



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:45 am GMT

PDB ID : 2V0T  
Title : THE A178L MUTATION IN THE C-TERMINAL HINGE OF THE FLEXIBLE LOOP-6 OF TRIOSEPHOSPHATE ISOMERASE (TIM) INDUCES A MORE CLOSED CONFORMATION OF THIS HINGE REGION IN DIMERIC AND MONOMERIC TIM  
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Deposited on : 2007-05-18  
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

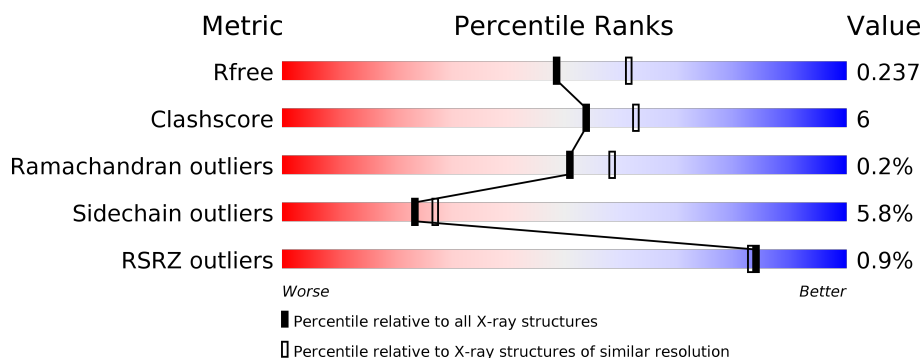
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
$R_{free}$	100719	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	250	<div> <div>%</div> <div> <div></div> <div>82%</div> <div>12%</div> <div>• •</div> </div> </div>
1	B	250	<div> <div>%</div> <div> <div></div> <div>83%</div> <div>16%</div> <div>•</div> </div> </div>
1	C	250	<div> <div></div> <div> <div>81%</div> <div>14%</div> <div>• •</div> </div> </div>
1	D	250	<div> <div>%</div> <div> <div></div> <div>88%</div> <div>9%</div> <div>• •</div> </div> </div>
1	E	250	<div> <div>%</div> <div> <div></div> <div>86%</div> <div>9%</div> <div>• •</div> </div> </div>
1	F	250	<div> <div></div> <div> <div>82%</div> <div>12%</div> <div>• •</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	250	
1	H	250	

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	1251	-	-	-	X
2	SO4	A	1252	-	-	-	X
2	SO4	B	1251	-	-	-	X
2	SO4	E	1251	-	-	-	X
2	SO4	G	1251	-	-	-	X
2	SO4	H	1251	-	-	-	X
3	EPE	D	1252	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16444 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 TRIOSEPHOSPHATE ISOMERASE GLYCOSOMAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	243	Total	C	N	O	S	0	0	0
			1849	1177	324	343	5			
1	B	249	Total	C	N	O	S	0	0	0
			1886	1200	331	350	5			
1	C	242	Total	C	N	O	S	0	1	0
			1851	1177	324	345	5			
1	D	249	Total	C	N	O	S	0	0	0
			1886	1200	331	350	5			
1	E	244	Total	C	N	O	S	0	0	0
			1853	1180	325	343	5			
1	F	242	Total	C	N	O	S	0	0	0
			1842	1172	323	342	5			
1	G	249	Total	C	N	O	S	0	0	0
			1886	1200	331	350	5			
1	H	242	Total	C	N	O	S	0	0	0
			1842	1172	323	342	5			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	178	LEU	ALA	ENGINEERED MUTATION	UNP P04789
B	178	LEU	ALA	ENGINEERED MUTATION	UNP P04789
C	178	LEU	ALA	ENGINEERED MUTATION	UNP P04789
D	178	LEU	ALA	ENGINEERED MUTATION	UNP P04789
E	178	LEU	ALA	ENGINEERED MUTATION	UNP P04789
F	178	LEU	ALA	ENGINEERED MUTATION	UNP P04789
G	178	LEU	ALA	ENGINEERED MUTATION	UNP P04789
H	178	LEU	ALA	ENGINEERED MUTATION	UNP P04789

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



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

- Molecule 3 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C<sub>8</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

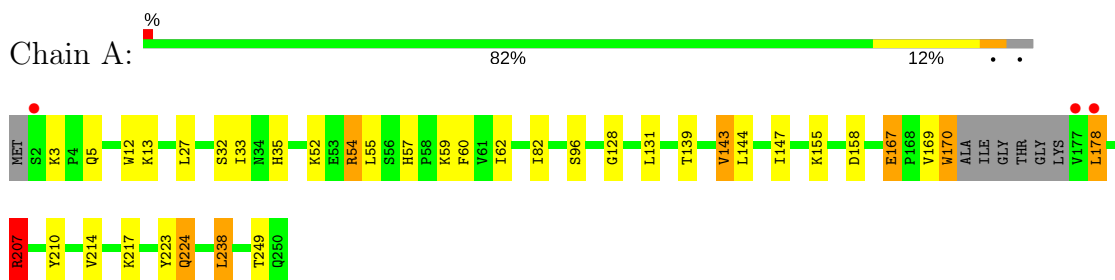
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	206	Total	O	0	0
			206	206		
4	B	196	Total	O	0	0
			196	196		
4	C	202	Total	O	0	0
			202	202		
4	D	214	Total	O	0	0
			214	214		
4	E	206	Total	O	0	0
			206	206		
4	F	187	Total	O	0	0
			187	187		
4	G	126	Total	O	0	0
			126	126		
4	H	132	Total	O	0	0
			132	132		

