



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:51 PM UTC

PDB ID : 4ISY / pdb_00004isy
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

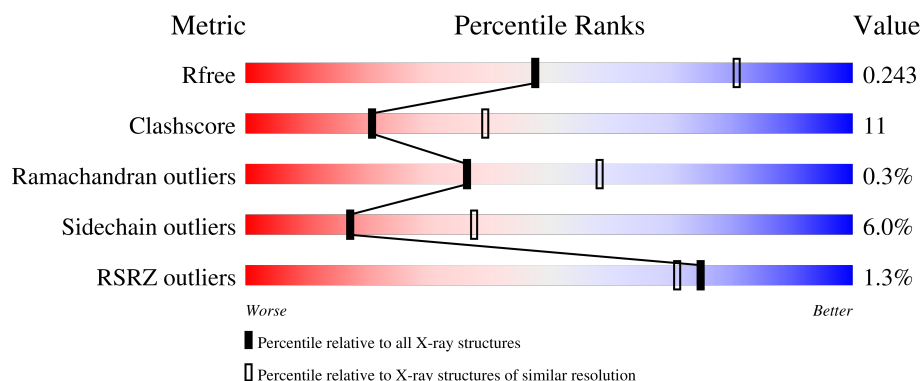
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	404	 2% 71% 22% • 6%
1	B	404	 73% 18% • 6%
1	C	404	 % 72% 20% • 5%
1	D	404	 2% 75% 17% • 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	C	403	-	-	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

Continued on next page...

Continued from previous page...

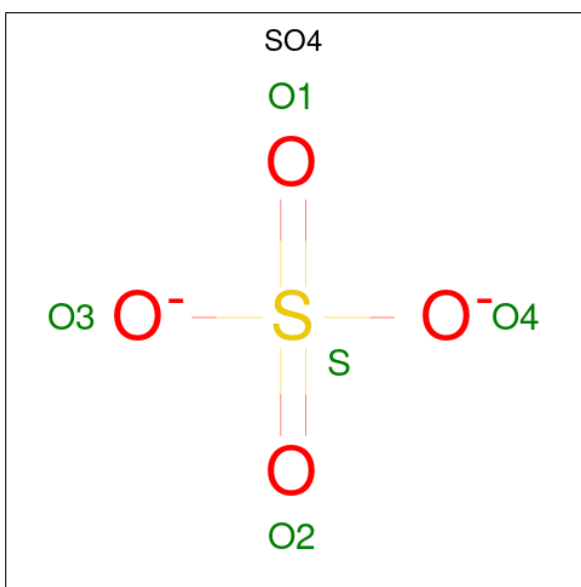
Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	HIS	-	expression tag	UNP O53272
B	0	GLY	-	expression tag	UNP O53272
B	1	SER	-	expression tag	UNP O53272
C	-10	MET	-	expression tag	UNP O53272
C	-9	ARG	-	expression tag	UNP O53272
C	-8	GLY	-	expression tag	UNP O53272
C	-7	SER	-	expression tag	UNP O53272
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 (CCD ID: GOL) (formula: $C_3H_8O_3$).



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		
2	C	1	Total	C	O	0	0
			6	3	3		

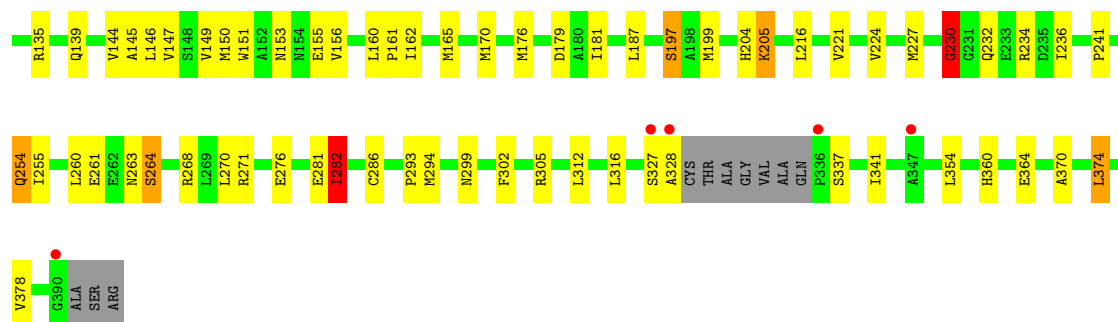
- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



