



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 25, 2024 – 10:16 PM EDT

PDB ID : 6SHI  
Title : Human kallikrein 7 with aromatic coumarinic ester compound 2 covalently bound to H57  
Authors : Hanke, S.; Straeter, N.  
Deposited on : 2019-08-06  
Resolution : 1.85 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

<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>.

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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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

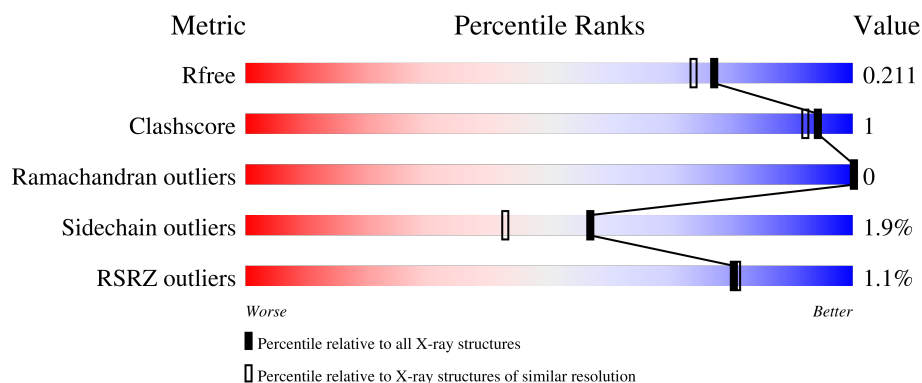
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 Å.

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



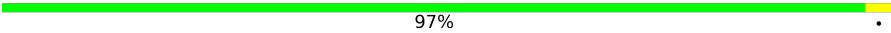
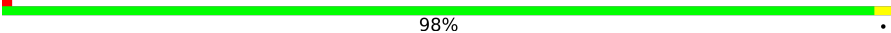
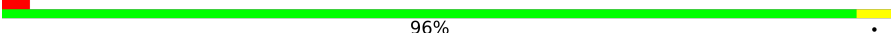
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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  $\geq 3$ , 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	224	<div> <div>%</div> <div>95%</div> <div>.</div> </div>
1	B	224	<div> <div>%</div> <div>98%</div> <div>.</div> </div>
1	C	224	<div> <div>96%</div> <div>.</div> </div>
1	D	224	<div> <div>%</div> <div>92%</div> <div>7%</div> <div>.</div> </div>
1	E	224	<div> <div>96%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	224	 97%
1	G	224	 98%
1	H	224	 96%

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
3	SH8	B	350[A]	-	-	-	X
3	SH8	B	350[B]	-	-	-	X
4	SO4	G	310	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16317 atoms, of which 56 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 Kallikrein-7.

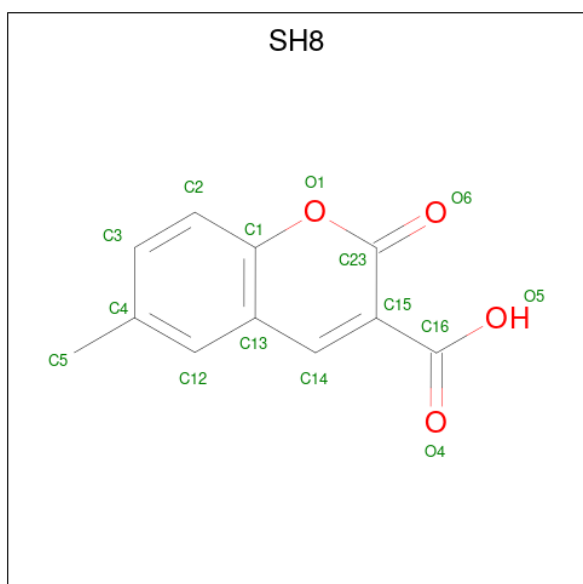
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	0	4	0
			1724	1074	312	320	18			
1	B	224	Total	C	N	O	S	0	4	0
			1699	1059	303	319	18			
1	C	224	Total	C	N	O	S	0	2	0
			1701	1057	308	318	18			
1	D	224	Total	C	N	O	S	0	2	0
			1709	1064	309	318	18			
1	E	224	Total	C	N	O	S	0	3	0
			1701	1062	304	317	18			
1	F	224	Total	C	N	O	S	0	2	0
			1696	1057	305	316	18			
1	G	224	Total	C	N	O	S	0	1	0
			1702	1059	309	316	18			
1	H	224	Total	C	N	O	S	0	1	0
			1697	1054	307	318	18			

