



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 04:09 PM UTC

PDB ID : 3FLO / pdb\_00003flo  
Title : Crystal structure of the carboxyl-terminal domain of yeast DNA polymerase alpha in complex with its B subunit  
Authors : Klinge, S.N.; Pellegrini, L.  
Deposited on : 2008-12-19  
Resolution : 2.50 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

<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 : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

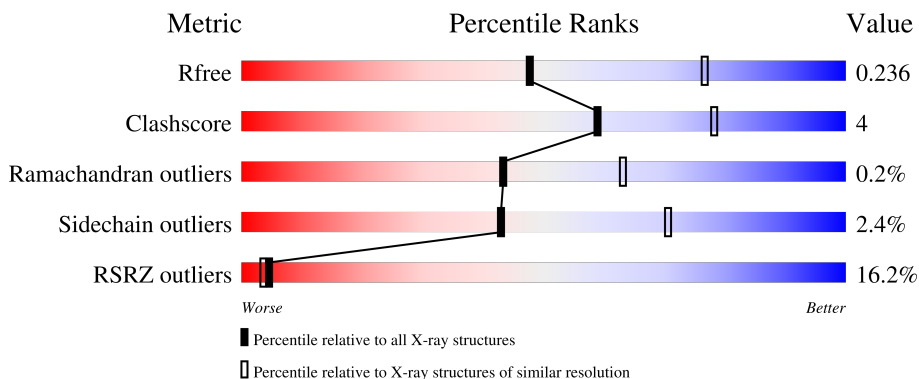
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 Å.

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







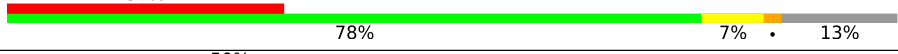


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	460	 2% (poor fit), 86% (0-1 outliers), 8% (2 outliers), 6% (3+ outliers)
1	C	460	 7% (poor fit), 80% (0-1 outliers), 13% (2 outliers), 6% (3+ outliers)
1	E	460	 24% (poor fit), 81% (0-1 outliers), 12% (2 outliers), 6% (3+ outliers)
1	G	460	 5% (poor fit), 82% (0-1 outliers), 12% (2 outliers), 6% (3+ outliers)
2	I	3	 100% (0 outliers)

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Mol	Chain	Length	Quality of chain
2	J	3	 100%
2	K	3	 100%
2	L	3	 100%
3	B	206	 3% 77% 8% • 13%
3	D	206	 31% 78% 7% • 13%
3	F	206	 50% 74% 11% • 13%
3	H	206	 21% 75% 12% 13%

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 20656 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 DNA polymerase alpha subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	433	3458	2208	589	651	10	0	3	0
1	C	433	3458	2208	589	651	10	0	3	0
1	E	433	3458	2208	589	651	10	0	3	0
1	G	433	3458	2208	589	651	10	0	3	0

- Molecule 2 is a protein called DNA polymerase alpha catalytic subunit A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	I	3	15	9	3	3	0	0	0
2	J	3	15	9	3	3	0	0	0
2	K	3	15	9	3	3	0	0	0
2	L	3	15	9	3	3	0	0	0

- Molecule 3 is a protein called DNA polymerase alpha catalytic subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	B	180	1471	925	247	287	12	0	1	0
3	D	180	1463	921	246	284	12	0	0	0
3	F	180	1463	921	246	284	12	0	0	0
3	H	180	1463	921	246	284	12	0	0	0

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



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	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		

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

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

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

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	2	Total Zn 2 2	0	0
5	D	2	Total Zn 2 2	0	0
5	F	2	Total Zn 2 2	0	0
5	H	2	Total Zn 2 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	135	Total O 135 135	0	0
6	B	79	Total O 79 79	0	0
6	C	106	Total O 106 106	0	0

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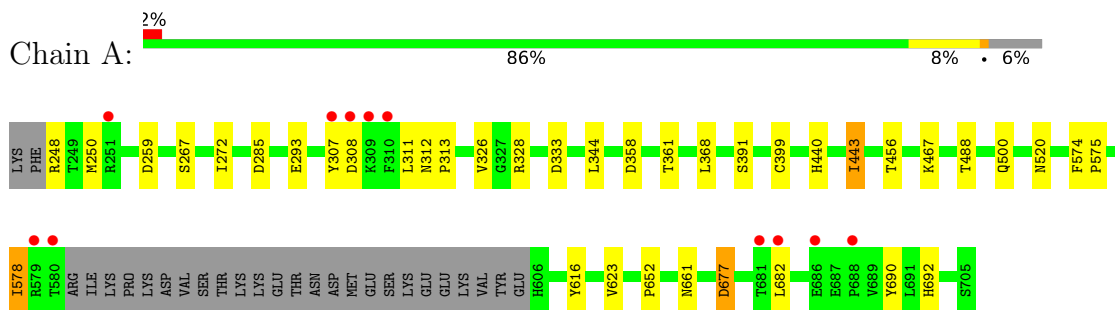
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	13	Total O 13 13	0	0
6	E	65	Total O 65 65	0	0
6	F	8	Total O 8 8	0	0
6	G	138	Total O 138 138	0	0
6	H	27	Total O 27 27	0	0

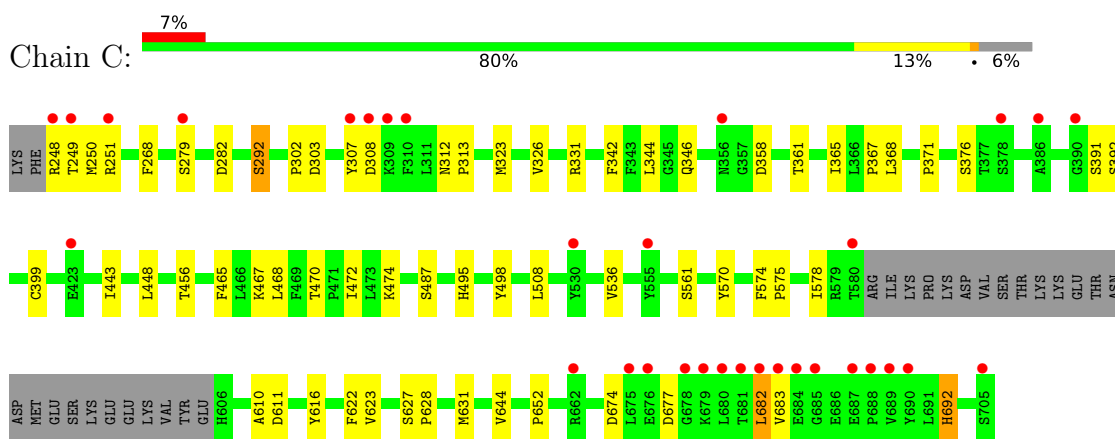
### 3 Residue-property plots [i](#)

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

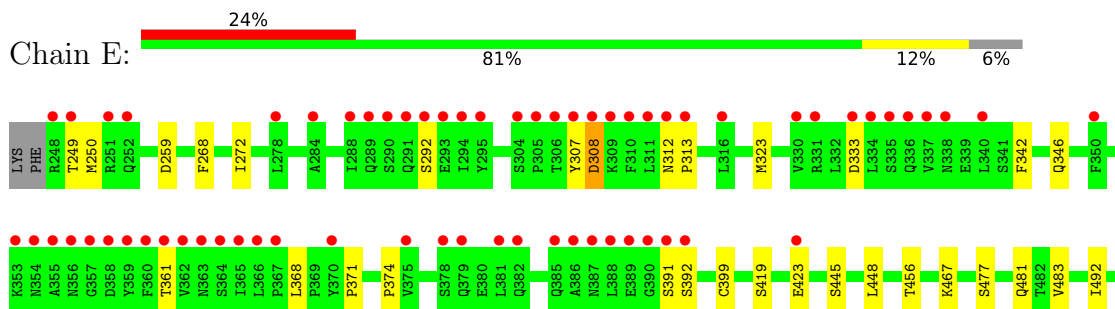
- Molecule 1: DNA polymerase alpha subunit B

