



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 13, 2026 – 08:07 PM UTC

PDB ID : 8R8B / pdb_00008r8b
Title : Wnt binding to COPalpha and COPBeta2 directs secretion on extracellular vesicles
Authors : Gurriaran-Rodriguez, U.; Datzkiw, D.; Radusky, L.G.; Fisher, F.; Xiao, F.; Ming, H.; De Repentigny, Y.; Kothary, R.; Serrano, L.; Rojas, A.L.; Hierro, A.; Rudnicki, M.A.
Deposited on : 2023-11-28
Resolution : 1.81 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

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>.

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)
Xtriage (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

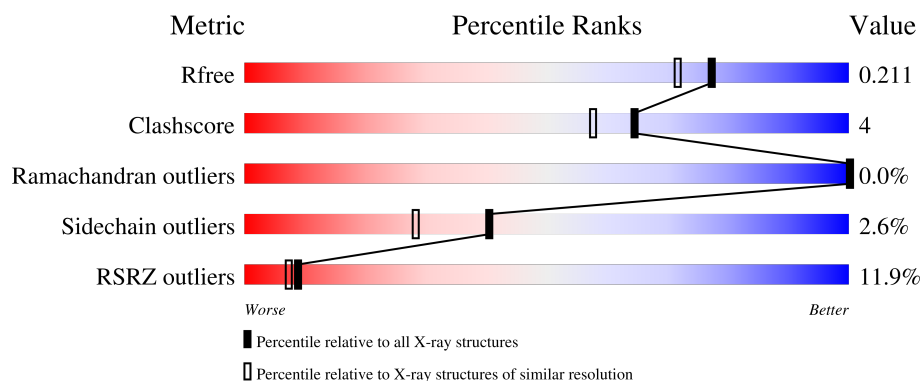
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.81 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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 ≥ 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	AAA	304	4% 89% 10% .
1	BBB	304	6% 84% 15% ..
1	CCC	304	8% 89% 9% .
1	DDD	304	5% 87% 12% ..

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Mol	Chain	Length	Quality of chain
1	EEE	304	6% 88% 11% .
1	FFF	304	7% 88% 10% ..
1	GGG	304	9% 89% 10% ..
1	HHH	304	14% 88% 11% .
1	III	304	11% 90% 10% .
1	JJJ	304	25% 87% 12% .
1	KKK	304	11% 88% 11% .
1	LLL	304	6% 86% 13% .
1	MMM	304	11% 87% 12% ..
1	NNN	304	9% 90% 10% .
1	OOO	304	9% 88% 12%
1	PPP	304	13% 82% 16% ..
1	QQQ	304	13% 88% 11% .
1	RRR	304	31% 89% 9% ..
1	SSS	304	16% 90% 8% .
1	TTT	304	10% 90% 9% .
1	UUU	304	13% 84% 15% .
1	VVV	304	22% 90% 9% .
1	WWW	304	18% 89% 11% .
1	XXX	304	11% 88% 11% .
2	aaa	6	83% 17%
2	bbb	6	67% 33%
2	ccc	6	17% 33% 67%
2	ddd	6	33% 67%
2	eee	6	67% 33%

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Mol	Chain	Length	Quality of chain
2	fff	6	
2	ggg	6	
2	hhh	6	
2	iii	6	
2	jjj	6	
2	kkk	6	
2	lll	6	
2	mmm	6	
2	nnn	6	
2	ooo	6	
2	ppp	6	
2	qqq	6	
2	rrr	6	
2	sss	6	
2	ttt	6	
2	uuu	6	
2	vvv	6	
2	www	6	
2	xxx	6	

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	SO4	EEE	405	-	-	X	-
3	SO4	NNN	403	-	-	X	-
3	SO4	OOO	403	-	-	X	-
4	GOL	XXX	411	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 64338 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 Coatomer subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	302	Total	C	N	O	S	0	1	0
			2433	1561	408	456	8			
1	BBB	302	Total	C	N	O	S	0	2	0
			2436	1562	408	458	8			
1	CCC	302	Total	C	N	O	S	0	1	0
			2433	1561	408	456	8			
1	DDD	302	Total	C	N	O	S	0	2	0
			2439	1566	409	456	8			
1	EEE	302	Total	C	N	O	S	0	0	0
			2429	1557	408	456	8			
1	FFF	302	Total	C	N	O	S	0	2	0
			2441	1566	409	458	8			
1	GGG	302	Total	C	N	O	S	0	1	0
			2432	1559	408	457	8			
1	HHH	302	Total	C	N	O	S	0	1	0
			2435	1562	409	456	8			
1	III	302	Total	C	N	O	S	0	0	0
			2429	1557	408	456	8			
1	JJJ	302	Total	C	N	O	S	0	0	0
			2429	1557	408	456	8			
1	KKK	302	Total	C	N	O	S	0	2	0
			2439	1564	408	459	8			
1	LLL	302	Total	C	N	O	S	0	0	0
			2429	1557	408	456	8			
1	MMM	302	Total	C	N	O	S	0	1	0
			2435	1561	408	458	8			
1	NNN	302	Total	C	N	O	S	0	2	0
			2439	1564	408	459	8			
1	OOO	303	Total	C	N	O	S	0	1	0
			2441	1565	409	459	8			
1	PPP	302	Total	C	N	O	S	0	1	0
			2438	1562	409	459	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	QQQ	302	Total	C	N	O	S	0	0	0
			2429	1557	408	456	8			
1	RRR	302	Total	C	N	O	S	0	0	0
			2429	1557	408	456	8			
1	SSS	300	Total	C	N	O	S	0	1	0
			2420	1553	405	454	8			
1	TTT	302	Total	C	N	O	S	0	0	0
			2429	1557	408	456	8			
1	UUU	303	Total	C	N	O	S	0	1	0
			2443	1565	409	461	8			
1	VVV	302	Total	C	N	O	S	0	0	0
			2429	1557	408	456	8			
1	WWW	302	Total	C	N	O	S	0	0	0
			2429	1557	408	456	8			
1	XXX	302	Total	C	N	O	S	0	0	0
			2429	1557	408	456	8			

- Molecule 2 is a protein called Small ribosomal subunit protein mS37.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	aaa	6	Total	C	N	O	0	0	0
			51	35	9	7			
2	bbb	6	Total	C	N	O	0	0	0
			51	35	9	7			
2	ccc	6	Total	C	N	O	0	0	0
			51	35	9	7			
2	ddd	6	Total	C	N	O	0	0	0
			51	35	9	7			
2	eee	6	Total	C	N	O	0	0	0
			51	35	9	7			
2	fff	6	Total	C	N	O	0	0	0
			51	35	9	7			
2	ggg	6	Total	C	N	O	0	0	0
			51	35	9	7			
2	hhh	6	Total	C	N	O	0	0	0
			51	35	9	7			
2	iii	6	Total	C	N	O	0	0	0
			51	35	9	7			
2	jjj	6	Total	C	N	O	0	0	0
			51	35	9	7			
2	kkk	6	Total	C	N	O	0	0	0
			51	35	9	7			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	lll	6	Total	C	N	O	0	0	0
			51	35	9	7			
2	mmm	6	Total	C	N	O	0	0	0
			51	35	9	7			
2	nnn	6	Total	C	N	O	0	0	0
			51	35	9	7			
2	ooo	6	Total	C	N	O	0	0	0
			51	35	9	7			
2	ppp	6	Total	C	N	O	0	0	0
			51	35	9	7			
2	qqq	6	Total	C	N	O	0	0	0
			51	35	9	7			
2	rrr	6	Total	C	N	O	0	0	0
			51	35	9	7			
2	sss	6	Total	C	N	O	0	0	0
			51	35	9	7			
2	ttt	6	Total	C	N	O	0	0	0
			51	35	9	7			
2	uuu	6	Total	C	N	O	0	0	0
			51	35	9	7			
2	vvv	6	Total	C	N	O	0	0	0
			51	35	9	7			
2	www	6	Total	C	N	O	0	0	0
			51	35	9	7			
2	xxx	6	Total	C	N	O	0	0	0
			51	35	9	7			

There are 24 discrepancies between the modelled and reference sequences:

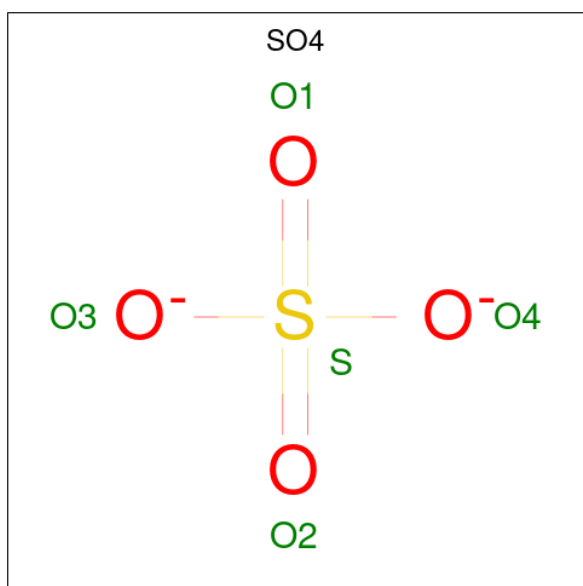
Chain	Residue	Modelled	Actual	Comment	Reference
aaa	196	ILE	VAL	conflict	UNP O75012
bbb	196	ILE	VAL	conflict	UNP O75012
ccc	196	ILE	VAL	conflict	UNP O75012
ddd	196	ILE	VAL	conflict	UNP O75012
eee	196	ILE	VAL	conflict	UNP O75012
fff	196	ILE	VAL	conflict	UNP O75012
ggg	196	ILE	VAL	conflict	UNP O75012
hhh	196	ILE	VAL	conflict	UNP O75012
iii	196	ILE	VAL	conflict	UNP O75012
jjj	196	ILE	VAL	conflict	UNP O75012
kkk	196	ILE	VAL	conflict	UNP O75012
lll	196	ILE	VAL	conflict	UNP O75012
mmm	196	ILE	VAL	conflict	UNP O75012

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Chain	Residue	Modelled	Actual	Comment	Reference
nnn	196	ILE	VAL	conflict	UNP O75012
ooo	196	ILE	VAL	conflict	UNP O75012
ppp	196	ILE	VAL	conflict	UNP O75012
qqq	196	ILE	VAL	conflict	UNP O75012
rrr	196	ILE	VAL	conflict	UNP O75012
sss	196	ILE	VAL	conflict	UNP O75012
ttt	196	ILE	VAL	conflict	UNP O75012
uuu	196	ILE	VAL	conflict	UNP O75012
vvv	196	ILE	VAL	conflict	UNP O75012
www	196	ILE	VAL	conflict	UNP O75012
xxx	196	ILE	VAL	conflict	UNP O75012

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	AAA	1	Total	O	S	0	0
			5	4	1		
3	AAA	1	Total	O	S	0	0
			5	4	1		
3	AAA	1	Total	O	S	0	0
			5	4	1		
3	AAA	1	Total	O	S	0	0
			5	4	1		
3	AAA	1	Total	O	S	0	0
			5	4	1		
3	AAA	1	Total	O	S	0	0
			5	4	1		
3	AAA	1	Total	O	S	0	0
			5	4	1		
3	BBB	1	Total	O	S	0	0
			5	4	1		
3	BBB	1	Total	O	S	0	0
			5	4	1		
3	BBB	1	Total	O	S	0	0
			5	4	1		
3	BBB	1	Total	O	S	0	0
			5	4	1		
3	BBB	1	Total	O	S	0	0
			5	4	1		
3	BBB	1	Total	O	S	0	0
			5	4	1		
3	CCC	1	Total	O	S	0	0
			5	4	1		
3	CCC	1	Total	O	S	0	0
			5	4	1		
3	CCC	1	Total	O	S	0	0
			5	4	1		
3	CCC	1	Total	O	S	0	0
			5	4	1		
3	CCC	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	CCC	1	Total	O	S	0	0
			5	4	1		
3	CCC	1	Total	O	S	0	0
			5	4	1		
3	DDD	1	Total	O	S	0	0
			5	4	1		
3	DDD	1	Total	O	S	0	0
			5	4	1		
3	DDD	1	Total	O	S	0	0
			5	4	1		
3	DDD	1	Total	O	S	0	0
			5	4	1		
3	DDD	1	Total	O	S	0	0
			5	4	1		
3	DDD	1	Total	O	S	0	0
			5	4	1		
3	DDD	1	Total	O	S	0	0
			5	4	1		
3	DDD	1	Total	O	S	0	0
			5	4	1		
3	EEE	1	Total	O	S	0	0
			5	4	1		
3	EEE	1	Total	O	S	0	0
			5	4	1		
3	EEE	1	Total	O	S	0	0
			5	4	1		
3	EEE	1	Total	O	S	0	0
			5	4	1		
3	EEE	1	Total	O	S	0	0
			5	4	1		
3	FFF	1	Total	O	S	0	0
			5	4	1		
3	FFF	1	Total	O	S	0	0
			5	4	1		
3	FFF	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	FFF	1	Total	O	S	0	0
			5	4	1		
3	FFF	1	Total	O	S	0	0
			5	4	1		
3	FFF	1	Total	O	S	0	0
			5	4	1		
3	FFF	1	Total	O	S	0	0
			5	4	1		
3	GGG	1	Total	O	S	0	0
			5	4	1		
3	GGG	1	Total	O	S	0	0
			5	4	1		
3	HHH	1	Total	O	S	0	0
			5	4	1		
3	HHH	1	Total	O	S	0	0
			5	4	1		
3	HHH	1	Total	O	S	0	0
			5	4	1		
3	HHH	1	Total	O	S	0	0
			5	4	1		
3	HHH	1	Total	O	S	0	0
			5	4	1		
3	HHH	1	Total	O	S	0	0
			5	4	1		
3	HHH	1	Total	O	S	0	0
			5	4	1		
3	HHH	1	Total	O	S	0	0
			5	4	1		
3	HHH	1	Total	O	S	0	0
			5	4	1		
3	III	1	Total	O	S	0	0
			5	4	1		
3	III	1	Total	O	S	0	0
			5	4	1		
3	III	1	Total	O	S	0	0
			5	4	1		
3	III	1	Total	O	S	0	0
			5	4	1		
3	III	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	III	1	Total	O	S	0	0
			5	4	1		
3	III	1	Total	O	S	0	0
			5	4	1		
3	III	1	Total	O	S	0	0
			5	4	1		
3	JJJ	1	Total	O	S	0	0
			5	4	1		
3	JJJ	1	Total	O	S	0	0
			5	4	1		
3	JJJ	1	Total	O	S	0	0
			5	4	1		
3	JJJ	1	Total	O	S	0	0
			5	4	1		
3	JJJ	1	Total	O	S	0	0
			5	4	1		
3	JJJ	1	Total	O	S	0	0
			5	4	1		
3	KKK	1	Total	O	S	0	0
			5	4	1		
3	KKK	1	Total	O	S	0	0
			5	4	1		
3	KKK	1	Total	O	S	0	0
			5	4	1		
3	KKK	1	Total	O	S	0	0
			5	4	1		
3	KKK	1	Total	O	S	0	0
			5	4	1		
3	KKK	1	Total	O	S	0	0
			5	4	1		
3	KKK	1	Total	O	S	0	0
			5	4	1		
3	KKK	1	Total	O	S	0	0
			5	4	1		
3	KKK	1	Total	O	S	0	0
			5	4	1		
3	LLL	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	LLL	1	Total	O	S	0	0
			5	4	1		
3	LLL	1	Total	O	S	0	0
			5	4	1		
3	LLL	1	Total	O	S	0	0
			5	4	1		
3	LLL	1	Total	O	S	0	0
			5	4	1		
3	LLL	1	Total	O	S	0	0
			5	4	1		
3	LLL	1	Total	O	S	0	0
			5	4	1		
3	LLL	1	Total	O	S	0	0
			5	4	1		
3	MMM	1	Total	O	S	0	0
			5	4	1		
3	MMM	1	Total	O	S	0	0
			5	4	1		
3	MMM	1	Total	O	S	0	0
			5	4	1		
3	MMM	1	Total	O	S	0	0
			5	4	1		
3	MMM	1	Total	O	S	0	0
			5	4	1		
3	MMM	1	Total	O	S	0	0
			5	4	1		
3	NNN	1	Total	O	S	0	0
			5	4	1		
3	NNN	1	Total	O	S	0	0
			5	4	1		
3	NNN	1	Total	O	S	0	0
			5	4	1		
3	NNN	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	NNN	1	Total	O	S	0	0
			5	4	1		
3	NNN	1	Total	O	S	0	0
			5	4	1		
3	NNN	1	Total	O	S	0	0
			5	4	1		
3	NNN	1	Total	O	S	0	0
			5	4	1		
3	NNN	1	Total	O	S	0	0
			5	4	1		
3	OOO	1	Total	O	S	0	0
			5	4	1		
3	OOO	1	Total	O	S	0	0
			5	4	1		
3	OOO	1	Total	O	S	0	0
			5	4	1		
3	OOO	1	Total	O	S	0	0
			5	4	1		
3	OOO	1	Total	O	S	0	0
			5	4	1		
3	OOO	1	Total	O	S	0	0
			5	4	1		
3	OOO	1	Total	O	S	0	0
			5	4	1		
3	OOO	1	Total	O	S	0	0
			5	4	1		
3	PPP	1	Total	O	S	0	0
			5	4	1		
3	PPP	1	Total	O	S	0	0
			5	4	1		
3	PPP	1	Total	O	S	0	0
			5	4	1		
3	PPP	1	Total	O	S	0	0
			5	4	1		
3	PPP	1	Total	O	S	0	0
			5	4	1		
3	PPP	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	PPP	1	Total	O	S	0	0
			5	4	1		
3	QQQ	1	Total	O	S	0	0
			5	4	1		
3	QQQ	1	Total	O	S	0	0
			5	4	1		
3	QQQ	1	Total	O	S	0	0
			5	4	1		
3	QQQ	1	Total	O	S	0	0
			5	4	1		
3	QQQ	1	Total	O	S	0	0
			5	4	1		
3	QQQ	1	Total	O	S	0	0
			5	4	1		
3	RRR	1	Total	O	S	0	0
			5	4	1		
3	RRR	1	Total	O	S	0	0
			5	4	1		
3	RRR	1	Total	O	S	0	0
			5	4	1		
3	RRR	1	Total	O	S	0	0
			5	4	1		
3	RRR	1	Total	O	S	0	0
			5	4	1		
3	RRR	1	Total	O	S	0	0
			5	4	1		
3	RRR	1	Total	O	S	0	0
			5	4	1		
3	SSS	1	Total	O	S	0	0
			5	4	1		
3	SSS	1	Total	O	S	0	0
			5	4	1		
3	SSS	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	SSS	1	Total	O	S	0	0
			5	4	1		
3	SSS	1	Total	O	S	0	0
			5	4	1		
3	SSS	1	Total	O	S	0	0
			5	4	1		
3	SSS	1	Total	O	S	0	0
			5	4	1		
3	SSS	1	Total	O	S	0	0
			5	4	1		
3	SSS	1	Total	O	S	0	0
			5	4	1		
3	SSS	1	Total	O	S	0	0
			5	4	1		
3	TTT	1	Total	O	S	0	0
			5	4	1		
3	TTT	1	Total	O	S	0	0
			5	4	1		
3	TTT	1	Total	O	S	0	0
			5	4	1		
3	TTT	1	Total	O	S	0	0
			5	4	1		
3	TTT	1	Total	O	S	0	0
			5	4	1		
3	TTT	1	Total	O	S	0	0
			5	4	1		
3	UUU	1	Total	O	S	0	0
			5	4	1		
3	UUU	1	Total	O	S	0	0
			5	4	1		
3	UUU	1	Total	O	S	0	0
			5	4	1		
3	UUU	1	Total	O	S	0	0
			5	4	1		
3	UUU	1	Total	O	S	0	0
			5	4	1		