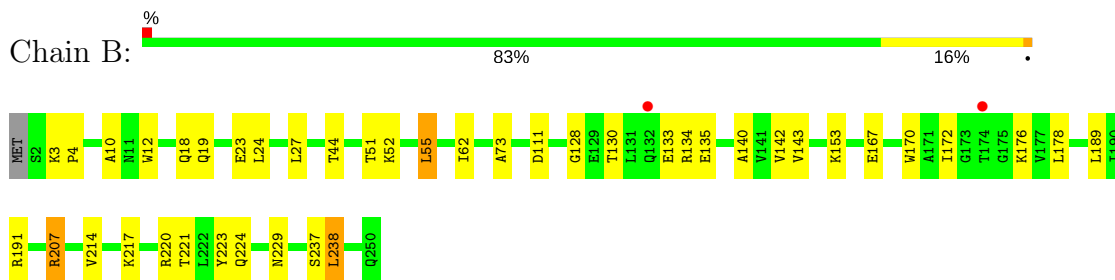
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

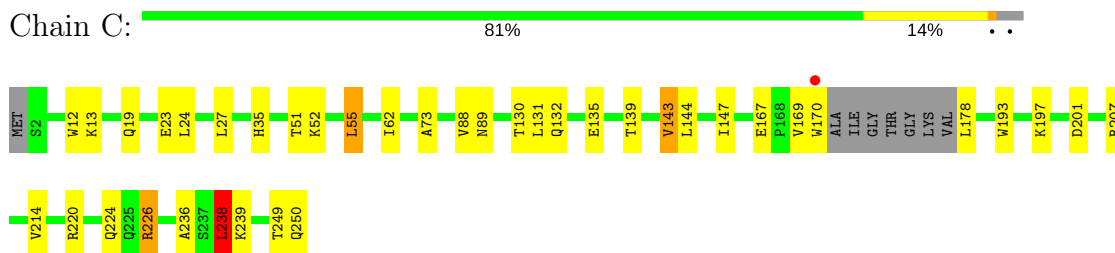
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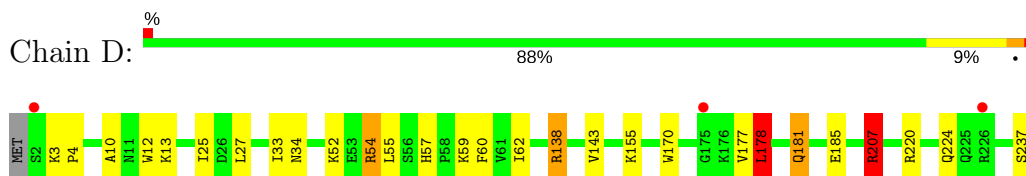
#### • Molecule 1: TRIOSEPHOSPHATE ISOMERASE GLYCOSOMAL



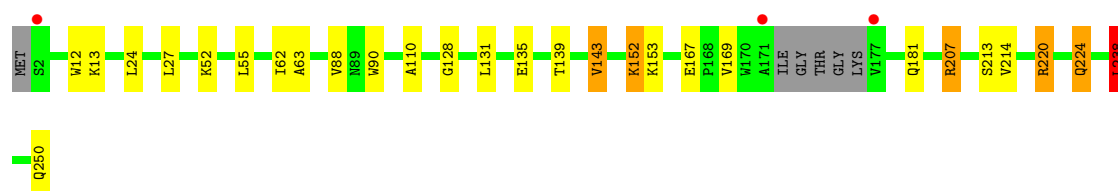
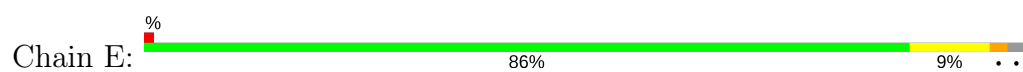
#### • Molecule 1: TRIOSEPHOSPHATE ISOMERASE GLYCOSOMAL



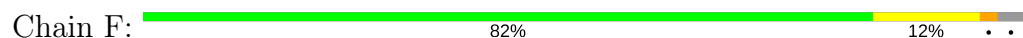
#### • Molecule 1: TRIOSEPHOSPHATE ISOMERASE GLYCOSOMAL



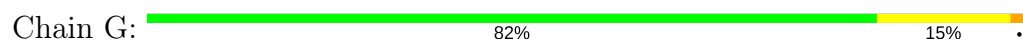
#### • Molecule 1: TRIOSEPHOSPHATE ISOMERASE GLYCOSOMAL



