



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:35 PM GMT

PDB ID : 4ISY  
Title : Crystal structure of IscS from Mycobacterium tuberculosis  
Authors : Rybniker, J.; Pojer, F.; Cole, S.T.  
Deposited on : 2013-01-17  
Resolution : 2.59 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

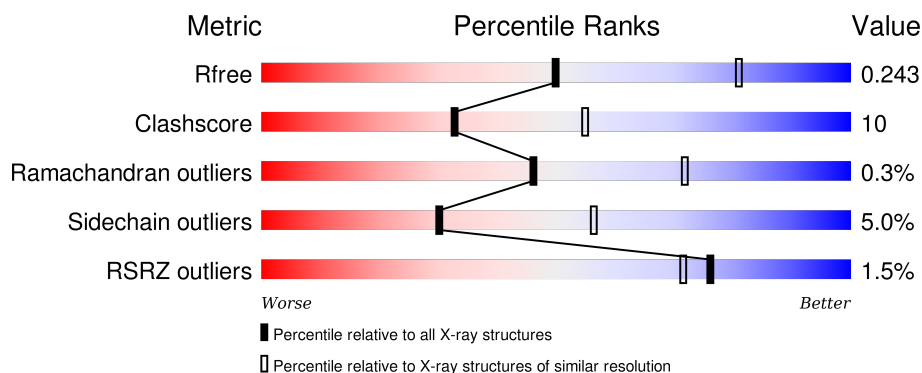
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.59 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	404	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 18%, green 74%, grey 1%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>74%</span> <span>18%</span> <span>• 6%</span> </div> </div>
1	B	404	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 16%, green 75%, grey 1%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>75%</span> <span>16%</span> <span>• 6%</span> </div> </div>
1	C	404	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 19%, green 75%, grey 1%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>75%</span> <span>19%</span> <span>• 5%</span> </div> </div>
1	D	404	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 14%, green 78%, grey 1%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>78%</span> <span>14%</span> <span>• 6%</span> </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	GOL	A	402	-	-	-	X
2	GOL	B	402	-	-	-	X
2	GOL	C	403	-	-	X	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11532 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 Cysteine desulfurase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	379	Total	C	N	O	P	S	0	0	0
			2795	1720	516	542	1	16			
1	B	379	Total	C	N	O	P	S	0	0	0
			2794	1719	516	542	1	16			
1	C	383	Total	C	N	O	P	S	0	0	0
			2814	1731	520	546	1	16			
1	D	381	Total	C	N	O	P	S	0	0	0
			2805	1726	518	544	1	16			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	EXPRESSION TAG	UNP O53272
A	-9	ARG	-	EXPRESSION TAG	UNP O53272
A	-8	GLY	-	EXPRESSION TAG	UNP O53272
A	-7	SER	-	EXPRESSION TAG	UNP O53272
A	-6	HIS	-	EXPRESSION TAG	UNP O53272
A	-5	HIS	-	EXPRESSION TAG	UNP O53272
A	-4	HIS	-	EXPRESSION TAG	UNP O53272
A	-3	HIS	-	EXPRESSION TAG	UNP O53272
A	-2	HIS	-	EXPRESSION TAG	UNP O53272
A	-1	HIS	-	EXPRESSION TAG	UNP O53272
A	0	GLY	-	EXPRESSION TAG	UNP O53272
A	1	SER	-	EXPRESSION TAG	UNP O53272
B	-10	MET	-	EXPRESSION TAG	UNP O53272
B	-9	ARG	-	EXPRESSION TAG	UNP O53272
B	-8	GLY	-	EXPRESSION TAG	UNP O53272
B	-7	SER	-	EXPRESSION TAG	UNP O53272
B	-6	HIS	-	EXPRESSION TAG	UNP O53272
B	-5	HIS	-	EXPRESSION TAG	UNP O53272
B	-4	HIS	-	EXPRESSION TAG	UNP O53272
B	-3	HIS	-	EXPRESSION TAG	UNP O53272
B	-2	HIS	-	EXPRESSION TAG	UNP O53272

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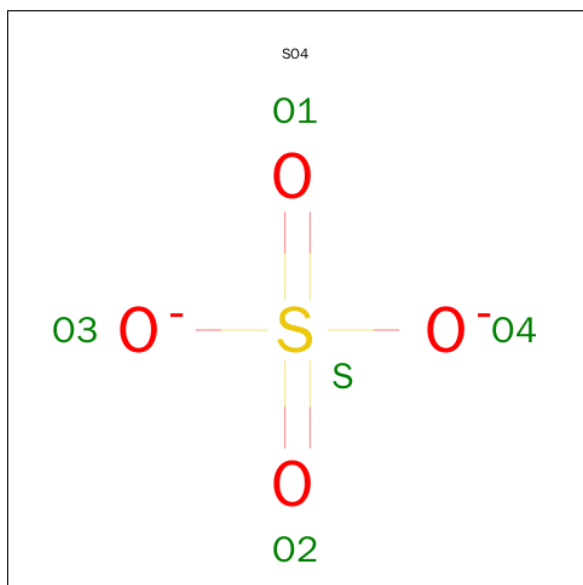
Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	HIS	-	EXPRESSION TAG	UNP O53272
B	0	GLY	-	EXPRESSION TAG	UNP O53272
B	1	SER	-	EXPRESSION TAG	UNP O53272
C	-10	MET	-	EXPRESSION TAG	UNP O53272
C	-9	ARG	-	EXPRESSION TAG	UNP O53272
C	-8	GLY	-	EXPRESSION TAG	UNP O53272
C	-7	SER	-	EXPRESSION TAG	UNP O53272
C	-6	HIS	-	EXPRESSION TAG	UNP O53272
C	-5	HIS	-	EXPRESSION TAG	UNP O53272
C	-4	HIS	-	EXPRESSION TAG	UNP O53272
C	-3	HIS	-	EXPRESSION TAG	UNP O53272
C	-2	HIS	-	EXPRESSION TAG	UNP O53272
C	-1	HIS	-	EXPRESSION TAG	UNP O53272
C	0	GLY	-	EXPRESSION TAG	UNP O53272
C	1	SER	-	EXPRESSION TAG	UNP O53272
D	-10	MET	-	EXPRESSION TAG	UNP O53272
D	-9	ARG	-	EXPRESSION TAG	UNP O53272
D	-8	GLY	-	EXPRESSION TAG	UNP O53272
D	-7	SER	-	EXPRESSION TAG	UNP O53272
D	-6	HIS	-	EXPRESSION TAG	UNP O53272
D	-5	HIS	-	EXPRESSION TAG	UNP O53272
D	-4	HIS	-	EXPRESSION TAG	UNP O53272
D	-3	HIS	-	EXPRESSION TAG	UNP O53272
D	-2	HIS	-	EXPRESSION TAG	UNP O53272
D	-1	HIS	-	EXPRESSION TAG	UNP O53272
D	0	GLY	-	EXPRESSION TAG	UNP O53272
D	1	SER	-	EXPRESSION TAG	UNP O53272

