



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 30, 2017 – 03:24 AM EDT

PDB ID : 3NSG  
Title : Crystal Structure of OmpF, an Outer Membrane Protein from Salmonella typhi  
Authors : Balasubramaniam, D.; Arockiasamy, A.; Sharma, A.; Krishnaswamy, S.  
Deposited on : unknown  
Resolution : 2.79 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

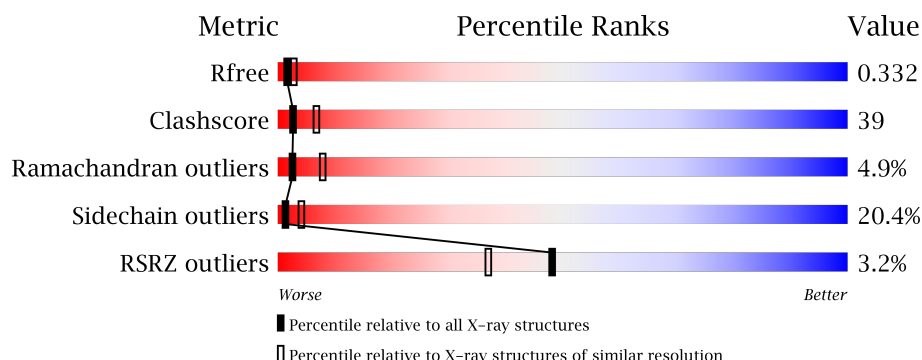
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.79 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))
$R_{free}$	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	341	<div> <div>4%</div> <div>35%</div> <div>48%</div> <div>16%</div> </div>
1	B	341	<div> <div>2%</div> <div>39%</div> <div>52%</div> <div>9%</div> </div>
1	C	341	<div> <div>3%</div> <div>39%</div> <div>49%</div> <div>11%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	353	-	-	-	X
2	SO4	A	354	-	-	-	X
2	SO4	A	358	-	-	-	X
2	SO4	A	361	-	-	X	-
2	SO4	A	366	-	-	-	X
2	SO4	B	345	-	-	X	-
2	SO4	B	349	-	-	-	X
2	SO4	C	343	-	-	-	X
2	SO4	C	348	-	-	-	X
2	SO4	C	362	-	-	-	X
2	SO4	C	363	-	-	-	X
2	SO4	C	364	-	-	-	X
2	SO4	C	368	-	-	-	X
2	SO4	C	370	-	-	X	-
3	GOL	A	370	-	-	-	X
3	GOL	A	371	-	-	-	X
3	GOL	A	375	-	-	-	X
3	GOL	B	365	-	-	X	-
3	GOL	B	373	-	-	-	X
3	GOL	C	1325	-	-	-	X
3	GOL	C	375	-	-	X	-
4	LDA	A	384	-	-	-	X
4	LDA	A	386	-	-	-	X
4	LDA	A	387	-	-	-	X
4	LDA	A	388	-	-	-	X
4	LDA	C	385	-	-	-	X
5	TAM	A	390	-	-	X	X
6	FLC	C	388	-	-	X	-

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 9432 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 Outer membrane protein F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	341	Total	C	N	O	Se	0	0	0
			2669	1662	453	547	7			
1	B	341	Total	C	N	O	Se	0	0	0
			2669	1662	453	547	7			
1	C	341	Total	C	N	O	Se	0	0	0
			2669	1662	453	547	7			

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



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

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

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

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

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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		

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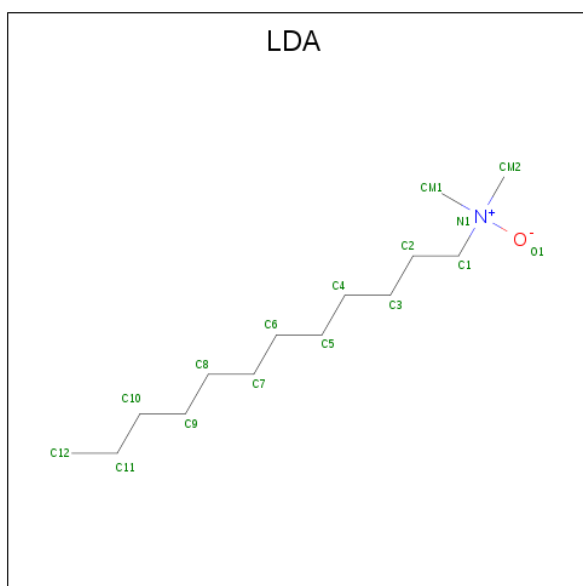
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula:  $C_{14}H_{31}NO$ ).



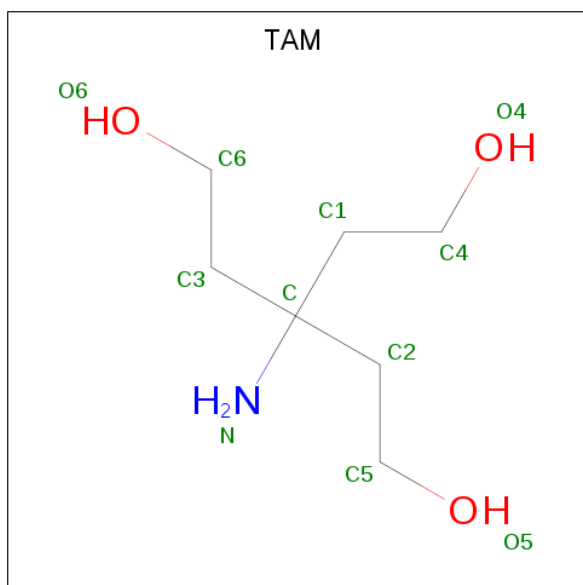
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			16	14	1	1		
4	A	1	Total	C	N	O	0	0
			16	14	1	1		
4	A	1	Total	C	N	O	0	0
			16	14	1	1		
4	A	1	Total	C	N	O	0	0
			16	14	1	1		
4	A	1	Total	C	N	O	0	0
			16	14	1	1		
4	B	1	Total	C	N	O	0	0
			16	14	1	1		
4	B	1	Total	C	N	O	0	0
			16	14	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			16	14	1	1		
4	B	1	Total	C	N	O	0	0
			16	14	1	1		
4	B	1	Total	C	N	O	0	0
			16	14	1	1		
4	B	1	Total	C	N	O	0	0
			16	14	1	1		
4	B	1	Total	C	N	O	0	0
			16	14	1	1		
4	C	1	Total	C	N	O	0	0
			16	14	1	1		
4	C	1	Total	C	N	O	0	0
			16	14	1	1		
4	C	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 5 is TRIS(HYDROXYETHYL)AMINOMETHANE (three-letter code: TAM) (formula:  $C_7H_{17}NO_3$ ).



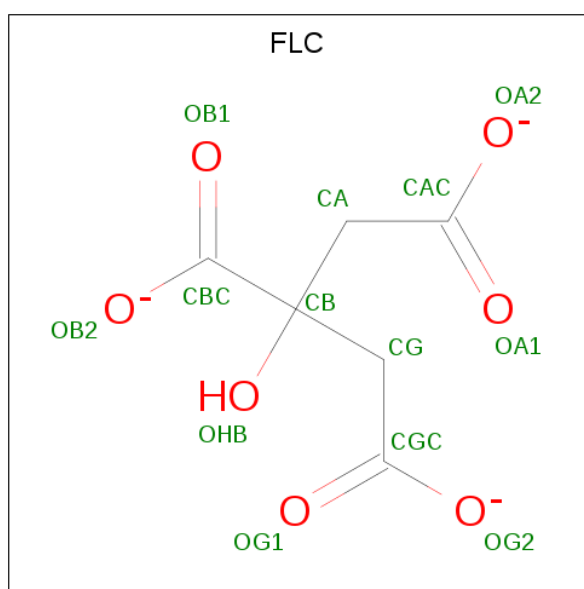
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			11	7	1	3		
5	A	1	Total	C	N	O	0	0
			11	7	1	3		

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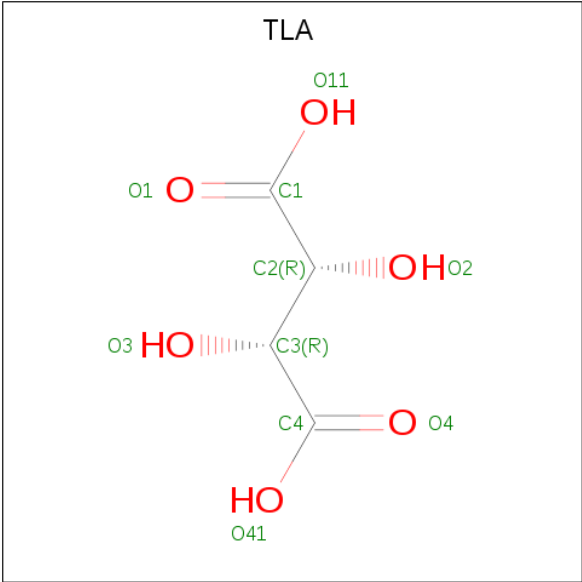
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			11	7	1	3		
5	C	1	Total	C	N	O	0	0
			11	7	1	3		
5	C	1	Total	C	N	O	0	0
			11	7	1	3		
5	C	1	Total	C	N	O	0	0
			11	7	1	3		

- Molecule 6 is CITRATE ANION (three-letter code: FLC) (formula:  $C_6H_5O_7$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			13	6	7		
6	C	1	Total	C	O	0	0
			13	6	7		
6	C	1	Total	C	O	0	0
			13	6	7		
6	C	1	Total	C	O	0	0
			13	6	7		

- Molecule 7 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula:  $C_4H_6O_6$ ).



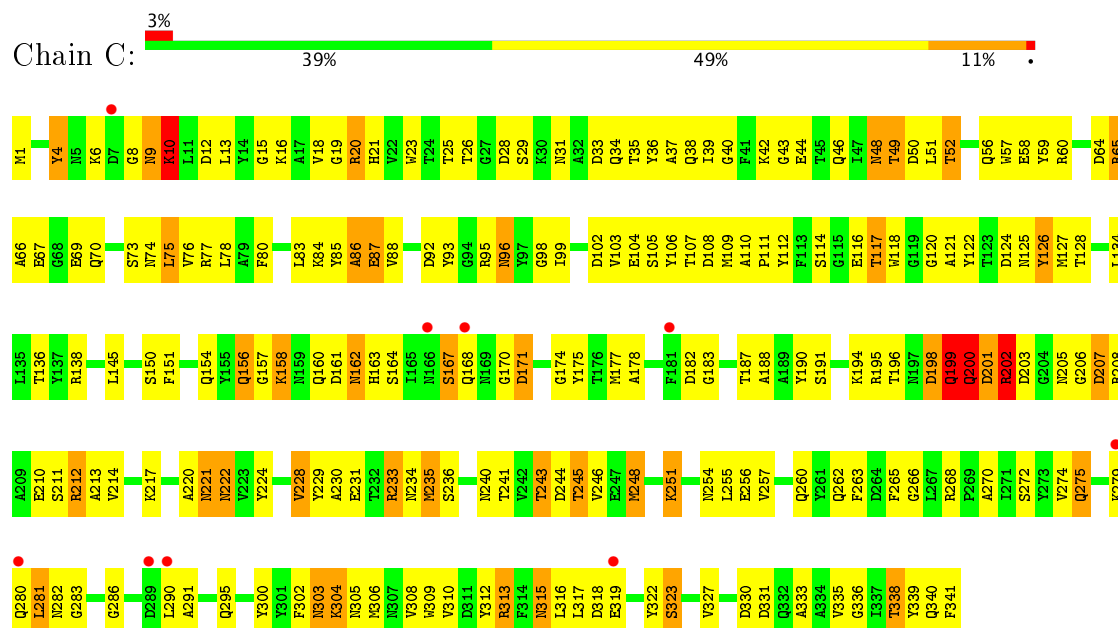
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			10	4	6		
7	B	1	Total	C	O	0	0
			10	4	6		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	134	Total	O	0	0
			134	134		
8	B	115	Total	O	0	0
			115	115		
8	C	138	Total	O	0	0
			138	138		



● Molecule 1: Outer membrane protein F





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.19Å 139.34Å 150.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.59 – 2.79 42.59 – 2.79	Depositor EDS
% Data completeness (in resolution range)	84.1 (42.59-2.79) 84.1 (42.59-2.79)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.44 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.255 , 0.337 0.253 , 0.332	Depositor DCC
$R_{free}$ test set	1898 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	45.9	Xtriage
Anisotropy	1.301	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 54.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	9432	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, LDA, TLA, SO4, TAM, FLC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.60	0/2717	0.75	0/3668
1	B	0.61	0/2717	0.75	0/3668
1	C	0.59	0/2717	0.73	0/3668
All	All	0.60	0/8151	0.74	0/11004

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2669	0	2464	246	0
1	B	2669	0	2464	219	0
1	C	2669	0	2464	231	0
2	A	135	0	0	6	0
2	B	110	0	0	4	0
2	C	155	0	0	6	0
3	A	84	0	112	4	0
3	B	66	0	88	6	0
3	C	78	0	104	8	0
4	A	96	0	186	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	112	0	217	10	0
4	C	64	0	124	15	0
5	A	22	0	34	11	0
5	B	11	0	17	0	0
5	C	33	0	51	12	0
6	A	13	0	5	0	0
6	C	39	0	15	6	0
7	A	10	0	4	0	0
7	B	10	0	4	1	0
8	A	134	0	0	11	0
8	B	115	0	0	7	0
8	C	138	0	0	11	0
All	All	9432	0	8353	687	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 39.