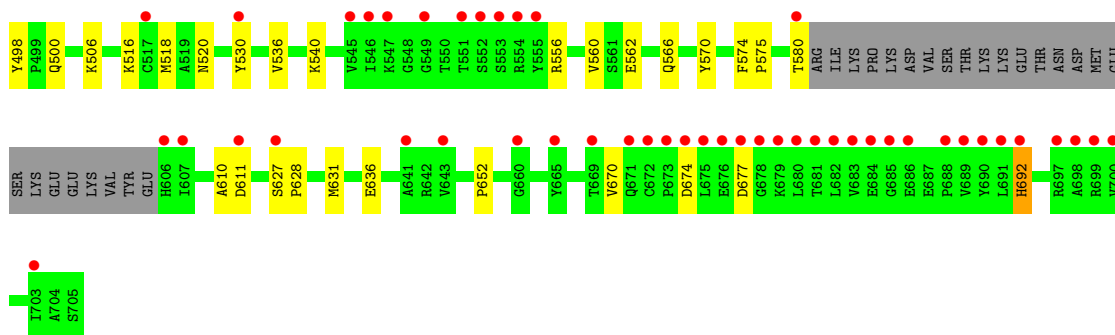


- Molecule 1: DNA polymerase alpha subunit B

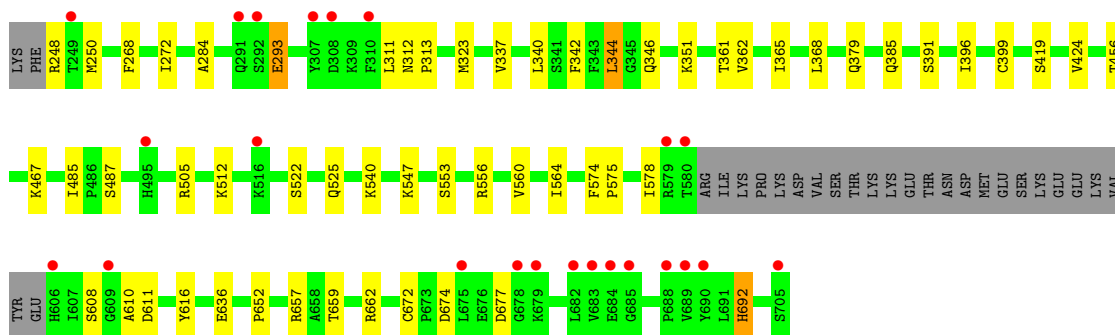
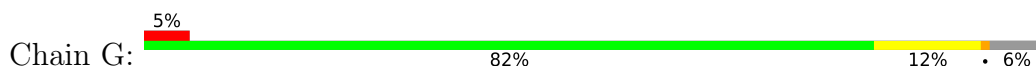


- Molecule 1: DNA polymerase alpha subunit B





- Molecule 1: DNA polymerase alpha subunit B



- Molecule 2: DNA polymerase alpha catalytic subunit A



There are no outlier residues recorded for this chain.

- Molecule 2: DNA polymerase alpha catalytic subunit A



There are no outlier residues recorded for this chain.

- Molecule 2: DNA polymerase alpha catalytic subunit A



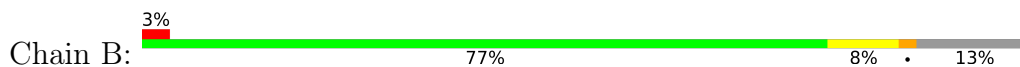
There are no outlier residues recorded for this chain.

- Molecule 2: DNA polymerase alpha catalytic subunit A



There are no outlier residues recorded for this chain.

- Molecule 3: DNA polymerase alpha catalytic subunit A





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.41Å 142.63Å 175.25Å 90.00° 102.33° 90.00°	Depositor
Resolution (Å)	31.90 – 2.50 31.90 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (31.90-2.50) 99.8 (31.90-2.50)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.59 (at 2.51Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.191 , 0.218 0.215 , 0.236	Depositor DCC
$R_{free}$ test set	7082 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	49.6	Xtrriage
Anisotropy	0.187	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 61.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.015 for h,-k,-h-l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	20656	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% 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 i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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	1.02	1/3537 (0.0%)	0.95	3/4801 (0.1%)
1	C	0.94	2/3537 (0.1%)	0.93	3/4801 (0.1%)
1	E	0.85	0/3537	0.88	1/4801 (0.0%)
1	G	1.02	4/3537 (0.1%)	0.98	5/4801 (0.1%)
3	B	1.01	0/1500	0.96	2/2024 (0.1%)
3	D	0.78	0/1492	0.91	3/2013 (0.1%)
3	F	0.76	0/1492	0.87	0/2013
3	H	0.83	1/1492 (0.1%)	0.92	1/2013 (0.0%)
All	All	0.93	8/20124 (0.0%)	0.93	18/27267 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	361	THR	CA-CB	7.28	1.63	1.53
1	G	362	VAL	CA-CB	5.60	1.60	1.54
1	G	485	ILE	CA-CB	5.53	1.58	1.54
1	C	623	VAL	CA-CB	5.53	1.60	1.54
3	H	1360	VAL	CA-CB	5.39	1.61	1.54
1	G	564	ILE	CA-CB	5.39	1.60	1.54
1	A	623	VAL	CA-CB	5.38	1.60	1.54
1	G	361	THR	CA-CB	5.05	1.60	1.53

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	692	HIS	N-CA-C	-7.78	99.77	110.35
1	A	692	HIS	N-CA-C	-6.80	100.37	110.23
1	G	578	ILE	CB-CA-C	-6.71	100.62	110.62
3	H	1349	ASP	CB-CA-C	-6.37	100.17	110.74
1	G	692	HIS	N-CA-C	-6.28	101.13	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1349	ASP	CB-CA-C	-6.17	100.49	110.74
1	C	692	HIS	N-CA-C	-6.02	101.50	110.23
1	G	692	HIS	CA-C-N	-5.98	114.95	123.20
1	G	692	HIS	C-N-CA	-5.98	114.95	123.20
3	D	1411	LEU	CA-C-N	5.89	125.57	119.56
3	D	1411	LEU	C-N-CA	5.89	125.57	119.56
3	D	1349	ASP	CB-CA-C	-5.75	98.99	110.42
1	C	692	HIS	CA-C-N	-5.62	115.49	123.03
1	C	692	HIS	C-N-CA	-5.62	115.49	123.03
1	G	608	SER	N-CA-C	5.59	115.62	108.24
1	A	692	HIS	CA-C-N	-5.39	115.76	123.20
1	A	692	HIS	C-N-CA	-5.39	115.76	123.20
3	B	1369	ASN	CB-CA-C	-5.39	102.17	110.26

There are no chirality outliers.

There are no planarity outliers.

## 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	3458	0	3444	22	0
1	C	3458	0	3444	37	0
1	E	3458	0	3444	49	0
1	G	3458	0	3444	30	0
2	I	15	0	5	0	0
2	J	15	0	5	0	0
2	K	15	0	5	0	0
2	L	15	0	5	0	0
3	B	1471	0	1422	11	0
3	D	1463	0	1419	10	0
3	F	1463	0	1419	17	0
3	H	1463	0	1419	13	0
4	A	65	0	0	1	0
4	B	30	0	0	0	0
4	C	55	0	0	1	0
4	D	20	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	60	0	0	1	0
4	F	20	0	0	0	0
4	G	55	0	0	1	0
4	H	20	0	0	0	0
5	B	2	0	0	0	0
5	D	2	0	0	0	0
5	F	2	0	0	0	0
5	H	2	0	0	0	0
6	A	135	0	0	1	0
6	B	79	0	0	0	0
6	C	106	0	0	1	0
6	D	13	0	0	0	0
6	E	65	0	0	0	0
6	F	8	0	0	0	0
6	G	138	0	0	1	0
6	H	27	0	0	0	0
All	All	20656	0	19475	175	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 4.