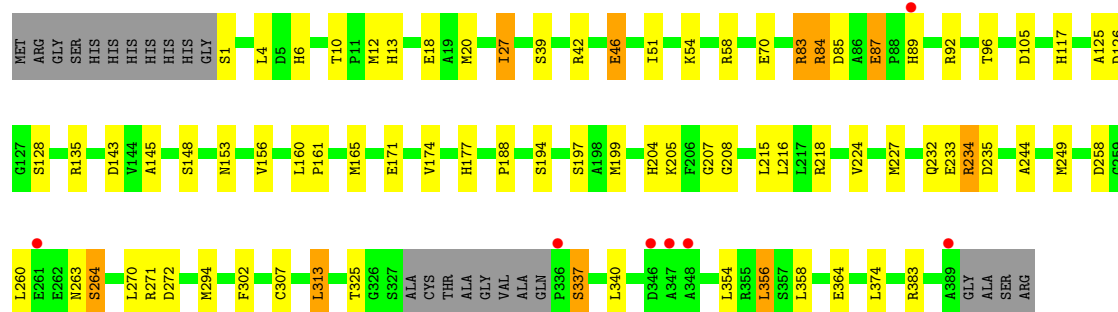
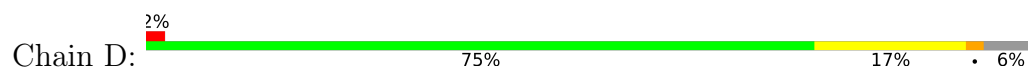
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	O	S	0	0
			5	4	1		

- 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		



• Molecule 1: Cysteine desulfurase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	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) 97.9 (45.22-2.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	29.3	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 23.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11532	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	1.09	8/2814 (0.3%)	1.20	10/3822 (0.3%)
1	B	1.17	5/2813 (0.2%)	1.25	10/3820 (0.3%)
1	C	1.15	5/2833 (0.2%)	1.20	6/3848 (0.2%)
1	D	1.17	5/2824 (0.2%)	1.18	10/3836 (0.3%)
All	All	1.15	23/11284 (0.2%)	1.21	36/15326 (0.2%)

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 (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	204	HIS	CG-ND1	-8.03	1.29	1.38
1	D	194	SER	C-O	-7.68	1.14	1.24
1	A	204	HIS	CG-ND1	-7.06	1.30	1.38
1	D	204	HIS	CD2-NE2	-6.93	1.30	1.37
1	C	204	HIS	CD2-NE2	-6.79	1.30	1.37
1	D	204	HIS	CG-ND1	-6.48	1.31	1.38
1	B	228	HIS	CG-CD2	6.03	1.42	1.35
1	A	204	HIS	CD2-NE2	-5.95	1.31	1.37
1	B	204	HIS	CG-ND1	-5.89	1.31	1.38
1	B	89	HIS	CG-CD2	5.79	1.42	1.35
1	B	204	HIS	CD2-NE2	-5.55	1.31	1.37
1	A	13	HIS	ND1-CE1	5.35	1.37	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	228	HIS	CE1-NE2	5.26	1.37	1.32
1	A	228	HIS	CE1-NE2	5.18	1.37	1.32
1	D	215	LEU	N-CA	-5.15	1.40	1.46
1	C	89	HIS	CG-CD2	5.14	1.41	1.35
1	A	13	HIS	CG-CD2	5.11	1.41	1.35
1	C	282	ILE	C-O	-5.10	1.18	1.24
1	A	117	HIS	CG-CD2	5.09	1.41	1.35
1	D	89	HIS	CG-CD2	5.07	1.41	1.35
1	C	187	LEU	C-O	-5.05	1.19	1.24
1	A	379	ALA	N-CA	5.03	1.52	1.46
1	A	161	PRO	CA-C	5.02	1.57	1.52

