



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:06 PM UTC

PDB ID : 7ZLX / pdb_00007zlx
Title : Crystal Structure of the TSG101-UEV domain:space group P21
Authors : Camara-Artigas, A.
Deposited on : 2022-04-16
Resolution : 2.25 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

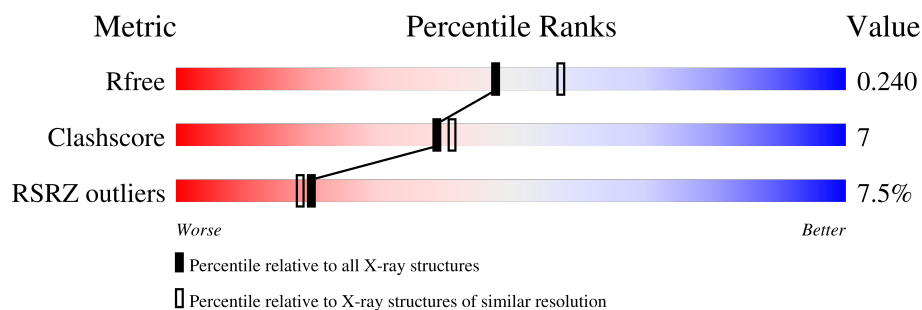
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	159	7% 84% 7% 9%
1	B	159	4% 79% 13% 9%
1	C	159	3% 82% 9% 8%
1	D	159	6% 72% 20% 8%
1	E	159	8% 79% 13% 8%
1	F	159	4% 81% 12% 7%
1	G	159	13% 76% 12% 12%

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Mol	Chain	Length	Quality of chain
1	H	159	 6% 72% 14% 13%
1	I	159	 10% 81% 13% 7%
1	J	159	 4% 75% 14% 10%
1	K	159	 9% 68% 18% 14%
1	L	159	 8% 76% 12% 12%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 25404 atoms, of which 11976 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 Tumor susceptibility gene 101 protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	144	Total	C	H	N	O	S	0	0	0
			2083	710	1002	165	200	6			
1	B	145	Total	C	H	N	O	S	0	0	0
			2104	712	1016	170	199	7			
1	C	146	Total	C	H	N	O	S	0	0	0
			2206	733	1083	177	206	7			
1	D	146	Total	C	H	N	O	S	0	0	0
			2164	726	1057	172	202	7			
1	E	147	Total	C	H	N	O	S	0	0	0
			2144	723	1041	169	204	7			
1	F	148	Total	C	H	N	O	S	0	0	0
			2145	723	1038	173	203	8			
1	G	140	Total	C	H	N	O	S	0	0	0
			1892	663	889	158	176	6			
1	H	138	Total	C	H	N	O	S	0	0	0
			1994	680	958	162	188	6			
1	I	148	Total	C	H	N	O	S	0	0	0
			2103	715	1013	168	199	8			
1	J	143	Total	C	H	N	O	S	0	0	0
			2018	694	963	161	193	7			
1	K	136	Total	C	H	N	O	S	0	0	0
			1965	672	947	156	184	6			
1	L	140	Total	C	H	N	O	S	0	0	0
			2013	689	969	165	184	6			

There are 168 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	initiating methionine	UNP Q99816
A	-12	ARG	-	expression tag	UNP Q99816
A	-11	GLY	-	expression tag	UNP Q99816
A	-10	SER	-	expression tag	UNP Q99816
A	-9	HIS	-	expression tag	UNP Q99816

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	HIS	-	expression tag	UNP Q99816
A	-7	HIS	-	expression tag	UNP Q99816
A	-6	HIS	-	expression tag	UNP Q99816
A	-5	HIS	-	expression tag	UNP Q99816
A	-4	HIS	-	expression tag	UNP Q99816
A	-3	GLY	-	expression tag	UNP Q99816
A	-2	MET	-	expression tag	UNP Q99816
A	-1	ALA	-	expression tag	UNP Q99816
A	0	SER	-	expression tag	UNP Q99816
B	-13	MET	-	initiating methionine	UNP Q99816
B	-12	ARG	-	expression tag	UNP Q99816
B	-11	GLY	-	expression tag	UNP Q99816
B	-10	SER	-	expression tag	UNP Q99816
B	-9	HIS	-	expression tag	UNP Q99816
B	-8	HIS	-	expression tag	UNP Q99816
B	-7	HIS	-	expression tag	UNP Q99816
B	-6	HIS	-	expression tag	UNP Q99816
B	-5	HIS	-	expression tag	UNP Q99816
B	-4	HIS	-	expression tag	UNP Q99816
B	-3	GLY	-	expression tag	UNP Q99816
B	-2	MET	-	expression tag	UNP Q99816
B	-1	ALA	-	expression tag	UNP Q99816
B	0	SER	-	expression tag	UNP Q99816
C	-13	MET	-	initiating methionine	UNP Q99816
C	-12	ARG	-	expression tag	UNP Q99816
C	-11	GLY	-	expression tag	UNP Q99816
C	-10	SER	-	expression tag	UNP Q99816
C	-9	HIS	-	expression tag	UNP Q99816
C	-8	HIS	-	expression tag	UNP Q99816
C	-7	HIS	-	expression tag	UNP Q99816
C	-6	HIS	-	expression tag	UNP Q99816
C	-5	HIS	-	expression tag	UNP Q99816
C	-4	HIS	-	expression tag	UNP Q99816
C	-3	GLY	-	expression tag	UNP Q99816
C	-2	MET	-	expression tag	UNP Q99816
C	-1	ALA	-	expression tag	UNP Q99816
C	0	SER	-	expression tag	UNP Q99816
D	-13	MET	-	initiating methionine	UNP Q99816
D	-12	ARG	-	expression tag	UNP Q99816
D	-11	GLY	-	expression tag	UNP Q99816
D	-10	SER	-	expression tag	UNP Q99816
D	-9	HIS	-	expression tag	UNP Q99816

