A:201:THR:O	1:A:611:ASN:ND2[1_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	A	623/643 (97%)	594 (95%)	28 (4%)	1 (0%)	47 76
1	B	623/643 (97%)	601 (96%)	22 (4%)	0	100 100
1	C	623/643 (97%)	601 (96%)	22 (4%)	0	100 100
1	D	623/643 (97%)	601 (96%)	22 (4%)	0	100 100
1	E	623/643 (97%)	603 (97%)	20 (3%)	0	100 100
1	F	623/643 (97%)	601 (96%)	22 (4%)	0	100 100
All	All	3738/3858 (97%)	3601 (96%)	136 (4%)	1 (0%)	100 100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	13	LEU

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar

resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	526/535 (98%)	494 (94%)	32 (6%)	18	49
1	B	526/535 (98%)	498 (95%)	28 (5%)	22	54
1	C	526/535 (98%)	501 (95%)	25 (5%)	25	58
1	D	526/535 (98%)	506 (96%)	20 (4%)	33	63
1	E	526/535 (98%)	508 (97%)	18 (3%)	37	66
1	F	526/535 (98%)	505 (96%)	21 (4%)	31	62
All	All	3156/3210 (98%)	3012 (95%)	144 (5%)	27	60

All (144) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	13	LEU
1	A	32	LEU
1	A	51	LEU
1	A	59	SER
1	A	61	GLU
1	A	86	PHE
1	A	102	ARG
1	A	139	ARG
1	A	158	LEU
1	A	187	ARG
1	A	270	GLN
1	A	292	VAL
1	A	299	HIS
1	A	311	GLN
1	A	339	GLN
1	A	350	SER
1	A	356	LEU
1	A	403	ASN
1	A	418	ASN
1	A	425	PRO
1	A	434	SER
1	A	495	GLN
1	A	499	HIS
1	A	529	LEU
1	A	545	THR

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Mol	Chain	Res	Type
1	A	546	LEU
1	A	569	ARG
1	A	571	VAL
1	A	584	THR
1	A	588	SER
1	A	625	VAL
1	B	6	LEU
1	B	7	VAL
1	B	13	LEU
1	B	39	LEU
1	B	48	LEU
1	B	51	LEU
1	B	80	VAL
1	B	85	GLN
1	B	102	ARG
1	B	107	ARG
1	B	139	ARG
1	B	158	LEU
1	B	215	MET
1	B	311	GLN
1	B	352	SER
1	B	368	GLN
1	B	390	VAL
1	B	442	ARG
1	B	495	GLN
1	B	499	HIS
1	B	529	LEU
1	B	560	TYR
1	B	571	VAL
1	B	584	THR
1	B	588	SER
1	B	607	ARG
1	B	625	VAL
1	B	634	GLN
1	C	13	LEU
1	C	18	LEU
1	C	51	LEU
1	C	102	ARG
1	C	128	SER
1	C	136	ARG
1	C	187	ARG
1	C	206	GLU

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Mol	Chain	Res	Type
1	C	207	ARG
1	C	215	MET
1	C	325	VAL
1	C	328	LEU
1	C	350	SER
1	C	352	SER
1	C	368	GLN
1	C	390	VAL
1	C	409	ARG
1	C	442	ARG
1	C	495	GLN
1	C	499	HIS
1	C	545	THR
1	C	546	LEU
1	C	588	SER
1	C	608	LEU
1	C	625	VAL
1	D	6	LEU
1	D	13	LEU
1	D	32	LEU
1	D	51	LEU
1	D	59	SER
1	D	83	HIS
1	D	102	ARG
1	D	139	ARG
1	D	215	MET
1	D	233	ARG
1	D	273	ARG
1	D	282	GLN
1	D	311	GLN
1	D	453	GLU
1	D	495	GLN
1	D	546	LEU
1	D	559	THR
1	D	560	TYR
1	D	588	SER
1	D	599	ASN
1	E	13	LEU
1	E	51	LEU
1	E	59	SER
1	E	68	ARG
1	E	78	SER

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Mol	Chain	Res	Type
1	E	215	MET
1	E	356	LEU
1	E	456	VAL
1	E	460	LEU
1	E	495	GLN
1	E	545	THR
1	E	559	THR
1	E	560	TYR
1	E	571	VAL
1	E	588	SER
1	E	610	LEU
1	E	625	VAL
1	E	634	GLN
1	F	13	LEU
1	F	51	LEU
1	F	59	SER
1	F	139	ARG
1	F	158	LEU
1	F	187	ARG
1	F	328	LEU
1	F	339	GLN
1	F	359	THR
1	F	368	GLN
1	F	442	ARG
1	F	491	LYS
1	F	495	GLN
1	F	545	THR
1	F	546	LEU
1	F	559	THR
1	F	560	TYR
1	F	607	ARG
1	F	608	LEU
1	F	609	ASP
1	F	617	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	270	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

258 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	B	738	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	C	712	-	4,4,4	0.15	0	6,6,6	0.04	0
2	SO4	C	738	-	4,4,4	0.15	0	6,6,6	0.05	0
2	SO4	E	709	-	4,4,4	0.14	0	6,6,6	0.04	0
2	SO4	D	728	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	E	701	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	F	741	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	A	706	-	4,4,4	0.15	0	6,6,6	0.07	0
2	SO4	A	721	-	4,4,4	0.14	0	6,6,6	0.04	0
2	SO4	E	712	-	4,4,4	0.14	0	6,6,6	0.04	0
2	SO4	D	715	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	F	702	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	F	723	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	A	724	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	F	714	-	4,4,4	0.14	0	6,6,6	0.04	0
2	SO4	A	725	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	F	721	-	4,4,4	0.14	0	6,6,6	0.04	0
