



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:05 PM GMT

PDB ID : 1DWK  
Title : STRUCTURE OF CYANASE WITH THE DI-ANION OXALATE BOUND  
AT THE ENZYME ACTIVE SITE  
Authors : Walsh, M.A.; Otwinowski, Z.; Perrakis, A.; Anderson, P.M.; Joachimiak, A.  
Deposited on : 1999-12-07  
Resolution : 1.65 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

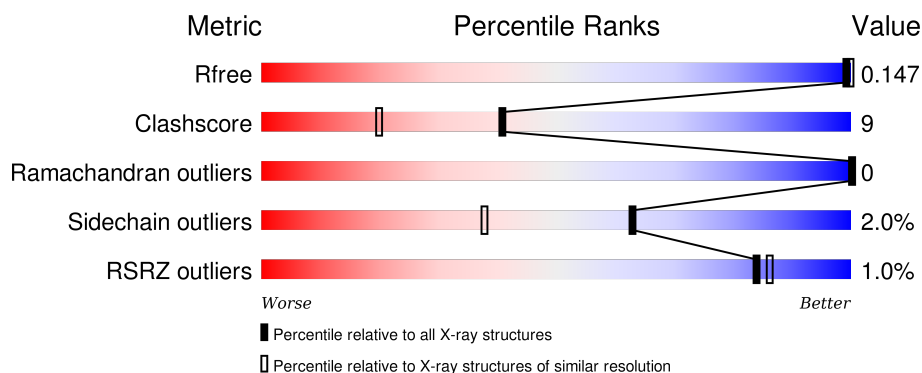
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.65 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))
$R_{free}$	91344	1226 (1.66-1.66)
Clashscore	102246	1323 (1.66-1.66)
Ramachandran outliers	100387	1295 (1.66-1.66)
Sidechain outliers	100360	1295 (1.66-1.66)
RSRZ outliers	91569	1227 (1.66-1.66)

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	156	<div> <div></div> <div>85%12%•</div> </div>
1	B	156	<div> <div></div> <div>83%14%•</div> </div>
1	C	156	<div> <div></div> <div>79%17%••</div> </div>
1	D	156	<div> <div></div> <div>85%12%•</div> </div>
1	E	156	<div> <div></div> <div>83%16%••</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	156	
1	G	156	
1	H	156	
1	I	156	
1	J	156	

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	1158	-	-	-	X
2	SO4	A	1159	-	-	-	X
2	SO4	C	1157	-	-	-	X
2	SO4	C	1158	-	-	-	X
2	SO4	D	1158	-	-	-	X
2	SO4	E	1158	-	-	-	X
2	SO4	E	1159	-	-	-	X
2	SO4	E	1160	-	-	-	X
2	SO4	F	1158	-	-	-	X
2	SO4	G	1157	-	-	-	X
2	SO4	H	1158	-	-	-	X
2	SO4	I	1158	-	-	-	X
2	SO4	J	1157	-	-	-	X
2	SO4	J	1158	-	-	-	X
3	OXL	A	1161	-	-	-	X
3	OXL	D	1159	-	-	-	X
3	OXL	E	1161	-	-	-	X
3	OXL	G	1159	-	-	-	X
3	OXL	I	1159	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14777 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 CYANATE HYDRATASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	156	Total	C	N	O	S	Se	0	10	0
			1229	791	201	232	1	4			
1	B	156	Total	C	N	O	S	Se	0	6	0
			1219	787	199	228	1	4			
1	C	156	Total	C	N	O	S	Se	0	8	0
			1223	790	200	228	1	4			
1	D	156	Total	C	N	O	S	Se	0	5	0
			1212	782	199	226	1	4			
1	E	156	Total	C	N	O	S	Se	0	6	0
			1217	783	199	230	1	4			
1	F	156	Total	C	N	O	S	Se	0	4	0
			1210	780	199	226	1	4			
1	G	156	Total	C	N	O	S	Se	0	7	0
			1219	784	200	230	1	4			
1	H	156	Total	C	N	O	S	Se	0	4	0
			1211	779	199	228	1	4			
1	I	156	Total	C	N	O	S	Se	0	2	0
			1204	774	199	226	1	4			
1	J	156	Total	C	N	O	S	Se	0	6	0
			1219	785	199	230	1	4			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP P00816
A	77	MSE	MET	MODIFIED RESIDUE	UNP P00816
A	94	MSE	MET	MODIFIED RESIDUE	UNP P00816
A	100	MSE	MET	MODIFIED RESIDUE	UNP P00816
B	1	MSE	MET	MODIFIED RESIDUE	UNP P00816
B	77	MSE	MET	MODIFIED RESIDUE	UNP P00816
B	94	MSE	MET	MODIFIED RESIDUE	UNP P00816
B	100	MSE	MET	MODIFIED RESIDUE	UNP P00816
C	1	MSE	MET	MODIFIED RESIDUE	UNP P00816

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Chain	Residue	Modelled	Actual	Comment	Reference
C	77	MSE	MET	MODIFIED RESIDUE	UNP P00816
C	94	MSE	MET	MODIFIED RESIDUE	UNP P00816
C	100	MSE	MET	MODIFIED RESIDUE	UNP P00816
D	1	MSE	MET	MODIFIED RESIDUE	UNP P00816
D	77	MSE	MET	MODIFIED RESIDUE	UNP P00816
D	94	MSE	MET	MODIFIED RESIDUE	UNP P00816
D	100	MSE	MET	MODIFIED RESIDUE	UNP P00816
E	1	MSE	MET	MODIFIED RESIDUE	UNP P00816
E	77	MSE	MET	MODIFIED RESIDUE	UNP P00816
E	94	MSE	MET	MODIFIED RESIDUE	UNP P00816
E	100	MSE	MET	MODIFIED RESIDUE	UNP P00816
F	1	MSE	MET	MODIFIED RESIDUE	UNP P00816
F	77	MSE	MET	MODIFIED RESIDUE	UNP P00816
F	94	MSE	MET	MODIFIED RESIDUE	UNP P00816
F	100	MSE	MET	MODIFIED RESIDUE	UNP P00816
G	1	MSE	MET	MODIFIED RESIDUE	UNP P00816
G	77	MSE	MET	MODIFIED RESIDUE	UNP P00816
G	94	MSE	MET	MODIFIED RESIDUE	UNP P00816
G	100	MSE	MET	MODIFIED RESIDUE	UNP P00816
H	1	MSE	MET	MODIFIED RESIDUE	UNP P00816
H	77	MSE	MET	MODIFIED RESIDUE	UNP P00816
H	94	MSE	MET	MODIFIED RESIDUE	UNP P00816
H	100	MSE	MET	MODIFIED RESIDUE	UNP P00816
I	1	MSE	MET	MODIFIED RESIDUE	UNP P00816
I	77	MSE	MET	MODIFIED RESIDUE	UNP P00816
I	94	MSE	MET	MODIFIED RESIDUE	UNP P00816
I	100	MSE	MET	MODIFIED RESIDUE	UNP P00816
J	1	MSE	MET	MODIFIED RESIDUE	UNP P00816
J	77	MSE	MET	MODIFIED RESIDUE	UNP P00816
J	94	MSE	MET	MODIFIED RESIDUE	UNP P00816
J	100	MSE	MET	MODIFIED RESIDUE	UNP P00816