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	209	PRO	CA-C-N	-9.52	111.10	120.52
1	A	209	PRO	C-N-CA	-9.52	111.10	120.52
1	C	108	ASN	N-CA-C	8.09	121.12	111.33
1	D	208	GLY	CA-C-N	7.54	125.17	119.66
1	D	208	GLY	C-N-CA	7.54	125.17	119.66
1	A	27	ILE	CB-CA-C	-6.83	101.35	110.98
1	A	228	HIS	CA-C-N	6.63	133.63	121.70
1	A	228	HIS	C-N-CA	6.63	133.63	121.70
1	B	126	ASP	N-CA-C	6.59	120.19	111.75
1	C	27	ILE	CB-CA-C	-6.48	101.17	110.83
1	C	31	SER	N-CA-C	-6.47	105.42	113.38
1	B	160	LEU	CA-C-N	-6.22	112.06	119.84
1	B	160	LEU	C-N-CA	-6.22	112.06	119.84
1	B	93	ILE	CB-CA-C	-6.20	102.41	110.84
1	B	209	PRO	CA-C-N	-6.19	114.39	120.52
1	B	209	PRO	C-N-CA	-6.19	114.39	120.52
1	A	353	SER	N-CA-C	6.03	119.88	110.17
1	B	325	THR	CB-CA-C	-5.99	99.18	110.67
1	D	125	ALA	CA-C-N	5.91	128.79	120.28
1	D	125	ALA	C-N-CA	5.91	128.79	120.28
1	A	299	ASN	N-CA-C	5.85	118.50	109.07
1	C	197	SER	N-CA-C	-5.64	105.12	112.23
1	B	228	HIS	CA-C-N	5.44	131.50	121.70
1	B	228	HIS	C-N-CA	5.44	131.50	121.70
1	B	353	SER	N-CA-C	5.40	118.61	109.76
1	D	87	GLU	CA-C-N	5.31	125.03	119.82
1	D	87	GLU	C-N-CA	5.31	125.03	119.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	83	ARG	N-CA-C	5.30	116.86	111.14
1	C	236	ILE	N-CA-C	-5.26	107.70	112.96
1	D	174	VAL	CA-C-N	-5.26	114.54	119.85
1	D	174	VAL	C-N-CA	-5.26	114.54	119.85
1	A	173	GLY	CA-C-N	-5.14	118.86	123.33
1	A	173	GLY	C-N-CA	-5.14	118.86	123.33
1	A	168	VAL	CB-CA-C	-5.05	105.25	112.22
1	D	337	SER	N-CA-C	5.05	117.48	109.96
1	D	224	VAL	N-CA-C	-5.03	104.30	108.63

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	2756	70	0
1	B	2794	0	2754	70	0
1	C	2814	0	2774	66	0
1	D	2805	0	2766	50	0
2	A	18	0	24	1	0
2	B	12	0	16	0	0
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	11114	249	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 11.