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-8	HIS	-	expression tag	UNP Q99816
D	-7	HIS	-	expression tag	UNP Q99816
D	-6	HIS	-	expression tag	UNP Q99816
D	-5	HIS	-	expression tag	UNP Q99816
D	-4	HIS	-	expression tag	UNP Q99816
D	-3	GLY	-	expression tag	UNP Q99816
D	-2	MET	-	expression tag	UNP Q99816
D	-1	ALA	-	expression tag	UNP Q99816
D	0	SER	-	expression tag	UNP Q99816
E	-13	MET	-	initiating methionine	UNP Q99816
E	-12	ARG	-	expression tag	UNP Q99816
E	-11	GLY	-	expression tag	UNP Q99816
E	-10	SER	-	expression tag	UNP Q99816
E	-9	HIS	-	expression tag	UNP Q99816
E	-8	HIS	-	expression tag	UNP Q99816
E	-7	HIS	-	expression tag	UNP Q99816
E	-6	HIS	-	expression tag	UNP Q99816
E	-5	HIS	-	expression tag	UNP Q99816
E	-4	HIS	-	expression tag	UNP Q99816
E	-3	GLY	-	expression tag	UNP Q99816
E	-2	MET	-	expression tag	UNP Q99816
E	-1	ALA	-	expression tag	UNP Q99816
E	0	SER	-	expression tag	UNP Q99816
F	-13	MET	-	initiating methionine	UNP Q99816
F	-12	ARG	-	expression tag	UNP Q99816
F	-11	GLY	-	expression tag	UNP Q99816
F	-10	SER	-	expression tag	UNP Q99816
F	-9	HIS	-	expression tag	UNP Q99816
F	-8	HIS	-	expression tag	UNP Q99816
F	-7	HIS	-	expression tag	UNP Q99816
F	-6	HIS	-	expression tag	UNP Q99816
F	-5	HIS	-	expression tag	UNP Q99816
F	-4	HIS	-	expression tag	UNP Q99816
F	-3	GLY	-	expression tag	UNP Q99816
F	-2	MET	-	expression tag	UNP Q99816
F	-1	ALA	-	expression tag	UNP Q99816
F	0	SER	-	expression tag	UNP Q99816
G	-13	MET	-	initiating methionine	UNP Q99816
G	-12	ARG	-	expression tag	UNP Q99816
G	-11	GLY	-	expression tag	UNP Q99816
G	-10	SER	-	expression tag	UNP Q99816
G	-9	HIS	-	expression tag	UNP Q99816

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-8	HIS	-	expression tag	UNP Q99816
G	-7	HIS	-	expression tag	UNP Q99816
G	-6	HIS	-	expression tag	UNP Q99816
G	-5	HIS	-	expression tag	UNP Q99816
G	-4	HIS	-	expression tag	UNP Q99816
G	-3	GLY	-	expression tag	UNP Q99816
G	-2	MET	-	expression tag	UNP Q99816
G	-1	ALA	-	expression tag	UNP Q99816
G	0	SER	-	expression tag	UNP Q99816
H	-13	MET	-	initiating methionine	UNP Q99816
H	-12	ARG	-	expression tag	UNP Q99816
H	-11	GLY	-	expression tag	UNP Q99816
H	-10	SER	-	expression tag	UNP Q99816
H	-9	HIS	-	expression tag	UNP Q99816
H	-8	HIS	-	expression tag	UNP Q99816
H	-7	HIS	-	expression tag	UNP Q99816
H	-6	HIS	-	expression tag	UNP Q99816
H	-5	HIS	-	expression tag	UNP Q99816
H	-4	HIS	-	expression tag	UNP Q99816
H	-3	GLY	-	expression tag	UNP Q99816
H	-2	MET	-	expression tag	UNP Q99816
H	-1	ALA	-	expression tag	UNP Q99816
H	0	SER	-	expression tag	UNP Q99816
I	-13	MET	-	initiating methionine	UNP Q99816
I	-12	ARG	-	expression tag	UNP Q99816
I	-11	GLY	-	expression tag	UNP Q99816
I	-10	SER	-	expression tag	UNP Q99816
I	-9	HIS	-	expression tag	UNP Q99816
I	-8	HIS	-	expression tag	UNP Q99816
I	-7	HIS	-	expression tag	UNP Q99816
I	-6	HIS	-	expression tag	UNP Q99816
I	-5	HIS	-	expression tag	UNP Q99816
I	-4	HIS	-	expression tag	UNP Q99816
I	-3	GLY	-	expression tag	UNP Q99816
I	-2	MET	-	expression tag	UNP Q99816
I	-1	ALA	-	expression tag	UNP Q99816
I	0	SER	-	expression tag	UNP Q99816
J	-13	MET	-	initiating methionine	UNP Q99816
J	-12	ARG	-	expression tag	UNP Q99816
J	-11	GLY	-	expression tag	UNP Q99816
J	-10	SER	-	expression tag	UNP Q99816
J	-9	HIS	-	expression tag	UNP Q99816