All (687) 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:A:198:ASP:HA	1:A:200:GLN:NE2	1.61	1.13
1:A:21:HIS:CE1	1:A:31:ASN:OD1	2.04	1.11
1:A:107:THR:HG21	1:A:256:GLU:OE1	1.56	1.05
1:A:117:THR:HG23	1:A:118:TRP:H	1.22	1.04
4:B:375:LDA:HM13	4:C:382:LDA:H21	1.38	1.03
5:C:387:TAM:H61	5:C:387:TAM:H51	1.38	1.03
1:A:125:ASN:O	1:A:128:THR:HG23	1.59	1.02
1:A:198:ASP:HA	1:A:200:GLN:HE22	0.84	1.00
1:B:195:ARG:HH12	1:B:206:GLY:HA2	1.26	1.00
5:A:390:TAM:C4	5:A:390:TAM:C5	2.40	0.99
1:C:241:THR:OG1	1:C:323:SER:HB2	1.61	0.99
5:C:387:TAM:C6	5:C:387:TAM:H51	1.93	0.97
1:C:244:ASP:OD1	6:C:388:FLC:HA2	1.64	0.96
5:A:390:TAM:H41	5:A:390:TAM:C5	1.95	0.96
1:A:9:ASN:HB3	1:A:45:THR:HA	1.48	0.95
1:C:128:THR:HG23	1:C:235:MSE:HE1	1.48	0.95
1:C:210:GLU:HB2	1:C:233:ARG:HB2	1.46	0.95
1:A:127:MSE:SE	1:A:154:GLN:OE1	2.34	0.95
1:A:117:THR:CG2	1:A:118:TRP:H	1.79	0.94
1:A:291:ALA:HA	1:A:317:LEU:HD11	1.49	0.94
1:B:139:ASN:HD22	1:B:151:PHE:HE2	1.13	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:255:LEU:HB3	1:C:275:GLN:HG2	1.47	0.94
1:C:65:ARG:CG	1:C:65:ARG:HH11	1.80	0.93
1:C:178:ALA:HB2	1:C:187:THR:HG23	1.51	0.92
1:B:252:THR:O	1:B:254:ASN:ND2	2.02	0.92
1:C:245:THR:HG22	3:C:375:GOL:H2	1.51	0.92
5:A:390:TAM:C4	5:A:390:TAM:H52	2.02	0.89
1:B:270:ALA:O	1:B:295:GLN:NE2	2.07	0.88
1:B:202:ARG:HB2	1:B:247:GLU:HB3	1.54	0.88
1:C:56:GLN:HB3	1:C:80:PHE:CZ	2.07	0.88
1:C:65:ARG:HH11	1:C:65:ARG:HG2	1.38	0.87
1:A:160:GLN:HA	1:A:168:GLN:HG2	1.58	0.85
1:C:128:THR:CG2	1:C:235:MSE:HE1	2.06	0.85
1:A:21:HIS:HE1	1:A:31:ASN:OD1	1.59	0.85
1:A:127:MSE:HG2	1:A:154:GLN:HE22	1.41	0.85
1:B:76:VAL:H	1:C:70:GLN:HE22	1.25	0.84
1:C:200:GLN:OE1	1:C:200:GLN:HA	1.76	0.84
1:B:1:MSE:O	1:B:2:GLU:HB2	1.77	0.84
1:B:312:TYR:CD2	1:B:333:ALA:HB2	2.13	0.84
5:A:390:TAM:O4	5:A:390:TAM:H52	1.77	0.83
1:C:272:SER:OG	1:C:295:GLN:HG3	1.78	0.83
1:C:26:THR:HG22	1:C:330:ASP:OD2	1.79	0.82
1:A:211:SER:OG	1:A:231:GLU:O	1.97	0.82
1:A:107:THR:CG2	1:A:256:GLU:OE1	2.28	0.82
1:A:115:GLY:O	1:A:120:GLY:HA3	1.81	0.80
1:A:127:MSE:HG2	1:A:154:GLN:NE2	1.97	0.80
1:A:260:GLN:HE21	1:A:270:ALA:HB2	1.46	0.80
1:B:139:ASN:ND2	1:B:142:PHE:HA	1.98	0.79
1:B:158:LYS:HE3	8:B:466:HOH:O	1.82	0.79
1:B:106:TYR:O	1:B:224:TYR:OH	2.00	0.79
1:A:67:GLU:O	1:C:75:LEU:HD22	1.82	0.79
1:B:76:VAL:H	1:C:70:GLN:NE2	1.82	0.78
5:A:390:TAM:O4	5:A:390:TAM:C2	2.30	0.78
1:B:130:ARG:NH2	1:C:67:GLU:OE2	2.16	0.78
5:A:390:TAM:O4	5:A:390:TAM:H21	1.83	0.78
1:C:10:LYS:NZ	1:C:42:LYS:HE2	1.99	0.78
5:A:390:TAM:H41	5:A:390:TAM:H51	1.66	0.77
1:C:77:ARG:O	1:C:95:ARG:HG2	1.83	0.77
1:A:4:TYR:HD1	1:B:1:MSE:HE1	1.48	0.77
1:A:18:VAL:O	1:A:35:THR:HG23	1.84	0.77
1:C:57:TRP:HA	1:C:78:LEU:O	1.84	0.77
1:C:200:GLN:O	1:C:202:ARG:N	2.18	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:ASP:OD1	1:C:66:ALA:HA	1.85	0.76
1:C:112:TYR:HB2	8:C:527:HOH:O	1.85	0.76
1:B:99:ILE:HD11	1:B:176:THR:HG22	1.67	0.76
1:A:93:TYR:OH	1:B:21:HIS:HD2	1.69	0.76
1:C:304:LYS:HE3	1:C:305:ASN:HD21	1.49	0.76
1:A:2:GLU:HA	1:A:12:ASP:HB2	1.68	0.75
1:A:207:ASP:HB3	2:A:361:SO4:O4	1.86	0.75
1:A:65:ARG:NH1	1:C:162:ASN:OD1	2.18	0.75
1:C:302:PHE:HE2	1:C:308:VAL:HG12	1.50	0.75
1:A:88:VAL:HG22	2:A:350:SO4:O3	1.87	0.75
1:B:163:HIS:HB3	1:B:167:SER:HB2	1.69	0.75
1:C:126:TYR:HB2	1:C:235:MSE:HE3	1.67	0.74
1:C:85:TYR:HB3	1:C:88:VAL:HG22	1.69	0.74
1:B:65:ARG:NH2	8:B:492:HOH:O	2.05	0.74
1:A:150:SER:OG	1:A:178:ALA:HB3	1.87	0.74
1:C:99:ILE:HB	1:C:154:GLN:HE21	1.52	0.74
1:B:76:VAL:N	1:C:70:GLN:HE22	1.85	0.74
1:C:65:ARG:HG2	1:C:65:ARG:NH1	1.97	0.74
1:C:98:GLY:HA3	1:C:127:MSE:HA	1.69	0.73
5:A:390:TAM:O4	5:A:390:TAM:C5	2.36	0.73
1:A:337:ILE:CD1	4:A:384:LDA:H122	2.19	0.73
1:B:103:VAL:O	1:B:106:TYR:HB2	1.89	0.72
5:A:390:TAM:H41	5:A:390:TAM:H52	1.62	0.72
1:C:241:THR:OG1	1:C:323:SER:CB	2.38	0.72
1:A:275:GLN:HA	1:A:291:ALA:O	1.89	0.72
1:B:26:THR:HG22	1:B:27:GLY:N	2.04	0.72
2:B:345:SO4:O3	8:B:474:HOH:O	2.08	0.72
1:A:48:ASN:HD22	1:A:49:THR:H	1.35	0.71
1:A:23:TRP:HZ2	4:A:384:LDA:HM13	1.52	0.71
1:B:195:ARG:NH1	1:B:206:GLY:HA2	2.04	0.71
1:C:134:LEU:HD23	1:C:156:GLN:HG3	1.71	0.71
5:C:387:TAM:H61	5:C:387:TAM:C5	2.18	0.71
1:A:204:GLY:O	8:A:485:HOH:O	2.08	0.70
1:A:43:GLY:HA3	1:B:339:TYR:CE2	2.26	0.70
1:C:110:ALA:HB3	1:C:114:SER:OG	1.91	0.70
1:C:99:ILE:HB	1:C:154:GLN:HG2	1.73	0.70
1:B:288:ALA:HB1	1:B:320:ASN:HD21	1.56	0.70
1:C:168:GLN:OE1	1:C:196:THR:HG21	1.91	0.70
1:B:130:ARG:HH21	1:C:67:GLU:CD	1.93	0.70
1:A:32:ALA:HA	4:C:385:LDA:H92	1.74	0.70
1:A:264:ASP:HB2	8:A:510:HOH:O	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:ASP:O	1:B:167:SER:HA	1.91	0.70
1:B:30:LYS:HD3	1:B:31:ASN:H	1.57	0.69
1:A:209:ALA:HA	1:A:234:ASN:HB2	1.74	0.69
1:B:3:ILE:HD11	1:B:13:LEU:HB2	1.75	0.69
1:C:244:ASP:OD1	6:C:388:FLC:CA	2.39	0.69
1:A:77:ARG:HH21	3:A:370:GOL:H32	1.57	0.69
1:C:99:ILE:H	1:C:154:GLN:NE2	1.91	0.69
1:A:217:LYS:CB	1:A:226:ALA:HB2	2.23	0.69
1:A:232:THR:HG21	1:A:236:SER:HB2	1.73	0.69
1:B:156:GLN:OE1	1:B:169:ASN:ND2	2.25	0.69
1:C:263:PHE:HB3	1:C:265:PHE:CE2	2.27	0.69
1:C:306:MSE:CE	1:C:339:TYR:HD1	2.06	0.69
1:A:207:ASP:HB3	2:A:361:SO4:S	2.34	0.68
1:B:258:VAL:HG22	1:B:272:SER:HB2	1.76	0.68
1:C:161:ASP:O	1:C:162:ASN:HB2	1.94	0.68
1:A:205:ASN:HB3	1:A:234:ASN:HD21	1.60	0.67
1:B:153:ILE:HD11	1:B:155:TYR:HE2	1.59	0.67
1:C:245:THR:CG2	3:C:375:GOL:H2	2.24	0.67
1:A:146:VAL:HG21	1:A:149:LEU:HB3	1.75	0.67
1:B:312:TYR:HD2	1:B:333:ALA:HB2	1.56	0.67
1:C:262:GLN:NE2	1:C:268:ARG:HD3	2.10	0.67
1:A:232:THR:HB	1:A:252:THR:HB	1.76	0.67
1:B:21:HIS:O	1:B:334:ALA:HB1	1.95	0.67
1:C:25:THR:HG22	4:C:383:LDA:H41	1.77	0.67
4:C:384:LDA:H41	4:C:384:LDA:HM13	1.77	0.67
1:C:86:ALA:O	1:C:87:GLU:HB2	1.94	0.67
1:A:149:LEU:HA	1:A:178:ALA:O	1.95	0.66
4:B:375:LDA:CM1	4:C:382:LDA:H21	2.21	0.66
1:C:306:MSE:HE2	1:C:339:TYR:HD1	1.59	0.66
1:B:77:ARG:O	1:B:95:ARG:HD2	1.96	0.66
1:A:20:ARG:HG3	1:A:34:GLN:O	1.96	0.66
1:C:99:ILE:N	1:C:154:GLN:NE2	2.44	0.66
1:C:194:LYS:HA	1:C:207:ASP:O	1.96	0.66
1:A:196:THR:O	1:A:199:GLN:HG3	1.95	0.66
1:C:136:THR:HG22	1:C:154:GLN:HB2	1.77	0.65
1:C:304:LYS:HE3	1:C:305:ASN:ND2	2.10	0.65
1:C:99:ILE:HB	1:C:154:GLN:NE2	2.11	0.65
1:C:4:TYR:O	1:C:10:LYS:HA	1.95	0.65
1:A:220:ALA:O	1:A:223:VAL:HG23	1.96	0.65
1:C:26:THR:CG2	1:C:330:ASP:OD2	2.44	0.65
1:B:134:LEU:HD22	1:B:154:GLN:HE21	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:ASN:CB	1:B:65:ARG:HH11	2.09	0.65
1:C:322:TYR:O	1:C:323:SER:C	2.34	0.65
1:A:104:GLU:HA	1:A:104:GLU:OE1	1.97	0.65
1:A:4:TYR:CD1	1:B:1:MSE:HE1	2.30	0.65
1:B:276:SER:HB2	1:B:291:ALA:HB3	1.78	0.65
1:C:222:ASN:HD22	1:C:222:ASN:N	1.95	0.64
1:A:117:THR:HA	1:A:326:TYR:CD1	2.33	0.64
1:A:77:ARG:O	1:A:78:LEU:HD23	1.97	0.64
1:B:127:MSE:HE1	1:B:174:GLY:HA3	1.79	0.64
1:A:20:ARG:NH1	1:A:36:TYR:CD2	2.65	0.64
1:A:93:TYR:OH	1:B:21:HIS:CD2	2.50	0.64
1:C:111:PRO:HA	2:C:348:SO4:O3	1.97	0.64
1:A:227:ALA:HB2	1:A:257:VAL:HG13	1.80	0.64
1:A:260:GLN:HE21	1:A:270:ALA:CB	2.10	0.64
1:B:99:ILE:HG22	1:B:127:MSE:CE	2.27	0.64
1:C:1:MSE:HB3	1:C:13:LEU:O	1.97	0.64
1:A:19:GLY:HA2	1:A:35:THR:HG23	1.80	0.63
1:A:110:ALA:HB3	1:A:114:SER:CB	2.28	0.63
1:A:204:GLY:O	1:A:206:GLY:N	2.31	0.63
1:B:120:GLY:O	1:B:122:TYR:N	2.27	0.63
1:A:91:ILE:HA	1:A:136:THR:O	1.99	0.63
1:A:57:TRP:HA	1:A:78:LEU:O	1.99	0.63
1:B:108:ASP:HA	1:B:114:SER:HB2	1.81	0.63
1:C:10:LYS:HZ1	1:C:42:LYS:HE2	1.62	0.63
1:C:315:ASN:N	1:C:331:ASP:OD1	2.23	0.63
1:A:117:THR:CG2	1:A:118:TRP:N	2.49	0.63
3:B:368:GOL:O2	8:B:414:HOH:O	2.16	0.63
1:B:101:TYR:O	1:B:101:TYR:CD2	2.51	0.63
1:A:302:PHE:HE2	1:A:308:VAL:HG12	1.64	0.62
1:C:207:ASP:OD1	1:C:208:ARG:HG2	1.98	0.62
1:A:4:TYR:O	1:A:10:LYS:HA	2.00	0.62
1:A:35:THR:HG22	1:A:36:TYR:N	2.13	0.62
1:A:161:ASP:HB2	8:A:461:HOH:O	1.98	0.62
1:A:299:THR:OG1	1:A:301:TYR:CE2	2.53	0.62
1:C:65:ARG:HD3	1:C:65:ARG:N	2.15	0.62
1:B:181:PHE:HB2	2:B:354:SO4:S	2.39	0.61
1:C:198:ASP:C	1:C:200:GLN:H	2.03	0.61
1:A:131:ALA:HB3	1:A:134:LEU:HD21	1.82	0.61
1:A:168:GLN:HB3	1:A:196:THR:HG21	1.82	0.61
1:A:202:ARG:NE	1:A:202:ARG:HA	2.15	0.61
1:B:327:VAL:O	1:B:327:VAL:CG2	2.49	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:377:LDA:H61	4:B:379:LDA:H71	1.82	0.61
1:C:241:THR:HG1	1:C:323:SER:HB2	1.65	0.61
1:B:20:ARG:HD2	1:B:34:GLN:HB3	1.82	0.61
1:C:48:ASN:HD21	1:C:51:LEU:HB2	1.64	0.61
1:B:206:GLY:O	1:B:207:ASP:HB2	2.00	0.61
1:B:192:ASN:ND2	1:B:210:GLU:OE2	2.34	0.61
1:C:50:ASP:HB3	1:C:85:TYR:CE1	2.36	0.61
1:C:19:GLY:HA2	1:C:35:THR:HG23	1.82	0.60
1:C:70:GLN:O	1:C:73:SER:HB2	2.01	0.60
1:A:189:ALA:O	1:A:212:ARG:HA	2.02	0.60
1:C:8:GLY:HA3	8:C:538:HOH:O	2.01	0.60
1:A:117:THR:HG23	1:A:118:TRP:N	2.04	0.60
1:A:260:GLN:NE2	1:A:270:ALA:HB2	2.16	0.60
1:A:65:ARG:CZ	1:C:162:ASN:OD1	2.49	0.60
1:A:1:MSE:HB2	1:A:341:PHE:HB2	1.84	0.60
1:A:251:LYS:O	1:A:278:GLY:HA2	2.02	0.60
1:A:82:GLY:C	1:A:83:LEU:HD23	2.21	0.60
1:B:30:LYS:HD3	1:B:31:ASN:N	2.16	0.60
1:A:26:THR:HB	1:A:330:ASP:HB3	1.83	0.59
1:B:158:LYS:NZ	1:B:160:GLN:OE1	2.33	0.59
1:B:139:ASN:OD1	3:B:365:GOL:H11	2.02	0.59
1:A:85:TYR:CD1	1:A:88:VAL:HG21	2.37	0.59
5:C:393:TAM:H62	8:C:484:HOH:O	2.01	0.59
1:A:22:VAL:HG21	1:A:112:TYR:CZ	2.38	0.59
1:B:139:ASN:HD21	1:B:142:PHE:HA	1.67	0.59
1:C:202:ARG:HB3	8:C:500:HOH:O	2.02	0.59
1:C:260:GLN:HB3	1:C:270:ALA:HA	1.85	0.59
1:A:110:ALA:HB3	1:A:114:SER:HB3	1.84	0.59
6:C:391:FLC:HG2	5:C:393:TAM:HN2	1.68	0.59
1:C:134:LEU:CD2	1:C:156:GLN:HG3	2.33	0.58
1:C:104:GLU:HG2	1:C:118:TRP:CZ2	2.38	0.58
1:C:116:GLU:OE2	1:C:313:ARG:NH1	2.31	0.58
1:C:272:SER:OG	1:C:295:GLN:CG	2.51	0.58
1:A:127:MSE:CG	1:A:154:GLN:HE22	2.13	0.58
1:A:131:ALA:HB3	1:A:134:LEU:HD11	1.85	0.58
1:B:231:GLU:OE2	1:B:233:ARG:NH2	2.35	0.58
1:C:157:GLY:HA2	1:C:171:ASP:OD2	2.03	0.58
1:A:299:THR:HG1	1:A:301:TYR:HE2	1.50	0.58
1:A:48:ASN:HD22	1:A:49:THR:N	2.00	0.58
1:B:99:ILE:HG22	1:B:127:MSE:HE3	1.84	0.58
1:C:306:MSE:CE	1:C:339:TYR:CD1	2.87	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:291:ALA:HA	1:C:317:LEU:HD12	1.84	0.58
1:C:306:MSE:HE1	1:C:339:TYR:CD1	2.39	0.58