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



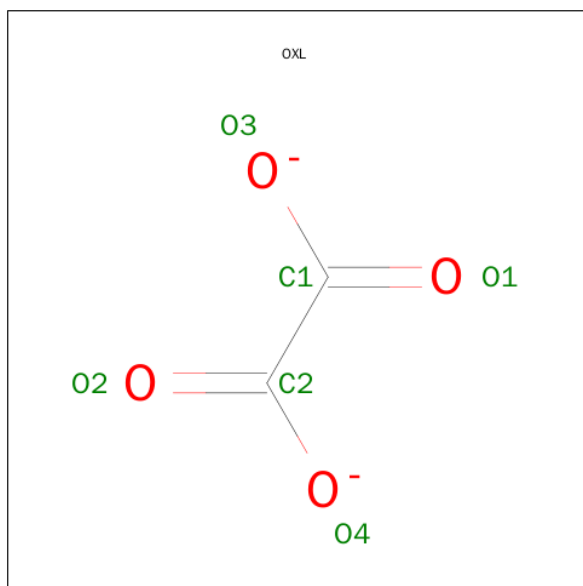
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	1
			10	8	2		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	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	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		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	F	1	Total	O	S	0	0
			5	4	1		
2	G	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	H	1	Total	O	S	0	0
			5	4	1		
2	I	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	J	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is OXALATE ION (three-letter code: OXL) (formula:  $C_2O_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	2	4		
3	D	1	Total	C	O	0	0
			6	2	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	E	1	Total	C	O	0	0
			6	2	4		
3	G	1	Total	C	O	0	0
			6	2	4		
3	I	1	Total	C	O	0	0
			6	2	4		

- Molecule 4 is water.

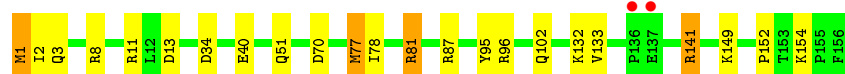
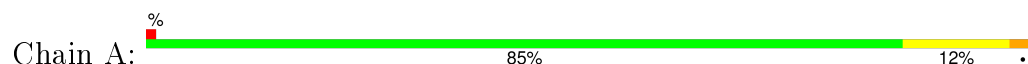
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	248	Total	O	0	0
			248	248		
4	B	263	Total	O	0	0
			263	263		
4	C	260	Total	O	0	0
			260	260		
4	D	243	Total	O	0	0
			243	243		
4	E	231	Total	O	0	0
			231	231		
4	F	230	Total	O	0	0
			230	230		
4	G	243	Total	O	0	0
			243	243		
4	H	217	Total	O	0	0
			217	217		
4	I	224	Total	O	0	0
			224	224		
4	J	248	Total	O	0	0
			248	248		
4	K	55	Total	O	0	0
			55	55		
4	L	2	Total	O	0	0
			2	2		



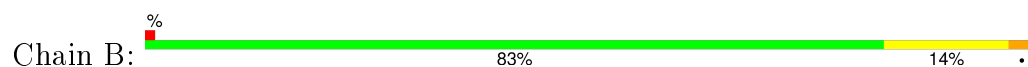
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

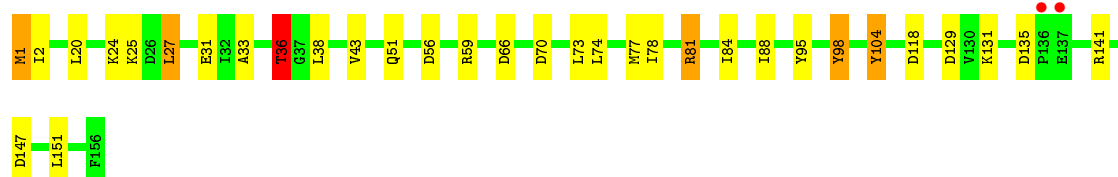
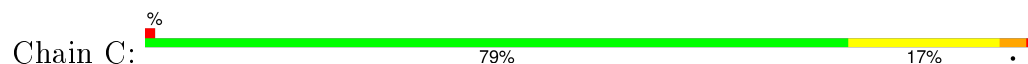
- Molecule 1: CYANATE HYDRATASE



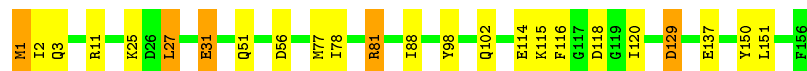
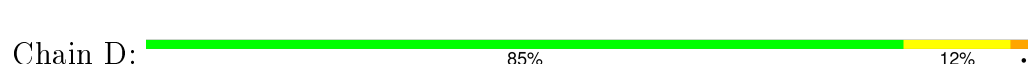
- Molecule 1: CYANATE HYDRATASE



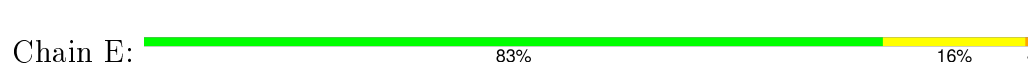
- Molecule 1: CYANATE HYDRATASE



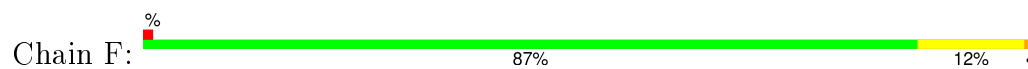
- Molecule 1: CYANATE HYDRATASE



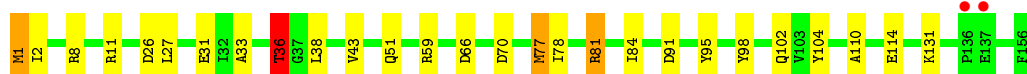
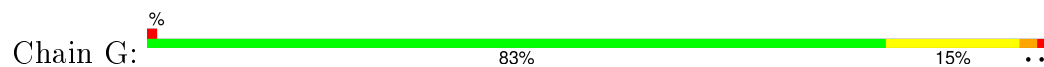
- Molecule 1: CYANATE HYDRATASE



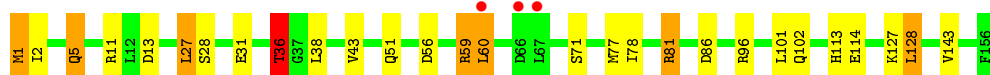
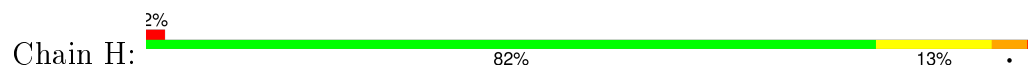
- Molecule 1: CYANATE HYDRATASE



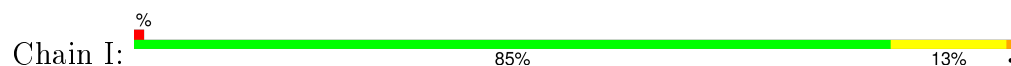
• Molecule 1: CYANATE HYDRATASE



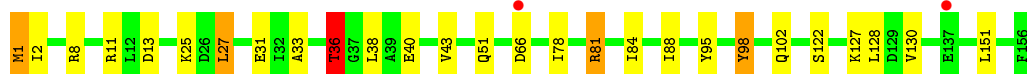
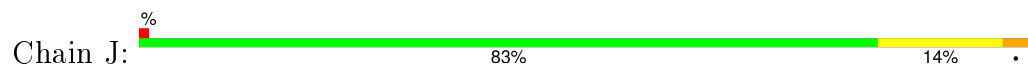
• Molecule 1: CYANATE HYDRATASE