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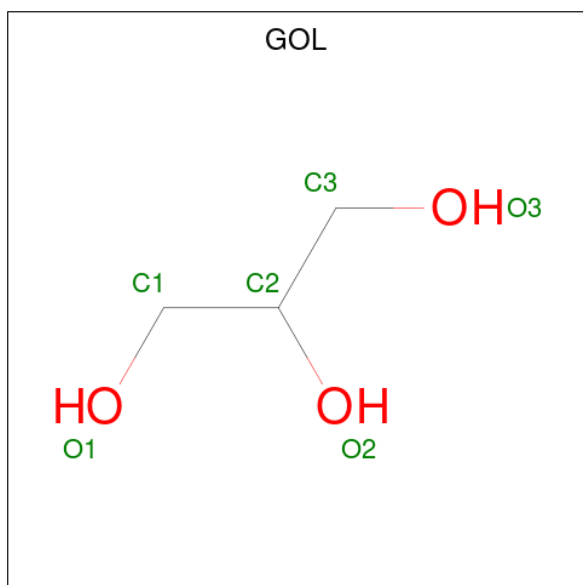
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	UUU	1	Total	O	S	0	0
			5	4	1		
3	UUU	1	Total	O	S	0	0
			5	4	1		
3	UUU	1	Total	O	S	0	0
			5	4	1		
3	UUU	1	Total	O	S	0	0
			5	4	1		
3	UUU	1	Total	O	S	0	0
			5	4	1		
3	VVV	1	Total	O	S	0	0
			5	4	1		
3	VVV	1	Total	O	S	0	0
			5	4	1		
3	VVV	1	Total	O	S	0	0
			5	4	1		
3	VVV	1	Total	O	S	0	0
			5	4	1		
3	VVV	1	Total	O	S	0	0
			5	4	1		
3	VVV	1	Total	O	S	0	0
			5	4	1		
3	WWW	1	Total	O	S	0	0
			5	4	1		
3	WWW	1	Total	O	S	0	0
			5	4	1		
3	WWW	1	Total	O	S	0	0
			5	4	1		
3	WWW	1	Total	O	S	0	0
			5	4	1		
3	XXX	1	Total	O	S	0	0
			5	4	1		
3	XXX	1	Total	O	S	0	0
			5	4	1		
3	XXX	1	Total	O	S	0	0
			5	4	1		
3	XXX	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	XXX	1	Total	O	S	0	0
			5	4	1		
3	XXX	1	Total	O	S	0	0
			5	4	1		
3	XXX	1	Total	O	S	0	0
			5	4	1		
3	XXX	1	Total	O	S	0	0
			5	4	1		
3	aaa	1	Total	O	S	0	0
			5	4	1		
3	ccc	1	Total	O	S	0	0
			5	4	1		
3	ggg	1	Total	O	S	0	0
			5	4	1		
3	ggg	1	Total	O	S	0	0
			5	4	1		
3	lll	1	Total	O	S	0	0
			5	4	1		
3	nnn	1	Total	O	S	0	0
			5	4	1		
3	vvv	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	AAA	1	Total 6	C 3	O 3	0	0
4	AAA	1	Total 6	C 3	O 3	0	0
4	AAA	1	Total 6	C 3	O 3	0	0
4	BBB	1	Total 6	C 3	O 3	0	0
4	BBB	1	Total 6	C 3	O 3	0	0
4	BBB	1	Total 6	C 3	O 3	0	0
4	CCC	1	Total 6	C 3	O 3	0	0
4	CCC	1	Total 6	C 3	O 3	0	0
4	CCC	1	Total 6	C 3	O 3	0	0
4	DDD	1	Total 6	C 3	O 3	0	0
4	DDD	1	Total 6	C 3	O 3	0	0
4	EEE	1	Total 6	C 3	O 3	0	0
4	EEE	1	Total 6	C 3	O 3	0	0
4	EEE	1	Total 6	C 3	O 3	0	0
4	FFF	1	Total 6	C 3	O 3	0	0
4	FFF	1	Total 6	C 3	O 3	0	0
4	FFF	1	Total 6	C 3	O 3	0	0
4	GGG	1	Total 6	C 3	O 3	0	0
4	GGG	1	Total 6	C 3	O 3	0	0
4	HHH	1	Total 6	C 3	O 3	0	0
4	HHH	1	Total 6	C 3	O 3	0	0
4	HHH	1	Total 6	C 3	O 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	HHH	1	Total	C	O	0	0
			6	3	3		
4	III	1	Total	C	O	0	0
			6	3	3		
4	III	1	Total	C	O	0	0
			6	3	3		
4	JJJ	1	Total	C	O	0	0
			6	3	3		
4	JJJ	1	Total	C	O	0	0
			6	3	3		
4	JJJ	1	Total	C	O	0	0
			6	3	3		
4	JJJ	1	Total	C	O	0	0
			6	3	3		
4	KKK	1	Total	C	O	0	0
			6	3	3		
4	KKK	1	Total	C	O	0	0
			6	3	3		
4	LLL	1	Total	C	O	0	0
			6	3	3		
4	MMM	1	Total	C	O	0	0
			6	3	3		
4	MMM	1	Total	C	O	0	0
			6	3	3		
4	MMM	1	Total	C	O	0	0
			6	3	3		
4	MMM	1	Total	C	O	0	0
			6	3	3		
4	NNN	1	Total	C	O	0	0
			6	3	3		
4	NNN	1	Total	C	O	0	0
			6	3	3		
4	OOO	1	Total	C	O	0	0
			6	3	3		
4	PPP	1	Total	C	O	0	0
			6	3	3		
4	PPP	1	Total	C	O	0	0
			6	3	3		
4	QQQ	1	Total	C	O	0	0
			6	3	3		
4	QQQ	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	RRR	1	Total	C	O	0	0
			6	3	3		
4	SSS	1	Total	C	O	0	0
			6	3	3		
4	SSS	1	Total	C	O	0	0
			6	3	3		
4	SSS	1	Total	C	O	0	0
			6	3	3		
4	TTT	1	Total	C	O	0	0
			6	3	3		
4	TTT	1	Total	C	O	0	0
			6	3	3		
4	UUU	1	Total	C	O	0	0
			6	3	3		
4	UUU	1	Total	C	O	0	0
			6	3	3		
4	UUU	1	Total	C	O	0	0
			6	3	3		
4	VVV	1	Total	C	O	0	0
			6	3	3		
4	WWW	1	Total	C	O	0	0
			6	3	3		
4	WWW	1	Total	C	O	0	0
			6	3	3		
4	XXX	1	Total	C	O	0	0
			6	3	3		
4	XXX	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AAA	162	Total	O	0	0
			162	162		
5	BBB	140	Total	O	0	0
			140	140		
5	CCC	119	Total	O	0	0
			119	119		
5	DDD	147	Total	O	0	0
			147	147		
5	EEE	138	Total	O	0	0
			138	138		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	FFF	147	Total 147	O 147	0	0
5	GGG	145	Total 145	O 145	0	0
5	HHH	142	Total 142	O 142	0	0
5	III	137	Total 137	O 137	0	0
5	JJJ	138	Total 138	O 138	0	0
5	KKK	144	Total 144	O 144	0	0
5	LLL	125	Total 125	O 125	0	0
5	MMM	151	Total 151	O 151	0	0
5	NNN	136	Total 136	O 136	0	0
5	OOO	142	Total 142	O 142	0	0
5	PPP	118	Total 118	O 118	0	0
5	QQQ	115	Total 115	O 115	0	0
5	RRR	118	Total 118	O 118	0	0
5	SSS	122	Total 122	O 122	0	0
5	TTT	131	Total 131	O 131	0	0
5	UUU	129	Total 129	O 129	0	0
5	VVV	125	Total 125	O 125	0	0
5	WWW	110	Total 110	O 110	0	0
5	XXX	114	Total 114	O 114	0	0
5	aaa	7	Total 7	O 7	0	0
5	bbb	3	Total 3	O 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	ccc	11	Total 11	O 11	0	0
5	ddd	6	Total 6	O 6	0	0
5	eee	3	Total 3	O 3	0	0
5	fff	8	Total 8	O 8	0	0
5	ggg	13	Total 13	O 13	0	0
5	hhh	4	Total 4	O 4	0	0
5	iii	7	Total 7	O 7	0	0
5	jjj	6	Total 6	O 6	0	0
5	kkk	5	Total 5	O 5	0	0
5	lll	7	Total 7	O 7	0	0
5	mmm	8	Total 8	O 8	0	0
5	nnn	7	Total 7	O 7	0	0
5	ooo	7	Total 7	O 7	0	0
5	ppp	5	Total 5	O 5	0	0
5	qqq	5	Total 5	O 5	0	0
5	rrr	6	Total 6	O 6	0	0
5	sss	4	Total 4	O 4	0	0
5	ttt	5	Total 5	O 5	0	0
5	uuu	9	Total 9	O 9	0	0
5	vvv	6	Total 6	O 6	0	0
5	www	6	Total 6	O 6	0	0

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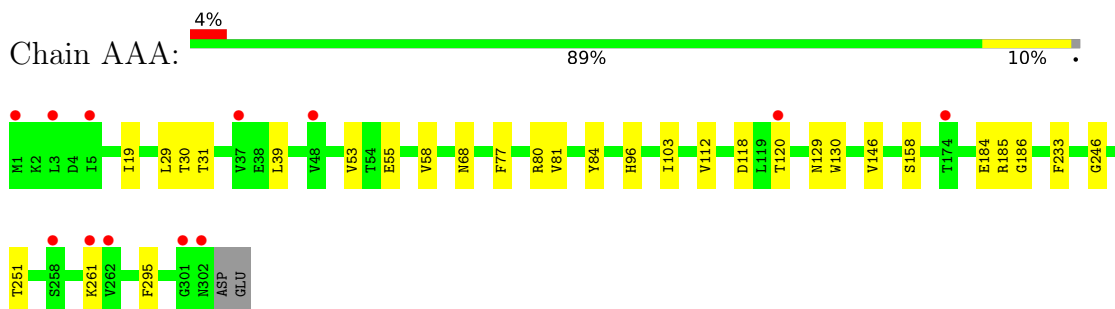
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	xxx	5	Total	O	0	0
			5	5		

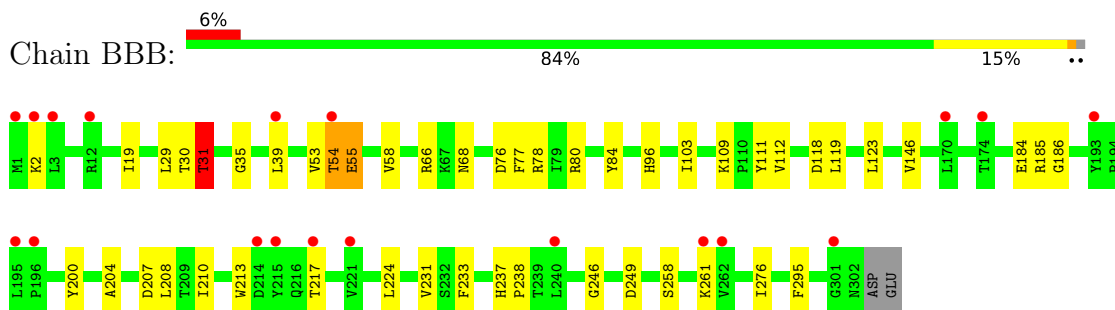
3 Residue-property plots [i](#)

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.

