



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 01:20 pm BST

PDB ID : 3QI6
Title : Crystal Structure of Cystathionine gamma-synthase MetB (Cgs) from Mycobacterium ulcerans Agy99
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2011-01-26
Resolution : 1.91 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

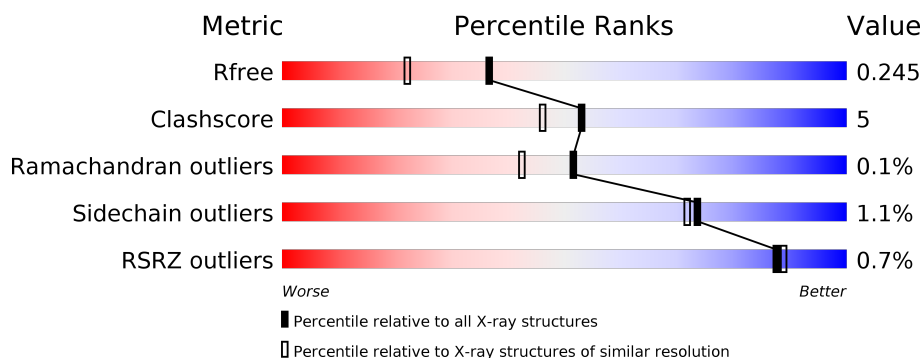
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.91 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}	130704	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RSRZ outliers	127900	7793 (1.94-1.90)

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 ≥ 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	392	
1	B	392	
1	C	392	
1	D	392	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12485 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 Cystathionine gamma-synthase MetB (Cgs).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	375	Total	C	N	O	P	S	0	6	0
			2754	1731	476	535	1	11			
1	B	374	Total	C	N	O	P	S	0	11	0
			2781	1753	481	535	1	11			
1	C	366	Total	C	N	O	P	S	0	8	0
			2700	1700	463	525	1	11			
1	D	373	Total	C	N	O	P	S	0	7	0
			2768	1742	486	528	1	11			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	EXPRESSION TAG	UNP A0PKT3
A	-2	PRO	-	EXPRESSION TAG	UNP A0PKT3
A	-1	GLY	-	EXPRESSION TAG	UNP A0PKT3
A	0	SER	-	EXPRESSION TAG	UNP A0PKT3
B	-3	GLY	-	EXPRESSION TAG	UNP A0PKT3
B	-2	PRO	-	EXPRESSION TAG	UNP A0PKT3
B	-1	GLY	-	EXPRESSION TAG	UNP A0PKT3
B	0	SER	-	EXPRESSION TAG	UNP A0PKT3
C	-3	GLY	-	EXPRESSION TAG	UNP A0PKT3
C	-2	PRO	-	EXPRESSION TAG	UNP A0PKT3
C	-1	GLY	-	EXPRESSION TAG	UNP A0PKT3
C	0	SER	-	EXPRESSION TAG	UNP A0PKT3
D	-3	GLY	-	EXPRESSION TAG	UNP A0PKT3
D	-2	PRO	-	EXPRESSION TAG	UNP A0PKT3
D	-1	GLY	-	EXPRESSION TAG	UNP A0PKT3
D	0	SER	-	EXPRESSION TAG	UNP A0PKT3

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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	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		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

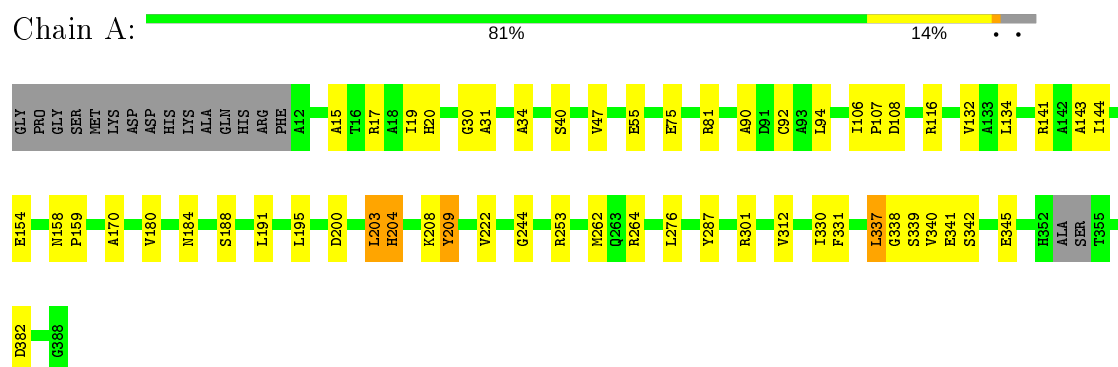
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	371	Total 371	O 371	0	0
6	B	382	Total 382	O 382	0	0
6	C	315	Total 315	O 315	0	0
6	D	372	Total 372	O 372	0	0