- Molecule 2 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



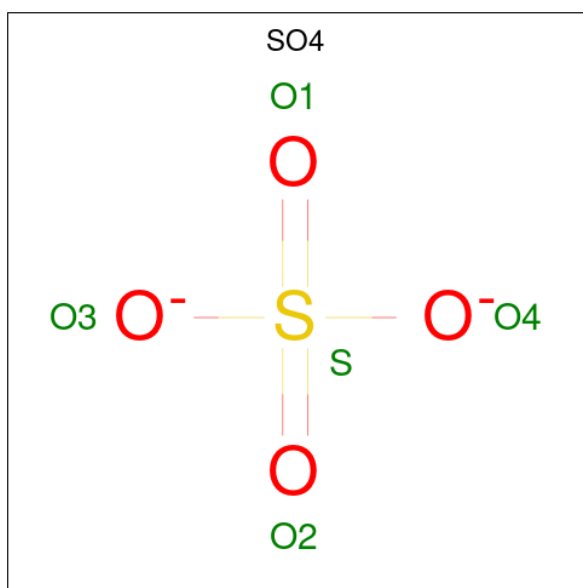
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			24	6	14	4		
2	B	1	Total	C	H	O	0	0
			24	6	14	4		
2	D	1	Total	C	H	O	0	0
			24	6	14	4		
2	F	1	Total	C	H	O	0	0
			24	6	14	4		

- Molecule 3 is 6-methyl-2-oxidanylidene-chromene-3-carboxylic acid (three-letter code: SH8) (formula:  $C_{11}H_8O_4$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 30 22 8	0	1
3	B	1	Total C O 30 22 8	0	1
3	C	1	Total C O 30 22 8	0	1
3	D	1	Total C O 30 22 8	0	1
3	E	1	Total C O 30 22 8	0	1
3	F	1	Total C O 30 22 8	0	1
3	G	1	Total C O 30 22 8	0	1
3	H	1	Total C O 30 22 8	0	1

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



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

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

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

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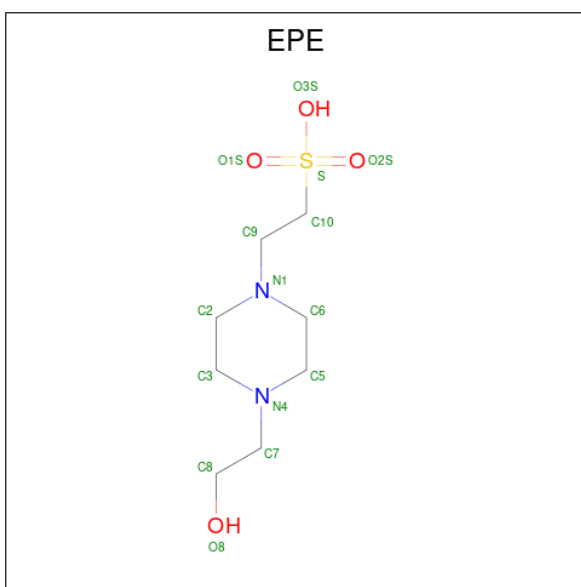
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	G	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 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
5	G	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
5	H	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	260	Total	O	0	1
			260	260		
6	B	249	Total	O	0	2
			249	249		
6	C	278	Total	O	0	2
			278	278		
6	D	235	Total	O	0	0
			235	235		
6	E	234	Total	O	0	1
			234	234		
6	F	280	Total	O	0	1
			280	280		
6	G	186	Total	O	0	0
			186	186		
6	H	165	Total	O	0	0
			165	165		

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

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Kallikrein-7



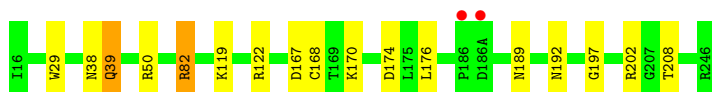
- Molecule 1: Kallikrein-7



- Molecule 1: Kallikrein-7



- Molecule 1: Kallikrein-7



- Molecule 1: Kallikrein-7



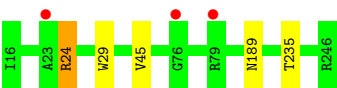
- Molecule 1: Kallikrein-7

Chain F:  97% .



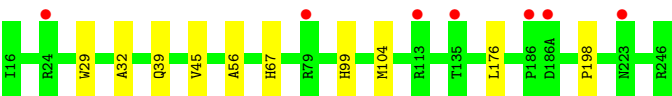
● Molecule 1: Kallikrein-7

Chain G:  98% .



● Molecule 1: Kallikrein-7

Chain H:  96% .