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-8	HIS	-	expression tag	UNP Q99816
J	-7	HIS	-	expression tag	UNP Q99816
J	-6	HIS	-	expression tag	UNP Q99816
J	-5	HIS	-	expression tag	UNP Q99816
J	-4	HIS	-	expression tag	UNP Q99816
J	-3	GLY	-	expression tag	UNP Q99816
J	-2	MET	-	expression tag	UNP Q99816
J	-1	ALA	-	expression tag	UNP Q99816
J	0	SER	-	expression tag	UNP Q99816
K	-13	MET	-	initiating methionine	UNP Q99816
K	-12	ARG	-	expression tag	UNP Q99816
K	-11	GLY	-	expression tag	UNP Q99816
K	-10	SER	-	expression tag	UNP Q99816
K	-9	HIS	-	expression tag	UNP Q99816
K	-8	HIS	-	expression tag	UNP Q99816
K	-7	HIS	-	expression tag	UNP Q99816
K	-6	HIS	-	expression tag	UNP Q99816
K	-5	HIS	-	expression tag	UNP Q99816
K	-4	HIS	-	expression tag	UNP Q99816
K	-3	GLY	-	expression tag	UNP Q99816
K	-2	MET	-	expression tag	UNP Q99816
K	-1	ALA	-	expression tag	UNP Q99816
K	0	SER	-	expression tag	UNP Q99816
L	-13	MET	-	initiating methionine	UNP Q99816
L	-12	ARG	-	expression tag	UNP Q99816
L	-11	GLY	-	expression tag	UNP Q99816
L	-10	SER	-	expression tag	UNP Q99816
L	-9	HIS	-	expression tag	UNP Q99816
L	-8	HIS	-	expression tag	UNP Q99816
L	-7	HIS	-	expression tag	UNP Q99816
L	-6	HIS	-	expression tag	UNP Q99816
L	-5	HIS	-	expression tag	UNP Q99816
L	-4	HIS	-	expression tag	UNP Q99816
L	-3	GLY	-	expression tag	UNP Q99816
L	-2	MET	-	expression tag	UNP Q99816
L	-1	ALA	-	expression tag	UNP Q99816
L	0	SER	-	expression tag	UNP Q99816

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		
2	L	1	Total	O	S	0	0
			5	4	1		

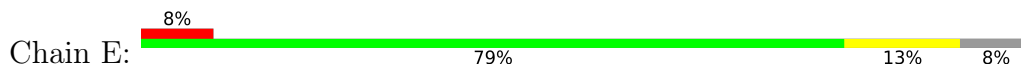
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	40	Total	O	0	0
			40	40		
3	B	65	Total	O	0	0
			65	65		

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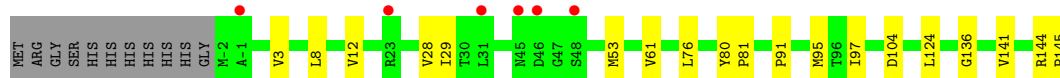
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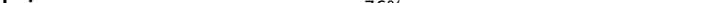
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	47	Total 47	O 47	0	0
3	D	61	Total 61	O 61	0	0
3	E	52	Total 52	O 52	0	0
3	F	54	Total 54	O 54	0	0
3	G	28	Total 28	O 28	0	0
3	H	41	Total 41	O 41	0	0
3	I	28	Total 28	O 28	0	0
3	J	39	Total 39	O 39	0	0
3	K	45	Total 45	O 45	0	0
3	L	23	Total 23	O 23	0	0



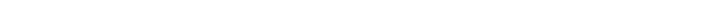


- Chain F: 

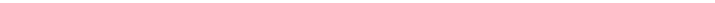


- Chain G:  13% 76% 12% 12%

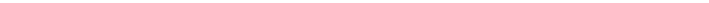


- Chain H:  6% 72% 14% 13%

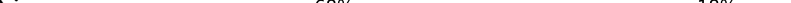


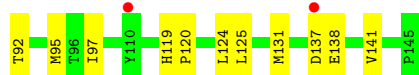
- Chain I:  10% 81% 13% 7%

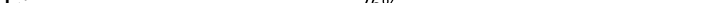


- Chain J:  4% 75% 14% 10%



- Chain K: 