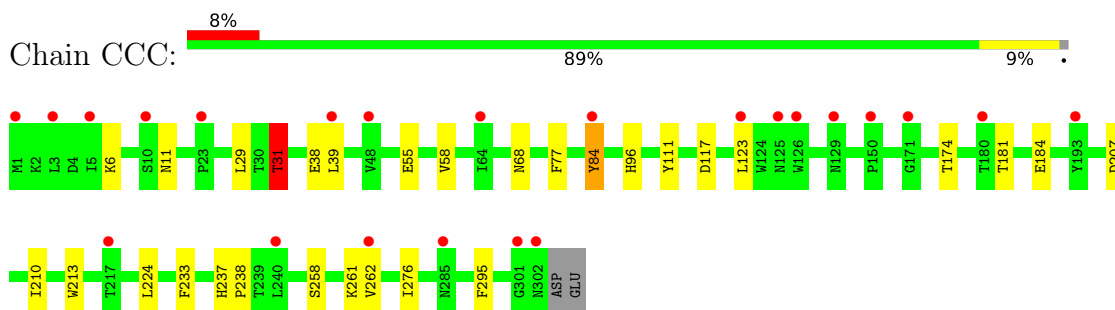
- Molecule 1: Coatomer subunit beta'



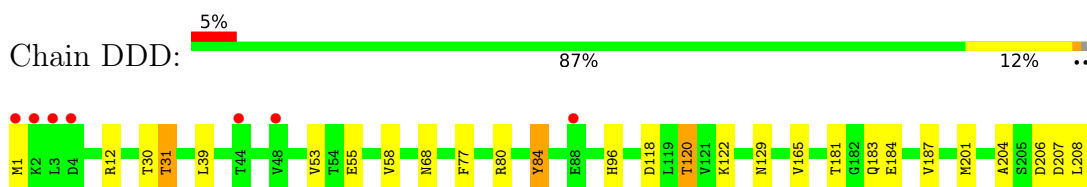
- Molecule 1: Coatomer subunit beta'

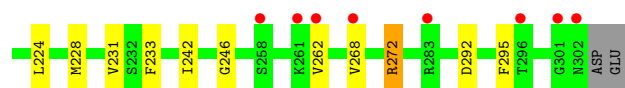


- Molecule 1: Coatomer subunit beta'

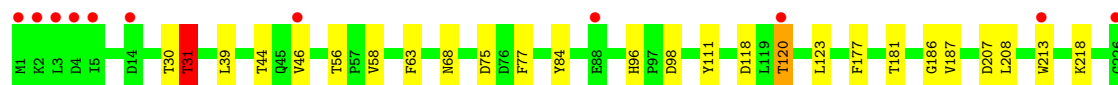
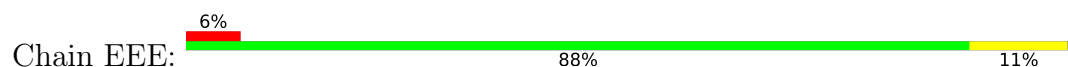


- Molecule 1: Coatomer subunit beta'

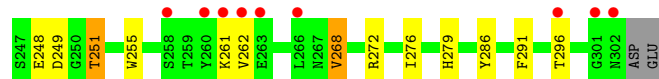




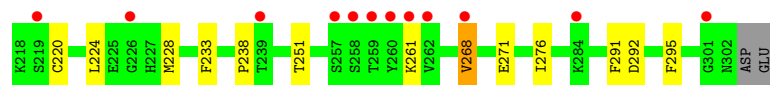
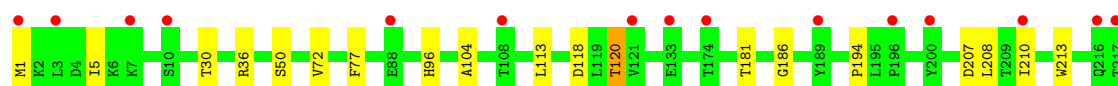
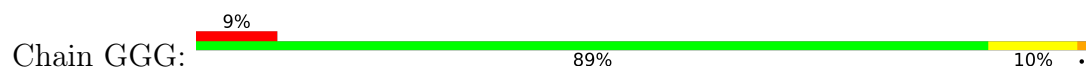
- Molecule 1: Coatomer subunit beta'



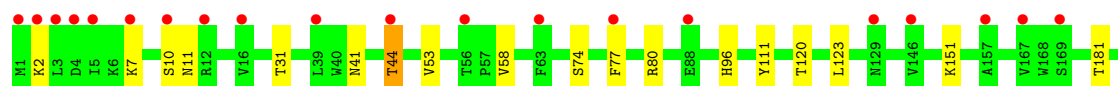
- Molecule 1: Coatomer subunit beta'



- Molecule 1: Coatomer subunit beta'

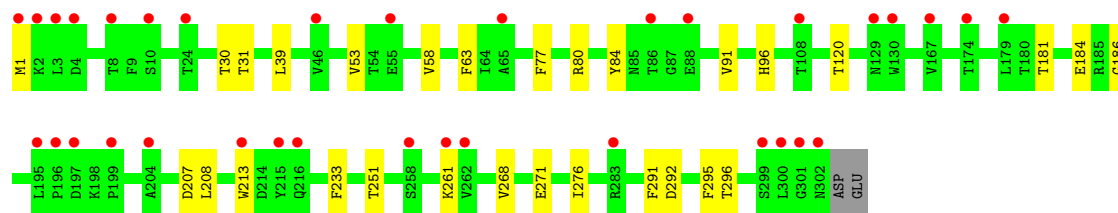


- Molecule 1: Coatomer subunit beta'

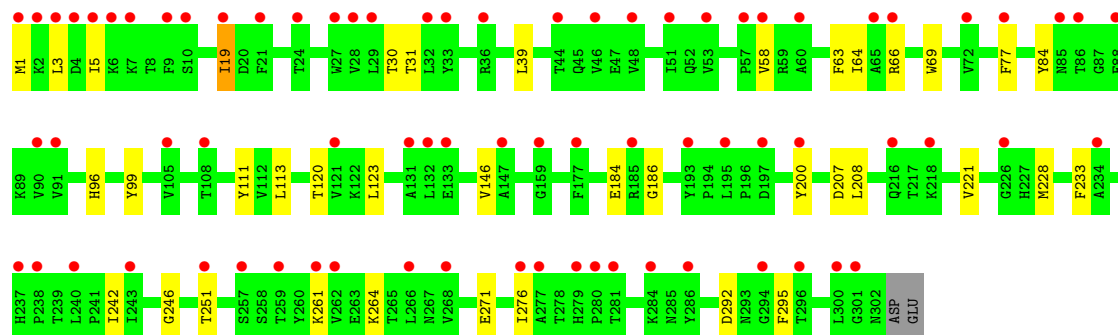


- Molecule 1: Coatomer subunit beta'

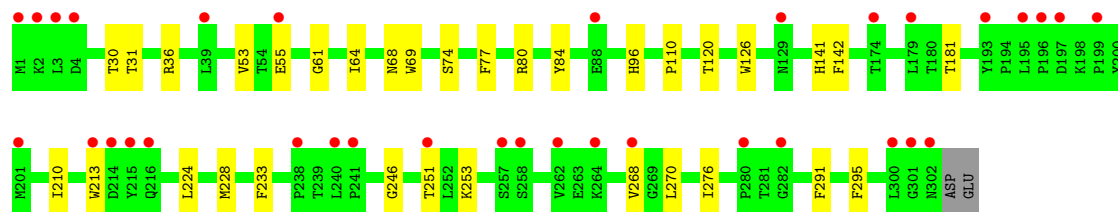




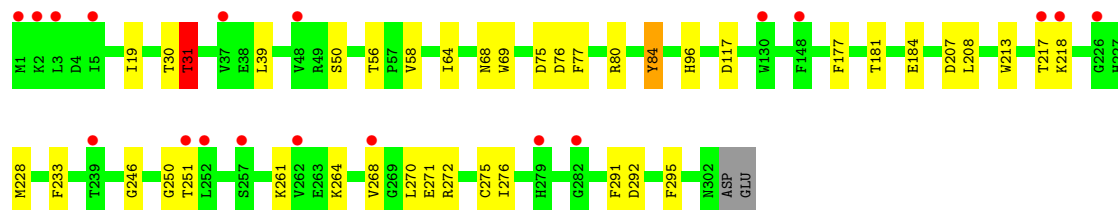
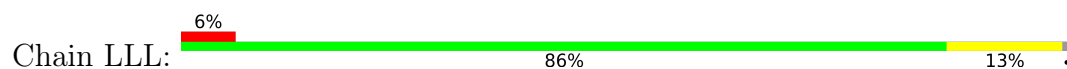
• Molecule 1: Coatomer subunit beta'



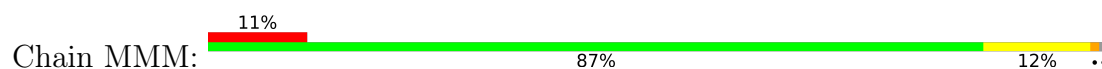
• Molecule 1: Coatomer subunit beta'

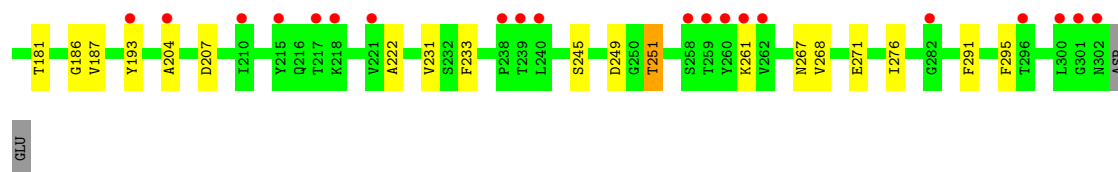


• Molecule 1: Coatomer subunit beta'

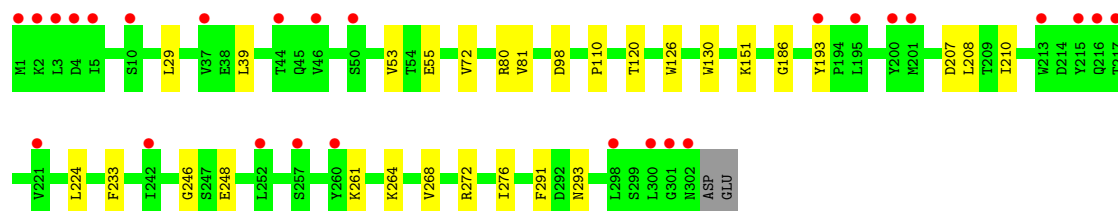


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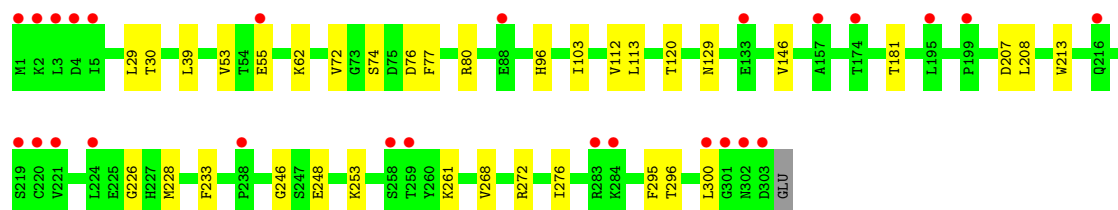




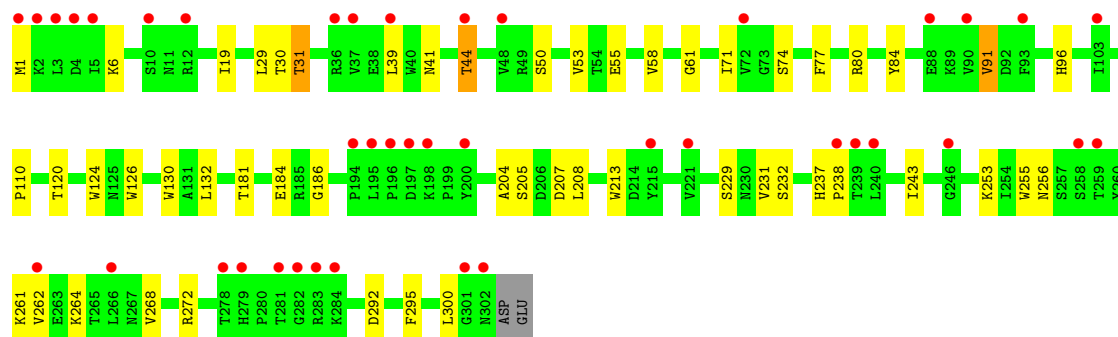
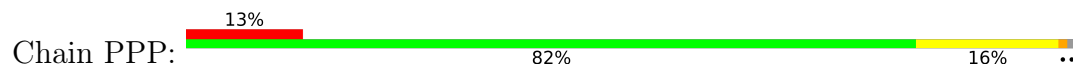
- Molecule 1: Coatomer subunit beta'



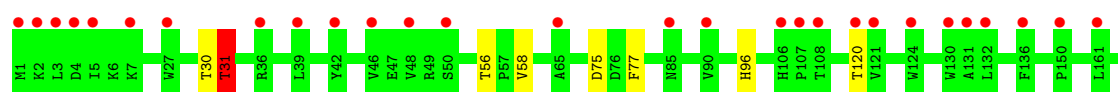
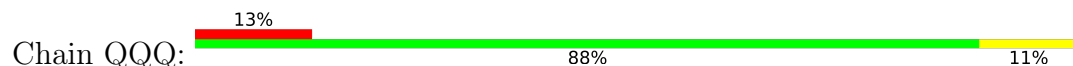
- Molecule 1: Coatomer subunit beta'

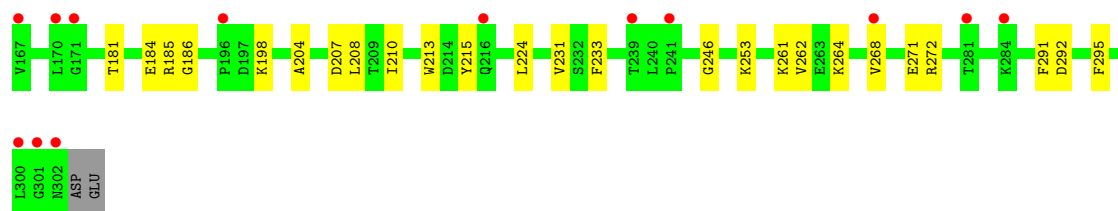


- Molecule 1: Coatomer subunit beta'

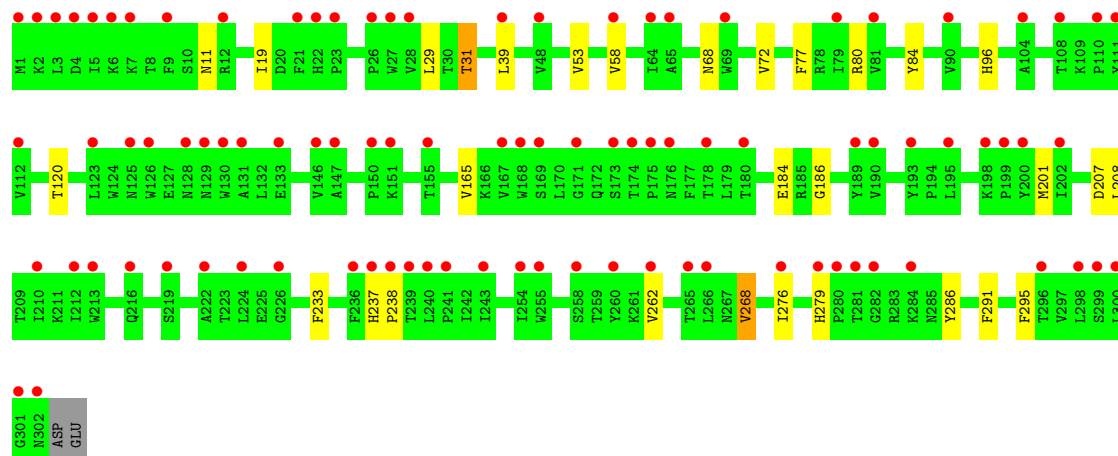


- Molecule 1: Coatomer subunit beta'

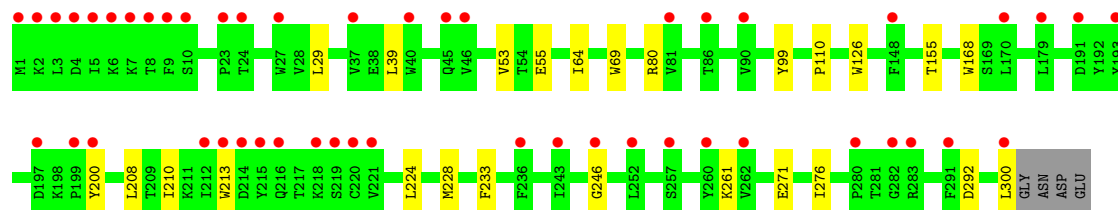




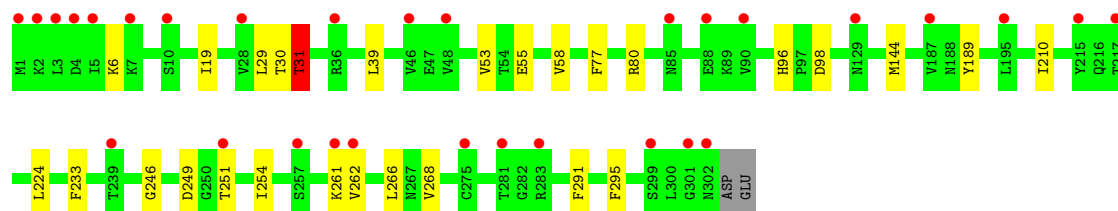
• Molecule 1: Coatomer subunit beta'



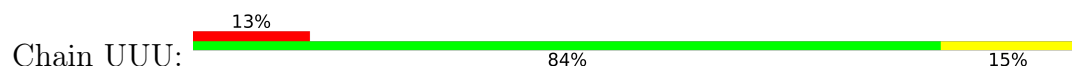
• Molecule 1: Coatomer subunit beta'

