



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 11:31 PM GMT

PDB ID : 1XCK  
Title : Crystal structure of apo GroEL  
Authors : Bartolucci, C.; Lamba, D.; Grazulis, S.; Manakova, E.; Heumann, H.  
Deposited on : 2004-09-02  
Resolution : 2.92 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  
<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

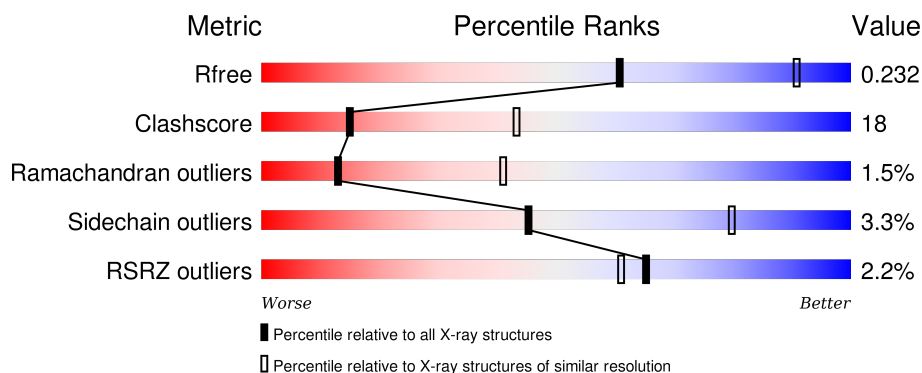
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.92 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.





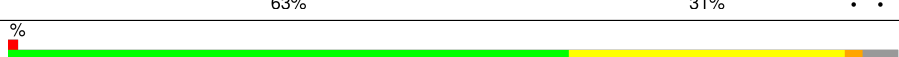

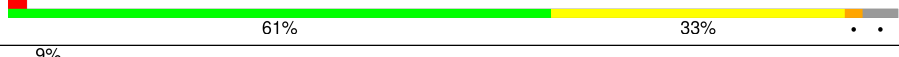
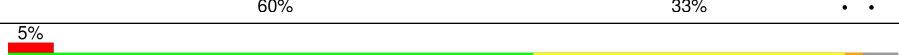
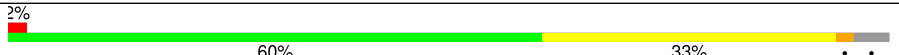


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1643 (2.94-2.90)
Clashscore	102246	1871 (2.94-2.90)
Ramachandran outliers	100387	1824 (2.94-2.90)
Sidechain outliers	100360	1826 (2.94-2.90)
RSRZ outliers	91569	1650 (2.94-2.90)

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	547	<div> <div>%</div> <div> <div></div> <div>66%</div> <div>27%</div> <div>• •</div> </div> </div>
1	B	547	<div> <div>3%</div> <div> <div></div> <div>64%</div> <div>29%</div> <div>• •</div> </div> </div>
1	C	547	<div> <div>2%</div> <div> <div></div> <div>63%</div> <div>30%</div> <div>• •</div> </div> </div>
1	D	547	<div> <div>%</div> <div> <div></div> <div>65%</div> <div>29%</div> <div>• •</div> </div> </div>
1	E	547	<div> <div>%</div> <div> <div></div> <div>65%</div> <div>28%</div> <div>• •</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	547	
1	G	547	
1	H	547	
1	I	547	
1	J	547	
1	K	547	
1	L	547	
1	M	547	
1	N	547	

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	B	1113	-	-	-	X
2	SO4	B	1136	-	-	X	-
2	SO4	C	1101	-	-	-	X
2	SO4	C	1133	-	-	-	X
2	SO4	D	1110	-	-	-	X
2	SO4	D	1128	-	-	-	X
2	SO4	G	1108	-	-	-	X
2	SO4	H	1120	-	-	-	X
2	SO4	I	1119	-	-	-	X
2	SO4	J	1111	-	-	-	X
2	SO4	J	1118	-	-	-	X
2	SO4	L	1116	-	-	-	X
2	SO4	M	1105	-	-	-	X
2	SO4	M	1126	-	-	-	X
3	K	H	3030	-	-	-	X
4	MPD	A	1511	-	-	-	X
4	MPD	B	1510	-	-	-	X
4	MPD	B	1512	-	-	-	X
4	MPD	C	1514	-	-	-	X
4	MPD	D	1508	-	-	-	X
4	MPD	E	1502	-	-	-	X
4	MPD	E	1503	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MPD	E	1504	-	-	-	X
4	MPD	E	1528	-	-	-	X
4	MPD	F	1501	-	-	-	X
4	MPD	F	1520	-	-	-	X
4	MPD	F	1522	-	-	-	X
4	MPD	G	1509	-	-	-	X
4	MPD	G	1519	-	-	-	X
4	MPD	I	1524	-	-	-	X
4	MPD	I	1530	-	-	-	X
4	MPD	J	1529	-	-	-	X
4	MPD	L	1500	-	-	-	X
4	MPD	M	1518	-	-	-	X
4	MPD	N	1515	-	-	-	X
4	MPD	N	1517	-	-	-	X
5	PEG	E	2100	-	-	-	X

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 55301 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 60 kDa chaperonin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	B	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	C	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	D	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	E	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	F	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	G	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	H	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	I	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	J	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	K	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	L	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	M	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	N	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	N	1	Total	O	S	0	0
			5	4	1		
2	M	1	Total	O	S	0	0
			5	4	1		
2	M	1	Total	O	S	0	0
			5	4	1		
2	A	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	D	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		
2	K	1	Total	O	S	0	0
			5	4	1		
2	N	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	K	0	0
			1	1		
3	J	1	Total	K	0	0
			1	1		
3	D	1	Total	K	0	0
			1	1		
3	K	1	Total	K	0	0
			1	1		
3	E	1	Total	K	0	0
			1	1		
3	H	1	Total	K	0	0
			1	1		
3	B	1	Total	K	0	0
			1	1		
3	I	1	Total	K	0	0
			1	1		
3	C	1	Total	K	0	0
			1	1		
3	A	1	Total	K	0	0
			1	1		
3	N	1	Total	K	0	0
			1	1		

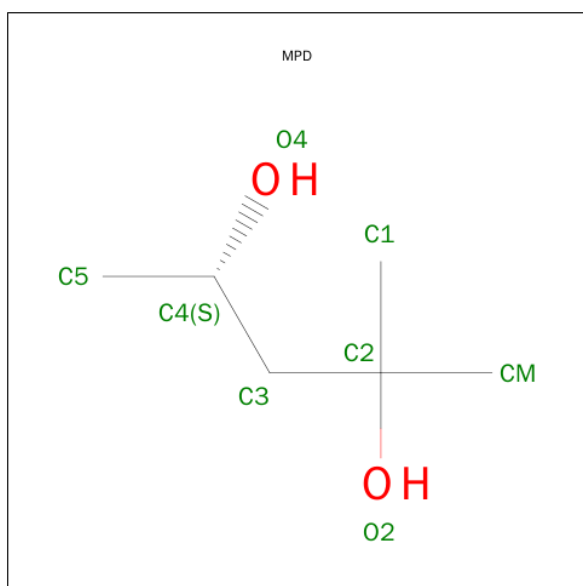
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	1	Total	K	0	0
			1	1		
3	F	1	Total	K	0	0
			1	1		
3	M	1	Total	K	0	0
			1	1		