All (175) 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:E:374:PRO:HB2	1:E:530:TYR:CE2	1.48	1.49
1:E:374:PRO:CB	1:E:530:TYR:CE2	2.01	1.42
1:A:399[B]:CYS:SG	1:A:652:PRO:HG2	1.87	1.13
1:E:374:PRO:CG	1:E:530:TYR:CD2	2.37	1.08
1:E:374:PRO:HG3	1:E:530:TYR:CD2	1.89	1.07
1:G:399[B]:CYS:SG	1:G:652:PRO:HG2	2.00	0.99
1:E:374:PRO:HB3	1:E:530:TYR:CE2	1.96	0.97
1:C:474:LYS:NZ	6:C:807:HOH:O	1.67	0.96
1:E:374:PRO:HB2	1:E:530:TYR:HE2	0.81	0.93
1:E:374:PRO:CB	1:E:530:TYR:CD2	2.55	0.90
1:E:399[B]:CYS:SG	1:E:652:PRO:HG2	2.13	0.88
1:G:250:MET:HE3	3:H:1452:CYS:HB2	1.59	0.84
1:E:272:ILE:HD11	1:E:368:LEU:HD23	1.60	0.83
1:E:570:TYR:HE1	1:E:631:MET:HE2	1.44	0.82
1:C:399[B]:CYS:SG	1:C:652:PRO:HG2	2.20	0.81
1:C:570:TYR:CE1	1:C:631:MET:HE2	2.17	0.79
3:B:1436:GLU:O	3:B:1440:THR:HG23	1.82	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399[B]:CYS:SG	1:A:652:PRO:CG	2.70	0.76
1:E:570:TYR:CE1	1:E:631:MET:HE2	2.20	0.76
1:G:293:GLU:OE1	1:G:351:LYS:NZ	2.19	0.75
1:C:250:MET:HE3	3:D:1452:CYS:HB2	1.69	0.74
1:E:374:PRO:CG	1:E:530:TYR:HD2	2.00	0.73
3:B:1284:GLU:HG2	3:B:1293:ARG:NH2	2.04	0.72
1:C:570:TYR:HE1	1:C:631:MET:HE2	1.55	0.72
1:E:307:TYR:HD1	1:E:308:ASP:O	1.74	0.69
3:H:1436:GLU:O	3:H:1440:THR:HG23	1.92	0.69
1:E:250:MET:HE3	3:F:1452:CYS:HB2	1.75	0.68
1:G:396:ILE:HD11	1:G:424:VAL:HG11	1.76	0.68
1:G:399[B]:CYS:SG	1:G:652:PRO:CG	2.79	0.68
1:E:399[B]:CYS:SG	1:E:652:PRO:CG	2.83	0.66
1:C:456:THR:O	1:C:467:LYS:HE3	1.99	0.63
1:E:307:TYR:CD1	1:E:308:ASP:O	2.52	0.62
1:E:272:ILE:HD11	1:E:368:LEU:CD2	2.29	0.62
3:B:1369:ASN:O	3:B:1370:ASP:C	2.44	0.61
3:H:1295:PRO:HB2	3:H:1409:ILE:HD13	1.84	0.59
1:A:661:ASN:ND2	4:A:50:SO4:O1	2.34	0.59
3:H:1438:MET:HA	3:H:1438:MET:HE2	1.86	0.58
1:C:292:SER:OG	4:C:69:SO4:S	2.62	0.57
1:G:248:ARG:HD2	1:G:616:TYR:CZ	2.41	0.56
1:E:456:THR:O	1:E:467:LYS:HE3	2.05	0.56
3:H:1369:ASN:O	3:H:1370:ASP:C	2.47	0.56
3:D:1369:ASN:O	3:D:1370:ASP:C	2.48	0.56
1:C:371:PRO:HG2	1:C:627:SER:HB3	1.88	0.56
1:G:337:VAL:HG11	1:G:365:ILE:HD11	1.87	0.55
1:G:674:ASP:HB3	1:G:677:ASP:HB2	1.87	0.55
1:E:448:LEU:HD13	3:F:1324:LEU:HG	1.88	0.54
1:E:371:PRO:HG2	1:E:627:SER:HB3	1.88	0.54
1:C:249:THR:HG23	1:C:251:ARG:HG3	1.90	0.53
1:G:284:ALA:HB1	6:G:1105:HOH:O	2.09	0.53
3:D:1436:GLU:O	3:D:1440:THR:HG23	2.10	0.52
3:D:1284:GLU:HG2	3:D:1293:ARG:NH2	2.24	0.52
1:G:659:THR:OG1	4:G:56:SO4:O1	2.25	0.52
3:H:1355:ILE:HD13	3:H:1369:ASN:OD1	2.09	0.52
3:F:1295:PRO:HB2	3:F:1409:ILE:HD13	1.92	0.51
3:H:1341:TYR:OH	3:H:1382:ASP:HB3	2.09	0.51
1:E:500:GLN:HB3	1:E:520:ASN:HB3	1.91	0.51
1:G:610:ALA:O	1:G:611:ASP:C	2.53	0.51
1:A:272:ILE:HD11	1:A:368:LEU:HD23	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:311:LEU:CD1	1:G:344:LEU:HD11	2.40	0.51
1:C:465:PHE:CE2	1:C:508:LEU:HD22	2.47	0.50
1:E:574:PHE:HA	1:E:575:PRO:C	2.37	0.49
1:C:443:ILE:HD13	1:C:448:LEU:HD21	1.95	0.49
1:G:657:ARG:HD2	1:G:662:ARG:O	2.13	0.48
3:D:1284:GLU:HG2	3:D:1293:ARG:CZ	2.43	0.48
1:G:456:THR:O	1:G:467:LYS:HE3	2.12	0.48
1:A:312:ASN:HB2	1:A:313:PRO:CD	2.44	0.48
1:C:628:PRO:HG3	1:C:631:MET:HE3	1.95	0.48
1:G:342:PHE:HA	1:G:346:GLN:OE1	2.12	0.48
1:E:498:TYR:CD2	1:E:536:VAL:CG2	2.97	0.48
1:E:483:VAL:HG13	1:E:518:MET:HG2	1.95	0.48
1:E:540:LYS:HD2	1:E:636:GLU:CD	2.38	0.48
1:E:250:MET:HE3	3:F:1452:CYS:CB	2.42	0.48
1:C:365:ILE:O	1:C:367:PRO:HD3	2.14	0.47
1:A:488:THR:HG23	6:A:753:HOH:O	2.13	0.47
1:C:248:ARG:HD2	1:C:616:TYR:CE2	2.49	0.47
3:F:1369:ASN:O	3:F:1370:ASP:C	2.57	0.47
1:C:682:LEU:HD12	1:C:683:VAL:N	2.30	0.47
3:D:1412:PRO:HA	3:D:1417:TYR:CG	2.50	0.47
1:C:376:SER:OG	1:C:692:HIS:NE2	2.38	0.47
3:F:1438:MET:HA	3:F:1438:MET:HE2	1.96	0.47
1:C:574:PHE:HA	1:C:575:PRO:C	2.40	0.46
3:F:1310:ASN:OD1	3:F:1310:ASN:N	2.48	0.46
1:A:285:ASP:OD2	1:A:328:ARG:NH2	2.48	0.46
1:E:374:PRO:HB3	1:E:530:TYR:CZ	2.46	0.46
1:G:505:ARG:CZ	1:G:512:LYS:HB2	2.44	0.46
1:C:249:THR:CG2	1:C:251:ARG:HG3	2.46	0.46
1:C:578:ILE:HD11	3:D:1343:ALA:HB1	1.98	0.46
1:C:498:TYR:CD2	1:C:536:VAL:CG2	2.98	0.46
3:H:1445:VAL:HG12	3:H:1449:LEU:HD12	1.98	0.46
3:H:1402:LYS:HD2	3:H:1428:LYS:HD2	1.97	0.46
1:C:561:SER:HB2	1:C:644:VAL:HG11	1.97	0.46
3:F:1346:LEU:HD23	3:F:1376:MET:HB3	1.97	0.46