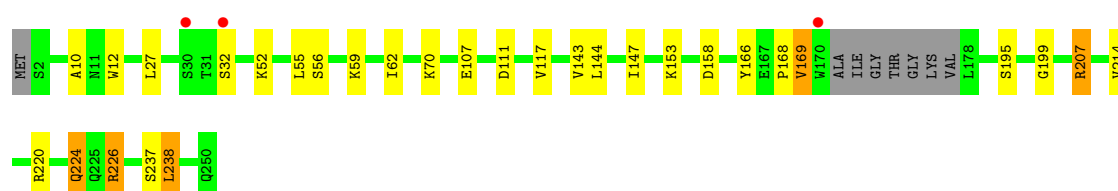
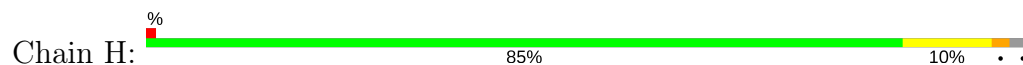
- Molecule 1: TRIOSEPHOSPHATE ISOMERASE GLYCOSOMAL



- Molecule 1: TRIOSEPHOSPHATE ISOMERASE GLYCOSOMAL



- Molecule 1: TRIOSEPHOSPHATE ISOMERASE GLYCOSOMAL





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.69Å 79.25Å 174.00Å 90.00° 99.22° 90.00°	Depositor
Resolution (Å)	19.81 – 2.20 19.81 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.81-2.20) 98.8 (19.81-2.20)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.59 (at 2.21Å)	Xtriage
Refinement program	REFMAC 5.3.0028	Depositor
R, $R_{free}$	0.178 , 0.238 0.178 , 0.237	Depositor DCC
$R_{free}$ test set	5153 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	20.7	Xtriage
Anisotropy	0.498	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 31.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	16444	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EPE, 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	0.69	0/1882	0.80	2/2551 (0.1%)
1	B	0.68	0/1920	0.77	2/2603 (0.1%)
1	C	0.75	0/1884	0.87	4/2553 (0.2%)
1	D	0.69	0/1920	0.76	4/2603 (0.2%)
1	E	0.70	0/1886	0.80	3/2558 (0.1%)
1	F	0.69	0/1875	0.77	4/2541 (0.2%)
1	G	0.62	0/1920	0.73	3/2603 (0.1%)
1	H	0.62	0/1875	0.70	2/2541 (0.1%)
All	All	0.68	0/15162	0.78	24/20553 (0.1%)

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	F	0	1

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	207	ARG	NE-CZ-NH1	-16.49	112.06	120.30
1	C	207	ARG	NE-CZ-NH2	14.34	127.47	120.30
1	A	207	ARG	NE-CZ-NH2	-11.40	114.60	120.30
1	E	207	ARG	NE-CZ-NH2	-10.19	115.21	120.30
1	B	207	ARG	NE-CZ-NH2	-9.97	115.31	120.30
1	A	207	ARG	NE-CZ-NH1	9.81	125.21	120.30
1	F	207	ARG	NE-CZ-NH2	-8.83	115.88	120.30
1	F	207	ARG	NE-CZ-NH1	8.82	124.71	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	207	ARG	NE-CZ-NH1	8.79	124.70	120.30
1	E	207	ARG	NE-CZ-NH1	8.62	124.61	120.30
1	D	207	ARG	NE-CZ-NH2	-8.51	116.04	120.30
1	C	207	ARG	CD-NE-CZ	8.24	135.14	123.60
1	H	207	ARG	NE-CZ-NH2	-8.05	116.27	120.30
1	G	207	ARG	NE-CZ-NH2	-7.61	116.50	120.30
1	F	138	ARG	NE-CZ-NH2	-6.75	116.92	120.30
1	D	207	ARG	NE-CZ-NH1	6.59	123.59	120.30
1	G	207	ARG	NE-CZ-NH1	6.51	123.55	120.30
1	C	238	LEU	CA-CB-CG	6.45	130.13	115.30
1	D	178	LEU	CA-CB-CG	6.30	129.80	115.30
1	H	207	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	F	201	ASP	CB-CG-OD1	5.71	123.44	118.30
1	D	138	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	E	238	LEU	CA-CB-CG	5.40	127.72	115.30
1	G	238	LEU	CA-CB-CG	5.09	127.00	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	169	VAL	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	1849	0	1880	20	0
1	B	1886	0	1923	25	0
1	C	1851	0	1876	29	0
1	D	1886	0	1923	15	0
1	E	1853	0	1885	22	0
1	F	1842	0	1871	27	0
1	G	1886	0	1923	27	0
1	H	1842	0	1871	24	0
2	A	10	0	0	0	0
2	B	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	10	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
3	C	15	0	17	0	0
3	D	15	0	17	0	0
4	A	206	0	0	2	0
4	B	196	0	0	2	0
4	C	202	0	0	2	0
4	D	214	0	0	2	0
4	E	206	0	0	3	0
4	F	187	0	0	4	0
4	G	126	0	0	5	0
4	H	132	0	0	1	0
All	All	16444	0	15186	184	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 6.