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:  $C_6H_{14}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	L	1	Total	C	O	0	0
			8	6	2		
4	F	1	Total	C	O	0	0
			8	6	2		
4	E	1	Total	C	O	0	0
			8	6	2		
4	E	1	Total	C	O	0	0
			8	6	2		
4	E	1	Total	C	O	0	0
			8	6	2		
4	I	1	Total	C	O	0	0
			8	6	2		
4	K	1	Total	C	O	0	0
			8	6	2		
4	A	1	Total	C	O	0	0
			8	6	2		

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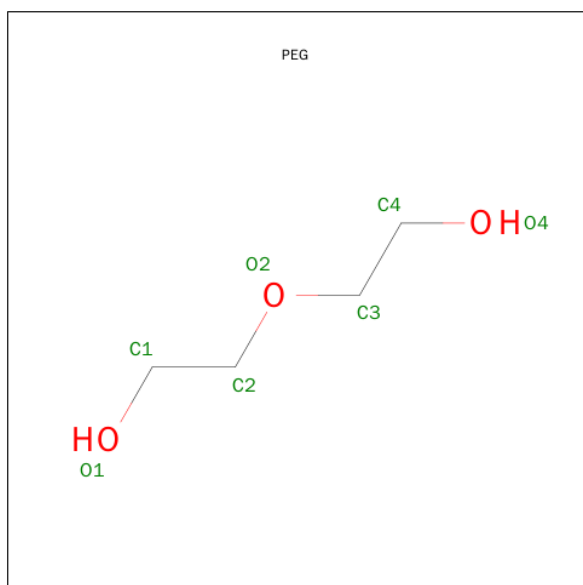
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			8	6	2		
4	G	1	Total	C	O	0	0
			8	6	2		
4	B	1	Total	C	O	0	0
			8	6	2		
4	A	1	Total	C	O	0	0
			8	6	2		
4	B	1	Total	C	O	0	0
			8	6	2		
4	B	1	Total	C	O	0	0
			8	6	2		
4	C	1	Total	C	O	0	0
			8	6	2		
4	N	1	Total	C	O	0	0
			8	6	2		
4	H	1	Total	C	O	0	0
			8	6	2		
4	N	1	Total	C	O	0	0
			8	6	2		
4	M	1	Total	C	O	0	0
			8	6	2		
4	G	1	Total	C	O	0	0
			8	6	2		
4	F	1	Total	C	O	0	0
			8	6	2		
4	E	1	Total	C	O	0	0
			8	6	2		
4	F	1	Total	C	O	0	0
			8	6	2		
4	B	1	Total	C	O	0	0
			8	6	2		
4	I	1	Total	C	O	0	0
			8	6	2		
4	H	1	Total	C	O	0	0
			8	6	2		
4	N	1	Total	C	O	0	0
			8	6	2		
4	K	1	Total	C	O	0	0
			8	6	2		
4	E	1	Total	C	O	0	0
			8	6	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	J	1	Total	C	O	0	0
			8	6	2		
4	I	1	Total	C	O	0	0
			8	6	2		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	E	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is water.

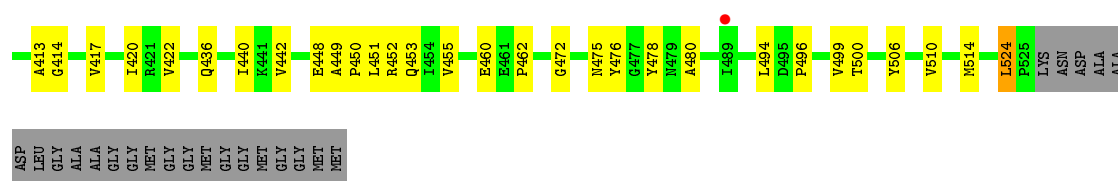
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	60	Total	O	0	0
			60	60		
6	B	76	Total	O	0	0
			76	76		
6	C	55	Total	O	0	0
			55	55		
6	D	79	Total	O	0	0
			79	79		
6	E	64	Total	O	0	0
			64	64		
6	F	65	Total	O	0	0
			65	65		

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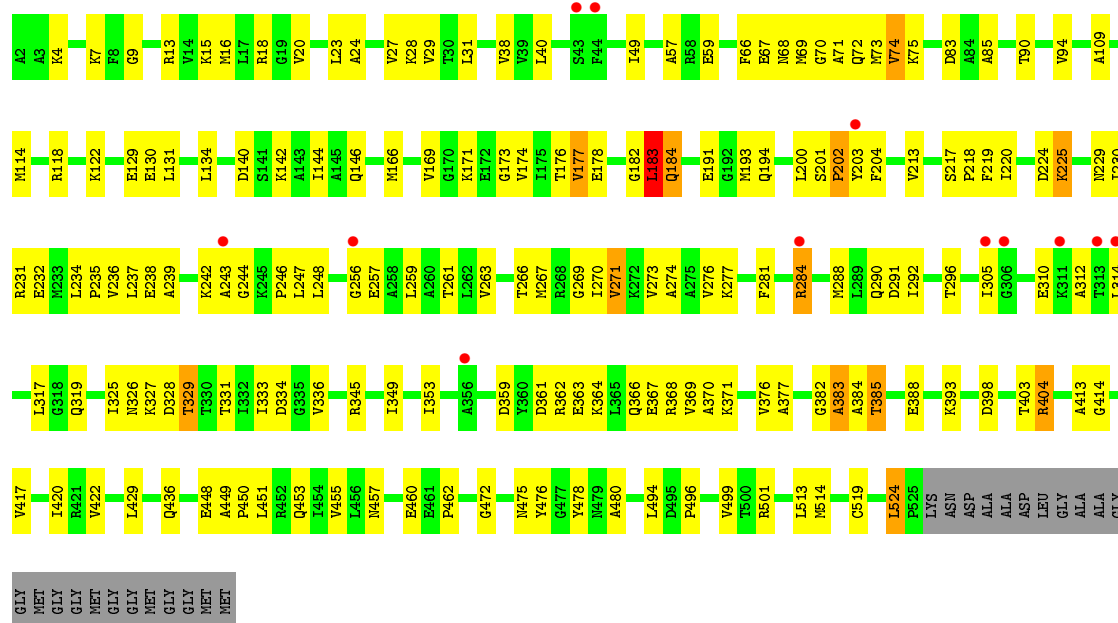
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	84	Total 84	O 84	0	0
6	H	61	Total 61	O 61	0	0
6	I	63	Total 63	O 63	0	0
6	J	45	Total 45	O 45	0	0
6	K	52	Total 52	O 52	0	0
6	L	32	Total 32	O 32	0	0
6	M	49	Total 49	O 49	0	0
6	N	62	Total 62	O 62	0	0

