



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2026 – 08:23 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 Full wwPDB X-ray Structure Validation 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:

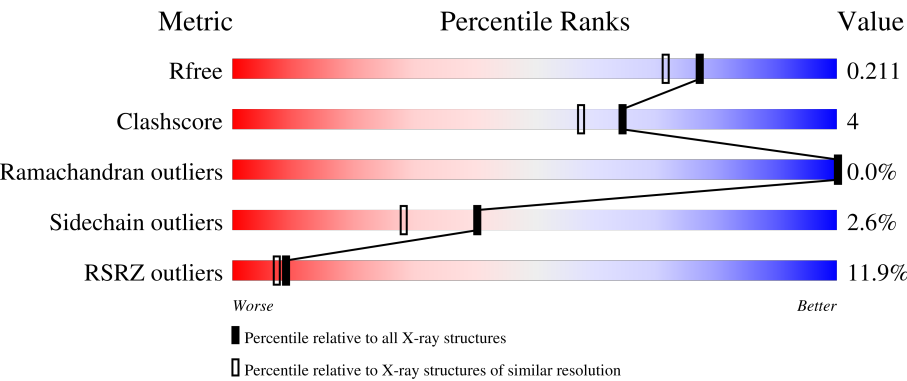
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

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	
1	FFF	304	
1	GGG	304	
1	HHH	304	
1	III	304	
1	JJJ	304	
1	KKK	304	
1	LLL	304	
1	MMM	304	
1	NNN	304	
1	OOO	304	
1	PPP	304	
1	QQQ	304	
1	RRR	304	
1	SSS	304	
1	TTT	304	
1	UUU	304	
1	VVV	304	
1	WWW	304	
1	XXX	304	
2	aaa	6	
2	bbb	6	
2	ccc	6	
2	ddd	6	
2	eee	6	

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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:

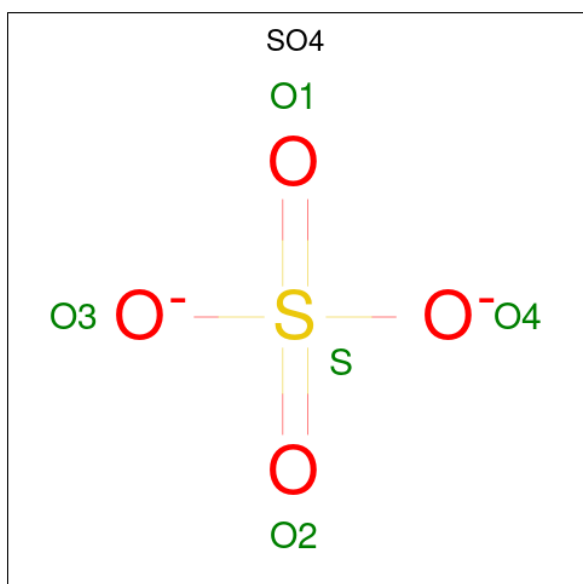
Chain	Residue	Modelled	Actual	Comment	Reference
aaa	196	ILE	VAL	conflict	UNP O75012
bbb	196	ILE	VAL	conflict	UNP O75012
ccc	196	ILE	VAL	conflict	UNP O75012
ddd	196	ILE	VAL	conflict	UNP O75012
eee	196	ILE	VAL	conflict	UNP O75012
fff	196	ILE	VAL	conflict	UNP O75012
ggg	196	ILE	VAL	conflict	UNP O75012
hhh	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 5 4 1	0	0
3	AAA	1	Total O S 5 4 1	0	0
3	AAA	1	Total O S 5 4 1	0	0
3	AAA	1	Total O S 5 4 1	0	0
3	AAA	1	Total O S 5 4 1	0	0
3	AAA	1	Total O S 5 4 1	0	0

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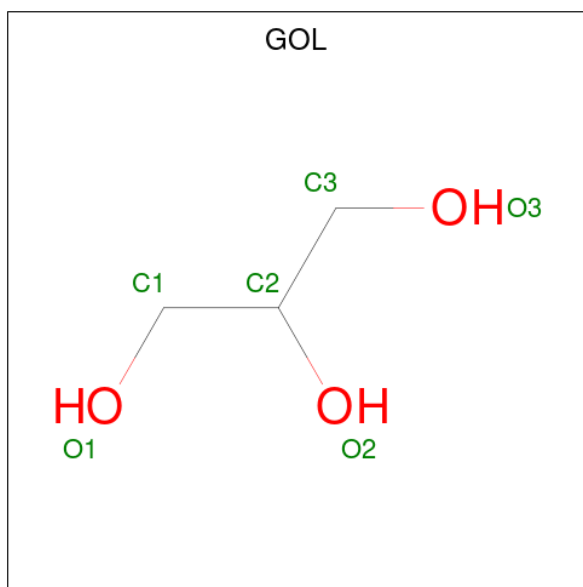
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			5	4	1		
3	UUU	1	Total	O	S	0	0
			5	4	1		
3	UUU	1	Total	O	S	0	0
			5	4	1		
3	UUU	1	Total	O	S	0	0
			5	4	1		
3	UUU	1	Total	O	S	0	0
			5	4	1		
3	VVV	1	Total	O	S	0	0
			5	4	1		
3	VVV	1	Total	O	S	0	0
			5	4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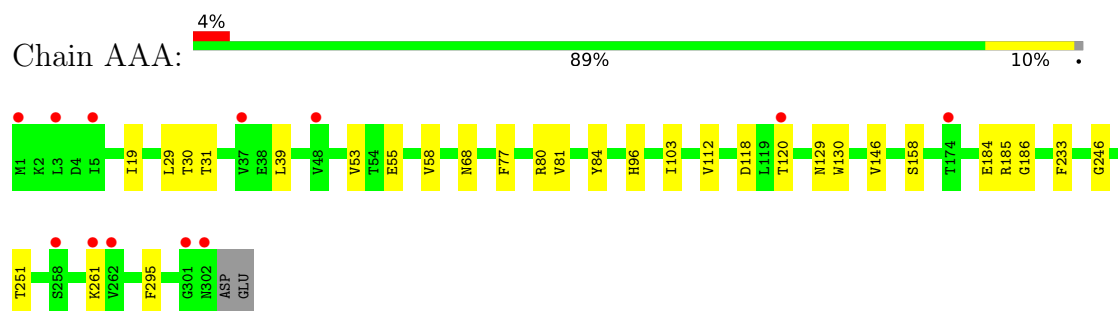
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	xxx	5	Total	O	0	0
			5	5		

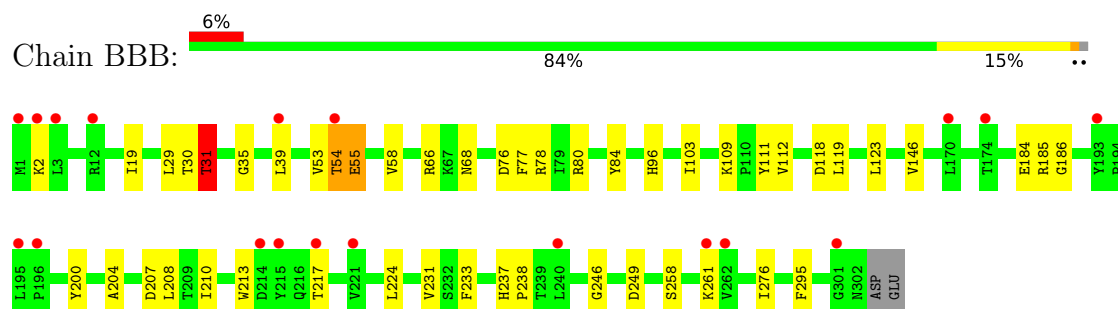
3 Residue-property plots [i](#)

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.

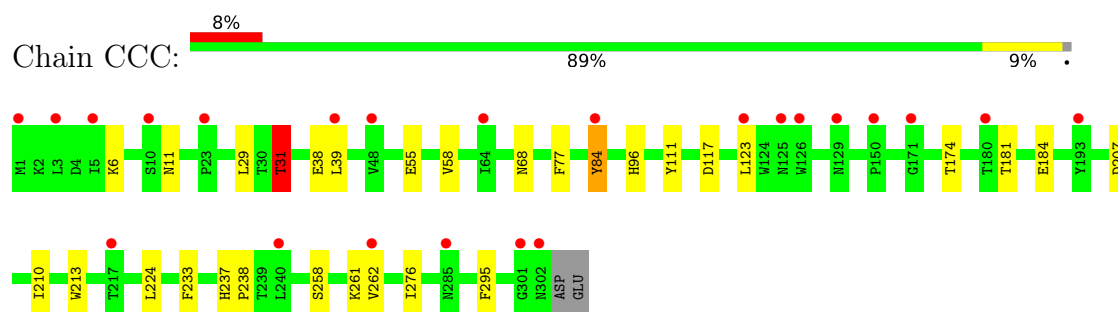
- Molecule 1: Coatomer subunit beta'



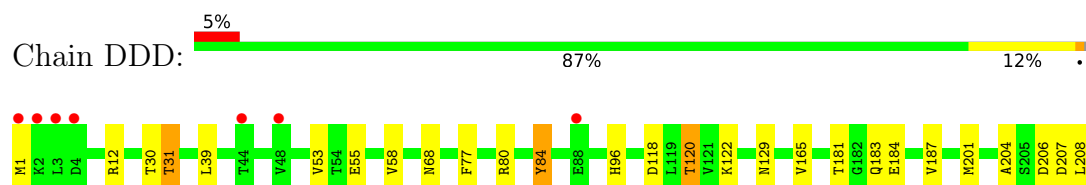
- Molecule 1: Coatomer subunit beta'

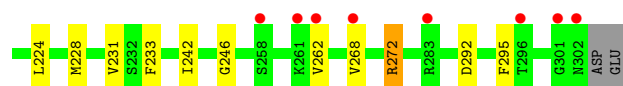


- Molecule 1: Coatomer subunit beta'

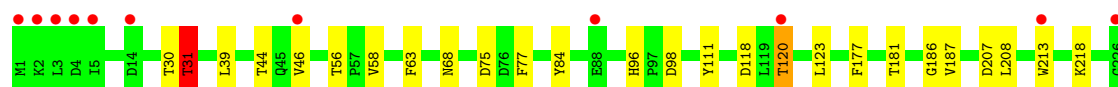
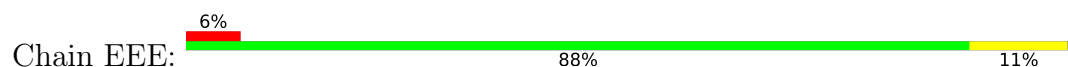


- Molecule 1: Coatomer subunit beta'





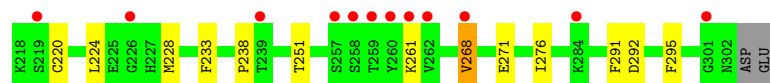
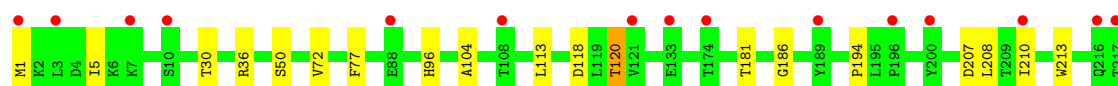
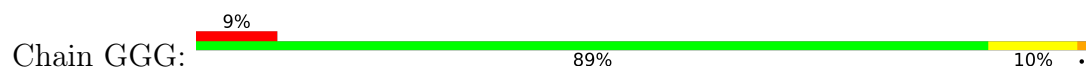
- Molecule 1: Coatomer subunit beta'



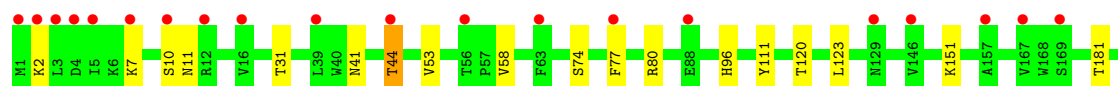
- Molecule 1: Coatomer subunit beta'



- Molecule 1: Coatomer subunit beta'

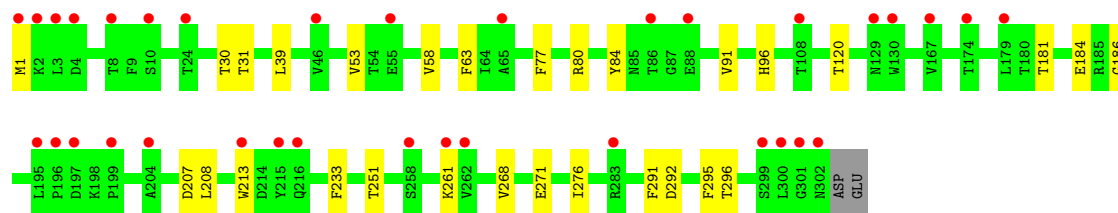


- Molecule 1: Coatomer subunit beta'

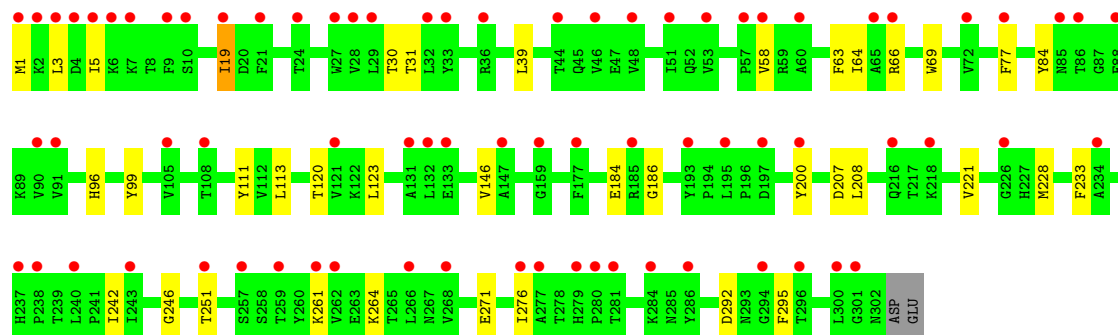


- Molecule 1: Coatomer subunit beta'

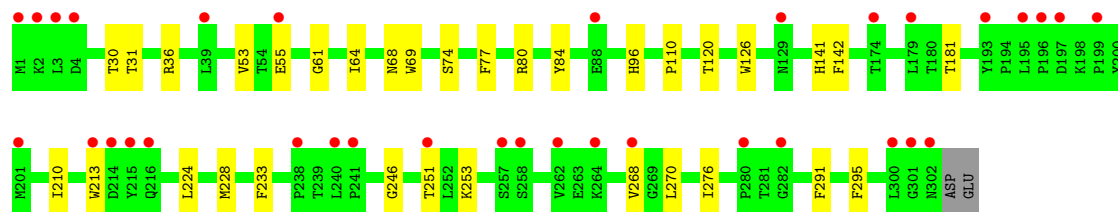




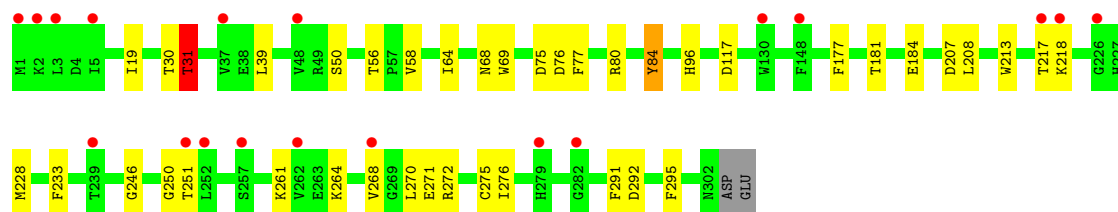
• Molecule 1: Coatomer subunit beta'