- Molecule 2 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
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

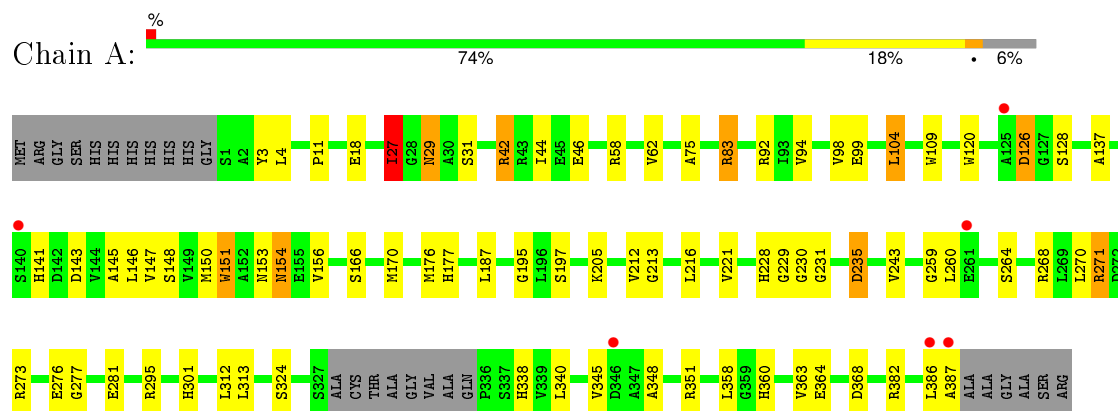
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	54	Total	O	0	0
			54	54		
4	B	68	Total	O	0	0
			68	68		
4	C	54	Total	O	0	0
			54	54		
4	D	95	Total	O	0	0
			95	95		

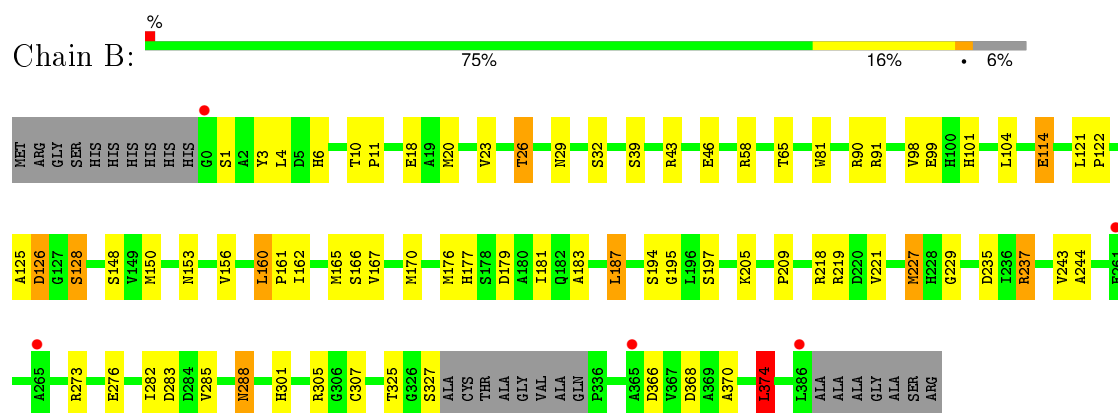
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

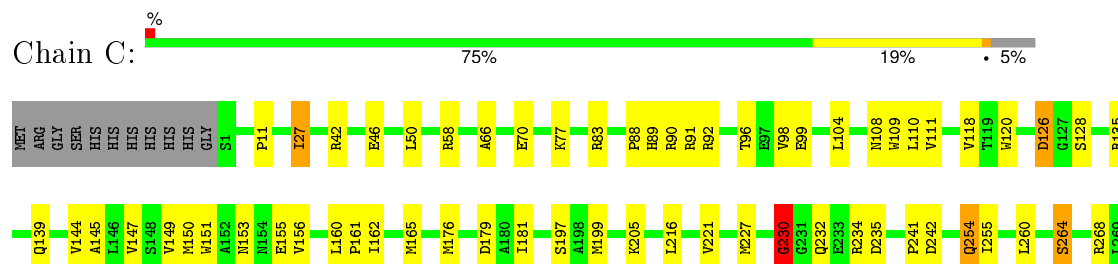
#### • Molecule 1: Cysteine desulfurase



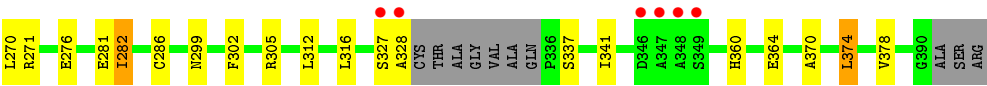
#### • Molecule 1: Cysteine desulfurase



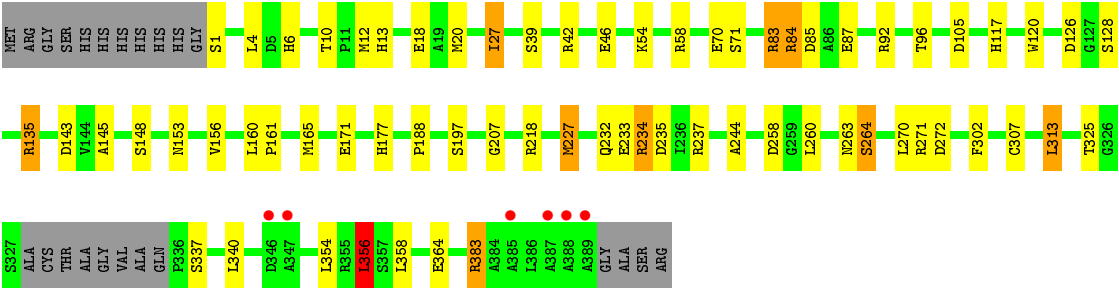
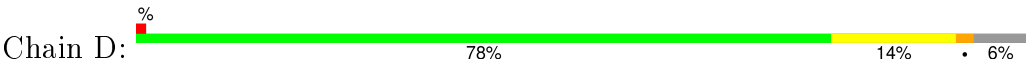
#### • Molecule 1: Cysteine desulfurase