1:G:312:ASN:HB2	1:G:313:PRO:CD	2.46	0.46
1:A:456:THR:O	1:A:467:LYS:HE3	2.16	0.46
1:A:677:ASP:C	1:A:677:ASP:OD1	2.59	0.46
1:E:628:PRO:HG2	1:E:631:MET:HE3	1.97	0.46
1:G:268:PHE:CE1	1:G:368:LEU:HD13	2.51	0.45
1:C:302:PRO:HD3	1:C:344:LEU:HD22	1.98	0.45
1:A:682:LEU:HD13	1:A:690:TYR:CZ	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:468:LEU:O	1:C:472:ILE:HD12	2.17	0.45
1:C:470:THR:O	1:C:474:LYS:HG3	2.17	0.45
3:H:1311:GLY:HA2	3:H:1434:ASN:ND2	2.32	0.45
1:C:622:PHE:CZ	1:C:631:MET:HE1	2.52	0.44
1:G:556:ARG:O	1:G:560:VAL:HG23	2.18	0.44
3:D:1349:ASP:HB2	3:D:1375:VAL:H	1.82	0.44
3:H:1311:GLY:HA2	3:H:1434:ASN:HD21	1.82	0.44
3:F:1386:TYR:CE2	3:F:1390:LEU:HD11	2.52	0.44
1:E:312:ASN:HB2	1:E:313:PRO:CD	2.48	0.44
1:C:342:PHE:HA	1:C:346:GLN:OE1	2.18	0.44
1:E:674:ASP:HB2	1:E:677:ASP:HB2	1.99	0.44
1:C:248:ARG:NH2	1:C:495[A]:HIS:HE1	2.16	0.44
1:C:307:TYR:HD1	1:C:308:ASP:O	2.01	0.44
3:F:1284:GLU:HG2	3:F:1293:ARG:NH2	2.32	0.44
3:B:1366:ARG:NH1	1:E:323:MET:HE3	2.33	0.44
1:C:248:ARG:HD2	1:C:616:TYR:CZ	2.53	0.44
1:C:674:ASP:HB3	1:C:677:ASP:OD2	2.18	0.44
1:A:250:MET:HE3	3:B:1452:CYS:HB2	1.99	0.43
1:A:307:TYR:HD1	1:A:308:ASP:O	2.01	0.43
1:E:268:PHE:CE1	1:E:368:LEU:HD13	2.54	0.43
1:E:342:PHE:HA	1:E:346:GLN:OE1	2.18	0.43
1:A:500:GLN:HB3	1:A:520:ASN:HB3	2.00	0.43
1:C:578:ILE:HD13	1:C:578:ILE:HG21	1.76	0.43
1:A:574:PHE:HA	1:A:575:PRO:C	2.43	0.43
3:B:1366:ARG:HH11	1:E:323:MET:HE3	1.83	0.43
3:F:1300:VAL:HA	3:F:1422:LEU:HD12	2.00	0.43
1:E:628:PRO:CG	1:E:631:MET:HE3	2.48	0.43
3:F:1334:ILE:HD11	3:F:1445:VAL:HG22	2.00	0.43
3:F:1423:THR:OG1	3:F:1426:SER:OG	2.25	0.43
1:C:279:SER:N	1:C:282:ASP:OD2	2.51	0.43
1:E:392:SER:HB2	1:E:670:VAL:O	2.19	0.42
1:A:259:ASP:OD2	1:E:259:ASP:OD2	2.37	0.42
1:A:333:ASP:HB3	1:A:361:THR:HA	2.00	0.42
1:C:312:ASN:HB2	1:C:313:PRO:CD	2.49	0.42
1:E:481:GLN:HE21	1:E:516:LYS:HG3	1.85	0.42
1:A:578:ILE:HD11	3:B:1343:ALA:HB1	2.01	0.42
1:C:610:ALA:O	1:C:611:ASP:C	2.61	0.42
1:A:311:LEU:HD11	1:A:344:LEU:HD11	2.01	0.42
3:D:1295:PRO:HB2	3:D:1409:ILE:HD13	2.02	0.42
1:E:374:PRO:HG2	1:E:530:TYR:HD2	1.81	0.42
1:G:574:PHE:HA	1:G:575:PRO:C	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:1416:ASP:O	3:F:1416:ASP:CG	2.62	0.42
3:H:1349:ASP:HB2	3:H:1375:VAL:H	1.85	0.42
1:C:323:MET:HE2	1:C:323:MET:HB3	1.79	0.41
1:E:323:MET:HB3	1:E:323:MET:HE2	1.80	0.41
1:G:340:LEU:HG	1:G:547:LYS:HB2	2.01	0.41
1:G:540:LYS:HD2	1:G:636:GLU:CD	2.44	0.41
3:H:1386:TYR:CZ	3:H:1390:LEU:HD11	2.55	0.41
1:A:307:TYR:CD1	1:A:308:ASP:O	2.73	0.41
1:A:440:HIS:HB3	1:A:443:ILE:HD12	2.02	0.41
1:C:268:PHE:CE1	1:C:368:LEU:HD13	2.54	0.41
1:A:248:ARG:HD2	1:A:616:TYR:CE2	2.55	0.41
1:G:311:LEU:HD13	1:G:344:LEU:HD11	2.03	0.41
1:E:249:THR:HA	3:F:1451:ASP:O	2.20	0.41
1:G:312:ASN:HB2	1:G:313:PRO:HD2	2.01	0.41
1:G:340:LEU:HD12	1:G:340:LEU:C	2.46	0.41
1:G:385:GLN:HG3	1:G:672:CYS:SG	2.61	0.41
1:G:311:LEU:CD1	1:G:344:LEU:CD1	2.98	0.41
1:E:506:LYS:HE2	4:E:26:SO4:O2	2.20	0.41
1:G:323:MET:HE2	1:G:323:MET:HB3	1.79	0.41
1:A:248:ARG:HD2	1:A:616:TYR:CZ	2.56	0.41
3:B:1327:THR:HB	3:B:1444:VAL:HG21	2.02	0.41
3:D:1417:TYR:CZ	3:D:1421:GLN:NE2	2.89	0.41
1:E:562:GLU:O	1:E:566:GLN:HG3	2.21	0.41
3:B:1346:LEU:HD11	3:B:1360:VAL:HG22	2.03	0.41
1:E:419:SER:O	1:E:423:GLU:HB2	2.21	0.41
3:B:1366:ARG:HH11	1:E:323:MET:CE	2.34	0.40
1:G:272:ILE:HD11	1:G:368:LEU:HD22	2.03	0.40
3:B:1349:ASP:HB2	3:B:1375:VAL:H	1.85	0.40
1:E:333:ASP:OD2	1:E:361:THR:OG1	2.37	0.40
1:E:445:SER:O	3:F:1329:GLN:NE2	2.53	0.40
1:E:610:ALA:O	1:E:611:ASP:C	2.63	0.40
3:F:1349:ASP:HB2	3:F:1375:VAL:H	1.86	0.40
1:G:248:ARG:HD2	1:G:616:TYR:CE2	2.56	0.40
1:C:303:ASP:OD2	1:C:331:ARG:NH1	2.53	0.40
1:E:556:ARG:O	1:E:560:VAL:HG23	2.21	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	432/460 (94%)	421 (98%)	10 (2%)	1 (0%)	43	63
1	C	432/460 (94%)	419 (97%)	12 (3%)	1 (0%)	43	63
1	E	432/460 (94%)	421 (98%)	10 (2%)	1 (0%)	43	63
1	G	432/460 (94%)	421 (98%)	10 (2%)	1 (0%)	43	63
3	B	179/206 (87%)	173 (97%)	6 (3%)	0	100	100
3	D	178/206 (86%)	171 (96%)	7 (4%)	0	100	100
3	F	178/206 (86%)	173 (97%)	5 (3%)	0	100	100
3	H	178/206 (86%)	172 (97%)	6 (3%)	0	100	100
All	All	2441/2664 (92%)	2371 (97%)	66 (3%)	4 (0%)	43	63