All (249) 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:HE1	1.21	1.17
1:B:99:GLU:HA	1:B:150:MET:CE	1.77	1.15
1:B:99:GLU:HA	1:B:150:MET:HE2	1.16	1.12
1:A:348:ALA:HA	1:A:351:ARG:HH21	0.99	1.10
1:C:99:GLU:HA	1:C:150:MET:HE2	1.33	1.04
1:B:161:PRO:HD2	1:B:165:MET:HE2	1.40	1.03
1:A:29:ASN:HD22	1:A:31:SER:H	1.06	1.00
1:A:98:VAL:O	1:A:150:MET:HE1	1.63	0.98
1:C:99:GLU:CA	1:C:150:MET:HE1	1.93	0.98
1:C:99:GLU:CA	1:C:150:MET:CE	2.41	0.97
1:B:98:VAL:O	1:B:150:MET:HE1	1.65	0.97
1:A:98:VAL:C	1:A:150:MET:HE1	1.90	0.95
1:A:99:GLU:HA	1:A:150:MET:CE	1.96	0.94
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:D:84:ARG:HG2	1:D:84:ARG:HH11	1.33	0.92
1:A:29:ASN:ND2	1:A:31:SER:H	1.70	0.89
1:A:99:GLU:HA	1:A:150:MET:HE1	1.52	0.89
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: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: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:A:99:GLU:CA	1:A:150:MET:HE1	2.14	0.78
1:A:83:ARG:CD	1:A:145:ALA:O	2.32	0.77
1:B:99:GLU:CA	1:B:150:MET:CE	2.60	0.77
1:C:98:VAL:O	1:C:150:MET:HE1	1.84	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:227:MET:HE2	1:D:70:GLU:HG3	1.76	0.67
1:A:99:GLU:HA	1:A:150:MET:HE2	1.75	0.67
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: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:A:166:SER:OG	1:A:195:GLY:HA3	1.96	0.65
1:B:81:TRP:HE1	1:B:114:GLU:HG2	1.60	0.65
1:C:281:GLU:C	1:C:282:ILE:HG12	2.21	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:B:91:ARG:HG3	1:B:91:ARG:HH11	1.63	0.64
1:C:83:ARG:HH11	2:C:403:GOL:C1	2.09	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:99:GLU:N	1:A:150:MET:HE1	2.12	0.63
1:B:12:MET:HE1	1:B:20:MET:CE	2.28	0.62
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: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
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:NZ	1:B:205:LLP:O3	2.30	0.60
1:B:12:MET:HE1	1:B:20:MET:HE1	1.84	0.59
1:A:154:ASN:H	1:A:154:ASN:HD22	1.50	0.59
1:B:126:ASP:HB3	1:B:128:SER:HB3	1.85	0.59
1:D:199:MET:HE2	1:D:216:LEU:HD12	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:98:VAL:HG23	1:A:150:MET:HE3	1.84	0.59
1:B:98:VAL:C	1:B:150:MET:CE	2.76	0.59
1:B:183:ALA:HB1	1:B:187:LEU:HD22	1.85	0.58
1:A:29:ASN:HD22	1:A:29:ASN:C	2.12	0.58
1:C:88:PRO:O	1:C:91:ARG:HD2	2.02	0.58
1:B:161:PRO:HD2	1:B:165:MET:CE	2.25	0.57
1:B:179:ASP:OD1	1:B:181:ILE:HD12	2.04	0.57
1:C:89:HIS:NE2	1:D:58:ARG:NH1	2.53	0.57
1:D:4:LEU:HD23	1:D:358:LEU:HD21	1.87	0.57
1:B:126:ASP:HB3	1:B:128:SER:H	1.68	0.57
1:D:313:LEU:HD13	1:D:325:THR:HG23	1.85	0.57
1:C:98:VAL:C	1:C:150:MET:HE1	2.30	0.57
1:B:187:LEU:C	1:B:187:LEU:HD23	2.29	0.57
1:B:150:MET:O	1:B:160:LEU:HD23	2.05	0.57
1:A:98:VAL:O	1:A:150:MET:CE	2.48	0.56
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:C:199:MET:HE2	1:C:216:LEU:HD22	1.88	0.56
1:A:153:ASN:ND2	1:A:156:VAL:H	1.99	0.56
1:A:98:VAL:C	1:A:150:MET:CE	2.73	0.55
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:B:98:VAL:C	1:B:150:MET:HE1	2.32	0.55
1:D:260:LEU:O	1:D:264:SER:HB2	2.07	0.54
1:B:229:GLY:CA	4:D:454:HOH:O	2.55	0.54
1:B:314:MET:SD	1:C:170:MET:HE1	2.48	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:D:84:ARG:NH1	1:D:85:ASP:OD1	2.41	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: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:A:273:ARG:NH2	1:A:368:ASP:OD1	2.33	0.53
1:C:160:LEU:N	1:C:160:LEU:HD12	2.24	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:161:PRO:HG2	1:D:165:MET:HE3	1.91	0.52
1:A:230:GLY:HA3	2:A:402:GOL:H31	1.91	0.52
1:B:58:ARG:HH22	1:B:219:ARG:HD2	1.74	0.52
1:B:167:VAL:HA	1:B:170:MET:HE3	1.90	0.52
1:D:83:ARG:CD	1:D:145:ALA:O	2.56	0.52
1:B:20:MET:HG3	1:B:244:ALA:HB1	1.91	0.52
1:C:293:PRO:O	1:C:294:MET:HE2	2.10	0.52
1:B:176:MET:HE2	1:B:196:LEU:HD21	1.92	0.51