1:B:123:THR:O	1:B:130:ARG:O	2.22	0.58
1:B:164:SER:O	1:B:166:ASN:N	2.37	0.58
1:C:99:ILE:H	1:C:154:GLN:HE21	1.49	0.58
1:C:335:VAL:HG22	1:C:336:GLY:N	2.19	0.57
1:B:26:THR:CG2	1:B:27:GLY:N	2.66	0.57
1:A:201:ASP:OD1	1:A:202:ARG:HG2	2.04	0.57
1:B:118:TRP:CG	1:B:119:GLY:N	2.72	0.57
1:A:162:ASN:CG	1:B:65:ARG:NH1	2.58	0.57
1:A:299:THR:OG1	1:A:301:TYR:HE2	1.88	0.57
1:B:233:ARG:O	1:B:250:ASN:HA	2.04	0.57
1:A:244:ASP:O	1:A:245:THR:CB	2.53	0.57
1:A:33:ASP:H	4:C:385:LDA:H111	1.68	0.57
1:B:297:GLY:HA3	1:B:311:ASP:HA	1.86	0.57
1:A:302:PHE:CE2	1:A:308:VAL:HG12	2.39	0.57
1:A:87:GLU:O	1:A:143:PHE:HD1	1.88	0.57
1:C:212:ARG:HG2	1:C:231:GLU:HB3	1.86	0.57
1:C:282:ASN:O	1:C:322:TYR:HE2	1.87	0.57
1:C:49:THR:HB	2:C:370:SO4:O3	2.04	0.57
1:A:337:ILE:HD13	4:A:384:LDA:H122	1.86	0.57
1:B:202:ARG:HB2	1:B:247:GLU:CB	2.31	0.57
1:A:117:THR:CG2	1:A:118:TRP:HD1	2.18	0.56
1:B:113:PHE:HD1	1:B:116:GLU:OE1	1.89	0.56
1:B:43:GLY:HA3	1:C:339:TYR:OH	2.06	0.56
1:C:234:ASN:O	1:C:248:MSE:HG2	2.06	0.56
1:B:116:GLU:O	1:B:121:ALA:HB2	2.06	0.56
1:B:313:ARG:NH2	1:B:327:VAL:HB	2.20	0.56
1:C:111:PRO:HB3	1:C:309:TRP:CD1	2.41	0.56
1:A:267:LEU:HD12	1:A:268:ARG:H	1.71	0.56
1:B:61:THR:HG22	1:B:74:ASN:HB3	1.87	0.56
1:A:33:ASP:OD1	1:A:35:THR:N	2.39	0.56
1:B:197:ASN:O	1:B:200:GLN:HG3	2.07	0.56
1:B:293:TYR:CE2	1:B:327:VAL:HG21	2.41	0.56
1:B:64:ASP:OD2	1:B:65:ARG:HD3	2.05	0.55
4:C:383:LDA:HM23	8:C:423:HOH:O	2.05	0.55
1:C:111:PRO:HD3	8:C:476:HOH:O	2.05	0.55
1:B:124:ASP:OD1	1:C:66:ALA:CA	2.53	0.55
1:B:202:ARG:CB	1:B:247:GLU:HB3	2.33	0.55
1:C:117:THR:OG1	1:C:118:TRP:N	2.39	0.55
1:A:177:MSE:O	1:A:187:THR:HG22	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:PHE:O	1:B:145:LEU:HB2	2.06	0.55
1:B:320:ASN:C	1:B:322:TYR:N	2.58	0.55
4:B:377:LDA:H31	4:B:379:LDA:H62	1.89	0.55
1:C:309:TRP:NE1	8:C:527:HOH:O	2.29	0.55
1:B:1:MSE:N	1:B:13:LEU:O	2.31	0.55
1:B:23:TRP:CD1	1:B:31:ASN:OD1	2.60	0.55
1:B:8:GLY:O	1:B:9:ASN:HB2	2.06	0.55
1:C:198:ASP:O	1:C:200:GLN:N	2.40	0.55
1:A:23:TRP:CZ2	4:A:384:LDA:HM13	2.38	0.54
1:B:66:ALA:O	1:B:70:GLN:HG3	2.08	0.54
1:A:217:LYS:HB3	1:A:226:ALA:HB2	1.89	0.54
1:A:70:GLN:NE2	1:C:76:VAL:H	2.05	0.54
1:B:139:ASN:HB3	1:B:151:PHE:CE2	2.42	0.54
1:C:281:LEU:H	1:C:281:LEU:HD13	1.71	0.54
1:A:117:THR:CG2	1:A:118:TRP:CD1	2.90	0.54
1:B:77:ARG:NH2	2:B:345:SO4:O4	2.33	0.54
1:A:131:ALA:CB	1:A:134:LEU:HD21	2.38	0.54
1:A:248:MSE:O	1:A:249:ALA:O	2.25	0.54
1:A:25:THR:HB	1:A:331:ASP:O	2.08	0.54
4:B:375:LDA:HM13	4:C:382:LDA:C2	2.25	0.54
1:C:103:VAL:HG11	1:C:213:ALA:HB1	1.90	0.54
1:C:98:GLY:HA3	1:C:127:MSE:CA	2.37	0.54
1:A:2:GLU:HA	1:A:12:ASP:CB	2.38	0.54
1:A:202:ARG:HD2	1:A:245:THR:CG2	2.38	0.54
1:A:78:LEU:CD2	1:A:130:ARG:HG2	2.37	0.54
1:A:195:ARG:HH21	1:A:248:MSE:HB2	1.72	0.54
1:A:1:MSE:HB3	1:A:341:PHE:HD2	1.73	0.54
1:C:93:TYR:HA	1:C:134:LEU:O	2.07	0.54
1:A:146:VAL:HG11	1:A:149:LEU:HB3	1.88	0.54
1:B:313:ARG:O	1:B:313:ARG:HG3	2.07	0.54
1:A:117:THR:HA	1:A:326:TYR:CE1	2.43	0.54
1:A:74:ASN:OD1	1:C:59:TYR:OH	2.14	0.54
1:C:240:ASN:O	1:C:243:THR:O	2.26	0.54
1:A:5:ASN:ND2	1:A:10:LYS:HB2	2.23	0.53
1:B:239:GLU:OE1	1:B:246:VAL:HG13	2.07	0.53
1:B:315:ASN:HD21	1:B:317:LEU:HB3	1.73	0.53
1:B:89:GLY:HA2	3:B:365:GOL:H12	1.90	0.53
5:C:387:TAM:H32	3:C:392:GOL:O2	2.07	0.53
1:A:47:ILE:HD11	1:B:306:MSE:HG2	1.91	0.53
1:A:172:GLY:HA3	1:A:193:SER:OG	2.08	0.53
1:A:207:ASP:HB3	2:A:361:SO4:O2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:306:MSE:HE1	1:B:339:TYR:CD1	2.43	0.53
1:C:23:TRP:CZ3	4:C:383:LDA:H82	2.43	0.53
1:A:101:TYR:CD1	1:A:104:GLU:HB3	2.43	0.53
1:B:169:ASN:ND2	8:B:401:HOH:O	2.40	0.53
1:A:110:ALA:HB3	1:A:114:SER:HB2	1.90	0.53
1:C:21:HIS:CG	4:C:384:LDA:H31	2.43	0.53
1:B:196:THR:HG22	1:B:198:ASP:H	1.74	0.53
1:B:306:MSE:CE	1:B:339:TYR:HD1	2.21	0.53
1:A:207:ASP:OD1	1:A:208:ARG:N	2.42	0.53
1:B:89:GLY:HA3	1:B:137:TYR:CE1	2.43	0.53
1:C:48:ASN:HD22	1:C:48:ASN:N	2.07	0.53
1:A:262:GLN:HG2	8:A:522:HOH:O	2.08	0.53
1:A:300:TYR:HE1	8:A:516:HOH:O	1.92	0.53
1:B:327:VAL:O	1:B:327:VAL:HG22	2.08	0.53
1:A:296:ALA:O	1:A:312:TYR:N	2.40	0.52
1:A:53:GLY:HA3	1:B:306:MSE:HE3	1.91	0.52
1:B:126:TYR:CE1	1:B:169:ASN:HB2	2.43	0.52
1:B:127:MSE:HE1	1:B:174:GLY:CA	2.38	0.52
1:A:232:THR:HB	1:A:252:THR:CB	2.38	0.52
1:B:145:LEU:HD12	4:B:376:LDA:H61	1.91	0.52
1:B:53:GLY:C	1:C:306:MSE:HE3	2.29	0.52
1:C:108:ASP:HA	1:C:114:SER:HB3	1.91	0.52
1:A:172:GLY:HA2	1:A:193:SER:HA	1.92	0.52
1:A:277:LYS:HG3	1:A:288:ALA:O	2.08	0.52
1:A:291:ALA:CA	1:A:317:LEU:HD11	2.33	0.52
1:B:2:GLU:HB3	3:B:364:GOL:H12	1.89	0.52
1:A:117:THR:HG22	1:A:118:TRP:CD1	2.44	0.52
1:B:250:ASN:O	1:B:251:LYS:O	2.28	0.52
1:B:261:TYR:O	1:B:269:PRO:HD2	2.10	0.52
1:C:255:LEU:HB3	1:C:275:GLN:CG	2.31	0.52
1:C:309:TRP:CD1	1:C:309:TRP:C	2.83	0.52
1:A:178:ALA:HA	1:A:187:THR:HG22	1.92	0.52
1:A:306:MSE:O	1:A:307:ASN:HB3	2.10	0.52
1:C:18:VAL:HG21	1:C:36:TYR:CZ	2.45	0.52
1:A:217:LYS:HB2	1:A:226:ALA:HB2	1.93	0.51
1:B:54:PHE:HE2	1:B:84:LYS:HB2	1.75	0.51
1:C:18:VAL:HG13	1:C:338:THR:HG22	1.92	0.51
1:A:111:PRO:HG3	1:A:299:THR:HG21	1.93	0.51
1:B:21:HIS:CE1	1:B:31:ASN:HD21	2.26	0.51
1:A:91:ILE:HD12	1:A:92:ASP:N	2.26	0.51
1:B:320:ASN:C	1:B:322:TYR:H	2.13	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:195:ARG:HH22	1:C:206:GLY:HA2	1.76	0.51
1:B:166:ASN:OD1	1:B:237:ILE:HD13	2.10	0.51
1:C:170:GLY:HA3	1:C:194:LYS:O	2.10	0.51
3:C:394:GOL:H2	8:C:488:HOH:O	2.11	0.51
1:C:107:THR:CG2	1:C:228:VAL:HG12	2.40	0.51
1:C:317:LEU:HD23	1:C:318:ASP:N	2.26	0.51
1:B:62:LYS:HB2	1:B:73:SER:HB2	1.92	0.51
1:B:42:LYS:NZ	1:B:42:LYS:CB	2.74	0.51
1:A:70:GLN:HE22	1:C:76:VAL:HG22	1.76	0.51
1:B:277:LYS:HE2	4:B:380:LDA:HM13	1.93	0.50
1:B:317:LEU:HD21	1:B:323:SER:OG	2.10	0.50
1:B:58:GLU:HB3	1:B:77:ARG:HG3	1.92	0.50
1:A:25:THR:HG21	1:A:312:TYR:OH	2.12	0.50
1:B:306:MSE:HE2	1:B:339:TYR:HD1	1.76	0.50
1:B:99:ILE:O	1:B:102:ASP:HB2	2.11	0.50
1:C:303:ASN:HB3	1:C:305:ASN:H	1.76	0.50
1:A:140:SER:O	1:A:150:SER:HB3	2.11	0.50
1:A:158:LYS:HE3	1:A:160:GLN:HB3	1.92	0.50
1:B:134:LEU:HD13	1:B:154:GLN:NE2	2.26	0.50
1:B:229:TYR:CE2	1:B:231:GLU:HG3	2.46	0.50
1:C:335:VAL:CG2	1:C:336:GLY:N	2.74	0.50
1:A:99:ILE:O	1:A:102:ASP:HB2	2.12	0.50
1:C:200:GLN:HG2	8:C:458:HOH:O	2.11	0.50
1:A:134:LEU:HD23	1:A:156:GLN:HG3	1.93	0.50
1:C:102:ASP:OD2	1:C:138:ARG:NH2	2.40	0.50
1:B:2:GLU:OE1	1:B:5:ASN:ND2	2.45	0.50
1:C:313:ARG:CZ	1:C:327:VAL:HG13	2.42	0.50
1:C:282:ASN:HA	2:C:365:SO4:O1	2.11	0.50
1:A:20:ARG:NH1	1:A:36:TYR:CE2	2.80	0.50
1:C:222:ASN:N	1:C:222:ASN:ND2	2.60	0.50
1:C:9:ASN:O	1:C:10:LYS:CB	2.60	0.50
1:A:180:GLU:HA	1:A:185:GLY:HA2	1.93	0.49
1:A:195:ARG:HD2	1:A:209:ALA:HB2	1.93	0.49
1:A:23:TRP:CD2	4:A:388:LDA:H82	2.47	0.49
1:A:91:ILE:HD12	1:A:91:ILE:C	2.32	0.49
1:C:281:LEU:HD13	1:C:281:LEU:N	2.27	0.49
1:A:146:VAL:HG23	1:A:147:ASP:N	2.27	0.49
1:B:89:GLY:HA2	3:B:365:GOL:C1	2.42	0.49
1:A:111:PRO:HG3	1:A:299:THR:CG2	2.43	0.49
1:A:20:ARG:NH1	1:A:36:TYR:HD2	2.10	0.49
1:A:267:LEU:HD12	1:A:268:ARG:N	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:ALA:HB3	1:A:69:GLU:OE2	2.12	0.49
1:B:265:PHE:HE1	1:B:267:LEU:HB2	1.77	0.49
7:B:383:TLA:O11	8:B:457:HOH:O	2.20	0.49
1:B:139:ASN:HD21	1:B:143:PHE:N	2.11	0.49
1:B:306:MSE:CE	1:B:339:TYR:CD1	2.96	0.49
3:C:375:GOL:O2	5:C:386:TAM:C2	2.60	0.49
1:C:50:ASP:CB	1:C:85:TYR:HE1	2.25	0.49
1:B:307:ASN:ND2	1:B:338:THR:CG2	2.75	0.49
1:B:95:ARG:HA	1:B:132:GLY:HA2	1.94	0.49
3:C:375:GOL:O2	5:C:386:TAM:H21	2.13	0.49
1:A:57:TRP:CZ2	1:A:59:TYR:HB2	2.48	0.49
1:A:1:MSE:O	1:A:13:LEU:O	2.31	0.49
1:B:127:MSE:CE	1:B:174:GLY:HA3	2.41	0.49
6:C:388:FLC:CBC	6:C:388:FLC:OG1	2.59	0.49
1:C:136:THR:HG22	1:C:154:GLN:CB	2.42	0.49
1:C:99:ILE:CB	1:C:154:GLN:HE21	2.23	0.49
1:C:195:ARG:HH21	1:C:203:ASP:HB3	1.78	0.49
1:C:241:THR:OG1	1:C:323:SER:CA	2.60	0.49
1:A:150:SER:OG	1:A:178:ALA:CB	2.60	0.49
1:A:87:GLU:O	1:A:143:PHE:CD1	2.66	0.49
1:B:26:THR:HG22	1:B:27:GLY:H	1.78	0.49
1:C:200:GLN:C	1:C:202:ARG:N	2.66	0.49
1:C:128:THR:HG21	1:C:235:MSE:HE1	1.93	0.49
1:C:265:PHE:HD2	1:C:265:PHE:H	1.59	0.49
1:A:275:GLN:HB2	1:A:292:LYS:HD2	1.93	0.48
1:C:110:ALA:O	1:C:111:PRO:C	2.48	0.48
1:A:106:TYR:CE2	1:A:217:LYS:HG2	2.47	0.48
1:B:21:HIS:CE1	1:B:31:ASN:ND2	2.81	0.48
4:C:382:LDA:H62	4:C:383:LDA:H111	1.94	0.48
1:B:26:THR:O	1:B:28:ASP:O	2.30	0.48
1:C:262:GLN:HB2	1:C:268:ARG:HD2	1.96	0.48
1:C:15:GLY:HA2	1:C:38:GLN:O	2.14	0.48
1:A:146:VAL:CG2	1:A:149:LEU:H	2.26	0.48
1:B:99:ILE:HG22	1:B:127:MSE:HE2	1.94	0.48
1:C:95:ARG:HH22	1:C:124:ASP:CG	2.16	0.48
1:A:24:THR:HB	1:A:30:LYS:H	1.78	0.48
1:A:69:GLU:OE1	1:C:164:SER:OG	2.31	0.48
1:B:26:THR:CG2	1:B:27:GLY:H	2.27	0.48
1:B:303:ASN:HB3	1:B:305:ASN:H	1.79	0.48
1:A:1:MSE:N	1:A:341:PHE:C	2.67	0.48
1:A:282:ASN:OD1	1:A:282:ASN:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:386:TAM:H22	5:C:386:TAM:H61	1.23	0.48
1:A:141:ASP:CG	1:A:144:GLY:H	2.17	0.48
1:B:199:GLN:O	1:B:203:ASP:HB3	2.13	0.48
1:B:21:HIS:O	1:B:334:ALA:CB	2.61	0.48
1:C:187:THR:HG22	1:C:188:ALA:N	2.29	0.48
1:C:279:LYS:O	1:C:280:GLN:HB2	2.13	0.48
1:A:95:ARG:NH2	1:A:124:ASP:OD1	2.47	0.48
1:B:137:TYR:HB3	1:B:153:ILE:HD13	1.96	0.48
1:C:201:ASP:O	1:C:202:ARG:C	2.51	0.47
1:A:20:ARG:HH11	1:A:36:TYR:HD2	1.62	0.47
1:A:238:VAL:HG13	1:A:325:SER:CB	2.43	0.47
1:A:320:ASN:HB2	1:A:323:SER:HB2	1.96	0.47
1:B:265:PHE:CE1	1:B:267:LEU:HB2	2.49	0.47
1:C:65:ARG:HG3	1:C:65:ARG:HH11	1.69	0.47
1:C:76:VAL:HG23	1:C:95:ARG:HD2	1.94	0.47
1:A:95:ARG:HG3	1:A:131:ALA:O	2.14	0.47
1:C:198:ASP:C	1:C:200:GLN:N	2.66	0.47
1:C:224:TYR:HB3	1:C:260:GLN:HG3	1.96	0.47
1:C:80:PHE:CD2	1:C:96:ASN:ND2	2.82	0.47
1:A:292:LYS:O	1:A:316:LEU:N	2.44	0.47
1:C:322:TYR:O	1:C:323:SER:O	2.32	0.47
1:A:279:LYS:O	1:A:280:GLN:HB2	2.14	0.47
1:B:229:TYR:HE2	1:B:231:GLU:HG3	1.78	0.47
1:C:263:PHE:HB3	1:C:265:PHE:HE2	1.74	0.47
1:A:244:ASP:O	1:A:245:THR:HB	2.15	0.47
1:A:78:LEU:HD21	1:A:130:ARG:HD2	1.97	0.47
1:A:18:VAL:HG12	1:A:20:ARG:HG2	1.95	0.47
1:A:330:ASP:OD2	1:A:330:ASP:N	2.48	0.47
1:C:33:ASP:C	1:C:34:GLN:HG2	2.35	0.47
1:A:76:VAL:HG13	1:B:70:GLN:HE22	1.79	0.47