All (184) 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:C:89:ASN:HB2	4:C:2097:HOH:O	1.52	1.10
1:E:153:LYS:HE2	4:E:2143:HOH:O	1.63	0.96
1:H:226:ARG:HH21	1:H:226:ARG:HG2	1.31	0.96
1:F:226:ARG:HH21	1:F:226:ARG:HG2	1.29	0.95
1:E:220:ARG:HH21	1:E:220:ARG:HG2	1.36	0.90
1:F:169:VAL:HG23	1:F:169:VAL:O	1.72	0.89
1:D:181:GLN:OE1	1:D:185:GLU:OE2	1.91	0.88
1:H:226:ARG:CG	1:H:226:ARG:HH21	1.95	0.79
1:H:224:GLN:HA	1:H:224:GLN:HE21	1.44	0.79
1:C:131:LEU:O	1:C:135:GLU:HG3	1.83	0.79
1:C:226:ARG:HH21	1:C:226:ARG:CG	1.97	0.78
1:B:111:ASP:OD1	1:B:153:LYS:HE3	1.83	0.77
1:F:220:ARG:NH2	1:F:224:GLN:HE22	1.83	0.77
1:G:153:LYS:HE2	4:G:2091:HOH:O	1.86	0.75
1:H:111:ASP:OD1	1:H:153:LYS:HD2	1.90	0.72
1:F:169:VAL:CG2	1:F:169:VAL:O	2.38	0.71
1:C:226:ARG:HH21	1:C:226:ARG:HG3	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:220:ARG:CG	1:E:220:ARG:HH21	2.04	0.70
1:B:111:ASP:OD1	1:B:153:LYS:CE	2.40	0.68
1:C:226:ARG:HH21	1:C:226:ARG:CB	2.05	0.68
1:F:52:LYS:HG3	1:F:62:ILE:HD13	1.77	0.66
1:C:12:TRP:CD1	1:C:238:LEU:HD13	2.32	0.65
1:F:226:ARG:NH2	1:F:226:ARG:HG2	2.07	0.65
1:C:169:VAL:O	1:C:170:TRP:CG	2.49	0.65
1:E:152:LYS:NZ	1:E:152:LYS:HB3	2.12	0.65
1:F:220:ARG:NH2	1:F:250:GLN:O	2.27	0.63
1:D:12:TRP:CD1	1:D:238:LEU:HD13	2.32	0.63
1:E:152:LYS:HZ2	1:E:152:LYS:CB	2.13	0.62
1:H:166:TYR:CE2	1:H:168:PRO:HG3	2.34	0.61
1:H:111:ASP:OD1	1:H:153:LYS:CD	2.49	0.60
1:E:12:TRP:CD1	1:E:238:LEU:HD13	2.37	0.60
1:F:128:GLY:HA3	1:F:167:GLU:O	2.02	0.60
1:F:33:ILE:HD12	1:F:57:HIS:CE1	2.36	0.59
1:B:18:GLN:NE2	4:B:2019:HOH:O	2.35	0.59
1:D:52:LYS:HG3	1:D:62:ILE:HD13	1.84	0.59
1:A:224:GLN:HA	1:A:224:GLN:HE21	1.67	0.59
1:B:12:TRP:CD1	1:B:238:LEU:HD13	2.38	0.59
1:H:52:LYS:HG3	1:H:62:ILE:HD13	1.85	0.58
1:E:131:LEU:O	1:E:135:GLU:HG3	2.03	0.58
1:B:52:LYS:HG3	1:B:62:ILE:HD13	1.86	0.58
1:G:131:LEU:HA	1:G:169:VAL:HG23	1.85	0.57
1:B:3:LYS:HB3	1:B:4:PRO:HD2	1.87	0.57
1:E:152:LYS:NZ	1:E:152:LYS:CB	2.67	0.57
1:C:193:TRP:CE2	1:C:197:LYS:HG3	2.39	0.57
1:C:132:GLN:NE2	1:F:132:GLN:HG2	2.20	0.56
1:F:34:ASN:ND2	4:F:2036:HOH:O	2.37	0.56
1:H:117:VAL:HG11	1:H:158:ASP:HB3	1.87	0.56
1:A:57:HIS:HB3	1:A:60:PHE:CD1	2.40	0.56
1:F:220:ARG:NH2	1:F:224:GLN:NE2	2.53	0.56
1:F:52:LYS:HG3	1:F:62:ILE:CD1	2.35	0.56
1:G:153:LYS:CE	4:G:2091:HOH:O	2.46	0.56
1:H:70:LYS:HD3	4:H:2004:HOH:O	2.06	0.56
1:E:153:LYS:NZ	4:E:2145:HOH:O	2.34	0.56
1:G:131:LEU:O	1:G:135:GLU:HG2	2.06	0.56
1:A:128:GLY:HA3	1:A:167:GLU:O	2.06	0.55
1:D:57:HIS:HB3	1:D:60:PHE:CD1	2.41	0.55
1:B:221:THR:HG23	4:B:2178:HOH:O	2.05	0.55
1:G:52:LYS:HG3	1:G:62:ILE:HD13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:25:ILE:HG21	1:D:54:ARG:HB3	1.90	0.54