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:A:126:ASP:HB3	1:A:128:SER:H	1.76	0.51
1:B:23:VAL:HG11	1:B:243:VAL:HG12	1.93	0.51
1:B:288:ASN:ND2	1:B:301:HIS:ND1	2.60	0.50
1:C:83:ARG:HD2	2:C:403:GOL:H12	1.93	0.50
1:C:96:THR:HG21	1:C:149:VAL:HG13	1.93	0.50
1:C:270:LEU:CD2	1:C:364:GLU:OE1	2.57	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: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:ND2	1:A:154:ASN:N	2.53	0.49
1:D:54:LYS:NZ	1:D:258:ASP:OD1	2.42	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:A:231:GLY:HA3	1:A:235:ASP:HA	1.95	0.49
1:A:42:ARG:O	1:A:46:GLU:HG3	2.13	0.48
1:C:327:SER:HB2	1:C:328:ALA:HB2	1.95	0.48
1:A:3:TYR:C	1:A:4:LEU:HD12	2.39	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:B:3:TYR:C	1:B:4:LEU:HD12	2.38	0.48
1:D:271:ARG:NH1	1:D:272:ASP:OD1	2.45	0.47
1:C:197:SER:HB3	1:C:221:VAL:HG21	1.96	0.47
1:D:92:ARG:NH1	1:D:143:ASP:OD2	2.47	0.47
1:D:233:GLU:O	1:D:235:ASP:N	2.48	0.47
1:B:46:GLU:CD	4:B:539:HOH:O	2.58	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:370:ALA:O	1:B:374:LEU:HB2	2.15	0.47
1:C:99:GLU:CD	1:C:150:MET:HE2	2.40	0.47
1:A:92:ARG:NH1	1:A:143:ASP:OD2	2.48	0.47
1:D:84:ARG:HG2	1:D:84:ARG:NH1	2.12	0.47
1:C:98:VAL:HG23	1:C:150:MET:HE3	1.97	0.47
1:C:135:ARG:HE	1:C:139:GLN:NE2	2.13	0.47
1:C:270:LEU:HD23	1:C:270:LEU:HA	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:A:99:GLU:CA	1:A:150:MET:CE	2.78	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:D:294:MET:HE2	1:D:294:MET:HA	1.97	0.46
1:C:126:ASP:HB3	1:C:128:SER:HB3	1.98	0.46
1:C:98:VAL:O	1:C:150:MET:CE	2.61	0.46
1:A:199:MET:HE2	1:A:216:LEU:HD12	1.97	0.45
1:C:98:VAL:C	1:C:150:MET:CE	2.89	0.45
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:B:121:LEU:HA	1:B:122:PRO:HD3	1.87	0.45
1:D:313:LEU:HD12	1:D:325:THR:HG23	1.94	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:A:197:SER:HB3	1:A:221:VAL:HG21	1.98	0.45
1:C:83:ARG:NH1	2:C:403:GOL:C1	2.80	0.45
1:A:259:GLY:O	1:A:260:LEU:C	2.58	0.45
1:A:104:LEU:HD11	1:A:338:HIS:CD2	2.52	0.44
1:D:51:ILE:HD13	1:D:249:MET:HE3	2.00	0.44
1:B:99:GLU:CA	1:B:150:MET:HE1	2.43	0.44
1:C:104:LEU:HA	1:C:104:LEU:HD23	1.62	0.44
1:D:4:LEU:HD23	1:D:358:LEU:CD2	2.48	0.44
1:D:313:LEU:HD12	1:D:325:THR:CG2	2.47	0.44
1:A:301:HIS:HE1	1:A:340:LEU:HD11	1.83	0.44
1:D:233:GLU:C	1:D:235:ASP:H	2.25	0.44
1:A:277:GLY:O	1:A:281:GLU:HG2	2.17	0.44
1:D:96:THR:HB	4:D:440:HOH:O	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:153:ASN:HD22	1:B:156:VAL:HG22	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:151:TRP:CE3	1:C:162:ILE:HG21	2.53	0.43
1:C:316:LEU:HD21	1:C:374:LEU:HD13	2.00	0.43
2:C:403:GOL:H2	4:C:540:HOH:O	2.18	0.43
1:D:148:SER:HA	1:D:177:HIS:O	2.18	0.43
1:B:98:VAL:C	1:B:150:MET:HE3	2.44	0.43
1:A:29:ASN:ND2	1:A:29:ASN:C	2.76	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:C:50:LEU:HD12	1:C:50:LEU:HA	1.80	0.43
1:D:233:GLU:C	1:D:235:ASP:N	2.74	0.43
1:A:264:SER:HB3	1:A:268:ARG:HH12	1.84	0.42
1:B:197:SER:HB3	1:B:221:VAL:HG21	2.01	0.42
1:A:99:GLU:CD	1:A:150:MET:HE2	2.44	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:B:187:LEU:HD23	1:B:187:LEU:O	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:A:313:LEU:HD23	1:A:314:MET:HE2	2.01	0.42
1:B:176:MET:HE2	1:B:196:LEU:CD2	2.50	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:B:98:VAL:HG23	1:B:150:MET:HE3	2.02	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:90:ARG:NH1	1:C:90:ARG:HG2	2.35	0.41
1:C:374:LEU:HD12	1:C:378:VAL:HG23	2.03	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:227:MET:HE2	1:D:70:GLU:HA	2.04	0.40
1:B:282:ILE:HD12	1:B:374:LEU:HD13	2.03	0.40
1:D:20:MET:HG2	1:D:244:ALA:O	2.20	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:270:LEU:HD21	1:D:364:GLU:OE1	2.21	0.40
1:B:29:ASN:HB3	1:B:32:SER:OG	2.22	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