1:B:23:TRP:HD1	1:B:31:ASN:OD1	1.97	0.47
1:B:53:GLY:HA3	1:C:306:MSE:HE3	1.97	0.47
1:A:160:GLN:NE2	8:A:476:HOH:O	2.47	0.46
1:A:238:VAL:HG13	1:A:325:SER:HB3	1.97	0.46
1:A:99:ILE:HG12	1:A:176:THR:HB	1.97	0.46
1:A:70:GLN:HE22	1:C:76:VAL:H	1.63	0.46
1:A:154:GLN:HG3	8:A:446:HOH:O	2.14	0.46
1:A:162:ASN:CB	1:B:65:ARG:NH1	2.77	0.46
1:C:220:ALA:O	1:C:221:ASN:C	2.53	0.46
1:A:119:GLY:HA2	1:A:128:THR:OG1	2.15	0.46
1:A:160:GLN:CA	1:A:168:GLN:HG2	2.39	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:ASN:HB2	1:A:250:ASN:OD1	2.15	0.46
1:A:279:LYS:HG2	1:A:286:GLY:O	2.15	0.46
1:A:35:THR:CG2	1:A:36:TYR:N	2.79	0.46
3:A:370:GOL:H12	5:A:390:TAM:O4	2.16	0.46
1:B:15:GLY:HA2	1:B:38:GLN:O	2.16	0.46
1:B:238:VAL:HG11	1:B:290:LEU:HD21	1.98	0.46
1:B:196:THR:HB	2:B:348:SO4:O3	2.15	0.46
1:B:141:ASP:HA	1:B:149:LEU:O	2.16	0.46
1:C:107:THR:HG23	1:C:228:VAL:HG12	1.96	0.46
1:A:306:MSE:HE2	1:C:83:LEU:HD21	1.97	0.46
1:A:202:ARG:HD2	1:A:245:THR:HG23	1.97	0.46
1:B:222:ASN:HB3	1:B:262:GLN:O	2.16	0.46
1:B:320:ASN:O	1:B:322:TYR:N	2.48	0.46
1:B:97:TYR:CZ	1:B:130:ARG:HD3	2.51	0.46
1:C:158:LYS:HD2	4:C:385:LDA:H61	1.98	0.46
1:C:99:ILE:N	1:C:154:GLN:HE21	2.10	0.46
1:A:9:ASN:CB	1:A:44:GLU:O	2.64	0.46
1:B:191:SER:O	1:B:210:GLU:HB2	2.15	0.46
1:C:120:GLY:O	1:C:122:TYR:N	2.49	0.46
1:C:182:ASP:HB3	1:C:183:GLY:H	1.57	0.46
1:C:86:ALA:O	1:C:87:GLU:CB	2.62	0.46
1:A:127:MSE:SE	1:A:154:GLN:CD	3.02	0.46
1:A:300:TYR:HD2	1:A:301:TYR:N	2.13	0.46
1:C:9:ASN:O	1:C:44:GLU:O	2.33	0.46
1:B:75:LEU:HB2	1:C:67:GLU:HG2	1.98	0.46
1:C:212:ARG:CG	1:C:231:GLU:HB3	2.46	0.46
1:C:251:LYS:HD2	1:C:280:GLN:HE22	1.81	0.46
1:A:200:GLN:N	1:A:200:GLN:HE21	2.14	0.46
1:C:263:PHE:CB	1:C:265:PHE:CE2	2.96	0.46
1:C:23:TRP:HZ3	1:C:335:VAL:HG12	1.80	0.46
1:C:103:VAL:HG12	1:C:104:GLU:N	2.31	0.45
1:B:30:LYS:HE2	1:B:30:LYS:HA	1.98	0.45
1:B:18:VAL:O	1:B:35:THR:HG23	2.17	0.45
1:C:103:VAL:O	1:C:106:TYR:HB2	2.16	0.45
1:C:109:MSE:CE	1:C:268:ARG:NH2	2.79	0.45
3:A:380:GOL:H31	8:A:500:HOH:O	2.16	0.45
1:B:203:ASP:N	1:B:203:ASP:OD1	2.48	0.45
1:B:288:ALA:HB1	1:B:320:ASN:ND2	2.29	0.45
5:C:393:TAM:H41	5:C:393:TAM:H21	1.61	0.45
1:B:77:ARG:O	1:B:78:LEU:HD23	2.16	0.45
1:B:164:SER:C	1:B:166:ASN:N	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:MSE:HG3	1:B:224:TYR:CE2	2.51	0.45
1:A:146:VAL:O	1:A:147:ASP:HB2	2.17	0.45
1:A:16:LYS:HB3	1:A:340:GLN:HB3	1.98	0.45
1:B:89:GLY:HA3	1:B:137:TYR:HE1	1.82	0.45
1:B:76:VAL:N	1:C:70:GLN:NE2	2.52	0.45
1:C:244:ASP:CG	6:C:388:FLC:HA2	2.34	0.45
1:B:42:LYS:HB3	1:B:42:LYS:HZ3	1.82	0.45
1:C:56:GLN:HB3	1:C:80:PHE:CE2	2.49	0.45
1:A:18:VAL:O	1:A:35:THR:CG2	2.60	0.45
1:B:7:ASP:O	1:B:9:ASN:ND2	2.50	0.45
1:A:104:GLU:O	1:A:105:SER:C	2.55	0.45
1:A:257:VAL:O	1:A:272:SER:HB2	2.17	0.45
1:A:309:TRP:C	1:A:309:TRP:CD1	2.90	0.45
1:B:91:ILE:HG12	4:C:384:LDA:C12	2.47	0.45
1:C:125:ASN:HA	8:C:477:HOH:O	2.17	0.45
1:C:151:PHE:HB3	1:C:177:MSE:HG3	1.98	0.45
1:C:262:GLN:NE2	1:C:268:ARG:CD	2.76	0.45
1:C:65:ARG:HD3	1:C:65:ARG:H	1.79	0.45
1:B:18:VAL:HG13	1:B:338:THR:HB	2.00	0.44
1:C:202:ARG:CD	3:C:375:GOL:H31	2.48	0.44
1:C:76:VAL:CG2	1:C:76:VAL:O	2.65	0.44
1:C:99:ILE:HG21	1:C:174:GLY:HA3	1.99	0.44
1:A:123:THR:O	1:A:129:SER:HB3	2.16	0.44
1:A:91:ILE:HD11	4:A:386:LDA:H91	1.98	0.44
1:B:124:ASP:OD1	1:C:66:ALA:CB	2.66	0.44
1:B:250:ASN:O	1:B:251:LYS:C	2.54	0.44
1:C:127:MSE:HG2	1:C:154:GLN:NE2	2.32	0.44
1:B:75:LEU:HA	1:C:70:GLN:HE21	1.82	0.44
1:A:202:ARG:HD2	1:A:245:THR:HG21	2.00	0.44
1:C:255:LEU:O	1:C:256:GLU:HG3	2.17	0.44
1:B:127:MSE:HE1	1:B:174:GLY:N	2.32	0.44
1:B:20:ARG:HD2	1:B:34:GLN:O	2.17	0.44
1:C:195:ARG:NH2	1:C:206:GLY:HA2	2.31	0.44
1:C:48:ASN:HB2	2:C:370:SO4:S	2.58	0.44
1:C:74:ASN:O	1:C:75:LEU:HD23	2.17	0.44
1:B:165:ILE:HG23	1:B:198:ASP:HB3	2.00	0.44
1:B:205:ASN:CG	8:B:433:HOH:O	2.56	0.44
1:C:99:ILE:HB	1:C:154:GLN:CG	2.43	0.44
1:A:238:VAL:O	1:A:246:VAL:HG23	2.17	0.44
1:A:9:ASN:HB2	8:A:409:HOH:O	2.17	0.44
1:B:197:ASN:C	1:B:199:GLN:H	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:156:GLN:HB3	1:C:156:GLN:HE21	1.65	0.44
1:B:43:GLY:HA3	1:C:339:TYR:CZ	2.52	0.44
1:C:98:GLY:HA2	1:C:154:GLN:HE22	1.82	0.44
1:A:101:TYR:HA	1:A:104:GLU:HB2	2.00	0.44
1:A:224:TYR:HE2	1:A:258:VAL:HG11	1.83	0.44
1:A:43:GLY:HA3	1:B:339:TYR:CZ	2.52	0.44
1:B:110:ALA:HB3	1:B:114:SER:N	2.33	0.44
1:B:113:PHE:CD1	1:B:116:GLU:OE1	2.69	0.44
1:B:325:SER:O	1:B:326:TYR:CB	2.65	0.44
1:B:313:ARG:NH2	1:B:332:GLN:OE1	2.51	0.44
1:A:162:ASN:HB3	1:B:65:ARG:HH11	1.83	0.44
1:C:282:ASN:O	1:C:322:TYR:CE2	2.69	0.44
1:C:52:THR:O	1:C:84:LYS:N	2.42	0.44
1:C:60:ARG:NH1	8:C:439:HOH:O	2.51	0.44
1:B:76:VAL:HG13	1:C:70:GLN:NE2	2.32	0.44
1:A:236:SER:HG	1:A:326:TYR:HH	1.65	0.44
1:C:213:ALA:HA	1:C:230:ALA:HA	1.99	0.44
1:A:181:PHE:CE1	1:A:184:PHE:HB2	2.53	0.43
1:A:24:THR:HB	1:A:30:LYS:N	2.33	0.43
1:C:23:TRP:CZ3	1:C:335:VAL:HG12	2.54	0.43
1:A:97:TYR:CE1	1:A:130:ARG:HD3	2.54	0.43
1:B:320:ASN:CB	1:B:323:SER:OG	2.65	0.43
1:C:190:TYR:CD1	1:C:191:SER:N	2.87	0.43
1:C:20:ARG:HD3	1:C:34:GLN:HB2	2.00	0.43
1:A:159:ASN:ND2	2:A:358:SO4:O2	2.52	0.43
1:B:171:ASP:OD1	1:B:171:ASP:N	2.46	0.43
1:C:222:ASN:HB3	1:C:262:GLN:O	2.19	0.43
1:C:16:LYS:NZ	2:C:343:SO4:O4	2.48	0.43
1:A:217:LYS:HB3	1:A:226:ALA:CB	2.49	0.43
1:B:141:ASP:OD1	3:B:365:GOL:C3	2.67	0.43
5:C:386:TAM:H21	5:C:386:TAM:H42	1.25	0.43
1:C:244:ASP:OD1	6:C:388:FLC:OB1	2.35	0.43
1:B:158:LYS:HA	1:B:169:ASN:O	2.19	0.43
1:B:84:LYS:HG3	1:B:90:SER:HB3	2.00	0.43
1:C:229:TYR:HA	1:C:254:ASN:O	2.19	0.43
1:A:239:GLU:HB2	8:A:443:HOH:O	2.17	0.43
1:A:22:VAL:HG22	1:A:334:ALA:HB2	2.01	0.43
1:B:170:GLY:HA3	1:B:194:LYS:O	2.18	0.43
1:B:200:GLN:C	1:B:201:ASP:O	2.56	0.43
1:B:255:LEU:O	1:B:256:GLU:HG3	2.18	0.43
1:B:320:ASN:HB3	1:B:323:SER:OG	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:ILE:HD11	1:C:306:MSE:HG2	2.01	0.43
1:C:312:TYR:CD1	1:C:333:ALA:HB2	2.54	0.43
1:B:321:ASP:C	1:B:322:TYR:HD1	2.22	0.43
1:C:309:TRP:HZ3	1:C:338:THR:CG2	2.31	0.43
1:A:233:ARG:NH2	2:A:363:SO4:S	2.87	0.42
1:B:164:SER:C	1:B:166:ASN:H	2.22	0.42
1:C:174:GLY:HA2	1:C:191:SER:HA	2.01	0.42
1:A:150:SER:O	1:A:178:ALA:N	2.52	0.42
1:A:307:ASN:OD1	1:A:307:ASN:C	2.58	0.42
1:B:164:SER:O	1:B:167:SER:N	2.50	0.42
1:C:104:GLU:HG2	1:C:118:TRP:CE2	2.54	0.42
1:A:198:ASP:CA	1:A:200:GLN:NE2	2.55	0.42
1:A:229:TYR:HA	1:A:254:ASN:O	2.19	0.42
1:B:320:ASN:ND2	1:B:322:TYR:HB2	2.34	0.42
5:C:387:TAM:H41	5:C:387:TAM:H22	1.66	0.42
1:A:78:LEU:HD23	1:A:130:ARG:HG2	2.01	0.42
1:B:19:GLY:HA2	1:B:35:THR:HG23	2.00	0.42
1:C:160:GLN:H	4:C:385:LDA:H81	1.84	0.42
1:A:339:TYR:CZ	1:C:43:GLY:HA3	2.55	0.42
1:C:50:ASP:CB	1:C:85:TYR:CE1	3.00	0.42
1:A:208:ARG:HB2	1:A:208:ARG:HE	1.72	0.42
1:A:211:SER:OG	1:A:232:THR:HA	2.20	0.42
1:B:56:GLN:CG	1:B:57:TRP:N	2.82	0.42
1:C:317:LEU:HD23	2:C:364:SO4:O1	2.19	0.42
1:B:57:TRP:CD1	1:C:37:ALA:HB3	2.55	0.42
1:A:208:ARG:NH2	3:A:375:GOL:H12	2.34	0.42
1:B:314:PHE:CZ	4:B:381:LDA:H42	2.55	0.42
1:C:199:GLN:HG2	1:C:203:ASP:HB2	2.02	0.42
1:C:190:TYR:HA	1:C:211:SER:O	2.19	0.42
1:C:65:ARG:N	1:C:65:ARG:CD	2.83	0.42
1:A:110:ALA:CB	1:A:114:SER:HB2	2.50	0.42
1:A:268:ARG:O	1:A:298:ALA:HA	2.20	0.42
1:A:281:LEU:HB2	1:A:322:TYR:OH	2.20	0.42
5:A:391:TAM:H52	5:A:391:TAM:H12	1.38	0.42
1:B:196:THR:O	1:B:199:GLN:HG2	2.20	0.42
1:C:201:ASP:HB3	1:C:246:VAL:O	2.20	0.42
1:A:95:ARG:HB2	1:B:63:ALA:HB1	2.02	0.42
1:C:13:LEU:HD12	1:C:40:GLY:O	2.20	0.42
1:A:66:ALA:HB2	1:C:167:SER:HB3	2.02	0.42
1:C:58:GLU:HB2	1:C:78:LEU:HD12	2.02	0.42
1:A:261:TYR:O	1:A:269:PRO:HD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:ASN:O	1:A:49:THR:C	2.57	0.41
1:B:20:ARG:HD2	1:B:34:GLN:CB	2.47	0.41
1:B:293:TYR:HB3	1:B:315:ASN:HA	2.01	0.41
1:A:126:TYR:HE2	1:A:248:MSE:CE	2.32	0.41
1:B:100:VAL:O	1:B:102:ASP:N	2.53	0.41
1:B:91:ILE:HG12	4:C:384:LDA:H123	2.02	0.41
1:A:91:ILE:HD13	1:A:135:LEU:HD11	2.02	0.41
1:C:164:SER:O	1:C:168:GLN:HG3	2.20	0.41
1:B:100:VAL:C	1:B:102:ASP:N	2.74	0.41
1:B:91:ILE:HD11	1:B:135:LEU:HD11	2.02	0.41
1:C:341:PHE:C	1:C:341:PHE:CD2	2.94	0.41
1:A:241:THR:HG22	1:A:321:ASP:O	2.21	0.41
1:C:118:TRP:HB3	1:C:254:ASN:ND2	2.35	0.41
1:A:313:ARG:O	1:A:313:ARG:HG3	2.21	0.41
1:C:136:THR:HG22	1:C:154:GLN:OE1	2.21	0.41
1:B:53:GLY:CA	1:C:306:MSE:HE3	2.50	0.41
1:A:111:PRO:HD2	1:A:311:ASP:OD2	2.20	0.41
1:B:78:LEU:HA	1:B:95:ARG:HG3	2.03	0.41
1:C:202:ARG:HD2	3:C:375:GOL:H31	2.03	0.41
1:C:266:GLY:HA3	1:C:300:TYR:CE1	2.56	0.41
1:B:115:GLY:O	1:B:120:GLY:HA3	2.20	0.41
1:B:254:ASN:HD22	1:B:254:ASN:N	2.19	0.41
1:B:62:LYS:HB2	1:B:73:SER:CB	2.50	0.41
1:B:93:TYR:CG	1:B:94:GLY:N	2.88	0.41
1:A:194:LYS:HA	1:A:208:ARG:HD3	2.02	0.41
1:B:317:LEU:CD2	1:B:323:SER:OG	2.69	0.41
1:B:22:VAL:HG23	1:B:334:ALA:HB2	2.03	0.41
1:A:238:VAL:HG12	1:A:239:GLU:H	1.86	0.41
1:A:262:GLN:HG3	1:A:262:GLN:O	2.19	0.41
1:B:101:TYR:HB2	1:B:128:THR:O	2.21	0.41
1:B:93:TYR:OH	1:C:33:ASP:OD1	2.39	0.41
1:A:11:LEU:O	1:A:12:ASP:HB3	2.21	0.40
1:A:142:PHE:CD1	1:A:149:LEU:HD23	2.56	0.40
1:C:281:LEU:HB2	1:C:322:TYR:CZ	2.56	0.40
1:A:67:GLU:OE1	1:C:77:ARG:HG2	2.21	0.40
1:A:117:THR:HA	1:A:326:TYR:HD1	1.82	0.40
1:A:146:VAL:HG23	1:A:147:ASP:H	1.86	0.40
1:B:226:ALA:O	1:B:257:VAL:HA	2.21	0.40
1:B:303:ASN:C	1:B:305:ASN:H	2.25	0.40
1:C:151:PHE:HA	1:C:177:MSE:HA	2.01	0.40
1:A:30:LYS:HE3	8:A:414:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:ASN:CG	1:B:65:ARG:HH12	2.25	0.40
1:B:134:LEU:HD23	1:B:156:GLN:HB2	2.03	0.40
1:B:205:ASN:HB2	1:B:234:ASN:ND2	2.37	0.40
4:B:380:LDA:HM22	4:B:380:LDA:H22	1.76	0.40
1:B:277:LYS:NZ	4:B:380:LDA:O1	2.45	0.40
1:C:21:HIS:NE2	1:C:31:ASN:OD1	2.45	0.40
1:C:39:ILE:HG22	1:C:59:TYR:HB3	2.03	0.40
1:A:91:ILE:CD1	1:A:135:LEU:HD11	2.50	0.40
1:B:210:GLU:OE1	1:B:212:ARG:NH1	2.55	0.40
1:B:68:GLY:C	1:B:69:GLU:HG3	2.41	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	339/341 (99%)	286 (84%)	39 (12%)	14 (4%)	3	11
1	B	339/341 (99%)	285 (84%)	37 (11%)	17 (5%)	2	7
1	C	339/341 (99%)	279 (82%)	41 (12%)	19 (6%)	2	6
All	All	1017/1023 (99%)	850 (84%)	117 (12%)	50 (5%)	2	8