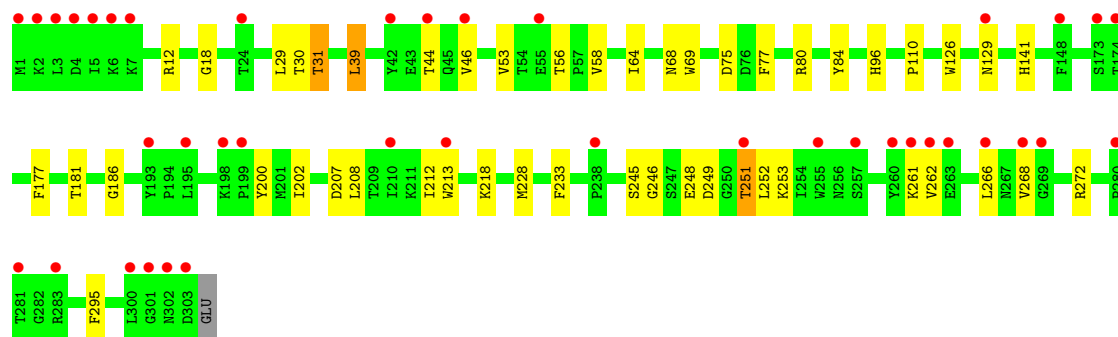


• Molecule 1: Coatomer subunit beta'

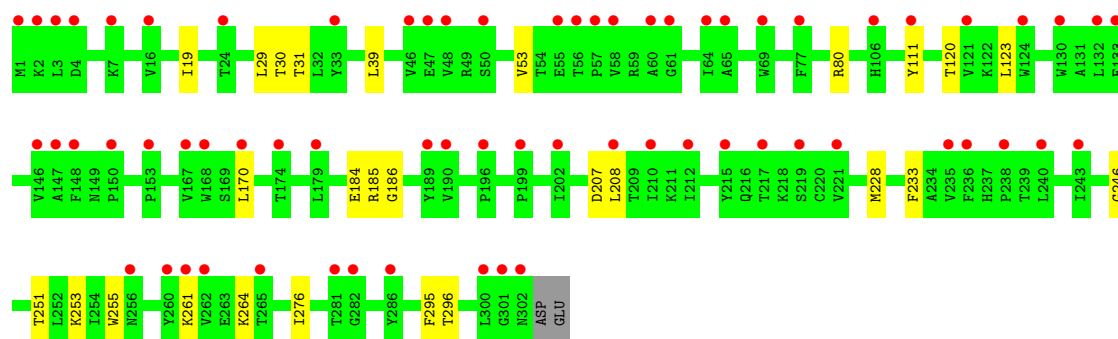


• Molecule 1: Coatomer subunit beta'

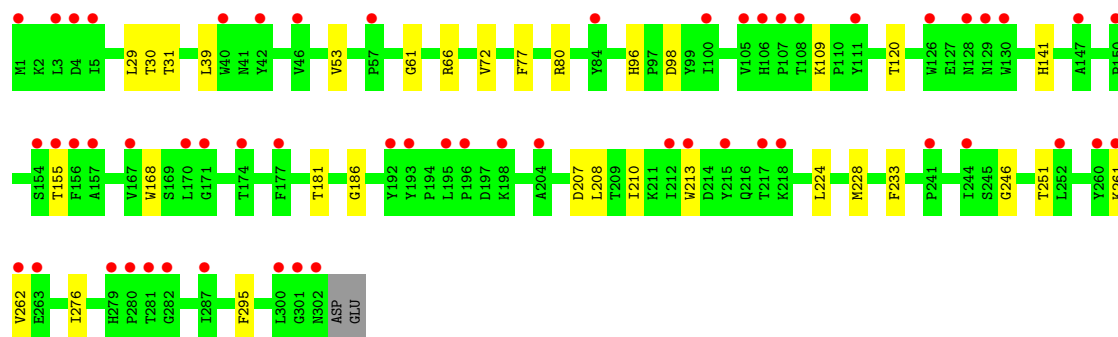




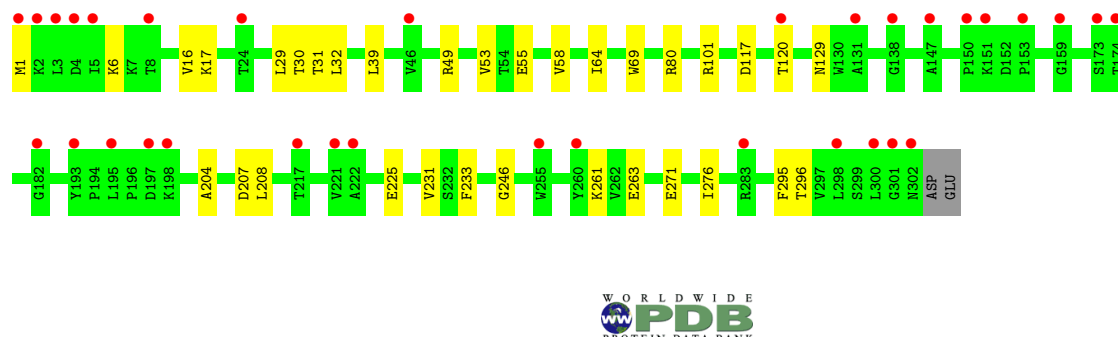
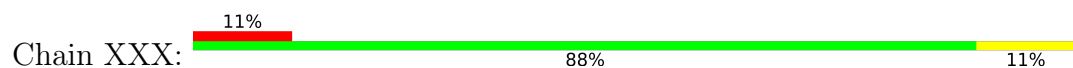
• Molecule 1: Coatomer subunit beta'



• Molecule 1: Coatomer subunit beta'



• Molecule 1: Coatomer subunit beta'



- Molecule 2: Small ribosomal subunit protein mS37

Chain aaa:  83% 17%



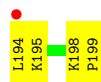
- Molecule 2: Small ribosomal subunit protein mS37

Chain bbb:  67% 33%

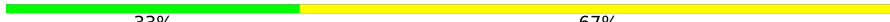


- Molecule 2: Small ribosomal subunit protein mS37

Chain ccc:  17% 33% 67%



- Molecule 2: Small ribosomal subunit protein mS37

Chain ddd:  33% 67%



- Molecule 2: Small ribosomal subunit protein mS37

Chain eee:  67% 33%



- Molecule 2: Small ribosomal subunit protein mS37

Chain fff:  67% 33%

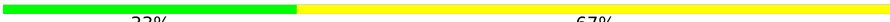


- Molecule 2: Small ribosomal subunit protein mS37

Chain ggg:  67% 33%



- Molecule 2: Small ribosomal subunit protein mS37

Chain hhh:  33% 67%



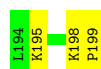
- Molecule 2: Small ribosomal subunit protein mS37

Chain iii:  67% 33%



- Molecule 2: Small ribosomal subunit protein mS37

Chain jjj:  50% 50%



- Molecule 2: Small ribosomal subunit protein mS37

Chain kkk:  67% 33%



- Molecule 2: Small ribosomal subunit protein mS37

Chain lll:  67% 33%



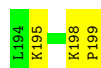
- Molecule 2: Small ribosomal subunit protein mS37

Chain mmm:  67% 33%



- Molecule 2: Small ribosomal subunit protein mS37

Chain nnn:  50% 50%



- Molecule 2: Small ribosomal subunit protein mS37

Chain ooo:  67% 33%



- Molecule 2: Small ribosomal subunit protein mS37

Chain ppp:  67% 33%



- Molecule 2: Small ribosomal subunit protein mS37

Chain qqq:  50% 50%



- Molecule 2: Small ribosomal subunit protein mS37

Chain rrr:  50% 50%



- Molecule 2: Small ribosomal subunit protein mS37

Chain sss:  33% 67%



- Molecule 2: Small ribosomal subunit protein mS37

Chain ttt:  17% 83%



- Molecule 2: Small ribosomal subunit protein mS37

Chain uuu:  67% 33%



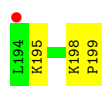
- Molecule 2: Small ribosomal subunit protein mS37

Chain vvv:  67% 33%



- Molecule 2: Small ribosomal subunit protein mS37

Chain www:  17% 50% 50%



- Molecule 2: Small ribosomal subunit protein mS37

Chain xxx:  50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	160.46Å 160.66Å 160.62Å 107.27° 107.16° 107.24°	Depositor
Resolution (Å)	49.38 – 1.81 49.38 – 1.81	Depositor EDS
% Data completeness (in resolution range)	72.4 (49.38-1.81) 89.6 (49.38-1.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.159 , 0.174 0.195 , 0.211	Depositor DCC
R_{free} test set	55123 reflections (4.54%)	wwPDB-VP
Wilson B-factor (Å ²)	37.1	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 29.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.247 for l,h,k 0.247 for k,l,h 0.002 for -l,-k,-h 0.013 for -k,-h,-l 0.000 for -h,-l,-k	Xtriage
Reported twinning fraction	0.263 for H, K, L 0.099 for -H, -L, -K 0.109 for -L, -K, -H 0.191 for K, L, H 0.198 for L, H, K 0.141 for -K, -H, -L	Depositor
Outliers	0 of 1088963 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	64338	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.78% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: GOL, 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	AAA	1.01	0/2505	1.24	1/3415 (0.0%)
1	BBB	1.01	0/2511	1.26	2/3423 (0.1%)
1	CCC	1.01	0/2505	1.25	1/3415 (0.0%)
1	DDD	1.00	0/2514	1.24	0/3427
1	EEE	1.01	0/2498	1.24	2/3405 (0.1%)
1	FFF	1.00	0/2516	1.23	1/3429 (0.0%)
1	GGG	1.01	0/2504	1.26	3/3413 (0.1%)
1	HHH	1.02	0/2507	1.25	0/3416
1	III	1.01	0/2498	1.25	1/3405 (0.0%)
1	JJJ	1.01	0/2498	1.24	1/3405 (0.0%)
1	KKK	1.01	0/2514	1.27	0/3427
1	LLL	1.00	0/2498	1.25	1/3405 (0.0%)
1	MMM	1.01	0/2507	1.25	3/3417 (0.1%)
1	NNN	1.02	0/2514	1.24	3/3427 (0.1%)
1	OOO	1.01	0/2513	1.24	0/3426
1	PPP	1.02	0/2507	1.23	1/3417 (0.0%)
1	QQQ	1.01	0/2498	1.24	2/3405 (0.1%)
1	RRR	1.02	0/2498	1.26	3/3405 (0.1%)
1	SSS	1.01	0/2492	1.25	0/3397
1	TTT	1.01	0/2498	1.25	1/3405 (0.0%)
1	UUU	1.01	0/2515	1.26	3/3428 (0.1%)
1	VVV	1.02	0/2498	1.26	1/3405 (0.0%)
1	WWW	1.02	0/2498	1.25	3/3405 (0.1%)
1	XXX	1.01	0/2498	1.26	2/3405 (0.1%)
2	aaa	0.95	0/51	1.37	0/64
2	bbb	0.97	0/51	1.51	0/64
2	ccc	0.86	0/51	1.29	0/64
2	ddd	0.88	0/51	1.25	0/64
2	eee	0.85	0/51	1.19	0/64
2	fff	0.92	0/51	1.23	0/64
2	ggg	0.90	0/51	1.30	0/64
2	hhh	0.97	0/51	1.50	0/64

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	iii	0.96	0/51	1.38	0/64
2	jjj	0.88	0/51	1.22	0/64
2	kkk	0.88	0/51	1.24	0/64
2	lll	0.90	0/51	1.18	0/64
2	mmm	0.89	0/51	1.27	0/64
2	nnn	0.92	0/51	1.34	0/64
2	ooo	0.99	0/51	1.44	0/64
2	ppp	0.97	0/51	1.39	0/64
2	qqq	0.88	0/51	1.21	0/64
2	rrr	0.92	0/51	1.33	0/64
2	sss	0.88	0/51	1.22	0/64
2	ttt	0.87	0/51	1.24	0/64
2	uuu	0.86	0/51	1.24	0/64
2	vvv	0.85	0/51	1.14	0/64
2	www	0.91	0/51	1.39	0/64
2	xxx	0.91	0/51	1.27	0/64
All	All	1.01	0/61328	1.25	35/83463 (0.0%)

There are no bond length outliers.

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	LLL	31	THR	CB-CA-C	7.81	122.41	110.62
1	QQQ	31	THR	CB-CA-C	7.24	121.19	110.62
1	EEE	31	THR	CB-CA-C	6.74	120.47	110.62
1	NNN	72	VAL	CA-C-N	5.93	125.68	121.65
1	NNN	72	VAL	C-N-CA	5.93	125.68	121.65

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	AAA	2433	0	2372	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	BBB	2436	0	2375	30	0
1	CCC	2433	0	2372	20	0
1	DDD	2439	0	2385	25	0
1	EEE	2429	0	2363	19	0
1	FFF	2441	0	2382	20	0
1	GGG	2432	0	2368	16	0
1	HHH	2435	0	2376	14	0
1	III	2429	0	2363	17	0
1	JJJ	2429	0	2363	24	0
1	KKK	2439	0	2376	18	0
1	LLL	2429	0	2363	26	0
1	MMM	2435	0	2369	23	0
1	NNN	2439	0	2376	15	0
1	OOO	2441	0	2376	21	0
1	PPP	2438	0	2368	24	0
1	QQQ	2429	0	2363	17	0
1	RRR	2429	0	2363	15	0
1	SSS	2420	0	2359	15	0
1	TTT	2429	0	2363	14	0
1	UUU	2443	0	2373	23	0
1	VVV	2429	0	2363	13	0
1	WWW	2429	0	2363	17	0
1	XXX	2429	0	2363	19	0
2	aaa	51	0	67	2	0
2	bbb	51	0	67	1	0
2	ccc	51	0	67	4	0
2	ddd	51	0	67	3	0
2	eee	51	0	67	1	0
2	fff	51	0	67	1	0
2	ggg	51	0	67	1	0
2	hhh	51	0	67	3	0
2	iii	51	0	67	1	0
2	jjj	51	0	67	2	0
2	kkk	51	0	67	1	0
2	lll	51	0	67	1	0
2	mmm	51	0	67	1	0
2	nnn	51	0	67	2	0
2	ooo	51	0	67	1	0
2	ppp	51	0	67	1	0
2	qqq	51	0	67	3	0
2	rrr	51	0	67	3	0
2	sss	51	0	67	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	ttt	51	0	67	5	0
2	uuu	51	0	67	1	0
2	vvv	51	0	67	1	0
2	www	51	0	67	2	0
2	xxx	51	0	67	2	0
3	AAA	70	0	0	0	0
3	BBB	35	0	0	0	0
3	CCC	40	0	0	0	0
3	DDD	50	0	0	1	0
3	EEE	30	0	0	4	0
3	FFF	35	0	0	0	0
3	GGG	10	0	0	0	0
3	HHH	50	0	0	0	0
3	III	40	0	0	0	0
3	JJJ	30	0	0	1	0
3	KKK	55	0	0	0	0
3	LLL	50	0	0	0	0
3	MMM	35	0	0	0	0
3	NNN	50	0	0	2	0
3	OOO	45	0	0	4	0
3	PPP	40	0	0	0	0
3	QQQ	40	0	0	1	0
3	RRR	45	0	0	0	0
3	SSS	55	0	0	0	0
3	TTT	35	0	0	0	0
3	UUU	60	0	0	0	0
3	VVV	30	0	0	0	0
3	WWW	20	0	0	0	0
3	XXX	45	0	0	0	0
3	aaa	5	0	0	0	0
3	ccc	5	0	0	0	0
3	ggg	10	0	0	0	0
3	lll	5	0	0	0	0
3	nnn	5	0	0	0	0
3	vvv	5	0	0	0	0
4	AAA	18	0	24	0	0
4	BBB	18	0	24	0	0
4	CCC	18	0	24	2	0
4	DDD	12	0	16	0	0
4	EEE	18	0	24	0	0
4	FFF	18	0	24	0	0
4	GGG	12	0	16	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	HHH	24	0	32	1	0
4	III	12	0	16	0	0
4	JJJ	24	0	32	0	0
4	KKK	12	0	16	0	0
4	LLL	6	0	8	0	0
4	MMM	24	0	32	3	0
4	NNN	12	0	16	0	0
4	OOO	6	0	8	0	0
4	PPP	12	0	16	0	0
4	QQQ	12	0	16	0	0
4	RRR	6	0	8	0	0
4	SSS	18	0	24	0	0
4	TTT	12	0	16	0	0
4	UUU	18	0	24	0	0
4	VVV	6	0	8	0	0
4	WWW	12	0	16	0	0
4	XXX	12	0	16	4	0
5	AAA	162	0	0	2	0
5	BBB	140	0	0	1	0
5	CCC	119	0	0	0	0
5	DDD	147	0	0	1	0
5	EEE	138	0	0	0	0
5	FFF	147	0	0	1	0
5	GGG	145	0	0	0	0
5	HHH	142	0	0	0	0
5	III	137	0	0	0	0
5	JJJ	138	0	0	0	0
5	KKK	144	0	0	1	0
5	LLL	125	0	0	2	0
5	MMM	151	0	0	0	0
5	NNN	136	0	0	1	0
5	OOO	142	0	0	2	0
5	PPP	118	0	0	0	0
5	QQQ	115	0	0	0	0
5	RRR	118	0	0	0	0
5	SSS	122	0	0	0	0
5	TTT	131	0	0	0	0
5	UUU	129	0	0	1	0
5	VVV	125	0	0	1	0
5	WWW	110	0	0	0	0
5	XXX	114	0	0	0	0
5	aaa	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	bbb	3	0	0	0	0
5	ccc	11	0	0	0	0
5	ddd	6	0	0	0	0
5	eee	3	0	0	0	0
5	fff	8	0	0	0	0
5	ggg	13	0	0	0	0
5	hhh	4	0	0	0	0
5	iii	7	0	0	0	0
5	jjj	6	0	0	0	0
5	kkk	5	0	0	0	0
5	lll	7	0	0	0	0
5	mmm	8	0	0	0	0
5	nnn	7	0	0	0	0
5	ooo	7	0	0	0	0
5	ppp	5	0	0	0	0
5	qqq	5	0	0	0	0
5	rrr	6	0	0	0	0
5	sss	4	0	0	0	0
5	ttt	5	0	0	0	0
5	uuu	9	0	0	0	0
5	vvv	6	0	0	0	0
5	www	6	0	0	0	0
5	xxx	5	0	0	0	0
All	All	64338	0	58921	472	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.