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%)	24	46
1	D	376/404 (93%)	362 (96%)	12 (3%)	2 (0%)	24	46
All	All	1502/1616 (93%)	1445 (96%)	53 (4%)	4 (0%)	36	58

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%)	267 (94%)	16 (6%)	18	40
1	B	283/298 (95%)	262 (93%)	21 (7%)	13	29
1	C	283/298 (95%)	267 (94%)	16 (6%)	18	40
1	D	283/298 (95%)	268 (95%)	15 (5%)	20	43
All	All	1132/1192 (95%)	1064 (94%)	68 (6%)	17	37

All (68) 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	51	ILE
1	A	146	LEU
1	A	154	ASN
1	A	170	MET
1	A	254	GLN
1	A	271	ARG
1	A	276	GLU
1	A	282	ILE
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	33	LEU
1	B	39	SER
1	B	46	GLU
1	B	51	ILE
1	B	126	ASP
1	B	128	SER
1	B	146	LEU
1	B	160	LEU
1	B	187	LEU
1	B	227	MET
1	B	276	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	288	ASN
1	B	305	ARG
1	B	307	CYS
1	B	354	LEU
1	B	373	VAL
1	B	374	LEU
1	B	386	LEU
1	C	9	THR
1	C	27	ILE
1	C	58	ARG
1	C	108	ASN
1	C	118	VAL
1	C	146	LEU
1	C	224	VAL
1	C	227	MET
1	C	254	GLN
1	C	261	GLU
1	C	263	ASN
1	C	264	SER
1	C	276	GLU
1	C	282	ILE
1	C	354	LEU
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	46	GLU
1	D	83	ARG
1	D	84	ARG
1	D	87	GLU
1	D	160	LEU
1	D	227	MET
1	D	264	SER
1	D	313	LEU
1	D	356	LEU
1	D	374	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	117	HIS
1	A	141	HIS
1	A	153	ASN
1	A	154	ASN
1	A	186	GLN
1	A	228	HIS
1	A	263	ASN
1	A	301	HIS
1	A	319	ASN
1	A	360	HIS
1	B	6	HIS
1	B	108	ASN
1	B	117	HIS
1	B	153	ASN
1	B	263	ASN
1	B	288	ASN
1	C	139	GLN
1	C	153	ASN
1	C	186	GLN
1	C	254	GLN
1	C	360	HIS
1	D	6	HIS
1	D	13	HIS
1	D	153	ASN
1	D	177	HIS
1	D	186	GLN
1	D	263	ASN

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	3.41	11 (47%)	25,32,34	2.03	9 (36%)
1	LLP	C	205	1	23,24,25	3.67	12 (52%)	25,32,34	1.92	6 (24%)
1	LLP	B	205	1	23,24,25	3.46	11 (47%)	25,32,34	2.34	8 (32%)
1	LLP	D	205	1	23,24,25	3.65	11 (47%)	25,32,34	2.17	6 (24%)

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	-	7/16/17/19	0/1/1/1
1	LLP	C	205	1	-	7/16/17/19	0/1/1/1
1	LLP	B	205	1	-	5/16/17/19	0/1/1/1
1	LLP	D	205	1	-	7/16/17/19	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	C2'-C2	-9.18	1.35	1.50
1	A	205	LLP	C2'-C2	-8.16	1.37	1.50
1	D	205	LLP	C2'-C2	-8.02	1.37	1.50
1	B	205	LLP	C2'-C2	-7.68	1.38	1.50
1	B	205	LLP	P-OP4	-6.38	1.40	1.60
1	C	205	LLP	C4-C4'	-6.30	1.33	1.46
1	A	205	LLP	P-OP1	-6.11	1.31	1.50
1	D	205	LLP	P-OP3	-6.09	1.32	1.54
1	B	205	LLP	C4'-NZ	5.74	1.46	1.27
1	A	205	LLP	C4'-NZ	5.70	1.46	1.27
1	D	205	LLP	P-OP2	-5.52	1.34	1.54
1	D	205	LLP	C4'-NZ	5.47	1.45	1.27
1	D	205	LLP	P-OP1	-5.22	1.34	1.50
1	A	205	LLP	P-OP2	-5.18	1.35	1.54
1	C	205	LLP	P-OP3	-5.10	1.35	1.54
1	C	205	LLP	C4'-NZ	5.09	1.44	1.27
1	D	205	LLP	C5'-C5	-5.04	1.37	1.50
1	C	205	LLP	C3-C2	-5.00	1.35	1.41
1	A	205	LLP	C4-C4'	-4.84	1.36	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	205	LLP	C4-C4'	-4.79	1.36	1.46
1	D	205	LLP	C3-C2	-4.74	1.36	1.41
1	D	205	LLP	P-OP4	-4.67	1.45	1.60
1	A	205	LLP	P-OP3	-4.64	1.37	1.54
1	B	205	LLP	P-OP2	-4.63	1.37	1.54
1	C	205	LLP	P-OP2	-4.60	1.37	1.54
1	B	205	LLP	C5'-C5	-4.48	1.39	1.50
1	D	205	LLP	C4-C4'	-4.42	1.37	1.46
1	C	205	LLP	C5'-C5	-4.41	1.39	1.50
1	C	205	LLP	P-OP1	-4.30	1.37	1.50
1	B	205	LLP	P-OP3	-4.26	1.39	1.54
1	A	205	LLP	C5'-C5	-4.06	1.40	1.50
1	B	205	LLP	P-OP1	-4.04	1.37	1.50
1	C	205	LLP	P-OP4	-3.91	1.48	1.60
1	B	205	LLP	C3-C2	-3.68	1.37	1.41
1	C	205	LLP	C4-C5	-3.67	1.36	1.42
1	A	205	LLP	C3-C2	-3.44	1.37	1.41
1	B	205	LLP	C4-C3	-3.31	1.35	1.41
1	A	205	LLP	P-OP4	-2.88	1.51	1.60
1	C	205	LLP	C4-C3	-2.79	1.36	1.41
1	A	205	LLP	CB-CA	-2.56	1.49	1.53
1	D	205	LLP	CB-CA	-2.53	1.49	1.53
1	A	205	LLP	C4-C3	-2.39	1.37	1.41
1	C	205	LLP	O3-C3	-2.37	1.31	1.36
1	B	205	LLP	C4-C5	-2.34	1.38	1.42
1	D	205	LLP	CA-N	-2.13	1.42	1.48