• Molecule 1: CYANATE HYDRATASE



• Molecule 1: CYANATE HYDRATASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.33Å 80.93Å 82.13Å 70.10° 71.95° 66.42°	Depositor
Resolution (Å)	20.00 – 1.65 19.98 – 1.65	Depositor EDS
% Data completeness (in resolution range)	95.4 (20.00-1.65) 87.1 (19.98-1.65)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.68 (at 1.65Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.146 , 0.181 0.143 , 0.147	Depositor DCC
$R_{free}$ test set	9561 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	11.0	Xtriage
Anisotropy	0.388	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 65.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 190228 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	14777	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.75% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: OXL, 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	0.83	2/1293 (0.2%)	1.37	13/1743 (0.7%)
1	B	0.86	2/1259 (0.2%)	1.35	15/1699 (0.9%)
1	C	0.85	2/1277 (0.2%)	1.47	17/1723 (1.0%)
1	D	0.86	1/1250 (0.1%)	1.40	13/1687 (0.8%)
1	E	0.85	0/1260	1.38	8/1700 (0.5%)
1	F	0.81	0/1243	1.36	8/1677 (0.5%)
1	G	0.84	2/1269 (0.2%)	1.38	15/1711 (0.9%)
1	H	0.90	1/1244 (0.1%)	1.58	17/1678 (1.0%)
1	I	0.83	1/1227 (0.1%)	1.31	8/1654 (0.5%)
1	J	0.82	2/1261 (0.2%)	1.40	9/1701 (0.5%)
All	All	0.84	13/12583 (0.1%)	1.40	123/16973 (0.7%)

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	C	1	0
1	H	0	1
All	All	1	1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1	MSE	CG-SE	-7.17	1.71	1.95
1	I	1	MSE	CG-SE	-7.12	1.71	1.95
1	B	1	MSE	CG-SE	-6.39	1.73	1.95
1	H	1	MSE	CG-SE	-6.06	1.74	1.95
1	C	1	MSE	SE-CE	-5.98	1.60	1.95
1	D	1	MSE	CG-SE	-5.90	1.75	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	77	MSE	SE-CE	-5.84	1.60	1.95
1	A	1	MSE	CG-SE	-5.67	1.76	1.95
1	B	69	GLU	CD-OE1	5.26	1.31	1.25
1	A	77	MSE	SE-CE	-5.22	1.64	1.95
1	G	1	MSE	CG-SE	-5.08	1.78	1.95
1	J	1	MSE	SE-CE	-5.05	1.65	1.95
1	J	1	MSE	CG-SE	-5.04	1.78	1.95

All (123) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1	MSE	CG-SE-CE	24.67	153.18	98.90
1	H	59	ARG	NE-CZ-NH2	-17.99	111.31	120.30
1	E	81	ARG	NE-CZ-NH2	-11.97	114.31	120.30
1	E	81	ARG	NE-CZ-NH1	11.92	126.26	120.30
1	D	137	GLU	OE1-CD-OE2	11.45	137.03	123.30
1	B	1	MSE	CG-SE-CE	10.75	122.56	98.90
1	I	1	MSE	CG-SE-CE	10.57	122.16	98.90
1	F	11	ARG	NE-CZ-NH1	10.50	125.55	120.30
1	G	8	ARG	NE-CZ-NH2	-10.50	115.05	120.30
1	D	129	ASP	CB-CG-OD1	-10.14	109.17	118.30
1	I	8	ARG	NE-CZ-NH1	10.09	125.35	120.30
1	J	1	MSE	CG-SE-CE	10.07	121.06	98.90
1	H	1	MSE	CG-SE-CE	9.46	119.71	98.90
1	H	11	ARG	NE-CZ-NH2	9.43	125.02	120.30
1	J	81	ARG	NE-CZ-NH1	9.12	124.86	120.30
1	A	1	MSE	CG-SE-CE	9.07	118.86	98.90
1	A	8	ARG	NE-CZ-NH2	-8.97	115.81	120.30
1	D	81	ARG	NE-CZ-NH2	-8.82	115.89	120.30
1	G	81	ARG	NE-CZ-NH1	8.79	124.70	120.30
1	I	8	ARG	NE-CZ-NH2	-8.68	115.96	120.30
1	A	34[A]	ASP	CB-CG-OD1	8.54	125.98	118.30
1	A	34[B]	ASP	CB-CG-OD1	8.54	125.98	118.30
1	I	11	ARG	NE-CZ-NH2	-8.37	116.11	120.30
1	E	36	THR	N-CA-CB	-8.35	94.44	110.30
1	H	13	ASP	CB-CG-OD1	8.28	125.75	118.30
1	B	56	ASP	CB-CG-OD1	8.23	125.70	118.30
1	J	11	ARG	NE-CZ-NH1	8.19	124.39	120.30
1	H	56	ASP	CB-CG-OD2	-8.15	110.96	118.30
1	J	36	THR	N-CA-CB	-8.14	94.84	110.30
1	J	13	ASP	CB-CG-OD1	8.00	125.50	118.30
1	F	8	ARG	NE-CZ-NH2	-7.96	116.32	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	141	ARG	NE-CZ-NH2	-7.79	116.41	120.30
1	H	59	ARG	NH1-CZ-NH2	7.72	127.89	119.40
1	G	36	THR	N-CA-CB	-7.68	95.70	110.30
1	G	59	ARG	NE-CZ-NH2	-7.50	116.55	120.30
1	C	66	ASP	CB-CG-OD1	7.50	125.05	118.30
1	E	36	THR	OG1-CB-CG2	7.42	127.06	110.00
1	J	36	THR	OG1-CB-CG2	7.38	126.97	110.00
1	F	141	ARG	NE-CZ-NH2	-7.16	116.72	120.30
1	F	8	ARG	NE-CZ-NH1	7.10	123.85	120.30
1	D	31	GLU	CA-CB-CG	7.09	129.01	113.40
1	G	1	MSE	CG-SE-CE	7.08	114.48	98.90
1	C	36	THR	N-CA-CB	-7.06	96.88	110.30
1	D	81	ARG	NE-CZ-NH1	7.05	123.83	120.30
1	C	36	THR	OG1-CB-CG2	6.99	126.09	110.00
1	G	8	ARG	NE-CZ-NH1	6.91	123.75	120.30
1	I	11	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	F	81	ARG	NE-CZ-NH1	6.85	123.72	120.30
1	D	137	GLU	CG-CD-OE2	-6.84	104.63	118.30
1	B	59	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	F	95	TYR	CB-CG-CD1	-6.80	116.92	121.00
1	D	150	TYR	CB-CG-CD1	6.79	125.08	121.00
1	D	11	ARG	NE-CZ-NH1	6.73	123.67	120.30
1	C	98	TYR	CB-CG-CD2	-6.72	116.97	121.00
1	C	70	ASP	CB-CG-OD2	-6.69	112.28	118.30
1	G	11	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	C	98	TYR	CB-CG-CD1	6.67	125.00	121.00
1	H	36	THR	O-C-N	-6.67	111.87	123.20
1	D	11	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	E	129	ASP	CB-CG-OD1	-6.57	112.39	118.30
1	A	95	TYR	CB-CG-CD1	-6.51	117.09	121.00
1	B	69	GLU	CB-CG-CD	6.50	131.76	114.20
1	C	56	ASP	CB-CG-OD1	6.37	124.03	118.30
1	D	1	MSE	CG-SE-CE	6.30	112.77	98.90
1	A	81	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	H	81	ARG	NE-CZ-NH1	6.25	123.43	120.30
1	G	31	GLU	OE1-CD-OE2	6.25	130.80	123.30
1	G	36	THR	OG1-CB-CG2	6.21	124.28	110.00
1	B	59	ARG	NE-CZ-NH2	-6.19	117.20	120.30
1	C	141	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	B	141	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	B	13	ASP	CB-CG-OD2	-5.96	112.94	118.30
1	E	69	GLU	OE1-CD-OE2	-5.95	116.16	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	5	GLN	CB-CA-C	-5.94	98.52	110.40
1	G	26	ASP	CB-CG-OD1	5.91	123.62	118.30
1	H	11	ARG	NH1-CZ-NH2	-5.83	112.99	119.40
1	H	86	ASP	CB-CG-OD1	5.82	123.54	118.30
1	D	150	TYR	CB-CG-CD2	-5.79	117.53	121.00
1	B	116	PHE	CB-CG-CD2	-5.77	116.76	120.80
1	I	150	TYR	CB-CG-CD1	5.75	124.45	121.00
1	H	59	ARG	CA-CB-CG	-5.74	100.77	113.40
1	B	87	ARG	NE-CZ-NH1	-5.72	117.44	120.30
1	C	95	TYR	CG-CD1-CE1	-5.68	116.76	121.30
1	B	150	TYR	CB-CG-CD2	-5.67	117.60	121.00
1	H	36	THR	C-N-CA	5.64	134.14	122.30
1	F	59	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	F	98	TYR	CG-CD1-CE1	-5.60	116.82	121.30
1	G	81	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	H	36	THR	N-CA-CB	-5.59	99.68	110.30
1	J	8	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	G	98	TYR	CG-CD1-CE1	-5.55	116.86	121.30
1	E	8	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	A	11	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	H	71	SER	O-C-N	-5.53	113.86	122.70
1	C	81	ARG	NE-CZ-NH2	-5.51	117.55	120.30
1	B	8	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	A	95	TYR	CZ-CE2-CD2	-5.47	114.88	119.80
1	H	27	LEU	CA-CB-CG	5.46	127.86	115.30
1	D	129	ASP	CB-CG-OD2	5.42	123.18	118.30
1	C	147	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	C	151	LEU	CB-CG-CD1	-5.41	101.80	111.00
1	B	104	TYR	CB-CG-CD1	-5.40	117.76	121.00
1	E	137	GLU	OE1-CD-OE2	-5.37	116.85	123.30
1	G	91	ASP	CB-CG-OD2	-5.36	113.47	118.30
1	J	95	TYR	CB-CG-CD1	-5.36	117.79	121.00
1	B	8	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	G	77	MSE	CG-SE-CE	-5.31	87.21	98.90
1	D	56	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	C	104	TYR	CB-CG-CD1	-5.28	117.83	121.00
1	C	118	ASP	CB-CG-OD2	-5.23	113.59	118.30
1	C	59	ARG	NE-CZ-NH1	-5.20	117.70	120.30
1	J	98	TYR	CB-CG-CD1	-5.19	117.89	121.00
1	H	96	ARG	NE-CZ-NH1	-5.15	117.72	120.30
1	C	135	ASP	CB-CG-OD1	-5.15	113.67	118.30
1	B	77	MSE	CG-SE-CE	-5.14	87.58	98.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	81	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	A	96	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	A	87	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	B	60	LEU	CA-CB-CG	5.09	127.01	115.30
1	A	13	ASP	CB-CG-OD2	-5.06	113.74	118.30
1	G	95	TYR	CG-CD1-CE1	-5.03	117.27	121.30
1	A	149	LYS	CD-CE-NZ	-5.01	100.17	111.70
1	I	98	TYR	CB-CG-CD2	-5.01	117.99	121.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	36	THR	CB