- Chain L: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	38.92Å 168.22Å 195.55Å 90.00° 92.91° 90.00°	Depositor
Resolution (Å)	39.06 – 2.25 39.06 – 2.25	Depositor EDS
% Data completeness (in resolution range)	90.2 (39.06-2.25) 90.2 (39.06-2.25)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 2.24Å)	Xtriage
Refinement program	PHENIX 1.20.4459	Depositor
R, R_{free}	0.226 , 0.244 (Not available) , 0.240	Depositor DCC
R_{free} test set	5170 reflections (4.35%)	wwPDB-VP
Wilson B-factor (Å ²)	34.2	Xtriage
Anisotropy	0.532	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 54.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.046 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	25404	wwPDB-VP
Average B, all atoms (Å ²)	48.0	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 19.83 % 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 9.9271e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.65	0/1114	0.86	0/1537
1	B	0.62	0/1121	0.88	0/1546
1	C	0.63	0/1156	0.88	1/1587 (0.1%)
1	D	0.65	0/1140	0.85	0/1569
1	E	0.67	1/1136 (0.1%)	0.89	0/1564
1	F	0.69	0/1140	0.92	0/1569
1	G	0.56	0/1035	0.82	0/1432
1	H	0.68	0/1067	0.96	3/1470 (0.2%)
1	I	0.59	0/1122	0.82	0/1548
1	J	0.57	0/1086	0.77	1/1500 (0.1%)
1	K	0.63	0/1049	0.84	0/1447
1	L	0.64	0/1077	0.92	1/1484 (0.1%)
All	All	0.63	1/13243 (0.0%)	0.87	6/18253 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	62	PRO	C-O	-5.66	1.19	1.24

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	121	GLN	CA-CB-CG	-5.53	103.05	114.10
1	H	102	HIS	N-CA-CB	-5.43	102.41	110.61
1	H	64	ARG	CA-C-N	-5.41	113.59	122.20
1	H	64	ARG	C-N-CA	-5.41	113.59	122.20
1	J	121	GLN	CA-CB-CG	-5.31	103.48	114.10
1	L	62	PRO	CB-CA-C	-5.13	105.26	111.46

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	A	1081	1002	1002	10	0
1	B	1088	1016	1018	11	0
1	C	1123	1083	1085	9	0
1	D	1107	1057	1059	21	0
1	E	1103	1041	1043	15	0
1	F	1107	1038	1040	14	0
1	G	1003	889	888	13	0
1	H	1036	958	957	19	0
1	I	1090	1013	1015	17	0
1	J	1055	963	964	17	0
1	K	1018	947	945	20	0
1	L	1044	969	968	15	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	F	5	0	0	0	0
2	G	5	0	0	0	0
2	H	5	0	0	0	0
2	I	5	0	0	0	0
2	J	5	0	0	0	0
2	L	5	0	0	0	0
3	A	40	0	0	0	0
3	B	65	0	0	0	0
3	C	47	0	0	0	0
3	D	61	0	0	0	0
3	E	52	0	0	0	0
3	F	54	0	0	0	0
3	G	28	0	0	0	0
3	H	41	0	0	0	0
3	I	28	0	0	0	0
3	J	39	0	0	0	0
3	K	45	0	0	0	0
3	L	23	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	13428	11976	11984	170	0

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 7.