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	205	LLP	C4-C3-C2	7.83	124.55	120.14
1	D	205	LLP	C4-C3-C2	6.92	124.04	120.14
1	C	205	LLP	C4-C3-C2	4.99	122.95	120.14
1	C	205	LLP	OP4-C5'-C5	4.60	117.97	109.36
1	D	205	LLP	OP4-C5'-C5	4.57	117.92	109.36
1	A	205	LLP	C4-C3-C2	4.37	122.60	120.14
1	A	205	LLP	OP4-P-OP1	-4.36	94.66	106.44
1	B	205	LLP	OP4-C5'-C5	3.95	116.75	109.36
1	A	205	LLP	C2'-C2-C3	-3.76	116.39	120.80
1	A	205	LLP	OP4-C5'-C5	3.74	116.37	109.36
1	B	205	LLP	C4-C4'-NZ	-3.24	109.09	124.04
1	B	205	LLP	C5-C4-C4'	3.15	126.33	121.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	205	LLP	C4-C4'-NZ	-3.10	109.74	124.04
1	C	205	LLP	C4-C4'-NZ	-3.08	109.82	124.04
1	A	205	LLP	C2'-C2-N1	3.00	123.30	117.64
1	A	205	LLP	C4-C4'-NZ	-2.87	110.79	124.04
1	D	205	LLP	OP4-P-OP1	-2.78	98.92	106.44
1	C	205	LLP	CE-NZ-C4'	-2.73	109.98	118.72
1	D	205	LLP	C5-C4-C4'	2.70	125.64	121.47
1	B	205	LLP	C3-C4-C4'	-2.45	115.98	120.40
1	A	205	LLP	C5-C4-C4'	2.38	125.14	121.47
1	B	205	LLP	OP2-P-OP4	-2.32	100.62	106.67
1	A	205	LLP	OP3-P-OP2	2.26	116.29	107.80
1	B	205	LLP	C2'-C2-N1	2.26	121.89	117.64
1	D	205	LLP	C3-C2-N1	-2.24	118.14	120.96
1	A	205	LLP	C3-C4-C4'	-2.14	116.54	120.40
1	B	205	LLP	OP4-P-OP1	-2.13	100.69	106.44
1	C	205	LLP	OP3-P-OP2	2.05	115.48	107.80
1	C	205	LLP	C3-C2-N1	-2.03	118.40	120.96

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	205	LLP	CG-CD-CE-NZ
1	B	205	LLP	C-CA-CB-CG
1	C	205	LLP	C4-C4'-NZ-CE
1	D	205	LLP	N-CA-CB-CG
1	D	205	LLP	C-CA-CB-CG
1	A	205	LLP	C4-C4'-NZ-CE
1	D	205	LLP	C4-C4'-NZ-CE
1	C	205	LLP	CG-CD-CE-NZ
1	D	205	LLP	CA-CB-CG-CD
1	D	205	LLP	C3-C4-C4'-NZ
1	C	205	LLP	CA-CB-CG-CD
1	B	205	LLP	C4-C4'-NZ-CE
1	A	205	LLP	C5'-OP4-P-OP2
1	A	205	LLP	CA-CB-CG-CD
1	B	205	LLP	C4-C5-C5'-OP4
1	D	205	LLP	CD-CE-NZ-C4'
1	B	205	LLP	N-CA-CB-CG
1	C	205	LLP	CD-CE-NZ-C4'
1	B	205	LLP	C3-C4-C4'-NZ
1	D	205	LLP	C5-C4-C4'-NZ