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	143	VAL	Mainchain

## 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	1229	0	1288	19	0
1	B	1219	0	1278	24	0
1	C	1223	0	1288	27	0
1	D	1212	0	1276	28	0
1	E	1217	0	1273	32	0
1	F	1210	0	1271	17	0
1	G	1219	0	1270	25	0
1	H	1211	0	1266	26	0
1	I	1204	0	1257	21	0
1	J	1219	0	1275	27	0
2	A	25	0	0	0	0
2	B	5	0	0	0	0
2	C	10	0	0	0	0
2	D	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	20	0	0	0	0
2	F	10	0	0	1	0
2	G	10	0	0	0	0
2	H	10	0	0	0	0
2	I	10	0	0	0	0
2	J	10	0	0	0	0
3	A	6	0	0	0	0
3	D	6	0	0	0	0
3	E	6	0	0	0	0
3	G	6	0	0	0	0
3	I	6	0	0	0	0
4	A	248	0	0	3	0
4	B	263	0	0	2	0
4	C	260	0	0	6	0
4	D	243	0	0	7	0
4	E	231	0	0	4	0
4	F	230	0	0	2	0
4	G	243	0	0	4	0
4	H	217	0	0	5	0
4	I	224	0	0	7	0
4	J	248	0	0	8	0
4	K	55	0	0	2	0
4	L	2	0	0	3	0
All	All	14777	0	12742	216	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 9.