3	TAM	A	749	-	7,10,10	0.55	0	9,12,12	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SO4	C	741	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	F	727	-	4,4,4	0.15	0	6,6,6	0.05	0
2	SO4	A	714	-	4,4,4	0.15	0	6,6,6	0.05	0
2	SO4	A	743	-	4,4,4	0.14	0	6,6,6	0.04	0
2	SO4	C	703	-	4,4,4	0.14	0	6,6,6	0.04	0
2	SO4	B	702	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	C	709	-	4,4,4	0.15	0	6,6,6	0.04	0
2	SO4	B	735	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	A	727	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	E	732	-	4,4,4	0.13	0	6,6,6	0.04	0
2	SO4	D	733	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	B	730	-	4,4,4	0.14	0	6,6,6	0.04	0
2	SO4	F	709	-	4,4,4	0.15	0	6,6,6	0.05	0
2	SO4	B	701	-	4,4,4	0.14	0	6,6,6	0.07	0
2	SO4	A	729	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	B	745	-	4,4,4	0.13	0	6,6,6	0.05	0
2	SO4	F	708	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	A	744	-	4,4,4	0.15	0	6,6,6	0.05	0
2	SO4	C	732	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	D	725	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	E	722	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	E	731	-	4,4,4	0.15	0	6,6,6	0.06	0
2	SO4	F	713	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	C	716	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	F	717	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	C	737	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	A	742	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	D	702	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	B	732	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	F	712	-	4,4,4	0.13	0	6,6,6	0.06	0
2	SO4	A	733	-	4,4,4	0.14	0	6,6,6	0.04	0
2	SO4	B	747	-	4,4,4	0.13	0	6,6,6	0.04	0
2	SO4	B	711	-	4,4,4	0.13	0	6,6,6	0.05	0
2	SO4	A	748	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	B	748	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	C	740	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	E	702	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	C	706	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	C	733	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	F	733	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	D	701	-	4,4,4	0.13	0	6,6,6	0.07	0
2	SO4	F	706	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	A	723	-	4,4,4	0.14	0	6,6,6	0.04	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SO4	D	736	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	F	743	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	D	704	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	B	750	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	E	714	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	D	723	-	4,4,4	0.14	0	6,6,6	0.04	0
2	SO4	D	724	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	C	718	-	4,4,4	0.13	0	6,6,6	0.05	0
2	SO4	B	733	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	F	725	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	D	711	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	A	701	-	4,4,4	0.14	0	6,6,6	0.04	0
2	SO4	D	719	-	4,4,4	0.15	0	6,6,6	0.04	0
2	SO4	C	714	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	E	704	-	4,4,4	0.14	0	6,6,6	0.04	0
2	SO4	C	739	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	E	723	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	B	741	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	F	722	-	4,4,4	0.14	0	6,6,6	0.04	0
2	SO4	C	702	-	4,4,4	0.15	0	6,6,6	0.07	0
2	SO4	F	744	-	4,4,4	0.14	0	6,6,6	0.04	0
2	SO4	D	714	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	D	731	-	4,4,4	0.15	0	6,6,6	0.04	0
2	SO4	D	709	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	E	711	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	F	724	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	E	719	-	4,4,4	0.14	0	6,6,6	0.07	0
2	SO4	B	714	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	C	717	-	4,4,4	0.13	0	6,6,6	0.05	0