All (50) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	113	PHE
1	A	205	ASN
1	A	208	ARG
1	A	245	THR
1	A	249	ALA
1	B	2	GLU
1	B	9	ASN

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Mol	Chain	Res	Type
1	B	207	ASP
1	B	251	LYS
1	B	326	TYR
1	C	6	LYS
1	C	9	ASN
1	C	126	TYR
1	C	201	ASP
1	C	202	ARG
1	C	251	LYS
1	C	286	GLY
1	A	114	SER
1	A	197	ASN
1	A	206	GLY
1	B	105	SER
1	B	206	GLY
1	B	283	GLY
1	C	10	LYS
1	C	87	GLU
1	C	199	GLN
1	C	200	GLN
1	C	236	SER
1	C	323	SER
1	A	4	TYR
1	A	7	ASP
1	A	148	GLY
1	A	233	ARG
1	B	240	ASN
1	C	86	ALA
1	C	221	ASN
1	B	7	ASP
1	B	101	TYR
1	B	117	THR
1	B	197	ASN
1	C	4	TYR
1	C	121	ALA
1	C	162	ASN
1	A	126	TYR
1	A	244	ASP
1	B	28	ASP
1	B	127	MSE
1	C	283	GLY
1	B	204	GLY

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Mol	Chain	Res	Type
1	B	327	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	271/265 (102%)	208 (77%)	63 (23%)	1	2
1	B	271/265 (102%)	223 (82%)	48 (18%)	2	6
1	C	271/265 (102%)	216 (80%)	55 (20%)	1	4
All	All	813/795 (102%)	647 (80%)	166 (20%)	1	4

All (166) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	4	TYR
1	A	5	ASN
1	A	6	LYS
1	A	9	ASN
1	A	10	LYS
1	A	20	ARG
1	A	24	THR
1	A	46	GLN
1	A	48	ASN
1	A	49	THR
1	A	52	THR
1	A	71	GLN
1	A	74	ASN
1	A	76	VAL
1	A	78	LEU
1	A	83	LEU
1	A	85	TYR
1	A	88	VAL
1	A	91	ILE
1	A	102	ASP

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Mol	Chain	Res	Type
1	A	104	GLU
1	A	109	MSE
1	A	112	TYR
1	A	117	THR
1	A	123	THR
1	A	128	THR
1	A	145	LEU
1	A	153	ILE
1	A	154	GLN
1	A	156	GLN
1	A	161	ASP
1	A	165	ILE
1	A	167	SER
1	A	171	ASP
1	A	177	MSE
1	A	193	SER
1	A	197	ASN
1	A	198	ASP
1	A	200	GLN
1	A	211	SER
1	A	212	ARG
1	A	223	VAL
1	A	225	LEU
1	A	228	VAL
1	A	235	MSE
1	A	246	VAL
1	A	252	THR
1	A	260	GLN
1	A	264	ASP
1	A	267	LEU
1	A	275	GLN
1	A	281	LEU
1	A	282	ASN
1	A	290	LEU
1	A	299	THR
1	A	300	TYR
1	A	308	VAL
1	A	311	ASP
1	A	313	ARG
1	A	315	ASN
1	A	330	ASP
1	A	335	VAL