All (170) 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:L:61:VAL:HG21	1:L:70:ILE:HD12	1.43	1.01
1:D:61:VAL:HG21	1:D:70:ILE:HD12	1.58	0.82
1:L:61:VAL:CG2	1:L:70:ILE:HD12	2.19	0.68
1:K:31:LEU:HD23	1:K:125:LEU:HD11	1.77	0.67
1:H:61:VAL:HG21	1:H:70:ILE:HD12	1.77	0.66
1:I:89:VAL:HG21	1:I:141:VAL:HG23	1.78	0.66
1:B:39:LEU:O	1:B:40:ASP:OD1	2.16	0.62
1:I:73:CYS:CB	1:I:90:LYS:HE2	2.30	0.62
1:I:83:ASN:ND2	1:K:79:THR:HG21	2.15	0.62
1:K:91:PRO:HG3	1:K:97:ILE:HG13	1.81	0.62
1:C:91:PRO:HG3	1:C:97:ILE:HG13	1.82	0.60
1:I:28:VAL:HG21	1:I:124:LEU:HB3	1.84	0.60
1:F:53:MET:HE3	1:F:76:LEU:HD12	1.84	0.60
1:E:61:VAL:HG12	1:E:136:GLY:HA2	1.82	0.60
1:J:72:ILE:HD13	1:J:131:MET:HE1	1.84	0.60
1:J:53:MET:CE	1:J:76:LEU:HD12	2.32	0.60
1:C:71:PRO:HB2	1:C:90:LYS:HE3	1.83	0.59
1:F:28:VAL:HG21	1:F:124:LEU:HB3	1.83	0.59
1:J:79:THR:HG21	1:L:83:ASN:ND2	2.17	0.59
1:K:12:VAL:CG1	1:K:53:MET:HE3	2.33	0.59
1:D:95:MET:SD	1:D:141:VAL:HG11	2.42	0.59
1:K:72:ILE:HD13	1:K:131:MET:HE1	1.85	0.59
1:K:95:MET:SD	1:K:141:VAL:HG11	2.44	0.58
1:E:118:LYS:O	1:E:121:GLN:HG2	2.04	0.58
1:E:28:VAL:HG21	1:E:124:LEU:HB3	1.86	0.57
1:E:8:LEU:O	1:E:12:VAL:HG22	2.05	0.57
1:C:90:LYS:O	1:C:90:LYS:HG2	2.05	0.57
1:H:63:TYR:CE2	1:H:64:ARG:HG3	2.40	0.56
1:I:73:CYS:HB3	1:I:90:LYS:HE2	1.87	0.56
1:E:80:TYR:CG	1:E:81:PRO:HA	2.41	0.56
1:B:91:PRO:HG3	1:B:97:ILE:HG13	1.88	0.56
1:G:25:THR:HG23	1:G:55:LEU:HD21	1.87	0.55
1:I:80:TYR:OH	1:I:124:LEU:HG	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:61:VAL:CG1	1:E:136:GLY:N	2.70	0.55
1:K:92:THR:OG1	1:K:95:MET:HE3	2.07	0.55
1:G:129:GLN:HG3	1:L:31:LEU:HD22	1.89	0.55
1:I:79:THR:HG21	1:K:83:ASN:ND2	2.21	0.54
1:D:92:THR:OG1	1:D:95:MET:HE3	2.06	0.54
1:I:89:VAL:HG21	1:I:141:VAL:CG2	2.37	0.54
1:J:127:LEU:C	1:J:127:LEU:HD13	2.33	0.54
1:E:61:VAL:HG12	1:E:136:GLY:CA	2.38	0.53
1:D:62:PRO:HB3	1:J:62:PRO:HG3	1.91	0.53
1:K:137:ASP:OD2	1:K:138:GLU:HG3	2.07	0.53
1:K:42:TYR:O	1:K:49:SER:HA	2.08	0.53
1:F:3:VAL:HG21	1:F:29:ILE:CD1	2.39	0.53
1:E:80:TYR:CD1	1:E:81:PRO:HA	2.44	0.52
1:B:80:TYR:CG	1:B:81:PRO:HA	2.45	0.52
1:L:39:LEU:HD23	1:L:52:LEU:C	2.34	0.52
1:D:144:ARG:HB2	1:D:145:PRO:HD2	1.91	0.52
1:I:53:MET:CE	1:I:76:LEU:HD12	2.39	0.52
1:H:116:GLU:O	1:H:116:GLU:HG2	2.08	0.52
1:J:131:MET:HA	1:J:134:VAL:HG22	1.92	0.52
1:L:80:TYR:CG	1:L:81:PRO:HA	2.44	0.52
1:A:142:PHE:HB3	1:L:142:PHE:HB3	1.91	0.51
1:D:53:MET:CE	1:D:76:LEU:HD12	2.40	0.51
1:I:3:VAL:CG1	1:I:8:LEU:HG	2.40	0.51
1:J:134:VAL:HG23	1:J:135:PHE:N	2.26	0.51
1:F:144:ARG:HB2	1:F:145:PRO:HD2	1.92	0.51
1:H:80:TYR:CD1	1:H:81:PRO:HA	2.45	0.51
1:E:91:PRO:HG3	1:E:97:ILE:HG13	1.92	0.51
1:H:80:TYR:CG	1:H:81:PRO:HA	2.46	0.51
1:J:80:TYR:CG	1:J:81:PRO:HA	2.45	0.51
1:F:80:TYR:CG	1:F:81:PRO:HA	2.46	0.51
1:F:80:TYR:CD1	1:F:81:PRO:HA	2.46	0.50
1:F:91:PRO:HG3	1:F:97:ILE:HG13	1.94	0.50
1:G:71:PRO:HD2	1:G:95:MET:HE1	1.93	0.50
1:J:91:PRO:HG3	1:J:97:ILE:HG13	1.93	0.50
1:L:80:TYR:CD1	1:L:81:PRO:HA	2.47	0.50
1:A:77:LEU:HD21	1:A:86:ILE:HD11	1.94	0.49
1:B:80:TYR:OH	1:B:124:LEU:HG	2.12	0.49
1:D:98:LYS:HE2	1:D:99:THR:O	2.13	0.49
1:F:3:VAL:HG21	1:F:29:ILE:HD12	1.95	0.49
1:A:80:TYR:CG	1:A:81:PRO:HA	2.47	0.49
1:A:95:MET:SD	1:A:141:VAL:HG11	2.52	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:92:THR:H	1:D:95:MET:HE3	1.78	0.49
1:G:80:TYR:CG	1:G:81:PRO:HA	2.48	0.48
1:J:53:MET:HE2	1:J:76:LEU:HD12	1.94	0.48
1:D:72:ILE:HG21	1:D:131:MET:CE	2.44	0.48
1:K:11:MET:HE2	1:K:53:MET:HG3	1.94	0.48
1:J:79:THR:HG21	1:L:83:ASN:HD22	1.76	0.48
1:B:144:ARG:HB2	1:B:145:PRO:HD2	1.94	0.48
1:E:74:LEU:HD22	1:E:87:CYS:SG	2.54	0.48
1:D:80:TYR:OH	1:D:124:LEU:HG	2.14	0.48
1:E:45:ASN:N	1:E:45:ASN:OD1	2.45	0.48
1:D:3:VAL:HG21	1:D:37:PRO:HG2	1.95	0.47