• Molecule 1: Coatomer subunit beta'

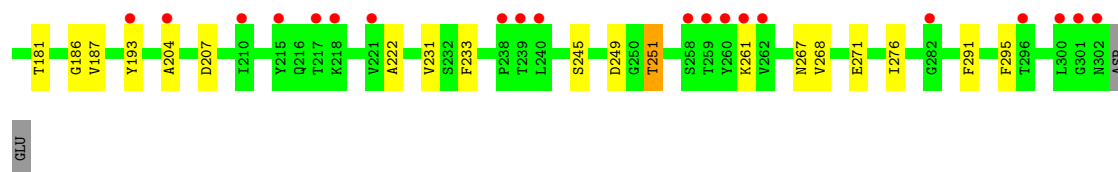


• Molecule 1: Coatomer subunit beta'

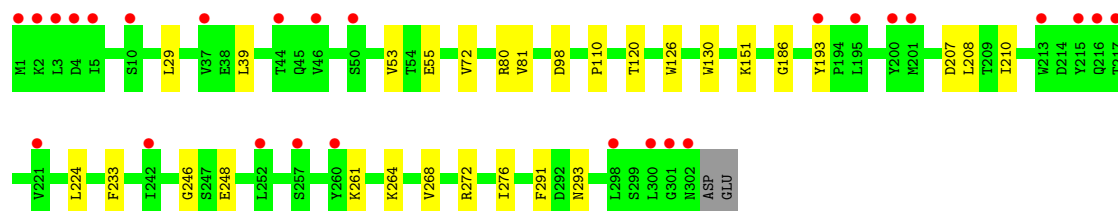


• Molecule 1: Coatomer subunit beta'

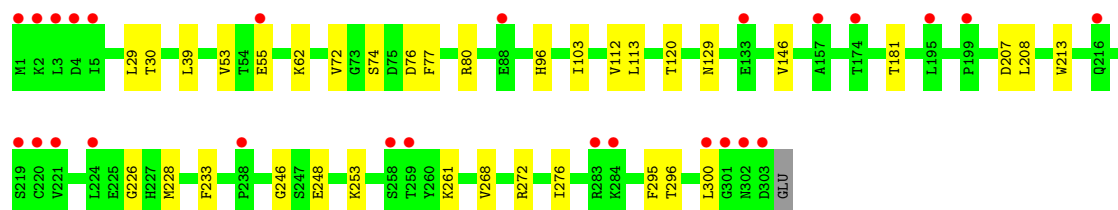




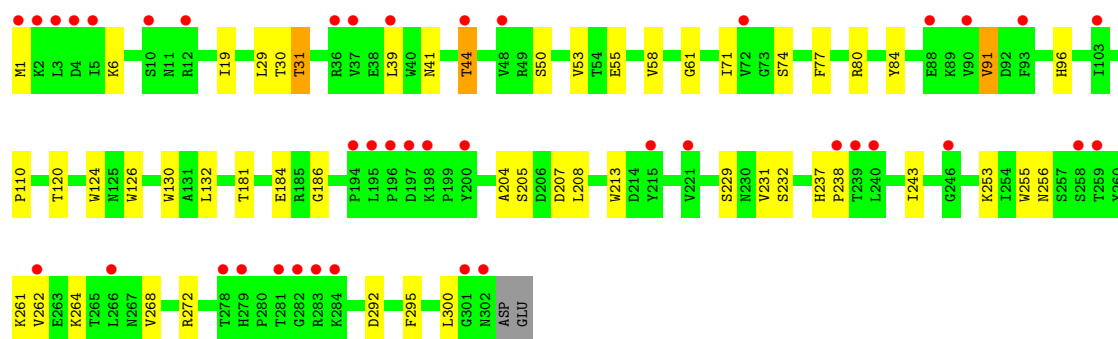
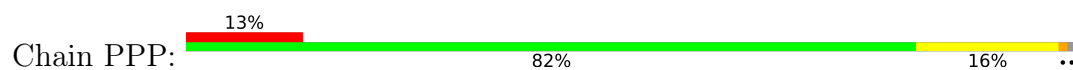
- Molecule 1: Coatomer subunit beta'



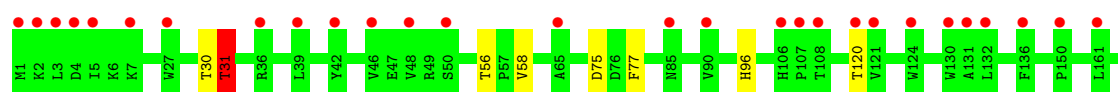
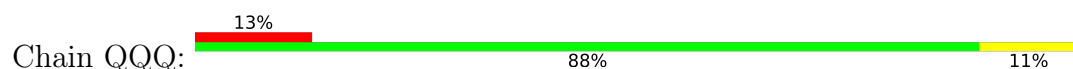
- Molecule 1: Coatomer subunit beta'

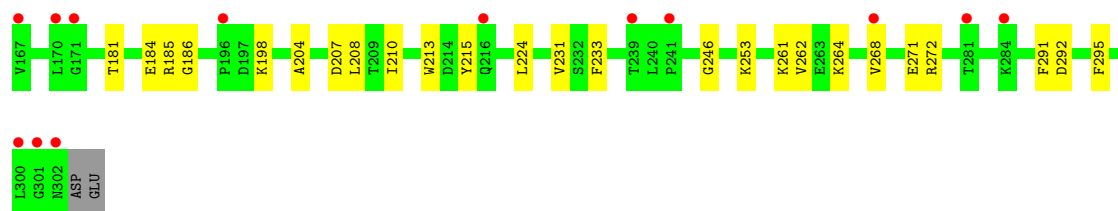


- Molecule 1: Coatomer subunit beta'



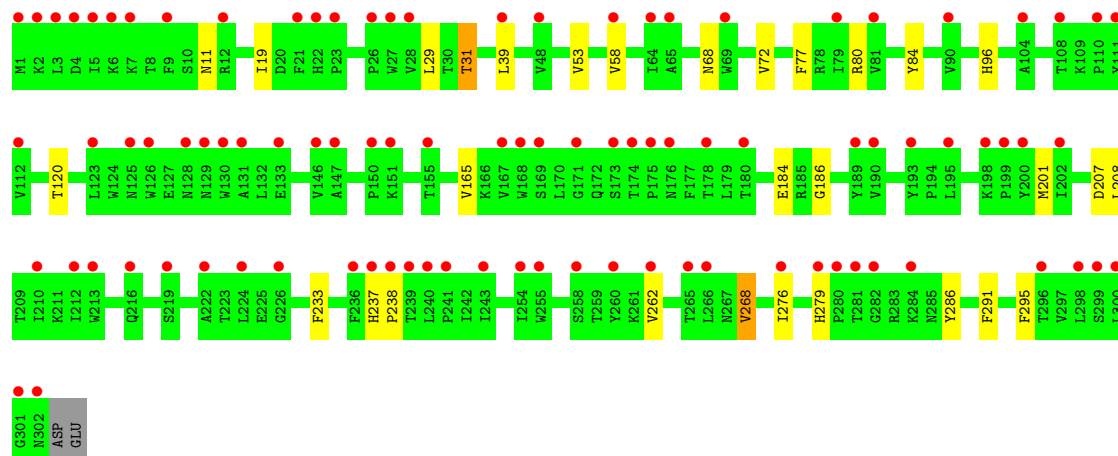
- Molecule 1: Coatomer subunit beta'





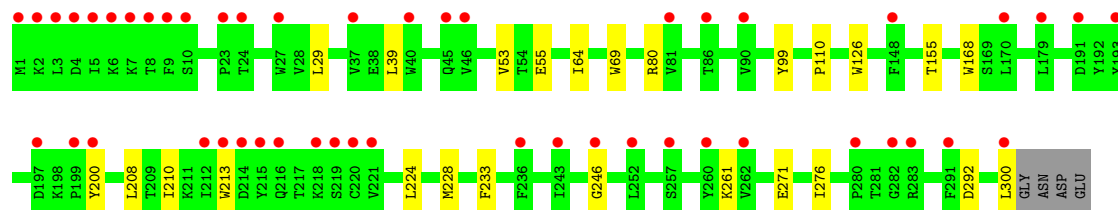
• Molecule 1: Coatomer subunit beta'

Chain RRR: 31% 89% 9%



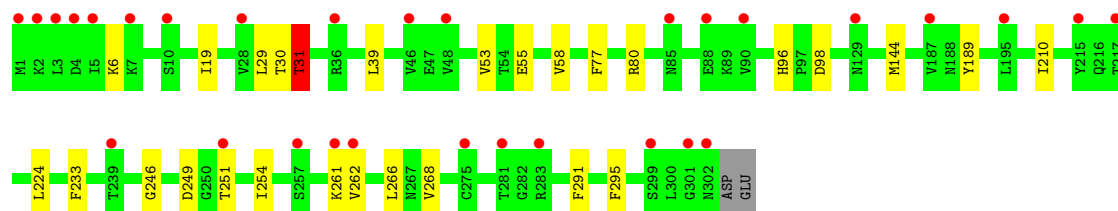
• Molecule 1: Coatomer subunit beta'

Chain SSS: 16% 90% 8%



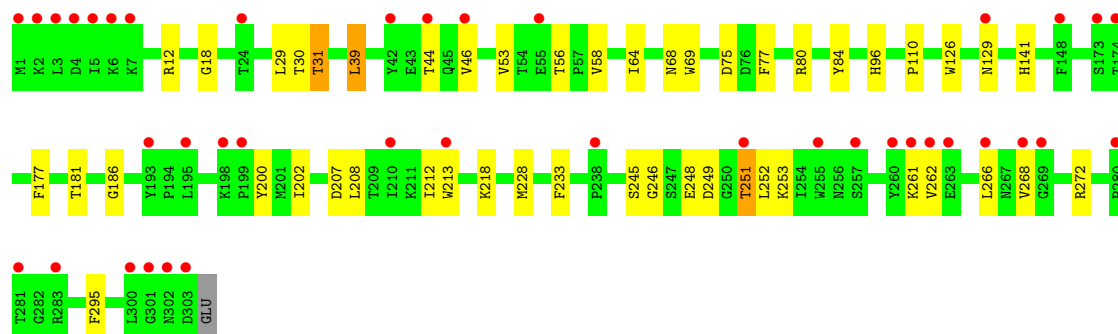
• Molecule 1: Coatomer subunit beta'

Chain TTT: 10% 90% 9%

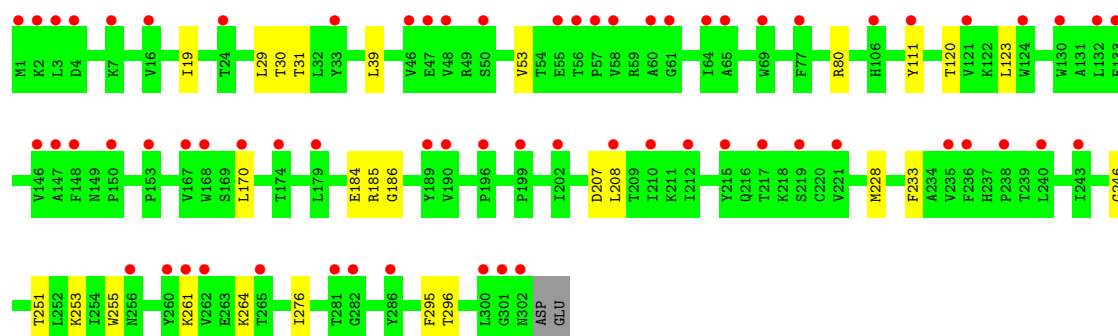


• Molecule 1: Coatomer subunit beta'

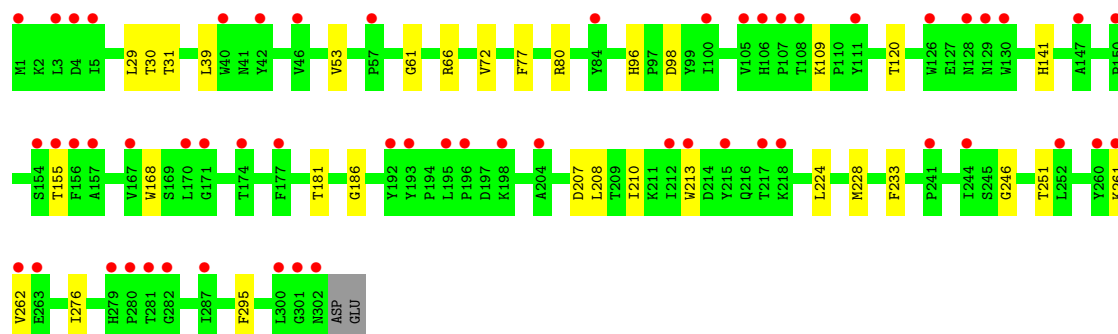
Chain UUU: 13% 84% 15%



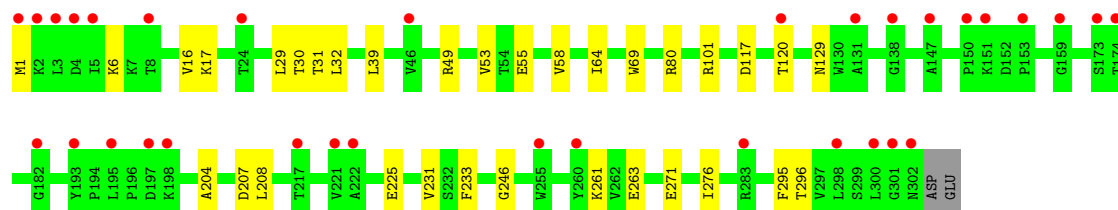
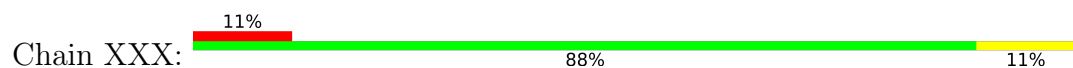
• Molecule 1: Coatomer subunit beta'



• Molecule 1: Coatomer subunit beta'



• Molecule 1: Coatomer subunit beta'



- Molecule 2: Small ribosomal subunit protein mS37

Chain aaa:  83% 17%



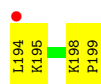
- Molecule 2: Small ribosomal subunit protein mS37

Chain bbb:  67% 33%

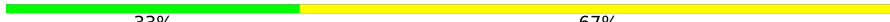


- Molecule 2: Small ribosomal subunit protein mS37

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%

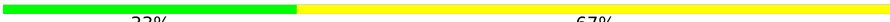


- Molecule 2: Small ribosomal subunit protein mS37

Chain ggg:  67% 33%



- Molecule 2: Small ribosomal subunit protein mS37

Chain hhh:  33% 67%



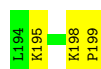
- Molecule 2: Small ribosomal subunit protein mS37

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%



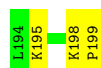
- Molecule 2: Small ribosomal subunit protein mS37

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%



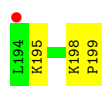
- Molecule 2: Small ribosomal subunit protein mS37

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.