● Molecule 1: Cysteine desulfurase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.81Å 78.13Å 92.77Å 94.54° 104.71° 98.57°	Depositor
Resolution (Å)	45.22 – 2.59 45.22 – 2.59	Depositor EDS
% Data completeness (in resolution range)	97.9 (45.22-2.59) 94.3 (45.22-2.59)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.62 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.186 , 0.245 0.184 , 0.243	Depositor DCC
$R_{free}$ test set	2811 reflections (5.46%)	DCC
Wilson B-factor (Å <sup>2</sup> )	29.3	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 26.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 54275 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	11532	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.36% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, LLP, SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.77	3/2814 (0.1%)	0.89	8/3822 (0.2%)
1	B	0.83	1/2813 (0.0%)	0.96	5/3820 (0.1%)
1	C	0.80	2/2833 (0.1%)	0.91	3/3848 (0.1%)
1	D	0.83	1/2824 (0.0%)	0.90	4/3836 (0.1%)
All	All	0.81	7/11284 (0.1%)	0.92	20/15326 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	D	0	1
All	All	0	2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	120	TRP	CD2-CE2	6.05	1.48	1.41
1	A	120	TRP	CD2-CE2	5.87	1.48	1.41
1	C	109	TRP	CD2-CE2	5.46	1.48	1.41
1	B	114	GLU	CD-OE1	-5.45	1.19	1.25
1	A	151	TRP	CD2-CE2	5.38	1.47	1.41
1	A	109	TRP	CD2-CE2	5.36	1.47	1.41
1	C	120	TRP	CD2-CE2	5.35	1.47	1.41

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	83	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	A	104	LEU	CA-CB-CG	5.96	129.01	115.30
1	A	58	ARG	NE-CZ-NH2	-5.87	117.37	120.30
1	D	356	LEU	CA-CB-CG	5.80	128.65	115.30
1	B	90	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	B	43	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	A	83	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	A	42	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	D	237	ARG	NE-CZ-NH1	-5.51	117.54	120.30
1	A	83	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	B	194	SER	C-N-CA	-5.48	110.79	122.30
1	C	126	ASP	CB-CG-OD1	-5.47	113.38	118.30
1	A	228	HIS	C-N-CA	5.40	133.63	122.30
1	D	227	MET	CG-SD-CE	5.40	108.84	100.20
1	C	242	ASP	CB-CG-OD1	5.27	123.05	118.30
1	C	27	ILE	CB-CA-C	-5.22	101.17	111.60
1	B	218	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	A	382	ARG	NE-CZ-NH2	-5.13	117.74	120.30
1	A	27	ILE	CB-CA-C	-5.12	101.35	111.60
1	B	374	LEU	CA-CB-CG	5.03	126.86	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	230	GLY	Peptide
1	D	307	CYS	Peptide

## 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	2795	0	2758	62	0
1	B	2794	0	2756	69	0
1	C	2814	0	2775	62	0
1	D	2805	0	2767	45	0
2	A	18	0	24	1	0
2	B	12	0	16	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	18	0	24	6	0
3	C	5	0	0	1	0
4	A	54	0	0	4	0
4	B	68	0	0	3	0
4	C	54	0	0	2	0
4	D	95	0	0	5	0
All	All	11532	0	11120	233	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 10.