1:I:79:THR:HG21	1:K:83:ASN:HD22	1.78	0.47
1:H:28:VAL:HG21	1:H:124:LEU:HB3	1.96	0.47
1:F:95:MET:HB3	1:F:141:VAL:HG13	1.95	0.47
1:K:119:HIS:ND1	1:K:120:PRO:HA	2.30	0.47
1:A:144:ARG:HB2	1:A:145:PRO:HD2	1.96	0.47
1:L:72:ILE:HD13	1:L:131:MET:HE1	1.96	0.47
1:E:80:TYR:CE2	1:E:81:PRO:HB3	2.50	0.47
1:G:22:VAL:O	1:G:26:VAL:HG23	2.14	0.47
1:H:53:MET:CE	1:H:76:LEU:HD12	2.45	0.47
1:D:119:HIS:ND1	1:D:120:PRO:HA	2.30	0.47
1:D:129:GLN:OE1	1:J:125:LEU:HD23	2.15	0.47
1:A:86:ILE:HG22	1:A:88:PHE:CE1	2.49	0.47
1:C:31:LEU:HD23	1:C:32:TYR:CE2	2.50	0.47
1:B:34:ASP:O	1:B:57:GLY:HA3	2.14	0.46
1:G:11:MET:HE1	1:G:37:PRO:C	2.40	0.46
1:G:80:TYR:CE2	1:G:81:PRO:HB3	2.50	0.46
1:D:92:THR:HG23	1:D:95:MET:CE	2.45	0.46
1:G:58:THR:HB	1:G:69:ASN:HB3	1.97	0.46
1:B:3:VAL:HG12	1:B:29:ILE:CD1	2.46	0.46
1:H:68:TYR:CD1	1:H:68:TYR:N	2.82	0.46
1:H:70:ILE:HD13	1:H:140:PRO:HD2	1.98	0.46
1:J:83:ASN:OD1	1:L:79:THR:HG21	2.14	0.46
1:K:80:TYR:CG	1:K:81:PRO:HA	2.50	0.46
1:A:77:LEU:HD21	1:A:86:ILE:CD1	2.46	0.46
1:H:63:TYR:HB3	1:H:68:TYR:CD1	2.50	0.46
1:L:39:LEU:HD23	1:L:39:LEU:HA	1.86	0.46
1:F:80:TYR:OH	1:F:124:LEU:HG	2.16	0.46
1:D:92:THR:HG23	1:D:95:MET:HE3	1.98	0.46
1:K:6:SER:C	1:K:8:LEU:H	2.22	0.46
1:E:34:ASP:O	1:E:57:GLY:HA3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:80:TYR:CG	1:C:81:PRO:HA	2.52	0.45
1:F:61:VAL:HG12	1:F:136:GLY:HA2	1.98	0.45
1:I:74:LEU:HD21	1:I:131:MET:HE1	1.98	0.45
1:J:104:ASP:C	1:J:104:ASP:OD1	2.58	0.45
1:F:53:MET:CE	1:F:76:LEU:HD12	2.46	0.45
1:I:80:TYR:CG	1:I:81:PRO:HA	2.51	0.45
1:H:34:ASP:O	1:H:57:GLY:HA3	2.16	0.45
1:F:8:LEU:O	1:F:12:VAL:HG22	2.17	0.45
1:K:12:VAL:HG11	1:K:53:MET:HE3	1.98	0.45
1:C:144:ARG:HB2	1:C:145:PRO:HD2	1.98	0.44
1:D:25:THR:HG23	1:D:55:LEU:HD21	1.99	0.44
1:L:95:MET:CE	1:L:141:VAL:HG21	2.47	0.44
1:D:34:ASP:OD2	1:D:58:THR:OG1	2.29	0.44
1:F:104:ASP:C	1:F:104:ASP:OD1	2.60	0.44
1:H:63:TYR:HB3	1:H:68:TYR:CE1	2.52	0.44
1:I:104:ASP:OD1	1:I:104:ASP:C	2.60	0.44
1:C:89:VAL:HG11	1:C:140:PRO:HB2	2.00	0.44
1:D:89:VAL:HG11	1:D:140:PRO:HB2	1.99	0.44
1:B:74:LEU:HD21	1:B:131:MET:HE1	1.99	0.44
1:E:26:VAL:O	1:E:30:THR:HG23	2.18	0.44
1:G:34:ASP:O	1:G:57:GLY:HA3	2.18	0.44
1:H:58:THR:HB	1:H:69:ASN:HB3	2.01	0.43
1:D:80:TYR:CG	1:D:81:PRO:HA	2.53	0.43
1:G:72:ILE:HD13	1:G:131:MET:HE1	1.98	0.43
1:D:91:PRO:HG3	1:D:97:ILE:HG13	2.00	0.43
1:G:142:PHE:HB3	1:I:142:PHE:HB3	2.00	0.43
1:C:80:TYR:OH	1:C:124:LEU:HG	2.19	0.43
1:B:53:MET:HE2	1:B:76:LEU:HD12	2.01	0.43
1:K:124:LEU:HD12	1:K:124:LEU:HA	1.86	0.43
1:H:42:TYR:O	1:H:49:SER:HA	2.18	0.43
1:H:80:TYR:CE2	1:H:81:PRO:HB3	2.53	0.43
1:I:86:ILE:HD13	1:I:86:ILE:N	2.34	0.43
1:G:80:TYR:OH	1:G:124:LEU:HG	2.18	0.42
1:B:24:GLU:OE1	1:B:123:ASP:HB2	2.19	0.42
1:K:34:ASP:OD2	1:K:58:THR:OG1	2.34	0.42
1:A:39:LEU:HD23	1:A:39:LEU:HA	1.85	0.42
1:I:85:PRO:C	1:I:86:ILE:HD13	2.44	0.42
1:J:42:TYR:O	1:J:49:SER:HA	2.20	0.42
1:G:80:TYR:CD1	1:G:81:PRO:HA	2.54	0.41
1:K:34:ASP:O	1:K:57:GLY:HA3	2.20	0.41
1:L:144:ARG:HB3	1:L:145:PRO:HD2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:VAL:O	1:B:53:MET:HA	2.20	0.41
1:H:116:GLU:O	1:H:116:GLU:CG	2.69	0.41
1:D:8:LEU:O	1:D:12:VAL:HG22	2.20	0.41
1:L:74:LEU:HD22	1:L:87:CYS:SG	2.61	0.41
1:H:63:TYR:CZ	1:H:64:ARG:HG3	2.55	0.41
1:K:72:ILE:CD1	1:K:131:MET:HE1	2.48	0.41
1:C:43:VAL:HG23	1:C:43:VAL:O	2.21	0.41
1:J:63:TYR:HB3	1:J:68:TYR:CE1	2.56	0.40
1:H:78:ASP:OD1	1:H:78:ASP:C	2.65	0.40
1:A:86:ILE:HG22	1:A:88:PHE:HE1	1.87	0.40
1:E:44:PHE:CD1	1:E:44:PHE:N	2.89	0.40
1:H:98:LYS:HE2	1:H:99:THR:O	2.21	0.40
1:J:96:THR:O	1:J:141:VAL:HA	2.21	0.40
1:A:80:TYR:CD1	1:A:81:PRO:HA	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 oligosaccharides in this entry.