The worst 5 of 472 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:BBB:54[B]:THR:HG21	1:BBB:76:ASP:OD2	1.71	0.89
1:DDD:184:GLU:HB3	4:XXX:411:GOL:H32	1.57	0.85
1:AAA:146[B]:VAL:HG22	5:AAA:624:HOH:O	1.76	0.85
1:XXX:31:THR:HG22	1:XXX:58:VAL:O	1.81	0.80
1:LLL:272:ARG:HD3	1:LLL:292:ASP:OD2	1.82	0.77

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AAA	301/304 (99%)	284 (94%)	17 (6%)	0	100	100
1	BBB	302/304 (99%)	285 (94%)	17 (6%)	0	100	100
1	CCC	301/304 (99%)	286 (95%)	15 (5%)	0	100	100
1	DDD	302/304 (99%)	287 (95%)	15 (5%)	0	100	100
1	EEE	300/304 (99%)	278 (93%)	22 (7%)	0	100	100
1	FFF	302/304 (99%)	286 (95%)	16 (5%)	0	100	100
1	GGG	301/304 (99%)	282 (94%)	19 (6%)	0	100	100
1	HHH	301/304 (99%)	280 (93%)	21 (7%)	0	100	100
1	III	300/304 (99%)	279 (93%)	21 (7%)	0	100	100
1	JJJ	300/304 (99%)	281 (94%)	19 (6%)	0	100	100
1	KKK	302/304 (99%)	283 (94%)	19 (6%)	0	100	100
1	LLL	300/304 (99%)	283 (94%)	17 (6%)	0	100	100
1	MMM	301/304 (99%)	284 (94%)	17 (6%)	0	100	100
1	NNN	302/304 (99%)	285 (94%)	17 (6%)	0	100	100
1	OOO	302/304 (99%)	286 (95%)	16 (5%)	0	100	100
1	PPP	301/304 (99%)	285 (95%)	16 (5%)	0	100	100
1	QQQ	300/304 (99%)	276 (92%)	23 (8%)	1 (0%)	36	25
1	RRR	300/304 (99%)	281 (94%)	19 (6%)	0	100	100
1	SSS	299/304 (98%)	279 (93%)	20 (7%)	0	100	100
1	TTT	300/304 (99%)	287 (96%)	13 (4%)	0	100	100
1	UUU	302/304 (99%)	289 (96%)	13 (4%)	0	100	100
1	VVV	300/304 (99%)	279 (93%)	21 (7%)	0	100	100
1	WWW	300/304 (99%)	285 (95%)	15 (5%)	0	100	100
1	XXX	300/304 (99%)	282 (94%)	18 (6%)	0	100	100
2	aaa	4/6 (67%)	4 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	bbb	4/6 (67%)	4 (100%)	0	0	100	100
2	ccc	4/6 (67%)	4 (100%)	0	0	100	100
2	ddd	4/6 (67%)	4 (100%)	0	0	100	100
2	eee	4/6 (67%)	4 (100%)	0	0	100	100
2	fff	4/6 (67%)	4 (100%)	0	0	100	100
2	ggg	4/6 (67%)	4 (100%)	0	0	100	100
2	hhh	4/6 (67%)	4 (100%)	0	0	100	100
2	iii	4/6 (67%)	4 (100%)	0	0	100	100
2	jjj	4/6 (67%)	4 (100%)	0	0	100	100
2	kkk	4/6 (67%)	4 (100%)	0	0	100	100
2	lll	4/6 (67%)	3 (75%)	1 (25%)	0	100	100
2	mmm	4/6 (67%)	4 (100%)	0	0	100	100
2	nnn	4/6 (67%)	4 (100%)	0	0	100	100
2	ooo	4/6 (67%)	4 (100%)	0	0	100	100
2	ppp	4/6 (67%)	4 (100%)	0	0	100	100
2	qqq	4/6 (67%)	4 (100%)	0	0	100	100
2	rrr	4/6 (67%)	4 (100%)	0	0	100	100
2	sss	4/6 (67%)	4 (100%)	0	0	100	100
2	ttt	4/6 (67%)	4 (100%)	0	0	100	100
2	uuu	4/6 (67%)	4 (100%)	0	0	100	100
2	vvv	4/6 (67%)	4 (100%)	0	0	100	100
2	www	4/6 (67%)	4 (100%)	0	0	100	100
2	xxx	4/6 (67%)	4 (100%)	0	0	100	100
All	All	7315/7440 (98%)	6887 (94%)	427 (6%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	QQQ	271	GLU

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	AAA	272/273 (100%)	267 (98%)	5 (2%)	51	43
1	BBB	273/273 (100%)	264 (97%)	9 (3%)	33	21
1	CCC	272/273 (100%)	264 (97%)	8 (3%)	37	25
1	DDD	273/273 (100%)	264 (97%)	9 (3%)	33	21
1	EEE	271/273 (99%)	266 (98%)	5 (2%)	51	43
1	FFF	273/273 (100%)	262 (96%)	11 (4%)	28	15
1	GGG	272/273 (100%)	266 (98%)	6 (2%)	45	34
1	HHH	272/273 (100%)	262 (96%)	10 (4%)	30	18
1	III	271/273 (99%)	265 (98%)	6 (2%)	45	34
1	JJJ	271/273 (99%)	265 (98%)	6 (2%)	45	34
1	KKK	273/273 (100%)	265 (97%)	8 (3%)	37	25
1	LLL	271/273 (99%)	262 (97%)	9 (3%)	33	21
1	MMM	272/273 (100%)	264 (97%)	8 (3%)	37	25
1	NNN	273/273 (100%)	268 (98%)	5 (2%)	51	43
1	OOO	273/273 (100%)	267 (98%)	6 (2%)	45	34
1	PPP	272/273 (100%)	256 (94%)	16 (6%)	18	7
1	QQQ	271/273 (99%)	263 (97%)	8 (3%)	36	24
1	RRR	271/273 (99%)	267 (98%)	4 (2%)	57	49
1	SSS	271/273 (99%)	268 (99%)	3 (1%)	65	60
1	TTT	271/273 (99%)	263 (97%)	8 (3%)	36	24
1	UUU	273/273 (100%)	262 (96%)	11 (4%)	28	15
1	VVV	271/273 (99%)	265 (98%)	6 (2%)	45	34
1	WWW	271/273 (99%)	267 (98%)	4 (2%)	57	49
1	XXX	271/273 (99%)	265 (98%)	6 (2%)	45	34
2	aaa	6/6 (100%)	6 (100%)	0	100	100
2	bbb	6/6 (100%)	6 (100%)	0	100	100
2	ccc	6/6 (100%)	6 (100%)	0	100	100
2	ddd	6/6 (100%)	6 (100%)	0	100	100
2	eee	6/6 (100%)	6 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	fff	6/6 (100%)	6 (100%)	0	100	100
2	ggg	6/6 (100%)	6 (100%)	0	100	100
2	hhh	6/6 (100%)	6 (100%)	0	100	100
2	iii	6/6 (100%)	6 (100%)	0	100	100
2	jjj	6/6 (100%)	6 (100%)	0	100	100
2	kkk	6/6 (100%)	6 (100%)	0	100	100
2	lll	6/6 (100%)	6 (100%)	0	100	100
2	mmm	6/6 (100%)	6 (100%)	0	100	100
2	nnn	6/6 (100%)	6 (100%)	0	100	100
2	ooo	6/6 (100%)	6 (100%)	0	100	100
2	ppp	6/6 (100%)	6 (100%)	0	100	100
2	qqq	6/6 (100%)	6 (100%)	0	100	100
2	rrr	6/6 (100%)	6 (100%)	0	100	100
2	sss	6/6 (100%)	6 (100%)	0	100	100
2	ttt	6/6 (100%)	6 (100%)	0	100	100
2	uuu	6/6 (100%)	6 (100%)	0	100	100
2	vvv	6/6 (100%)	6 (100%)	0	100	100
2	www	6/6 (100%)	6 (100%)	0	100	100
2	xxx	6/6 (100%)	6 (100%)	0	100	100
All	All	6668/6696 (100%)	6491 (97%)	177 (3%)	40	27

5 of 177 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	PPP	74	SER
1	TTT	31	THR
1	PPP	229	SER
1	QQQ	215	TYR
1	UUU	12	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 ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