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	391	SER
1	A	391	SER
1	C	391	SER
1	E	391	SER

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	392/416 (94%)	385 (98%)	7 (2%)	51	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	392/416 (94%)	386 (98%)	6 (2%)	57 80
1	E	392/416 (94%)	386 (98%)	6 (2%)	57 80
1	G	392/416 (94%)	383 (98%)	9 (2%)	44 72
3	B	169/193 (88%)	161 (95%)	8 (5%)	23 47
3	D	168/193 (87%)	162 (96%)	6 (4%)	31 58
3	F	168/193 (87%)	160 (95%)	8 (5%)	23 46
3	H	168/193 (87%)	164 (98%)	4 (2%)	43 70
All	All	2241/2436 (92%)	2187 (98%)	54 (2%)	43 70

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	267	SER
1	A	293	GLU
1	A	326	VAL
1	A	358	ASP
1	A	443	ILE
1	A	578	ILE
1	A	677	ASP
3	B	1273	ASP
3	B	1292	LYS
3	B	1293	ARG
3	B	1310	ASN
3	B	1356	VAL
3	B	1409	ILE
3	B	1440	THR
3	B	1451	ASP
1	C	292	SER
1	C	326	VAL
1	C	358	ASP
1	C	392	SER
1	C	487	SER
1	C	682	LEU
3	D	1273	ASP
3	D	1284	GLU
3	D	1353	CYS
3	D	1356	VAL
3	D	1369	ASN
3	D	1452	CYS
1	E	292	SER

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Mol	Chain	Res	Type
1	E	308	ASP
1	E	477	SER
1	E	492	ILE
1	E	580	THR
1	E	692	HIS
3	F	1346	LEU
3	F	1349	ASP
3	F	1356	VAL
3	F	1369	ASN
3	F	1370	ASP
3	F	1399	GLU
3	F	1414	ASP
3	F	1452	CYS
1	G	293	GLU
1	G	344	LEU
1	G	379	GLN
1	G	419	SER
1	G	487	SER
1	G	522	SER
1	G	525	GLN
1	G	553	SER
1	G	692	HIS
3	H	1273	ASP
3	H	1284	GLU
3	H	1292	LYS
3	H	1356	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	275	HIS
1	A	372	ASN
1	A	422	ASN
1	A	509	GLN
3	B	1433	GLN
1	C	382	GLN
1	C	606	HIS
3	D	1421	GLN
3	D	1433	GLN
1	E	255	GLN
1	E	289	GLN
1	E	363	ASN

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Mol	Chain	Res	Type
1	E	481	GLN
1	E	514	ASN
1	E	667	GLN
3	F	1329	GLN
3	F	1450	ASN
1	G	372	ASN
3	H	1433	GLN
3	H	1434	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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

Of 73 ligands modelled in this entry, 8 are monoatomic - leaving 65 for Mogul analysis.

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	E	22	-	4,4,4	0.25	0	6,6,6	0.29	0
4	SO4	E	45	-	4,4,4	0.31	0	6,6,6	0.12	0
4	SO4	E	58	-	4,4,4	0.29	0	6,6,6	0.18	0
4	SO4	G	55	-	4,4,4	0.37	0	6,6,6	0.45	0
4	SO4	B	62	-	4,4,4	0.36	0	6,6,6	0.58	0
4	SO4	E	24	-	4,4,4	0.22	0	6,6,6	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	SO4	C	53	-	4,4,4	0.29	0	6,6,6	0.35	0
4	SO4	A	49	-	4,4,4	0.25	0	6,6,6	0.49	0
4	SO4	C	9	-	4,4,4	0.28	0	6,6,6	0.18	0
4	SO4	H	65	-	4,4,4	0.31	0	6,6,6	0.48	0
4	SO4	C	11	-	4,4,4	0.24	0	6,6,6	0.55	0
4	SO4	E	44	-	4,4,4	0.27	0	6,6,6	0.19	0
4	SO4	B	37	-	4,4,4	0.25	0	6,6,6	0.24	0
4	SO4	G	1	-	4,4,4	0.25	0	6,6,6	0.29	0
4	SO4	D	39	-	4,4,4	0.23	0	6,6,6	0.25	0
4	SO4	G	17	-	4,4,4	0.28	0	6,6,6	0.34	0
4	SO4	G	51	-	4,4,4	0.26	0	6,6,6	0.22	0
4	SO4	A	30	-	4,4,4	0.18	0	6,6,6	0.64	0
4	SO4	E	20	-	4,4,4	0.24	0	6,6,6	0.21	0
4	SO4	D	63	-	4,4,4	0.32	0	6,6,6	0.25	0
4	SO4	A	3	-	4,4,4	0.30	0	6,6,6	0.53	0
4	SO4	B	38	-	4,4,4	0.24	0	6,6,6	0.23	0
4	SO4	E	26	-	4,4,4	0.33	0	6,6,6	0.38	0
4	SO4	C	15	-	4,4,4	0.33	0	6,6,6	0.60	0
4	SO4	B	68	-	4,4,4	0.38	0	6,6,6	0.38	0
4	SO4	A	50	-	4,4,4	0.20	0	6,6,6	0.24	0
4	SO4	A	5	-	4,4,4	0.32	0	6,6,6	0.21	0
4	SO4	C	46	-	4,4,4	0.30	0	6,6,6	0.20	0
4	SO4	E	4	-	4,4,4	0.23	0	6,6,6	0.19	0
4	SO4	E	33	-	4,4,4	0.22	0	6,6,6	0.37	0
4	SO4	F	41	-	4,4,4	0.25	0	6,6,6	0.13	0
4	SO4	G	27	-	4,4,4	0.27	0	6,6,6	0.42	0
4	SO4	A	12	-	4,4,4	0.27	0	6,6,6	0.29	0
4	SO4	G	56	-	4,4,4	0.27	0	6,6,6	0.25	0
4	SO4	E	54	-	4,4,4	0.26	0	6,6,6	0.21	0
4	SO4	A	31	-	4,4,4	0.33	0	6,6,6	0.39	0
4	SO4	G	18	-	4,4,4	0.24	0	6,6,6	0.52	0
4	SO4	B	57	-	4,4,4	0.31	0	6,6,6	0.23	0
4	SO4	D	40	-	4,4,4	0.26	0	6,6,6	0.17	0
4	SO4	G	42	-	4,4,4	0.29	0	6,6,6	0.24	0
4	SO4	G	7	-	4,4,4	0.28	0	6,6,6	0.36	0
4	SO4	G	16	-	4,4,4	0.24	0	6,6,6	0.26	0
4	SO4	A	32	-	4,4,4	0.29	0	6,6,6	0.15	0
4	SO4	A	34	-	4,4,4	0.25	0	6,6,6	0.19	0
4	SO4	C	43	-	4,4,4	0.26	0	6,6,6	0.20	0
4	SO4	H	61	-	4,4,4	0.25	0	6,6,6	0.25	0
4	SO4	C	10	-	4,4,4	0.24	0	6,6,6	0.27	0
4	SO4	E	25	-	4,4,4	0.20	0	6,6,6	0.21	0
4	SO4	C	8	-	4,4,4	0.39	0	6,6,6	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	SO4	G	2	-	4,4,4	0.26	0	6,6,6	0.31	0
4	SO4	B	59	-	4,4,4	0.31	0	6,6,6	0.45	0
4	SO4	C	69	-	4,4,4	0.74	0	6,6,6	0.35	0
4	SO4	A	48	-	4,4,4	0.18	0	6,6,6	0.55	0
4	SO4	C	52	-	4,4,4	0.27	0	6,6,6	0.29	0
4	SO4	D	67	-	4,4,4	0.30	0	6,6,6	0.36	0
4	SO4	F	64	-	4,4,4	0.33	0	6,6,6	0.16	0
4	SO4	F	28	-	4,4,4	0.29	0	6,6,6	0.18	0
4	SO4	C	6	-	4,4,4	0.23	0	6,6,6	0.19	0
4	SO4	A	13	-	4,4,4	0.20	0	6,6,6	0.53	0
4	SO4	A	35	-	4,4,4	0.26	0	6,6,6	0.22	0
4	SO4	A	47	-	4,4,4	0.32	0	6,6,6	0.27	0
4	SO4	E	23	-	4,4,4	0.32	0	6,6,6	0.23	0
4	SO4	H	19	-	4,4,4	0.17	0	6,6,6	0.22	0
4	SO4	F	66	-	4,4,4	0.31	0	6,6,6	0.32	0
4	SO4	H	60	-	4,4,4	0.29	0	6,6,6	0.28	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	26	SO4	1	0
4	A	50	SO4	1	0
4	G	56	SO4	1	0
4	C	69	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	433/460 (94%)	-0.07	11 (2%) 58 54	7, 37, 95, 141	3 (0%)
1	C	433/460 (94%)	0.31	32 (7%) 20 18	13, 49, 109, 165	3 (0%)
1	E	433/460 (94%)	1.10	112 (25%) 1 1	19, 67, 153, 211	3 (0%)
1	G	433/460 (94%)	-0.01	23 (5%) 32 28	11, 38, 94, 143	3 (0%)
2	I	0/3	-	-	-	-
2	J	0/3	-	-	-	-
2	K	0/3	-	-	-	-
2	L	0/3	-	-	-	-
3	B	180/206 (87%)	0.08	7 (3%) 43 38	19, 46, 77, 87	1 (0%)
3	D	180/206 (87%)	1.57	63 (35%) 1 1	35, 82, 176, 213	0
3	F	180/206 (87%)	2.49	104 (57%) 0 0	50, 103, 210, 256	0
3	H	180/206 (87%)	1.04	44 (24%) 2 1	30, 68, 151, 189	0
All	All	2452/2676 (91%)	0.61	396 (16%) 4 3	7, 52, 139, 256	13 (0%)