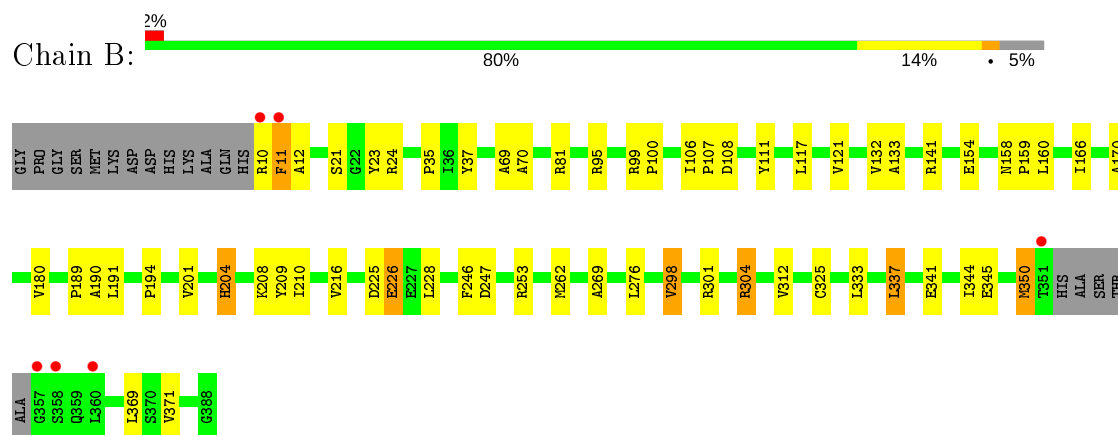
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

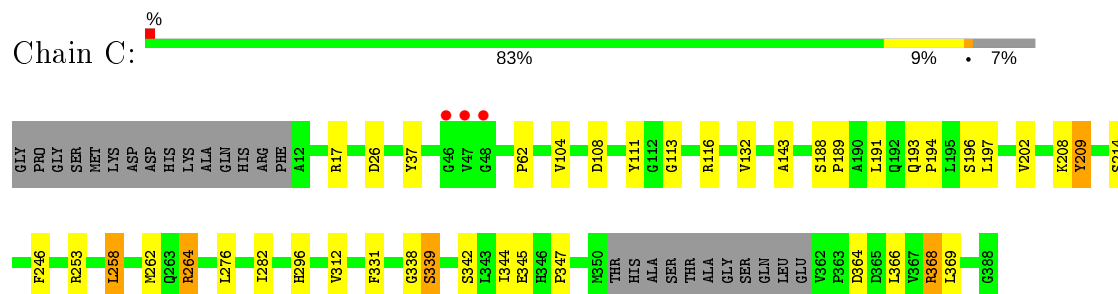
• Molecule 1: Cystathionine gamma-synthase MetB (Cgs)



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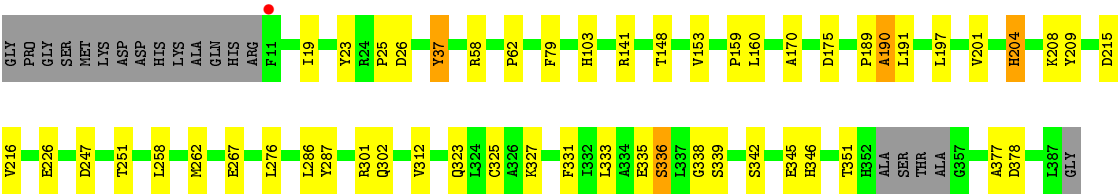
● Molecule 1: Cystathionine gamma-synthase MetB (Cgs)

Chain D:

82%

13%

5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.96Å 106.92Å 100.31Å 90.00° 113.67° 90.00°	Depositor
Resolution (Å)	44.47 – 1.91 44.47 – 1.91	Depositor EDS
% Data completeness (in resolution range)	97.9 (44.47-1.91) 97.2 (44.47-1.91)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.60 (at 1.91Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.200 , 0.241 0.206 , 0.245	Depositor DCC
R_{free} test set	5969 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	15.4	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 19.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.38$	Xtriage
Estimated twinning fraction	0.259 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12485	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.21 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.1079e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: GOL, SO4, LLP, EDO, NA

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	1.30	12/2799 (0.4%)	1.06	10/3821 (0.3%)
1	B	1.31	13/2838 (0.5%)	1.08	10/3871 (0.3%)
1	C	1.21	3/2751 (0.1%)	1.05	8/3755 (0.2%)
1	D	1.29	12/2813 (0.4%)	1.04	4/3835 (0.1%)
All	All	1.28	40/11201 (0.4%)	1.06	32/15282 (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	A	0	1
1	B	0	2
1	D	0	1
All	All	0	4