2	SO4	A	736	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	B	709	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	B	739	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	C	731	-	4,4,4	0.14	0	6,6,6	0.04	0
2	SO4	F	720	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	D	721	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	F	715	-	4,4,4	0.15	0	6,6,6	0.04	0
2	SO4	F	705	-	4,4,4	0.13	0	6,6,6	0.06	0
2	SO4	C	734	-	4,4,4	0.14	0	6,6,6	0.04	0
2	SO4	A	739	-	4,4,4	0.13	0	6,6,6	0.08	0
2	SO4	F	729	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	C	704	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	C	729	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	A	719	-	4,4,4	0.13	0	6,6,6	0.04	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SO4	A	726	-	4,4,4	0.14	0	6,6,6	0.07	0
2	SO4	F	742	-	4,4,4	0.14	0	6,6,6	0.07	0
2	SO4	B	708	-	4,4,4	0.15	0	6,6,6	0.06	0
2	SO4	D	726	-	4,4,4	0.14	0	6,6,6	0.04	0
2	SO4	C	711	-	4,4,4	0.15	0	6,6,6	0.05	0
2	SO4	C	721	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	A	731	-	4,4,4	0.14	0	6,6,6	0.07	0
2	SO4	C	727	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	B	703	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	B	704	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	F	732	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	E	718	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	B	723	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	F	728	-	4,4,4	0.14	0	6,6,6	0.07	0
2	SO4	A	730	-	4,4,4	0.15	0	6,6,6	0.05	0
2	SO4	E	733	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	D	730	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	D	706	-	4,4,4	0.14	0	6,6,6	0.04	0
2	SO4	F	737	-	4,4,4	0.14	0	6,6,6	0.04	0
2	SO4	C	735	-	4,4,4	0.14	0	6,6,6	0.04	0
2	SO4	B	726	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	C	720	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	A	720	-	4,4,4	0.14	0	6,6,6	0.04	0
2	SO4	B	749	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	F	710	-	4,4,4	0.15	0	6,6,6	0.05	0
2	SO4	F	738	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	A	728	-	4,4,4	0.14	0	6,6,6	0.04	0
3	TAM	D	735	-	7,10,10	0.55	0	9,12,12	0.88	0
2	SO4	D	720	-	4,4,4	0.15	0	6,6,6	0.04	0
2	SO4	A	703	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	F	701	-	4,4,4	0.14	0	6,6,6	0.04	0
2	SO4	E	706	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	A	715	-	4,4,4	0.14	0	6,6,6	0.04	0
2	SO4	D	703	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	D	705	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	B	720	-	4,4,4	0.14	0	6,6,6	0.07	0
2	SO4	A	713	-	4,4,4	0.14	0	6,6,6	0.04	0
2	SO4	B	716	-	4,4,4	0.13	0	6,6,6	0.05	0
2	SO4	F	707	-	4,4,4	0.14	0	6,6,6	0.04	0
2	SO4	A	738	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	B	721	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	A	745	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	B	705	-	4,4,4	0.14	0	6,6,6	0.04	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SO4	B	718	-	4,4,4	0.14	0	6,6,6	0.04	0
2	SO4	A	702	-	4,4,4	0.13	0	6,6,6	0.04	0
2	SO4	B	743	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	C	705	-	4,4,4	0.15	0	6,6,6	0.06	0
2	SO4	C	726	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	D	708	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	E	725	-	4,4,4	0.14	0	6,6,6	0.08	0
2	SO4	E	703	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	F	736	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	E	717	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	B	707	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	E	727	-	4,4,4	0.15	0	6,6,6	0.05	0
2	SO4	F	739	-	4,4,4	0.14	0	6,6,6	0.04	0
2	SO4	B	706	-	4,4,4	0.13	0	6,6,6	0.06	0
2	SO4	A	732	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	D	729	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	D	716	-	4,4,4	0.14	0	6,6,6	0.04	0