All (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
1	PPP	186	GLY	CA-C-O	-5.81	118.22	122.23
1	RRR	72	VAL	CA-C-N	5.79	125.59	121.65
1	RRR	72	VAL	C-N-CA	5.79	125.59	121.65
1	III	186	GLY	CA-C-O	-5.76	118.25	122.23
1	WWW	72	VAL	CA-C-N	5.67	125.51	121.65
1	WWW	72	VAL	C-N-CA	5.67	125.51	121.65
1	GGG	72	VAL	CA-C-N	5.64	125.49	121.65
1	GGG	72	VAL	C-N-CA	5.64	125.49	121.65
1	FFF	186	GLY	CA-C-O	-5.64	118.07	122.52
1	JJJ	186	GLY	CA-C-O	-5.63	118.35	122.23
1	QQQ	186	GLY	CA-C-O	-5.61	118.41	122.45
1	BBB	31	THR	CB-CA-C	5.57	120.59	111.23
1	BBB	186	GLY	CA-C-O	-5.55	118.45	122.45
1	UUU	186	GLY	CA-C-O	-5.52	118.48	122.45
1	VVV	186	GLY	CA-C-O	-5.50	118.65	122.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	EEE	186	GLY	CA-C-O	-5.49	118.50	122.45
1	TTT	31	THR	CB-CA-C	5.42	120.34	111.23
1	CCC	31	THR	CB-CA-C	5.40	119.48	111.17
1	WWW	186	GLY	CA-C-O	-5.37	118.28	122.52
1	AAA	186	GLY	CA-C-O	-5.36	118.29	122.52
1	MMM	186	GLY	CA-C-O	-5.29	118.34	122.52
1	RRR	186	GLY	CA-C-O	-5.28	118.35	122.52
1	GGG	186	GLY	CA-C-O	-5.25	118.38	122.52
1	NNN	186	GLY	CA-C-O	-5.23	118.39	122.52
1	XXX	17	LYS	CA-C-N	5.12	125.13	121.65
1	XXX	17	LYS	C-N-CA	5.12	125.13	121.65
1	UUU	245	SER	CA-C-N	5.09	125.11	121.65
1	UUU	245	SER	C-N-CA	5.09	125.11	121.65
1	MMM	245	SER	CA-C-N	5.02	125.06	121.65
1	MMM	245	SER	C-N-CA	5.02	125.06	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