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.64Å 116.96Å 291.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.60 – 1.85 47.08 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.60-1.85) 99.8 (47.08-1.85)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.16 (at 1.84Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, $R_{free}$	0.176 , 0.208 0.179 , 0.211	Depositor DCC
$R_{free}$ test set	2682 reflections (1.51%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.7	Xtriage
Anisotropy	0.506	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 55.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	16317	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% 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: SH8, EPE, SO4, PGE

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	0.68	1/1772 (0.1%)	0.74	4/2406 (0.2%)
1	B	0.65	0/1744	0.67	0/2371
1	C	0.70	0/1740	0.69	0/2365
1	D	0.75	0/1751	0.68	0/2379
1	E	0.68	0/1743	0.69	0/2371
1	F	0.71	0/1738	0.67	0/2364
1	G	0.68	0/1741	0.67	0/2365
1	H	0.61	0/1736	0.65	0/2361
All	All	0.68	1/13965 (0.0%)	0.68	4/18982 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	179	SER	CB-OG	-5.48	1.35	1.42

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	128	ARG	NE-CZ-NH1	7.30	123.95	120.30
1	A	128	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	A	235[A]	THR	CA-C-O	5.44	131.52	120.10
1	A	235[B]	THR	CA-C-O	5.44	131.52	120.10

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	1724	0	1710	4	0
1	B	1699	0	1659	3	0
1	C	1701	0	1661	3	0
1	D	1709	0	1683	10	0
1	E	1701	0	1667	6	0
1	F	1696	0	1659	4	0
1	G	1702	0	1672	1	0
1	H	1697	0	1652	6	0
2	A	10	14	14	1	0
2	B	10	14	14	0	0
2	D	10	14	14	0	0
2	F	10	14	14	1	0
3	A	30	0	0	0	0
3	B	30	0	0	0	0
3	C	30	0	0	0	0
3	D	30	0	0	0	0
3	E	30	0	0	0	0
3	F	30	0	0	0	0
3	G	30	0	0	0	0
3	H	30	0	0	0	0
4	A	50	0	0	1	0
4	B	60	0	0	0	0
4	C	60	0	0	0	0
4	D	55	0	0	0	0
4	E	40	0	0	0	0
4	F	55	0	0	0	0
4	G	55	0	0	0	0
4	H	60	0	0	0	0
5	G	15	0	17	0	0
5	H	15	0	17	1	0
6	A	260	0	0	1	0
6	B	249	0	0	1	0
6	C	278	0	0	0	0
6	D	235	0	0	2	0
6	E	234	0	0	4	0
6	F	280	0	0	1	0
6	G	186	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	H	165	0	0	1	0
All	All	16261	56	13453	36	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 1.

The worst 5 of 36 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:G:24:ARG:HE	1:G:24:ARG:H	1.38	0.70
1:D:122:ARG:HD3	1:D:208:THR:HG22	1.79	0.64
1:D:82:ARG:HD3	1:F:128:ARG:HG2	1.86	0.57
1:D:82:ARG:CD	1:F:128:ARG:HG2	2.35	0.57
1:E:82:ARG:HD3	6:E:441:HOH:O	2.08	0.52

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	226/224 (101%)	222 (98%)	4 (2%)	0	100	100
1	B	225/224 (100%)	221 (98%)	4 (2%)	0	100	100
1	C	223/224 (100%)	221 (99%)	2 (1%)	0	100	100
1	D	224/224 (100%)	222 (99%)	2 (1%)	0	100	100
1	E	225/224 (100%)	222 (99%)	3 (1%)	0	100	100
1	F	224/224 (100%)	222 (99%)	2 (1%)	0	100	100
1	G	223/224 (100%)	220 (99%)	3 (1%)	0	100	100
1	H	223/224 (100%)	219 (98%)	4 (2%)	0	100	100
All	All	1793/1792 (100%)	1769 (99%)	24 (1%)	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	197/194 (102%)	193 (98%)	4 (2%)	55	40
1	B	192/194 (99%)	191 (100%)	1 (0%)	88	86
1	C	192/194 (99%)	188 (98%)	4 (2%)	53	38
1	D	194/194 (100%)	187 (96%)	7 (4%)	35	18
1	E	192/194 (99%)	187 (97%)	5 (3%)	46	30
1	F	191/194 (98%)	188 (98%)	3 (2%)	62	49
1	G	192/194 (99%)	187 (97%)	5 (3%)	46	30
1	H	191/194 (98%)	189 (99%)	2 (1%)	76	69
All	All	1541/1552 (99%)	1510 (98%)	31 (2%)	57	40

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	192	ASN
1	G	189	ASN
1	E	45[A]	VAL
1	H	29	TRP
1	G	24	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