All (216) 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:D:1:MSE:HE3	1:D:2:ILE:HG22	1.22	1.18
1:I:1:MSE:HE2	1:I:2:ILE:HG22	1.25	1.16
1:B:1:MSE:HE3	1:B:2:ILE:HG22	1.21	1.13
1:H:2:ILE:HD11	1:H:78[A]:ILE:HD11	1.31	1.13
1:G:1:MSE:HE3	1:G:2:ILE:HG22	1.21	1.13
1:D:2:ILE:HD11	1:D:78[A]:ILE:HD11	1.29	1.13
1:J:2:ILE:HD11	1:J:78[A]:ILE:HD11	1.31	1.12
1:I:2:ILE:HD11	1:I:78:ILE:HD11	1.32	1.11
1:F:2:ILE:HD11	1:F:78[A]:ILE:HD11	1.32	1.08
1:H:1:MSE:HE3	1:H:2:ILE:HG22	1.24	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:2:ILE:HD11	1:G:78[A]:ILE:HD11	1.31	1.06
1:C:1:MSE:HE3	1:I:114:GLU:HG3	1.39	1.05
1:E:2:ILE:HD11	1:E:78[A]:ILE:HD11	1.39	1.05
1:C:2:ILE:HD11	1:C:78[A]:ILE:HD11	1.40	1.03
1:B:1:MSE:CE	1:B:2:ILE:HG22	1.92	1.00
1:A:2:ILE:HD11	1:A:78[B]:ILE:HD11	1.43	1.00
1:B:2:ILE:HD11	1:B:78[A]:ILE:HD11	1.42	0.99
1:E:27[B]:LEU:HD23	1:E:31[B]:GLU:CD	1.83	0.99
1:E:27[B]:LEU:HD23	1:E:31[B]:GLU:OE1	1.65	0.97
1:A:1:MSE:CE	1:A:2:ILE:HG22	1.98	0.94
1:J:25:LYS:HE2	4:J:2065:HOH:O	1.68	0.92
1:A:1:MSE:HE2	1:A:2:ILE:HG22	1.49	0.92
1:J:1:MSE:HE3	1:J:2:ILE:HG22	1.49	0.92
1:E:114:GLU:HG3	1:F:1:MSE:HE1	1.50	0.91
1:H:1:MSE:CE	1:H:2:ILE:HG22	2.01	0.90
1:J:1:MSE:CE	1:J:2:ILE:HG22	2.02	0.88
1:I:1:MSE:CE	1:I:2:ILE:HG22	2.03	0.88
1:C:1:MSE:CE	1:I:114:GLU:HG3	2.05	0.87
1:D:1:MSE:CE	1:D:2:ILE:HG22	2.05	0.86
1:C:1:MSE:SE	4:J:2042:HOH:O	2.44	0.84
1:D:115:LYS:HG3	4:D:2185:HOH:O	1.78	0.82
1:D:1:MSE:HE3	1:D:2:ILE:CG2	2.08	0.81
4:C:2040:HOH:O	1:G:1:MSE:SE	2.49	0.79
1:G:1:MSE:CE	1:G:2:ILE:HG22	2.10	0.78
1:E:24:LYS:HG3	4:E:2061:HOH:O	1.84	0.78
1:C:25:LYS:HE2	4:C:2070:HOH:O	1.85	0.77
4:A:2036:HOH:O	1:B:1:MSE:SE	2.52	0.77
1:H:2:ILE:CD1	1:H:78[A]:ILE:HD11	2.12	0.77
1:G:1:MSE:CE	1:H:114:GLU:HG3	2.16	0.76
1:F:1:MSE:SE	4:G:2040:HOH:O	2.54	0.76
4:H:2025:HOH:O	1:I:1:MSE:SE	2.53	0.75
1:I:1:MSE:HE3	4:I:2004:HOH:O	1.88	0.74
1:E:27[B]:LEU:CD2	1:E:31[B]:GLU:OE1	2.35	0.74
1:E:27[B]:LEU:HD22	1:E:31[B]:GLU:HG3	1.70	0.74
1:J:66:ASP:HB3	4:J:2146:HOH:O	1.88	0.74
1:I:140:GLU:HG2	4:I:2196:HOH:O	1.88	0.73
1:G:1:MSE:HE3	1:G:2:ILE:CG2	2.12	0.72
1:D:115:LYS:HE2	4:D:2185:HOH:O	1.90	0.72
1:F:2:ILE:HD11	1:F:78[A]:ILE:CD1	2.17	0.72
4:C:2120:HOH:O	1:I:151:LEU:HD13	1.92	0.70
1:D:1:MSE:SE	4:F:2037:HOH:O	2.59	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:LYS:HD2	4:C:2129:HOH:O	1.90	0.70
1:F:137:GLU:HG2	4:F:2207:HOH:O	1.92	0.69
1:B:78[A]:ILE:HD13	1:D:118:ASP:HB2	1.76	0.68
1:D:2:ILE:HD11	1:D:78[A]:ILE:CD1	2.16	0.68
1:H:59:ARG:HH11	1:H:59:ARG:HG2	1.61	0.66
1:A:1:MSE:SE	4:I:2028:HOH:O	2.63	0.66
1:G:1:MSE:HE1	1:H:114:GLU:HG3	1.77	0.65
1:C:77:MSE:SE	4:C:2174:HOH:O	2.65	0.65
1:E:114:GLU:HG3	1:F:1:MSE:CE	2.27	0.63
1:B:114:GLU:HG3	1:D:1:MSE:CE	2.30	0.61
1:A:133[A]:VAL:HG21	4:D:2230:HOH:O	2.00	0.61
1:E:27[B]:LEU:CD2	1:E:31[B]:GLU:CD	2.65	0.61
1:A:1:MSE:HE3	1:A:2:ILE:HG22	1.80	0.60
1:B:78[A]:ILE:HD13	1:D:118:ASP:CB	2.30	0.60
1:J:36:THR:CG2	1:J:38:LEU:H	2.15	0.60
1:F:1:MSE:HE3	1:F:2:ILE:HG22	1.84	0.60
1:C:27[A]:LEU:HD12	1:C:31:GLU:CD	2.22	0.60
1:E:36:THR:CG2	1:E:38:LEU:H	2.15	0.60
1:H:36:THR:CG2	1:H:38:LEU:H	2.15	0.60
1:C:36:THR:CG2	1:C:38:LEU:H	2.14	0.59
1:C:20:LEU:HG	1:C:24:LYS:HE3	1.82	0.59
1:E:151:LEU:HD23	4:E:2222:HOH:O	2.03	0.59
1:B:2:ILE:HD11	1:B:78[A]:ILE:CD1	2.25	0.59
1:C:36:THR:HG23	1:C:38:LEU:H	1.66	0.59
1:B:1:MSE:HE1	4:D:2190:HOH:O	2.03	0.59
1:G:1:MSE:HE2	1:H:114:GLU:HG3	1.82	0.59
1:D:27[A]:LEU:HD12	4:D:2076:HOH:O	2.03	0.58
1:G:36:THR:HG21	1:G:43:VAL:HG21	1.84	0.58
1:D:120:ILE:HD11	1:D:151:LEU:HD12	1.87	0.57
1:G:2:ILE:CD1	1:G:78[A]:ILE:HD11	2.22	0.57
1:E:25:LYS:HB3	1:E:27[A]:LEU:HD13	1.87	0.56
1:H:59:ARG:NH1	1:H:59:ARG:HG2	2.19	0.56
1:E:25:LYS:HE2	4:E:2062:HOH:O	2.05	0.56
1:G:131:LYS:HG3	4:G:2208:HOH:O	2.05	0.56
1:C:25:LYS:HB2	1:C:27[A]:LEU:HD22	1.87	0.56
1:E:27[B]:LEU:CD2	1:E:31[B]:GLU:HG3	2.35	0.56
1:H:36:THR:HG22	4:K:2052:HOH:O	2.06	0.56
1:E:51:GLN:NE2	1:E:81:ARG:HH21	2.05	0.55
1:J:151:LEU:HD22	4:L:2001:HOH:O	2.07	0.55
1:I:131:LYS:HD2	4:I:2089:HOH:O	2.07	0.55
1:J:40[B]:GLU:OE2	4:J:2102:HOH:O	2.18	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:51:GLN:NE2	1:F:81:ARG:HH21	2.04	0.55
1:E:33:ALA:O	1:E:36:THR:HB	2.08	0.54
1:J:51:GLN:NE2	1:J:81:ARG:HH21	2.05	0.54
1:C:73:LEU:HD12	4:C:2178:HOH:O	2.08	0.54
1:J:151:LEU:HD13	4:L:2001:HOH:O	2.07	0.54
1:A:132[B]:LYS:HG3	1:D:116:PHE:CE1	2.43	0.54
1:J:36:THR:HG21	1:J:43:VAL:HG21	1.90	0.54
1:J:130:VAL:O	4:J:2102:HOH:O	2.19	0.54
1:G:36:THR:CG2	1:G:38:LEU:H	2.22	0.53
1:J:2:ILE:HD11	1:J:78[A]:ILE:CD1	2.21	0.53
1:I:2:ILE:HD11	1:I:78:ILE:CD1	2.21	0.53
1:G:51:GLN:NE2	1:G:81:ARG:HH21	2.07	0.53
1:I:51:GLN:NE2	1:I:81:ARG:HH21	2.07	0.52
1:G:78[A]:ILE:HD12	1:H:113:HIS:HB3	1.91	0.52
1:E:88:ILE:HD12	1:E:98:TYR:CZ	2.45	0.51
1:B:25:LYS:HB2	1:B:27[B]:LEU:HD22	1.93	0.51
1:J:2:ILE:CD1	1:J:78[A]:ILE:HD11	2.22	0.51
1:E:27[B]:LEU:CD2	1:E:31[B]:GLU:CG	2.89	0.51
1:E:20:LEU:HD12	4:E:2061:HOH:O	2.10	0.51
1:E:36:THR:HG22	1:E:38:LEU:H	1.75	0.51
1:H:36:THR:HG22	1:H:38:LEU:H	1.75	0.51
1:B:88:ILE:HD12	1:B:98:TYR:CZ	2.45	0.51
1:G:77:MSE:HG2	4:G:2156:HOH:O	2.11	0.51
1:B:78[A]:ILE:CD1	1:D:118:ASP:HB2	2.41	0.50
1:C:51:GLN:NE2	1:C:81:ARG:HH21	2.10	0.50
1:D:25:LYS:HB3	1:D:27[A]:LEU:HD13	1.92	0.50