All (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
1:UUU:31:THR:HG22	1:UUU:58:VAL:HB	1.70	0.73
1:MMM:77:PHE:HB3	1:MMM:96:HIS:O	1.90	0.71
1:CCC:207:ASP:HB2	4:CCC:410:GOL:H31	1.72	0.71
1:DDD:77:PHE:HB3	1:DDD:96:HIS:O	1.91	0.70
1:PPP:272:ARG:HD3	1:PPP:292:ASP:OD2	1.91	0.70
1:JJJ:77:PHE:HB3	1:JJJ:96:HIS:O	1.92	0.69
1:PPP:205:SER:O	1:PPP:231:VAL:HG12	1.92	0.68
1:KKK:77:PHE:HB3	1:KKK:96:HIS:O	1.93	0.67
1:EEE:77:PHE:HB3	1:EEE:96:HIS:O	1.95	0.66
1:EEE:233:PHE:CZ	1:EEE:246:GLY:HA3	2.30	0.66
1:BBB:77:PHE:HB3	1:BBB:96:HIS:O	1.94	0.66
3:EEE:405:SO4:O3	2:hhh:196:ILE:HG12	1.97	0.65
1:RRR:77:PHE:HB3	1:RRR:96:HIS:O	1.97	0.65
1:RRR:31:THR:HG22	1:RRR:58:VAL:HB	1.78	0.64
1:WWW:29:LEU:HD13	1:WWW:39:LEU:HD21	1.77	0.64
1:OOO:80:ARG:N	3:OOO:403:SO4:O3	2.31	0.63
1:OOO:296:THR:HG21	5:OOO:629:HOH:O	1.97	0.63
1:UUU:18:GLY:HA3	5:UUU:503:HOH:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:77:PHE:HB3	1:AAA:96:HIS:O	1.99	0.62
1:VVV:111:TYR:HB3	1:VVV:123:LEU:HD11	1.82	0.61
1:KKK:268:VAL:HG11	1:KKK:291:PHE:CE2	2.35	0.61
1:LLL:233:PHE:CZ	1:LLL:246:GLY:HA3	2.36	0.61
1:DDD:184:GLU:OE1	4:XXX:411:GOL:H31	2.02	0.60
1:HHH:77:PHE:HB3	1:HHH:96:HIS:O	2.01	0.60
1:CCC:31:THR:CG2	1:CCC:58:VAL:O	2.48	0.60
1:FFF:77:PHE:HB3	1:FFF:96:HIS:O	2.02	0.59
1:MMM:31:THR:HG22	1:MMM:58:VAL:HB	1.82	0.59
1:PPP:77:PHE:HB3	1:PPP:96:HIS:O	2.02	0.59
1:AAA:31:THR:HG22	1:AAA:58:VAL:HB	1.84	0.59
1:CCC:77:PHE:HB3	1:CCC:96:HIS:O	2.02	0.59
1:SSS:53:VAL:HG13	1:SSS:80:ARG:HD2	1.83	0.59
1:DDD:272:ARG:HD2	1:DDD:292:ASP:OD2	2.02	0.59
1:CCC:31:THR:HG23	1:CCC:58:VAL:O	2.03	0.59
1:EEE:31:THR:HG23	1:EEE:58:VAL:O	2.03	0.58
1:QQQ:272:ARG:CD	1:QQQ:292:ASP:OD2	2.51	0.58
1:QQQ:272:ARG:HD2	1:QQQ:292:ASP:OD2	2.03	0.58
1:BBB:31:THR:HG23	1:BBB:58:VAL:O	2.03	0.57
1:VVV:185:ARG:NH1	5:VVV:501:HOH:O	2.37	0.57
1:WWW:53:VAL:HG13	1:WWW:80:ARG:HD2	1.86	0.57
1:XXX:30:THR:HG21	1:XXX:295:PHE:CD2	2.39	0.57
1:DDD:272:ARG:NH2	3:DDD:401:SO4:O2	2.35	0.57
1:QQQ:272:ARG:NH2	3:QQQ:404:SO4:O2	2.34	0.57
1:TTT:77:PHE:HB3	1:TTT:96:HIS:O	2.04	0.57
1:III:39:LEU:HD11	1:III:63:PHE:CZ	2.40	0.57
1:WWW:98:ASP:OD1	2:www:195:LYS:NZ	2.31	0.57
1:CCC:207:ASP:CB	4:CCC:410:GOL:H31	2.35	0.57
1:QQQ:184:GLU:O	1:SSS:228:MET:HA	2.05	0.56
1:GGG:77:PHE:HB3	1:GGG:96:HIS:O	2.05	0.56
1:JJJ:31:THR:HG22	1:JJJ:58:VAL:O	2.06	0.56
1:BBB:146:VAL:HB	5:BBB:617:HOH:O	2.06	0.56
1:GGG:268:VAL:HG11	1:GGG:291:PHE:CZ	2.40	0.56
1:LLL:77:PHE:HB3	1:LLL:96:HIS:O	2.05	0.56
1:WWW:31:THR:HG21	1:WWW:61:GLY:HA3	1.88	0.56
1:LLL:31:THR:CG2	1:LLL:58:VAL:O	2.54	0.55
1:PPP:272:ARG:HD2	2:xxx:194:LEU:HB3	1.86	0.55
1:OOO:62:LYS:NZ	5:OOO:502:HOH:O	2.36	0.55
1:OOO:233:PHE:CZ	1:OOO:246:GLY:HA3	2.42	0.55
1:EEE:31:THR:CG2	1:EEE:58:VAL:O	2.54	0.55
1:III:31:THR:HG22	1:III:58:VAL:HB	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:19:ILE:HA	1:BBB:29:LEU:O	2.07	0.55
1:KKK:141:HIS:HD1	1:KKK:142:PHE:H	1.54	0.55
1:QQQ:31:THR:CG2	1:QQQ:58:VAL:O	2.54	0.55
1:GGG:207:ASP:O	1:GGG:208:LEU:HB2	2.05	0.55
1:QQQ:31:THR:HG23	1:QQQ:58:VAL:O	2.06	0.55
1:GGG:271:GLU:OE1	2:aaa:194:LEU:N	2.40	0.55
1:NNN:29:LEU:HD13	1:NNN:39:LEU:HD21	1.88	0.55
1:TTT:53:VAL:HG13	1:TTT:80:ARG:HD2	1.88	0.55
1:III:53:VAL:HG13	1:III:80:ARG:HD2	1.89	0.54
1:HHH:31:THR:HG22	1:HHH:58:VAL:O	2.06	0.54
1:WWW:77:PHE:HB3	1:WWW:96:HIS:O	2.07	0.54
2:iii:198:LYS:N	2:iii:199:PRO:HD2	2.22	0.54
1:JJJ:207:ASP:O	1:JJJ:208:LEU:HB2	2.07	0.54
1:FFF:233:PHE:CZ	1:FFF:276:ILE:HB	2.43	0.54
1:MMM:267:ASN:HB3	4:MMM:408:GOL:H2	1.90	0.54
1:PPP:30:THR:HG21	1:PPP:295:PHE:CD2	2.43	0.54
1:KKK:31:THR:HG21	1:KKK:61:GLY:HA3	1.90	0.53
1:PPP:31:THR:HG23	1:PPP:58:VAL:O	2.07	0.53
1:BBB:78:ARG:HD3	1:BBB:80:ARG:NH2	2.24	0.53
1:RRR:68:ASN:HA	1:RRR:84:TYR:CZ	2.43	0.53
1:TTT:30:THR:HG21	1:TTT:295:PHE:CD2	2.44	0.53
1:GGG:118:ASP:OD1	1:GGG:120:THR:HB	2.08	0.53
1:KKK:53:VAL:HG13	1:KKK:80:ARG:HD2	1.90	0.53
1:BBB:29:LEU:HD13	1:BBB:39:LEU:HD21	1.90	0.53
1:FFF:29:LEU:HD13	1:FFF:39:LEU:HD21	1.89	0.53
1:KKK:233:PHE:CZ	1:KKK:246:GLY:HA3	2.43	0.53
1:KKK:233:PHE:CE1	1:KKK:276:ILE:HB	2.44	0.53
1:PPP:41:ASN:HB3	1:PPP:44:THR:HG22	1.91	0.53
1:DDD:30:THR:HG21	1:DDD:295:PHE:CD2	2.44	0.53
1:MMM:271:GLU:OE1	2:sss:194:LEU:N	2.42	0.53
1:XXX:29:LEU:HD13	1:XXX:39:LEU:HD21	1.92	0.52
1:BBB:31:THR:CG2	1:BBB:58:VAL:O	2.57	0.52
1:III:31:THR:HG22	1:III:58:VAL:O	2.08	0.52
1:LLL:31:THR:HG23	1:LLL:58:VAL:O	2.09	0.52
1:BBB:233:PHE:CZ	1:BBB:246:GLY:HA3	2.44	0.52
1:FFF:18:GLY:CA	1:FFF:31:THR:HG22	2.39	0.52
1:XXX:233:PHE:CZ	1:XXX:246:GLY:HA3	2.44	0.52
1:XXX:208:LEU:O	4:XXX:411:GOL:O2	2.24	0.52
1:III:207:ASP:O	1:III:208:LEU:HB2	2.09	0.52
1:UUU:64:ILE:HB	1:UUU:69:TRP:HB2	1.92	0.52
1:WWW:233:PHE:CZ	1:WWW:246:GLY:HA3	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XXX:101:ARG:HD3	1:XXX:117:ASP:OD1	2.09	0.52
1:AAA:184:GLU:O	1:GGG:228:MET:HA	2.10	0.52
1:DDD:233:PHE:CZ	1:DDD:246:GLY:HA3	2.45	0.52
1:OOO:29:LEU:HD13	1:OOO:39:LEU:HD21	1.93	0.51
1:FFF:31:THR:OG1	1:FFF:58:VAL:HB	2.09	0.51
1:MMM:41:ASN:HB3	1:MMM:44:THR:HG22	1.93	0.51
1:OOO:53:VAL:HG13	1:OOO:80:ARG:HD2	1.92	0.51
1:KKK:268:VAL:HG11	1:KKK:291:PHE:CZ	2.46	0.51
1:SSS:29:LEU:HD13	1:SSS:39:LEU:HD21	1.93	0.51
2:xxx:198:LYS:N	2:xxx:199:PRO:CD	2.74	0.51
1:KKK:233:PHE:CZ	1:KKK:276:ILE:HB	2.46	0.51
1:TTT:268:VAL:HG21	1:TTT:291:PHE:CZ	2.46	0.51
1:JJJ:184:GLU:O	1:KKK:228:MET:HA	2.11	0.51
1:RRR:53:VAL:HG13	1:RRR:80:ARG:HD2	1.92	0.51
1:WWW:30:THR:HG21	1:WWW:295:PHE:CD2	2.46	0.51
1:AAA:53:VAL:HG13	1:AAA:80:ARG:HD2	1.91	0.50
1:JJJ:292:ASP:OD2	2:ccc:194:LEU:N	2.44	0.50
1:UUU:207:ASP:O	1:UUU:208:LEU:HB2	2.10	0.50
1:OOO:53:VAL:CG1	3:OOO:403:SO4:O4	2.59	0.50
1:FFF:233:PHE:CZ	1:FFF:246:GLY:HA3	2.47	0.50
1:III:233:PHE:CE1	1:III:276:ILE:HB	2.46	0.50
1:HHH:11:ASN:HB3	1:HHH:295:PHE:CE2	2.47	0.50
1:UUU:77:PHE:HB3	1:UUU:96:HIS:O	2.12	0.50
1:VVV:253:LYS:HD2	1:VVV:255:TRP:CZ2	2.45	0.50
1:BBB:54[A]:THR:HG22	1:BBB:55:GLU:H	1.76	0.50
2:fff:198:LYS:N	2:fff:199:PRO:CD	2.74	0.50
2:kkk:198:LYS:N	2:kkk:199:PRO:CD	2.75	0.50
1:CCC:184:GLU:O	1:JJJ:228:MET:HA	2.12	0.50
1:EEE:177:PHE:CG	1:EEE:218:LYS:HE3	2.46	0.50
1:EEE:207:ASP:O	1:EEE:208:LEU:HB2	2.11	0.50
1:CCC:68:ASN:HA	1:CCC:84:TYR:CZ	2.46	0.50
1:EEE:111:TYR:HB3	1:EEE:123:LEU:HD11	1.93	0.50
1:FFF:55[B]:GLU:OE1	1:FFF:55[B]:GLU:HA	2.12	0.50
1:DDD:204:ALA:HB1	1:DDD:231:VAL:HG12	1.94	0.50
1:EEE:68:ASN:HA	1:EEE:84:TYR:CZ	2.47	0.50
1:SSS:233:PHE:CZ	1:SSS:246:GLY:HA3	2.47	0.50
1:WWW:29:LEU:HD13	1:WWW:39:LEU:CD2	2.41	0.50
1:KKK:210:ILE:HB	1:KKK:224:LEU:HB2	1.94	0.49
1:QQQ:268:VAL:HG21	1:QQQ:291:PHE:CZ	2.47	0.49
1:UUU:233:PHE:CZ	1:UUU:246:GLY:HA3	2.46	0.49
1:FFF:207:ASP:O	1:FFF:208:LEU:HB2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:JJJ:113:LEU:HB3	1:JJJ:146:VAL:HG11	1.93	0.49
1:RRR:268:VAL:HG11	1:RRR:291:PHE:CZ	2.47	0.49
1:WWW:207:ASP:O	1:WWW:208:LEU:HB2	2.11	0.49
2:uuu:198:LYS:N	2:uuu:199:PRO:CD	2.75	0.49
1:QQQ:185:ARG:HG2	1:SSS:208:LEU:HD11	1.94	0.49
1:JJJ:1:MET:HE1	1:JJJ:242:ILE:CG2	2.42	0.49
1:MMM:11:ASN:HB3	1:MMM:295:PHE:CE2	2.47	0.49
1:XXX:233:PHE:CE1	1:XXX:276:ILE:HB	2.47	0.49
1:DDD:272:ARG:CD	1:DDD:292:ASP:OD2	2.61	0.49
1:EEE:271:GLU:HB3	3:EEE:405:SO4:O4	2.12	0.49
1:HHH:41:ASN:HB3	1:HHH:44:THR:HG22	1.94	0.49
1:LLL:233:PHE:CE1	1:LLL:276:ILE:HB	2.48	0.49
1:PPP:91:VAL:HG21	1:PPP:130:TRP:NE1	2.28	0.49
2:lll:198:LYS:N	2:lll:199:PRO:CD	2.76	0.49
1:JJJ:30:THR:HG21	1:JJJ:295:PHE:CD2	2.48	0.49
1:LLL:30:THR:HG21	1:LLL:295:PHE:CD2	2.48	0.49
1:OOO:30:THR:HG21	1:OOO:295:PHE:CD2	2.48	0.49
1:PPP:53:VAL:CG1	1:PPP:80:ARG:HD2	2.43	0.49
1:DDD:118:ASP:OD1	1:DDD:120:THR:HB	2.13	0.48
1:NNN:53:VAL:HG13	1:NNN:80:ARG:HD2	1.95	0.48
1:QQQ:233:PHE:CZ	1:QQQ:246:GLY:HA3	2.48	0.48
1:AAA:233:PHE:CZ	1:AAA:246:GLY:HA3	2.48	0.48
1:CCC:210:ILE:HB	1:CCC:224:LEU:HB2	1.95	0.48
1:QQQ:77:PHE:HB3	1:QQQ:96:HIS:O	2.11	0.48
1:SSS:64:ILE:HB	1:SSS:69:TRP:HB2	1.95	0.48
1:NNN:268:VAL:HG21	1:NNN:291:PHE:CZ	2.48	0.48
1:CCC:29:LEU:HD13	1:CCC:39:LEU:CD2	2.43	0.48
1:AAA:29:LEU:HD13	1:AAA:39:LEU:HD21	1.96	0.48
1:LLL:76:ASP:OD2	1:LLL:80:ARG:NH2	2.45	0.48
1:NNN:210:ILE:HB	1:NNN:224:LEU:HB2	1.96	0.48
1:BBB:111:TYR:HB3	1:BBB:123:LEU:HD11	1.96	0.48
1:SSS:99:TYR:CZ	2:sss:195:LYS:HD3	2.48	0.48
1:TTT:210:ILE:HB	1:TTT:224:LEU:HB2	1.96	0.48
1:VVV:207:ASP:O	1:VVV:208:LEU:HB2	2.13	0.48
1:VVV:233:PHE:CE1	1:VVV:276:ILE:HB	2.49	0.48
2:www:198:LYS:N	2:www:199:PRO:CD	2.76	0.48
1:BBB:53:VAL:CG1	1:BBB:80:ARG:HD2	2.44	0.48
1:JJJ:1:MET:HE1	1:JJJ:242:ILE:HG21	1.95	0.48
1:SSS:200:TYR:HA	1:SSS:213:TRP:O	2.14	0.48
2:qqq:198:LYS:N	2:qqq:199:PRO:CD	2.77	0.48
1:NNN:233:PHE:CZ	1:NNN:246:GLY:HA3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:NNN:293:ASN:ND2	5:NNN:501:HOH:O	2.32	0.48
2:jjj:198:LYS:N	2:jjj:199:PRO:CD	2.77	0.48
1:HHH:237:HIS:CG	1:HHH:238:PRO:HD2	2.49	0.47
1:AAA:158:SER:CB	5:AAA:624:HOH:O	2.62	0.47
1:BBB:233:PHE:CE1	1:BBB:276:ILE:HB	2.49	0.47
1:BBB:249:ASP:HB2	1:UUU:141:HIS:HE2	1.79	0.47
1:CCC:237:HIS:CG	1:CCC:238:PRO:HD2	2.49	0.47
1:III:77:PHE:HB3	1:III:96:HIS:O	2.14	0.47
1:III:184:GLU:O	1:WWW:228:MET:HA	2.14	0.47
1:KKK:268:VAL:HG13	5:KKK:502:HOH:O	2.13	0.47
1:LLL:117:ASP:O	5:LLL:501:HOH:O	2.20	0.47
1:TTT:31:THR:HG23	1:TTT:58:VAL:HG12	1.96	0.47
2:mmm:198:LYS:N	2:mmm:199:PRO:CD	2.77	0.47
1:HHH:233:PHE:CE1	1:HHH:276:ILE:HB	2.49	0.47
1:MMM:268:VAL:HG21	1:MMM:291:PHE:CZ	2.49	0.47
1:PPP:207:ASP:O	1:PPP:208:LEU:HB2	2.13	0.47
1:UUU:181:THR:HA	1:UUU:213:TRP:CZ2	2.50	0.47
1:DDD:53:VAL:CG1	1:DDD:80:ARG:HD2	2.44	0.47
1:LLL:184:GLU:O	1:OOO:228:MET:HA	2.14	0.47
1:SSS:110:PRO:HA	1:SSS:126:TRP:CZ2	2.48	0.47
1:PPP:29:LEU:HD13	1:PPP:39:LEU:CD2	2.44	0.47
1:RRR:29:LEU:HD13	1:RRR:39:LEU:CD2	2.44	0.47
1:CCC:11:ASN:HB3	1:CCC:295:PHE:CE2	2.49	0.47
1:LLL:56:THR:HB	1:LLL:75:ASP:HB2	1.96	0.47
1:KKK:68:ASN:HA	1:KKK:84:TYR:CZ	2.49	0.47
1:QQQ:56:THR:HB	1:QQQ:75:ASP:HB2	1.97	0.47
1:TTT:98:ASP:OD1	2:ttt:195:LYS:NZ	2.36	0.47
1:XXX:53:VAL:HG13	1:XXX:80:ARG:HD2	1.95	0.47
2:ggg:198:LYS:N	2:ggg:199:PRO:CD	2.78	0.47
1:LLL:272:ARG:HD2	2:rrr:194:LEU:HB3	1.97	0.47
1:XXX:31:THR:CG2	1:XXX:58:VAL:HG12	2.45	0.47
1:BBB:204:ALA:HB1	1:BBB:231:VAL:HG12	1.96	0.47
1:EEE:56:THR:HB	1:EEE:75:ASP:HB2	1.96	0.47
1:LLL:181:THR:HA	1:LLL:213:TRP:CZ2	2.49	0.47
1:OOO:233:PHE:CE1	1:OOO:276:ILE:HB	2.50	0.47
1:FFF:68:ASN:HA	1:FFF:84:TYR:CZ	2.50	0.47
1:TTT:31:THR:CG2	1:TTT:58:VAL:O	2.63	0.47
1:OOO:77:PHE:HB3	1:OOO:96:HIS:O	2.15	0.46
1:TTT:19:ILE:HA	1:TTT:29:LEU:O	2.15	0.46
1:FFF:268:VAL:HG22	5:FFF:528:HOH:O	2.16	0.46
1:GGG:268:VAL:HG11	1:GGG:291:PHE:CE2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:LLL:272:ARG:CD	1:LLL:292:ASP:OD2	2.59	0.46
1:VVV:233:PHE:CZ	1:VVV:246:GLY:HA3	2.50	0.46
1:XXX:271:GLU:OE1	2:ddd:194:LEU:N	2.48	0.46
1:BBB:210:ILE:HB	1:BBB:224:LEU:HB2	1.96	0.46
1:XXX:207:ASP:O	1:XXX:208:LEU:HB2	2.15	0.46
1:AAA:19:ILE:HA	1:AAA:29:LEU:O	2.15	0.46
1:XXX:204:ALA:HB1	1:XXX:231:VAL:HG12	1.97	0.46
1:DDD:1:MET:HE1	1:DDD:242:ILE:CG2	2.46	0.46
1:JJJ:233:PHE:CE1	1:JJJ:276:ILE:HB	2.51	0.46
1:NNN:233:PHE:CE1	1:NNN:276:ILE:HB	2.50	0.46
1:TTT:31:THR:HG23	1:TTT:58:VAL:O	2.16	0.46