263 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	$\# Z > 2$
3	SO4	KKK	410	-	4,4,4	0.35	0	6,6,6	0.07	0
3	SO4	OOO	407	-	4,4,4	0.34	0	6,6,6	0.07	0
3	SO4	PPP	402	-	4,4,4	0.35	0	6,6,6	0.07	0
3	SO4	UUU	405	-	4,4,4	0.34	0	6,6,6	0.08	0
3	SO4	HHH	407	-	4,4,4	0.34	0	6,6,6	0.08	0
4	GOL	SSS	412	-	5,5,5	0.09	0	5,5,5	0.31	0
3	SO4	EEE	406	-	4,4,4	0.34	0	6,6,6	0.08	0
3	SO4	LLL	409	-	4,4,4	0.35	0	6,6,6	0.07	0
4	GOL	KKK	413	-	5,5,5	0.10	0	5,5,5	0.37	0
3	SO4	SSS	403	-	4,4,4	0.34	0	6,6,6	0.08	0
3	SO4	HHH	403	-	4,4,4	0.34	0	6,6,6	0.07	0
4	GOL	AAA	415	-	5,5,5	0.09	0	5,5,5	0.27	0
4	GOL	JJJ	409	-	5,5,5	0.08	0	5,5,5	0.26	0
3	SO4	FFF	406	-	4,4,4	0.35	0	6,6,6	0.07	0
3	SO4	EEE	403	-	4,4,4	0.33	0	6,6,6	0.08	0
3	SO4	HHH	401	-	4,4,4	0.36	0	6,6,6	0.08	0
4	GOL	WWW	406	-	5,5,5	0.08	0	5,5,5	0.28	0
3	SO4	LLL	403	-	4,4,4	0.34	0	6,6,6	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	MMM	403	-	4,4,4	0.32	0	6,6,6	0.07	0
4	GOL	XXX	410	-	5,5,5	0.10	0	5,5,5	0.32	0
3	SO4	QQQ	402	-	4,4,4	0.35	0	6,6,6	0.08	0
3	SO4	OOO	406	-	4,4,4	0.35	0	6,6,6	0.08	0
4	GOL	EEE	409	-	5,5,5	0.10	0	5,5,5	0.27	0
3	SO4	AAA	405	-	4,4,4	0.34	0	6,6,6	0.06	0
3	SO4	BBB	403	-	4,4,4	0.36	0	6,6,6	0.06	0
3	SO4	TTT	406	-	4,4,4	0.34	0	6,6,6	0.07	0
3	SO4	UUU	408	-	4,4,4	0.34	0	6,6,6	0.07	0
4	GOL	HHH	411	-	5,5,5	0.11	0	5,5,5	0.41	0
3	SO4	DDD	404	-	4,4,4	0.35	0	6,6,6	0.07	0
3	SO4	EEE	405	-	4,4,4	0.39	0	6,6,6	0.04	0
3	SO4	OOO	409	-	4,4,4	0.35	0	6,6,6	0.07	0
3	SO4	III	402	-	4,4,4	0.34	0	6,6,6	0.08	0
3	SO4	NNN	408	-	4,4,4	0.35	0	6,6,6	0.08	0
4	GOL	EEE	408	-	5,5,5	0.09	0	5,5,5	0.26	0
3	SO4	HHH	405	-	4,4,4	0.34	0	6,6,6	0.08	0
4	GOL	III	410	-	5,5,5	0.10	0	5,5,5	0.26	0
4	GOL	KKK	412	-	5,5,5	0.08	0	5,5,5	0.27	0
3	SO4	PPP	401	-	4,4,4	0.34	0	6,6,6	0.07	0
3	SO4	KKK	406	-	4,4,4	0.35	0	6,6,6	0.07	0
3	SO4	NNN	405	-	4,4,4	0.36	0	6,6,6	0.09	0
3	SO4	PPP	403	-	4,4,4	0.34	0	6,6,6	0.07	0
3	SO4	III	406	-	4,4,4	0.34	0	6,6,6	0.08	0
4	GOL	PPP	410	-	5,5,5	0.10	0	5,5,5	0.33	0
3	SO4	TTT	402	-	4,4,4	0.34	0	6,6,6	0.07	0
3	SO4	XXX	409	-	4,4,4	0.34	0	6,6,6	0.07	0
3	SO4	AAA	413	-	4,4,4	0.34	0	6,6,6	0.06	0
3	SO4	aaa	201	-	4,4,4	0.33	0	6,6,6	0.06	0
3	SO4	NNN	403	-	4,4,4	0.38	0	6,6,6	0.07	0
3	SO4	MMM	406	-	4,4,4	0.34	0	6,6,6	0.08	0
3	SO4	HHH	402	-	4,4,4	0.34	0	6,6,6	0.08	0
4	GOL	GGG	403	-	5,5,5	0.09	0	5,5,5	0.28	0
3	SO4	XXX	403	-	4,4,4	0.35	0	6,6,6	0.07	0
3	SO4	CCC	407	-	4,4,4	0.35	0	6,6,6	0.07	0
3	SO4	TTT	404	-	4,4,4	0.34	0	6,6,6	0.07	0
3	SO4	SSS	411	-	4,4,4	0.34	0	6,6,6	0.07	0
3	SO4	SSS	408	-	4,4,4	0.34	0	6,6,6	0.07	0
3	SO4	FFF	405	-	4,4,4	0.34	0	6,6,6	0.08	0
3	SO4	RRR	408	-	4,4,4	0.34	0	6,6,6	0.08	0
3	SO4	VVV	402	-	4,4,4	0.34	0	6,6,6	0.08	0
3	SO4	RRR	405	-	4,4,4	0.34	0	6,6,6	0.08	0
3	SO4	ggg	202	-	4,4,4	0.36	0	6,6,6	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	BBB	402	-	4,4,4	0.35	0	6,6,6	0.07	0
3	SO4	TTT	405	-	4,4,4	0.34	0	6,6,6	0.07	0
4	GOL	SSS	413	-	5,5,5	0.10	0	5,5,5	0.28	0
4	GOL	EEE	407	-	5,5,5	0.10	0	5,5,5	0.33	0
3	SO4	LLL	408	-	4,4,4	0.35	0	6,6,6	0.08	0
3	SO4	JJJ	402	-	4,4,4	0.35	0	6,6,6	0.08	0
3	SO4	KKK	404	-	4,4,4	0.36	0	6,6,6	0.07	0
3	SO4	NNN	410	-	4,4,4	0.35	0	6,6,6	0.07	0
4	GOL	FFF	410	-	5,5,5	0.11	0	5,5,5	0.25	0
3	SO4	AAA	411	-	4,4,4	0.35	0	6,6,6	0.07	0
3	SO4	SSS	406	-	4,4,4	0.35	0	6,6,6	0.07	0
3	SO4	HHH	406	-	4,4,4	0.34	0	6,6,6	0.08	0
4	GOL	BBB	409	-	5,5,5	0.10	0	5,5,5	0.26	0
3	SO4	III	401	-	4,4,4	0.34	0	6,6,6	0.07	0
4	GOL	JJJ	407	-	5,5,5	0.09	0	5,5,5	0.26	0
3	SO4	UUU	409	-	4,4,4	0.34	0	6,6,6	0.07	0
4	GOL	QQQ	410	-	5,5,5	0.10	0	5,5,5	0.26	0
3	SO4	AAA	408	-	4,4,4	0.34	0	6,6,6	0.08	0
3	SO4	PPP	406	-	4,4,4	0.34	0	6,6,6	0.08	0
3	SO4	AAA	409	-	4,4,4	0.34	0	6,6,6	0.08	0
3	SO4	NNN	402	-	4,4,4	0.33	0	6,6,6	0.08	0
3	SO4	KKK	407	-	4,4,4	0.34	0	6,6,6	0.08	0
3	SO4	RRR	407	-	4,4,4	0.34	0	6,6,6	0.07	0
3	SO4	JJJ	405	-	4,4,4	0.34	0	6,6,6	0.07	0
3	SO4	QQQ	404	-	4,4,4	0.35	0	6,6,6	0.09	0
3	SO4	TTT	401	-	4,4,4	0.35	0	6,6,6	0.07	0
3	SO4	XXX	407	-	4,4,4	0.33	0	6,6,6	0.07	0
4	GOL	RRR	410	-	5,5,5	0.09	0	5,5,5	0.24	0
3	SO4	DDD	408	-	4,4,4	0.34	0	6,6,6	0.08	0
3	SO4	KKK	403	-	4,4,4	0.34	0	6,6,6	0.07	0
4	GOL	MMM	411	-	5,5,5	0.10	0	5,5,5	0.28	0
3	SO4	HHH	404	-	4,4,4	0.33	0	6,6,6	0.07	0
3	SO4	VVV	404	-	4,4,4	0.34	0	6,6,6	0.08	0
3	SO4	LLL	410	-	4,4,4	0.34	0	6,6,6	0.08	0
3	SO4	KKK	401	-	4,4,4	0.34	0	6,6,6	0.07	0
4	GOL	BBB	410	-	5,5,5	0.09	0	5,5,5	0.29	0
4	GOL	UUU	413	-	5,5,5	0.10	0	5,5,5	0.28	0
3	SO4	RRR	403	-	4,4,4	0.33	0	6,6,6	0.07	0
3	SO4	PPP	404	-	4,4,4	0.34	0	6,6,6	0.08	0
3	SO4	UUU	404	-	4,4,4	0.33	0	6,6,6	0.07	0
3	SO4	III	405	-	4,4,4	0.34	0	6,6,6	0.06	0
3	SO4	TTT	403	-	4,4,4	0.34	0	6,6,6	0.08	0
3	SO4	XXX	406	-	4,4,4	0.34	0	6,6,6	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	NNN	409	-	4,4,4	0.35	0	6,6,6	0.08	0
3	SO4	KKK	405	-	4,4,4	0.35	0	6,6,6	0.08	0
4	GOL	CCC	409	-	5,5,5	0.09	0	5,5,5	0.25	0
4	GOL	FFF	409	-	5,5,5	0.10	0	5,5,5	0.25	0
3	SO4	AAA	412	-	4,4,4	0.38	0	6,6,6	0.08	0
3	SO4	JJJ	404	-	4,4,4	0.35	0	6,6,6	0.07	0
3	SO4	XXX	405	-	4,4,4	0.34	0	6,6,6	0.05	0
3	SO4	JJJ	406	-	4,4,4	0.34	0	6,6,6	0.08	0
4	GOL	OOO	410	-	5,5,5	0.10	0	5,5,5	0.33	0
3	SO4	AAA	410	-	4,4,4	0.34	0	6,6,6	0.08	0
3	SO4	QQQ	406	-	4,4,4	0.34	0	6,6,6	0.07	0
4	GOL	CCC	411	-	5,5,5	0.09	0	5,5,5	0.24	0
3	SO4	OOO	404	-	4,4,4	0.33	0	6,6,6	0.09	0
3	SO4	XXX	402	-	4,4,4	0.34	0	6,6,6	0.07	0
3	SO4	vvv	201	-	4,4,4	0.34	0	6,6,6	0.07	0
3	SO4	SSS	404	-	4,4,4	0.35	0	6,6,6	0.06	0
3	SO4	MMM	404	-	4,4,4	0.34	0	6,6,6	0.08	0
4	GOL	HHH	413	-	5,5,5	0.08	0	5,5,5	0.25	0
3	SO4	DDD	402	-	4,4,4	0.36	0	6,6,6	0.08	0
3	SO4	DDD	407	-	4,4,4	0.34	0	6,6,6	0.08	0
4	GOL	WWW	405	-	5,5,5	0.08	0	5,5,5	0.24	0
3	SO4	KKK	402	-	4,4,4	0.35	0	6,6,6	0.07	0
3	SO4	QQQ	407	-	4,4,4	0.34	0	6,6,6	0.07	0
3	SO4	AAA	403	-	4,4,4	0.35	0	6,6,6	0.07	0
3	SO4	KKK	408	-	4,4,4	0.36	0	6,6,6	0.07	0
3	SO4	CCC	408	-	4,4,4	0.34	0	6,6,6	0.07	0
3	SO4	JJJ	403	-	4,4,4	0.34	0	6,6,6	0.07	0
3	SO4	KKK	411	-	4,4,4	0.34	0	6,6,6	0.07	0
3	SO4	III	407	-	4,4,4	0.36	0	6,6,6	0.07	0
3	SO4	XXX	404	-	4,4,4	0.34	0	6,6,6	0.07	0
3	SO4	AAA	401	-	4,4,4	0.35	0	6,6,6	0.10	0
3	SO4	DDD	410	-	4,4,4	0.35	0	6,6,6	0.07	0
3	SO4	NNN	406	-	4,4,4	0.33	0	6,6,6	0.07	0
3	SO4	PPP	408	-	4,4,4	0.35	0	6,6,6	0.08	0
4	GOL	MMM	409	-	5,5,5	0.09	0	5,5,5	0.30	0
3	SO4	EEE	401	-	4,4,4	0.35	0	6,6,6	0.07	0
3	SO4	QQQ	401	-	4,4,4	0.35	0	6,6,6	0.07	0
4	GOL	DDD	412	-	5,5,5	0.09	0	5,5,5	0.25	0
3	SO4	WWW	403	-	4,4,4	0.33	0	6,6,6	0.07	0
3	SO4	JJJ	401	-	4,4,4	0.33	0	6,6,6	0.09	0
3	SO4	OOO	403	-	4,4,4	0.42	0	6,6,6	0.08	0
4	GOL	HHH	412	-	5,5,5	0.10	0	5,5,5	0.32	0
3	SO4	DDD	409	-	4,4,4	0.34	0	6,6,6	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	WWW	404	-	4,4,4	0.34	0	6,6,6	0.08	0
3	SO4	LLL	407	-	4,4,4	0.34	0	6,6,6	0.08	0
4	GOL	NNN	411	-	5,5,5	0.09	0	5,5,5	0.33	0
4	GOL	QQQ	409	-	5,5,5	0.09	0	5,5,5	0.24	0
3	SO4	SSS	407	-	4,4,4	0.34	0	6,6,6	0.08	0
3	SO4	QQQ	405	-	4,4,4	0.35	0	6,6,6	0.07	0
4	GOL	NNN	412	-	5,5,5	0.09	0	5,5,5	0.30	0
4	GOL	UUU	414	-	5,5,5	0.09	0	5,5,5	0.26	0
3	SO4	CCC	401	-	4,4,4	0.34	0	6,6,6	0.07	0
4	GOL	LLL	411	-	5,5,5	0.09	0	5,5,5	0.26	0
3	SO4	RRR	401	-	4,4,4	0.35	0	6,6,6	0.08	0
3	SO4	SSS	410	-	4,4,4	0.35	0	6,6,6	0.08	0
4	GOL	FFF	408	-	5,5,5	0.07	0	5,5,5	0.26	0
3	SO4	MMM	401	-	4,4,4	0.34	0	6,6,6	0.08	0
3	SO4	AAA	402	-	4,4,4	0.36	0	6,6,6	0.06	0
3	SO4	AAA	407	-	4,4,4	0.35	0	6,6,6	0.07	0
3	SO4	LLL	404	-	4,4,4	0.34	0	6,6,6	0.07	0
3	SO4	BBB	401	-	4,4,4	0.34	0	6,6,6	0.08	0
3	SO4	XXX	401	-	4,4,4	0.36	0	6,6,6	0.06	0
3	SO4	LLL	406	-	4,4,4	0.34	0	6,6,6	0.07	0
3	SO4	ccc	201	-	4,4,4	0.35	0	6,6,6	0.07	0
4	GOL	TTT	409	-	5,5,5	0.10	0	5,5,5	0.30	0
4	GOL	JJJ	408	-	5,5,5	0.11	0	5,5,5	0.29	0
4	GOL	MMM	410	-	5,5,5	0.09	0	5,5,5	0.26	0
3	SO4	QQQ	408	-	4,4,4	0.35	0	6,6,6	0.08	0
3	SO4	LLL	405	-	4,4,4	0.34	0	6,6,6	0.06	0
3	SO4	VVV	401	-	4,4,4	0.34	0	6,6,6	0.08	0
3	SO4	ggg	201	-	4,4,4	0.34	0	6,6,6	0.07	0
4	GOL	UUU	415	-	5,5,5	0.08	0	5,5,5	0.27	0
3	SO4	EEE	404	-	4,4,4	0.34	0	6,6,6	0.07	0
3	SO4	BBB	405	-	4,4,4	0.35	0	6,6,6	0.07	0
3	SO4	VVV	403	-	4,4,4	0.34	0	6,6,6	0.07	0
3	SO4	GGG	401	-	4,4,4	0.35	0	6,6,6	0.07	0
3	SO4	SSS	401	-	4,4,4	0.36	0	6,6,6	0.07	0
3	SO4	KKK	409	-	4,4,4	0.34	0	6,6,6	0.08	0
3	SO4	CCC	403	-	4,4,4	0.36	0	6,6,6	0.07	0
3	SO4	TTT	407	-	4,4,4	0.35	0	6,6,6	0.07	0
4	GOL	HHH	414	-	5,5,5	0.09	0	5,5,5	0.27	0
3	SO4	RRR	409	-	4,4,4	0.35	0	6,6,6	0.08	0
3	SO4	BBB	407	-	4,4,4	0.34	0	6,6,6	0.07	0
4	GOL	PPP	409	-	5,5,5	0.09	0	5,5,5	0.25	0
4	GOL	MMM	408	-	5,5,5	0.10	0	5,5,5	0.33	0
4	GOL	TTT	408	-	5,5,5	0.11	0	5,5,5	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	III	408	-	4,4,4	0.34	0	6,6,6	0.08	0
3	SO4	FFF	402	-	4,4,4	0.34	0	6,6,6	0.08	0
3	SO4	DDD	403	-	4,4,4	0.35	0	6,6,6	0.08	0
3	SO4	GGG	402	-	4,4,4	0.34	0	6,6,6	0.07	0
3	SO4	UUU	411	-	4,4,4	0.35	0	6,6,6	0.07	0
4	GOL	BBB	408	-	5,5,5	0.10	0	5,5,5	0.24	0
3	SO4	UUU	403	-	4,4,4	0.36	0	6,6,6	0.07	0
3	SO4	QQQ	403	-	4,4,4	0.34	0	6,6,6	0.08	0
3	SO4	NNN	401	-	4,4,4	0.35	0	6,6,6	0.07	0
3	SO4	OOO	402	-	4,4,4	0.35	0	6,6,6	0.07	0
3	SO4	PPP	407	-	4,4,4	0.35	0	6,6,6	0.07	0
3	SO4	UUU	412	-	4,4,4	0.35	0	6,6,6	0.07	0
3	SO4	DDD	405	-	4,4,4	0.34	0	6,6,6	0.08	0
3	SO4	XXX	408	-	4,4,4	0.34	0	6,6,6	0.08	0
3	SO4	AAA	414	-	4,4,4	0.35	0	6,6,6	0.07	0
3	SO4	III	201	-	4,4,4	0.34	0	6,6,6	0.06	0
3	SO4	FFF	401	-	4,4,4	0.35	0	6,6,6	0.08	0
3	SO4	III	404	-	4,4,4	0.34	0	6,6,6	0.07	0
3	SO4	NNN	407	-	4,4,4	0.34	0	6,6,6	0.07	0
4	GOL	GGG	404	-	5,5,5	0.09	0	5,5,5	0.28	0
4	GOL	JJJ	410	-	5,5,5	0.10	0	5,5,5	0.25	0
3	SO4	AAA	404	-	4,4,4	0.34	0	6,6,6	0.08	0
3	SO4	OOO	401	-	4,4,4	0.35	0	6,6,6	0.06	0
3	SO4	HHH	409	-	4,4,4	0.34	0	6,6,6	0.08	0
4	GOL	III	409	-	5,5,5	0.10	0	5,5,5	0.28	0
3	SO4	SSS	402	-	4,4,4	0.34	0	6,6,6	0.09	0
3	SO4	CCC	402	-	4,4,4	0.34	0	6,6,6	0.07	0
3	SO4	DDD	406	-	4,4,4	0.34	0	6,6,6	0.08	0
3	SO4	OOO	405	-	4,4,4	0.34	0	6,6,6	0.07	0
3	SO4	UUU	402	-	4,4,4	0.34	0	6,6,6	0.08	0
4	GOL	VVV	407	-	5,5,5	0.09	0	5,5,5	0.28	0
3	SO4	FFF	407	-	4,4,4	0.35	0	6,6,6	0.07	0
3	SO4	MMM	402	-	4,4,4	0.34	0	6,6,6	0.07	0
3	SO4	HHH	410	-	4,4,4	0.34	0	6,6,6	0.07	0
3	SO4	MMM	407	-	4,4,4	0.33	0	6,6,6	0.07	0
3	SO4	NNN	404	-	4,4,4	0.33	0	6,6,6	0.07	0
3	SO4	PPP	405	-	4,4,4	0.34	0	6,6,6	0.08	0
3	SO4	III	403	-	4,4,4	0.34	0	6,6,6	0.08	0
3	SO4	LLL	402	-	4,4,4	0.35	0	6,6,6	0.07	0
3	SO4	LLL	401	-	4,4,4	0.35	0	6,6,6	0.08	0
3	SO4	RRR	406	-	4,4,4	0.35	0	6,6,6	0.10	0
3	SO4	HHH	408	-	4,4,4	0.34	0	6,6,6	0.08	0
3	SO4	VVV	406	-	4,4,4	0.34	0	6,6,6	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	SSS	405	-	4,4,4	0.34	0	6,6,6	0.07	0
4	GOL	SSS	414	-	5,5,5	0.09	0	5,5,5	0.26	0
3	SO4	WWW	402	-	4,4,4	0.34	0	6,6,6	0.08	0
3	SO4	CCC	405	-	4,4,4	0.35	0	6,6,6	0.07	0
3	SO4	CCC	406	-	4,4,4	0.34	0	6,6,6	0.07	0
3	SO4	FFF	404	-	4,4,4	0.35	0	6,6,6	0.09	0
3	SO4	OOO	408	-	4,4,4	0.35	0	6,6,6	0.07	0
3	SO4	nnn	201	-	4,4,4	0.37	0	6,6,6	0.08	0
3	SO4	UUU	410	-	4,4,4	0.35	0	6,6,6	0.07	0
4	GOL	AAA	417	-	5,5,5	0.10	0	5,5,5	0.27	0
3	SO4	MMM	405	-	4,4,4	0.35	0	6,6,6	0.08	0
3	SO4	BBB	406	-	4,4,4	0.34	0	6,6,6	0.07	0
3	SO4	RRR	402	-	4,4,4	0.34	0	6,6,6	0.08	0
4	GOL	AAA	416	-	5,5,5	0.08	0	5,5,5	0.26	0
3	SO4	UUU	407	-	4,4,4	0.34	0	6,6,6	0.07	0
3	SO4	UUU	406	-	4,4,4	0.34	0	6,6,6	0.07	0
4	GOL	CCC	410	-	5,5,5	0.10	0	5,5,5	0.36	0
3	SO4	EEE	402	-	4,4,4	0.34	0	6,6,6	0.08	0
3	SO4	AAA	406	-	4,4,4	0.34	0	6,6,6	0.06	0
3	SO4	WWW	401	-	4,4,4	0.34	0	6,6,6	0.09	0
3	SO4	DDD	401	-	4,4,4	0.35	0	6,6,6	0.10	0
3	SO4	RRR	404	-	4,4,4	0.34	0	6,6,6	0.07	0
3	SO4	CCC	404	-	4,4,4	0.34	0	6,6,6	0.07	0
3	SO4	FFF	403	-	4,4,4	0.35	0	6,6,6	0.07	0
3	SO4	VVV	405	-	4,4,4	0.34	0	6,6,6	0.07	0
4	GOL	XXX	411	-	5,5,5	0.11	0	5,5,5	0.39	0
3	SO4	UUU	401	-	4,4,4	0.34	0	6,6,6	0.07	0
4	GOL	DDD	411	-	5,5,5	0.08	0	5,5,5	0.29	0
3	SO4	SSS	409	-	4,4,4	0.34	0	6,6,6	0.07	0
3	SO4	BBB	404	-	4,4,4	0.34	0	6,6,6	0.07	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
4	GOL	BBB	409	-	-	2/4/4/4	-
4	GOL	GGG	404	-	-	0/4/4/4	-
4	GOL	JJJ	410	-	-	0/4/4/4	-
4	GOL	MMM	409	-	-	4/4/4/4	-
4	GOL	DDD	412	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	SSS	412	-	-	4/4/4/4	-
4	GOL	III	409	-	-	0/4/4/4	-
4	GOL	HHH	412	-	-	2/4/4/4	-
4	GOL	JJJ	407	-	-	0/4/4/4	-
4	GOL	KKK	413	-	-	4/4/4/4	-
4	GOL	QQQ	410	-	-	1/4/4/4	-
4	GOL	NNN	411	-	-	2/4/4/4	-
4	GOL	QQQ	409	-	-	2/4/4/4	-
4	GOL	AAA	415	-	-	4/4/4/4	-
4	GOL	JJJ	409	-	-	4/4/4/4	-
4	GOL	VVV	407	-	-	0/4/4/4	-
4	GOL	RRR	410	-	-	0/4/4/4	-
4	GOL	NNN	412	-	-	4/4/4/4	-
4	GOL	UUU	414	-	-	2/4/4/4	-
4	GOL	WWW	406	-	-	2/4/4/4	-
4	GOL	XXX	410	-	-	2/4/4/4	-
4	GOL	EEE	409	-	-	1/4/4/4	-
4	GOL	HHH	411	-	-	4/4/4/4	-
4	GOL	LLL	411	-	-	0/4/4/4	-
4	GOL	MMM	411	-	-	3/4/4/4	-
4	GOL	FFF	408	-	-	2/4/4/4	-
4	GOL	EEE	408	-	-	0/4/4/4	-
4	GOL	BBB	410	-	-	3/4/4/4	-
4	GOL	III	410	-	-	3/4/4/4	-
4	GOL	KKK	412	-	-	2/4/4/4	-
4	GOL	UUU	413	-	-	4/4/4/4	-
4	GOL	SSS	414	-	-	2/4/4/4	-
4	GOL	TTT	409	-	-	2/4/4/4	-
4	GOL	JJJ	408	-	-	2/4/4/4	-
4	GOL	MMM	410	-	-	1/4/4/4	-
4	GOL	UUU	415	-	-	0/4/4/4	-
4	GOL	FFF	409	-	-	0/4/4/4	-
4	GOL	AAA	417	-	-	2/4/4/4	-
4	GOL	CCC	409	-	-	2/4/4/4	-
4	GOL	PPP	410	-	-	2/4/4/4	-
4	GOL	HHH	414	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	OOO	410	-	-	3/4/4/4	-
4	GOL	GGG	403	-	-	2/4/4/4	-
4	GOL	CCC	411	-	-	0/4/4/4	-
4	GOL	AAA	416	-	-	2/4/4/4	-
4	GOL	CCC	410	-	-	2/4/4/4	-
4	GOL	PPP	409	-	-	2/4/4/4	-
4	GOL	MMM	408	-	-	4/4/4/4	-
4	GOL	TTT	408	-	-	2/4/4/4	-
4	GOL	HHH	413	-	-	2/4/4/4	-
4	GOL	WWW	405	-	-	3/4/4/4	-
4	GOL	XXX	411	-	-	4/4/4/4	-
4	GOL	BBB	408	-	-	2/4/4/4	-
4	GOL	SSS	413	-	-	3/4/4/4	-
4	GOL	DDD	411	-	-	2/4/4/4	-
4	GOL	EEE	407	-	-	4/4/4/4	-
4	GOL	FFF	410	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 113 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	AAA	415	GOL	O1-C1-C2-C3
4	AAA	415	GOL	C1-C2-C3-O3
4	BBB	408	GOL	O1-C1-C2-O2
4	BBB	408	GOL	O1-C1-C2-C3
4	BBB	409	GOL	O1-C1-C2-C3