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Mol	Chain	Res	Type
1	B	3	ILE
1	B	4	TYR
1	B	6	LYS
1	B	10	LYS
1	B	13	LEU
1	B	20	ARG
1	B	24	THR
1	B	28	ASP
1	B	30	LYS
1	B	42	LYS
1	B	47	ILE
1	B	52	THR
1	B	65	ARG
1	B	71	GLN
1	B	74	ASN
1	B	76	VAL
1	B	83	LEU
1	B	87	GLU
1	B	92	ASP
1	B	146	VAL
1	B	153	ILE
1	B	171	ASP
1	B	175	TYR
1	B	182	ASP
1	B	187	THR
1	B	191	SER
1	B	193	SER
1	B	208	ARG
1	B	212	ARG
1	B	225	LEU
1	B	241	THR
1	B	242	VAL
1	B	243	THR
1	B	246	VAL
1	B	248	MSE
1	B	257	VAL
1	B	264	ASP
1	B	272	SER
1	B	274	VAL
1	B	276	SER
1	B	289	ASP
1	B	303	ASN

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Mol	Chain	Res	Type
1	B	310	VAL
1	B	313	ARG
1	B	321	ASP
1	B	326	TYR
1	B	327	VAL
1	B	338	THR
1	C	10	LYS
1	C	12	ASP
1	C	20	ARG
1	C	28	ASP
1	C	29	SER
1	C	46	GLN
1	C	48	ASN
1	C	49	THR
1	C	52	THR
1	C	64	ASP
1	C	65	ARG
1	C	69	GLU
1	C	75	LEU
1	C	92	ASP
1	C	96	ASN
1	C	105	SER
1	C	117	THR
1	C	145	LEU
1	C	150	SER
1	C	156	GLN
1	C	158	LYS
1	C	163	HIS
1	C	167	SER
1	C	171	ASP
1	C	175	TYR
1	C	198	ASP
1	C	199	GLN
1	C	200	GLN
1	C	202	ARG
1	C	205	ASN
1	C	207	ASP
1	C	212	ARG
1	C	214	VAL
1	C	217	LYS
1	C	222	ASN
1	C	228	VAL

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Mol	Chain	Res	Type
1	C	233	ARG
1	C	235	MSE
1	C	243	THR
1	C	245	THR
1	C	248	MSE
1	C	257	VAL
1	C	274	VAL
1	C	275	GLN
1	C	281	LEU
1	C	290	LEU
1	C	303	ASN
1	C	304	LYS
1	C	310	VAL
1	C	313	ARG
1	C	315	ASN
1	C	316	LEU
1	C	319	GLU
1	C	338	THR
1	C	340	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	9	ASN
1	A	21	HIS
1	A	48	ASN
1	A	70	GLN
1	A	159	ASN
1	A	166	ASN
1	A	200	GLN
1	A	234	ASN
1	A	240	ASN
1	A	260	GLN
1	A	275	GLN
1	A	305	ASN
1	A	315	ASN
1	B	5	ASN
1	B	9	ASN
1	B	21	HIS
1	B	31	ASN
1	B	56	GLN

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Mol	Chain	Res	Type
1	B	70	GLN
1	B	154	GLN
1	B	159	ASN
1	B	200	GLN
1	B	282	ASN
1	B	307	ASN
1	B	315	ASN
1	B	320	ASN
1	C	5	ASN
1	C	48	ASN
1	C	56	GLN
1	C	70	GLN
1	C	154	GLN
1	C	156	GLN
1	C	159	ASN
1	C	166	ASN
1	C	169	ASN
1	C	205	ASN
1	C	222	ASN
1	C	254	ASN
1	C	262	GLN
1	C	275	GLN
1	C	280	GLN
1	C	282	ASN
1	C	303	ASN
1	C	305	ASN
1	C	315	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