All (396) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	1451	ASP	8.2
3	F	1433	GLN	7.8
3	F	1427	ILE	6.7
3	F	1300	VAL	6.4
3	F	1431	THR	6.2
1	E	676	GLU	6.2
3	F	1309	TYR	6.1
1	E	677	ASP	6.0
3	F	1422	LEU	5.9
1	E	291	GLN	5.9
1	E	675	LEU	5.8
3	F	1452	CYS	5.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	B	1451	ASP	5.5
3	F	1410	TYR	5.3
3	F	1426	SER	5.2
3	F	1290	CYS	5.2
3	H	1422	LEU	5.1
1	E	292	SER	5.0
3	F	1429	ALA	5.0
3	F	1423	THR	5.0
3	F	1412	PRO	5.0
3	F	1304	TYR	5.0
3	F	1411	LEU	5.0
3	F	1421	GLN	5.0
3	D	1452	CYS	4.9
3	F	1305	TYR	4.9
1	E	310	PHE	4.9
3	D	1412	PRO	4.9
3	D	1422	LEU	4.8
3	F	1402	LYS	4.8
3	D	1411	LEU	4.8
1	E	679	LYS	4.7
3	D	1427	ILE	4.7
3	F	1409	ILE	4.7
1	C	678	GLY	4.7
1	E	336	GLN	4.6
1	E	678	GLY	4.6
3	F	1301	SER	4.6
3	F	1294	PHE	4.6
3	F	1417	TYR	4.5
3	D	1451	ASP	4.5
3	D	1274	VAL	4.5
3	H	1274	VAL	4.5
1	E	549	GLY	4.4
3	D	1404	GLN	4.4
3	F	1424	GLU	4.4
3	D	1415	LEU	4.4
1	G	579	ARG	4.4
3	F	1428	LYS	4.4
3	F	1302	SER	4.3
1	E	680	LEU	4.3
3	F	1415	LEU	4.3
3	F	1425	SER	4.3
3	F	1404	GLN	4.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	F	1307	VAL	4.2
3	F	1406	LEU	4.2
3	H	1415	LEU	4.2
1	E	363	ASN	4.2
3	F	1430	LEU	4.2
3	F	1299	ILE	4.1
1	E	689	VAL	4.1
3	F	1292	LYS	4.1
3	H	1451	ASP	4.1
1	E	335	SER	4.1
3	F	1405	GLU	4.1
3	D	1417	TYR	4.1
1	E	337	VAL	4.1
1	C	688	PRO	4.1
3	F	1297	GLY	4.1
3	D	1300	VAL	4.1
1	C	249	THR	4.0
1	E	289	GLN	4.0
1	G	310	PHE	4.0
3	F	1318	GLU	4.0
1	E	555	TYR	3.9
3	F	1407	LYS	3.9
1	E	355	ALA	3.9
1	E	688	PRO	3.9
1	E	530	TYR	3.8
1	E	673	PRO	3.8
3	F	1296	PHE	3.8
1	C	684	GLU	3.8
3	F	1420	GLU	3.8
3	D	1431	THR	3.8
3	D	1304	TYR	3.8
1	E	389	GLU	3.8
1	E	674	ASP	3.8
1	E	682	LEU	3.8
1	E	358	ASP	3.7
1	E	361	THR	3.7
3	F	1314	CYS	3.7
3	H	1412	PRO	3.7
3	F	1313	GLN	3.6
3	F	1316	HIS	3.6
3	F	1277	PHE	3.6
3	F	1312	LEU	3.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	E	356	ASN	3.6
3	D	1303	ASN	3.5
1	E	359	TYR	3.5
1	G	682	LEU	3.5
1	E	390	GLY	3.5
3	F	1386	TYR	3.5
3	F	1352	THR	3.5
1	E	313	PRO	3.5
1	E	357	GLY	3.5
3	F	1315	LYS	3.5
3	F	1298	GLY	3.4
3	D	1406	LEU	3.4
3	F	1408	PRO	3.4
1	C	685	GLY	3.4
1	E	607	ILE	3.4
3	D	1309	TYR	3.4
3	H	1419	LYS	3.4
3	D	1424	GLU	3.4
1	C	310	PHE	3.3
1	E	338	ASN	3.3
3	F	1403	LYS	3.3
1	E	546	ILE	3.3
3	F	1450	ASN	3.3
3	F	1280	THR	3.3
3	D	1419	LYS	3.3
3	F	1347	GLN	3.3
1	E	387	ASN	3.3
1	A	682	LEU	3.3
3	F	1306	ARG	3.3
1	C	683	VAL	3.3
3	D	1423	THR	3.3
1	G	516	LYS	3.3
1	E	308	ASP	3.2
1	C	248	ARG	3.2
3	H	1417	TYR	3.2
3	D	1398	CYS	3.2
3	F	1432	GLU	3.2
3	D	1409	ILE	3.2
1	C	680	LEU	3.2
3	H	1452	CYS	3.2
3	F	1400	LYS	3.2
1	E	249	THR	3.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	F	1351	SER	3.2
3	D	1273	ASP	3.2
3	H	1416	ASP	3.2
3	D	1410	TYR	3.2
3	H	1410	TYR	3.2
1	E	551	THR	3.2
1	E	698	ALA	3.1
1	E	364	SER	3.1
3	D	1301	SER	3.1
1	E	683	VAL	3.1
3	H	1427	ILE	3.1
3	B	1420	GLU	3.1
3	D	1408	PRO	3.1
3	D	1425	SER	3.1
1	E	340	LEU	3.1
3	F	1274	VAL	3.1
3	D	1299	ILE	3.1
1	E	362	VAL	3.1
1	A	310	PHE	3.1
3	F	1368	LEU	3.1
1	E	365	ILE	3.1
3	D	1420	GLU	3.0
3	B	1452	CYS	3.0
3	F	1295	PRO	3.0
3	F	1320	LEU	3.0
1	A	251	ARG	3.0
3	F	1435	ARG	3.0
1	E	288	ILE	3.0
1	C	307	TYR	3.0
3	F	1418	PRO	3.0
3	F	1321	PHE	3.0
3	F	1293	ARG	3.0
3	H	1426	SER	3.0
1	G	685	GLY	3.0
1	C	580	THR	3.0
1	E	690	TYR	3.0
1	E	547	LYS	3.0
3	H	1428	LYS	3.0
1	E	278	LEU	2.9
3	F	1303	ASN	2.9
3	H	1420	GLU	2.9
1	C	679	LYS	2.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	D	1426	SER	2.9
1	E	309	LYS	2.9
3	D	1403	LYS	2.9
1	C	682	LEU	2.9
1	E	334	LEU	2.9
3	F	1285	LEU	2.9
3	F	1395	LEU	2.9
1	C	308	ASP	2.9
3	H	1425	SER	2.9
3	F	1317	CYS	2.9