There are no ring outliers.

11 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	EEE	405	SO4	4	0
3	NNN	403	SO4	2	0
3	JJJ	402	SO4	1	0
3	QQQ	404	SO4	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	MMM	411	GOL	1	0
4	HHH	413	GOL	1	0
3	OOO	403	SO4	4	0
4	MMM	408	GOL	2	0
4	CCC	410	GOL	2	0
3	DDD	401	SO4	1	0
4	XXX	411	GOL	4	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, 95th 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 ²)	Q<0.9
1	AAA	302/304 (99%)	0.66	12 (3%) 42 41	12, 24, 36, 50	1 (0%)
1	BBB	302/304 (99%)	0.86	19 (6%) 26 24	18, 28, 40, 57	2 (0%)
1	CCC	302/304 (99%)	0.91	23 (7%) 20 18	15, 30, 40, 53	1 (0%)
1	DDD	302/304 (99%)	0.69	15 (4%) 34 33	17, 25, 37, 55	2 (0%)
1	EEE	302/304 (99%)	0.75	17 (5%) 30 29	17, 26, 38, 57	0
1	FFF	302/304 (99%)	0.83	21 (6%) 22 21	18, 27, 41, 57	2 (0%)
1	GGG	302/304 (99%)	1.00	27 (8%) 15 13	20, 31, 43, 50	1 (0%)
1	HHH	302/304 (99%)	1.22	42 (13%) 6 5	22, 33, 47, 52	1 (0%)
1	III	302/304 (99%)	1.11	34 (11%) 10 8	22, 33, 46, 53	0
1	JJJ	302/304 (99%)	1.46	75 (24%) 2 1	25, 37, 49, 56	0
1	KKK	302/304 (99%)	1.03	34 (11%) 10 8	19, 29, 45, 55	2 (0%)
1	LLL	302/304 (99%)	0.86	19 (6%) 26 24	19, 28, 41, 55	0
1	MMM	302/304 (99%)	1.16	32 (10%) 11 9	23, 33, 46, 61	1 (0%)
1	NNN	302/304 (99%)	0.96	27 (8%) 15 13	15, 29, 40, 54	2 (0%)
1	OOO	303/304 (99%)	0.93	26 (8%) 16 14	17, 29, 40, 55	1 (0%)
1	PPP	302/304 (99%)	1.23	41 (13%) 7 5	16, 34, 49, 60	1 (0%)
1	QQQ	302/304 (99%)	1.14	41 (13%) 7 5	22, 32, 43, 61	0
1	RRR	302/304 (99%)	1.58	94 (31%) 1 1	25, 38, 50, 58	0
1	SSS	300/304 (98%)	1.24	49 (16%) 4 3	22, 33, 46, 58	1 (0%)
1	TTT	302/304 (99%)	0.94	30 (9%) 13 11	20, 29, 43, 54	0
1	UUU	303/304 (99%)	1.08	40 (13%) 7 6	19, 30, 45, 60	1 (0%)
1	VVV	302/304 (99%)	1.38	67 (22%) 2 2	22, 37, 49, 65	0
1	WWW	302/304 (99%)	1.23	56 (18%) 3 2	22, 33, 45, 58	0
1	XXX	302/304 (99%)	1.09	33 (10%) 10 9	19, 31, 41, 64	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	aaa	6/6 (100%)	-0.13	0 100 100	20, 22, 22, 24	0
2	bbb	6/6 (100%)	0.22	0 100 100	24, 25, 29, 30	0
2	ccc	6/6 (100%)	0.36	1 (16%) 4 3	25, 26, 29, 31	0
2	ddd	6/6 (100%)	0.29	0 100 100	22, 23, 25, 26	0
2	eee	6/6 (100%)	0.50	0 100 100	21, 22, 27, 28	0
2	fff	6/6 (100%)	0.27	0 100 100	26, 27, 29, 30	0
2	ggg	6/6 (100%)	0.51	0 100 100	25, 26, 27, 28	0
2	hhh	6/6 (100%)	0.50	0 100 100	27, 27, 30, 31	0
2	iii	6/6 (100%)	0.67	0 100 100	26, 28, 32, 34	0
2	jjj	6/6 (100%)	0.91	0 100 100	30, 30, 34, 37	0
2	kkk	6/6 (100%)	0.48	0 100 100	27, 29, 32, 32	0
2	lll	6/6 (100%)	1.01	0 100 100	25, 27, 30, 32	0
2	mmm	6/6 (100%)	0.35	0 100 100	28, 29, 30, 31	0
2	nnn	6/6 (100%)	0.48	0 100 100	24, 25, 28, 28	0
2	ooo	6/6 (100%)	0.45	0 100 100	25, 27, 30, 31	0
2	ppp	6/6 (100%)	0.63	0 100 100	29, 31, 32, 32	0
2	qqq	6/6 (100%)	0.41	0 100 100	25, 26, 30, 32	0
2	rrr	6/6 (100%)	0.60	0 100 100	28, 29, 31, 33	0
2	sss	6/6 (100%)	0.82	0 100 100	28, 30, 31, 32	0
2	ttt	6/6 (100%)	0.02	0 100 100	22, 23, 27, 28	0
2	uuu	6/6 (100%)	0.21	0 100 100	28, 30, 30, 31	0
2	vvv	6/6 (100%)	0.85	0 100 100	29, 31, 33, 35	0
2	www	6/6 (100%)	0.88	1 (16%) 4 3	28, 29, 34, 35	0
2	xxx	6/6 (100%)	0.67	0 100 100	25, 26, 32, 32	0
All	All	7392/7440 (99%)	1.05	876 (11%) 9 7	12, 31, 45, 65	19 (0%)

The worst 5 of 876 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	MMM	3	LEU	5.4
1	XXX	3	LEU	4.9
1	OOO	301	GLY	4.7
1	XXX	301	GLY	4.6
1	NNN	5	ILE	4.5