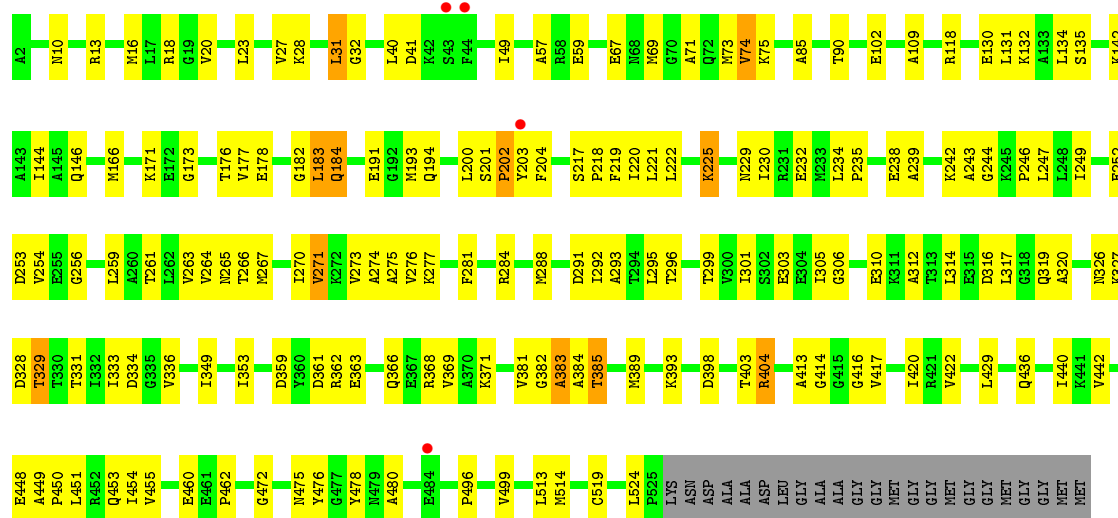




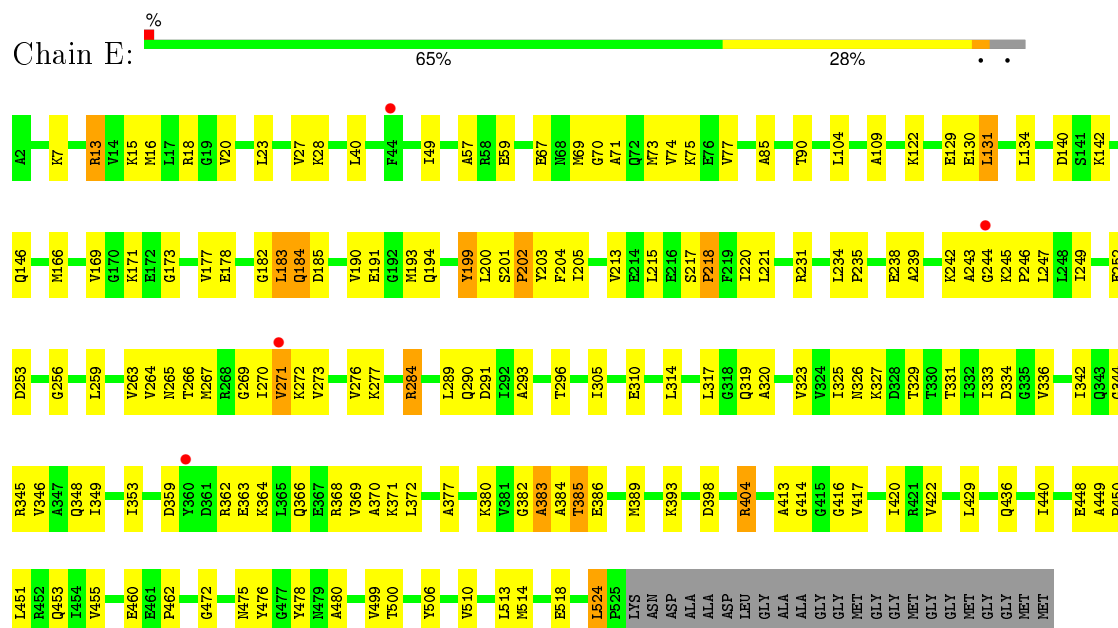
- Molecule 1: 60 kDa chaperonin



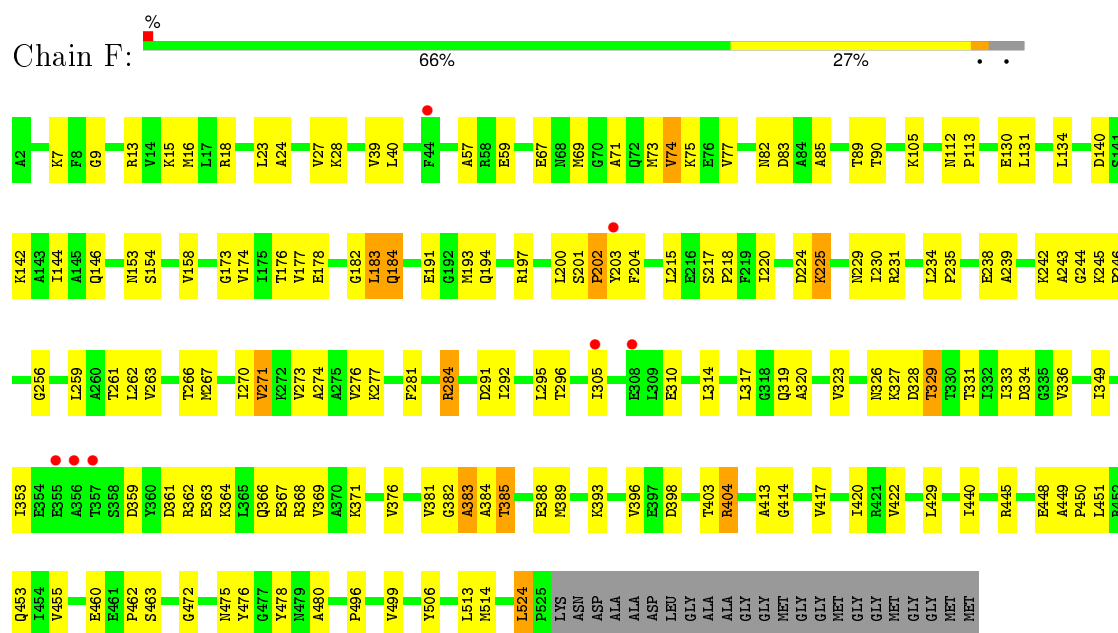
- Molecule 1: 60 kDa chaperonin



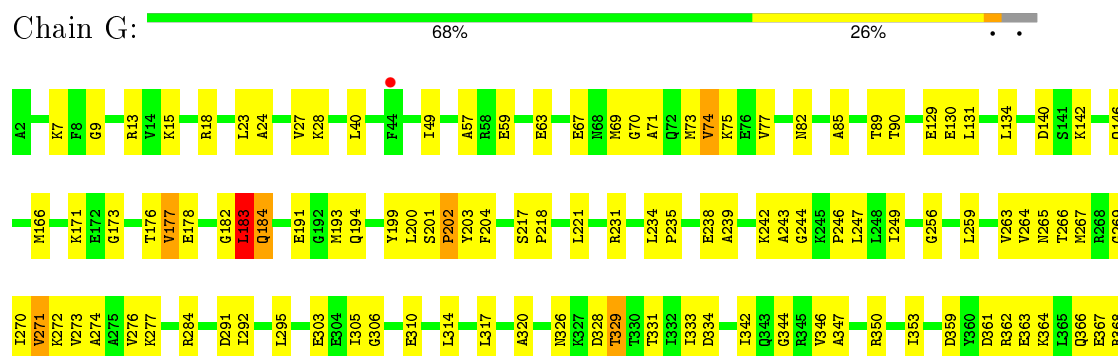
- Molecule 1: 60 kDa chaperonin

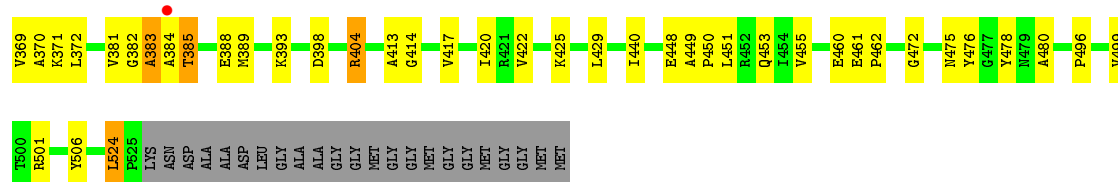


- Molecule 1: 60 kDa chaperonin

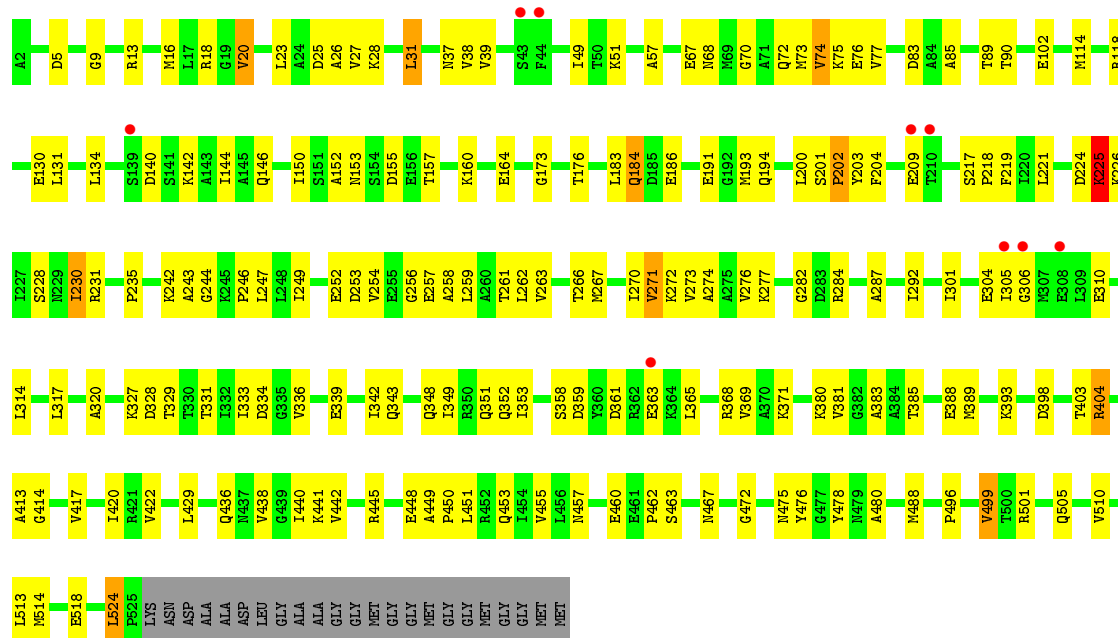


- Molecule 1: 60 kDa chaperonin

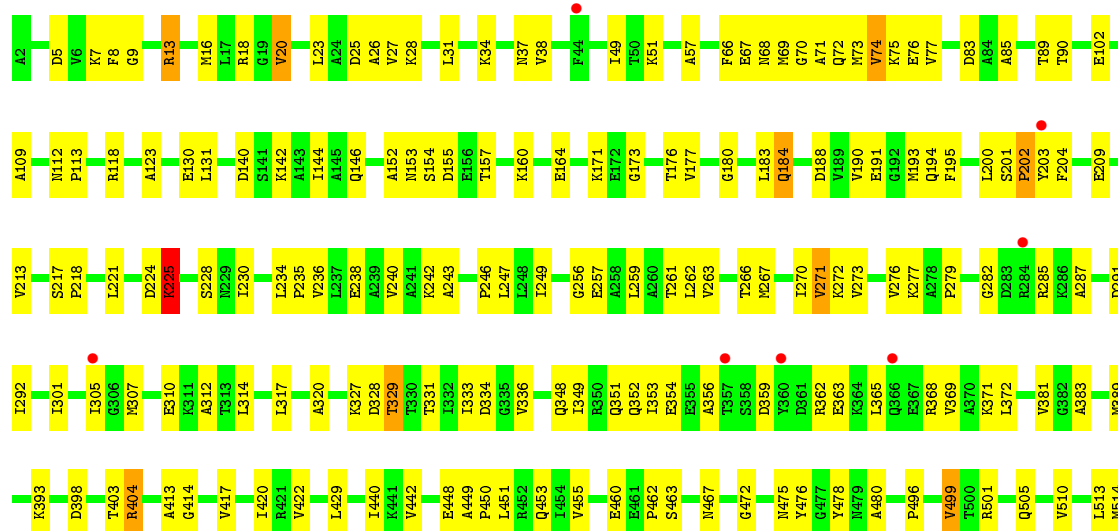




• Molecule 1: 60 kDa chaperonin

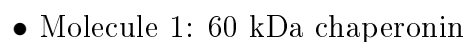
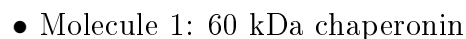


• Molecule 1: 60 kDa chaperonin









	M488	K380	R284	E209	R118	A2
	P496	V381	Q290	A212	A123	D5
	V499	A383	D291	I292	E130	V6
	T500	M389	A293	P218	L131	K7
	V510	K392	T296	F219	L134	G9
	M514	K393	E304	I220	D140	R13
	E518	V396	I305	L221	S141	M16
	L524	E397	G306	A223	K142	L17
	P525	D398	M307	D224	A143	R18
LYS	ASN	T403	E310	K225	I144	G19
ASP	ASP	R404	L314	S228	A145	V20
ALA	ALA	A413	L317	N229	Q146	A24