1	E	311	LEU	2.9
3	H	1411	LEU	2.9
1	C	251	ARG	2.8
1	C	689	VAL	2.8
1	E	545	VAL	2.8
1	C	681	THR	2.8
1	C	675	LEU	2.8
1	E	392	SER	2.8
3	H	1303	ASN	2.8
1	E	382	GLN	2.8
3	F	1370	ASP	2.8
3	F	1286	SER	2.8
1	E	381	LEU	2.8
3	D	1429	ALA	2.8
1	E	293	GLU	2.8
3	D	1428	LYS	2.8
3	F	1413	ASP	2.8
3	D	1277	PHE	2.8
3	D	1297	GLY	2.8
1	G	292	SER	2.8
3	F	1310	ASN	2.8
3	F	1369	ASN	2.8
3	H	1450	ASN	2.8
3	D	1320	LEU	2.8
3	D	1402	LYS	2.8
3	H	1402	LYS	2.8
3	D	1305	TYR	2.7
3	D	1450	ASN	2.7
3	F	1283	LEU	2.7
3	H	1404	GLN	2.7
1	G	683	VAL	2.7
1	C	386	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
3	H	1275	GLU	2.7
1	G	495[A]	HIS	2.7
1	G	688	PRO	2.7
1	A	307	TYR	2.7
1	G	307	TYR	2.7
3	D	1302	SER	2.7
3	D	1430	LEU	2.7
3	F	1419	LYS	2.7
1	E	386	ALA	2.7
3	D	1435	ARG	2.7
1	E	423	GLU	2.7
3	D	1316	HIS	2.7
1	E	660	GLY	2.7
1	E	290	SER	2.7
1	E	691	LEU	2.7
1	E	307	TYR	2.7
1	E	611	ASP	2.6
1	A	309	LYS	2.6
1	C	309	LYS	2.6
3	H	1403	LYS	2.6
3	D	1401	ASN	2.6
1	E	643	VAL	2.6
1	G	684	GLU	2.6
1	E	353	LYS	2.6
3	H	1292	LYS	2.6
3	D	1307	VAL	2.6
1	A	688	PRO	2.6
1	E	681	THR	2.6
1	E	248	ARG	2.6
1	E	333	ASP	2.6
3	F	1279	ASP	2.6
1	E	388	LEU	2.6
3	F	1275	GLU	2.6
3	F	1308	SER	2.6
1	A	580	THR	2.6
1	E	251	ARG	2.5
1	E	697	ARG	2.5
3	D	1294	PHE	2.5
1	E	671	GLN	2.5
1	E	552	SER	2.5
1	G	580	THR	2.5
3	H	1293	ARG	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	D	1413	ASP	2.5
3	H	1430	LEU	2.5
1	E	375	VAL	2.5
1	G	249	THR	2.5
1	E	331	ARG	2.5
3	D	1407	LYS	2.5
3	F	1348	CYS	2.5
3	F	1288	PRO	2.5
1	A	308	ASP	2.5
1	G	679	LYS	2.5
1	C	356	ASN	2.5
1	E	391	SER	2.5
3	D	1317	CYS	2.4
1	A	686	GLU	2.4
1	G	678	GLY	2.4
3	D	1405	GLU	2.4
1	E	294	ILE	2.4
3	D	1278	LYS	2.4
3	D	1400	LYS	2.4
1	E	306	THR	2.4
1	C	687	GLU	2.4
1	E	252	GLN	2.4
1	E	665	TYR	2.4
3	F	1346	LEU	2.4
1	C	676	GLU	2.4
3	D	1416	ASP	2.4
3	F	1291	ASP	2.4
3	H	1382	ASP	2.4
3	H	1316	HIS	2.4
1	C	530	TYR	2.4
1	E	360	PHE	2.4
1	E	684	GLU	2.4
3	H	1418	PRO	2.4
1	C	378	SER	2.4
3	H	1273	ASP	2.4
3	H	1304	TYR	2.4
3	F	1281	VAL	2.4
3	H	1424	GLU	2.4
1	E	669	THR	2.3
3	H	1423	THR	2.3
3	D	1314	CYS	2.3
3	F	1287	CYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	370	TYR	2.3
1	E	686	GLU	2.3
1	C	705	SER	2.3
3	D	1286	SER	2.3
3	D	1293	ARG	2.3
3	F	1355	ILE	2.3
3	H	1300	VAL	2.3
1	C	423	GLU	2.3
1	E	305	PRO	2.3
1	E	606	HIS	2.3
3	D	1292	LYS	2.3
1	E	330	VAL	2.3
3	H	1406	LEU	2.3
3	D	1432	GLU	2.3
1	C	555	TYR	2.3
3	F	1282	THR	2.2
3	F	1373	THR	2.2
1	E	685	GLY	2.2
1	G	609	GLY	2.2
1	E	553	SER	2.2
1	C	662	ARG	2.2
1	G	689	VAL	2.2
3	F	1375	VAL	2.2
1	E	312	ASN	2.2
1	E	385	GLN	2.2
1	E	580	THR	2.2
3	H	1431	THR	2.2
3	F	1374	GLY	2.2
1	E	366	LEU	2.2
3	H	1318	GLU	2.2
3	H	1399	GLU	2.2
1	E	699	ARG	2.2
3	F	1276	ARG	2.2
1	E	284	ALA	2.2
1	E	641	ALA	2.2
3	F	1383	LYS	2.2
1	E	672	CYS	2.2
3	H	1421	GLN	2.2
1	E	316	LEU	2.2
1	E	627	SER	2.2
3	H	1315	LYS	2.2
1	C	390	GLY	2.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	E	378	SER	2.2
1	E	354	ASN	2.1
3	B	1450	ASN	2.1
3	D	1386	TYR	2.1
3	H	1409	ILE	2.1
1	E	517	CYS	2.1
3	F	1398	CYS	2.1
3	D	1284	GLU	2.1
3	D	1306	ARG	2.1
1	A	681	THR	2.1
3	D	1312	LEU	2.1
3	B	1386	TYR	2.1
1	G	308	ASP	2.1
1	G	705	SER	2.1
1	G	291	GLN	2.1
3	B	1274	VAL	2.1
3	F	1354	GLY	2.1
1	E	554	ARG	2.1
3	B	1309	TYR	2.1
3	H	1370	ASP	2.1
1	G	606	HIS	2.1
1	E	350	PHE	2.1
1	E	379	GLN	2.1
1	G	675	LEU	2.1
3	F	1437	LEU	2.1
3	F	1311	GLY	2.1
3	D	1318	GLU	2.1
3	H	1299	ILE	2.1
1	E	295	TYR	2.1
3	F	1416	ASP	2.1
1	C	279	SER	2.1
1	E	304	SER	2.1
1	E	367	PRO	2.1
1	E	700	VAL	2.0
1	A	579	ARG	2.0
3	F	1449	LEU	2.0
3	F	1439	GLU	2.0
3	F	1440	THR	2.0
1	G	690	TYR	2.0
3	D	1349	ASP	2.0