2	SO4	A	710	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	B	712	-	4,4,4	0.15	0	6,6,6	0.06	0
2	SO4	A	704	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	A	711	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	F	731	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	F	740	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	A	747	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	E	721	-	4,4,4	0.14	0	6,6,6	0.04	0
2	SO4	A	740	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	E	716	-	4,4,4	0.13	0	6,6,6	0.05	0
2	SO4	F	735	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	F	730	-	4,4,4	0.13	0	6,6,6	0.05	0
2	SO4	E	724	-	4,4,4	0.14	0	6,6,6	0.04	0
2	SO4	B	727	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	C	744	-	4,4,4	0.14	0	6,6,6	0.04	0
2	SO4	E	715	-	4,4,4	0.14	0	6,6,6	0.04	0
2	SO4	C	701	-	4,4,4	0.14	0	6,6,6	0.04	0
2	SO4	B	731	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	B	713	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	B	717	-	4,4,4	0.14	0	6,6,6	0.04	0
2	SO4	E	707	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	E	720	-	4,4,4	0.14	0	6,6,6	0.04	0
2	SO4	A	718	-	4,4,4	0.13	0	6,6,6	0.05	0
2	SO4	A	735	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	E	726	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	D	718	-	4,4,4	0.14	0	6,6,6	0.05	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SO4	C	715	-	4,4,4	0.13	0	6,6,6	0.04	0
2	SO4	D	722	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	F	726	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	F	716	-	4,4,4	0.14	0	6,6,6	0.04	0
2	SO4	C	736	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	D	732	-	4,4,4	0.13	0	6,6,6	0.04	0
2	SO4	B	710	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	B	729	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	C	710	-	4,4,4	0.14	0	6,6,6	0.04	0
2	SO4	C	723	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	D	734	-	4,4,4	0.14	0	6,6,6	0.04	0
2	SO4	B	724	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	C	724	-	4,4,4	0.14	0	6,6,6	0.04	0
2	SO4	C	742	-	4,4,4	0.15	0	6,6,6	0.05	0
2	SO4	A	716	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	C	725	-	4,4,4	0.14	0	6,6,6	0.04	0
2	SO4	A	746	-	4,4,4	0.15	0	6,6,6	0.05	0
2	SO4	B	715	-	4,4,4	0.13	0	6,6,6	0.04	0
2	SO4	D	707	-	4,4,4	0.14	0	6,6,6	0.04	0
2	SO4	E	730	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	A	741	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	B	734	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	D	713	-	4,4,4	0.14	0	6,6,6	0.04	0
2	SO4	C	707	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	C	719	-	4,4,4	0.14	0	6,6,6	0.04	0
2	SO4	C	730	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	B	744	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	D	717	-	4,4,4	0.14	0	6,6,6	0.04	0
2	SO4	D	712	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	E	734	-	4,4,4	0.13	0	6,6,6	0.04	0
2	SO4	B	742	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	D	727	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	E	728	-	4,4,4	0.14	0	6,6,6	0.04	0
2	SO4	C	728	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	A	709	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	E	705	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	B	736	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	A	707	-	4,4,4	0.14	0	6,6,6	0.04	0
2	SO4	A	722	-	4,4,4	0.14	0	6,6,6	0.04	0
2	SO4	F	734	-	4,4,4	0.14	0	6,6,6	0.07	0
2	SO4	E	713	-	4,4,4	0.13	0	6,6,6	0.05	0
2	SO4	A	737	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	E	708	-	4,4,4	0.14	0	6,6,6	0.05	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SO4	B	722	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	F	703	-	4,4,4	0.14	0	6,6,6	0.07	0
2	SO4	F	704	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	A	708	-	4,4,4	0.14	0	6,6,6	0.10	0
2	SO4	F	719	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	A	734	-	4,4,4	0.14	0	6,6,6	0.04	0