1:G:178:LEU:HG	1:G:182:GLN:HB2	1.89	0.54
1:C:220:ARG:NH2	1:C:250:GLN:O	2.40	0.54
1:G:12:TRP:CD1	1:G:238:LEU:HD13	2.43	0.54
1:E:152:LYS:HZ2	1:E:152:LYS:HB3	1.72	0.54
1:B:220:ARG:O	1:B:224:GLN:HG2	2.06	0.54
1:H:226:ARG:NH2	1:H:226:ARG:CG	2.64	0.54
1:H:224:GLN:HA	1:H:224:GLN:NE2	2.17	0.54
1:C:139:THR:O	1:C:143:VAL:HG13	2.08	0.53
1:C:169:VAL:O	1:C:170:TRP:CD1	2.60	0.53
1:C:226:ARG:HG3	1:C:226:ARG:NH2	2.24	0.53
1:C:19:GLN:O	1:C:23:GLU:HG3	2.09	0.53
1:F:141:VAL:HG23	4:F:2136:HOH:O	2.08	0.53
1:G:50:MET:HB2	4:G:2027:HOH:O	2.09	0.52
1:F:247:LYS:O	1:F:250:GLN:HG3	2.08	0.52
1:C:52:LYS:HG3	1:C:62:ILE:HD13	1.91	0.52
1:G:193:TRP:CE2	1:G:197:LYS:HG3	2.44	0.52
1:G:139:THR:O	1:G:143:VAL:HG13	2.10	0.51
1:G:12:TRP:O	1:G:15:ASN:HB2	2.10	0.51
1:H:52:LYS:HG3	1:H:62:ILE:CD1	2.40	0.51
1:D:10:ALA:HB1	1:D:237:SER:HB2	1.93	0.51
1:E:220:ARG:CG	1:E:220:ARG:NH2	2.69	0.51
1:F:12:TRP:CD1	1:F:238:LEU:HD13	2.46	0.51
1:H:12:TRP:CD1	1:H:238:LEU:HD13	2.46	0.50
1:H:169:VAL:HG23	1:H:169:VAL:O	2.11	0.50
1:B:52:LYS:HG3	1:B:62:ILE:CD1	2.41	0.50
1:B:133:GLU:CD	1:B:142:VAL:HG21	2.31	0.50
1:E:110:ALA:HB3	1:E:153:LYS:HE3	1.94	0.50
1:G:169:VAL:HG13	1:G:176:LYS:H	1.76	0.50
1:G:52:LYS:HG3	1:G:62:ILE:CD1	2.42	0.50
1:A:12:TRP:CD1	1:A:238:LEU:HD13	2.47	0.49
1:F:181:GLN:H	1:F:181:GLN:NE2	2.10	0.49
1:H:220:ARG:O	1:H:224:GLN:HG2	2.12	0.49
1:A:52:LYS:HG3	1:A:62:ILE:HD13	1.95	0.49
1:D:170:TRP:CZ2	1:D:178:LEU:HD22	2.47	0.49
1:F:181:GLN:H	1:F:181:GLN:CD	2.15	0.49
1:H:224:GLN:CA	1:H:224:GLN:HE21	2.21	0.49
1:D:52:LYS:HG3	1:D:62:ILE:CD1	2.43	0.49
1:H:111:ASP:OD1	1:H:153:LYS:HE3	2.13	0.49
1:A:3:LYS:NZ	1:A:223:TYR:O	2.46	0.48
1:B:133:GLU:OE1	1:B:142:VAL:HG11	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:52:LYS:HG3	1:E:62:ILE:HD13	1.95	0.48
1:E:62:ILE:HD11	1:E:88:VAL:HG22	1.94	0.48
1:D:13:LYS:HD3	1:F:73:ALA:HA	1.95	0.48
1:F:52:LYS:O	4:F:2057:HOH:O	2.19	0.48
1:G:169:VAL:HG13	1:G:176:LYS:N	2.28	0.48
1:A:33:ILE:O	1:A:59:LYS:NZ	2.46	0.48
1:C:62:ILE:HD11	1:C:88:VAL:HG22	1.94	0.48
1:F:139:THR:O	1:F:143:VAL:HG13	2.14	0.48
1:G:141:VAL:HG23	4:G:2085:HOH:O	2.14	0.48
1:H:10:ALA:HB1	1:H:237:SER:HB2	1.95	0.48
1:C:236:ALA:HA	1:C:239:LYS:HD2	1.96	0.47
1:G:161:LYS:HE2	4:G:2074:HOH:O	2.14	0.47
1:G:174:THR:HB	1:G:175:GLY:H	1.50	0.47
1:E:220:ARG:O	1:E:224:GLN:HG2	2.14	0.47
1:F:221:THR:HG23	4:F:2170:HOH:O	2.16	0.46
1:D:10:ALA:CB	1:D:237:SER:HB2	2.46	0.46
1:F:35:HIS:HE1	1:F:249:THR:OG1	1.99	0.46
1:C:130:THR:HA	1:C:169:VAL:HB	1.98	0.45
1:E:128:GLY:HA3	1:E:167:GLU:O	2.16	0.45
1:A:131:LEU:HB2	1:A:170:TRP:HB3	1.99	0.45
1:F:131:LEU:H	1:F:170:TRP:C	2.19	0.45
1:A:13:LYS:HD3	1:B:73:ALA:HA	1.99	0.45
1:D:33:ILE:O	1:D:59:LYS:NZ	2.50	0.45