3	F	1273	ASP	2.0
1	E	692	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
3	H	1398	CYS	2.0
3	F	1377	ARG	2.0
3	F	1401	ASN	2.0
1	E	703	ILE	2.0
3	H	1279	ASP	2.0
1	C	690	TYR	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 oligosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B	59	5/5	0.40	0.19	120,120,121,122	0
4	SO4	B	38	5/5	0.42	0.12	139,139,139,139	0
4	SO4	A	47	5/5	0.42	0.16	136,137,137,138	0
4	SO4	E	44	5/5	0.49	0.09	148,148,148,148	0
4	SO4	A	34	5/5	0.50	0.14	144,144,145,145	0
4	SO4	E	54	5/5	0.50	0.15	129,129,129,130	0
4	SO4	G	17	5/5	0.50	0.16	122,122,123,123	0
4	SO4	H	60	5/5	0.50	0.14	129,129,130,130	0
4	SO4	G	42	5/5	0.51	0.16	105,106,107,107	0
4	SO4	E	45	5/5	0.53	0.14	140,140,140,141	0
4	SO4	F	28	5/5	0.54	0.14	136,136,137,137	0
4	SO4	F	41	5/5	0.58	0.12	144,144,144,144	0
4	SO4	B	57	5/5	0.60	0.12	123,123,123,124	0
4	SO4	A	31	5/5	0.60	0.14	102,102,103,104	0
4	SO4	C	53	5/5	0.60	0.17	119,119,120,120	0
4	SO4	E	20	5/5	0.60	0.13	117,117,118,118	0
4	SO4	G	56	5/5	0.62	0.12	135,135,135,136	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	SO4	E	26	5/5	0.63	0.12	112,112,113,114	0
4	SO4	A	50	5/5	0.63	0.14	136,136,136,137	0
4	SO4	C	43	5/5	0.64	0.11	120,120,120,121	0
4	SO4	D	39	5/5	0.65	0.09	133,133,134,134	0
4	SO4	G	55	5/5	0.65	0.15	101,103,104,105	0
4	SO4	E	22	5/5	0.66	0.22	121,122,122,123	0
4	SO4	C	46	5/5	0.67	0.13	127,127,128,128	0
4	SO4	D	63	5/5	0.69	0.14	121,122,122,123	0
4	SO4	H	19	5/5	0.69	0.09	123,124,124,124	0
4	SO4	D	40	5/5	0.69	0.10	119,120,120,121	0
4	SO4	C	52	5/5	0.70	0.23	125,125,126,126	0
4	SO4	E	58	5/5	0.70	0.08	123,123,124,124	0
4	SO4	A	49	5/5	0.73	0.14	112,112,112,113	0
4	SO4	B	68	5/5	0.75	0.17	111,112,112,113	0
4	SO4	C	8	5/5	0.75	0.19	93,93,94,94	0
4	SO4	G	18	5/5	0.75	0.12	101,102,102,103	0
4	SO4	C	9	5/5	0.75	0.11	114,114,115,115	0
4	SO4	G	2	5/5	0.76	0.10	106,106,107,107	0
4	SO4	A	13	5/5	0.76	0.11	99,100,101,101	0
4	SO4	A	35	5/5	0.76	0.17	137,137,137,138	0
4	SO4	D	67	5/5	0.76	0.15	117,118,120,120	0
4	SO4	B	37	5/5	0.77	0.11	118,119,120,120	0
4	SO4	G	51	5/5	0.77	0.23	125,126,127,127	0
4	SO4	E	4	5/5	0.77	0.13	123,123,124,124	0
4	SO4	G	27	5/5	0.78	0.26	91,91,92,93	0
4	SO4	H	61	5/5	0.78	0.14	111,111,112,112	0
4	SO4	E	24	5/5	0.79	0.12	105,106,107,107	0
4	SO4	C	11	5/5	0.79	0.10	97,97,98,99	0
4	SO4	E	33	5/5	0.79	0.13	116,117,117,117	0
4	SO4	A	5	5/5	0.79	0.19	96,97,97,98	0
4	SO4	H	65	5/5	0.79	0.15	105,106,106,107	0
4	SO4	A	32	5/5	0.80	0.12	138,139,139,140	0
4	SO4	F	66	5/5	0.80	0.11	121,121,122,122	0
4	SO4	G	16	5/5	0.81	0.11	114,114,115,115	0
4	SO4	A	30	5/5	0.81	0.19	96,97,97,98	0
4	SO4	A	48	5/5	0.81	0.18	98,100,101,102	0
4	SO4	G	7	5/5	0.81	0.17	87,87,88,88	0
4	SO4	A	12	5/5	0.82	0.10	117,117,118,118	0
4	SO4	C	10	5/5	0.82	0.13	128,128,128,129	0
4	SO4	C	15	5/5	0.83	0.23	89,89,90,91	0
4	SO4	C	69	5/5	0.83	0.20	81,82,82,83	0
4	SO4	B	62	5/5	0.83	0.15	97,97,98,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	SO4	E	23	5/5	0.84	0.22	91,92,92,93	0
5	ZN	F	1	1/1	0.84	0.10	72,72,72,72	0
4	SO4	E	25	5/5	0.86	0.11	110,111,111,111	0
4	SO4	F	64	5/5	0.88	0.09	115,115,115,116	0
4	SO4	C	6	5/5	0.91	0.13	120,121,121,121	0
4	SO4	A	3	5/5	0.91	0.18	93,94,95,95	0
4	SO4	G	1	5/5	0.94	0.15	89,90,91,92	0
5	ZN	D	1	1/1	0.95	0.06	70,70,70,70	0
5	ZN	F	2	1/1	0.97	0.04	68,68,68,68	0
5	ZN	B	2	1/1	0.98	0.04	63,63,63,63	0
5	ZN	D	2	1/1	0.98	0.04	66,66,66,66	0
5	ZN	H	1	1/1	0.98	0.04	67,67,67,67	0
5	ZN	H	2	1/1	0.98	0.05	61,61,61,61	0
5	ZN	B	1	1/1	0.99	0.08	59,59,59,59	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.