All (233) 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:C:99:GLU:HA	1:C:150:MET:CE	1.49	1.41
1:C:99:GLU:HA	1:C:150:MET:HE2	1.19	1.19
1:B:99:GLU:HA	1:B:150:MET:CE	1.77	1.15
1:A:348:ALA:HA	1:A:351:ARG:HH21	0.99	1.10
1:B:99:GLU:HA	1:B:150:MET:HE2	1.25	1.08
1:C:99:GLU:HA	1:C:150:MET:HE1	1.35	1.07
1:A:99:GLU:CA	1:A:150:MET:HE1	1.90	1.01
1:A:99:GLU:HA	1:A:150:MET:HE1	1.02	1.00
1:A:29:ASN:HD22	1:A:31:SER:H	1.06	1.00
1:C:99:GLU:CA	1:C:150:MET:CE	2.41	0.97
1:A:348:ALA:HA	1:A:351:ARG:NH2	1.79	0.94
1:A:271:ARG:NH1	1:A:295:ARG:HD3	1.83	0.94
1:A:99:GLU:HA	1:A:150:MET:CE	1.96	0.93
1:D:84:ARG:HH11	1:D:84:ARG:HG2	1.33	0.92
1:C:98:VAL:O	1:C:150:MET:HE1	1.69	0.92
1:A:29:ASN:ND2	1:A:31:SER:H	1.70	0.89
1:C:99:GLU:CA	1:C:150:MET:HE1	2.03	0.88
1:D:153:ASN:HD22	1:D:156:VAL:H	1.19	0.88
1:B:23:VAL:O	1:B:26:THR:HB	1.72	0.87
1:B:153:ASN:HD22	1:B:156:VAL:H	1.24	0.85
1:A:98:VAL:O	1:A:150:MET:HE3	1.76	0.84
1:A:270:LEU:HD21	1:A:364:GLU:OE1	1.77	0.84
1:A:153:ASN:HD22	1:A:156:VAL:H	1.25	0.82
1:A:83:ARG:HD3	1:A:145:ALA:O	1.80	0.82
1:B:98:VAL:O	1:B:150:MET:HE1	1.80	0.81
1:B:161:PRO:HD2	1:B:165:MET:HE2	1.64	0.80
1:A:98:VAL:C	1:A:150:MET:HE3	2.03	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:153:ASN:HD22	1:C:156:VAL:H	1.29	0.79
1:C:83:ARG:HH11	2:C:403:GOL:H12	1.48	0.78
1:B:99:GLU:CA	1:B:150:MET:CE	2.60	0.77
1:A:83:ARG:CD	1:A:145:ALA:O	2.32	0.77
1:D:83:ARG:HD2	1:D:145:ALA:O	1.84	0.77
1:C:161:PRO:O	1:C:165:MET:HG3	1.84	0.77
1:C:270:LEU:HD21	1:C:364:GLU:OE1	1.85	0.76
1:A:154:ASN:H	1:A:154:ASN:ND2	1.79	0.75
1:B:325:THR:HG22	1:B:327:SER:H	1.52	0.74
1:B:153:ASN:ND2	1:B:156:VAL:H	1.86	0.74
1:C:42:ARG:O	1:C:46:GLU:HG3	1.87	0.73
1:B:183:ALA:HB1	1:B:187:LEU:CD2	2.19	0.72
1:C:179:ASP:OD1	1:C:181:ILE:HD12	1.89	0.72
1:D:313:LEU:CD1	1:D:325:THR:HG23	2.20	0.72
1:B:98:VAL:O	1:B:150:MET:CE	2.38	0.70
1:A:271:ARG:HH12	1:A:295:ARG:HD3	1.55	0.70
1:B:99:GLU:HA	1:B:150:MET:HE1	1.72	0.69
1:C:153:ASN:ND2	1:C:156:VAL:H	1.92	0.68
1:A:62:VAL:HG22	1:A:216:LEU:CD2	2.24	0.68
1:B:65:THR:HA	1:B:237:ARG:NH1	2.09	0.67
1:B:229:GLY:HA2	4:D:454:HOH:O	1.95	0.67
1:C:98:VAL:C	1:C:150:MET:HE1	2.14	0.66
1:B:161:PRO:HD2	1:B:165:MET:CE	2.25	0.66
1:D:153:ASN:ND2	1:D:156:VAL:H	1.92	0.66
1:B:6:HIS:HD2	1:B:10:THR:OG1	1.79	0.65
1:B:81:TRP:HE1	1:B:114:GLU:HG2	1.60	0.65
1:A:166:SER:OG	1:A:195:GLY:HA3	1.96	0.65
1:A:29:ASN:HD22	1:A:31:SER:N	1.89	0.64
1:A:27:ILE:HD13	4:A:519:HOH:O	1.97	0.64
1:C:83:ARG:HH11	2:C:403:GOL:C1	2.09	0.64
1:B:91:ARG:HH11	1:B:91:ARG:HG3	1.63	0.64
1:B:183:ALA:HB1	1:B:187:LEU:HD21	1.80	0.64
1:B:273:ARG:NH2	1:B:368:ASP:OD1	2.29	0.64
1:A:229:GLY:HA2	4:A:502:HOH:O	1.98	0.64
1:A:229:GLY:CA	4:A:502:HOH:O	2.46	0.62
1:C:111:VAL:HG21	1:C:118:VAL:CG2	2.29	0.62
1:B:162:ILE:HG23	1:B:176:MET:HE1	1.79	0.62
1:A:271:ARG:HH11	1:A:295:ARG:HD3	1.62	0.61
1:C:205:LLP:NZ	1:C:205:LLP:O3	2.30	0.61
1:A:270:LEU:CD2	1:A:364:GLU:OE1	2.47	0.61
1:C:181:ILE:HD13	1:C:205:LLP:C6	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:281:GLU:C	1:C:282:ILE:HG12	2.21	0.61
1:D:6:HIS:HD2	1:D:10:THR:OG1	1.82	0.61
1:D:148:SER:OG	1:D:177:HIS:HD2	1.83	0.61
1:D:263:ASN:HB3	4:D:475:HOH:O	2.00	0.60
1:B:11:PRO:HG3	1:D:27:ILE:HG21	1.83	0.60
1:A:94:VAL:HB	1:A:147:VAL:HG22	1.84	0.60
1:A:205:LLP:NZ	1:A:205:LLP:O3	2.29	0.60
1:B:81:TRP:HE1	1:B:114:GLU:CG	2.15	0.60
1:B:205:LLP:O3	1:B:205:LLP:NZ	2.30	0.60
1:A:98:VAL:O	1:A:150:MET:CE	2.48	0.59
1:A:154:ASN:HD22	1:A:154:ASN:H	1.50	0.59
1:B:126:ASP:HB3	1:B:128:SER:HB3	1.85	0.59