2	SO4	A	750	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	B	728	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	C	722	-	4,4,4	0.15	0	6,6,6	0.04	0
2	SO4	C	743	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	F	711	-	4,4,4	0.14	0	6,6,6	0.08	0
2	SO4	D	710	-	4,4,4	0.15	0	6,6,6	0.05	0
2	SO4	C	708	-	4,4,4	0.14	0	6,6,6	0.04	0
2	SO4	B	746	-	4,4,4	0.15	0	6,6,6	0.06	0
2	SO4	E	729	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	A	705	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	A	717	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	B	737	-	4,4,4	0.15	0	6,6,6	0.05	0
2	SO4	B	740	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	B	719	-	4,4,4	0.14	0	6,6,6	0.03	0
2	SO4	A	712	-	4,4,4	0.14	0	6,6,6	0.04	0
2	SO4	B	725	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	C	713	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	E	710	-	4,4,4	0.15	0	6,6,6	0.05	0
2	SO4	F	718	-	4,4,4	0.14	0	6,6,6	0.05	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
3	TAM	D	735	-	-	7/12/12/12	-
3	TAM	A	749	-	-	9/12/12/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	749	TAM	C2-C-C1-C4
3	A	749	TAM	C3-C-C1-C4
3	A	749	TAM	N-C-C1-C4
3	A	749	TAM	C1-C-C2-C5
3	A	749	TAM	C3-C-C2-C5
3	A	749	TAM	N-C-C2-C5
3	A	749	TAM	C1-C-C3-C6
3	A	749	TAM	C2-C-C3-C6
3	A	749	TAM	N-C-C3-C6
3	D	735	TAM	C2-C-C1-C4
3	D	735	TAM	C3-C-C1-C4
3	D	735	TAM	N-C-C1-C4
3	D	735	TAM	C1-C-C3-C6
3	D	735	TAM	C2-C-C3-C6
3	D	735	TAM	N-C-C3-C6
3	D	735	TAM	C-C3-C6-O6

There are no ring outliers.

45 monomers are involved in 55 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	712	SO4	1	0
2	F	714	SO4	1	0
3	A	749	TAM	2	0
2	C	741	SO4	1	0
2	F	727	SO4	1	0
2	B	735	SO4	2	0
2	B	701	SO4	1	0
2	B	732	SO4	2	0
2	B	711	SO4	1	0
2	D	736	SO4	1	0
2	B	750	SO4	1	0
2	D	723	SO4	1	0
2	D	724	SO4	1	0
2	A	701	SO4	1	0
2	C	739	SO4	2	0
2	D	731	SO4	1	0
2	C	717	SO4	1	0
2	B	739	SO4	3	0
2	C	731	SO4	3	0
2	F	715	SO4	1	0
2	A	739	SO4	1	0
2	A	730	SO4	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	726	SO4	1	0
3	D	735	TAM	2	0
2	A	715	SO4	1	0
2	D	705	SO4	1	0
2	F	707	SO4	1	0
2	A	702	SO4	1	0
2	C	705	SO4	1	0
2	D	708	SO4	1	0
2	D	716	SO4	1	0
2	E	716	SO4	1	0
2	C	701	SO4	1	0
2	B	717	SO4	1	0
2	D	722	SO4	1	0
2	C	736	SO4	1	0
2	B	710	SO4	1	0
2	C	710	SO4	1	0
2	D	734	SO4	1	0
2	C	719	SO4	1	0
2	F	703	SO4	1	0
2	A	708	SO4	1	0
2	D	710	SO4	1	0
2	B	740	SO4	1	0
2	B	719	SO4	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	A	627/643 (97%)	-0.25	4 (0%)	89	90	53, 88, 124, 190	0
1	B	627/643 (97%)	-0.26	4 (0%)	89	90	57, 95, 134, 217	0
1	C	627/643 (97%)	-0.33	5 (0%)	86	87	59, 88, 131, 223	0
1	D	627/643 (97%)	0.04	12 (1%)	66	65	73, 112, 189, 244	0
1	E	627/643 (97%)	-0.03	16 (2%)	56	53	68, 106, 183, 227	0
1	F	627/643 (97%)	-0.16	9 (1%)	75	75	63, 94, 184, 255	0
All	All	3762/3858 (97%)	-0.16	50 (1%)	77	77	53, 97, 171, 255	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	338	SER	4.1
1	A	338	SER	4.0
1	E	590	SER	3.9
1	E	82	GLY	3.8
1	D	589	GLY	3.7
1	D	607	ARG	3.6
1	E	599	ASN	3.6
1	F	613	GLY	3.4
1	E	328	LEU	3.3
1	D	201	THR	3.3
1	E	613	GLY	3.1
1	E	201	THR	3.1
1	D	600	GLY	3.0
1	E	83	HIS	2.9
1	E	549	GLY	2.9
1	A	61	GLU	2.9
1	F	602	ILE	2.9
1	D	328	LEU	2.8
1	E	476	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	202	LEU	2.8
1	D	599	ASN	2.8
1	A	5	ARG	2.7
1	B	202	LEU	2.7
1	F	338	SER	2.6
1	E	620	ALA	2.6
1	F	614	GLY	2.5
1	D	202	LEU	2.5
1	F	591	ALA	2.5
1	E	606	GLY	2.4
1	E	608	LEU	2.4
1	F	599	ASN	2.4
1	C	201	THR	2.4
1	C	203	GLY	2.3
1	F	339	GLN	2.3
1	B	291	VAL	2.3
1	E	202	LEU	2.3
1	E	44	PRO	2.3
1	D	615	ALA	2.2
1	E	592	PHE	2.2
1	D	340	PHE	2.2
1	F	594	LEU	2.1
1	E	639	PRO	2.1
1	D	620	ALA	2.1
1	D	341	GLU	2.1
1	F	592	PHE	2.1
1	B	201	THR	2.0
1	B	207	ARG	2.0
1	D	210	PHE	2.0
1	A	324	VAL	2.0
1	C	328	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{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	E	726	5/5	0.44	0.27	219,222,224,224	0
2	SO4	A	739	5/5	0.46	0.53	210,216,220,226	0