1:B:10:ALA:HB1	1:B:237:SER:HB2	1.99	0.45
1:A:54:ARG:HD2	4:A:2067:HOH:O	2.16	0.45
1:B:133:GLU:HB3	1:B:142:VAL:HG21	1.99	0.45
1:F:217:LYS:H	1:F:217:LYS:HD2	1.82	0.45
1:G:51:THR:O	1:G:55:LEU:HB2	2.17	0.45
1:A:35:HIS:HE1	1:A:249:THR:OG1	2.00	0.45
1:G:3:LYS:NZ	1:G:223:TYR:O	2.50	0.44
1:G:177:VAL:HG12	1:G:213:SER:HB3	1.99	0.44
1:C:51:THR:O	1:C:55:LEU:HB2	2.17	0.44
1:D:138:ARG:NH2	4:D:2141:HOH:O	2.50	0.44
1:C:226:ARG:NH2	1:C:226:ARG:CB	2.79	0.44
1:A:139:THR:O	1:A:143:VAL:HG13	2.17	0.44
1:B:3:LYS:NZ	1:B:223:TYR:O	2.50	0.44
1:A:82:ILE:HD13	1:B:44:THR:HG21	1.98	0.44
1:E:224:GLN:H	1:E:224:GLN:HG2	1.65	0.44
1:A:178:LEU:HG	1:A:210:TYR:OH	2.19	0.43
1:C:226:ARG:NH2	1:C:226:ARG:CG	2.67	0.43
1:A:96:SER:CB	1:A:169:VAL:HG22	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:35:HIS:CD2	1:G:250:GLN:HG2	2.54	0.43
1:G:5:GLN:OE1	1:G:207:ARG:NH2	2.52	0.43
1:C:73:ALA:HA	1:E:13:LYS:HD3	2.01	0.43
1:A:5:GLN:OE1	1:A:207:ARG:NH2	2.52	0.43
1:B:220:ARG:O	1:B:220:ARG:HD2	2.19	0.43
1:C:226:ARG:HG2	4:C:2183:HOH:O	2.18	0.43
1:B:130:THR:C	1:B:170:TRP:HB3	2.40	0.42
1:C:62:ILE:CD1	1:C:88:VAL:HG22	2.49	0.42
1:D:220:ARG:O	1:D:224:GLN:HG2	2.18	0.42
1:H:144:LEU:HA	1:H:147:ILE:HG22	2.01	0.42
1:F:130:THR:HA	1:F:170:TRP:C	2.40	0.42
1:H:111:ASP:OD1	1:H:153:LYS:CE	2.67	0.42
1:A:207:ARG:HD3	4:A:2166:HOH:O	2.19	0.42
1:C:144:LEU:HA	1:C:147:ILE:HG22	2.00	0.42
1:G:144:LEU:HA	1:G:147:ILE:HG22	2.01	0.42
1:E:181:GLN:HB2	4:E:2161:HOH:O	2.20	0.42
1:A:144:LEU:HA	1:A:147:ILE:HG22	2.02	0.42
1:C:220:ARG:O	1:C:224:GLN:HG2	2.19	0.42
1:E:110:ALA:HB1	1:E:153:LYS:HG3	2.01	0.42
1:H:55:LEU:HD23	1:H:56:SER:N	2.35	0.42
1:B:19:GLN:O	1:B:23:GLU:HG3	2.20	0.41
1:G:111:ASP:OD1	1:G:153:LYS:HD2	2.20	0.41
1:G:168:PRO:CB	1:G:178:LEU:HD22	2.50	0.41
1:A:57:HIS:HB3	1:A:60:PHE:HD1	1.83	0.41
1:C:52:LYS:HG3	1:C:62:ILE:CD1	2.50	0.41
1:H:195:SER:HA	1:H:199:GLY:O	2.20	0.41
1:B:24:LEU:HD11	1:B:238:LEU:HA	2.01	0.41
1:C:226:ARG:HB3	1:C:226:ARG:NH2	2.35	0.41
1:C:35:HIS:HE1	1:C:249:THR:OG1	2.02	0.41
1:B:51:THR:O	1:B:55:LEU:HB2	2.20	0.41
1:B:128:GLY:HA3	1:B:167:GLU:O	2.20	0.41
1:B:111:ASP:OD1	1:B:153:LYS:CD	2.68	0.41
1:B:191:ARG:NH2	1:B:229:ASN:OD1	2.46	0.41
1:H:10:ALA:CB	1:H:237:SER:HB2	2.51	0.41
1:B:140:ALA:HA	1:B:189:LEU:HD21	2.02	0.41
1:D:207:ARG:HD3	4:D:2155:HOH:O	2.21	0.41
1:D:3:LYS:HA	1:D:4:PRO:HD2	1.88	0.41
1:E:139:THR:O	1:E:143:VAL:HG13	2.21	0.41
1:F:155:LYS:HA	1:F:155:LYS:HD3	1.70	0.41
1:G:68:ILE:O	1:G:79:SER:HA	2.20	0.41
1:H:226:ARG:NH2	1:H:226:ARG:HG2	2.14	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:LYS:O	1:A:158:ASP:HB2	2.22	0.40
1:E:63:ALA:HA	1:E:90:TRP:O	2.22	0.40
1:G:155:LYS:HA	1:G:155:LYS:HD3	1.88	0.40