1:VVV:123:LEU:HD22	1:VVV:170:LEU:HD22	1.98	0.46
1:HHH:151:LYS:NZ	1:HHH:193:TYR:O	2.48	0.46
1:MMM:222:ALA:HA	4:MMM:411:GOL:H32	1.98	0.46
1:TTT:233:PHE:CZ	1:TTT:246:GLY:HA3	2.51	0.46
1:AAA:118:ASP:OD1	1:AAA:120:THR:HG22	2.15	0.46
1:BBB:54[A]:THR:HG21	1:BBB:76:ASP:OD2	2.16	0.46
1:III:39:LEU:HD11	1:III:63:PHE:CE1	2.51	0.46
1:UUU:110:PRO:HA	1:UUU:126:TRP:CZ2	2.51	0.46
2:sss:198:LYS:N	2:sss:199:PRO:CD	2.79	0.46
2:ccc:198:LYS:N	2:ccc:199:PRO:CD	2.78	0.46
1:MMM:53:VAL:HG13	1:MMM:80:ARG:HD2	1.98	0.45
1:OOO:248:GLU:O	1:OOO:272:ARG:HG2	2.16	0.45
1:VVV:53:VAL:CG1	1:VVV:80:ARG:HD2	2.46	0.45
1:JJJ:19:ILE:HD12	1:JJJ:30:THR:HG22	1.98	0.45
1:OOO:113:LEU:HB3	1:OOO:146[B]:VAL:HG11	1.99	0.45
1:RRR:279:HIS:HB2	1:RRR:286:TYR:HB2	1.98	0.45
1:UUU:30:THR:HG21	1:UUU:295:PHE:CD2	2.50	0.45
2:ppp:198:LYS:N	2:ppp:199:PRO:CD	2.78	0.45
1:BBB:31:THR:HG23	1:BBB:58:VAL:HG12	1.98	0.45
1:LLL:207:ASP:O	1:LLL:208:LEU:HB2	2.17	0.45
2:eee:198:LYS:N	2:eee:199:PRO:CD	2.80	0.45
1:LLL:31:THR:HG23	1:LLL:58:VAL:HG12	1.97	0.45
1:NNN:151:LYS:NZ	3:NNN:403:SO4:O2	2.49	0.45
1:NNN:193:TYR:O	3:NNN:403:SO4:O4	2.33	0.45
1:EEE:272:ARG:N	3:EEE:405:SO4:O4	2.50	0.45
1:CCC:31:THR:HG22	1:CCC:58:VAL:O	2.15	0.45
1:JJJ:39:LEU:HD22	1:JJJ:63:PHE:HZ	1.80	0.45
1:OOO:74:SER:OG	1:OOO:76:ASP:OD1	2.34	0.45
1:TTT:249:ASP:HB2	1:WWW:141:HIS:HE2	1.80	0.45
1:CCC:117:ASP:OD2	2:ccc:195:LYS:HE3	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EEE:118:ASP:OD1	1:EEE:120:THR:HG22	2.17	0.45
1:FFF:268:VAL:HG21	1:FFF:291:PHE:CZ	2.52	0.45
1:GGG:30:THR:HG21	1:GGG:295:PHE:CD2	2.51	0.45
1:GGG:233:PHE:CE1	1:GGG:276:ILE:HB	2.51	0.45
1:MMM:249:ASP:OD1	1:MMM:251:THR:HB	2.16	0.45
1:UUU:228:MET:HA	1:VVV:184:GLU:O	2.16	0.45
1:VVV:29:LEU:HA	1:VVV:39:LEU:HD23	1.98	0.45
1:FFF:242:ILE:HA	1:FFF:255:TRP:O	2.17	0.45
1:NNN:98:ASP:OD1	2:nnn:195:LYS:NZ	2.50	0.45
1:RRR:207:ASP:C	1:RRR:208:LEU:HG	2.42	0.45
1:UUU:252:LEU:HB2	1:UUU:266:LEU:HB2	1.99	0.45
1:DDD:68:ASN:HA	1:DDD:84:TYR:CZ	2.52	0.45
1:KKK:110:PRO:HA	1:KKK:126:TRP:CZ2	2.52	0.45
1:OOO:226:GLY:O	1:OOO:253:LYS:HD3	2.17	0.45
1:RRR:233:PHE:CE1	1:RRR:276:ILE:HB	2.51	0.45
1:AAA:68:ASN:HA	1:AAA:84:TYR:CZ	2.52	0.44
1:UUU:53:VAL:HG13	1:UUU:80:ARG:HD2	1.99	0.44
1:VVV:30:THR:HG21	1:VVV:295:PHE:CD1	2.52	0.44
1:BBB:30:THR:HG21	1:BBB:295:PHE:CD2	2.52	0.44
1:DDD:31:THR:CG2	1:DDD:58:VAL:HG12	2.47	0.44
1:TTT:144:MET:HE2	2:ttt:197:LYS:HE2	1.99	0.44
1:UUU:68:ASN:HA	1:UUU:84:TYR:CZ	2.52	0.44
2:vvv:198:LYS:N	2:vvv:199:PRO:CD	2.80	0.44
1:AAA:29:LEU:HD13	1:AAA:39:LEU:CD2	2.48	0.44
1:DDD:165:VAL:HG11	1:DDD:201:MET:HE1	1.99	0.44
1:EEE:30:THR:HG21	1:EEE:295:PHE:CD2	2.53	0.44
1:GGG:292:ASP:OD2	2:aaa:194:LEU:N	2.50	0.44
1:OOO:103:ILE:HG23	1:OOO:112:VAL:HG13	1.99	0.44
1:PPP:19:ILE:HA	1:PPP:29:LEU:O	2.18	0.44
2:ttt:198:LYS:N	2:ttt:199:PRO:CD	2.80	0.44
1:DDD:183:GLN:HA	1:DDD:207:ASP:OD2	2.18	0.44
1:PPP:110:PRO:HA	1:PPP:126:TRP:CZ2	2.53	0.44
1:DDD:207:ASP:O	1:DDD:208:LEU:HB2	2.16	0.44
1:MMM:233:PHE:CE1	1:MMM:276:ILE:HB	2.53	0.44
1:CCC:224:LEU:N	1:CCC:224:LEU:HD12	2.32	0.44
1:DDD:53:VAL:HG13	1:DDD:80:ARG:HD2	2.00	0.44
1:SSS:271:GLU:OE1	2:qqq:194:LEU:N	2.51	0.44
2:ooo:198:LYS:N	2:ooo:199:PRO:CD	2.81	0.44
1:NNN:248:GLU:O	1:NNN:272:ARG:HG2	2.17	0.44
1:QQQ:207:ASP:O	1:QQQ:208:LEU:HB2	2.18	0.44
1:XXX:16:VAL:HG22	1:XXX:32:LEU:CD2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:OOO:72:VAL:O	3:OOO:403:SO4:O3	2.36	0.44
2:nnn:198:LYS:N	2:nnn:199:PRO:CD	2.81	0.44
1:GGG:104:ALA:HB3	1:GGG:113:LEU:HB2	2.00	0.44
1:LLL:228:MET:HA	1:RRR:184:GLU:O	2.18	0.44
1:UUU:177:PHE:CG	1:UUU:218:LYS:HE3	2.52	0.44
1:JJJ:64:ILE:HB	1:JJJ:69:TRP:HB2	2.00	0.43
1:KKK:64:ILE:HB	1:KKK:69:TRP:HB2	1.99	0.43
1:PPP:243:ILE:HB	1:PPP:255:TRP:HB2	2.00	0.43
1:WWW:181:THR:HA	1:WWW:213:TRP:CZ2	2.53	0.43
1:JJJ:31:THR:CG2	1:JJJ:58:VAL:HG12	2.48	0.43
1:RRR:11:ASN:HB3	1:RRR:295:PHE:CE1	2.53	0.43
1:FFF:66:ARG:NH1	1:FFF:109:LYS:O	2.51	0.43
1:QQQ:30:THR:HG21	1:QQQ:295:PHE:CD2	2.53	0.43
1:BBB:118:ASP:C	1:BBB:119:LEU:HG	2.44	0.43
1:EEE:268:VAL:HG21	1:EEE:291:PHE:CZ	2.53	0.43
1:FFF:249:ASP:OD1	1:FFF:251:THR:HB	2.17	0.43
1:HHH:207:ASP:O	1:HHH:208:LEU:HB2	2.17	0.43
1:JJJ:111:TYR:HB3	1:JJJ:123:LEU:HD11	2.01	0.43
1:RRR:165:VAL:HG11	1:RRR:201:MET:HE1	1.99	0.43
1:AAA:81:VAL:HG21	1:AAA:130:TRP:CH2	2.54	0.43
1:DDD:31:THR:HG22	1:DDD:58:VAL:HG12	2.00	0.43
1:NNN:207:ASP:O	1:NNN:208:LEU:HB2	2.17	0.43
1:XXX:225:GLU:CB	4:XXX:411:GOL:H2	2.49	0.43
2:bbb:198:LYS:N	2:bbb:199:PRO:CD	2.82	0.43
1:CCC:233:PHE:CE1	1:CCC:276:ILE:HB	2.53	0.43
1:DDD:228:MET:HA	1:PPP:184:GLU:O	2.18	0.43
1:XXX:64:ILE:HB	1:XXX:69:TRP:HB2	2.00	0.43
1:BBB:66:ARG:NH2	1:BBB:109:LYS:O	2.51	0.43
1:GGG:181:THR:HA	1:GGG:213:TRP:CH2	2.54	0.43
1:JJJ:66:ARG:N	3:JJJ:402:SO4:O2	2.49	0.43
1:LLL:268:VAL:HG21	1:LLL:291:PHE:CZ	2.54	0.43
1:MMM:267:ASN:HD22	4:MMM:408:GOL:C2	2.31	0.43
1:PPP:1:MET:HE3	1:PPP:256:ASN:HD22	1.82	0.43
1:KKK:53:VAL:CG1	1:KKK:80:ARG:HD2	2.48	0.43
1:AAA:103:ILE:HG23	1:AAA:112:VAL:HG13	2.01	0.43
1:EEE:181:THR:HA	1:EEE:213:TRP:CZ2	2.53	0.43
3:EEE:405:SO4:O4	2:hhh:194:LEU:O	2.35	0.43
1:OOO:207:ASP:O	1:OOO:208:LEU:HB2	2.18	0.43
1:WWW:66:ARG:NH2	1:WWW:109:LYS:O	2.52	0.43
1:WWW:155:THR:HA	1:WWW:168:TRP:O	2.19	0.43
1:DDD:210:ILE:HB	1:DDD:224:LEU:HB2	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EEE:233:PHE:CE1	1:EEE:276:ILE:HB	2.54	0.42
1:JJJ:3:LEU:HB3	1:JJJ:5:ILE:HD11	2.01	0.42
1:CCC:181:THR:HA	1:CCC:213:TRP:CZ2	2.54	0.42
1:HHH:181:THR:HA	1:HHH:213:TRP:CZ2	2.54	0.42
2:hhh:198:LYS:N	2:hhh:199:PRO:CD	2.82	0.42
2:rrr:198:LYS:N	2:rrr:199:PRO:CD	2.82	0.42
1:CCC:39:LEU:N	1:CCC:39:LEU:HD23	2.34	0.42
1:PPP:91:VAL:HG21	1:PPP:130:TRP:CD1	2.53	0.42
1:CCC:111:TYR:HB3	1:CCC:123:LEU:HD11	2.01	0.42
1:MMM:44:THR:HG23	1:MMM:46:VAL:HB	2.02	0.42
1:WWW:233:PHE:CE1	1:WWW:276:ILE:HB	2.53	0.42
1:LLL:268:VAL:HG22	5:LLL:505:HOH:O	2.20	0.42
1:MMM:151:LYS:NZ	1:MMM:193:TYR:O	2.53	0.42
1:QQQ:210:ILE:HB	1:QQQ:224:LEU:HB2	2.02	0.42
1:BBB:207:ASP:O	1:BBB:208:LEU:HB2	2.17	0.42
1:DDD:181:THR:HG21	1:DDD:187:VAL:HG21	2.02	0.42
1:EEE:181:THR:HG21	1:EEE:187:VAL:HG21	2.02	0.42
1:JJJ:99:TYR:CZ	2:jjj:195:LYS:HD2	2.55	0.42
1:LLL:19:ILE:HG22	1:LLL:275:CYS:SG	2.60	0.42
1:QQQ:204:ALA:HB1	1:QQQ:231:VAL:HG12	2.02	0.42
1:BBB:53:VAL:HG13	1:BBB:80:ARG:HD2	2.00	0.42
1:FFF:248:GLU:O	1:FFF:272:ARG:HG2	2.19	0.42
1:LLL:31:THR:HG22	1:LLL:58:VAL:O	2.19	0.42
1:NNN:233:PHE:CZ	1:NNN:276:ILE:HB	2.55	0.42
1:OOO:74:SER:OG	3:OOO:403:SO4:O1	2.31	0.42
1:SSS:292:ASP:OD2	2:qqq:194:LEU:N	2.52	0.42
1:CCC:31:THR:HG23	1:CCC:58:VAL:HG12	2.01	0.42
1:MMM:68:ASN:HA	1:MMM:84:TYR:CZ	2.55	0.42
1:BBB:184:GLU:O	1:VVV:228:MET:HA	2.19	0.42
1:GGG:210:ILE:HB	1:GGG:224:LEU:HB2	2.01	0.42
1:PPP:204:ALA:HB1	1:PPP:231:VAL:HG13	2.02	0.42
1:TTT:254:ILE:HD11	1:TTT:266:LEU:HD11	2.02	0.42
1:UUU:200:TYR:HA	1:UUU:213:TRP:O	2.19	0.42
1:VVV:19:ILE:HA	1:VVV:29:LEU:O	2.20	0.42
1:BBB:237:HIS:CG	1:BBB:238:PRO:HD2	2.55	0.42
1:DDD:120:THR:CG2	1:DDD:122:LYS:HG3	2.50	0.42
1:III:268:VAL:HG21	1:III:291:PHE:CZ	2.55	0.42
1:MMM:29:LEU:HD13	1:MMM:39:LEU:HD21	2.02	0.42
1:MMM:204:ALA:HB1	1:MMM:231:VAL:HG12	2.02	0.42
1:RRR:39:LEU:N	1:RRR:39:LEU:HD23	2.34	0.42
1:BBB:68:ASN:HA	1:BBB:84:TYR:CZ	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:JJJ:233:PHE:CZ	1:JJJ:246:GLY:HA3	2.55	0.41
1:MMM:29:LEU:HD13	1:MMM:39:LEU:CD2	2.50	0.41
1:QQQ:181:THR:HA	1:QQQ:213:TRP:CZ2	2.55	0.41
1:XXX:31:THR:HG21	1:XXX:58:VAL:HG12	2.01	0.41
1:BBB:103:ILE:HG23	1:BBB:112:VAL:HG13	2.01	0.41
1:KKK:181:THR:HA	1:KKK:213:TRP:CZ2	2.55	0.41
1:MMM:53:VAL:CG1	1:MMM:80:ARG:HD2	2.50	0.41
1:PPP:181:THR:HA	1:PPP:213:TRP:CZ2	2.55	0.41
1:WWW:210:ILE:HB	1:WWW:224:LEU:HB2	2.02	0.41
1:HHH:10:SER:OG	1:HHH:296:THR:HG23	2.19	0.41
1:III:1:MET:HE3	1:III:1:MET:HB2	1.90	0.41
1:NNN:110:PRO:HA	1:NNN:126:TRP:CH2	2.54	0.41
1:QQQ:31:THR:HG23	1:QQQ:58:VAL:HG12	2.02	0.41
1:RRR:19:ILE:HA	1:RRR:29:LEU:O	2.20	0.41
1:JJJ:200:TYR:CE1	1:JJJ:221:VAL:HG21	2.55	0.41
1:PPP:55[B]:GLU:HG2	1:WWW:77:PHE:CE1	2.55	0.41
1:UUU:29:LEU:HD13	1:UUU:39:LEU:CD2	2.51	0.41
2:ddd:198:LYS:N	2:ddd:199:PRO:CD	2.84	0.41
1:HHH:53:VAL:CG1	1:HHH:80:ARG:HD2	2.51	0.41
1:LLL:64:ILE:HB	1:LLL:69:TRP:HB2	2.01	0.41
1:AAA:31:THR:HG22	1:AAA:58:VAL:O	2.19	0.41
1:HHH:31:THR:HG23	1:HHH:58:VAL:HB	2.02	0.41
1:PPP:237:HIS:CG	1:PPP:238:PRO:HD2	2.55	0.41
1:SSS:233:PHE:CE1	1:SSS:276:ILE:HB	2.56	0.41
1:NNN:81:VAL:HG21	1:NNN:130:TRP:CH2	2.56	0.41
1:RRR:237:HIS:CG	1:RRR:238:PRO:HD2	2.56	0.41
1:XXX:39:LEU:HD12	1:XXX:49:ARG:HB3	2.02	0.41
1:DDD:206:ASP:OD2	2:ddd:197:LYS:HE2	2.21	0.41
1:EEE:44:THR:HG22	1:EEE:46:VAL:HG23	2.02	0.41
1:III:30:THR:HG21	1:III:295:PHE:CD2	2.56	0.41
1:JJJ:39:LEU:HD22	1:JJJ:63:PHE:CZ	2.56	0.41
1:JJJ:271:GLU:OE1	2:ccc:194:LEU:N	2.54	0.41
1:LLL:250:GLY:HA2	1:LLL:271:GLU:O	2.21	0.41
1:LLL:292:ASP:OD2	2:rrr:194:LEU:N	2.54	0.41
1:BBB:35:GLY:HA2	1:BBB:58:VAL:HG23	2.03	0.41
1:EEE:39:LEU:CD2	1:EEE:63:PHE:CZ	3.04	0.41
1:III:181:THR:HA	1:III:213:TRP:CH2	2.56	0.41
1:III:181:THR:HA	1:III:213:TRP:CZ2	2.56	0.41
1:KKK:30:THR:HG21	1:KKK:295:PHE:CD2	2.56	0.41
1:HHH:185:ARG:NH2	4:HHH:413:GOL:O3	2.54	0.41
1:SSS:99:TYR:CG	2:sss:195:LYS:HE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:UUU:249:ASP:OD1	1:UUU:251:THR:HB	2.21	0.41
1:XXX:1:MET:HE2	1:XXX:263:GLU:HG3	2.02	0.41
1:CCC:38:GLU:C	1:CCC:39:LEU:HD23	2.46	0.40
1:FFF:120:THR:HG21	1:FFF:122:LYS:HE3	2.03	0.40
1:GGG:36:ARG:NE	1:GGG:50:SER:OG	2.55	0.40
1:LLL:68:ASN:HA	1:LLL:84:TYR:CZ	2.56	0.40
1:UUU:53:VAL:CG1	1:UUU:80:ARG:HD2	2.50	0.40
1:AAA:30:THR:HG21	1:AAA:295:PHE:CD2	2.56	0.40
1:FFF:18:GLY:HA3	1:FFF:31:THR:HG22	2.03	0.40
1:GGG:194:PRO:HG3	1:GGG:238:PRO:HA	2.03	0.40
1:III:31:THR:CG2	1:III:58:VAL:HB	2.50	0.40
1:JJJ:113:LEU:CB	1:JJJ:146:VAL:HG11	2.51	0.40
1:OOO:233:PHE:CZ	1:OOO:276:ILE:HB	2.56	0.40
1:PPP:53:VAL:HG12	1:PPP:80:ARG:HD2	2.04	0.40
1:PPP:61:GLY:HA2	1:PPP:71:ILE:O	2.21	0.40
1:PPP:124:TRP:CZ3	1:PPP:132:LEU:HB2	2.56	0.40
1:FFF:233:PHE:CE1	1:FFF:276:ILE:HB	2.57	0.40
1:III:271:GLU:OE1	2:ttt:194:LEU:N	2.54	0.40
1:III:292:ASP:OD2	2:ttt:194:LEU:N	2.54	0.40
1:LLL:177:PHE:CG	1:LLL:218:LYS:HE3	2.55	0.40
1:MMM:19:ILE:HA	1:MMM:29:LEU:O	2.21	0.40
1:UUU:228:MET:SD	1:UUU:249:ASP:HB3	2.61	0.40
1:DDD:12:ARG:NH2	5:DDD:513:HOH:O	2.55	0.40
1:FFF:68:ASN:HA	1:FFF:84:TYR:OH	2.22	0.40
1:FFF:279:HIS:HB2	1:FFF:286:TYR:HB2	2.03	0.40
1:MMM:31:THR:HG23	1:MMM:37:VAL:HG12	2.04	0.40
1:SSS:155:THR:HA	1:SSS:168:TRP:O	2.21	0.40
1:SSS:210:ILE:HB	1:SSS:224:LEU:HB2	2.04	0.40
1:UUU:202:ILE:HD12	1:UUU:212:ILE:CD1	2.51	0.40
1:UUU:248:GLU:O	1:UUU:272:ARG:HG2	2.21	0.40
1:XXX:233:PHE:CZ	1:XXX:276:ILE:HB	2.56	0.40
1:BBB:29:LEU:HD13	1:BBB:39:LEU:CD2	2.51	0.40
1:BBB:200:TYR:HA	1:BBB:213:TRP:O	2.22	0.40
1:GGG:213:TRP:CZ3	1:GGG:220:CYS:HB2	2.57	0.40
1:HHH:111:TYR:HB3	1:HHH:123:LEU:HD11	2.03	0.40
1:MMM:181:THR:HG21	1:MMM:187:VAL:HG21	2.03	0.40
1:MMM:233:PHE:CZ	1:MMM:276:ILE:HB	2.56	0.40
1:OOO:181:THR:HA	1:OOO:213:TRP:CZ2	2.56	0.40
1:UUU:56:THR:HB	1:UUU:75:ASP:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	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