ALA	G414	G414	T325	I230	I150	V27
ASP	V417	V417	N326	R231	S151	K28
LEU	I420	I420	K327	P235	A152	K34
GLY	R421	R421	D328	E238	S154	N37
ALA	V422	V422	T329	A239	D155	S43
ALA	L429	L429	T330	V240	E156	F44
GLY	GLY	GLY	T331	A241	T157	I49
GLY	GLY	GLY	I332	K242	K160	K51
MET	MET	I440	I333	A243	E164	A57
GLY	GLY	K441	D334	G245	T50	F66
GLY	GLY	V442	G335	P246	V169	E67
MET	MET	R445	V336	L247	G170	G70
GLY	GLY	E448	I342	L248	K171	A71
MET	MET	A449	R345	I249	E172	Q72
GLY	GLY	P450	V346	A251	G173	M73
MET	MET	L451	A347	G256	T176	V74
MET	MET	R452	Q348	E257	V177	K75
		Q453	I349	A258	T181	E76
		V455	R350	L259	G182	V77
		I456	Q351	A260	L183	D83
		M457	Q352	T261	Q184	A84
		E460	I353	L262	D185	A85
		B461	A356	V263	E186	T89
		P462	D359	T266	E191	T90
		S463	Y360	M267	G192	V94
		M467	E363	G269	M193	E102
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		M475	L365	V271	F195	P113
		Y476	V369	K272	Y199	
		G477	A370	V273	L200	
		Y478	K371	V276	S201	
		M479	A377	K277	P202	
		A480		P279	Y203	
					F204	
					I205	