109 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	$\# Z  > 2$
4	SO4	C	313	-	4,4,4	0.05	0	6,6,6	0.28	0
4	SO4	B	307	-	4,4,4	0.30	0	6,6,6	0.15	0
4	SO4	G	309	-	4,4,4	0.12	0	6,6,6	0.09	0
4	SO4	D	310	-	4,4,4	0.37	0	6,6,6	0.52	0
5	EPE	H	301	-	15,15,15	0.91	1 (6%)	18,20,20	0.36	0
4	SO4	D	309	-	4,4,4	0.23	0	6,6,6	1.13	1 (16%)
3	SH8	B	350[B]	1	16,16,16	0.64	1 (6%)	22,23,23	0.83	0
4	SO4	D	311	-	4,4,4	0.33	0	6,6,6	0.28	0
3	SH8	H	350[B]	1	16,16,16	1.55	2 (12%)	22,23,23	1.49	2 (9%)
5	EPE	G	301	-	15,15,15	1.15	1 (6%)	18,20,20	0.27	0
4	SO4	G	306	-	4,4,4	0.13	0	6,6,6	0.10	0
4	SO4	F	309	-	4,4,4	0.22	0	6,6,6	0.26	0
4	SO4	A	307	-	4,4,4	0.14	0	6,6,6	0.16	0
4	SO4	F	303	-	4,4,4	0.34	0	6,6,6	0.23	0
4	SO4	F	312	-	4,4,4	0.26	0	6,6,6	0.99	1 (16%)
4	SO4	B	306	-	4,4,4	0.69	0	6,6,6	0.84	0
3	SH8	B	350[A]	1	16,16,16	0.60	0	22,23,23	0.77	0
4	SO4	D	308	-	4,4,4	0.61	0	6,6,6	0.68	0
4	SO4	E	307	-	4,4,4	0.22	0	6,6,6	0.13	0
3	SH8	H	350[A]	1	16,16,16	1.56	2 (12%)	22,23,23	1.47	2 (9%)
4	SO4	D	306	-	4,4,4	0.83	0	6,6,6	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SH8	D	350[B]	1	16,16,16	1.53	2 (12%)	22,23,23	1.49	2 (9%)
4	SO4	B	309	-	4,4,4	0.18	0	6,6,6	0.14	0
4	SO4	H	309	-	4,4,4	0.13	0	6,6,6	0.11	0
3	SH8	G	350[B]	1	16,16,16	0.57	0	22,23,23	0.88	1 (4%)
4	SO4	C	312	-	4,4,4	0.21	0	6,6,6	0.13	0
4	SO4	C	305	-	4,4,4	0.65	0	6,6,6	0.67	0
4	SO4	D	304	-	4,4,4	0.16	0	6,6,6	0.23	0
4	SO4	C	304	-	4,4,4	0.18	0	6,6,6	0.21	0
4	SO4	D	313	-	4,4,4	0.15	0	6,6,6	0.12	0
4	SO4	H	303	-	4,4,4	0.35	0	6,6,6	0.36	0
3	SH8	D	350[A]	1	16,16,16	1.54	2 (12%)	22,23,23	1.52	2 (9%)
4	SO4	F	306	-	4,4,4	0.53	0	6,6,6	0.89	0
4	SO4	A	306	-	4,4,4	0.48	0	6,6,6	0.78	0
4	SO4	B	304	-	4,4,4	0.30	0	6,6,6	0.37	0
4	SO4	E	309	-	4,4,4	0.15	0	6,6,6	0.16	0
3	SH8	A	350[A]	1	16,16,16	1.55	2 (12%)	22,23,23	1.46	2 (9%)
2	PGE	A	301	-	9,9,9	0.51	0	8,8,8	0.27	0
4	SO4	H	308	-	4,4,4	0.15	0	6,6,6	0.20	0
4	SO4	C	306	-	4,4,4	0.49	0	6,6,6	0.60	0
4	SO4	H	305	-	4,4,4	0.52	0	6,6,6	0.55	0
4	SO4	G	310	-	4,4,4	0.15	0	6,6,6	0.05	0
4	SO4	A	312	-	4,4,4	0.16	0	6,6,6	0.05	0
4	SO4	G	303	-	4,4,4	0.40	0	6,6,6	0.36	0
4	SO4	H	306	-	4,4,4	0.10	0	6,6,6	0.26	0
3	SH8	F	350[B]	1	16,16,16	1.52	2 (12%)	22,23,23	1.51	2 (9%)
4	SO4	E	308	-	4,4,4	0.35	0	6,6,6	1.06	1 (16%)
3	SH8	E	350[B]	1	16,16,16	1.52	2 (12%)	22,23,23	1.52	2 (9%)
2	PGE	F	301	-	9,9,9	0.34	0	8,8,8	0.44	0
4	SO4	D	305	-	4,4,4	0.27	0	6,6,6	0.27	0
4	SO4	E	305	-	4,4,4	0.19	0	6,6,6	0.12	0
4	SO4	H	311	-	4,4,4	0.13	0	6,6,6	0.15	0
3	SH8	C	350[B]	1	16,16,16	0.59	0	22,23,23	0.97	1 (4%)
4	SO4	H	307	-	4,4,4	0.16	0	6,6,6	0.10	0
4	SO4	A	309	-	4,4,4	0.39	0	6,6,6	0.34	0
2	PGE	B	302	-	9,9,9	0.38	0	8,8,8	0.58	0
4	SO4	C	309	-	4,4,4	0.31	0	6,6,6	0.15	0
3	SH8	E	350[A]	1	16,16,16	1.53	2 (12%)	22,23,23	1.63	3 (13%)
4	SO4	A	305	-	4,4,4	0.12	0	6,6,6	0.15	0
4	SO4	B	303	-	4,4,4	0.53	0	6,6,6	0.36	0
4	SO4	B	308	-	4,4,4	0.21	0	6,6,6	0.10	0