1:A:348:ALA:CA	1:A:351:ARG:HH21	1.93	0.59
1:C:83:ARG:HD3	1:C:145:ALA:O	2.03	0.59
1:B:183:ALA:HB1	1:B:187:LEU:HD22	1.85	0.58
1:C:88:PRO:O	1:C:91:ARG:HD2	2.02	0.58
1:B:179:ASP:OD1	1:B:181:ILE:HD12	2.04	0.57
1:D:4:LEU:HD23	1:D:358:LEU:HD21	1.87	0.57
1:C:89:HIS:NE2	1:D:58:ARG:NH1	2.53	0.57
1:A:98:VAL:C	1:A:150:MET:CE	2.73	0.57
1:D:313:LEU:HD13	1:D:325:THR:HG23	1.85	0.57
1:B:126:ASP:HB3	1:B:128:SER:H	1.68	0.57
1:B:150:MET:O	1:B:160:LEU:HD23	2.05	0.57
1:A:166:SER:OG	1:A:195:GLY:CA	2.53	0.56
1:D:126:ASP:HB3	1:D:128:SER:H	1.69	0.56
1:A:83:ARG:HD2	1:A:145:ALA:O	2.03	0.56
1:A:153:ASN:ND2	1:A:156:VAL:H	1.99	0.56
1:A:62:VAL:HG22	1:A:216:LEU:HD21	1.87	0.55
1:B:166:SER:OG	1:B:195:GLY:HA3	2.06	0.55
1:C:370:ALA:O	1:C:374:LEU:HB2	2.06	0.55
1:D:260:LEU:O	1:D:264:SER:HB2	2.07	0.54
1:B:98:VAL:C	1:B:150:MET:CE	2.76	0.54
1:B:229:GLY:CA	4:D:454:HOH:O	2.55	0.54
1:D:84:ARG:NH1	1:D:85:ASP:OD1	2.41	0.54
1:B:166:SER:OG	1:B:195:GLY:CA	2.56	0.54
1:C:254:GLN:HE21	1:C:255:ILE:HG13	1.73	0.54
1:A:151:TRP:NE1	1:A:187:LEU:HD11	2.22	0.54
1:B:4:LEU:HD11	1:B:366:ASP:HB3	1.88	0.54
1:B:229:GLY:HA3	1:D:105:ASP:OD2	2.08	0.53
1:C:260:LEU:O	1:C:264:SER:HB2	2.08	0.53
1:A:29:ASN:HD22	1:A:29:ASN:C	2.12	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:354:LEU:HD23	1:D:356:LEU:HD11	1.90	0.53
1:A:147:VAL:CG1	1:A:176:MET:HG3	2.38	0.53
1:C:160:LEU:HD12	1:C:160:LEU:N	2.24	0.53
1:A:273:ARG:NH2	1:A:368:ASP:OD1	2.33	0.53
1:B:58:ARG:HH22	1:B:219:ARG:HD2	1.74	0.52
1:A:230:GLY:HA3	2:A:402:GOL:H31	1.91	0.52
1:C:99:GLU:CA	1:C:150:MET:HE2	2.13	0.52
1:D:83:ARG:CD	1:D:145:ALA:O	2.56	0.52
1:B:167:VAL:HA	1:B:170:MET:HE3	1.90	0.52
1:B:99:GLU:CA	1:B:150:MET:HE1	2.33	0.52
1:B:187:LEU:C	1:B:187:LEU:HD23	2.29	0.52
1:B:20:MET:HG3	1:B:244:ALA:HB1	1.91	0.52
1:D:302:PHE:HE2	1:D:356:LEU:HD22	1.75	0.51
1:B:282:ILE:CD1	1:B:374:LEU:HD13	2.41	0.51
1:C:11:PRO:O	1:C:360:HIS:HE1	1.93	0.51
1:D:354:LEU:CD2	1:D:356:LEU:HD11	2.41	0.51
1:B:153:ASN:ND2	1:B:156:VAL:HG22	2.26	0.51
1:B:23:VAL:HG11	1:B:243:VAL:HG12	1.93	0.51
1:A:126:ASP:HB3	1:A:128:SER:H	1.76	0.51
1:C:83:ARG:HD2	2:C:403:GOL:H12	1.93	0.50
1:C:270:LEU:CD2	1:C:364:GLU:OE1	2.57	0.50
1:B:288:ASN:ND2	1:B:301:HIS:ND1	2.60	0.50
1:C:96:THR:HG21	1:C:149:VAL:HG13	1.93	0.50
1:B:91:ARG:HG3	1:B:91:ARG:NH1	2.25	0.50
1:A:229:GLY:HA3	4:A:502:HOH:O	2.11	0.50
1:D:197:SER:HA	1:D:218:ARG:HD3	1.93	0.50
1:B:98:VAL:C	1:B:150:MET:HE3	2.32	0.50
1:B:11:PRO:HG3	1:D:27:ILE:CG2	2.42	0.50
1:B:81:TRP:NE1	1:B:114:GLU:HG2	2.26	0.49
1:A:154:ASN:N	1:A:154:ASN:ND2	2.53	0.49
1:A:147:VAL:HG12	1:A:176:MET:HG3	1.93	0.49
1:A:313:LEU:HD11	1:A:324:SER:HA	1.94	0.49
1:C:271:ARG:HD3	1:C:299:ASN:O	2.12	0.49
1:B:325:THR:HG22	1:B:325:THR:O	2.12	0.49
1:A:231:GLY:HA3	1:A:235:ASP:HA	1.95	0.49
1:C:327:SER:HB2	1:C:328:ALA:HB2	1.95	0.48
1:A:42:ARG:O	1:A:46:GLU:HG3	2.13	0.48
1:C:153:ASN:ND2	1:C:155:GLU:H	2.11	0.48
1:A:11:PRO:O	1:A:360:HIS:HE1	1.96	0.48
1:D:54:LYS:NZ	1:D:258:ASP:OD1	2.42	0.47
1:D:271:ARG:NH1	1:D:272:ASP:OD1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:92:ARG:NH1	1:D:143:ASP:OD2	2.47	0.47
1:C:197:SER:HB3	1:C:221:VAL:HG21	1.96	0.47
1:B:227:MET:HE2	1:D:70:GLU:HA	1.96	0.47
1:C:199:MET:HE2	1:C:216:LEU:HD22	1.96	0.47
1:D:233:GLU:O	1:D:235:ASP:N	2.48	0.47
1:B:370:ALA:O	1:B:374:LEU:HB2	2.15	0.47
1:B:325:THR:O	1:B:325:THR:CG2	2.63	0.47
1:D:84:ARG:NH1	1:D:84:ARG:HG2	2.12	0.47
1:A:92:ARG:NH1	1:A:143:ASP:OD2	2.48	0.47
1:C:135:ARG:HE	1:C:139:GLN:NE2	2.13	0.47