There are no symmetry-related clashes.

## 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	239/250 (96%)	235 (98%)	4 (2%)	0	100	100
1	B	247/250 (99%)	240 (97%)	7 (3%)	0	100	100
1	C	239/250 (96%)	236 (99%)	2 (1%)	1 (0%)	38	41
1	D	247/250 (99%)	243 (98%)	4 (2%)	0	100	100
1	E	240/250 (96%)	233 (97%)	7 (3%)	0	100	100
1	F	238/250 (95%)	233 (98%)	4 (2%)	1 (0%)	38	41
1	G	247/250 (99%)	240 (97%)	7 (3%)	0	100	100
1	H	238/250 (95%)	228 (96%)	9 (4%)	1 (0%)	38	41
All	All	1935/2000 (97%)	1888 (98%)	44 (2%)	3 (0%)	51	58

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	169	VAL
1	H	169	VAL
1	C	13	LYS

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	194/198 (98%)	181 (93%)	13 (7%)	19	21
1	B	197/198 (100%)	185 (94%)	12 (6%)	22	25
1	C	194/198 (98%)	184 (95%)	10 (5%)	27	32
1	D	197/198 (100%)	186 (94%)	11 (6%)	25	29
1	E	194/198 (98%)	181 (93%)	13 (7%)	19	21
1	F	193/198 (98%)	182 (94%)	11 (6%)	24	28
1	G	197/198 (100%)	186 (94%)	11 (6%)	25	29
1	H	193/198 (98%)	183 (95%)	10 (5%)	27	32
All	All	1559/1584 (98%)	1468 (94%)	91 (6%)	23	27

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	32	SER
1	A	54	ARG
1	A	55	LEU
1	A	143	VAL
1	A	167	GLU
1	A	170	TRP
1	A	178	LEU
1	A	207	ARG
1	A	214	VAL
1	A	217	LYS
1	A	224	GLN
1	A	238	LEU
1	B	27	LEU
1	B	55	LEU
1	B	134	ARG
1	B	135	GLU
1	B	143	VAL
1	B	172	ILE

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Mol	Chain	Res	Type
1	B	176	LYS
1	B	178	LEU
1	B	207	ARG
1	B	214	VAL
1	B	217	LYS
1	B	238	LEU
1	C	24	LEU
1	C	27	LEU
1	C	55	LEU
1	C	143	VAL
1	C	167	GLU
1	C	178	LEU
1	C	201	ASP
1	C	214	VAL
1	C	226	ARG
1	C	238	LEU
1	D	27	LEU
1	D	34	ASN
1	D	54	ARG
1	D	55	LEU
1	D	143	VAL
1	D	155	LYS
1	D	177	VAL
1	D	178	LEU
1	D	181	GLN
1	D	207	ARG
1	D	238	LEU
1	E	24	LEU
1	E	27	LEU
1	E	55	LEU
1	E	143	VAL
1	E	152	LYS
1	E	169	VAL
1	E	207	ARG
1	E	213	SER
1	E	214	VAL
1	E	220	ARG
1	E	224	GLN
1	E	238	LEU
1	E	250	GLN
1	F	19	GLN
1	F	24	LEU

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Mol	Chain	Res	Type
1	F	27	LEU
1	F	143	VAL
1	F	169	VAL
1	F	170	TRP
1	F	207	ARG
1	F	214	VAL
1	F	217	LYS
1	F	226	ARG
1	F	238	LEU
1	G	24	LEU
1	G	27	LEU
1	G	55	LEU
1	G	143	VAL
1	G	174	THR
1	G	178	LEU
1	G	201	ASP
1	G	207	ARG
1	G	214	VAL
1	G	226	ARG
1	G	238	LEU
1	H	27	LEU
1	H	32	SER
1	H	59	LYS
1	H	107	GLU
1	H	143	VAL
1	H	207	ARG
1	H	214	VAL
1	H	224	GLN
1	H	226	ARG
1	H	238	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	34	ASN
1	A	35	HIS
1	B	18	GLN
1	B	34	ASN
1	B	224	GLN
1	C	34	ASN
1	C	35	HIS

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Mol	Chain	Res	Type
1	C	89	ASN
1	C	250	GLN
1	D	19	GLN
1	D	34	ASN
1	D	35	HIS
1	D	181	GLN
1	E	19	GLN
1	E	35	HIS
1	E	224	GLN
1	F	19	GLN
1	F	35	HIS
1	F	181	GLN
1	F	224	GLN
1	F	250	GLN
1	G	19	GLN
1	G	35	HIS
1	G	224	GLN
1	H	35	HIS
1	H	224	GLN
1	H	250	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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