2	SO4	A	748	5/5	0.50	0.72	219,222,226,226	0
2	SO4	B	721	5/5	0.57	0.57	199,209,211,212	0
2	SO4	E	709	5/5	0.59	0.37	190,199,199,202	0
2	SO4	C	716	5/5	0.62	0.32	198,199,205,208	0
2	SO4	F	725	5/5	0.62	0.57	218,219,223,223	0
3	TAM	D	735	11/11	0.62	0.46	135,150,173,175	0
2	SO4	A	722	5/5	0.63	0.40	196,198,200,207	0
2	SO4	F	741	5/5	0.63	0.53	215,219,221,223	0
2	SO4	A	723	5/5	0.63	0.38	219,222,224,227	0
2	SO4	E	729	5/5	0.64	0.62	213,220,223,223	0
2	SO4	B	747	5/5	0.65	0.37	234,234,235,237	0
2	SO4	C	728	5/5	0.65	0.31	197,203,204,205	0
2	SO4	F	742	5/5	0.66	0.53	225,229,229,230	0
2	SO4	A	728	5/5	0.67	0.65	206,210,213,214	0
2	SO4	C	735	5/5	0.68	0.31	220,225,227,230	0
2	SO4	E	714	5/5	0.68	0.35	225,226,228,231	0
2	SO4	D	728	5/5	0.69	0.48	211,215,216,219	0
2	SO4	B	744	5/5	0.69	0.38	212,215,218,220	0
2	SO4	C	743	5/5	0.69	0.53	196,196,203,206	0
2	SO4	C	727	5/5	0.70	0.50	173,181,183,190	0
2	SO4	A	727	5/5	0.70	0.48	180,185,189,194	0
2	SO4	D	720	5/5	0.70	0.21	194,203,204,208	0
2	SO4	B	730	5/5	0.71	0.24	188,188,196,202	0
2	SO4	F	731	5/5	0.71	0.41	181,185,187,196	0
2	SO4	C	721	5/5	0.71	0.36	204,207,211,211	0
2	SO4	C	726	5/5	0.71	0.46	170,181,188,197	0
2	SO4	D	729	5/5	0.71	0.36	191,195,198,199	0
2	SO4	E	730	5/5	0.72	0.47	215,216,219,225	0
2	SO4	F	717	5/5	0.72	0.38	177,182,190,197	0
2	SO4	E	705	5/5	0.72	0.26	156,173,175,179	0
2	SO4	B	717	5/5	0.72	0.27	190,193,197,201	0
2	SO4	C	703	5/5	0.72	0.26	155,163,182,184	0
2	SO4	B	745	5/5	0.72	0.34	212,213,215,217	0
2	SO4	B	746	5/5	0.72	0.49	185,200,201,206	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	F	724	5/5	0.73	0.33	181,187,189,195	0
2	SO4	C	742	5/5	0.74	0.31	198,199,207,208	0
2	SO4	F	726	5/5	0.74	0.22	165,179,184,186	0
2	SO4	A	746	5/5	0.74	0.44	187,191,195,196	0
2	SO4	B	723	5/5	0.74	0.36	199,200,202,205	0
2	SO4	C	714	5/5	0.74	0.52	180,187,188,189	0
2	SO4	E	720	5/5	0.74	0.40	168,179,184,185	0
2	SO4	D	733	5/5	0.75	0.26	180,188,190,191	0
2	SO4	D	726	5/5	0.75	0.44	177,177,182,192	0
2	SO4	A	737	5/5	0.75	0.39	180,182,192,196	0
2	SO4	B	720	5/5	0.75	0.28	186,188,197,200	0
2	SO4	B	749	5/5	0.76	0.53	173,182,190,192	0
2	SO4	E	728	5/5	0.76	0.35	154,167,175,182	0
2	SO4	D	723	5/5	0.76	0.20	231,231,232,234	0
2	SO4	F	733	5/5	0.76	0.97	214,219,221,225	0
2	SO4	A	720	5/5	0.76	0.32	178,182,186,193	0
2	SO4	C	704	5/5	0.76	0.27	126,159,168,170	0
2	SO4	B	738	5/5	0.76	0.36	180,182,187,195	0
2	SO4	E	701	5/5	0.77	0.28	176,178,186,188	0
2	SO4	F	722	5/5	0.77	0.39	164,169,176,186	0
2	SO4	A	725	5/5	0.77	0.33	191,197,199,206	0
2	SO4	B	741	5/5	0.77	0.24	215,220,223,224	0
2	SO4	A	714	5/5	0.77	0.42	165,171,178,185	0
2	SO4	C	732	5/5	0.77	0.46	196,201,206,207	0
2	SO4	C	720	5/5	0.77	0.13	178,180,182,186	0
2	SO4	F	740	5/5	0.77	0.29	215,216,217,219	0
2	SO4	C	740	5/5	0.77	0.32	191,191,196,202	0
2	SO4	A	747	5/5	0.77	0.39	197,199,200,204	0
2	SO4	D	734	5/5	0.77	0.28	184,191,202,202	0
2	SO4	B	718	5/5	0.78	0.33	150,151,166,172	0
2	SO4	C	733	5/5	0.78	0.46	232,232,235,237	0
2	SO4	E	715	5/5	0.78	0.40	198,199,202,203	0
2	SO4	F	720	5/5	0.78	0.28	169,177,181,193	0
2	SO4	D	725	5/5	0.78	0.29	199,200,202,202	0
2	SO4	C	729	5/5	0.78	0.27	172,180,190,203	0
2	SO4	D	715	5/5	0.78	0.28	207,209,211,213	0
2	SO4	C	734	5/5	0.79	0.54	187,195,197,201	0
2	SO4	A	734	5/5	0.79	0.41	174,174,188,192	0
2	SO4	D	712	5/5	0.79	0.25	144,157,162,171	0
2	SO4	D	714	5/5	0.79	0.35	199,202,204,209	0
2	SO4	A	741	5/5	0.79	0.56	214,215,219,219	0
2	SO4	A	729	5/5	0.80	0.23	227,228,228,228	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	B	739	5/5	0.80	0.42	206,207,212,212	0
2	SO4	B	710	5/5	0.80	0.25	146,152,154,164	0
2	SO4	E	733	5/5	0.80	0.33	184,186,189,195	0
2	SO4	F	710	5/5	0.80	0.19	171,178,179,181	0
2	SO4	C	741	5/5	0.80	0.59	207,208,209,211	0
2	SO4	F	719	5/5	0.80	0.45	179,181,185,186	0
2	SO4	C	722	5/5	0.80	0.44	185,189,190,191	0
2	SO4	B	742	5/5	0.80	0.95	218,221,224,224	0
2	SO4	B	715	5/5	0.81	0.29	193,194,197,202	0
2	SO4	D	717	5/5	0.81	0.24	184,190,191,196	0