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	262.80Å 283.60Å 135.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.71 – 2.92 33.65 – 2.92	Depositor EDS
% Data completeness (in resolution range)	83.8 (33.71-2.92) 83.9 (33.65-2.92)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.43 (at 2.90Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.203 , 0.235 0.202 , 0.232	Depositor DCC
$R_{free}$ test set	18290 reflections (9.93%)	DCC
Wilson B-factor (Å <sup>2</sup> )	53.1	Xtriage
Anisotropy	0.625	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 42.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 184155 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	55301	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MPD, PEG, K, 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	0.40	0/3883	0.69	3/5243 (0.1%)
1	B	0.40	0/3883	0.64	2/5243 (0.0%)
1	C	0.39	0/3883	0.64	1/5243 (0.0%)
1	D	0.40	0/3883	0.64	3/5243 (0.1%)
1	E	0.39	0/3883	0.69	3/5243 (0.1%)
1	F	0.39	0/3883	0.64	2/5243 (0.0%)
1	G	0.40	0/3883	0.64	2/5243 (0.0%)
1	H	0.37	0/3883	0.66	3/5243 (0.1%)
1	I	0.37	0/3883	0.61	2/5243 (0.0%)
1	J	0.37	0/3883	0.61	2/5243 (0.0%)
1	K	0.37	0/3883	0.61	2/5243 (0.0%)
1	L	0.38	0/3883	0.66	3/5243 (0.1%)
1	M	0.37	0/3883	0.61	2/5243 (0.0%)
1	N	0.36	0/3883	0.60	2/5243 (0.0%)
All	All	0.38	0/54362	0.64	32/73402 (0.0%)

There are no bond length outliers.

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	13	ARG	NE-CZ-NH2	-14.67	112.97	120.30
1	H	13	ARG	NE-CZ-NH2	-14.55	113.03	120.30
1	A	13	ARG	NE-CZ-NH2	-13.99	113.31	120.30
1	E	13	ARG	NE-CZ-NH1	13.46	127.03	120.30
1	L	13	ARG	NE-CZ-NH2	-13.45	113.58	120.30

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	3855	0	3976	121	0
1	B	3855	0	3976	146	0
1	C	3855	0	3976	155	0
1	D	3855	0	3976	126	0
1	E	3855	0	3976	139	0
1	F	3855	0	3976	127	0
1	G	3855	0	3976	117	0
1	H	3855	0	3976	150	0
1	I	3855	0	3976	152	0
1	J	3855	0	3976	146	0
1	K	3855	0	3976	154	0
1	L	3855	0	3976	163	0
1	M	3855	0	3976	175	0
1	N	3855	0	3976	175	0
2	A	20	0	0	0	0
2	B	25	0	0	2	0
2	C	20	0	0	0	0
2	D	25	0	0	0	0
2	E	10	0	0	0	0
2	F	10	0	0	1	0
2	G	15	0	0	0	0
2	H	15	0	0	0	0
2	I	10	0	0	0	0
2	J	20	0	0	0	0
2	K	10	0	0	0	0
2	L	10	0	0	0	0
2	M	15	0	0	0	0
2	N	10	0	0	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
4	A	16	0	28	0	0
4	B	32	0	56	2	0
4	C	8	0	14	2	0
4	D	8	0	14	0	0
4	E	40	0	70	1	0
4	F	24	0	42	1	0
4	G	16	0	28	1	0
4	H	16	0	28	2	0
4	I	24	0	42	0	0
4	J	8	0	14	0	0
4	K	16	0	28	2	0
4	L	8	0	14	0	0
4	M	8	0	14	3	0
4	N	24	0	42	9	0
5	E	7	0	10	0	0
6	A	60	0	0	1	0
6	B	76	0	0	3	0
6	C	55	0	0	2	0
6	D	79	0	0	5	0
6	E	64	0	0	1	0
6	F	65	0	0	1	0
6	G	84	0	0	2	0
6	H	61	0	0	2	0
6	I	63	0	0	2	0
6	J	45	0	0	5	0
6	K	52	0	0	3	0
6	L	32	0	0	1	0
6	M	49	0	0	3	0
6	N	62	0	0	1	0
All	All	55301	0	56108	1943	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 18.

The worst 5 of 1943 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:B:270:ILE:HG23	1:C:231:ARG:HH12	1.20	1.03
1:B:329:THR:HG22	6:B:3165:HOH:O	1.60	1.01
1:D:242:LYS:HG2	1:E:231:ARG:NH2	1.78	0.97
1:B:326:ASN:HD22	1:B:329:THR:HB	1.31	0.94
1:K:272:LYS:NZ	1:L:229:ASN:HD21	1.65	0.94

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	522/547 (95%)	488 (94%)	26 (5%)	8 (2%)	13	41
1	B	522/547 (95%)	485 (93%)	28 (5%)	9 (2%)	11	37
1	C	522/547 (95%)	489 (94%)	24 (5%)	9 (2%)	11	37
1	D	522/547 (95%)	488 (94%)	25 (5%)	9 (2%)	11	37
1	E	522/547 (95%)	487 (93%)	28 (5%)	7 (1%)	15	45
1	F	522/547 (95%)	493 (94%)	20 (4%)	9 (2%)	11	37
1	G	522/547 (95%)	488 (94%)	26 (5%)	8 (2%)	13	41
1	H	522/547 (95%)	491 (94%)	23 (4%)	8 (2%)	13	41
1	I	522/547 (95%)	491 (94%)	25 (5%)	6 (1%)	17	50
1	J	522/547 (95%)	490 (94%)	26 (5%)	6 (1%)	17	50
1	K	522/547 (95%)	491 (94%)	23 (4%)	8 (2%)	13	41
1	L	522/547 (95%)	488 (94%)	26 (5%)	8 (2%)	13	41
1	M	522/547 (95%)	492 (94%)	22 (4%)	8 (2%)	13	41
1	N	522/547 (95%)	491 (94%)	23 (4%)	8 (2%)	13	41
All	All	7308/7658 (95%)	6852 (94%)	345 (5%)	111 (2%)	13	41

5 of 111 Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	A	184	GLN
1	B	183	LEU
1	B	184	GLN
1	C	183	LEU
1	C	184	GLN

### 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	404/414 (98%)	393 (97%)	11 (3%)	52	84
1	B	404/414 (98%)	393 (97%)	11 (3%)	52	84
1	C	404/414 (98%)	391 (97%)	13 (3%)	46	81
1	D	404/414 (98%)	393 (97%)	11 (3%)	52	84
1	E	404/414 (98%)	392 (97%)	12 (3%)	48	82
1	F	404/414 (98%)	392 (97%)	12 (3%)	48	82
1	G	404/414 (98%)	391 (97%)	13 (3%)	46	81
1	H	404/414 (98%)	390 (96%)	14 (4%)	43	78
1	I	404/414 (98%)	390 (96%)	14 (4%)	43	78
1	J	404/414 (98%)	388 (96%)	16 (4%)	38	73
1	K	404/414 (98%)	389 (96%)	15 (4%)	41	76
1	L	404/414 (98%)	390 (96%)	14 (4%)	43	78
1	M	404/414 (98%)	388 (96%)	16 (4%)	38	73
1	N	404/414 (98%)	389 (96%)	15 (4%)	41	76
All	All	5656/5796 (98%)	5469 (97%)	187 (3%)	45	80

5 of 187 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	74	VAL
1	I	329	THR
1	N	20	VAL