1:H:51:GLN:NE2	1:H:81:ARG:HH21	2.09	0.50
1:D:51:GLN:NE2	1:D:81:ARG:HH21	2.09	0.50
1:A:51:GLN:NE2	1:A:81:ARG:HH21	2.10	0.50
1:H:36:THR:HG21	1:H:43:VAL:HG21	1.93	0.50
1:A:1:MSE:HE3	4:A:2004:HOH:O	2.12	0.50
1:E:151:LEU:HD13	4:L:2002:HOH:O	2.12	0.50
1:B:1:MSE:CE	1:D:114:GLU:HG3	2.41	0.49
1:B:114:GLU:HG3	1:D:1:MSE:HE1	1.93	0.49
1:D:115:LYS:NZ	4:D:2192:HOH:O	2.43	0.49
1:J:88:ILE:HD12	1:J:98:TYR:CZ	2.48	0.49
1:D:77:MSE:HG2	4:D:2151:HOH:O	2.13	0.49
1:G:33:ALA:O	1:G:36:THR:HB	2.13	0.49
1:C:1:MSE:HE1	4:I:2172:HOH:O	2.13	0.49
1:C:24:LYS:HE2	1:G:70:ASP:OD1	2.13	0.49
1:G:66:ASP:HB3	4:G:2141:HOH:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:GLU:HG3	1:D:1:MSE:HE2	1.96	0.48
1:F:1:MSE:HE3	1:F:2:ILE:CG2	2.43	0.48
1:B:69:GLU:HG3	4:B:2168:HOH:O	2.13	0.48
1:J:36:THR:HG23	1:J:38:LEU:H	1.77	0.48
1:E:77:MSE:HE2	1:E:77:MSE:HB3	1.52	0.48
1:C:1:MSE:HE1	4:I:2170:HOH:O	2.13	0.48
1:A:1:MSE:HE1	4:J:2197:HOH:O	2.13	0.48
1:E:36:THR:HG23	1:E:38:LEU:HB2	1.96	0.48
1:B:74:LEU:HA	1:B:77:MSE:HG3	1.96	0.47
1:B:51:GLN:NE2	1:B:81:ARG:HH21	2.12	0.47
1:E:78[A]:ILE:HD12	1:F:113:HIS:HB3	1.95	0.47
1:G:36:THR:HG22	1:G:38:LEU:H	1.79	0.47
1:J:36:THR:HG22	1:J:38:LEU:H	1.78	0.47
1:G:114:GLU:HG3	1:H:1:MSE:CE	2.44	0.47
1:A:77:MSE:HG2	4:A:2162:HOH:O	2.14	0.47
1:H:77:MSE:HE1	4:H:2009:HOH:O	2.15	0.47
1:C:77:MSE:HE2	1:C:77:MSE:HB3	1.65	0.47
1:I:59:ARG:HD3	4:I:2116:HOH:O	2.15	0.47
1:J:33:ALA:O	1:J:36:THR:HB	2.15	0.46
1:G:77:MSE:HE2	1:G:77:MSE:HB3	1.46	0.46
1:C:25:LYS:CB	1:C:27[A]:LEU:HD22	2.45	0.46
1:B:77:MSE:HE2	1:B:77:MSE:HB3	1.45	0.46
1:C:84:ILE:HD11	1:H:101[B]:LEU:HG	1.98	0.46
1:F:77:MSE:HE2	1:F:77:MSE:HB3	1.66	0.46
1:D:88:ILE:HD12	1:D:98:TYR:CZ	2.50	0.46
1:H:59:ARG:NH1	1:H:59:ARG:CG	2.78	0.46
1:H:28:SER:OG	1:H:31[A]:GLU:HG3	2.16	0.46
1:F:1:MSE:CE	1:F:2:ILE:HG22	2.46	0.46
1:I:74:LEU:HA	1:I:77:MSE:HG3	1.98	0.45
1:C:88[A]:ILE:HD12	1:C:98:TYR:CZ	2.52	0.45
1:H:36:THR:HG23	1:H:38:LEU:H	1.81	0.45
1:B:135:ASP:HB2	1:B:141:ARG:HG3	1.98	0.45
1:E:128[A]:LEU:HD21	1:G:104:TYR:CD1	2.51	0.45
1:E:29:PHE:CE2	1:G:110:ALA:HB1	2.52	0.45
1:H:5:GLN:HG3	4:H:2028:HOH:O	2.17	0.45
1:E:36:THR:HG21	1:E:43:VAL:HG21	1.97	0.45
1:I:2:ILE:CD1	1:I:78:ILE:HD11	2.24	0.45
1:A:1:MSE:HE3	1:A:2:ILE:H	1.82	0.45
1:A:40:GLU:HG2	4:K:2006:HOH:O	2.16	0.45
1:B:77:MSE:SE	4:B:2092:HOH:O	2.85	0.44
1:F:25:LYS:HB2	1:F:27:LEU:HD22	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:77:MSE:HE2	1:D:77:MSE:HB3	1.72	0.44
1:E:101[B]:LEU:HG	1:G:84:ILE:HD11	1.98	0.44
1:C:74:LEU:HA	1:C:77:MSE:HG3	2.00	0.44
1:H:127:LYS:NZ	4:H:2179:HOH:O	2.50	0.44
1:B:113:HIS:HB3	1:D:78[A]:ILE:HD12	1.99	0.44
1:A:77:MSE:HE2	1:A:77:MSE:HB3	1.57	0.44
1:J:1:MSE:HE2	1:J:2:ILE:HG22	1.91	0.44
1:F:35:GLY:N	2:F:1158:SO4:O4	2.39	0.44
1:A:2:ILE:CD1	1:A:78[B]:ILE:HD11	2.32	0.44
1:B:24:LYS:HE2	1:E:70:ASP:OD1	2.17	0.44
1:D:27[B]:LEU:CD2	1:D:31:GLU:HG3	2.48	0.43
1:B:1:MSE:HE2	1:D:114:GLU:HG3	2.00	0.43
1:I:115:LYS:NZ	4:J:2102:HOH:O	2.51	0.43
1:C:2:ILE:HD11	1:C:78[A]:ILE:CD1	2.29	0.43
1:I:120:ILE:HD11	1:I:151:LEU:HD12	2.00	0.43
1:E:36:THR:HG23	1:E:38:LEU:H	1.80	0.43
1:J:122:SER:HB2	1:J:151:LEU:HD12	2.00	0.43
1:H:60:LEU:HD22	4:H:2070:HOH:O	2.17	0.43
1:A:133[A]:VAL:CG2	1:A:141:ARG:HB2	2.49	0.42
1:I:101[B]:LEU:HG	1:J:84:ILE:HD11	2.00	0.42
1:C:33:ALA:O	1:C:36:THR:HG22	2.20	0.42
1:J:1:MSE:HE3	1:J:2:ILE:H	1.84	0.42
1:F:3:GLN:HB3	1:F:77:MSE:HE3	2.02	0.42
1:H:28:SER:HG	1:H:31[A]:GLU:HG3	1.84	0.42
1:C:129:ASP:OD2	1:C:131:LYS:HE2	2.20	0.41
1:E:25:LYS:CB	1:E:27[A]:LEU:HD13	2.49	0.41
1:J:151:LEU:HD21	4:J:2235:HOH:O	2.20	0.41
1:C:104:TYR:CD1	1:H:128[A]:LEU:HD21	2.55	0.41
1:F:152:PRO:CG	1:F:154:LYS:HZ3	2.34	0.41
1:A:3:GLN:HB3	1:A:77:MSE:HE3	2.03	0.41
1:I:126:PHE:HE2	1:I:128[A]:LEU:HD22	1.86	0.41
1:E:114:GLU:CG	1:F:1:MSE:HE1	2.36	0.41
1:J:36:THR:HG23	1:J:38:LEU:HB2	2.03	0.41
1:J:2:ILE:HD13	1:J:2:ILE:HG21	1.84	0.40
1:A:152:PRO:CG	1:A:154:LYS:HE2	2.51	0.40
1:C:36:THR:HG21	1:C:43:VAL:HG21	2.03	0.40
1:D:3:GLN:HB3	1:D:77:MSE:HE3	2.03	0.40
1:J:27[B]:LEU:HD23	1:J:31[B]:GLU:CD	2.42	0.40
1:A:70:ASP:OD1	1:I:24:LYS:HE2	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	164/156 (105%)	161 (98%)	3 (2%)	0	100	100
1	B	160/156 (103%)	157 (98%)	3 (2%)	0	100	100
1	C	162/156 (104%)	159 (98%)	3 (2%)	0	100	100
1	D	159/156 (102%)	156 (98%)	3 (2%)	0	100	100
1	E	160/156 (103%)	157 (98%)	3 (2%)	0	100	100
1	F	158/156 (101%)	155 (98%)	3 (2%)	0	100	100
1	G	161/156 (103%)	158 (98%)	3 (2%)	0	100	100
1	H	158/156 (101%)	155 (98%)	3 (2%)	0	100	100
1	I	156/156 (100%)	152 (97%)	4 (3%)	0	100	100
1	J	160/156 (103%)	157 (98%)	3 (2%)	0	100	100
All	All	1598/1560 (102%)	1567 (98%)	31 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	137/123 (111%)	136 (99%)	1 (1%)	88	78
1	B	133/123 (108%)	131 (98%)	2 (2%)	72	51
1	C	135/123 (110%)	132 (98%)	3 (2%)	60	32
1	D	132/123 (107%)	128 (97%)	4 (3%)	48	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	133/123 (108%)	131 (98%)	2 (2%)	72	51
1	F	131/123 (106%)	129 (98%)	2 (2%)	72	51
1	G	134/123 (109%)	132 (98%)	2 (2%)	72	51
1	H	131/123 (106%)	125 (95%)	6 (5%)	33	8
1	I	129/123 (105%)	128 (99%)	1 (1%)	86	76
1	J	133/123 (108%)	126 (95%)	7 (5%)	28	6
All	All	1328/1230 (108%)	1298 (98%)	30 (2%)	63	30