147 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	$\# Z  > 2$
2	SO4	A	342	-	4,4,4	0.18	0	6,6,6	0.10	0
2	SO4	A	343	-	4,4,4	0.12	0	6,6,6	0.19	0
2	SO4	A	344	-	4,4,4	0.18	0	6,6,6	0.13	0
2	SO4	A	345	-	4,4,4	0.23	0	6,6,6	0.11	0
2	SO4	A	346	-	4,4,4	0.26	0	6,6,6	0.17	0
2	SO4	A	347	-	4,4,4	0.22	0	6,6,6	0.11	0
2	SO4	A	348	-	4,4,4	0.20	0	6,6,6	0.15	0
2	SO4	A	349	-	4,4,4	0.31	0	6,6,6	0.13	0
2	SO4	A	350	-	4,4,4	0.20	0	6,6,6	0.15	0
2	SO4	A	351	-	4,4,4	0.17	0	6,6,6	0.13	0
2	SO4	A	352	-	4,4,4	0.18	0	6,6,6	0.18	0
2	SO4	A	353	-	4,4,4	0.18	0	6,6,6	0.17	0
2	SO4	A	354	-	4,4,4	0.19	0	6,6,6	0.13	0
2	SO4	A	355	-	4,4,4	0.25	0	6,6,6	0.24	0
2	SO4	A	356	-	4,4,4	0.24	0	6,6,6	0.28	0
2	SO4	A	357	-	4,4,4	0.13	0	6,6,6	0.22	0
2	SO4	A	358	-	4,4,4	0.16	0	6,6,6	0.23	0
2	SO4	A	359	-	4,4,4	0.18	0	6,6,6	0.13	0
2	SO4	A	360	-	4,4,4	0.21	0	6,6,6	0.09	0
2	SO4	A	361	-	4,4,4	0.14	0	6,6,6	0.19	0
2	SO4	A	362	-	4,4,4	0.16	0	6,6,6	0.18	0
2	SO4	A	363	-	4,4,4	0.21	0	6,6,6	0.11	0
2	SO4	A	364	-	4,4,4	0.15	0	6,6,6	0.08	0
2	SO4	A	365	-	4,4,4	0.19	0	6,6,6	0.10	0
2	SO4	A	366	-	4,4,4	0.26	0	6,6,6	0.10	0
2	SO4	A	367	-	4,4,4	0.20	0	6,6,6	0.19	0
2	SO4	A	369	-	4,4,4	0.32	0	6,6,6	0.10	0
3	GOL	A	370	-	5,5,5	0.35	0	5,5,5	0.26	0
3	GOL	A	371	-	5,5,5	0.42	0	5,5,5	0.21	0
3	GOL	A	372	-	5,5,5	0.35	0	5,5,5	0.25	0
3	GOL	A	373	-	5,5,5	0.30	0	5,5,5	0.23	0
3	GOL	A	374	-	5,5,5	0.36	0	5,5,5	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GOL	A	375	-	5,5,5	0.34	0	5,5,5	0.55	0
3	GOL	A	376	-	5,5,5	0.34	0	5,5,5	0.35	0
3	GOL	A	377	-	5,5,5	0.34	0	5,5,5	0.35	0
3	GOL	A	378	-	5,5,5	0.25	0	5,5,5	0.26	0
3	GOL	A	379	-	5,5,5	0.33	0	5,5,5	0.26	0
3	GOL	A	380	-	5,5,5	0.36	0	5,5,5	0.39	0
3	GOL	A	381	-	5,5,5	0.31	0	5,5,5	0.30	0
3	GOL	A	382	-	5,5,5	0.31	0	5,5,5	0.18	0
3	GOL	A	383	-	5,5,5	0.36	0	5,5,5	0.35	0
4	LDA	A	384	-	13,15,15	2.29	2 (15%)	14,17,17	0.94	1 (7%)
4	LDA	A	385	-	13,15,15	2.38	1 (7%)	14,17,17	0.63	0
4	LDA	A	386	-	13,15,15	2.33	2 (15%)	14,17,17	0.71	0
4	LDA	A	387	-	13,15,15	2.29	1 (7%)	14,17,17	0.80	1 (7%)
4	LDA	A	388	-	13,15,15	2.32	1 (7%)	14,17,17	0.83	0
4	LDA	A	389	-	13,15,15	2.27	1 (7%)	14,17,17	0.71	0
5	TAM	A	390	-	7,10,10	0.47	0	9,12,12	0.44	0
5	TAM	A	391	-	7,10,10	0.54	0	9,12,12	0.54	0
6	FLC	A	392	-	3,12,12	2.02	1 (33%)	3,17,17	2.89	2 (66%)
7	TLA	A	393	-	3,9,9	0.64	0	6,12,12	0.70	0
2	SO4	B	342	-	4,4,4	0.16	0	6,6,6	0.15	0
2	SO4	B	343	-	4,4,4	0.17	0	6,6,6	0.12	0
2	SO4	B	344	-	4,4,4	0.17	0	6,6,6	0.17	0
2	SO4	B	345	-	4,4,4	0.30	0	6,6,6	0.15	0
2	SO4	B	346	-	4,4,4	0.17	0	6,6,6	0.16	0
2	SO4	B	347	-	4,4,4	0.21	0	6,6,6	0.35	0
2	SO4	B	348	-	4,4,4	0.18	0	6,6,6	0.38	0
2	SO4	B	349	-	4,4,4	0.13	0	6,6,6	0.17	0
2	SO4	B	350	-	4,4,4	0.21	0	6,6,6	0.10	0
2	SO4	B	351	-	4,4,4	0.46	0	6,6,6	0.36	0
2	SO4	B	352	-	4,4,4	0.19	0	6,6,6	0.10	0
2	SO4	B	353	-	4,4,4	0.15	0	6,6,6	0.18	0
2	SO4	B	354	-	4,4,4	0.18	0	6,6,6	0.06	0
2	SO4	B	355	-	4,4,4	0.20	0	6,6,6	0.13	0
2	SO4	B	356	-	4,4,4	0.27	0	6,6,6	0.08	0
2	SO4	B	357	-	4,4,4	0.20	0	6,6,6	0.09	0
2	SO4	B	358	-	4,4,4	0.19	0	6,6,6	0.09	0
2	SO4	B	359	-	4,4,4	0.16	0	6,6,6	0.15	0
2	SO4	B	360	-	4,4,4	0.20	0	6,6,6	0.09	0
2	SO4	B	361	-	4,4,4	0.17	0	6,6,6	0.15	0
2	SO4	B	362	-	4,4,4	0.17	0	6,6,6	0.11	0
2	SO4	B	363	-	4,4,4	0.15	0	6,6,6	0.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GOL	B	364	-	5,5,5	0.42	0	5,5,5	0.20	0
3	GOL	B	365	-	5,5,5	0.22	0	5,5,5	0.49	0
3	GOL	B	366	-	5,5,5	0.45	0	5,5,5	0.66	0
3	GOL	B	367	-	5,5,5	0.33	0	5,5,5	0.36	0
3	GOL	B	368	-	5,5,5	0.38	0	5,5,5	0.19	0
3	GOL	B	369	-	5,5,5	0.38	0	5,5,5	0.39	0
3	GOL	B	370	-	5,5,5	0.32	0	5,5,5	0.28	0
3	GOL	B	371	-	5,5,5	0.38	0	5,5,5	0.44	0
3	GOL	B	372	-	5,5,5	0.37	0	5,5,5	0.46	0
3	GOL	B	373	-	5,5,5	0.37	0	5,5,5	0.19	0
3	GOL	B	374	-	5,5,5	0.37	0	5,5,5	0.17	0
4	LDA	B	375	-	13,15,15	2.49	1 (7%)	14,17,17	1.11	2 (14%)
4	LDA	B	376	-	13,15,15	2.40	2 (15%)	14,17,17	0.64	0
4	LDA	B	377	-	13,15,15	2.22	1 (7%)	14,17,17	0.74	0
4	LDA	B	378	-	13,15,15	2.37	1 (7%)	14,17,17	0.53	0
4	LDA	B	379	-	13,15,15	2.34	1 (7%)	14,17,17	0.78	0
4	LDA	B	380	-	13,15,15	2.38	1 (7%)	14,17,17	0.82	0
4	LDA	B	381	-	13,15,15	2.15	1 (7%)	14,17,17	0.80	1 (7%)
5	TAM	B	382	-	7,10,10	0.56	0	9,12,12	0.39	0
7	TLA	B	383	-	3,9,9	0.56	0	6,12,12	1.38	1 (16%)
3	GOL	C	1325	-	5,5,5	0.27	0	5,5,5	0.27	0
2	SO4	C	342	-	4,4,4	0.21	0	6,6,6	0.20	0
2	SO4	C	343	-	4,4,4	0.17	0	6,6,6	0.11	0
2	SO4	C	344	-	4,4,4	0.25	0	6,6,6	0.14	0
2	SO4	C	345	-	4,4,4	0.17	0	6,6,6	0.19	0
2	SO4	C	346	-	4,4,4	0.19	0	6,6,6	0.11	0
2	SO4	C	347	-	4,4,4	0.17	0	6,6,6	0.22	0
2	SO4	C	348	-	4,4,4	0.22	0	6,6,6	0.17	0
2	SO4	C	349	-	4,4,4	0.22	0	6,6,6	0.12	0
2	SO4	C	350	-	4,4,4	0.22	0	6,6,6	0.11	0
2	SO4	C	351	-	4,4,4	0.22	0	6,6,6	0.20	0
2	SO4	C	352	-	4,4,4	0.18	0	6,6,6	0.23	0
2	SO4	C	353	-	4,4,4	0.17	0	6,6,6	0.13	0
2	SO4	C	354	-	4,4,4	0.22	0	6,6,6	0.11	0
2	SO4	C	355	-	4,4,4	0.19	0	6,6,6	0.18	0
2	SO4	C	356	-	4,4,4	0.21	0	6,6,6	0.13	0
2	SO4	C	357	-	4,4,4	0.16	0	6,6,6	0.19	0
2	SO4	C	358	-	4,4,4	0.17	0	6,6,6	0.16	0
2	SO4	C	359	-	4,4,4	0.21	0	6,6,6	0.06	0
2	SO4	C	360	-	4,4,4	0.14	0	6,6,6	0.07	0
2	SO4	C	361	-	4,4,4	0.18	0	6,6,6	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	C	362	-	4,4,4	0.16	0	6,6,6	0.12	0
2	SO4	C	363	-	4,4,4	0.19	0	6,6,6	0.09	0
2	SO4	C	364	-	4,4,4	0.12	0	6,6,6	0.22	0
2	SO4	C	365	-	4,4,4	0.19	0	6,6,6	0.13	0
2	SO4	C	366	-	4,4,4	0.18	0	6,6,6	0.13	0
2	SO4	C	367	-	4,4,4	0.18	0	6,6,6	0.18	0
2	SO4	C	368	-	4,4,4	0.16	0	6,6,6	0.12	0
2	SO4	C	369	-	4,4,4	0.16	0	6,6,6	0.18	0
2	SO4	C	370	-	4,4,4	0.30	0	6,6,6	0.19	0
2	SO4	C	371	-	4,4,4	0.18	0	6,6,6	0.10	0
2	SO4	C	372	-	4,4,4	0.27	0	6,6,6	0.12	0
3	GOL	C	373	-	5,5,5	0.34	0	5,5,5	0.23	0
3	GOL	C	374	-	5,5,5	0.35	0	5,5,5	0.45	0
3	GOL	C	375	-	5,5,5	0.29	0	5,5,5	0.25	0
3	GOL	C	376	-	5,5,5	0.39	0	5,5,5	0.14	0
3	GOL	C	377	-	5,5,5	0.38	0	5,5,5	0.29	0
3	GOL	C	378	-	5,5,5	0.38	0	5,5,5	0.33	0
3	GOL	C	379	-	5,5,5	0.33	0	5,5,5	0.25	0
3	GOL	C	380	-	5,5,5	0.36	0	5,5,5	0.20	0
3	GOL	C	381	-	5,5,5	0.38	0	5,5,5	0.37	0
4	LDA	C	382	-	13,15,15	2.32	1 (7%)	14,17,17	0.48	0
4	LDA	C	383	-	13,15,15	2.32	1 (7%)	14,17,17	0.88	0
4	LDA	C	384	-	13,15,15	2.43	2 (15%)	14,17,17	0.81	0
4	LDA	C	385	-	13,15,15	2.34	2 (15%)	14,17,17	0.68	0
5	TAM	C	386	-	7,10,10	0.54	0	9,12,12	0.68	0
5	TAM	C	387	-	7,10,10	0.65	0	9,12,12	0.65	0
6	FLC	C	388	-	3,12,12	1.96	1 (33%)	3,17,17	2.03	1 (33%)
6	FLC	C	389	-	3,12,12	0.64	0	3,17,17	2.79	1 (33%)
3	GOL	C	390	-	5,5,5	0.34	0	5,5,5	0.28	0
6	FLC	C	391	-	3,12,12	0.93	0	3,17,17	4.39	3 (100%)
3	GOL	C	392	-	5,5,5	0.35	0	5,5,5	0.17	0
5	TAM	C	393	-	7,10,10	0.48	0	9,12,12	0.68	0
3	GOL	C	394	-	5,5,5	0.31	0	5,5,5	0.59	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	342	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	343	-	-	0/0/0/0	0/0/0/0
2	SO4	A	344	-	-	0/0/0/0	0/0/0/0
2	SO4	A	345	-	-	0/0/0/0	0/0/0/0
2	SO4	A	346	-	-	0/0/0/0	0/0/0/0
2	SO4	A	347	-	-	0/0/0/0	0/0/0/0
2	SO4	A	348	-	-	0/0/0/0	0/0/0/0
2	SO4	A	349	-	-	0/0/0/0	0/0/0/0
2	SO4	A	350	-	-	0/0/0/0	0/0/0/0
2	SO4	A	351	-	-	0/0/0/0	0/0/0/0
2	SO4	A	352	-	-	0/0/0/0	0/0/0/0
2	SO4	A	353	-	-	0/0/0/0	0/0/0/0
2	SO4	A	354	-	-	0/0/0/0	0/0/0/0
2	SO4	A	355	-	-	0/0/0/0	0/0/0/0
2	SO4	A	356	-	-	0/0/0/0	0/0/0/0
2	SO4	A	357	-	-	0/0/0/0	0/0/0/0
2	SO4	A	358	-	-	0/0/0/0	0/0/0/0
2	SO4	A	359	-	-	0/0/0/0	0/0/0/0
2	SO4	A	360	-	-	0/0/0/0	0/0/0/0
2	SO4	A	361	-	-	0/0/0/0	0/0/0/0
2	SO4	A	362	-	-	0/0/0/0	0/0/0/0
2	SO4	A	363	-	-	0/0/0/0	0/0/0/0
2	SO4	A	364	-	-	0/0/0/0	0/0/0/0
2	SO4	A	365	-	-	0/0/0/0	0/0/0/0
2	SO4	A	366	-	-	0/0/0/0	0/0/0/0
2	SO4	A	367	-	-	0/0/0/0	0/0/0/0
2	SO4	A	369	-	-	0/0/0/0	0/0/0/0
3	GOL	A	370	-	-	0/4/4/4	0/0/0/0
3	GOL	A	371	-	-	0/4/4/4	0/0/0/0
3	GOL	A	372	-	-	0/4/4/4	0/0/0/0
3	GOL	A	373	-	-	0/4/4/4	0/0/0/0
3	GOL	A	374	-	-	0/4/4/4	0/0/0/0
3	GOL	A	375	-	-	0/4/4/4	0/0/0/0
3	GOL	A	376	-	-	0/4/4/4	0/0/0/0
3	GOL	A	377	-	-	0/4/4/4	0/0/0/0
3	GOL	A	378	-	-	0/4/4/4	0/0/0/0
3	GOL	A	379	-	-	0/4/4/4	0/0/0/0
3	GOL	A	380	-	-	0/4/4/4	0/0/0/0
3	GOL	A	381	-	-	0/4/4/4	0/0/0/0
3	GOL	A	382	-	-	0/4/4/4	0/0/0/0
3	GOL	A	383	-	-	0/4/4/4	0/0/0/0
4	LDA	A	384	-	-	0/13/13/13	0/0/0/0
4	LDA	A	385	-	-	0/13/13/13	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	LDA	A	386	-	-	0/13/13/13	0/0/0/0
4	LDA	A	387	-	-	0/13/13/13	0/0/0/0
4	LDA	A	388	-	-	0/13/13/13	0/0/0/0
4	LDA	A	389	-	-	0/13/13/13	0/0/0/0
5	TAM	A	390	-	-	0/12/12/12	0/0/0/0
5	TAM	A	391	-	-	0/12/12/12	0/0/0/0
6	FLC	A	392	-	-	0/6/16/16	0/0/0/0
7	TLA	A	393	-	-	0/4/12/12	0/0/0/0
2	SO4	B	342	-	-	0/0/0/0	0/0/0/0
2	SO4	B	343	-	-	0/0/0/0	0/0/0/0
2	SO4	B	344	-	-	0/0/0/0	0/0/0/0
2	SO4	B	345	-	-	0/0/0/0	0/0/0/0
2	SO4	B	346	-	-	0/0/0/0	0/0/0/0
2	SO4	B	347	-	-	0/0/0/0	0/0/0/0
2	SO4	B	348	-	-	0/0/0/0	0/0/0/0
2	SO4	B	349	-	-	0/0/0/0	0/0/0/0
2	SO4	B	350	-	-	0/0/0/0	0/0/0/0
2	SO4	B	351	-	-	0/0/0/0	0/0/0/0
2	SO4	B	352	-	-	0/0/0/0	0/0/0/0
2	SO4	B	353	-	-	0/0/0/0	0/0/0/0
2	SO4	B	354	-	-	0/0/0/0	0/0/0/0
2	SO4	B	355	-	-	0/0/0/0	0/0/0/0
2	SO4	B	356	-	-	0/0/0/0	0/0/0/0
2	SO4	B	357	-	-	0/0/0/0	0/0/0/0
2	SO4	B	358	-	-	0/0/0/0	0/0/0/0
2	SO4	B	359	-	-	0/0/0/0	0/0/0/0
2	SO4	B	360	-	-	0/0/0/0	0/0/0/0
2	SO4	B	361	-	-	0/0/0/0	0/0/0/0
2	SO4	B	362	-	-	0/0/0/0	0/0/0/0
2	SO4	B	363	-	-	0/0/0/0	0/0/0/0
3	GOL	B	364	-	-	0/4/4/4	0/0/0/0
3	GOL	B	365	-	-	0/4/4/4	0/0/0/0
3	GOL	B	366	-	-	0/4/4/4	0/0/0/0
3	GOL	B	367	-	-	0/4/4/4	0/0/0/0
3	GOL	B	368	-	-	0/4/4/4	0/0/0/0
3	GOL	B	369	-	-	0/4/4/4	0/0/0/0
3	GOL	B	370	-	-	0/4/4/4	0/0/0/0
3	GOL	B	371	-	-	0/4/4/4	0/0/0/0
3	GOL	B	372	-	-	0/4/4/4	0/0/0/0
3	GOL	B	373	-	-	0/4/4/4	0/0/0/0
3	GOL	B	374	-	-	0/4/4/4	0/0/0/0
4	LDA	B	375	-	-	0/13/13/13	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	LDA	B	376	-	-	0/13/13/13	0/0/0/0
4	LDA	B	377	-	-	0/13/13/13	0/0/0/0
4	LDA	B	378	-	-	0/13/13/13	0/0/0/0
4	LDA	B	379	-	-	0/13/13/13	0/0/0/0
4	LDA	B	380	-	-	0/13/13/13	0/0/0/0
4	LDA	B	381	-	-	0/13/13/13	0/0/0/0
5	TAM	B	382	-	-	0/12/12/12	0/0/0/0
7	TLA	B	383	-	-	0/4/12/12	0/0/0/0
3	GOL	C	1325	-	-	0/4/4/4	0/0/0/0
2	SO4	C	342	-	-	0/0/0/0	0/0/0/0
2	SO4	C	343	-	-	0/0/0/0	0/0/0/0
2	SO4	C	344	-	-	0/0/0/0	0/0/0/0
2	SO4	C	345	-	-	0/0/0/0	0/0/0/0
2	SO4	C	346	-	-	0/0/0/0	0/0/0/0
2	SO4	C	347	-	-	0/0/0/0	0/0/0/0
2	SO4	C	348	-	-	0/0/0/0	0/0/0/0
2	SO4	C	349	-	-	0/0/0/0	0/0/0/0
2	SO4	C	350	-	-	0/0/0/0	0/0/0/0
2	SO4	C	351	-	-	0/0/0/0	0/0/0/0
2	SO4	C	352	-	-	0/0/0/0	0/0/0/0
2	SO4	C	353	-	-	0/0/0/0	0/0/0/0
2	SO4	C	354	-	-	0/0/0/0	0/0/0/0
2	SO4	C	355	-	-	0/0/0/0	0/0/0/0
2	SO4	C	356	-	-	0/0/0/0	0/0/0/0
2	SO4	C	357	-	-	0/0/0/0	0/0/0/0
2	SO4	C	358	-	-	0/0/0/0	0/0/0/0
2	SO4	C	359	-	-	0/0/0/0	0/0/0/0
2	SO4	C	360	-	-	0/0/0/0	0/0/0/0
2	SO4	C	361	-	-	0/0/0/0	0/0/0/0
2	SO4	C	362	-	-	0/0/0/0	0/0/0/0
2	SO4	C	363	-	-	0/0/0/0	0/0/0/0
2	SO4	C	364	-	-	0/0/0/0	0/0/0/0
2	SO4	C	365	-	-	0/0/0/0	0/0/0/0
2	SO4	C	366	-	-	0/0/0/0	0/0/0/0
2	SO4	C	367	-	-	0/0/0/0	0/0/0/0
2	SO4	C	368	-	-	0/0/0/0	0/0/0/0
2	SO4	C	369	-	-	0/0/0/0	0/0/0/0
2	SO4	C	370	-	-	0/0/0/0	0/0/0/0
2	SO4	C	371	-	-	0/0/0/0	0/0/0/0
2	SO4	C	372	-	-	0/0/0/0	0/0/0/0
3	GOL	C	373	-	-	0/4/4/4	0/0/0/0
3	GOL	C	374	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	C	375	-	-	0/4/4/4	0/0/0/0
3	GOL	C	376	-	-	0/4/4/4	0/0/0/0
3	GOL	C	377	-	-	0/4/4/4	0/0/0/0
3	GOL	C	378	-	-	0/4/4/4	0/0/0/0
3	GOL	C	379	-	-	0/4/4/4	0/0/0/0
3	GOL	C	380	-	-	0/4/4/4	0/0/0/0
3	GOL	C	381	-	-	0/4/4/4	0/0/0/0
4	LDA	C	382	-	-	0/13/13/13	0/0/0/0
4	LDA	C	383	-	-	0/13/13/13	0/0/0/0
4	LDA	C	384	-	-	0/13/13/13	0/0/0/0
4	LDA	C	385	-	-	0/13/13/13	0/0/0/0
5	TAM	C	386	-	-	0/12/12/12	0/0/0/0
5	TAM	C	387	-	-	0/12/12/12	0/0/0/0
6	FLC	C	388	-	-	0/6/16/16	0/0/0/0
6	FLC	C	389	-	-	0/6/16/16	0/0/0/0
3	GOL	C	390	-	-	0/4/4/4	0/0/0/0
6	FLC	C	391	-	-	0/6/16/16	0/0/0/0
3	GOL	C	392	-	-	0/4/4/4	0/0/0/0
5	TAM	C	393	-	-	0/12/12/12	0/0/0/0
3	GOL	C	394	-	-	0/4/4/4	0/0/0/0

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	375	LDA	O1-N1	-8.74	1.24	1.42
4	C	384	LDA	O1-N1	-8.37	1.25	1.42
4	B	376	LDA	O1-N1	-8.36	1.25	1.42
4	B	378	LDA	O1-N1	-8.31	1.25	1.42
4	B	380	LDA	O1-N1	-8.29	1.25	1.42
4	A	385	LDA	O1-N1	-8.26	1.25	1.42
4	B	379	LDA	O1-N1	-8.19	1.26	1.42
4	C	385	LDA	O1-N1	-8.15	1.26	1.42
4	A	388	LDA	O1-N1	-8.13	1.26	1.42
4	C	383	LDA	O1-N1	-8.12	1.26	1.42
4	C	382	LDA	O1-N1	-8.11	1.26	1.42
4	A	387	LDA	O1-N1	-8.08	1.26	1.42
4	A	386	LDA	O1-N1	-8.08	1.26	1.42
4	A	384	LDA	O1-N1	-7.92	1.26	1.42
4	A	389	LDA	O1-N1	-7.89	1.26	1.42
4	B	377	LDA	O1-N1	-7.58	1.27	1.42
4	B	381	LDA	O1-N1	-7.50	1.27	1.42
4	C	384	LDA	C1-N1	-2.44	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	384	LDA	C1-N1	-2.24	1.46	1.51
4	A	386	LDA	C1-N1	-2.16	1.46	1.51
4	C	385	LDA	C1-N1	-2.03	1.46	1.51
4	B	376	LDA	C1-N1	-2.01	1.46	1.51
6	A	392	FLC	CG-CB	2.92	1.59	1.54
6	C	388	FLC	OHB-CB	3.02	1.47	1.43

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	392	FLC	CB-CA-CAC	-3.50	109.49	114.95
6	C	388	FLC	CB-CG-CGC	-3.41	109.62	114.95
7	B	383	TLA	C1-C2-C3	-3.17	106.28	113.11
4	B	375	LDA	CM2-N1-CM1	-2.37	106.46	110.99
4	A	384	LDA	CM2-N1-CM1	-2.28	106.62	110.99
4	B	381	LDA	CM2-N1-CM1	-2.22	106.73	110.99
6	C	391	FLC	CB-CG-CGC	2.21	118.40	114.95
4	A	387	LDA	CM2-N1-C1	2.25	114.96	110.23
4	B	375	LDA	CM2-N1-C1	2.73	115.98	110.23
6	A	392	FLC	CG-CB-CA	3.32	118.02	109.75
6	C	389	FLC	CG-CB-CA	4.41	120.74	109.75
6	C	391	FLC	CB-CA-CAC	4.65	122.22	114.95
6	C	391	FLC	CG-CB-CA	5.60	123.68	109.75