4	SO4	H	310	-	4,4,4	0.13	0	6,6,6	0.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	SO4	F	310	-	4,4,4	0.33	0	6,6,6	0.42	0
4	SO4	A	303	-	4,4,4	0.40	0	6,6,6	0.23	0
3	SH8	G	350[A]	1	16,16,16	0.66	0	22,23,23	1.05	1 (4%)
4	SO4	D	307	-	4,4,4	0.53	0	6,6,6	0.77	0
4	SO4	F	311	-	4,4,4	0.19	0	6,6,6	0.08	0
4	SO4	A	304	-	4,4,4	0.24	0	6,6,6	0.20	0
4	SO4	G	307	-	4,4,4	0.14	0	6,6,6	0.07	0
4	SO4	H	313	-	4,4,4	0.15	0	6,6,6	0.07	0
4	SO4	E	303	-	4,4,4	0.35	0	6,6,6	0.12	0
2	PGE	D	301	-	9,9,9	0.25	0	8,8,8	0.12	0
4	SO4	B	310	-	4,4,4	0.17	0	6,6,6	0.07	0
4	SO4	F	308	-	4,4,4	0.61	0	6,6,6	0.76	0
4	SO4	H	314	-	4,4,4	0.14	0	6,6,6	0.13	0
4	SO4	G	304	-	4,4,4	0.15	0	6,6,6	0.15	0
4	SO4	C	308	-	4,4,4	0.28	0	6,6,6	0.25	0
4	SO4	H	304	-	4,4,4	0.08	0	6,6,6	0.16	0
4	SO4	F	313	-	4,4,4	0.18	0	6,6,6	0.16	0
4	SO4	G	311	-	4,4,4	0.14	0	6,6,6	0.07	0
3	SH8	F	350[A]	1	16,16,16	1.53	2 (12%)	22,23,23	1.53	2 (9%)
4	SO4	D	303	-	4,4,4	0.38	0	6,6,6	0.45	0
4	SO4	E	306	-	4,4,4	0.40	0	6,6,6	0.20	0
4	SO4	B	314	-	4,4,4	0.40	0	6,6,6	1.72	2 (33%)
4	SO4	F	307	-	4,4,4	0.46	0	6,6,6	0.74	0
4	SO4	C	302	-	4,4,4	0.39	0	6,6,6	0.26	0
4	SO4	C	303	-	4,4,4	0.24	0	6,6,6	0.29	0
4	SO4	G	313	-	4,4,4	0.16	0	6,6,6	0.08	0
3	SH8	C	350[A]	1	16,16,16	0.71	0	22,23,23	0.91	1 (4%)
4	SO4	C	307	-	4,4,4	0.13	0	6,6,6	0.10	0
4	SO4	B	311	-	4,4,4	0.19	0	6,6,6	0.13	0
4	SO4	B	313	-	4,4,4	0.15	0	6,6,6	0.06	0
4	SO4	D	312	-	4,4,4	0.32	0	6,6,6	0.55	0
4	SO4	G	305	-	4,4,4	0.21	0	6,6,6	0.17	0
4	SO4	H	312	-	4,4,4	0.14	0	6,6,6	0.06	0
4	SO4	C	310	-	4,4,4	0.33	0	6,6,6	0.27	0
4	SO4	E	302	-	4,4,4	0.44	0	6,6,6	0.13	0
4	SO4	F	305	-	4,4,4	0.27	0	6,6,6	0.17	0
4	SO4	B	305	-	4,4,4	0.30	0	6,6,6	0.19	0
4	SO4	G	308	-	4,4,4	0.28	0	6,6,6	0.51	0
4	SO4	C	311	-	4,4,4	0.56	0	6,6,6	0.34	0
4	SO4	A	310	-	4,4,4	0.13	0	6,6,6	0.29	0
4	SO4	A	311	-	4,4,4	0.17	0	6,6,6	0.24	0
4	SO4	F	304	-	4,4,4	0.30	0	6,6,6	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	SO4	A	308	-	4,4,4	0.72	0	6,6,6	0.57	0
3	SH8	A	350[B]	1	16,16,16	1.53	2 (12%)	22,23,23	1.48	2 (9%)
4	SO4	G	312	-	4,4,4	0.17	0	6,6,6	0.10	0
4	SO4	E	304	-	4,4,4	0.41	0	6,6,6	0.41	0
4	SO4	B	312	-	4,4,4	0.13	0	6,6,6	0.09	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SH8	G	350[A]	1	-	4/4/4/4	0/2/2/2
3	SH8	A	350[A]	1	-	4/4/4/4	0/2/2/2
2	PGE	A	301	-	-	2/7/7/7	-
5	EPE	H	301	-	-	5/9/19/19	0/1/1/1
3	SH8	B	350[B]	1	-	2/4/4/4	0/2/2/2
2	PGE	D	301	-	-	3/7/7/7	-
3	SH8	H	350[B]	1	-	4/4/4/4	0/2/2/2
5	EPE	G	301	-	-	5/9/19/19	0/1/1/1
3	SH8	F	350[B]	1	-	4/4/4/4	0/2/2/2
3	SH8	B	350[A]	1	-	4/4/4/4	0/2/2/2
3	SH8	E	350[B]	1	-	4/4/4/4	0/2/2/2
2	PGE	F	301	-	-	4/7/7/7	-
3	SH8	H	350[A]	1	-	4/4/4/4	0/2/2/2
3	SH8	C	350[B]	1	-	4/4/4/4	0/2/2/2
3	SH8	D	350[B]	1	-	2/4/4/4	0/2/2/2
3	SH8	F	350[A]	1	-	4/4/4/4	0/2/2/2
3	SH8	G	350[B]	1	-	4/4/4/4	0/2/2/2
2	PGE	B	302	-	-	3/7/7/7	-
3	SH8	E	350[A]	1	-	4/4/4/4	0/2/2/2
3	SH8	A	350[B]	1	-	4/4/4/4	0/2/2/2
3	SH8	D	350[A]	1	-	4/4/4/4	0/2/2/2
3	SH8	C	350[A]	1	-	4/4/4/4	0/2/2/2