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	102	GLN
1	B	60	LEU
1	B	102	GLN
1	C	27[A]	LEU
1	C	27[B]	LEU
1	C	36	THR
1	D	27[A]	LEU
1	D	27[B]	LEU
1	D	102	GLN
1	D	129	ASP
1	E	36	THR
1	E	102	GLN
1	F	27	LEU
1	F	102	GLN
1	G	36	THR
1	G	102	GLN
1	H	27	LEU
1	H	36	THR
1	H	60	LEU
1	H	102	GLN
1	H	128[A]	LEU
1	H	128[B]	LEU
1	I	102	GLN
1	J	27[A]	LEU
1	J	27[B]	LEU
1	J	36	THR
1	J	102	GLN
1	J	127	LYS
1	J	128[A]	LEU

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Mol	Chain	Res	Type
1	J	128[B]	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
1	A	102	GLN
1	B	51	GLN
1	B	102	GLN
1	C	51	GLN
1	C	102	GLN
1	D	51	GLN
1	D	102	GLN
1	E	51	GLN
1	E	102	GLN
1	F	51	GLN
1	F	102	GLN
1	G	51	GLN
1	G	102	GLN
1	H	51	GLN
1	H	76	GLN
1	H	102	GLN
1	I	51	GLN
1	I	102	GLN
1	J	51	GLN
1	J	102	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 ⓘ