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Mol	Chain	Res	Type
1	H	209	GLU
1	H	404	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 96 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	326	ASN
1	G	475	ASN
1	M	351	GLN
1	F	366	GLN
1	G	265	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 89 ligands modelled in this entry, 14 are monoatomic - leaving 75 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	$\# Z  > 2$
2	SO4	A	1107	-	4,4,4	0.26	0	6,6,6	0.11	0
2	SO4	A	1115	-	4,4,4	0.22	0	6,6,6	0.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	A	1121	-	4,4,4	0.26	0	6,6,6	0.13	0
2	SO4	A	1139	-	4,4,4	0.22	0	6,6,6	0.12	0
4	MPD	A	1507	-	6,7,7	0.36	0	7,10,10	0.54	0
4	MPD	A	1511	-	6,7,7	0.52	0	7,10,10	0.51	0
2	SO4	B	1113	-	4,4,4	0.22	0	6,6,6	0.08	0
2	SO4	B	1114	-	4,4,4	0.22	0	6,6,6	0.06	0
2	SO4	B	1130	-	4,4,4	0.24	0	6,6,6	0.12	0
2	SO4	B	1135	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	B	1136	-	4,4,4	0.25	0	6,6,6	0.10	0
4	MPD	B	1510	-	6,7,7	0.35	0	7,10,10	0.51	0
4	MPD	B	1512	-	6,7,7	0.43	0	7,10,10	0.45	0
4	MPD	B	1513	-	6,7,7	0.39	0	7,10,10	0.57	0
4	MPD	B	1523	-	6,7,7	0.52	0	7,10,10	0.49	0
2	SO4	C	1101	-	4,4,4	0.27	0	6,6,6	0.06	0
2	SO4	C	1124	-	4,4,4	0.25	0	6,6,6	0.09	0
2	SO4	C	1133	-	4,4,4	0.21	0	6,6,6	0.12	0
2	SO4	C	1137	-	4,4,4	0.25	0	6,6,6	0.12	0
4	MPD	C	1514	-	6,7,7	0.35	0	7,10,10	0.39	0
2	SO4	D	1110	-	4,4,4	0.27	0	6,6,6	0.08	0
2	SO4	D	1112	-	4,4,4	0.28	0	6,6,6	0.13	0
2	SO4	D	1128	-	4,4,4	0.22	0	6,6,6	0.10	0
2	SO4	D	1129	-	4,4,4	0.22	0	6,6,6	0.11	0
2	SO4	D	1138	-	4,4,4	0.25	0	6,6,6	0.07	0
4	MPD	D	1508	-	6,7,7	0.43	0	7,10,10	0.41	0
2	SO4	E	1123	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	E	1140	-	4,4,4	0.26	0	6,6,6	0.15	0
4	MPD	E	1502	-	6,7,7	0.45	0	7,10,10	0.50	0
4	MPD	E	1503	-	6,7,7	0.42	0	7,10,10	0.49	0
4	MPD	E	1504	-	6,7,7	0.44	0	7,10,10	0.63	0
4	MPD	E	1521	-	6,7,7	0.39	0	7,10,10	0.55	0
4	MPD	E	1528	-	6,7,7	0.50	0	7,10,10	0.51	0
5	PEG	E	2100	-	6,6,6	0.82	0	5,5,5	1.56	1 (20%)
2	SO4	F	1125	-	4,4,4	0.26	0	6,6,6	0.09	0
2	SO4	F	1141	-	4,4,4	0.27	0	6,6,6	0.08	0
4	MPD	F	1501	-	6,7,7	0.49	0	7,10,10	0.38	0
4	MPD	F	1520	-	6,7,7	0.42	0	7,10,10	0.52	0
4	MPD	F	1522	-	6,7,7	0.38	0	7,10,10	0.46	0
2	SO4	G	1108	-	4,4,4	0.23	0	6,6,6	0.12	0
2	SO4	G	1109	-	4,4,4	0.22	0	6,6,6	0.12	0
2	SO4	G	1132	-	4,4,4	0.24	0	6,6,6	0.09	0
4	MPD	G	1509	-	6,7,7	0.51	0	7,10,10	0.54	0
4	MPD	G	1519	-	6,7,7	0.36	0	7,10,10	0.45	0
2	SO4	H	1103	-	4,4,4	0.28	0	6,6,6	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	H	1120	-	4,4,4	0.25	0	6,6,6	0.10	0
2	SO4	H	1142	-	4,4,4	0.25	0	6,6,6	0.09	0
4	MPD	H	1516	-	6,7,7	0.43	0	7,10,10	0.51	0
4	MPD	H	1525	-	6,7,7	0.44	0	7,10,10	0.51	0
2	SO4	I	1119	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	I	1143	-	4,4,4	0.24	0	6,6,6	0.10	0
4	MPD	I	1505	-	6,7,7	0.36	0	7,10,10	0.57	0
4	MPD	I	1524	-	6,7,7	0.37	0	7,10,10	0.45	0
4	MPD	I	1530	-	6,7,7	0.49	0	7,10,10	0.58	0
2	SO4	J	1111	-	4,4,4	0.20	0	6,6,6	0.06	0
2	SO4	J	1118	-	4,4,4	0.23	0	6,6,6	0.11	0
2	SO4	J	1127	-	4,4,4	0.23	0	6,6,6	0.09	0
2	SO4	J	1144	-	4,4,4	0.25	0	6,6,6	0.09	0
4	MPD	J	1529	-	6,7,7	0.45	0	7,10,10	0.47	0
2	SO4	K	1134	-	4,4,4	0.27	0	6,6,6	0.10	0
2	SO4	K	1145	-	4,4,4	0.27	0	6,6,6	0.08	0
4	MPD	K	1506	-	6,7,7	0.53	0	7,10,10	0.39	0
4	MPD	K	1527	-	6,7,7	0.38	0	7,10,10	0.46	0
2	SO4	L	1116	-	4,4,4	0.24	0	6,6,6	0.06	0
2	SO4	L	1117	-	4,4,4	0.24	0	6,6,6	0.10	0
4	MPD	L	1500	-	6,7,7	0.54	0	7,10,10	0.57	0
2	SO4	M	1105	-	4,4,4	0.25	0	6,6,6	0.14	0
2	SO4	M	1106	-	4,4,4	0.22	0	6,6,6	0.07	0
2	SO4	M	1126	-	4,4,4	0.21	0	6,6,6	0.13	0
4	MPD	M	1518	-	6,7,7	0.53	0	7,10,10	0.41	0
2	SO4	N	1104	-	4,4,4	0.27	0	6,6,6	0.17	0
2	SO4	N	1146	-	4,4,4	0.26	0	6,6,6	0.13	0
4	MPD	N	1515	-	6,7,7	0.55	0	7,10,10	0.55	0
4	MPD	N	1517	-	6,7,7	0.50	0	7,10,10	0.53	0
4	MPD	N	1526	-	6,7,7	0.41	0	7,10,10	0.46	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	1107	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1115	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1121	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1139	-	-	0/0/0/0	0/0/0/0
4	MPD	A	1507	-	-	0/5/5/5	0/0/0/0
4	MPD	A	1511	-	-	0/5/5/5	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	B	1113	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1114	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1130	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1135	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1136	-	-	0/0/0/0	0/0/0/0
4	MPD	B	1510	-	-	0/5/5/5	0/0/0/0
4	MPD	B	1512	-	-	0/5/5/5	0/0/0/0
4	MPD	B	1513	-	-	0/5/5/5	0/0/0/0
4	MPD	B	1523	-	-	0/5/5/5	0/0/0/0
2	SO4	C	1101	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1124	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1133	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1137	-	-	0/0/0/0	0/0/0/0
4	MPD	C	1514	-	-	0/5/5/5	0/0/0/0
2	SO4	D	1110	-	-	0/0/0/0	0/0/0/0
2	SO4	D	1112	-	-	0/0/0/0	0/0/0/0
2	SO4	D	1128	-	-	0/0/0/0	0/0/0/0
2	SO4	D	1129	-	-	0/0/0/0	0/0/0/0
2	SO4	D	1138	-	-	0/0/0/0	0/0/0/0
4	MPD	D	1508	-	-	0/5/5/5	0/0/0/0
2	SO4	E	1123	-	-	0/0/0/0	0/0/0/0
2	SO4	E	1140	-	-	0/0/0/0	0/0/0/0
4	MPD	E	1502	-	-	0/5/5/5	0/0/0/0
4	MPD	E	1503	-	-	0/5/5/5	0/0/0/0
4	MPD	E	1504	-	-	0/5/5/5	0/0/0/0
4	MPD	E	1521	-	-	0/5/5/5	0/0/0/0
4	MPD	E	1528	-	-	0/5/5/5	0/0/0/0
5	PEG	E	2100	-	-	0/4/4/4	0/0/0/0
2	SO4	F	1125	-	-	0/0/0/0	0/0/0/0
2	SO4	F	1141	-	-	0/0/0/0	0/0/0/0
4	MPD	F	1501	-	-	0/5/5/5	0/0/0/0
4	MPD	F	1520	-	-	0/5/5/5	0/0/0/0
4	MPD	F	1522	-	-	0/5/5/5	0/0/0/0
2	SO4	G	1108	-	-	0/0/0/0	0/0/0/0
2	SO4	G	1109	-	-	0/0/0/0	0/0/0/0
2	SO4	G	1132	-	-	0/0/0/0	0/0/0/0
4	MPD	G	1509	-	-	0/5/5/5	0/0/0/0
4	MPD	G	1519	-	-	0/5/5/5	0/0/0/0
2	SO4	H	1103	-	-	0/0/0/0	0/0/0/0
2	SO4	H	1120	-	-	0/0/0/0	0/0/0/0
2	SO4	H	1142	-	-	0/0/0/0	0/0/0/0
4	MPD	H	1516	-	-	0/5/5/5	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MPD	H	1525	-	-	0/5/5/5	0/0/0/0
2	SO4	I	1119	-	-	0/0/0/0	0/0/0/0
2	SO4	I	1143	-	-	0/0/0/0	0/0/0/0
4	MPD	I	1505	-	-	0/5/5/5	0/0/0/0
4	MPD	I	1524	-	-	0/5/5/5	0/0/0/0
4	MPD	I	1530	-	-	0/5/5/5	0/0/0/0
2	SO4	J	1111	-	-	0/0/0/0	0/0/0/0
2	SO4	J	1118	-	-	0/0/0/0	0/0/0/0
2	SO4	J	1127	-	-	0/0/0/0	0/0/0/0
2	SO4	J	1144	-	-	0/0/0/0	0/0/0/0
4	MPD	J	1529	-	-	0/5/5/5	0/0/0/0
2	SO4	K	1134	-	-	0/0/0/0	0/0/0/0
2	SO4	K	1145	-	-	0/0/0/0	0/0/0/0
4	MPD	K	1506	-	-	0/5/5/5	0/0/0/0
4	MPD	K	1527	-	-	0/5/5/5	0/0/0/0
2	SO4	L	1116	-	-	0/0/0/0	0/0/0/0
2	SO4	L	1117	-	-	0/0/0/0	0/0/0/0
4	MPD	L	1500	-	-	0/5/5/5	0/0/0/0
2	SO4	M	1105	-	-	0/0/0/0	0/0/0/0
2	SO4	M	1106	-	-	0/0/0/0	0/0/0/0
2	SO4	M	1126	-	-	0/0/0/0	0/0/0/0
4	MPD	M	1518	-	-	0/5/5/5	0/0/0/0
2	SO4	N	1104	-	-	0/0/0/0	0/0/0/0
2	SO4	N	1146	-	-	0/0/0/0	0/0/0/0
4	MPD	N	1515	-	-	0/5/5/5	0/0/0/0
4	MPD	N	1517	-	-	0/5/5/5	0/0/0/0
4	MPD	N	1526	-	-	0/5/5/5	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	2100	PEG	O2-C2-C1	2.41	121.54	110.43