2	SO4	D	719	5/5	0.81	0.23	166,173,181,187	0
2	SO4	A	713	5/5	0.81	0.32	149,162,171,177	0
2	SO4	B	727	5/5	0.81	0.49	212,212,217,217	0
2	SO4	B	740	5/5	0.81	0.41	211,217,219,220	0
2	SO4	E	724	5/5	0.82	0.37	188,193,196,197	0
2	SO4	B	743	5/5	0.82	0.50	185,192,193,195	0
2	SO4	D	706	5/5	0.82	0.30	140,149,153,159	0
2	SO4	A	724	5/5	0.82	0.50	197,200,204,208	0
2	SO4	E	708	5/5	0.82	0.23	155,158,161,163	0
2	SO4	A	717	5/5	0.82	0.32	176,189,190,194	0
2	SO4	B	729	5/5	0.82	0.28	147,164,172,185	0
2	SO4	A	712	5/5	0.82	0.30	170,171,173,174	0
2	SO4	E	719	5/5	0.82	0.30	133,141,159,172	0
3	TAM	A	749	11/11	0.82	0.46	103,136,167,169	0
2	SO4	B	735	5/5	0.82	0.39	195,200,200,201	0
2	SO4	F	723	5/5	0.83	0.35	194,194,199,201	0
2	SO4	C	723	5/5	0.83	0.23	139,151,156,162	0
2	SO4	D	721	5/5	0.83	0.26	198,200,200,202	0
2	SO4	D	701	5/5	0.83	0.28	127,151,156,161	0
2	SO4	A	742	5/5	0.83	0.52	216,219,221,224	0
2	SO4	B	716	5/5	0.83	0.46	173,183,191,191	0
2	SO4	C	737	5/5	0.83	0.22	148,162,164,164	0
2	SO4	E	716	5/5	0.83	0.28	181,183,187,192	0
2	SO4	B	708	5/5	0.83	0.20	139,154,160,166	0
2	SO4	F	743	5/5	0.83	0.34	230,230,233,236	0
2	SO4	A	743	5/5	0.83	0.33	190,191,196,201	0
2	SO4	C	709	5/5	0.83	0.28	165,168,177,183	0
2	SO4	D	732	5/5	0.84	0.24	160,163,173,174	0
2	SO4	E	731	5/5	0.84	0.38	134,153,160,166	0
2	SO4	C	712	5/5	0.84	0.22	201,210,212,215	0
2	SO4	A	715	5/5	0.84	0.26	208,213,215,217	0
2	SO4	C	739	5/5	0.84	0.52	215,215,218,220	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	A	710	5/5	0.85	0.16	154,158,169,179	0
2	SO4	D	703	5/5	0.85	0.18	167,180,183,185	0
2	SO4	C	713	5/5	0.85	0.35	172,185,186,190	0
2	SO4	A	716	5/5	0.85	0.22	153,161,165,171	0
2	SO4	E	711	5/5	0.85	0.41	168,169,175,175	0
2	SO4	B	728	5/5	0.85	0.35	172,187,193,193	0
2	SO4	E	732	5/5	0.85	0.22	162,164,171,183	0
2	SO4	F	738	5/5	0.85	0.46	190,196,205,205	0
2	SO4	F	739	5/5	0.85	0.33	210,213,215,216	0
2	SO4	A	732	5/5	0.85	0.39	175,179,181,188	0
2	SO4	C	730	5/5	0.85	0.23	185,186,191,194	0
2	SO4	F	712	5/5	0.85	0.41	127,128,147,167	0
2	SO4	A	709	5/5	0.85	0.18	126,132,158,163	0
2	SO4	C	710	5/5	0.85	0.31	182,188,189,193	0
2	SO4	E	722	5/5	0.85	0.33	178,185,187,195	0
2	SO4	E	702	5/5	0.86	0.15	162,169,177,179	0
2	SO4	D	713	5/5	0.86	0.22	159,168,170,175	0
2	SO4	E	706	5/5	0.86	0.24	155,158,163,167	0
2	SO4	B	714	5/5	0.86	0.50	157,163,167,172	0
2	SO4	D	727	5/5	0.86	0.28	181,189,190,198	0
2	SO4	B	722	5/5	0.86	0.30	179,180,185,185	0
2	SO4	A	745	5/5	0.86	0.51	146,152,162,167	0
2	SO4	F	705	5/5	0.86	0.13	124,147,160,172	0
2	SO4	D	730	5/5	0.86	0.43	159,159,166,174	0
2	SO4	D	731	5/5	0.86	0.42	191,199,202,205	0
2	SO4	C	718	5/5	0.86	0.18	181,192,195,196	0
2	SO4	C	719	5/5	0.86	0.25	159,167,172,179	0
2	SO4	B	724	5/5	0.86	0.36	189,196,200,200	0
2	SO4	A	721	5/5	0.86	0.22	191,194,201,204	0
2	SO4	A	740	5/5	0.87	0.25	205,209,211,212	0
2	SO4	B	731	5/5	0.87	0.23	186,187,191,195	0
2	SO4	F	707	5/5	0.87	0.14	174,177,182,188	0
2	SO4	F	727	5/5	0.87	0.24	203,206,208,215	0
2	SO4	F	708	5/5	0.87	0.18	134,156,161,173	0
2	SO4	C	708	5/5	0.87	0.21	181,192,193,195	0
2	SO4	F	736	5/5	0.87	0.41	130,141,152,156	0
2	SO4	F	737	5/5	0.87	0.51	167,177,182,188	0
2	SO4	E	713	5/5	0.87	0.32	207,210,212,213	0
2	SO4	F	715	5/5	0.87	0.28	207,210,212,214	0
2	SO4	B	734	5/5	0.87	0.37	205,209,211,212	0
2	SO4	A	718	5/5	0.87	0.17	180,181,183,186	0
2	SO4	D	722	5/5	0.87	0.29	190,194,195,198	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	F	721	5/5	0.87	0.20	193,197,201,201	0
2	SO4	E	717	5/5	0.87	0.24	194,195,198,203	0
2	SO4	B	703	5/5	0.87	0.24	105,135,151,162	0
2	SO4	D	716	5/5	0.88	0.15	182,185,186,186	0
2	SO4	F	706	5/5	0.88	0.19	139,147,152,153	0
2	SO4	D	702	5/5	0.88	0.21	128,148,152,163	0
2	SO4	C	715	5/5	0.88	0.39	185,188,198,199	0
2	SO4	B	737	5/5	0.88	0.40	193,197,199,202	0
2	SO4	B	725	5/5	0.88	0.67	184,188,192,202	0
2	SO4	A	730	5/5	0.88	0.15	141,151,158,158	0
2	SO4	F	716	5/5	0.88	0.21	176,178,180,181	0