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	350[A]	SH8	O4-C16	5.16	1.36	1.22
3	H	350[B]	SH8	O4-C16	5.12	1.36	1.22
3	A	350[A]	SH8	O4-C16	5.09	1.36	1.22
3	E	350[A]	SH8	O4-C16	5.06	1.36	1.22
3	E	350[B]	SH8	O4-C16	5.05	1.36	1.22

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	350[B]	SH8	O4-C16-C15	-5.30	110.83	122.46
3	D	350[A]	SH8	O4-C16-C15	-5.26	110.90	122.46
3	F	350[A]	SH8	O4-C16-C15	-5.20	111.05	122.46
3	D	350[B]	SH8	O4-C16-C15	-5.18	111.09	122.46
3	H	350[B]	SH8	O4-C16-C15	-5.16	111.14	122.46

There are no chirality outliers.

5 of 82 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	350[A]	SH8	C23-C15-C16-O5
3	A	350[A]	SH8	C14-C15-C16-O5
3	A	350[A]	SH8	C23-C15-C16-O4
3	A	350[A]	SH8	C14-C15-C16-O4
3	A	350[B]	SH8	C23-C15-C16-O5

There are no ring outliers.

4 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	301	EPE	1	0
2	A	301	PGE	1	0
2	F	301	PGE	1	0
4	A	308	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	224/224 (100%)	-0.38	2 (0%) 84 84	16, 24, 41, 71	0
1	B	224/224 (100%)	-0.30	3 (1%) 77 78	16, 24, 42, 76	1 (0%)
1	C	224/224 (100%)	-0.23	1 (0%) 92 92	16, 25, 44, 68	1 (0%)
1	D	224/224 (100%)	-0.29	2 (0%) 84 84	18, 28, 48, 62	0
1	E	224/224 (100%)	-0.40	1 (0%) 92 92	17, 25, 43, 68	0
1	F	224/224 (100%)	-0.31	0 100 100	17, 26, 43, 68	0
1	G	224/224 (100%)	0.18	3 (1%) 77 78	23, 35, 52, 78	0
1	H	224/224 (100%)	0.17	7 (3%) 49 47	23, 37, 54, 75	0
All	All	1792/1792 (100%)	-0.20	19 (1%) 80 81	16, 28, 48, 78	2 (0%)

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	246	ARG	4.8
1	H	186(A)	ASP	3.7
1	A	246	ARG	3.4
1	H	79	ARG	2.8
1	C	246	ARG	2.7

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

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.



## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<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	B-factors(Å <sup>2</sup> )	Q<0.9
4	SO4	F	312	5/5	0.48	0.36	149,150,150,150	0
4	SO4	A	312	5/5	0.59	0.39	165,165,165,165	0
4	SO4	G	310	5/5	0.60	0.46	203,203,204,204	0
4	SO4	A	311	5/5	0.66	0.20	75,76,80,81	0
5	EPE	G	301	15/15	0.67	0.35	103,104,111,111	0
2	PGE	A	301	10/10	0.70	0.21	38,40,42,45	0
5	EPE	H	301	15/15	0.71	0.32	69,73,74,75	0
2	PGE	D	301	10/10	0.73	0.25	46,47,49,51	0
4	SO4	F	311	5/5	0.73	0.36	102,102,103,104	0
3	SH8	B	350[B]	15/15	0.75	0.47	28,39,41,41	15
3	SH8	B	350[A]	15/15	0.75	0.47	25,29,30,30	15
4	SO4	H	307	5/5	0.77	0.23	106,107,107,107	0
3	SH8	A	350[A]	15/15	0.78	0.38	25,28,31,31	15
3	SH8	A	350[B]	15/15	0.78	0.38	29,33,37,38	15
3	SH8	C	350[A]	15/15	0.81	0.45	26,31,34,35	15
3	SH8	C	350[B]	15/15	0.81	0.45	20,35,38,40	15
2	PGE	B	302	10/10	0.81	0.28	42,44,47,48	0
4	SO4	G	309	5/5	0.81	0.37	118,119,119,120	0
4	SO4	G	306	5/5	0.82	0.21	120,120,120,121	0
4	SO4	B	308	5/5	0.82	0.20	90,91,92,93	0
4	SO4	B	311	5/5	0.82	0.21	103,103,104,104	0
4	SO4	D	312	5/5	0.82	0.46	94,94,95,96	0
3	SH8	F	350[A]	15/15	0.82	0.43	27,28,30,30	15
3	SH8	F	350[B]	15/15	0.82	0.43	27,34,40,41	15
3	SH8	H	350[B]	15/15	0.83	0.46	28,37,39,40	15
3	SH8	D	350[A]	15/15	0.83	0.48	29,34,36,37	15
3	SH8	D	350[B]	15/15	0.83	0.48	30,39,44,45	15
3	SH8	G	350[A]	15/15	0.83	0.52	32,37,38,39	15
3	SH8	G	350[B]	15/15	0.83	0.52	28,37,42,42	15
4	SO4	B	313	5/5	0.83	0.22	117,118,118,118	0
4	SO4	D	309	5/5	0.83	0.17	83,84,86,88	0
3	SH8	H	350[A]	15/15	0.83	0.46	29,32,35,36	15
4	SO4	H	313	5/5	0.84	0.31	95,95,96,97	0
4	SO4	H	314	5/5	0.84	0.32	95,95,96,97	0
4	SO4	B	314	5/5	0.85	0.16	85,87,87,87	0
3	SH8	E	350[B]	15/15	0.85	0.33	18,33,40,42	15
3	SH8	E	350[A]	15/15	0.85	0.33	23,29,34,34	15