All (177) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	55	GLU
1	AAA	129	ASN
1	AAA	185	ARG
1	AAA	251	THR
1	AAA	261	LYS
1	BBB	2	LYS
1	BBB	31	THR
1	BBB	54[A]	THR
1	BBB	54[B]	THR
1	BBB	55	GLU
1	BBB	185	ARG

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Mol	Chain	Res	Type
1	BBB	217	THR
1	BBB	258	SER
1	BBB	261	LYS
1	CCC	6	LYS
1	CCC	31	THR
1	CCC	55	GLU
1	CCC	84	TYR
1	CCC	174	THR
1	CCC	258	SER
1	CCC	261	LYS
1	CCC	262	VAL
1	DDD	31	THR
1	DDD	39	LEU
1	DDD	55	GLU
1	DDD	84	TYR
1	DDD	120	THR
1	DDD	129	ASN
1	DDD	262	VAL
1	DDD	268	VAL
1	DDD	272	ARG
1	EEE	31	THR
1	EEE	98	ASP
1	EEE	120	THR
1	EEE	261	LYS
1	EEE	262	VAL
1	FFF	44	THR
1	FFF	55[A]	GLU
1	FFF	55[B]	GLU
1	FFF	66	ARG
1	FFF	74	SER
1	FFF	120	THR
1	FFF	251	THR
1	FFF	261	LYS
1	FFF	262	VAL
1	FFF	268	VAL
1	FFF	296	THR
1	GGG	1	MET
1	GGG	5	ILE
1	GGG	120	THR
1	GGG	251	THR
1	GGG	261	LYS
1	GGG	268	VAL

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Mol	Chain	Res	Type
1	HHH	2	LYS
1	HHH	7[A]	LYS
1	HHH	7[B]	LYS
1	HHH	44	THR
1	HHH	74	SER
1	HHH	120	THR
1	HHH	229	SER
1	HHH	251	THR
1	HHH	253	LYS
1	HHH	261	LYS
1	III	84	TYR
1	III	91	VAL
1	III	120	THR
1	III	251	THR
1	III	261	LYS
1	III	296	THR
1	JJJ	19	ILE
1	JJJ	84	TYR
1	JJJ	120	THR
1	JJJ	251	THR
1	JJJ	261	LYS
1	JJJ	264	LYS
1	KKK	36	ARG
1	KKK	55[A]	GLU
1	KKK	55[B]	GLU
1	KKK	74	SER
1	KKK	120	THR
1	KKK	251	THR
1	KKK	253	LYS
1	KKK	270	LEU
1	LLL	31	THR
1	LLL	39	LEU
1	LLL	50	SER
1	LLL	84	TYR
1	LLL	217	THR
1	LLL	251	THR
1	LLL	261	LYS
1	LLL	264	LYS
1	LLL	270	LEU
1	MMM	44	THR
1	MMM	55	GLU
1	MMM	74	SER

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Mol	Chain	Res	Type
1	MMM	84	TYR
1	MMM	120	THR
1	MMM	207	ASP
1	MMM	251	THR
1	MMM	261	LYS
1	NNN	55[A]	GLU
1	NNN	55[B]	GLU
1	NNN	120	THR
1	NNN	261	LYS
1	NNN	264	LYS
1	OOO	55	GLU
1	OOO	120	THR
1	OOO	129	ASN
1	OOO	261	LYS
1	OOO	268	VAL
1	OOO	300	LEU
1	PPP	6	LYS
1	PPP	31	THR
1	PPP	44	THR
1	PPP	50	SER
1	PPP	74	SER
1	PPP	84	TYR
1	PPP	91	VAL
1	PPP	120	THR
1	PPP	229	SER
1	PPP	232	SER
1	PPP	253	LYS
1	PPP	261	LYS
1	PPP	262	VAL
1	PPP	264	LYS
1	PPP	268	VAL
1	PPP	300	LEU
1	QQQ	31	THR
1	QQQ	120	THR
1	QQQ	198	LYS
1	QQQ	215	TYR
1	QQQ	253	LYS
1	QQQ	261	LYS
1	QQQ	262	VAL
1	QQQ	264	LYS
1	RRR	31	THR
1	RRR	120	THR

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Mol	Chain	Res	Type
1	RRR	262	VAL
1	RRR	268	VAL
1	SSS	55	GLU
1	SSS	261	LYS
1	SSS	300	LEU
1	TTT	6	LYS
1	TTT	31	THR
1	TTT	39	LEU
1	TTT	55	GLU
1	TTT	189	TYR
1	TTT	251	THR
1	TTT	261	LYS
1	TTT	262	VAL
1	UUU	12	ARG
1	UUU	31	THR
1	UUU	39	LEU
1	UUU	44	THR
1	UUU	46	VAL
1	UUU	129	ASN
1	UUU	251	THR
1	UUU	253	LYS
1	UUU	261	LYS
1	UUU	262	VAL
1	UUU	268	VAL
1	VVV	31	THR
1	VVV	120	THR
1	VVV	251	THR
1	VVV	261	LYS
1	VVV	264	LYS
1	VVV	296	THR
1	WWW	120	THR
1	WWW	251	THR
1	WWW	261	LYS
1	WWW	262	VAL
1	XXX	6	LYS
1	XXX	55	GLU
1	XXX	120	THR
1	XXX	129	ASN
1	XXX	261	LYS
1	XXX	296	THR

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.

All (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
4	CCC	409	GOL	O1-C1-C2-C3
4	DDD	411	GOL	C1-C2-C3-O3
4	DDD	412	GOL	C1-C2-C3-O3
4	EEE	407	GOL	O1-C1-C2-C3
4	EEE	407	GOL	C1-C2-C3-O3
4	HHH	411	GOL	O1-C1-C2-O2
4	HHH	411	GOL	O1-C1-C2-C3
4	HHH	412	GOL	C1-C2-C3-O3
4	HHH	413	GOL	O1-C1-C2-O2
4	HHH	413	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
4	JJJ	409	GOL	O1-C1-C2-C3
4	KKK	413	GOL	C1-C2-C3-O3
4	MMM	408	GOL	O1-C1-C2-C3
4	MMM	409	GOL	O1-C1-C2-C3
4	MMM	409	GOL	C1-C2-C3-O3
4	MMM	411	GOL	O1-C1-C2-C3
4	OOO	410	GOL	C1-C2-C3-O3
4	QQQ	409	GOL	O1-C1-C2-C3
4	SSS	412	GOL	O1-C1-C2-C3
4	SSS	412	GOL	C1-C2-C3-O3
4	SSS	413	GOL	O1-C1-C2-C3
4	SSS	414	GOL	C1-C2-C3-O3
4	TTT	408	GOL	O1-C1-C2-C3
4	TTT	409	GOL	O1-C1-C2-C3
4	UUU	413	GOL	C1-C2-C3-O3
4	UUU	414	GOL	O1-C1-C2-O2
4	WWW	406	GOL	C1-C2-C3-O3
4	XXX	410	GOL	C1-C2-C3-O3
4	AAA	416	GOL	O2-C2-C3-O3
4	AAA	417	GOL	O2-C2-C3-O3
4	DDD	412	GOL	O2-C2-C3-O3
4	EEE	407	GOL	O2-C2-C3-O3
4	KKK	413	GOL	O2-C2-C3-O3
4	MMM	408	GOL	O1-C1-C2-O2
4	MMM	409	GOL	O2-C2-C3-O3
4	SSS	414	GOL	O2-C2-C3-O3
4	UUU	413	GOL	O2-C2-C3-O3
4	XXX	410	GOL	O2-C2-C3-O3
4	AAA	416	GOL	C1-C2-C3-O3
4	AAA	417	GOL	C1-C2-C3-O3
4	CCC	410	GOL	C1-C2-C3-O3
4	FFF	408	GOL	C1-C2-C3-O3
4	GGG	403	GOL	O1-C1-C2-C3
4	HHH	411	GOL	C1-C2-C3-O3
4	III	410	GOL	O1-C1-C2-C3
4	JJJ	409	GOL	C1-C2-C3-O3
4	KKK	413	GOL	O1-C1-C2-C3
4	MMM	408	GOL	C1-C2-C3-O3
4	NNN	411	GOL	O1-C1-C2-C3
4	NNN	412	GOL	O1-C1-C2-C3
4	NNN	412	GOL	C1-C2-C3-O3
4	PPP	409	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
4	PPP	410	GOL	O1-C1-C2-C3
4	UUU	413	GOL	O1-C1-C2-C3
4	UUU	414	GOL	O1-C1-C2-C3
4	XXX	411	GOL	O1-C1-C2-C3
4	AAA	415	GOL	O1-C1-C2-O2
4	AAA	415	GOL	O2-C2-C3-O3
4	BBB	409	GOL	O1-C1-C2-O2
4	CCC	410	GOL	O2-C2-C3-O3
4	DDD	411	GOL	O2-C2-C3-O3
4	EEE	407	GOL	O1-C1-C2-O2
4	MMM	408	GOL	O2-C2-C3-O3
4	MMM	409	GOL	O1-C1-C2-O2
4	OOO	410	GOL	O2-C2-C3-O3
4	QQQ	409	GOL	O1-C1-C2-O2
4	SSS	412	GOL	O1-C1-C2-O2
4	SSS	412	GOL	O2-C2-C3-O3
4	SSS	413	GOL	O1-C1-C2-O2
4	GGG	403	GOL	O1-C1-C2-O2
4	HHH	412	GOL	O2-C2-C3-O3
4	NNN	411	GOL	O1-C1-C2-O2
4	NNN	412	GOL	O1-C1-C2-O2
4	TTT	408	GOL	O1-C1-C2-O2
4	TTT	409	GOL	O1-C1-C2-O2
4	WWW	406	GOL	O2-C2-C3-O3
4	JJJ	408	GOL	O1-C1-C2-C3
4	BBB	410	GOL	O1-C1-C2-O2
4	HHH	411	GOL	O2-C2-C3-O3
4	III	410	GOL	O1-C1-C2-O2
4	JJJ	409	GOL	O2-C2-C3-O3
4	KKK	413	GOL	O1-C1-C2-O2
4	NNN	412	GOL	O2-C2-C3-O3
4	XXX	411	GOL	O2-C2-C3-O3
4	EEE	409	GOL	O2-C2-C3-O3
4	JJJ	408	GOL	O2-C2-C3-O3
4	JJJ	409	GOL	O1-C1-C2-O2
4	MMM	411	GOL	O1-C1-C2-O2
4	OOO	410	GOL	O1-C1-C2-O2
4	PPP	409	GOL	O1-C1-C2-O2
4	QQQ	410	GOL	O1-C1-C2-O2
4	BBB	410	GOL	C1-C2-C3-O3
4	MMM	410	GOL	C1-C2-C3-O3
4	WWW	405	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	CCC	409	GOL	O1-C1-C2-O2
4	MMM	411	GOL	O2-C2-C3-O3
4	XXX	411	GOL	O1-C1-C2-O2
4	UUU	413	GOL	O1-C1-C2-O2
4	KKK	412	GOL	O1-C1-C2-C3
4	XXX	411	GOL	C1-C2-C3-O3
4	FFF	408	GOL	O2-C2-C3-O3
4	PPP	410	GOL	O1-C1-C2-O2
4	SSS	413	GOL	O2-C2-C3-O3
4	WWW	405	GOL	O2-C2-C3-O3
4	BBB	410	GOL	O1-C1-C2-C3
4	III	410	GOL	O2-C2-C3-O3
4	WWW	405	GOL	O1-C1-C2-O2
4	KKK	412	GOL	O1-C1-C2-O2

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
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%)