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, 95th 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($\text{\AA}^2$)	Q<0.9
3	SO4	TTT	406	5/5	0.65	0.23	68,70,70,71	0
3	SO4	RRR	406	5/5	0.68	0.26	55,55,55,56	5
3	SO4	SSS	411	5/5	0.77	0.17	70,70,70,70	5
3	SO4	SSS	407	5/5	0.77	0.16	77,77,78,78	0
3	SO4	FFF	407	5/5	0.79	0.24	36,36,36,36	5
4	GOL	UUU	414	6/6	0.79	0.25	50,50,51,51	0
3	SO4	PPP	406	5/5	0.80	0.17	60,61,61,61	5
3	SO4	FFF	404	5/5	0.80	0.27	48,48,49,49	5
3	SO4	NNN	408	5/5	0.81	0.30	33,33,33,33	5
3	SO4	GGG	401	5/5	0.81	0.16	46,47,48,48	5
3	SO4	HHH	410	5/5	0.81	0.15	60,61,61,61	5
3	SO4	UUU	410	5/5	0.81	0.28	48,48,49,49	5
3	SO4	VVV	403	5/5	0.81	0.16	68,68,69,69	0
3	SO4	SSS	406	5/5	0.81	0.18	68,68,68,69	0
3	SO4	DDD	406	5/5	0.82	0.16	65,66,66,67	0
3	SO4	RRR	401	5/5	0.82	0.16	65,66,66,66	0
3	SO4	UUU	405	5/5	0.82	0.15	56,56,57,57	0
3	SO4	AAA	409	5/5	0.82	0.13	59,59,59,60	0
3	SO4	AAA	410	5/5	0.82	0.18	49,49,49,50	5
4	GOL	DDD	411	6/6	0.82	0.19	55,55,55,55	0
4	GOL	TTT	408	6/6	0.82	0.16	32,33,33,34	0
3	SO4	PPP	405	5/5	0.82	0.23	53,53,54,54	5
3	SO4	XXX	406	5/5	0.83	0.18	56,56,57,58	0
3	SO4	TTT	407	5/5	0.83	0.23	35,35,36,36	5
4	GOL	DDD	412	6/6	0.83	0.19	39,40,41,42	0
4	GOL	EEE	408	6/6	0.83	0.24	37,37,37,37	6
4	GOL	GGG	403	6/6	0.83	0.16	33,34,35,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	LLL	410	5/5	0.83	0.18	55,55,56,56	5
3	SO4	XXX	404	5/5	0.83	0.17	68,68,69,70	0
3	SO4	OOO	407	5/5	0.84	0.23	43,43,44,44	5
3	SO4	KKK	411	5/5	0.84	0.15	46,47,47,47	5
3	SO4	OOO	406	5/5	0.84	0.18	44,44,44,44	5
4	GOL	AAA	415	6/6	0.84	0.17	30,32,32,33	0
4	GOL	HHH	412	6/6	0.84	0.15	33,33,33,33	0
4	GOL	SSS	412	6/6	0.84	0.18	42,43,43,44	0
4	GOL	SSS	413	6/6	0.84	0.18	47,47,47,47	0
4	GOL	AAA	417	6/6	0.84	0.15	31,32,33,33	0
4	GOL	CCC	410	6/6	0.84	0.13	34,34,35,35	0
4	GOL	VVV	407	6/6	0.84	0.18	29,30,30,30	0
3	SO4	DDD	407	5/5	0.85	0.16	45,45,45,46	5
3	SO4	MMM	406	5/5	0.85	0.14	54,54,54,54	5
3	SO4	HHH	405	5/5	0.85	0.14	63,64,65,65	0
3	SO4	HHH	407	5/5	0.85	0.16	57,58,58,58	0
3	SO4	FFF	405	5/5	0.85	0.15	47,47,48,48	5
3	SO4	UUU	408	5/5	0.85	0.23	36,37,37,37	5
3	SO4	UUU	409	5/5	0.85	0.11	68,68,69,69	0
4	GOL	JJJ	410	6/6	0.85	0.17	39,40,41,41	0
4	GOL	PPP	410	6/6	0.85	0.16	35,36,37,37	0
3	SO4	JJJ	404	5/5	0.85	0.14	66,66,66,66	0
3	SO4	JJJ	406	5/5	0.85	0.12	60,61,61,61	5
3	SO4	KKK	406	5/5	0.85	0.18	36,36,37,37	5
3	SO4	EEE	406	5/5	0.85	0.17	43,43,43,43	5
3	SO4	LLL	407	5/5	0.85	0.17	49,49,50,50	5
3	SO4	KKK	408	5/5	0.86	0.22	39,39,40,40	5
3	SO4	KKK	409	5/5	0.86	0.16	47,47,47,47	5
4	GOL	FFF	409	6/6	0.86	0.17	54,54,54,54	0
3	SO4	XXX	407	5/5	0.86	0.14	54,54,55,56	0
3	SO4	nnn	201	5/5	0.86	0.20	38,38,39,39	5
3	SO4	NNN	406	5/5	0.86	0.16	26,27,27,27	5
4	GOL	MMM	411	6/6	0.86	0.20	54,54,55,55	0
4	GOL	AAA	416	6/6	0.86	0.14	35,35,36,36	0
3	SO4	DDD	408	5/5	0.86	0.12	60,60,61,61	5
4	GOL	BBB	409	6/6	0.86	0.18	34,35,35,35	0
4	GOL	BBB	410	6/6	0.86	0.17	53,54,54,55	0
3	SO4	CCC	401	5/5	0.86	0.14	54,54,54,55	0
3	SO4	WWW	402	5/5	0.86	0.14	63,64,64,64	0
4	GOL	WWW	405	6/6	0.86	0.17	28,28,28,28	6
3	SO4	III	404	5/5	0.87	0.11	56,56,57,57	0
3	SO4	III	406	5/5	0.87	0.15	53,53,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	SSS	408	5/5	0.87	0.14	42,42,42,43	5
3	SO4	III	407	5/5	0.87	0.25	27,27,28,28	5
3	SO4	TTT	404	5/5	0.87	0.16	65,66,67,67	0
4	GOL	KKK	412	6/6	0.87	0.14	35,37,37,38	0
4	GOL	KKK	413	6/6	0.87	0.17	34,35,36,37	6
4	GOL	MMM	408	6/6	0.87	0.17	38,39,40,40	0
3	SO4	TTT	405	5/5	0.87	0.14	59,59,60,60	0
4	GOL	NNN	412	6/6	0.87	0.16	46,47,47,48	0
3	SO4	LLL	406	5/5	0.87	0.19	37,37,38,38	5
4	GOL	RRR	410	6/6	0.87	0.19	49,49,49,49	0
3	SO4	CCC	406	5/5	0.87	0.16	50,50,51,51	5
3	SO4	HHH	408	5/5	0.87	0.21	52,52,53,53	5
3	SO4	QQQ	406	5/5	0.87	0.15	58,58,59,59	5
3	SO4	MMM	401	5/5	0.87	0.14	53,53,53,54	0
3	SO4	BBB	405	5/5	0.87	0.15	43,43,43,43	5
3	SO4	SSS	405	5/5	0.87	0.12	59,60,60,61	0
3	SO4	MMM	407	5/5	0.88	0.13	43,43,43,44	5
3	SO4	LLL	409	5/5	0.88	0.20	46,47,47,48	5
3	SO4	OOO	408	5/5	0.88	0.19	47,47,47,47	5
3	SO4	RRR	407	5/5	0.88	0.14	53,53,53,53	5
4	GOL	PPP	409	6/6	0.88	0.13	34,35,36,36	0
3	SO4	VVV	406	5/5	0.88	0.13	62,62,62,62	5
3	SO4	AAA	414	5/5	0.88	0.17	34,35,35,36	5
4	GOL	HHH	413	6/6	0.88	0.19	37,37,38,38	6
4	GOL	III	409	6/6	0.88	0.15	34,35,36,37	0
4	GOL	SSS	414	6/6	0.88	0.16	47,48,48,48	0
4	GOL	III	410	6/6	0.88	0.14	29,30,30,30	0
4	GOL	JJJ	409	6/6	0.88	0.14	41,41,41,42	0
3	SO4	OOO	404	5/5	0.88	0.15	36,37,37,37	5
3	SO4	QQQ	405	5/5	0.88	0.11	58,58,59,59	0
3	SO4	RRR	409	5/5	0.89	0.15	59,60,60,60	5
3	SO4	SSS	404	5/5	0.89	0.11	42,42,42,43	0
3	SO4	AAA	407	5/5	0.89	0.15	33,33,33,33	5
3	SO4	XXX	409	5/5	0.89	0.16	45,45,45,46	5
4	GOL	EEE	409	6/6	0.89	0.18	47,47,47,47	0
3	SO4	III	201	5/5	0.89	0.13	40,40,41,42	0
4	GOL	FFF	410	6/6	0.89	0.13	26,26,26,26	0
3	SO4	EEE	405	5/5	0.89	0.25	26,26,27,27	5
4	GOL	HHH	411	6/6	0.89	0.14	30,31,32,35	0
3	SO4	MMM	404	5/5	0.89	0.14	65,65,65,65	0
3	SO4	DDD	404	5/5	0.89	0.12	46,46,48,48	0
3	SO4	FFF	402	5/5	0.89	0.13	42,42,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	UUU	413	6/6	0.89	0.13	32,33,33,34	0
4	GOL	BBB	408	6/6	0.89	0.13	28,29,29,30	0
4	GOL	UUU	415	6/6	0.89	0.19	45,45,45,45	6
3	SO4	NNN	404	5/5	0.89	0.12	53,53,54,54	0
3	SO4	PPP	401	5/5	0.89	0.12	47,47,49,49	0
4	GOL	XXX	411	6/6	0.89	0.15	30,30,30,30	0
3	SO4	KKK	401	5/5	0.90	0.12	46,46,47,47	0
3	SO4	LLL	408	5/5	0.90	0.14	53,53,53,53	5
3	SO4	NNN	410	5/5	0.90	0.16	44,44,45,45	5
3	SO4	RRR	408	5/5	0.90	0.14	55,55,55,55	5
3	SO4	AAA	403	5/5	0.90	0.13	58,58,58,58	0
4	GOL	NNN	411	6/6	0.90	0.11	26,27,28,28	0
3	SO4	HHH	404	5/5	0.90	0.12	39,40,41,41	0
3	SO4	HHH	409	5/5	0.90	0.12	47,48,48,48	5
3	SO4	WWW	404	5/5	0.90	0.12	55,55,56,56	5
4	GOL	QQQ	410	6/6	0.90	0.14	34,35,36,36	0
3	SO4	KKK	410	5/5	0.90	0.20	38,38,38,39	5
3	SO4	MMM	405	5/5	0.90	0.18	48,48,48,48	5
3	SO4	AAA	412	5/5	0.90	0.17	23,24,25,25	5
4	GOL	GGG	404	6/6	0.90	0.13	45,45,45,45	0
3	SO4	LLL	405	5/5	0.90	0.14	43,44,44,45	5
3	SO4	PPP	408	5/5	0.90	0.10	57,57,57,57	5
3	SO4	NNN	403	5/5	0.90	0.13	41,42,44,45	0
4	GOL	HHH	414	6/6	0.90	0.15	42,43,43,44	0
3	SO4	III	402	5/5	0.90	0.12	55,55,56,56	0
3	SO4	QQQ	408	5/5	0.90	0.14	51,51,51,52	5
4	GOL	WWW	406	6/6	0.90	0.14	46,46,46,46	0
3	SO4	UUU	404	5/5	0.90	0.12	46,46,46,46	0
3	SO4	AAA	413	5/5	0.91	0.15	39,39,40,40	5
3	SO4	WWW	403	5/5	0.91	0.14	34,35,35,35	5
3	SO4	CCC	408	5/5	0.91	0.11	52,52,52,52	5
3	SO4	XXX	403	5/5	0.91	0.12	42,43,43,43	0
3	SO4	AAA	406	5/5	0.91	0.11	47,48,49,49	0
3	SO4	NNN	409	5/5	0.91	0.15	31,31,31,32	5
4	GOL	JJJ	408	6/6	0.91	0.17	48,48,49,49	0
3	SO4	AAA	404	5/5	0.91	0.13	20,20,20,20	5
3	SO4	XXX	408	5/5	0.91	0.21	23,23,23,24	5
3	SO4	BBB	406	5/5	0.91	0.15	48,48,48,49	5
3	SO4	OOO	405	5/5	0.91	0.10	48,49,49,49	0
3	SO4	GGG	402	5/5	0.91	0.17	37,38,39,39	0
4	GOL	MMM	409	6/6	0.91	0.14	34,37,37,39	0
4	GOL	MMM	410	6/6	0.91	0.13	36,36,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	vvv	201	5/5	0.91	0.16	29,29,29,29	5
3	SO4	HHH	403	5/5	0.91	0.10	51,51,52,52	0
3	SO4	SSS	409	5/5	0.91	0.12	44,44,44,44	5
3	SO4	SSS	410	5/5	0.91	0.16	50,50,50,50	5
3	SO4	JJJ	401	5/5	0.91	0.11	44,44,45,45	0
3	SO4	OOO	409	5/5	0.91	0.11	57,57,57,57	5
3	SO4	JJJ	403	5/5	0.91	0.11	45,45,45,45	0
3	SO4	BBB	407	5/5	0.91	0.12	42,42,43,43	5
4	GOL	CCC	411	6/6	0.91	0.13	27,28,28,29	0
3	SO4	JJJ	405	5/5	0.91	0.13	53,53,53,53	5
3	SO4	AAA	408	5/5	0.91	0.12	45,45,47,47	0
3	SO4	QQQ	401	5/5	0.91	0.11	41,42,42,43	0
3	SO4	HHH	406	5/5	0.91	0.10	40,40,42,42	0
4	GOL	FFF	408	6/6	0.91	0.10	24,24,25,25	0
3	SO4	KKK	405	5/5	0.91	0.14	31,31,32,32	5
3	SO4	QQQ	407	5/5	0.91	0.11	58,59,59,59	5
3	SO4	CCC	405	5/5	0.91	0.10	62,62,63,63	0
3	SO4	KKK	407	5/5	0.91	0.11	52,52,53,54	0
4	GOL	CCC	409	6/6	0.92	0.12	27,27,28,28	0
3	SO4	ggg	201	5/5	0.92	0.13	36,37,37,38	0
3	SO4	SSS	402	5/5	0.92	0.13	34,35,36,37	0
3	SO4	QQQ	403	5/5	0.92	0.13	38,38,38,39	0
4	GOL	TTT	409	6/6	0.92	0.12	39,40,40,40	0
3	SO4	XXX	402	5/5	0.92	0.11	41,41,42,42	0
3	SO4	RRR	405	5/5	0.92	0.15	28,28,28,29	5
3	SO4	FFF	406	5/5	0.92	0.11	47,47,47,48	5
3	SO4	III	403	5/5	0.92	0.10	47,48,48,48	0
3	SO4	VVV	405	5/5	0.92	0.12	38,39,39,40	5
3	SO4	NNN	402	5/5	0.92	0.10	42,42,43,43	0
3	SO4	AAA	411	5/5	0.92	0.27	47,47,48,48	5
3	SO4	UUU	412	5/5	0.93	0.11	44,44,44,44	5
4	GOL	QQQ	409	6/6	0.93	0.12	36,37,37,37	0
3	SO4	VVV	401	5/5	0.93	0.13	38,38,39,39	5
3	SO4	NNN	405	5/5	0.93	0.10	26,26,27,27	5
3	SO4	VVV	404	5/5	0.93	0.11	38,38,38,39	5
3	SO4	KKK	402	5/5	0.93	0.12	39,40,41,41	0
3	SO4	NNN	407	5/5	0.93	0.10	48,48,48,49	0
3	SO4	III	408	5/5	0.93	0.15	42,42,42,43	5
3	SO4	HHH	402	5/5	0.93	0.10	44,44,44,44	0
3	SO4	LLL	402	5/5	0.93	0.10	48,48,48,49	0
3	SO4	RRR	403	5/5	0.93	0.10	36,37,38,38	0
3	SO4	OOO	403	5/5	0.93	0.30	33,34,34,35	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	JJJ	402	5/5	0.93	0.10	49,49,50,50	0
3	SO4	DDD	409	5/5	0.93	0.10	45,46,46,46	5
4	GOL	OOO	410	6/6	0.93	0.09	21,22,23,23	0
3	SO4	UUU	411	5/5	0.93	0.14	43,43,43,44	5
3	SO4	XXX	405	5/5	0.94	0.11	36,37,38,38	0
3	SO4	UUU	407	5/5	0.94	0.09	50,50,51,52	0
3	SO4	FFF	403	5/5	0.94	0.10	41,41,43,43	0
3	SO4	SSS	403	5/5	0.94	0.08	47,48,48,48	0
3	SO4	AAA	405	5/5	0.94	0.15	30,30,31,31	5
3	SO4	aaa	201	5/5	0.94	0.11	35,36,36,38	0
3	SO4	ccc	201	5/5	0.94	0.10	49,49,50,50	0
3	SO4	AAA	402	5/5	0.94	0.10	34,34,34,35	0
3	SO4	BBB	403	5/5	0.94	0.12	40,40,41,41	0
3	SO4	DDD	410	5/5	0.94	0.10	48,49,49,50	5
3	SO4	VVV	402	5/5	0.94	0.09	49,49,49,49	0
3	SO4	EEE	403	5/5	0.94	0.12	35,36,37,37	0
3	SO4	BBB	404	5/5	0.94	0.09	46,47,48,48	0
3	SO4	III	401	5/5	0.94	0.12	34,35,35,35	0
3	SO4	RRR	402	5/5	0.94	0.10	24,24,25,25	5
3	SO4	PPP	402	5/5	0.94	0.10	42,42,43,43	0
3	SO4	PPP	403	5/5	0.94	0.09	44,45,45,46	0
3	SO4	PPP	404	5/5	0.94	0.11	30,31,31,31	5
3	SO4	DDD	405	5/5	0.94	0.10	50,50,51,52	0
4	GOL	LLL	411	6/6	0.94	0.09	24,24,24,25	0
3	SO4	CCC	403	5/5	0.94	0.10	38,38,38,40	0
4	GOL	XXX	410	6/6	0.94	0.08	21,22,22,23	0
3	SO4	PPP	407	5/5	0.94	0.10	44,44,44,44	5
3	SO4	CCC	402	5/5	0.95	0.12	34,35,36,36	0
3	SO4	SSS	401	5/5	0.95	0.11	39,39,40,41	0
3	SO4	TTT	403	5/5	0.95	0.09	42,42,42,43	0
3	SO4	EEE	402	5/5	0.95	0.09	39,39,40,40	0
3	SO4	DDD	401	5/5	0.95	0.10	36,37,37,37	0
3	SO4	HHH	401	5/5	0.95	0.10	40,41,41,42	0
3	SO4	CCC	404	5/5	0.95	0.11	37,38,38,38	0
3	SO4	UUU	401	5/5	0.95	0.16	30,30,31,32	0
3	SO4	QQQ	402	5/5	0.95	0.09	46,46,46,46	0
3	SO4	CCC	407	5/5	0.95	0.14	44,44,44,44	5
3	SO4	WWW	401	5/5	0.95	0.10	39,39,40,40	0
3	SO4	LLL	404	5/5	0.95	0.12	33,35,36,36	0
3	SO4	MMM	402	5/5	0.95	0.07	49,49,49,50	0
4	GOL	JJJ	407	6/6	0.95	0.10	32,33,33,33	0
4	GOL	EEE	407	6/6	0.95	0.10	25,25,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	TTT	401	5/5	0.96	0.10	34,35,36,37	0
3	SO4	TTT	402	5/5	0.96	0.11	29,30,31,31	0
3	SO4	OOO	401	5/5	0.96	0.10	35,35,37,37	0
3	SO4	OOO	402	5/5	0.96	0.11	36,36,37,38	0
3	SO4	EEE	404	5/5	0.96	0.10	38,39,39,40	0
3	SO4	III	405	5/5	0.96	0.08	44,45,45,47	0
3	SO4	MMM	403	5/5	0.96	0.14	37,38,39,41	0
3	SO4	ggg	202	5/5	0.96	0.09	22,23,23,23	5
3	SO4	EEE	401	5/5	0.96	0.09	39,40,40,40	0
3	SO4	UUU	403	5/5	0.96	0.10	42,42,43,43	0
3	SO4	KKK	403	5/5	0.96	0.08	35,36,36,37	0
3	SO4	RRR	404	5/5	0.96	0.14	25,26,26,26	5
3	SO4	UUU	406	5/5	0.96	0.13	38,39,39,39	0
3	SO4	DDD	403	5/5	0.96	0.08	40,40,41,41	0
3	SO4	DDD	402	5/5	0.96	0.09	43,43,44,44	0
3	SO4	LLL	403	5/5	0.96	0.09	39,39,40,40	0
3	SO4	QQQ	404	5/5	0.96	0.08	43,43,44,44	0
3	SO4	UUU	402	5/5	0.97	0.07	40,41,41,41	0
3	SO4	FFF	401	5/5	0.97	0.09	38,38,39,39	0
3	SO4	BBB	402	5/5	0.97	0.07	39,40,40,41	0
3	SO4	AAA	401	5/5	0.97	0.08	19,20,20,20	5
3	SO4	NNN	401	5/5	0.97	0.08	28,28,29,29	0
3	SO4	BBB	401	5/5	0.97	0.09	31,32,32,32	0
3	SO4	KKK	404	5/5	0.97	0.09	36,36,37,37	0
3	SO4	XXX	401	5/5	0.97	0.09	36,36,37,38	0
3	SO4	LLL	401	5/5	0.98	0.05	42,42,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.