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

42 monomers are involved in 87 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	350	SO4	1	0
2	A	358	SO4	1	0
2	A	361	SO4	3	0
2	A	363	SO4	1	0
3	A	370	GOL	2	0
3	A	375	GOL	1	0
3	A	380	GOL	1	0
4	A	384	LDA	4	0
4	A	386	LDA	1	0
4	A	388	LDA	1	0
5	A	390	TAM	10	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	391	TAM	1	0
2	B	345	SO4	2	0
2	B	348	SO4	1	0
2	B	354	SO4	1	0
3	B	364	GOL	1	0
3	B	365	GOL	4	0
3	B	368	GOL	1	0
4	B	375	LDA	3	0
4	B	376	LDA	1	0
4	B	377	LDA	2	0
4	B	379	LDA	2	0
4	B	380	LDA	3	0
4	B	381	LDA	1	0
7	B	383	TLA	1	0
2	C	343	SO4	1	0
2	C	348	SO4	1	0
2	C	364	SO4	1	0
2	C	365	SO4	1	0
2	C	370	SO4	2	0
3	C	375	GOL	6	0
4	C	382	LDA	4	0
4	C	383	LDA	4	0
4	C	384	LDA	4	0
4	C	385	LDA	4	0
5	C	386	TAM	4	0
5	C	387	TAM	5	0
6	C	388	FLC	5	0
6	C	391	FLC	1	0
3	C	392	GOL	1	0
5	C	393	TAM	3	0
3	C	394	GOL	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	334/341 (97%)	0.17	15 (4%) 34 24	34, 57, 80, 91	0
1	B	334/341 (97%)	0.13	8 (2%) 59 49	34, 56, 68, 88	0
1	C	334/341 (97%)	0.20	9 (2%) 55 44	34, 58, 81, 92	0
All	All	1002/1023 (97%)	0.17	32 (3%) 48 37	34, 57, 79, 92	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	289	ASP	5.8
1	A	320	ASN	5.3
1	B	7	ASP	4.6
1	A	288	ALA	4.5
1	B	4	TYR	3.5
1	A	321	ASP	3.3
1	B	6	LYS	3.2
1	A	6	LYS	3.0
1	A	241	THR	3.0
1	C	290	LEU	2.9
1	B	8	GLY	2.8
1	A	319	GLU	2.8
1	C	181	PHE	2.7
1	C	166	ASN	2.7
1	A	229	TYR	2.6
1	C	280	GLN	2.6
1	A	318	ASP	2.5
1	C	279	LYS	2.4
1	C	289	ASP	2.4
1	A	13	LEU	2.4
1	B	202	ARG	2.3
1	A	3	ILE	2.2
1	A	239	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	168	GLN	2.1
1	A	209	ALA	2.1
1	B	328	GLY	2.1
1	A	317	LEU	2.1
1	B	27	GLY	2.1
1	C	319	GLU	2.1
1	B	318	ASP	2.0
1	C	7	ASP	2.0
1	A	290	LEU	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	TAM	A	390	11/11	0.73	0.79	29.25	19,21,22,22	11
3	GOL	B	373	6/6	0.63	0.71	10.89	107,108,109,109	0
2	SO4	C	343	5/5	0.89	0.34	7.83	126,126,127,127	0
3	GOL	C	1325	6/6	0.79	0.48	7.31	113,114,115,115	0
2	SO4	C	364	5/5	0.81	0.59	6.86	143,143,144,144	0
2	SO4	A	353	5/5	0.93	0.32	6.78	129,130,130,130	0
3	GOL	A	370	6/6	0.86	0.31	6.16	82,83,84,84	0
4	LDA	A	384	16/16	0.92	0.42	5.99	51,59,71,71	0
4	LDA	A	388	16/16	0.83	0.32	5.61	101,107,115,115	0
4	LDA	A	387	16/16	0.75	0.39	5.03	65,82,95,96	0
2	SO4	C	368	5/5	0.88	0.45	4.60	114,114,114,114	0
4	LDA	C	385	16/16	0.73	0.40	3.80	91,97,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	A	366	5/5	0.77	0.35	3.64	167,167,167,167	0
2	SO4	A	358	5/5	0.83	0.32	3.63	126,126,126,126	0
3	GOL	A	371	6/6	0.78	0.35	3.51	85,85,86,86	0
2	SO4	B	349	5/5	0.90	0.30	3.04	104,105,105,105	0
3	GOL	A	375	6/6	0.86	0.35	2.99	81,81,82,82	0
2	SO4	A	354	5/5	0.87	0.24	2.69	122,122,123,123	0
2	SO4	C	348	5/5	0.85	0.27	2.65	98,98,99,99	0
2	SO4	C	362	5/5	0.88	0.36	2.34	148,149,149,149	0
2	SO4	C	363	5/5	0.81	0.23	2.26	144,144,145,145	0
4	LDA	A	386	16/16	0.94	0.28	2.22	46,49,61,62	0
2	SO4	A	360	5/5	0.90	0.23	1.80	120,120,121,121	0
2	SO4	C	367	5/5	0.96	0.39	1.67	99,100,100,100	0
2	SO4	B	348	5/5	0.94	0.21	1.52	107,107,107,108	0
2	SO4	C	365	5/5	0.96	0.35	1.45	100,100,101,101	0
4	LDA	C	383	16/16	0.90	0.24	1.45	35,48,68,69	0
2	SO4	A	349	5/5	0.91	0.19	1.26	113,113,113,114	0
4	LDA	B	380	16/16	0.89	0.22	0.89	80,84,86,86	0
2	SO4	B	346	5/5	0.88	0.19	0.53	144,144,144,144	0
3	GOL	B	365	6/6	0.92	0.16	0.28	78,78,79,80	0
4	LDA	C	384	16/16	0.96	0.19	-0.17	41,45,58,58	0
4	LDA	B	379	16/16	0.81	0.22	-	73,87,96,96	0
5	TAM	C	386	11/11	0.73	0.28	-	50,51,51,52	11
3	GOL	A	372	6/6	0.65	0.35	-	86,88,88,88	0
2	SO4	B	356	5/5	0.89	0.33	-	139,139,139,139	0
2	SO4	C	350	5/5	0.89	0.25	-	146,146,147,147	0
2	SO4	B	354	5/5	0.90	0.26	-	153,153,153,153	0
2	SO4	C	371	5/5	0.84	0.17	-	137,137,137,137	0
2	SO4	B	350	5/5	0.80	0.28	-	159,159,159,159	0
2	SO4	B	357	5/5	0.85	0.32	-	113,113,113,114	0
2	SO4	B	359	5/5	0.96	0.29	-	108,108,108,108	0
3	GOL	B	366	6/6	0.83	0.39	-	56,60,61,63	0
2	SO4	B	351	5/5	0.69	0.59	-	174,174,175,175	0
2	SO4	C	347	5/5	0.85	0.31	-	119,119,119,119	0
2	SO4	C	344	5/5	0.97	0.10	-	82,82,83,84	0
3	GOL	B	367	6/6	0.67	0.31	-	85,85,86,86	0
2	SO4	A	352	5/5	0.93	0.43	-	113,113,113,114	0
3	GOL	A	383	6/6	0.78	0.31	-	90,91,91,92	0
2	SO4	A	367	5/5	0.90	0.25	-	114,114,115,115	0
2	SO4	A	355	5/5	0.92	0.18	-	133,133,133,133	0
6	FLC	C	388	13/13	0.81	0.45	-	42,44,46,46	0
5	TAM	C	387	11/11	0.88	0.24	-	21,23,24,26	11
2	SO4	C	359	5/5	0.79	0.57	-	143,144,144,144	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GOL	A	378	6/6	0.50	0.89	-	118,119,119,119	0
2	SO4	B	353	5/5	0.86	0.33	-	121,121,121,121	0
3	GOL	A	382	6/6	0.77	0.25	-	82,84,84,86	0
2	SO4	C	352	5/5	0.85	0.14	-	112,112,112,112	0
3	GOL	C	392	6/6	0.77	0.36	-	104,105,105,105	0
3	GOL	C	376	6/6	0.32	0.47	-	134,135,135,135	0
3	GOL	A	380	6/6	0.91	0.19	-	76,77,77,77	0
2	SO4	C	356	5/5	0.86	0.43	-	113,113,114,114	0
2	SO4	A	369	5/5	0.33	0.71	-	164,164,164,164	0
2	SO4	A	364	5/5	0.81	0.24	-	145,145,145,145	0
2	SO4	A	342	5/5	0.90	0.30	-	132,132,132,132	0
3	GOL	B	372	6/6	0.82	0.43	-	74,75,76,76	0
2	SO4	A	344	5/5	0.91	0.26	-	105,105,106,106	0
2	SO4	C	345	5/5	0.89	0.17	-	113,113,113,114	0
4	LDA	A	389	16/16	0.71	0.48	-	75,93,105,106	0
2	SO4	B	355	5/5	0.78	0.38	-	142,142,142,142	0
7	TLA	A	393	10/10	0.79	0.32	-	125,126,126,127	0
2	SO4	C	360	5/5	0.48	0.36	-	170,170,170,170	0
3	GOL	A	379	6/6	0.82	0.18	-	82,84,85,85	0
2	SO4	B	361	5/5	0.77	0.22	-	143,143,144,144	0
3	GOL	C	379	6/6	0.44	0.86	-	122,123,124,124	0
3	GOL	C	373	6/6	0.86	0.33	-	70,72,72,73	0
3	GOL	B	364	6/6	0.81	0.30	-	99,100,101,101	0
3	GOL	C	375	6/6	0.75	0.22	-	117,119,119,120	0
2	SO4	A	346	5/5	0.92	0.16	-	105,105,105,106	0
2	SO4	B	352	5/5	0.96	0.18	-	102,102,102,102	0
4	LDA	C	382	16/16	0.90	0.33	-	43,56,67,67	0
2	SO4	A	357	5/5	0.94	0.25	-	106,106,107,107	0
2	SO4	C	361	5/5	0.85	0.24	-	122,123,123,123	0
2	SO4	A	356	5/5	0.90	0.28	-	104,104,104,104	0
2	SO4	C	342	5/5	0.95	0.23	-	83,83,84,86	0
2	SO4	B	363	5/5	0.88	0.29	-	123,123,123,123	0
3	GOL	B	369	6/6	0.72	0.28	-	80,82,84,85	0
2	SO4	C	346	5/5	0.88	0.43	-	124,125,125,125	0
6	FLC	C	389	13/13	0.79	0.33	-	95,97,98,99	0
2	SO4	B	343	5/5	0.66	0.45	-	151,151,151,151	0
3	GOL	A	374	6/6	0.88	0.40	-	81,83,83,84	0
2	SO4	A	347	5/5	0.90	0.31	-	103,104,104,104	0
2	SO4	B	347	5/5	0.88	0.21	-	98,99,99,100	0
3	GOL	C	394	6/6	0.59	0.24	-	67,69,70,70	0
2	SO4	C	366	5/5	0.70	0.35	-	148,148,148,148	0
2	SO4	A	362	5/5	0.88	0.24	-	133,134,134,134	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	A	365	5/5	0.77	0.37	-	131,131,132,132	0
2	SO4	A	363	5/5	0.81	0.18	-	138,138,138,139	0
2	SO4	A	343	5/5	0.88	0.24	-	142,142,142,142	0
2	SO4	C	369	5/5	0.80	0.34	-	114,114,114,114	0
3	GOL	C	390	6/6	0.79	0.26	-	94,96,97,97	0
3	GOL	B	374	6/6	0.79	0.69	-	84,85,86,87	0
2	SO4	B	344	5/5	0.78	0.41	-	134,134,134,134	0
3	GOL	C	374	6/6	0.86	0.17	-	91,91,92,92	0
2	SO4	B	360	5/5	0.92	0.16	-	113,113,113,113	0
2	SO4	C	355	5/5	0.93	0.19	-	109,110,110,110	0
2	SO4	C	351	5/5	0.87	0.29	-	105,106,107,107	0
2	SO4	A	351	5/5	0.86	0.44	-	128,128,128,128	0
3	GOL	C	377	6/6	0.76	0.29	-	97,97,99,99	0
4	LDA	A	385	16/16	0.57	0.75	-	106,112,117,117	0
2	SO4	A	361	5/5	0.94	0.30	-	126,127,127,127	0
3	GOL	B	368	6/6	0.80	0.33	-	87,88,88,89	0
6	FLC	C	391	13/13	0.81	0.15	-	85,87,87,88	0
4	LDA	B	377	16/16	0.72	0.33	-	87,101,108,108	0
3	GOL	A	377	6/6	0.48	0.33	-	82,83,84,84	0
3	GOL	A	376	6/6	0.71	0.26	-	101,102,102,102	0
5	TAM	C	393	11/11	0.67	0.21	-	60,61,61,61	11
3	GOL	C	381	6/6	0.94	0.31	-	77,78,78,79	0
2	SO4	A	350	5/5	0.73	0.70	-	143,144,144,144	0
2	SO4	A	359	5/5	0.80	0.35	-	136,136,136,136	0
3	GOL	A	381	6/6	0.77	0.35	-	95,96,96,97	0
3	GOL	C	378	6/6	0.69	0.37	-	83,85,85,86	0
2	SO4	C	372	5/5	0.82	0.28	-	134,134,134,135	0
7	TLA	B	383	10/10	0.87	0.23	-	76,79,80,80	0
3	GOL	B	370	6/6	0.88	0.31	-	85,85,86,86	0
3	GOL	C	380	6/6	0.86	0.23	-	96,96,97,97	0
4	LDA	B	375	16/16	0.94	0.31	-	57,60,62,62	0
6	FLC	A	392	13/13	0.73	0.45	-	120,120,121,121	0
2	SO4	C	370	5/5	0.86	0.21	-	139,139,139,139	0
2	SO4	B	358	5/5	0.86	0.45	-	110,110,110,110	0
4	LDA	B	378	16/16	0.85	0.34	-	73,84,95,95	0
2	SO4	C	358	5/5	0.93	0.12	-	120,120,120,120	0
2	SO4	A	348	5/5	0.90	0.16	-	141,141,141,141	0
3	GOL	A	373	6/6	0.88	0.24	-	89,90,90,90	0
3	GOL	B	371	6/6	0.76	0.43	-	88,89,89,89	0
2	SO4	B	342	5/5	0.94	0.35	-	101,101,101,101	0
2	SO4	B	362	5/5	0.80	0.54	-	148,148,148,149	0
2	SO4	B	345	5/5	0.80	0.35	-	106,106,107,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	C	354	5/5	0.81	0.60	-	152,152,152,153	0
5	TAM	A	391	11/11	0.71	0.30	-	62,63,63,64	11
4	LDA	B	376	16/16	0.91	0.37	-	72,76,81,81	0
2	SO4	C	357	5/5	0.88	0.18	-	119,120,120,120	0
4	LDA	B	381	16/16	0.56	0.47	-	83,90,105,105	0
2	SO4	C	353	5/5	0.78	0.31	-	128,128,128,128	0
2	SO4	A	345	5/5	0.87	0.18	-	112,112,112,112	0
5	TAM	B	382	11/11	0.73	0.19	-	52,54,55,55	11
2	SO4	C	349	5/5	0.92	0.28	-	96,97,97,97	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.