All (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

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Mol	Chain	Res	Type	RSRZ
1	FFF	262	VAL	4.4
1	RRR	3	LEU	4.4
1	XXX	2	LYS	4.4
1	GGG	301	GLY	4.4
1	RRR	282	GLY	4.4
1	HHH	215	TYR	4.4
1	FFF	261	LYS	4.4
1	HHH	193	TYR	4.3
1	UUU	303	ASP	4.3
1	MMM	4	ASP	4.3
1	CCC	171	GLY	4.3
1	SSS	46	VAL	4.2
1	MMM	301	GLY	4.2
1	QQQ	3	LEU	4.2
1	JJJ	257	SER	4.2
1	MMM	261	LYS	4.1
1	SSS	3	LEU	4.1
1	III	301	GLY	4.1
1	III	196	PRO	4.1
1	VVV	302	ASN	4.1
1	JJJ	1	MET	4.1
1	VVV	1	MET	4.1
1	MMM	262	VAL	4.0
1	TTT	4	ASP	4.0
1	GGG	258	SER	4.0
1	JJJ	268	VAL	4.0
1	RRR	301	GLY	4.0
1	RRR	5	ILE	4.0
1	VVV	301	GLY	3.9
1	QQQ	5	ILE	3.9
1	XXX	5	ILE	3.9
1	KKK	3	LEU	3.9
1	KKK	2	LYS	3.9
1	EEE	2	LYS	3.8
1	RRR	281	THR	3.8
1	JJJ	195	LEU	3.8
1	NNN	301	GLY	3.8
1	PPP	301	GLY	3.8
1	HHH	1	MET	3.8
1	BBB	2	LYS	3.8
1	PPP	2	LYS	3.7
1	UUU	3	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	UUU	5	ILE	3.7
1	HHH	262	VAL	3.7
1	RRR	198	LYS	3.7
1	QQQ	65	ALA	3.7
1	UUU	129	ASN	3.7
1	KKK	193	TYR	3.6
1	RRR	110	PRO	3.6
1	MMM	258	SER	3.6
1	LLL	1	MET	3.6
1	NNN	300	LEU	3.6
1	PPP	282	GLY	3.6
1	JJJ	46	VAL	3.6
1	UUU	262	VAL	3.6
1	GGG	217	THR	3.6
1	RRR	279	HIS	3.6
1	PPP	195	LEU	3.6
1	KKK	301	GLY	3.5
1	MMM	1	MET	3.5
1	HHH	146	VAL	3.5
1	OOO	5	ILE	3.5
1	RRR	210	ILE	3.5
1	DDD	301	GLY	3.5
1	GGG	226	GLY	3.5
1	TTT	301	GLY	3.5
1	TTT	5	ILE	3.5
1	XXX	46	VAL	3.5
1	CCC	3	LEU	3.5
1	TTT	3	LEU	3.5
1	EEE	4	ASP	3.5
1	LLL	2	LYS	3.5
1	WWW	129	ASN	3.4
1	QQQ	171	GLY	3.4
1	III	3	LEU	3.4
1	RRR	298	LEU	3.4
1	SSS	219	SER	3.4
1	RRR	193	TYR	3.4
1	WWW	5	ILE	3.4
1	RRR	146	VAL	3.4
2	www	194	LEU	3.4
1	TTT	281	THR	3.4
1	GGG	1	MET	3.4
1	GGG	268	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	NNN	193	TYR	3.3
1	HHH	221	VAL	3.3
1	HHH	282	GLY	3.3
1	UUU	173	SER	3.3
1	HHH	3	LEU	3.3
1	QQQ	150	PRO	3.3
1	UUU	199	PRO	3.3
1	CCC	302	ASN	3.3
1	LLL	257	SER	3.3
1	III	262	VAL	3.3
1	PPP	262	VAL	3.3
1	WWW	3	LEU	3.3
1	MMM	238	PRO	3.3
1	RRR	260	TYR	3.2
1	VVV	121	VAL	3.2
1	JJJ	296	THR	3.2
1	TTT	195	LEU	3.2
1	XXX	217	THR	3.2
1	WWW	302	ASN	3.2
1	BBB	3	LEU	3.2
1	JJJ	159	GLY	3.2
1	QQQ	2	LYS	3.2
1	RRR	27	TRP	3.2
1	JJJ	60	ALA	3.2
1	PPP	215	TYR	3.2
1	VVV	57	PRO	3.2
1	JJJ	262	VAL	3.2
1	WWW	262	VAL	3.2
1	DDD	261	LYS	3.2
1	MMM	2	LYS	3.2
1	XXX	1	MET	3.2
1	RRR	239	THR	3.1
1	JJJ	216	GLN	3.1
1	OOO	199	PRO	3.1
1	UUU	193	TYR	3.1
1	BBB	262	VAL	3.1
1	BBB	1	MET	3.1
1	RRR	108	THR	3.1
1	EEE	5	ILE	3.1
1	SSS	199	PRO	3.1
1	VVV	111	TYR	3.1
1	RRR	300	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	TTT	262	VAL	3.1
1	VVV	167	VAL	3.1
1	SSS	4	ASP	3.1
1	JJJ	281	THR	3.1
1	RRR	150	PRO	3.1
1	FFF	301	GLY	3.1
1	QQQ	301	GLY	3.1
1	TTT	46	VAL	3.1
1	RRR	280	PRO	3.1
1	MMM	210	ILE	3.0
1	NNN	195	LEU	3.0
1	RRR	240	LEU	3.0
1	KKK	1	MET	3.0
1	XXX	302	ASN	3.0
1	AAA	174	THR	3.0
1	AAA	301	GLY	3.0
1	PPP	238	PRO	3.0
1	OOO	2	LYS	3.0
1	JJJ	251	THR	3.0
1	PPP	44	THR	3.0
1	PPP	198	LYS	3.0
1	SSS	2	LYS	3.0
1	JJJ	5	ILE	3.0
1	TTT	129	ASN	3.0
1	PPP	3	LEU	3.0
1	UUU	268	VAL	3.0
1	VVV	260	TYR	3.0
1	III	4	ASP	3.0
1	JJJ	2	LYS	3.0
1	OOO	174	THR	3.0
1	RRR	2	LYS	3.0
1	VVV	2	LYS	3.0
1	FFF	1	MET	3.0
1	III	1	MET	3.0
1	HHH	300	LEU	2.9
1	WWW	195	LEU	2.9
1	HHH	258	SER	2.9
1	VVV	215	TYR	2.9
1	XXX	193	TYR	2.9
1	VVV	261	LYS	2.9
1	FFF	174	THR	2.9
1	HHH	296	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	LLL	217	THR	2.9
1	WWW	301	GLY	2.9
1	NNN	1	MET	2.9
1	PPP	196	PRO	2.9
1	WWW	1	MET	2.9
1	KKK	129	ASN	2.9
1	OOO	302	ASN	2.9
1	UUU	257	SER	2.9
1	XXX	173	SER	2.9
1	NNN	46	VAL	2.9
1	HHH	301	GLY	2.9
1	OOO	133	GLU	2.9
1	QQQ	108	THR	2.9
1	RRR	175	PRO	2.9
1	XXX	150	PRO	2.9
1	AAA	5	ILE	2.9
1	DDD	3	LEU	2.9
1	SSS	300	LEU	2.9
1	PPP	1	MET	2.9
1	VVV	133	GLU	2.9
1	III	46	VAL	2.9
1	KKK	268	VAL	2.9
1	QQQ	90	VAL	2.9
1	VVV	61	GLY	2.9
1	VVV	174	THR	2.9
1	UUU	302	ASN	2.9
1	MMM	217	THR	2.8
1	TTT	302	ASN	2.8
1	RRR	28	VAL	2.8
1	III	215	TYR	2.8
1	SSS	215	TYR	2.8
1	DDD	4	ASP	2.8
1	SSS	280	PRO	2.8
1	VVV	58	VAL	2.8
1	III	2	LYS	2.8
1	KKK	55[A]	GLU	2.8
1	JJJ	147	ALA	2.8
1	MMM	300	LEU	2.8
1	RRR	195	LEU	2.8
1	EEE	296	THR	2.8
1	HHH	203	THR	2.8
1	III	86	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	TTT	239	THR	2.8
1	UUU	281	THR	2.8
1	XXX	198	LYS	2.8
1	QQQ	121	VAL	2.8
1	SSS	81	VAL	2.8
1	PPP	4	ASP	2.8
1	KKK	258	SER	2.8
1	WWW	157	ALA	2.8
1	JJJ	85	ASN	2.8
1	NNN	2	LYS	2.8
1	SSS	218	LYS	2.8
1	HHH	56	THR	2.8
1	NNN	298	LEU	2.8
1	RRR	224	LEU	2.8
1	EEE	1	MET	2.8
1	DDD	262	VAL	2.8
1	FFF	258	SER	2.7
1	BBB	193	TYR	2.7
1	MMM	193	TYR	2.7
1	HHH	7[A]	LYS	2.7
1	RRR	1	MET	2.7
1	WWW	212	ILE	2.7
1	QQQ	46	VAL	2.7
1	RRR	167	VAL	2.7
1	VVV	48	VAL	2.7
1	WWW	105	VAL	2.7
1	UUU	213	TRP	2.7
1	III	129	ASN	2.7
1	GGG	133	GLU	2.7
1	VVV	47	GLU	2.7
1	WWW	111	TYR	2.7
1	MMM	282	GLY	2.7
1	XXX	4	ASP	2.7
1	CCC	39	LEU	2.7
1	KKK	240	LEU	2.7
1	SSS	170	LEU	2.7
1	HHH	5	ILE	2.7
1	VVV	210	ILE	2.7
1	HHH	216	GLN	2.7
1	AAA	302	ASN	2.7
1	FFF	263	GLU	2.7
1	QQQ	7	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	TTT	48	VAL	2.7
1	VVV	46	VAL	2.7
1	DDD	1	MET	2.7
1	QQQ	4	ASP	2.7
1	BBB	174	THR	2.7
1	III	8	THR	2.7
1	QQQ	120	THR	2.7
1	LLL	252	LEU	2.7
1	OOO	195	LEU	2.7
1	RRR	238	PRO	2.7
1	SSS	179	LEU	2.7
1	UUU	195	LEU	2.7
1	HHH	88	GLU	2.7
1	LLL	5	ILE	2.7
1	JJJ	237	HIS	2.7
1	BBB	221	VAL	2.7
1	VVV	221	VAL	2.7
1	CCC	301	GLY	2.6
1	QQQ	131	ALA	2.6
1	SSS	1	MET	2.6
1	KKK	214	ASP	2.6
1	SSS	193	TYR	2.6
1	UUU	4	ASP	2.6
1	JJJ	259	THR	2.6
1	RRR	236	PHE	2.6
1	UUU	174	THR	2.6
1	HHH	2	LYS	2.6
1	JJJ	7	LYS	2.6
1	NNN	10	SER	2.6
1	RRR	241	PRO	2.6
1	III	195	LEU	2.6
1	JJJ	3	LEU	2.6
1	JJJ	132	LEU	2.6
1	KKK	302	ASN	2.6
1	VVV	179	LEU	2.6
1	RRR	254	ILE	2.6
1	GGG	121	VAL	2.6
1	PPP	90	VAL	2.6
1	TTT	1	MET	2.6
1	KKK	4	ASP	2.6
1	VVV	65	ALA	2.6
1	NNN	215	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	GGG	239	THR	2.6
1	XXX	24	THR	2.6
1	FFF	173	SER	2.6
1	PPP	10	SER	2.6
1	RRR	173	SER	2.6
1	XXX	255	TRP	2.6
1	VVV	236	PHE	2.6
1	WWW	156	PHE	2.6
1	JJJ	280	PRO	2.6
1	PPP	240	LEU	2.6
1	JJJ	51	ILE	2.6
1	III	216	GLN	2.6
1	OOO	303	ASP	2.6
1	SSS	246	GLY	2.6
1	DDD	268	VAL	2.6
1	RRR	131	ALA	2.6
1	WWW	167	VAL	2.6
1	AAA	261	LYS	2.6
1	SSS	7	LYS	2.6
1	BBB	217	THR	2.6
1	LLL	251	THR	2.6
1	MMM	296	THR	2.6
1	OOO	219	SER	2.6
1	PPP	239	THR	2.6
1	RRR	258	SER	2.6
1	RRR	299	SER	2.6
1	TTT	251	THR	2.6
1	WWW	174	THR	2.6
1	RRR	168	TRP	2.6
1	GGG	3	LEU	2.6
1	KKK	195	LEU	2.6
1	NNN	216	GLN	2.6
1	VVV	55	GLU	2.6
1	JJJ	218	LYS	2.6
1	UUU	261	LYS	2.6
1	SSS	37	VAL	2.6
1	SSS	90	VAL	2.6
1	RRR	169	SER	2.6
1	JJJ	24	THR	2.6
1	KKK	199	PRO	2.5
1	KKK	215	TYR	2.5
1	MMM	215	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	VVV	238	PRO	2.5
1	GGG	216	GLN	2.5
1	EEE	88	GLU	2.5
1	CCC	123	LEU	2.5
1	CCC	240	LEU	2.5
1	EEE	240	LEU	2.5
1	FFF	3	LEU	2.5
1	HHH	4	ASP	2.5
1	KKK	300	LEU	2.5
1	OOO	4	ASP	2.5
1	KKK	213	TRP	2.5
1	JJJ	226	GLY	2.5
1	PPP	5	ILE	2.5
1	VVV	202	ILE	2.5
1	FFF	302	ASN	2.5
1	RRR	65	ALA	2.5
1	AAA	258	SER	2.5
1	TTT	257	SER	2.5
1	CCC	48	VAL	2.5
1	JJJ	58	VAL	2.5
1	MMM	90	VAL	2.5
1	JJJ	44	THR	2.5
1	KKK	174	THR	2.5
1	WWW	155	THR	2.5
1	FFF	199	PRO	2.5
1	OOO	238	PRO	2.5
1	QQQ	1	MET	2.5
1	PPP	88	GLU	2.5
1	UUU	238	PRO	2.5
1	RRR	111	TYR	2.5
1	SSS	236	PHE	2.5
1	AAA	3	LEU	2.5
1	XXX	300	LEU	2.5
1	UUU	269	GLY	2.5
1	UUU	301	GLY	2.5
1	WWW	171	GLY	2.5
1	MMM	126	TRP	2.5
1	RRR	128	ASN	2.5
1	RRR	302	ASN	2.5
1	TTT	299	SER	2.5
1	RRR	104	ALA	2.5
1	FFF	46	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	GGG	108	THR	2.5
1	MMM	259	THR	2.5
1	NNN	37	VAL	2.5
1	QQQ	167	VAL	2.5
1	RRR	58	VAL	2.5
1	RRR	90	VAL	2.5
1	RRR	7	LYS	2.5
1	GGG	189	TYR	2.5
1	JJJ	301	GLY	2.5
1	KKK	179	LEU	2.5
1	VVV	3	LEU	2.5
1	CCC	129	ASN	2.5
1	MMM	302	ASN	2.5
1	HHH	10	SER	2.5
1	FFF	45	GLN	2.5
1	WWW	40	TRP	2.5
1	JJJ	28	VAL	2.5
1	JJJ	48	VAL	2.5
1	JJJ	53	VAL	2.5
1	QQQ	284	LYS	2.5
1	KKK	238	PRO	2.5
1	VVV	196	PRO	2.5
1	HHH	12	ARG	2.4
1	KKK	282	GLY	2.4
1	PPP	283	ARG	2.4
1	RRR	226	GLY	2.4
1	HHH	302	ASN	2.4
1	SSS	200	TYR	2.4
1	TTT	85	ASN	2.4
1	VVV	189	TYR	2.4
1	OOO	88	GLU	2.4
1	OOO	258	SER	2.4
1	CCC	64	ILE	2.4
1	RRR	243	ILE	2.4
1	FFF	2	LYS	2.4
1	UUU	44	THR	2.4
1	VVV	130	TRP	2.4
1	VVV	168	TRP	2.4
1	EEE	262	VAL	2.4
1	WWW	57	PRO	2.4
1	BBB	215	TYR	2.4
1	CCC	1	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	GGG	219	SER	2.4
1	JJJ	266	LEU	2.4
1	MMM	111	TYR	2.4
1	MMM	240	LEU	2.4
1	UUU	300	LEU	2.4
1	VVV	132	LEU	2.4
1	SSS	148	PHE	2.4
1	VVV	77	PHE	2.4
1	GGG	210	ILE	2.4
1	SSS	212	ILE	2.4
1	DDD	296	THR	2.4
1	NNN	217	THR	2.4
1	QQQ	239	THR	2.4
1	RRR	180	THR	2.4
1	VVV	24	THR	2.4
1	WWW	108	THR	2.4
1	HHH	204	ALA	2.4
1	JJJ	65	ALA	2.4
1	KKK	196	PRO	2.4
1	QQQ	107	PRO	2.4
1	RRR	23	PRO	2.4