2	SO4	A	707	5/5	0.88	0.19	122,137,139,145	0
2	SO4	B	705	5/5	0.88	0.15	157,176,179,182	0
2	SO4	D	718	5/5	0.89	0.29	185,191,193,195	0
2	SO4	F	718	5/5	0.89	0.22	137,162,163,170	0
2	SO4	F	709	5/5	0.89	0.35	122,144,149,162	0
2	SO4	A	704	5/5	0.89	0.15	152,156,158,164	0
2	SO4	C	702	5/5	0.89	0.17	121,142,146,150	0
2	SO4	F	732	5/5	0.89	0.34	197,198,202,204	0
2	SO4	C	738	5/5	0.89	0.39	153,156,164,177	0
2	SO4	F	735	5/5	0.89	0.24	155,157,170,173	0
2	SO4	E	725	5/5	0.89	0.33	113,141,161,162	0
2	SO4	C	705	5/5	0.90	0.18	164,165,169,173	0
2	SO4	D	709	5/5	0.90	0.20	173,182,183,184	0
2	SO4	E	704	5/5	0.90	0.18	146,160,168,173	0
2	SO4	C	707	5/5	0.90	0.18	175,176,179,181	0
2	SO4	B	726	5/5	0.90	0.26	189,189,191,191	0
2	SO4	A	705	5/5	0.90	0.24	86,138,150,150	0
2	SO4	B	733	5/5	0.90	0.15	137,146,159,166	0
2	SO4	F	703	5/5	0.90	0.28	128,136,151,164	0
2	SO4	F	728	5/5	0.90	0.20	106,143,151,154	0
2	SO4	F	729	5/5	0.90	0.63	183,187,189,195	0
2	SO4	A	719	5/5	0.90	0.19	183,187,189,189	0
2	SO4	B	702	5/5	0.90	0.14	142,156,162,166	0
2	SO4	A	736	5/5	0.91	0.26	169,172,175,179	0
2	SO4	A	711	5/5	0.91	0.19	158,164,167,168	0
2	SO4	D	710	5/5	0.91	0.14	149,155,163,166	0
2	SO4	A	731	5/5	0.92	0.32	105,141,156,167	0
2	SO4	A	744	5/5	0.92	0.35	160,164,174,177	0
2	SO4	A	703	5/5	0.92	0.30	61,134,142,143	0
2	SO4	C	706	5/5	0.92	0.13	136,153,156,171	0
2	SO4	C	724	5/5	0.92	0.13	110,133,140,151	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	E	712	5/5	0.92	0.18	81,127,142,146	0
2	SO4	A	706	5/5	0.92	0.20	114,137,140,143	0
2	SO4	E	734	5/5	0.92	0.47	155,166,167,172	0
2	SO4	D	705	5/5	0.92	0.13	158,162,165,165	0
2	SO4	A	702	5/5	0.93	0.14	104,126,131,147	0
2	SO4	B	706	5/5	0.93	0.24	93,105,129,147	0
2	SO4	B	732	5/5	0.93	0.14	160,168,174,180	0
2	SO4	B	707	5/5	0.93	0.17	145,146,149,151	0
2	SO4	D	736	5/5	0.93	0.14	138,150,161,164	0
2	SO4	A	735	5/5	0.93	0.17	106,108,127,148	0
2	SO4	A	738	5/5	0.93	0.46	169,172,178,180	0
2	SO4	B	736	5/5	0.93	0.40	175,177,180,181	0
2	SO4	B	713	5/5	0.93	0.15	147,147,157,167	0
2	SO4	B	704	5/5	0.93	0.24	162,164,171,174	0
2	SO4	E	707	5/5	0.93	0.14	149,158,163,175	0
2	SO4	F	730	5/5	0.93	0.16	154,160,163,168	0
2	SO4	F	702	5/5	0.93	0.16	105,117,131,138	0
2	SO4	D	704	5/5	0.94	0.16	152,161,164,168	0
2	SO4	B	709	5/5	0.94	0.17	140,142,145,147	0
2	SO4	E	723	5/5	0.94	0.23	165,178,181,182	0
2	SO4	A	708	5/5	0.94	0.21	70,101,110,118	0
2	SO4	F	714	5/5	0.94	0.21	158,164,165,169	0
2	SO4	F	744	5/5	0.94	0.13	136,137,148,165	0
2	SO4	D	707	5/5	0.94	0.13	148,159,164,177	0
2	SO4	C	744	5/5	0.94	0.22	112,118,128,135	0
2	SO4	A	733	5/5	0.95	0.20	100,112,123,127	0
2	SO4	C	725	5/5	0.95	0.20	66,108,123,139	0
2	SO4	F	704	5/5	0.95	0.36	182,184,188,188	0
2	SO4	E	710	5/5	0.95	0.10	120,129,133,142	0
2	SO4	A	701	5/5	0.95	0.08	88,115,123,135	0
2	SO4	F	734	5/5	0.95	0.10	121,134,137,146	0
2	SO4	B	712	5/5	0.96	0.17	75,101,119,123	0
2	SO4	C	701	5/5	0.96	0.10	109,120,128,131	0
2	SO4	E	718	5/5	0.96	0.08	132,145,148,149	0
2	SO4	C	731	5/5	0.96	0.18	104,117,126,133	0
2	SO4	F	701	5/5	0.96	0.15	101,129,134,142	0
2	SO4	B	719	5/5	0.96	0.13	97,113,130,146	0
2	SO4	E	721	5/5	0.96	0.16	93,121,124,141	0
2	SO4	D	724	5/5	0.96	0.11	120,126,129,140	0
2	SO4	B	748	5/5	0.97	0.17	139,153,155,157	0
2	SO4	E	703	5/5	0.97	0.14	139,146,149,154	0
2	SO4	B	711	5/5	0.97	0.13	95,109,121,132	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	D	708	5/5	0.97	0.16	76,91,106,110	0
2	SO4	C	736	5/5	0.98	0.10	118,130,139,147	0
2	SO4	B	701	5/5	0.98	0.08	105,108,120,126	0
2	SO4	B	750	5/5	0.98	0.22	73,92,99,102	0
2	SO4	A	726	5/5	0.98	0.10	105,108,123,129	0
2	SO4	A	750	5/5	0.98	0.19	84,92,100,101	0
2	SO4	D	711	5/5	0.98	0.17	122,124,125,126	0
2	SO4	C	711	5/5	0.98	0.15	89,92,110,125	0
2	SO4	C	717	5/5	0.98	0.08	108,135,145,152	0
2	SO4	F	711	5/5	0.98	0.18	77,86,97,119	0
2	SO4	E	727	5/5	0.98	0.15	111,112,119,134	0
2	SO4	F	713	5/5	0.98	0.11	102,116,124,127	0

6.5 Other polymers (i)

There are no such residues in this entry.