1:B:98:VAL:HG23	1:B:150:MET:HE3	1.97	0.46
1:C:270:LEU:HA	1:C:270:LEU:HD23	1.77	0.46
1:C:92:ARG:HB3	1:C:144:VAL:HA	1.97	0.46
1:A:154:ASN:HD22	1:A:154:ASN:N	2.14	0.46
1:D:234:ARG:O	1:D:235:ASP:CB	2.63	0.46
1:C:230:GLY:HA3	1:C:232:GLN:OE1	2.15	0.46
1:C:126:ASP:HB3	1:C:128:SER:HB3	1.98	0.46
1:D:337:SER:HB3	1:D:340:LEU:HD12	1.98	0.45
1:D:383:ARG:NE	4:D:452:HOH:O	2.48	0.45
1:D:313:LEU:HD12	1:D:325:THR:HG23	1.94	0.45
1:B:121:LEU:HA	1:B:122:PRO:HD3	1.87	0.45
1:C:92:ARG:NH2	3:C:401:SO4:O2	2.49	0.45
1:A:44:ILE:HD12	1:A:243:VAL:HA	1.98	0.45
1:C:99:GLU:N	1:C:150:MET:HE1	2.32	0.45
1:C:83:ARG:NH1	2:C:403:GOL:C1	2.80	0.45
1:A:197:SER:HB3	1:A:221:VAL:HG21	1.98	0.45
1:A:104:LEU:HD11	1:A:338:HIS:CD2	2.52	0.44
1:D:313:LEU:HD12	1:D:325:THR:CG2	2.47	0.44
1:D:4:LEU:HD23	1:D:358:LEU:CD2	2.48	0.44
1:C:104:LEU:HD23	1:C:104:LEU:HA	1.62	0.44
1:A:301:HIS:HE1	1:A:340:LEU:HD11	1.83	0.44
1:B:3:TYR:C	1:B:4:LEU:HD12	2.38	0.44
1:D:96:THR:HB	4:D:440:HOH:O	2.17	0.44
1:A:277:GLY:O	1:A:281:GLU:HG2	2.17	0.44
1:B:282:ILE:HG22	1:B:285:VAL:CG2	2.48	0.44
1:D:13:HIS:CD2	1:D:207:GLY:HA3	2.53	0.44
1:C:135:ARG:HE	1:C:139:GLN:HE21	1.66	0.43
1:C:305:ARG:HG3	1:C:305:ARG:HH11	1.83	0.43
1:B:98:VAL:O	1:B:150:MET:HE3	2.18	0.43
1:B:153:ASN:HD22	1:B:156:VAL:HG22	1.84	0.43
2:C:403:GOL:H2	4:C:540:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:316:LEU:HD21	1:C:374:LEU:HD13	2.00	0.43
1:C:151:TRP:CE3	1:C:162:ILE:HG21	2.53	0.43
1:D:148:SER:HA	1:D:177:HIS:O	2.18	0.43
1:A:3:TYR:C	1:A:4:LEU:HD12	2.39	0.43
1:C:264:SER:HB3	1:C:268:ARG:HH12	1.82	0.43
1:C:286:CYS:O	1:C:302:PHE:HA	2.19	0.43
1:D:161:PRO:HG2	1:D:165:MET:HE2	2.01	0.43
1:C:50:LEU:HD12	1:C:50:LEU:HA	1.80	0.43
1:A:264:SER:HB3	1:A:268:ARG:HH12	1.84	0.42
1:B:46:GLU:CD	4:B:539:HOH:O	2.58	0.42
1:B:197:SER:HB3	1:B:221:VAL:HG21	2.01	0.42
1:B:162:ILE:HD13	1:B:165:MET:HE3	2.01	0.42
1:C:83:ARG:NH1	2:C:403:GOL:H12	2.26	0.42
1:C:312:LEU:HD12	1:C:312:LEU:O	2.19	0.42
1:C:199:MET:CE	1:C:216:LEU:HD22	2.49	0.42
1:A:259:GLY:O	1:A:260:LEU:C	2.58	0.42
1:B:187:LEU:O	1:B:187:LEU:HD23	2.19	0.42
1:A:387:ALA:HB3	1:D:188:PRO:HG2	2.01	0.42
1:B:283:ASP:HA	4:B:565:HOH:O	2.20	0.42
1:A:75:ALA:CB	1:A:177:HIS:CD2	3.03	0.42
1:C:77:LYS:HA	1:C:110:LEU:HD11	2.02	0.41
1:C:337:SER:O	1:C:341:ILE:HG12	2.20	0.41
1:D:92:ARG:HA	1:D:117:HIS:O	2.19	0.41
1:D:135:ARG:NH2	1:D:171:GLU:OE1	2.53	0.41
1:C:147:VAL:HB	1:C:176:MET:HG3	2.02	0.41
1:B:101:HIS:HA	1:B:104:LEU:HB2	2.02	0.41
1:B:148:SER:HA	1:B:177:HIS:O	2.21	0.41
1:A:137:ALA:O	1:A:141:HIS:HD2	2.04	0.41
1:C:66:ALA:N	1:C:70:GLU:OE1	2.44	0.41
1:C:241:PRO:HA	4:C:544:HOH:O	2.21	0.41
1:C:374:LEU:HD12	1:C:378:VAL:HG23	2.03	0.41
1:C:90:ARG:HG2	1:C:90:ARG:NH1	2.35	0.41
1:A:212:VAL:HG22	1:A:213:GLY:N	2.36	0.41
1:A:148:SER:HA	1:A:177:HIS:O	2.22	0.40
1:B:125:ALA:HB1	4:B:528:HOH:O	2.21	0.40
1:B:282:ILE:HD12	1:B:374:LEU:HD13	2.03	0.40
1:D:161:PRO:HD2	1:D:165:MET:HE3	2.03	0.40
1:D:270:LEU:HD21	1:D:364:GLU:OE1	2.21	0.40
1:D:20:MET:HG2	1:D:244:ALA:O	2.20	0.40
1:B:282:ILE:HD11	1:B:374:LEU:HD13	2.04	0.40
1:D:42:ARG:O	1:D:46:GLU:HG3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:ASN:HB3	1:B:32:SER:OG	2.22	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	374/404 (93%)	360 (96%)	14 (4%)	0	100	100
1	B	374/404 (93%)	362 (97%)	12 (3%)	0	100	100
1	C	378/404 (94%)	361 (96%)	15 (4%)	2 (0%)	34	60
1	D	376/404 (93%)	362 (96%)	12 (3%)	2 (0%)	34	60
All	All	1502/1616 (93%)	1445 (96%)	53 (4%)	4 (0%)	46	72