1	RRR	199	PRO	2.4
1	XXX	153	PRO	2.4
1	III	55	GLU	2.4
1	III	88	GLU	2.4
1	MMM	221	VAL	2.4
1	PPP	221	VAL	2.4
1	UUU	46	VAL	2.4
1	WWW	213	TRP	2.4
1	RRR	216	GLN	2.4
1	WWW	300	LEU	2.4
1	CCC	193	TYR	2.4
1	FFF	260	TYR	2.4
1	JJJ	193	TYR	2.4
1	NNN	260	TYR	2.4
1	WWW	4	ASP	2.4
1	NNN	44	THR	2.4
1	PPP	281	THR	2.4
1	QQQ	36	ARG	2.4
1	QQQ	281	THR	2.4
1	RRR	155	THR	2.4
1	SSS	24	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	SSS	283	ARG	2.4
1	WWW	281	THR	2.4
1	CCC	5	ILE	2.4
1	JJJ	243	ILE	2.4
1	XXX	147	ALA	2.4
1	QQQ	196	PRO	2.4
1	VVV	150	PRO	2.4
1	RRR	125	ASN	2.4
1	AAA	37	VAL	2.4
1	BBB	301	GLY	2.4
1	LLL	262	VAL	2.4
1	NNN	221	VAL	2.4
1	PPP	37	VAL	2.4
1	QQQ	48	VAL	2.4
1	SSS	262	VAL	2.4
1	JJJ	10	SER	2.4
1	PPP	258	SER	2.4
1	QQQ	50	SER	2.4
1	SSS	10	SER	2.4
1	DDD	2	LYS	2.4
1	MMM	218	LYS	2.4
1	BBB	214	ASP	2.3
1	BBB	195	LEU	2.3
1	HHH	39	LEU	2.3
1	JJJ	300	LEU	2.3
1	KKK	39	LEU	2.3
1	JJJ	77	PHE	2.3
1	SSS	9	PHE	2.3
1	CCC	217	THR	2.3
1	III	108	THR	2.3
1	VVV	217	THR	2.3
1	SSS	216	GLN	2.3
1	JJJ	131	ALA	2.3
1	WWW	147	ALA	2.3
1	WWW	244	ILE	2.3
1	DDD	302	ASN	2.3
1	PPP	302	ASN	2.3
1	QQQ	302	ASN	2.3
1	RRR	129	ASN	2.3
1	FFF	238	PRO	2.3
1	SSS	23	PRO	2.3
1	RRR	151	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	EEE	46	VAL	2.3
1	HHH	167	VAL	2.3
1	LLL	268	VAL	2.3
1	RRR	219	SER	2.3
1	WWW	46	VAL	2.3
1	MMM	88[A]	GLU	2.3
1	OOO	3	LEU	2.3
1	RRR	266	LEU	2.3
1	MMM	260	TYR	2.3
1	RRR	174	THR	2.3
1	VVV	281	THR	2.3
1	WWW	260	TYR	2.3
1	XXX	120	THR	2.3
1	HHH	218	LYS	2.3
1	JJJ	261	LYS	2.3
1	TTT	2	LYS	2.3
1	TTT	7	LYS	2.3
1	HHH	169	SER	2.3
1	VVV	219	SER	2.3
1	CCC	262	VAL	2.3
1	OOO	221	VAL	2.3
1	SSS	197	ASP	2.3
1	VVV	4	ASP	2.3
1	VVV	190	VAL	2.3
1	XXX	197	ASP	2.3
1	JJJ	27	TRP	2.3
1	JJJ	29	LEU	2.3
1	RRR	255	TRP	2.3
1	WWW	252	LEU	2.3
1	XXX	298	LEU	2.3
1	HHH	44	THR	2.3
1	NNN	302	ASN	2.3
1	UUU	24	THR	2.3
1	VVV	256	ASN	2.3
1	FFF	193	TYR	2.3
1	JJJ	21	PHE	2.3
1	UUU	42	TYR	2.3
1	TTT	261	LYS	2.3
1	VVV	147	ALA	2.3
1	WWW	196	PRO	2.3
1	JJJ	276	ILE	2.3
1	LLL	282	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	RRR	171	GLY	2.3
1	XXX	283	ARG	2.3
1	DDD	88	GLU	2.3
1	JJJ	197	ASP	2.3
1	PPP	197	ASP	2.3
1	JJJ	105	VAL	2.3
1	PPP	48	VAL	2.3
1	RRR	112	VAL	2.3
1	VVV	235	VAL	2.3
1	XXX	221	VAL	2.3
1	HHH	129	ASN	2.3
1	MMM	129	ASN	2.3
1	PPP	279	HIS	2.3
1	RRR	176	ASN	2.3
1	BBB	261	LYS	2.3
1	FFF	266	LEU	2.3
1	HHH	261	LYS	2.3
1	III	24	THR	2.3
1	III	261	LYS	2.3
1	NNN	252	LEU	2.3
1	VVV	300	LEU	2.3
1	JJJ	66	ARG	2.2
1	LLL	130	TRP	2.2
1	QQQ	124	TRP	2.2
1	VVV	69	TRP	2.2
1	VVV	124	TRP	2.2
1	JJJ	294	GLY	2.2
1	PPP	200	TYR	2.2
1	RRR	133	GLU	2.2
1	RRR	147	ALA	2.2
1	RRR	189	TYR	2.2
1	UUU	260	TYR	2.2
1	WWW	282	GLY	2.2
1	XXX	182	GLY	2.2
1	CCC	10	SER	2.2
1	III	258	SER	2.2
1	SSS	257	SER	2.2
1	RRR	4	ASP	2.2
1	RRR	79	ILE	2.2
1	VVV	64	ILE	2.2
1	KKK	216	GLN	2.2
1	OOO	216	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	RRR	262	VAL	2.2
1	QQQ	106	HIS	2.2
1	RRR	22	HIS	2.2
1	RRR	237	HIS	2.2
1	WWW	198	LYS	2.2
1	OOO	220	CYS	2.2
1	SSS	8	THR	2.2
1	WWW	217	THR	2.2
1	UUU	55[A]	GLU	2.2
1	VVV	208	LEU	2.2
1	CCC	23	PRO	2.2
1	HHH	241	PRO	2.2
1	VVV	282	GLY	2.2
1	HHH	222	ALA	2.2
1	JJJ	277	ALA	2.2
1	NNN	4	ASP	2.2
1	WWW	154	SER	2.2
1	CCC	126	TRP	2.2
1	EEE	213	TRP	2.2
1	HHH	63	PHE	2.2
1	JJJ	286	TYR	2.2
1	NNN	213	TRP	2.2
1	RRR	69	TRP	2.2
1	WWW	84	TYR	2.2
1	XXX	260	TYR	2.2
1	HHH	198	LYS	2.2
1	NNN	201	MET	2.2
1	SSS	6	LYS	2.2
1	UUU	2	LYS	2.2
1	UUU	198	LYS	2.2
1	KKK	262	VAL	2.2
1	QQQ	268	VAL	2.2
1	TTT	88	GLU	2.2
1	BBB	54[A]	THR	2.2
1	DDD	44	THR	2.2
1	EEE	259	THR	2.2
1	III	174	THR	2.2
1	SSS	86	THR	2.2
1	TTT	217	THR	2.2
1	VVV	56	THR	2.2
1	EEE	3	LEU	2.2
1	MMM	123	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	WWW	170	LEU	2.2
1	GGG	10	SER	2.2
1	TTT	10	SER	2.2
1	HHH	280	PRO	2.2
1	III	199	PRO	2.2
1	JJJ	238	PRO	2.2
1	VVV	199	PRO	2.2
1	III	65	ALA	2.2
1	VVV	60	ALA	2.2
1	CCC	84	TYR	2.2
1	JJJ	177	PHE	2.2
1	VVV	33	TYR	2.2
1	JJJ	19	ILE	2.2
1	VVV	243	ILE	2.2
1	WWW	100	ILE	2.2
1	PPP	284	LYS	2.2
1	QQQ	27	TRP	2.2
1	CCC	125	ASN	2.2
1	III	302	ASN	2.2
1	WWW	279	HIS	2.2
1	GGG	88	GLU	2.2
1	WWW	263	GLU	2.2
1	TTT	187	VAL	2.2
1	VVV	262	VAL	2.2
1	AAA	120	THR	2.2
1	JJJ	108	THR	2.2
1	MMM	239	THR	2.2
1	XXX	8	THR	2.2
1	KKK	197	ASP	2.2
1	LLL	226	GLY	2.2
1	OOO	300	LEU	2.2
1	QQQ	132	LEU	2.2
1	RRR	39	LEU	2.2
1	RRR	123	LEU	2.2
1	SSS	252	LEU	2.2
1	UUU	266	LEU	2.2
2	ccc	194	LEU	2.2
1	CCC	150	PRO	2.2
1	QQQ	241	PRO	2.2
1	UUU	280	PRO	2.2
1	XXX	131	ALA	2.2
1	GGG	7	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	JJJ	6	LYS	2.2
1	OOO	284	LYS	2.2
1	TTT	283	ARG	2.2
1	WWW	218	LYS	2.2
1	AAA	1	MET	2.1
1	JJJ	279	HIS	2.1
1	OOO	1	MET	2.1
1	UUU	1	MET	2.1
1	JJJ	9	PHE	2.1
1	JJJ	33	TYR	2.1
1	KKK	88	GLU	2.1
1	RRR	9	PHE	2.1
1	RRR	21	PHE	2.1
1	WWW	177	PHE	2.1
1	SSS	260	TYR	2.1
1	NNN	242	ILE	2.1
1	RRR	202	ILE	2.1
1	RRR	276	ILE	2.1
1	SSS	243	ILE	2.1
1	SSS	45	GLN	2.1
1	WWW	126	TRP	2.1
1	AAA	48	VAL	2.1
1	FFF	296	THR	2.1
1	GGG	174	THR	2.1
1	JJJ	91	VAL	2.1
1	JJJ	121	VAL	2.1
1	LLL	37	VAL	2.1
1	PPP	259	THR	2.1
1	RRR	190	VAL	2.1
1	SSS	221	VAL	2.1
1	UUU	251	THR	2.1
1	VVV	16	VAL	2.1
1	DDD	258	SER	2.1
1	III	10	SER	2.1
1	SSS	220	CYS	2.1
1	DDD	283	ARG	2.1
1	III	179	LEU	2.1
1	JJJ	240	LEU	2.1
1	NNN	3	LEU	2.1
1	PPP	36	ARG	2.1
1	PPP	39	LEU	2.1
1	QQQ	161	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	QQQ	170	LEU	2.1
1	VVV	240	LEU	2.1
1	JJJ	284	LYS	2.1
1	UUU	7	LYS	2.1
1	WWW	241	PRO	2.1
1	JJJ	88	GLU	2.1
1	RRR	222	ALA	2.1
1	QQQ	216	GLN	2.1
1	JJJ	200	TYR	2.1
1	NNN	200	TYR	2.1
1	PPP	103	ILE	2.1
1	QQQ	42	TYR	2.1
1	RRR	64	ILE	2.1
1	WWW	42	TYR	2.1
1	SSS	191	ASP	2.1
1	GGG	259	THR	2.1
1	PPP	278	THR	2.1
1	RRR	265	THR	2.1
1	UUU	255	TRP	2.1
1	VVV	265	THR	2.1
1	WWW	130	TRP	2.1
1	BBB	12	ARG	2.1
1	EEE	226	GLY	2.1
1	EEE	301	GLY	2.1
1	JJJ	36	ARG	2.1
1	PPP	246	GLY	2.1
1	XXX	159	GLY	2.1
1	GGG	261	LYS	2.1
1	LLL	218	LYS	2.1
1	RRR	6	LYS	2.1
1	JJJ	133	GLU	2.1
1	BBB	196	PRO	2.1
1	TTT	275	CYS	2.1
1	BBB	240	LEU	2.1
1	WWW	128	ASN	2.1
1	XXX	195	LEU	2.1
1	FFF	147	ALA	2.1
1	HHH	157	ALA	2.1
1	JJJ	234	ALA	2.1
1	OOO	157	ALA	2.1
1	XXX	222	ALA	2.1
1	MMM	93	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	SSS	291	PHE	2.1
1	GGG	200	TYR	2.1
1	JJJ	4	ASP	2.1
1	RRR	200	TYR	2.1
1	SSS	214	ASP	2.1
1	TTT	215	TYR	2.1
1	UUU	210	ILE	2.1
1	VVV	286	TYR	2.1
1	EEE	257	SER	2.1
1	NNN	50	SER	2.1
1	OOO	283	ARG	2.1
1	VVV	50	SER	2.1
1	OOO	55	GLU	2.1
1	OOO	259	THR	2.1
1	RRR	178	THR	2.1
1	RRR	296	THR	2.1
1	SSS	282	GLY	2.1
1	AAA	262	VAL	2.1
1	GGG	262	VAL	2.1
1	HHH	16	VAL	2.1
1	III	130	TRP	2.1
1	III	213	TRP	2.1
1	LLL	48	VAL	2.1
1	QQQ	85	ASN	2.1
1	RRR	48	VAL	2.1
1	RRR	126	TRP	2.1
1	RRR	130	TRP	2.1
1	SSS	213	TRP	2.1
1	JJJ	57	PRO	2.1
1	KKK	280	PRO	2.1
1	WWW	107	PRO	2.1
1	WWW	150	PRO	2.1
1	BBB	39	LEU	2.1
1	III	300	LEU	2.1
1	JJJ	32	LEU	2.1
1	LLL	3	LEU	2.1
1	PPP	266	LEU	2.1
1	QQQ	39	LEU	2.1
1	QQQ	300	LEU	2.1
1	MMM	204	ALA	2.1
1	WWW	204	ALA	2.1
1	PPP	12	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	LLL	148	PHE	2.0
1	MMM	133	GLU	2.0
1	QQQ	136	PHE	2.0
1	RRR	212	ILE	2.0
1	RRR	284	LYS	2.0
1	UUU	263	GLU	2.0
1	GGG	257	SER	2.0
1	KKK	257	SER	2.0
1	VVV	7	LYS	2.0
1	HHH	200	TYR	2.0
1	HHH	260	TYR	2.0
1	WWW	192	TYR	2.0
1	CCC	180	THR	2.0
1	KKK	201	MET	2.0
1	XXX	174	THR	2.0
1	LLL	279	HIS	2.0
1	VVV	106	HIS	2.0
1	WWW	106	HIS	2.0
1	XXX	138	GLY	2.0
1	CCC	285	ASN	2.0
1	DDD	48	VAL	2.0
1	GGG	196	PRO	2.0
1	III	167	VAL	2.0
1	KKK	241	PRO	2.0
1	TTT	28	VAL	2.0
1	BBB	170	LEU	2.0
1	OOO	224	LEU	2.0
1	QQQ	130	TRP	2.0
1	RRR	213	TRP	2.0
1	SSS	27	TRP	2.0
1	SSS	40	TRP	2.0
1	VVV	170	LEU	2.0
1	III	204	ALA	2.0
1	EEE	14	ASP	2.0
1	III	197	ASP	2.0
1	RRR	12	ARG	2.0
1	TTT	36	ARG	2.0
1	UUU	283	ARG	2.0
1	GGG	284	LYS	2.0
1	KKK	264	LYS	2.0
1	UUU	6	LYS	2.0
1	WWW	261	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	XXX	151	LYS	2.0
1	III	299	SER	2.0
1	NNN	257	SER	2.0
1	HHH	77	PHE	2.0
1	PPP	93	PHE	2.0
1	SSS	5	ILE	2.0
1	UUU	148	PHE	2.0
1	VVV	148	PHE	2.0
1	VVV	212	ILE	2.0
1	WWW	287	ILE	2.0
1	EEE	120	THR	2.0
1	JJJ	86	THR	2.0
1	KKK	251	THR	2.0
1	LLL	239	THR	2.0
1	FFF	200	TYR	2.0
1	GGG	260	TYR	2.0
1	WWW	193	TYR	2.0
1	WWW	215	TYR	2.0
1	PPP	194	PRO	2.0
1	RRR	26	PRO	2.0
1	VVV	153	PRO	2.0
1	WWW	280	PRO	2.0
1	HHH	297	VAL	2.0
1	III	283	ARG	2.0
1	JJJ	72	VAL	2.0
1	JJJ	90	VAL	2.0
1	JJJ	185	ARG	2.0
1	PPP	72	VAL	2.0
1	RRR	81	VAL	2.0
1	TTT	90	VAL	2.0
1	VVV	146	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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(Å 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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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.