5.6 Ligand geometry

10 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	H	201	-	4,4,4	0.26	0	6,6,6	0.52	0
2	SO4	B	201	-	4,4,4	0.32	0	6,6,6	0.44	0
2	SO4	J	201	-	4,4,4	0.33	0	6,6,6	0.28	0
2	SO4	I	201	-	4,4,4	0.46	0	6,6,6	0.41	0
2	SO4	F	201	-	4,4,4	0.46	0	6,6,6	0.09	0
2	SO4	A	201	-	4,4,4	0.36	0	6,6,6	0.58	0
2	SO4	G	201	-	4,4,4	0.26	0	6,6,6	0.31	0
2	SO4	C	201	-	4,4,4	0.33	0	6,6,6	0.14	0
2	SO4	L	201	-	4,4,4	0.41	0	6,6,6	0.28	0
2	SO4	D	201	-	4,4,4	0.27	0	6,6,6	0.28	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	144/159 (90%)	0.48	11 (7%) 20 18	27, 44, 70, 98	0
1	B	145/159 (91%)	0.29	7 (4%) 35 35	26, 41, 64, 92	0
1	C	146/159 (91%)	0.34	5 (3%) 48 48	27, 42, 79, 94	0
1	D	146/159 (91%)	0.43	9 (6%) 26 24	28, 41, 66, 94	0
1	E	147/159 (92%)	0.52	12 (8%) 17 16	31, 44, 73, 112	0
1	F	148/159 (93%)	0.54	6 (4%) 41 41	29, 44, 73, 107	0
1	G	140/159 (88%)	0.99	21 (15%) 5 5	40, 56, 83, 103	0
1	H	138/159 (86%)	0.57	9 (6%) 25 23	34, 47, 72, 84	0
1	I	148/159 (93%)	0.67	16 (10%) 11 10	34, 50, 81, 103	0
1	J	143/159 (89%)	0.61	7 (4%) 35 34	34, 50, 68, 86	0
1	K	136/159 (85%)	0.64	14 (10%) 12 11	34, 46, 74, 85	0
1	L	140/159 (88%)	0.76	12 (8%) 16 15	42, 55, 78, 102	0
All	All	1721/1908 (90%)	0.57	129 (7%) 20 18	26, 47, 75, 112	0