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	234	ARG
1	D	232	GLN
1	C	234	ARG
1	C	230	GLY

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	283/298 (95%)	268 (95%)	15 (5%)	28	53
1	B	283/298 (95%)	266 (94%)	17 (6%)	24	47
1	C	283/298 (95%)	273 (96%)	10 (4%)	43	71
1	D	283/298 (95%)	268 (95%)	15 (5%)	28	53
All	All	1132/1192 (95%)	1075 (95%)	57 (5%)	30	56

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	GLU
1	A	27	ILE
1	A	29	ASN
1	A	126	ASP
1	A	146	LEU
1	A	154	ASN
1	A	170	MET
1	A	235	ASP
1	A	271	ARG
1	A	276	GLU
1	A	312	LEU
1	A	345	VAL
1	A	358	LEU
1	A	363	VAL
1	A	386	LEU
1	B	1	SER
1	B	18	GLU
1	B	26	THR
1	B	39	SER
1	B	126	ASP
1	B	128	SER
1	B	160	LEU
1	B	187	LEU
1	B	209	PRO
1	B	227	MET
1	B	235	ASP
1	B	237	ARG
1	B	276	GLU
1	B	288	ASN
1	B	305	ARG
1	B	307	CYS
1	B	374	LEU
1	C	27	ILE

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Mol	Chain	Res	Type
1	C	58	ARG
1	C	108	ASN
1	C	227	MET
1	C	235	ASP
1	C	254	GLN
1	C	264	SER
1	C	276	GLU
1	C	282	ILE
1	C	374	LEU
1	D	1	SER
1	D	12	MET
1	D	18	GLU
1	D	27	ILE
1	D	39	SER
1	D	71	SER
1	D	84	ARG
1	D	87	GLU
1	D	135	ARG
1	D	160	LEU
1	D	227	MET
1	D	264	SER
1	D	313	LEU
1	D	356	LEU
1	D	383	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	141	HIS
1	A	153	ASN
1	A	154	ASN
1	A	186	GLN
1	A	263	ASN
1	A	288	ASN
1	A	360	HIS
1	B	6	HIS
1	B	108	ASN
1	B	153	ASN
1	B	263	ASN
1	B	288	ASN
1	C	139	GLN

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Mol	Chain	Res	Type
1	C	153	ASN
1	C	254	GLN
1	C	288	ASN
1	C	360	HIS
1	D	6	HIS
1	D	13	HIS
1	D	101	HIS
1	D	153	ASN
1	D	177	HIS
1	D	263	ASN
1	D	288	ASN
1	D	360	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	LLP	A	205	1	23,24,25	3.50	11 (47%)	28,32,34	1.93	9 (32%)
1	LLP	B	205	1	23,24,25	3.52	11 (47%)	28,32,34	1.88	8 (28%)
1	LLP	C	205	1	23,24,25	3.79	12 (52%)	28,32,34	1.76	5 (17%)
1	LLP	D	205	1	23,24,25	3.77	11 (47%)	28,32,34	1.84	6 (21%)

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
1	LLP	A	205	1	-	0/15/17/19	0/1/1/1
1	LLP	B	205	1	-	0/15/17/19	0/1/1/1
1	LLP	C	205	1	-	0/15/17/19	0/1/1/1
1	LLP	D	205	1	-	0/15/17/19	0/1/1/1

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	205	LLP	C4-C4'	-7.73	1.33	1.46
1	C	205	LLP	C2'-C2	-7.24	1.35	1.50
1	C	205	LLP	C3-C2	-7.22	1.35	1.40
1	D	205	LLP	C3-C2	-6.83	1.36	1.40
1	A	205	LLP	C2'-C2	-6.44	1.37	1.50
1	D	205	LLP	C2'-C2	-6.32	1.37	1.50
1	D	205	LLP	P-OP3	-6.28	1.32	1.54
1	B	205	LLP	C2'-C2	-6.05	1.38	1.50
1	A	205	LLP	P-OP1	-5.99	1.31	1.51
1	B	205	LLP	P-OP4	-5.99	1.40	1.60
1	A	205	LLP	C4-C4'	-5.94	1.36	1.46
1	B	205	LLP	C4-C4'	-5.89	1.36	1.46
1	D	205	LLP	P-OP2	-5.68	1.34	1.54
1	D	205	LLP	C4-C4'	-5.43	1.37	1.46
1	A	205	LLP	P-OP2	-5.33	1.35	1.54
1	C	205	LLP	P-OP3	-5.25	1.35	1.54
1	B	205	LLP	C3-C2	-5.24	1.37	1.40
1	D	205	LLP	P-OP1	-5.15	1.34	1.51
1	A	205	LLP	C3-C2	-4.88	1.37	1.40
1	A	205	LLP	P-OP3	-4.77	1.37	1.54
1	B	205	LLP	P-OP2	-4.77	1.37	1.54
1	C	205	LLP	P-OP2	-4.73	1.37	1.54
1	D	205	LLP	C5'-C5	-4.55	1.37	1.50
1	D	205	LLP	P-OP4	-4.38	1.45	1.60
1	B	205	LLP	P-OP3	-4.38	1.39	1.54
1	C	205	LLP	P-OP1	-4.28	1.37	1.51
1	A	205	LLP	CB-CA	-4.20	1.49	1.53
1	D	205	LLP	CB-CA	-4.15	1.49	1.53
1	B	205	LLP	C5'-C5	-4.05	1.39	1.50
1	B	205	LLP	P-OP1	-4.04	1.37	1.51
1	B	205	LLP	C4-C3	-4.02	1.35	1.40
1	C	205	LLP	C5'-C5	-3.98	1.39	1.50
1	C	205	LLP	C4-C5	-3.76	1.36	1.42
1	A	205	LLP	C5'-C5	-3.67	1.40	1.50
1	C	205	LLP	P-OP4	-3.66	1.48	1.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	205	LLP	C4-C3	-3.34	1.36	1.40
1	A	205	LLP	C4-C3	-2.83	1.37	1.40
1	A	205	LLP	P-OP4	-2.69	1.51	1.60
1	B	205	LLP	C4-C5	-2.39	1.38	1.42
1	C	205	LLP	O3-C3	-2.38	1.31	1.37
1	D	205	LLP	C4-C3	-2.07	1.38	1.40
1	C	205	LLP	C4'-NZ	5.59	1.44	1.27
1	D	205	LLP	C4'-NZ	6.02	1.45	1.27
1	A	205	LLP	C4'-NZ	6.28	1.46	1.27
1	B	205	LLP	C4'-NZ	6.32	1.46	1.27