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	A	205	LLP	CD-CE-NZ-C4'
1	A	205	LLP	C3-C4-C4'-NZ
1	C	205	LLP	C5'-OP4-P-OP1
1	A	205	LLP	C4-C5-C5'-OP4
1	C	205	LLP	C3-C4-C4'-NZ
1	C	205	LLP	N-CA-CB-CG

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	C	205	LLP	2	0
1	B	205	LLP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	B	401	-	5,5,5	0.40	0	5,5,5	0.44	0
3	SO4	C	401	-	4,4,4	0.53	0	6,6,6	0.73	0
2	GOL	A	401	-	5,5,5	0.37	0	5,5,5	0.64	0
2	GOL	C	404	-	5,5,5	0.39	0	5,5,5	0.37	0
2	GOL	A	402	-	5,5,5	0.75	0	5,5,5	0.83	0
2	GOL	A	403	-	5,5,5	0.47	0	5,5,5	0.42	0
2	GOL	C	403	-	5,5,5	0.53	0	5,5,5	0.71	0
2	GOL	B	402	-	5,5,5	0.70	0	5,5,5	0.84	0
2	GOL	C	402	-	5,5,5	0.47	0	5,5,5	0.47	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	B	401	-	-	2/4/4/4	-
2	GOL	A	401	-	-	1/4/4/4	-
2	GOL	C	404	-	-	2/4/4/4	-
2	GOL	A	402	-	-	4/4/4/4	-
2	GOL	A	403	-	-	2/4/4/4	-
2	GOL	C	403	-	-	0/4/4/4	-
2	GOL	B	402	-	-	3/4/4/4	-
2	GOL	C	402	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	402	GOL	O1-C1-C2-C3
2	A	403	GOL	O1-C1-C2-O2
2	A	403	GOL	O1-C1-C2-C3
2	B	401	GOL	C1-C2-C3-O3
2	C	402	GOL	C1-C2-C3-O3
2	C	404	GOL	C1-C2-C3-O3
2	A	402	GOL	C1-C2-C3-O3
2	A	402	GOL	O1-C1-C2-O2
2	B	401	GOL	O2-C2-C3-O3
2	C	402	GOL	O2-C2-C3-O3
2	C	404	GOL	O2-C2-C3-O3
2	A	401	GOL	O2-C2-C3-O3
2	B	402	GOL	O1-C1-C2-O2
2	A	402	GOL	O2-C2-C3-O3
2	B	402	GOL	O1-C1-C2-C3
2	B	402	GOL	O2-C2-C3-O3

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	401	SO4	1	0
2	A	402	GOL	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	378/404 (93%)	0.15	7 (1%) 66 61	17, 30, 55, 73	0
1	B	378/404 (93%)	-0.19	1 (0%) 90 88	13, 23, 44, 56	0
1	C	382/404 (94%)	-0.11	5 (1%) 75 71	14, 25, 47, 73	0
1	D	380/404 (94%)	-0.17	7 (1%) 67 63	12, 23, 49, 84	0
All	All	1518/1616 (93%)	-0.08	20 (1%) 75 71	12, 25, 49, 84	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	387	ALA	5.0
1	C	328	ALA	4.9
1	A	336	PRO	3.5
1	A	327	SER	3.1
1	D	89	HIS	3.1
1	A	386	LEU	3.1
1	D	346	ASP	2.9
1	D	389	ALA	2.8
1	B	386	LEU	2.7
1	D	347	ALA	2.6
1	D	336	PRO	2.4
1	C	347	ALA	2.4
1	C	336	PRO	2.3
1	D	261	GLU	2.2
1	C	390	GLY	2.2
1	A	140	SER	2.2
1	A	139	GLN	2.1
1	D	348	ALA	2.1
1	C	327	SER	2.1
1	A	142	ASP	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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	LLP	A	205	24/25	0.92	0.11	25,27,28,29	0
1	LLP	B	205	24/25	0.93	0.10	18,22,25,29	0
1	LLP	C	205	24/25	0.93	0.10	18,21,26,27	0
1	LLP	D	205	24/25	0.95	0.09	18,21,22,23	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GOL	B	402	6/6	0.79	0.22	49,58,60,67	0
2	GOL	C	402	6/6	0.79	0.17	55,61,64,66	0
2	GOL	C	404	6/6	0.84	0.13	49,53,56,56	0
2	GOL	A	403	6/6	0.85	0.19	39,43,48,48	0
2	GOL	A	401	6/6	0.86	0.15	38,47,51,52	0
2	GOL	C	403	6/6	0.87	0.13	34,40,42,45	0
2	GOL	B	401	6/6	0.89	0.13	39,57,61,68	0
2	GOL	A	402	6/6	0.90	0.14	41,54,57,59	0
3	SO4	C	401	5/5	0.94	0.08	45,46,55,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.