All (129) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	6	SER	6.0
1	A	41	SER	4.4
1	F	-1	ALA	4.4
1	C	46	ASP	4.4
1	A	46	ASP	4.4
1	K	8	LEU	4.4
1	D	46	ASP	4.3
1	E	-1	ALA	4.2
1	K	44	PHE	4.2
1	F	45	ASN	4.2
1	I	43	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
1	G	46	ASP	4.0
1	C	0	SER	4.0
1	A	40	ASP	4.0
1	G	48	SER	4.0
1	F	46	ASP	3.8
1	G	45	ASN	3.8
1	E	43	VAL	3.8
1	G	6	SER	3.7
1	I	45	ASN	3.6
1	H	44	PHE	3.6
1	A	3	VAL	3.6
1	K	43	VAL	3.5
1	J	-1	ALA	3.5
1	B	41	SER	3.5
1	K	49	SER	3.4
1	E	40	ASP	3.3
1	I	46	ASP	3.3
1	L	56	THR	3.3
1	H	43	VAL	3.3
1	J	48	SER	3.3
1	I	-1	ALA	3.3
1	F	31	LEU	3.2
1	K	137	ASP	3.2
1	H	6	SER	3.2
1	J	49	SER	3.1
1	G	143	SER	3.1
1	D	44	PHE	3.1
1	J	56	THR	3.1
1	F	48	SER	3.0
1	E	49	SER	3.0
1	L	45	ASN	3.0
1	G	43	VAL	2.9
1	I	0	SER	2.9
1	B	45	ASN	2.9
1	L	46	ASP	2.9
1	C	3	VAL	2.9
1	A	101	LYS	2.8
1	G	7	GLN	2.8
1	E	50	ARG	2.8
1	I	48	SER	2.8
1	G	44	PHE	2.8
1	E	46	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	I	93	SER	2.8
1	E	45	ASN	2.7
1	D	34	ASP	2.7
1	J	0	SER	2.7
1	E	32	TYR	2.6
1	H	67	THR	2.6
1	A	49	SER	2.6
1	G	11	MET	2.6
1	H	4	SER	2.6
1	D	18	ARG	2.6
1	B	40	ASP	2.6
1	I	49	SER	2.6
1	C	45	ASN	2.5
1	L	48	SER	2.5
1	E	34	ASP	2.5
1	A	145	PRO	2.5
1	I	145	PRO	2.5
1	L	49	SER	2.5
1	E	44	PHE	2.5
1	H	143	SER	2.5
1	K	27	ASN	2.5
1	L	137	ASP	2.5
1	G	73	CYS	2.4
1	K	56	THR	2.4
1	I	97	ILE	2.4
1	I	-2	MET	2.4
1	G	34	ASP	2.4
1	D	48	SER	2.4
1	G	97	ILE	2.4
1	J	41	SER	2.4
1	L	44	PHE	2.4
1	D	19	ASP	2.4
1	K	41	SER	2.4
1	H	39	LEU	2.4
1	I	31	LEU	2.4
1	F	23	ARG	2.4
1	B	48	SER	2.3
1	E	41	SER	2.3
1	L	43	VAL	2.3
1	B	46	ASP	2.3
1	I	34	ASP	2.3
1	L	110	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	129	GLN	2.3
1	B	43	VAL	2.3
1	G	67	THR	2.3
1	D	0	SER	2.3
1	A	45	ASN	2.2
1	A	143	SER	2.2
1	G	13	SER	2.2
1	L	41	SER	2.2
1	L	73	CYS	2.2
1	K	7	GLN	2.2
1	A	2	ALA	2.2
1	D	3	VAL	2.2
1	H	123	ASP	2.2
1	J	3	VAL	2.2
1	K	66	ASN	2.2
1	K	67	THR	2.2
1	A	34	ASP	2.1
1	D	1	MET	2.1
1	E	26	VAL	2.1
1	K	34	ASP	2.1
1	G	41	SER	2.1
1	I	96	THR	2.1
1	G	123	ASP	2.1
1	G	63	TYR	2.1
1	G	145	PRO	2.1
1	C	43	VAL	2.1
1	H	38	VAL	2.1
1	B	1	MET	2.0
1	G	51	GLU	2.0
1	K	110	TYR	2.0
1	L	38	VAL	2.0
1	I	44	PHE	2.0
1	I	51	GLU	2.0
1	G	39	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	L	201	5/5	0.79	0.14	61,68,82,85	0
2	SO4	F	201	5/5	0.88	0.15	54,55,57,61	0
2	SO4	D	201	5/5	0.91	0.10	47,48,60,61	0
2	SO4	A	201	5/5	0.92	0.10	41,46,49,56	0
2	SO4	H	201	5/5	0.93	0.13	56,58,68,68	0
2	SO4	J	201	5/5	0.95	0.10	47,50,60,63	0
2	SO4	I	201	5/5	0.96	0.09	38,42,61,64	0
2	SO4	C	201	5/5	0.96	0.10	51,51,61,69	0
2	SO4	B	201	5/5	0.96	0.09	43,43,49,52	0
2	SO4	G	201	5/5	0.97	0.08	43,54,59,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.