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	205	LLP	OP4-P-OP1	-4.90	94.66	107.14
1	A	205	LLP	C2'-C2-C3	-3.85	116.39	121.04
1	D	205	LLP	OP4-P-OP1	-3.23	98.92	107.14
1	B	205	LLP	C3-C4-C4'	-3.23	115.98	120.16
1	C	205	LLP	CE-NZ-C4'	-3.11	109.98	118.97
1	C	205	LLP	O-C-CA	-3.05	117.54	125.49
1	B	205	LLP	C4-C4'-NZ	-2.87	109.09	125.06
1	A	205	LLP	C3-C4-C4'	-2.80	116.54	120.16
1	A	205	LLP	O-C-CA	-2.76	118.31	125.49
1	D	205	LLP	C4-C4'-NZ	-2.75	109.74	125.06
1	C	205	LLP	C4-C4'-NZ	-2.74	109.82	125.06
1	A	205	LLP	C4-C4'-NZ	-2.56	110.79	125.06
1	B	205	LLP	OP4-P-OP1	-2.53	100.69	107.14
1	D	205	LLP	C3-C4-C4'	-2.34	117.14	120.16
1	B	205	LLP	OP2-P-OP4	-2.06	100.62	106.56
1	C	205	LLP	OP3-P-OP2	2.13	115.48	107.38
1	A	205	LLP	OP3-P-OP2	2.34	116.29	107.38
1	A	205	LLP	C2'-C2-N1	2.41	123.30	117.95
1	B	205	LLP	C5'-C5-C4	2.49	125.66	121.47
1	B	205	LLP	OP2-P-OP1	2.50	118.62	110.58
1	A	205	LLP	C5-C4-C4'	2.52	125.14	121.52
1	D	205	LLP	C5-C4-C4'	2.87	125.64	121.52
1	D	205	LLP	C5'-C5-C4	3.09	126.66	121.47
1	B	205	LLP	C5-C4-C4'	3.35	126.33	121.52
1	A	205	LLP	OP4-C5'-C5	4.46	116.37	108.99
1	B	205	LLP	OP4-C5'-C5	4.70	116.75	108.99
1	D	205	LLP	OP4-C5'-C5	5.40	117.92	108.99
1	C	205	LLP	OP4-C5'-C5	5.43	117.97	108.99



There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	205	LLP	1	0
1	B	205	LLP	1	0
1	C	205	LLP	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

9 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	GOL	A	401	-	5,5,5	0.35	0	5,5,5	0.53	0
2	GOL	A	402	-	5,5,5	0.68	0	5,5,5	0.81	0
2	GOL	A	403	-	5,5,5	0.41	0	5,5,5	0.35	0
2	GOL	B	401	-	5,5,5	0.35	0	5,5,5	0.40	0
2	GOL	B	402	-	5,5,5	0.62	0	5,5,5	0.77	0
3	SO4	C	401	-	4,4,4	0.51	0	6,6,6	0.77	0
2	GOL	C	402	-	5,5,5	0.40	0	5,5,5	0.44	0
2	GOL	C	403	-	5,5,5	0.47	0	5,5,5	0.66	0
2	GOL	C	404	-	5,5,5	0.34	0	5,5,5	0.29	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	GOL	A	401	-	-	0/4/4/4	0/0/0/0
2	GOL	A	402	-	-	0/4/4/4	0/0/0/0
2	GOL	A	403	-	-	0/4/4/4	0/0/0/0
2	GOL	B	401	-	-	0/4/4/4	0/0/0/0
2	GOL	B	402	-	-	0/4/4/4	0/0/0/0
3	SO4	C	401	-	-	0/0/0/0	0/0/0/0
2	GOL	C	402	-	-	0/4/4/4	0/0/0/0
2	GOL	C	403	-	-	0/4/4/4	0/0/0/0
2	GOL	C	404	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	402	GOL	1	0
3	C	401	SO4	1	0
2	C	403	GOL	6	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	378/404 (93%)	-0.02	6 (1%) 74 69	17, 30, 55, 73	0
1	B	378/404 (93%)	-0.30	5 (1%) 79 75	13, 23, 44, 56	0
1	C	382/404 (94%)	-0.21	6 (1%) 74 69	14, 25, 47, 73	0
1	D	380/404 (94%)	-0.18	6 (1%) 74 69	12, 23, 49, 84	0
All	All	1518/1616 (93%)	-0.18	23 (1%) 76 71	12, 25, 49, 84	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	388	ALA	4.7
1	D	387	ALA	4.3
1	D	347	ALA	3.3
1	D	346	ASP	3.2
1	C	346	ASP	3.1
1	A	261	GLU	3.1
1	D	385	ALA	2.8
1	A	140	SER	2.7
1	A	386	LEU	2.6
1	A	387	ALA	2.6
1	C	347	ALA	2.6
1	B	386	LEU	2.4
1	A	125	ALA	2.4
1	B	261	GLU	2.4
1	C	328	ALA	2.4
1	A	346	ASP	2.4
1	C	348	ALA	2.3
1	D	389	ALA	2.2
1	B	0	GLY	2.1
1	B	265	ALA	2.1
1	B	365	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	327	SER	2.1
1	C	349	SER	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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
1	LLP	A	205	24/25	0.95	0.15	-	25,27,28,29	0
1	LLP	D	205	24/25	0.97	0.11	-	18,21,22,23	0
1	LLP	B	205	24/25	0.96	0.12	-	18,22,25,29	0
1	LLP	C	205	24/25	0.96	0.11	-	18,21,26,27	0

## 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
2	GOL	B	402	6/6	0.82	0.26	6.41	49,58,60,67	0
2	GOL	C	403	6/6	0.90	0.19	5.56	34,40,42,45	0
2	GOL	A	402	6/6	0.87	0.30	2.35	41,54,57,59	0
2	GOL	A	403	6/6	0.85	0.27	1.84	39,43,48,48	0
3	SO4	C	401	5/5	0.97	0.13	-	45,46,55,56	0
2	GOL	C	404	6/6	0.74	0.24	-	49,53,56,56	0
2	GOL	C	402	6/6	0.81	0.28	-	55,61,64,66	0
2	GOL	A	401	6/6	0.86	0.25	-	38,47,51,52	0
2	GOL	B	401	6/6	0.86	0.21	-	39,57,61,68	0

## 6.5 Other polymers

There are no such residues in this entry.