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1136	SO4	2	0
4	B	1510	MPD	2	0
4	C	1514	MPD	2	0
4	E	1502	MPD	1	0
2	F	1141	SO4	1	0
4	F	1522	MPD	1	0
4	G	1509	MPD	1	0
4	H	1516	MPD	2	0
4	K	1506	MPD	2	0
4	M	1518	MPD	3	0
2	N	1146	SO4	1	0
4	N	1515	MPD	5	0
4	N	1517	MPD	2	0
4	N	1526	MPD	2	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	524/547 (95%)	-0.22	4 (0%) 87 86	15, 40, 73, 90	0
1	B	524/547 (95%)	-0.02	16 (3%) 52 46	15, 43, 75, 91	0
1	C	524/547 (95%)	-0.14	12 (2%) 64 59	17, 43, 75, 90	0
1	D	524/547 (95%)	-0.26	4 (0%) 87 86	15, 41, 73, 90	0
1	E	524/547 (95%)	-0.22	4 (0%) 87 86	17, 42, 74, 90	0
1	F	524/547 (95%)	-0.20	7 (1%) 79 78	16, 41, 75, 90	0
1	G	524/547 (95%)	-0.28	2 (0%) 93 92	16, 40, 73, 88	0
1	H	524/547 (95%)	-0.04	9 (1%) 73 70	20, 48, 89, 101	0
1	I	524/547 (95%)	-0.17	7 (1%) 79 78	21, 49, 89, 101	0
1	J	524/547 (95%)	-0.17	6 (1%) 82 80	19, 48, 89, 102	0
1	K	524/547 (95%)	-0.11	9 (1%) 73 70	20, 48, 89, 102	0
1	L	524/547 (95%)	0.18	47 (8%) 12 7	19, 49, 91, 103	0
1	M	524/547 (95%)	0.02	25 (4%) 34 29	20, 49, 90, 103	0
1	N	524/547 (95%)	-0.11	9 (1%) 73 70	21, 49, 89, 102	0
All	All	7336/7658 (95%)	-0.13	161 (2%) 65 61	15, 45, 84, 103	0

The worst 5 of 161 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	313	THR	6.4
1	L	203	TYR	5.8
1	L	312	ALA	5.2
1	M	44	PHE	5.0
1	L	266	THR	5.0