12 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	A	1251	-	4,4,4	0.19	0	6,6,6	0.41	0
2	SO4	A	1252	-	4,4,4	0.27	0	6,6,6	0.46	0
2	SO4	B	1251	-	4,4,4	0.31	0	6,6,6	0.23	0
2	SO4	C	1251	-	4,4,4	0.24	0	6,6,6	0.32	0
3	EPE	C	1252	-	15,15,15	1.45	1 (6%)	18,20,20	3.12	6 (33%)
2	SO4	D	1251	-	4,4,4	0.10	0	6,6,6	0.40	0
3	EPE	D	1252	-	15,15,15	1.00	1 (6%)	18,20,20	2.17	2 (11%)
2	SO4	E	1251	-	4,4,4	0.15	0	6,6,6	0.50	0
2	SO4	E	1252	-	4,4,4	0.34	0	6,6,6	0.63	0
2	SO4	F	1251	-	4,4,4	0.16	0	6,6,6	0.34	0
2	SO4	G	1251	-	4,4,4	0.20	0	6,6,6	0.58	0
2	SO4	H	1251	-	4,4,4	0.16	0	6,6,6	0.26	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
2	SO4	A	1251	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1252	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1251	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1251	-	-	0/0/0/0	0/0/0/0
3	EPE	C	1252	-	-	0/9/19/19	0/1/1/1
2	SO4	D	1251	-	-	0/0/0/0	0/0/0/0
3	EPE	D	1252	-	-	0/9/19/19	0/1/1/1
2	SO4	E	1251	-	-	0/0/0/0	0/0/0/0
2	SO4	E	1252	-	-	0/0/0/0	0/0/0/0
2	SO4	F	1251	-	-	0/0/0/0	0/0/0/0
2	SO4	G	1251	-	-	0/0/0/0	0/0/0/0
2	SO4	H	1251	-	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1252	EPE	C10-S	3.16	1.82	1.77
3	C	1252	EPE	C10-S	5.17	1.85	1.77

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1252	EPE	O1S-S-C10	-7.80	100.09	106.79
3	C	1252	EPE	O2S-S-C10	-6.88	100.88	106.79
3	D	1252	EPE	O1S-S-C10	-6.00	101.64	106.79
3	C	1252	EPE	O3S-S-C10	-5.24	99.62	106.06
3	D	1252	EPE	O2S-S-C10	-4.94	102.55	106.79
3	C	1252	EPE	C7-N4-C5	-2.96	103.66	111.26
3	C	1252	EPE	C5-N4-C3	2.23	113.91	108.87
3	C	1252	EPE	O3S-S-O2S	3.45	119.27	111.37

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 [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	243/250 (97%)	-0.35	3 (1%) 79 77	6, 12, 21, 32	0
1	B	249/250 (99%)	-0.35	2 (0%) 86 85	6, 12, 28, 39	0
1	C	242/250 (96%)	-0.37	1 (0%) 92 91	8, 12, 20, 45	0
1	D	249/250 (99%)	-0.34	3 (1%) 79 77	6, 12, 19, 27	0
1	E	244/250 (97%)	-0.35	3 (1%) 79 77	6, 13, 21, 29	0
1	F	242/250 (96%)	-0.38	1 (0%) 92 91	6, 12, 19, 34	0
1	G	249/250 (99%)	-0.15	1 (0%) 92 91	8, 13, 18, 28	0
1	H	242/250 (96%)	-0.20	3 (1%) 79 77	7, 13, 20, 34	0
All	All	1960/2000 (98%)	-0.31	17 (0%) 84 83	6, 12, 21, 45	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	170	TRP	4.5
1	F	170	TRP	3.8
1	A	177	VAL	3.3
1	H	170	TRP	3.0
1	B	132	GLN	2.7
1	H	32	SER	2.6
1	G	34	ASN	2.6
1	A	178	LEU	2.5
1	A	2	SER	2.4
1	E	177	VAL	2.4
1	D	2	SER	2.3
1	E	171	ALA	2.3
1	H	30	SER	2.3
1	B	174	THR	2.2
1	D	175	GLY	2.1
1	D	226	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	2	SER	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	SO4	E	1251	5/5	0.97	0.20	6.74	35,36,37,37	0
3	EPE	D	1252	15/15	0.93	0.27	2.97	38,45,52,53	0
2	SO4	A	1251	5/5	0.98	0.11	2.88	29,30,31,31	0
2	SO4	G	1251	5/5	0.95	0.21	2.72	40,42,42,44	0
2	SO4	H	1251	5/5	0.97	0.16	2.58	39,41,42,42	0
2	SO4	A	1252	5/5	0.96	0.27	2.40	34,37,37,38	0
2	SO4	B	1251	5/5	0.98	0.13	2.02	23,24,25,25	0
2	SO4	D	1251	5/5	0.99	0.17	1.69	16,16,19,19	0
2	SO4	E	1252	5/5	0.95	0.17	1.17	25,27,32,32	0
3	EPE	C	1252	15/15	0.97	0.15	0.96	9,16,25,30	0
2	SO4	F	1251	5/5	0.99	0.13	0.78	34,34,34,35	0
2	SO4	C	1251	5/5	0.98	0.16	0.36	21,21,23,24	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.