29 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	1157	-	4,4,4	0.90	0	6,6,6	0.70	0
2	SO4	A	1158	-	4,4,4	0.69	0	6,6,6	0.60	0
2	SO4	A	1159	-	4,4,4	0.62	0	6,6,6	0.73	0
2	SO4	A	1160[A]	-	4,4,4	1.61	1 (25%)	6,6,6	0.51	0
2	SO4	A	1160[B]	-	4,4,4	1.06	0	6,6,6	0.34	0
3	OXL	A	1161	-	0,5,5	0.00	-	0,6,6	0.00	-
2	SO4	B	1157	-	4,4,4	1.21	1 (25%)	6,6,6	0.76	0
2	SO4	C	1157	-	4,4,4	1.41	1 (25%)	6,6,6	0.81	0
2	SO4	C	1158	-	4,4,4	0.69	0	6,6,6	1.04	1 (16%)
2	SO4	D	1157	-	4,4,4	0.87	0	6,6,6	0.43	0
2	SO4	D	1158	-	4,4,4	1.27	1 (25%)	6,6,6	0.54	0
3	OXL	D	1159	-	0,5,5	0.00	-	0,6,6	0.00	-
2	SO4	E	1157	-	4,4,4	1.14	0	6,6,6	0.59	0
2	SO4	E	1158	-	4,4,4	0.91	0	6,6,6	0.51	0
2	SO4	E	1159	-	4,4,4	0.81	0	6,6,6	0.64	0
2	SO4	E	1160	-	4,4,4	1.29	1 (25%)	6,6,6	0.37	0
3	OXL	E	1161	-	0,5,5	0.00	-	0,6,6	0.00	-
2	SO4	F	1157	-	4,4,4	1.09	1 (25%)	6,6,6	0.39	0
2	SO4	F	1158	-	4,4,4	0.78	0	6,6,6	0.88	0
2	SO4	G	1157	-	4,4,4	0.98	0	6,6,6	0.43	0
2	SO4	G	1158	-	4,4,4	1.01	0	6,6,6	0.63	0
3	OXL	G	1159	-	0,5,5	0.00	-	0,6,6	0.00	-
2	SO4	H	1157	-	4,4,4	1.17	0	6,6,6	0.71	0
2	SO4	H	1158	-	4,4,4	0.93	0	6,6,6	0.38	0
2	SO4	I	1157	-	4,4,4	1.17	1 (25%)	6,6,6	0.73	0
2	SO4	I	1158	-	4,4,4	1.05	0	6,6,6	0.81	0
3	OXL	I	1159	-	0,5,5	0.00	-	0,6,6	0.00	-
2	SO4	J	1157	-	4,4,4	1.13	0	6,6,6	0.55	0
2	SO4	J	1158	-	4,4,4	0.99	0	6,6,6	0.72	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	1157	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1158	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1159	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1160[A]	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1160[B]	-	-	0/0/0/0	0/0/0/0
3	OXL	A	1161	-	-	0/0/4/4	0/0/0/0
2	SO4	B	1157	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1157	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1158	-	-	0/0/0/0	0/0/0/0
2	SO4	D	1157	-	-	0/0/0/0	0/0/0/0
2	SO4	D	1158	-	-	0/0/0/0	0/0/0/0
3	OXL	D	1159	-	-	0/0/4/4	0/0/0/0
2	SO4	E	1157	-	-	0/0/0/0	0/0/0/0
2	SO4	E	1158	-	-	0/0/0/0	0/0/0/0
2	SO4	E	1159	-	-	0/0/0/0	0/0/0/0
2	SO4	E	1160	-	-	0/0/0/0	0/0/0/0
3	OXL	E	1161	-	-	0/0/4/4	0/0/0/0
2	SO4	F	1157	-	-	0/0/0/0	0/0/0/0
2	SO4	F	1158	-	-	0/0/0/0	0/0/0/0
2	SO4	G	1157	-	-	0/0/0/0	0/0/0/0
2	SO4	G	1158	-	-	0/0/0/0	0/0/0/0
3	OXL	G	1159	-	-	0/0/4/4	0/0/0/0
2	SO4	H	1157	-	-	0/0/0/0	0/0/0/0
2	SO4	H	1158	-	-	0/0/0/0	0/0/0/0
2	SO4	I	1157	-	-	0/0/0/0	0/0/0/0
2	SO4	I	1158	-	-	0/0/0/0	0/0/0/0
3	OXL	I	1159	-	-	0/0/4/4	0/0/0/0
2	SO4	J	1157	-	-	0/0/0/0	0/0/0/0
2	SO4	J	1158	-	-	0/0/0/0	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1157	SO4	O4-S	2.04	1.54	1.47
2	D	1158	SO4	O1-S	2.16	1.54	1.47
2	I	1157	SO4	O4-S	2.21	1.55	1.47
2	B	1157	SO4	O4-S	2.29	1.55	1.47
2	E	1160	SO4	O4-S	2.45	1.56	1.47
2	C	1157	SO4	O4-S	2.71	1.57	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1160[A]	SO4	O2-S	2.84	1.56	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1158	SO4	O4-S-O3	2.14	117.69	108.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	1158	SO4	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	152/156 (97%)	-0.37	2 (1%) 79 82	6, 12, 20, 38	0
1	B	152/156 (97%)	-0.46	1 (0%) 89 90	7, 11, 20, 38	0
1	C	152/156 (97%)	-0.45	2 (1%) 79 82	7, 11, 21, 37	0
1	D	152/156 (97%)	-0.43	0 100 100	7, 12, 21, 26	0
1	E	152/156 (97%)	-0.43	0 100 100	7, 12, 21, 25	0
1	F	152/156 (97%)	-0.39	1 (0%) 89 90	7, 13, 23, 33	0
1	G	152/156 (97%)	-0.35	2 (1%) 79 82	7, 12, 22, 37	0
1	H	152/156 (97%)	-0.20	3 (1%) 68 71	6, 13, 28, 36	0
1	I	152/156 (97%)	-0.39	2 (1%) 79 82	7, 12, 24, 37	0
1	J	152/156 (97%)	-0.39	2 (1%) 79 82	7, 12, 21, 36	0
All	All	1520/1560 (97%)	-0.39	15 (0%) 84 86	6, 12, 22, 38	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	136	PRO	4.1
1	A	136	PRO	3.8
1	H	60	LEU	3.0
1	B	136	PRO	3.0
1	H	66	ASP	2.9
1	C	137	GLU	2.9
1	I	137	GLU	2.8
1	J	137	GLU	2.8
1	I	136	PRO	2.4
1	H	67	LEU	2.3
1	F	137	GLU	2.3
1	A	137	GLU	2.2
1	G	136	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	137	GLU	2.1
1	J	66	ASP	2.1

## 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	C	1157	5/5	0.97	0.17	13.21	25,31,32,33	0
2	SO4	A	1158	5/5	0.99	0.19	8.55	21,27,28,29	0
2	SO4	J	1157	5/5	0.96	0.19	6.57	29,32,35,36	0
2	SO4	E	1158	5/5	0.99	0.17	6.21	24,27,30,31	0
2	SO4	C	1158	5/5	0.99	0.15	5.95	23,27,28,28	0
2	SO4	D	1158	5/5	0.76	0.26	5.87	58,59,59,60	0
2	SO4	A	1159	5/5	0.99	0.15	5.86	22,26,28,28	0
2	SO4	I	1158	5/5	0.84	0.27	5.78	58,60,60,61	0
2	SO4	G	1157	5/5	0.98	0.18	5.52	32,32,35,36	0
3	OXL	A	1161	6/6	0.90	0.16	5.44	7,15,17,17	0
3	OXL	G	1159	6/6	0.93	0.12	4.27	6,15,16,16	0
3	OXL	I	1159	6/6	0.92	0.12	4.25	7,14,15,15	0
2	SO4	F	1158	5/5	0.90	0.23	3.66	60,61,61,61	0
2	SO4	E	1160	5/5	0.64	0.28	3.51	59,59,60,62	0
2	SO4	H	1158	5/5	0.79	0.23	3.21	61,61,62,63	0
2	SO4	E	1159	5/5	0.99	0.12	3.04	23,27,29,30	0
3	OXL	E	1161	6/6	0.92	0.12	2.98	9,16,16,17	0
3	OXL	D	1159	6/6	0.93	0.12	2.94	8,15,15,17	0
2	SO4	J	1158	5/5	0.83	0.20	2.17	55,55,56,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	A	1160[A]	5/5	0.91	0.16	1.71	27,29,30,32	5
2	SO4	A	1160[B]	5/5	0.91	0.16	1.71	21,21,23,23	5
2	SO4	G	1158	5/5	0.92	0.15	0.84	44,45,46,46	0
2	SO4	I	1157	5/5	0.98	0.20	-	28,30,34,34	0
2	SO4	F	1157	5/5	0.98	0.17	-	35,37,39,40	0
2	SO4	A	1157	5/5	0.97	0.14	-	23,25,29,30	0
2	SO4	E	1157	5/5	0.98	0.19	-	27,30,33,33	0
2	SO4	D	1157	5/5	0.98	0.17	-	24,26,30,31	0
2	SO4	B	1157	5/5	0.97	0.17	-	25,32,33,34	0
2	SO4	H	1157	5/5	0.97	0.18	-	33,35,38,38	0

## 6.5 Other polymers

There are no such residues in this entry.