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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MPD	F	1522	8/8	0.84	0.40	14.44	70,73,74,75	0
4	MPD	I	1530	8/8	0.88	0.30	12.16	58,59,62,62	0
4	MPD	B	1510	8/8	0.89	0.36	10.56	76,76,77,77	0
4	MPD	E	1528	8/8	0.87	0.31	10.55	63,65,69,70	0
4	MPD	N	1517	8/8	0.88	0.33	10.44	67,69,70,71	0
4	MPD	F	1520	8/8	0.86	0.31	9.00	41,47,56,57	0
4	MPD	G	1509	8/8	0.90	0.32	8.85	55,57,62,65	0
4	MPD	M	1518	8/8	0.91	0.28	8.79	64,65,65,66	0
4	MPD	B	1512	8/8	0.83	0.34	8.51	69,72,73,74	0
2	SO4	H	1120	5/5	0.91	0.38	8.25	107,108,109,109	0
2	SO4	D	1110	5/5	0.85	0.27	7.75	113,114,115,115	0
4	MPD	J	1529	8/8	0.96	0.27	7.52	55,56,57,57	0
4	MPD	F	1501	8/8	0.89	0.37	7.48	54,59,66,68	0
4	MPD	E	1504	8/8	0.90	0.31	7.25	52,53,57,59	0
4	MPD	L	1500	8/8	0.91	0.29	7.07	43,46,49,49	0
4	MPD	G	1519	8/8	0.87	0.26	7.06	57,59,60,60	0
4	MPD	C	1514	8/8	0.88	0.28	6.53	59,60,66,66	0
4	MPD	A	1511	8/8	0.93	0.25	5.78	42,43,45,45	0
2	SO4	I	1119	5/5	0.92	0.32	5.72	105,106,106,107	0
2	SO4	M	1105	5/5	0.86	0.38	5.68	124,125,125,125	0
2	SO4	L	1116	5/5	0.89	0.33	5.64	114,115,115,115	0
4	MPD	E	1503	8/8	0.95	0.36	4.73	56,56,59,59	0
2	SO4	C	1101	5/5	0.89	0.27	4.36	101,102,103,103	0
3	K	H	3030	1/1	0.74	0.28	4.08	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	C	1133	5/5	0.80	0.31	3.96	139,139,140,140	0
2	SO4	B	1113	5/5	0.85	0.25	3.54	112,113,114,114	0
4	MPD	D	1508	8/8	0.78	0.38	3.13	78,80,81,81	0
2	SO4	D	1128	5/5	0.88	0.33	3.07	118,118,118,119	0
2	SO4	G	1108	5/5	0.89	0.26	2.98	116,117,117,118	0
4	MPD	E	1502	8/8	0.85	0.29	2.93	73,75,79,81	0
5	PEG	E	2100	7/7	0.69	0.23	2.91	83,86,88,89	0
4	MPD	I	1524	8/8	0.75	0.29	2.80	75,80,83,83	0
2	SO4	M	1126	5/5	0.87	0.23	2.59	115,115,116,116	0
4	MPD	N	1515	8/8	0.91	0.23	2.59	67,69,70,70	0
2	SO4	J	1118	5/5	0.95	0.26	2.14	104,104,104,105	0
2	SO4	J	1111	5/5	0.88	0.21	2.04	111,112,112,112	0
4	MPD	B	1523	8/8	0.91	0.35	1.88	77,77,79,79	0
4	MPD	K	1506	8/8	0.93	0.21	1.70	46,50,50,51	0
2	SO4	K	1134	5/5	0.91	0.20	1.54	109,109,109,110	0
2	SO4	N	1104	5/5	0.88	0.23	1.28	108,108,108,108	0
2	SO4	B	1114	5/5	0.90	0.21	1.26	130,130,131,132	0
4	MPD	H	1525	8/8	0.87	0.25	1.14	74,75,75,75	0
4	MPD	H	1516	8/8	0.94	0.16	1.04	48,49,49,49	0
2	SO4	J	1127	5/5	0.94	0.31	0.51	137,137,137,138	0
2	SO4	H	1103	5/5	0.87	0.19	0.30	116,116,117,117	0
2	SO4	F	1125	5/5	0.90	0.16	0.11	110,111,111,111	0
2	SO4	A	1107	5/5	0.90	0.22	-0.08	128,129,129,129	0
2	SO4	D	1112	5/5	0.94	0.16	-0.14	88,90,90,90	0
2	SO4	A	1121	5/5	0.94	0.18	-0.45	98,98,99,99	0
3	K	L	3070	1/1	0.89	0.13	-0.51	71,71,71,71	0
2	SO4	G	1109	5/5	0.94	0.14	-1.05	85,85,86,86	0
2	SO4	C	1137	5/5	0.87	0.34	-	139,140,140,140	0
3	K	A	3010	1/1	0.84	0.29	-	88,88,88,88	0
4	MPD	E	1521	8/8	0.79	0.30	-	80,81,84,84	0
2	SO4	M	1106	5/5	0.77	0.31	-	147,147,147,147	0
4	MPD	N	1526	8/8	0.73	0.43	-	85,86,87,87	0
3	K	I	3040	1/1	0.74	0.21	-	94,94,94,94	0
2	SO4	H	1142	5/5	0.90	0.28	-	120,120,121,121	0
3	K	G	3130	1/1	0.89	0.35	-	79,79,79,79	0
2	SO4	F	1141	5/5	0.88	0.29	-	103,104,104,104	0
2	SO4	B	1130	5/5	0.88	0.46	-	132,133,133,133	0
2	SO4	A	1139	5/5	0.84	0.31	-	124,124,125,125	0
2	SO4	E	1123	5/5	0.88	0.31	-	137,137,137,137	0
2	SO4	N	1146	5/5	0.83	0.32	-	135,135,136,136	0
3	K	K	3050	1/1	0.89	0.15	-	91,91,91,91	0
2	SO4	C	1124	5/5	0.82	0.40	-	133,133,134,134	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	G	1132	5/5	0.81	0.27	-	145,146,146,146	0
2	SO4	L	1117	5/5	0.75	0.42	-	146,146,147,147	0
2	SO4	K	1145	5/5	0.84	0.31	-	127,127,128,128	0
2	SO4	D	1138	5/5	0.83	0.35	-	134,134,134,135	0
2	SO4	E	1140	5/5	0.87	0.36	-	135,135,136,136	0
2	SO4	B	1136	5/5	0.87	0.48	-	130,130,130,130	0
4	MPD	B	1513	8/8	0.92	0.31	-	45,51,55,56	0
2	SO4	I	1143	5/5	0.90	0.29	-	120,121,121,121	0
4	MPD	K	1527	8/8	0.84	0.34	-	99,101,102,102	0
2	SO4	J	1144	5/5	0.89	0.27	-	129,129,130,131	0
2	SO4	D	1129	5/5	0.82	0.29	-	144,144,144,144	0
3	K	E	3110	1/1	0.92	0.18	-	80,80,80,80	0
4	MPD	A	1507	8/8	0.89	0.26	-	56,59,60,62	0
3	K	D	3020	1/1	0.88	0.13	-	65,65,65,65	0
3	K	M	3080	1/1	0.77	0.19	-	87,87,87,87	0
2	SO4	B	1135	5/5	0.79	0.31	-	137,138,139,139	0
3	K	C	3100	1/1	0.86	0.24	-	78,78,78,78	0
2	SO4	A	1115	5/5	0.58	0.49	-	157,157,158,158	0
3	K	J	3060	1/1	0.79	0.16	-	78,78,78,78	0
3	K	F	3120	1/1	0.79	0.24	-	81,81,81,81	0
3	K	B	3140	1/1	0.81	0.18	-	70,70,70,70	0
4	MPD	I	1505	8/8	0.87	0.36	-	63,66,68,68	0
3	K	N	3090	1/1	0.93	0.14	-	67,67,67,67	0

## 6.5 Other polymers

There are no such residues in this entry.