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	SO4	H	311	5/5	0.85	0.37	103,103,104,106	0
4	SO4	G	313	5/5	0.86	0.37	116,117,118,118	0
4	SO4	B	310	5/5	0.86	0.38	94,95,96,97	0
4	SO4	C	312	5/5	0.86	0.20	88,89,89,91	0
4	SO4	G	305	5/5	0.86	0.24	86,86,87,88	0
4	SO4	B	307	5/5	0.86	0.22	68,68,69,71	0
2	PGE	F	301	10/10	0.86	0.19	37,42,46,47	0
4	SO4	E	307	5/5	0.86	0.20	85,87,89,89	0
4	SO4	G	312	5/5	0.87	0.24	98,98,98,99	0
4	SO4	A	310	5/5	0.88	0.17	68,72,74,76	0
4	SO4	C	309	5/5	0.88	0.19	59,61,62,63	0
4	SO4	E	308	5/5	0.89	0.25	70,71,73,75	0
4	SO4	B	312	5/5	0.89	0.20	92,93,94,94	0
4	SO4	D	313	5/5	0.89	0.19	90,90,90,91	0
4	SO4	E	305	5/5	0.89	0.27	79,82,82,83	0
4	SO4	C	311	5/5	0.89	0.23	52,52,57,59	0
4	SO4	H	309	5/5	0.90	0.31	108,108,108,108	0
4	SO4	F	310	5/5	0.90	0.29	93,93,94,95	0
4	SO4	D	310	5/5	0.90	0.25	87,88,88,89	0
4	SO4	G	308	5/5	0.90	0.34	96,96,97,98	0
4	SO4	H	306	5/5	0.90	0.22	57,60,63,64	0
4	SO4	C	308	5/5	0.90	0.21	54,56,59,62	0
4	SO4	E	306	5/5	0.91	0.26	47,50,56,56	0
4	SO4	C	313	5/5	0.91	0.25	65,66,70,74	0
4	SO4	F	313	5/5	0.91	0.21	82,82,83,83	0
4	SO4	F	306	5/5	0.92	0.27	69,69,70,70	0
4	SO4	C	310	5/5	0.92	0.18	47,54,58,60	0
4	SO4	G	311	5/5	0.92	0.34	94,94,95,96	0
4	SO4	A	306	5/5	0.92	0.18	60,61,66,66	0
4	SO4	G	307	5/5	0.92	0.14	87,87,88,89	0
4	SO4	H	305	5/5	0.92	0.14	77,78,78,81	0
4	SO4	D	311	5/5	0.92	0.29	79,80,81,83	0
4	SO4	F	307	5/5	0.93	0.10	57,59,62,64	0
4	SO4	E	304	5/5	0.93	0.18	50,53,57,58	0
4	SO4	D	307	5/5	0.93	0.19	45,49,54,56	0
4	SO4	E	309	5/5	0.93	0.36	75,75,75,77	0
4	SO4	A	309	5/5	0.93	0.31	48,50,57,57	0
4	SO4	G	304	5/5	0.93	0.16	77,78,79,79	0
4	SO4	B	305	5/5	0.94	0.11	46,49,52,56	0
4	SO4	H	312	5/5	0.94	0.18	87,87,88,89	0
4	SO4	C	307	5/5	0.94	0.13	75,75,76,78	0
4	SO4	C	306	5/5	0.95	0.26	70,71,73,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	SO4	B	309	5/5	0.95	0.29	67,68,70,70	0
4	SO4	H	310	5/5	0.95	0.32	91,91,91,91	0
4	SO4	A	307	5/5	0.95	0.17	69,70,73,74	0
4	SO4	D	305	5/5	0.95	0.11	43,44,46,48	0
4	SO4	C	304	5/5	0.95	0.09	45,48,50,53	0
4	SO4	C	305	5/5	0.95	0.09	64,67,68,69	0
4	SO4	F	308	5/5	0.95	0.10	44,48,50,51	0
4	SO4	F	309	5/5	0.95	0.21	59,60,63,65	0
4	SO4	D	308	5/5	0.96	0.29	55,56,59,60	0
4	SO4	B	306	5/5	0.96	0.09	60,61,62,63	0
4	SO4	F	304	5/5	0.96	0.13	44,45,47,50	0
4	SO4	H	308	5/5	0.96	0.23	91,91,92,93	0
4	SO4	A	304	5/5	0.97	0.11	35,39,43,44	0
4	SO4	A	308	5/5	0.97	0.07	47,51,52,53	0
4	SO4	D	304	5/5	0.97	0.14	60,60,64,65	0
4	SO4	D	306	5/5	0.98	0.15	44,49,51,52	0
4	SO4	A	305	5/5	0.98	0.15	63,63,64,66	0
4	SO4	H	304	5/5	0.98	0.06	44,44,49,49	0
4	SO4	B	304	5/5	0.98	0.06	30,31,33,35	0
4	SO4	F	305	5/5	0.98	0.10	48,48,50,51	0
4	SO4	E	302	5/5	0.99	0.09	32,34,35,37	0
4	SO4	F	303	5/5	0.99	0.08	36,37,38,40	0
4	SO4	E	303	5/5	0.99	0.09	40,40,45,49	0
4	SO4	C	302	5/5	0.99	0.08	36,36,38,39	0
4	SO4	G	303	5/5	0.99	0.07	40,40,40,44	0
4	SO4	C	303	5/5	0.99	0.08	30,30,31,32	0
4	SO4	H	303	5/5	0.99	0.10	35,35,37,41	0
4	SO4	B	303	5/5	0.99	0.08	29,32,33,36	0
4	SO4	A	303	5/5	0.99	0.08	30,32,36,36	0
4	SO4	D	303	5/5	0.99	0.08	26,30,33,34	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.