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	170	ALA	CA-CB	7.42	1.68	1.52
1	B	70	ALA	CA-CB	7.09	1.67	1.52
1	C	104	VAL	CB-CG2	7.03	1.67	1.52
1	B	154	GLU	CB-CG	-6.78	1.39	1.52
1	C	26	ASP	CB-CG	-6.50	1.38	1.51
1	A	90	ALA	CA-CB	6.47	1.66	1.52
1	D	23	TYR	CD1-CE1	-6.35	1.29	1.39
1	D	170	ALA	CA-CB	6.26	1.65	1.52
1	D	190	ALA	CA-CB	6.20	1.65	1.52
1	A	340	VAL	CB-CG2	6.18	1.65	1.52
1	D	287	TYR	CD2-CE2	6.17	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	154	GLU	CD-OE1	6.16	1.32	1.25
1	A	203	LEU	CG-CD2	6.08	1.74	1.51
1	A	34	ALA	CA-CB	6.01	1.65	1.52
1	B	210	ILE	C-O	-6.00	1.11	1.23
1	A	92	CYS	CB-SG	-5.87	1.72	1.81
1	B	371	VAL	CB-CG2	5.83	1.65	1.52
1	D	26	ASP	CB-CG	-5.82	1.39	1.51
1	B	216	VAL	CB-CG1	5.69	1.64	1.52
1	A	40	SER	CB-OG	5.52	1.49	1.42
1	B	69	ALA	CA-CB	5.49	1.64	1.52
1	B	201	VAL	CB-CG1	5.47	1.64	1.52
1	A	154	GLU	CB-CG	-5.45	1.41	1.52
1	C	209	TYR	CD1-CE1	5.39	1.47	1.39
1	A	209	TYR	CD1-CE1	-5.35	1.31	1.39
1	A	55	GLU	CG-CD	5.32	1.59	1.51
1	D	251	THR	C-O	5.26	1.33	1.23
1	D	23	TYR	CD2-CE2	-5.25	1.31	1.39
1	B	298	VAL	CB-CG2	5.23	1.63	1.52
1	A	81	ARG	CB-CG	-5.23	1.38	1.52
1	D	37	TYR	CD2-CE2	-5.22	1.31	1.39
1	A	287	TYR	CG-CD2	-5.21	1.32	1.39
1	D	287	TYR	CD1-CE1	5.20	1.47	1.39
1	B	180	VAL	CB-CG2	5.19	1.63	1.52
1	D	153	VAL	C-O	5.13	1.33	1.23
1	D	201	VAL	CB-CG1	5.13	1.63	1.52
1	B	23	TYR	CD2-CE2	-5.12	1.31	1.39
1	A	15	ALA	CA-CB	5.10	1.63	1.52
1	B	269	ALA	CA-CB	5.04	1.63	1.52
1	D	377	ALA	CA-CB	5.03	1.63	1.52

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	58	ARG	NE-CZ-NH2	10.38	125.49	120.30
1	A	108	ASP	CB-CG-OD1	8.63	126.06	118.30
1	B	108	ASP	CB-CG-OD1	7.44	125.00	118.30
1	A	108	ASP	CB-CG-OD2	-7.01	111.99	118.30
1	A	301	ARG	NE-CZ-NH2	-6.91	116.84	120.30
1	D	58	ARG	NE-CZ-NH1	-6.71	116.95	120.30
1	B	81	ARG	NE-CZ-NH2	-6.69	116.95	120.30
1	B	108	ASP	CB-CG-OD2	-6.65	112.31	118.30
1	B	95	ARG	NE-CZ-NH2	-6.64	116.98	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	201	VAL	CB-CA-C	-6.63	98.80	111.40
1	A	264	ARG	NE-CZ-NH1	6.29	123.45	120.30
1	C	368	ARG	NE-CZ-NH1	6.09	123.34	120.30
1	C	282	ILE	CG1-CB-CG2	-6.03	98.14	111.40
1	A	134	LEU	CB-CG-CD1	-6.01	100.78	111.00
1	A	17	ARG	NE-CZ-NH1	6.01	123.30	120.30
1	C	258	LEU	CB-CG-CD1	5.91	121.05	111.00
1	B	99	ARG	NE-CZ-NH1	5.83	123.21	120.30
1	D	215	ASP	CB-CG-OD2	-5.74	113.14	118.30
1	C	364	ASP	CB-CG-OD1	-5.70	113.17	118.30
1	B	304	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	C	253	ARG	NE-CZ-NH2	5.58	123.09	120.30
1	A	253	ARG	NE-CZ-NH2	5.57	123.09	120.30
1	C	116	ARG	NE-CZ-NH1	5.57	123.09	120.30
1	B	95	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	A	116	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	C	108	ASP	CB-CG-OD1	5.36	123.12	118.30
1	C	368	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	B	253	ARG	NE-CZ-NH1	-5.28	117.66	120.30
1	A	200	ASP	CB-CG-OD1	-5.26	113.57	118.30
1	A	94	LEU	CB-CG-CD2	-5.20	102.15	111.00
1	B	253	ARG	NE-CZ-NH2	5.15	122.88	120.30
1	D	175	ASP	CB-CG-OD1	5.07	122.86	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	204	HIS	Peptide
1	B	204	HIS	Peptide
1	B	350	MET	Peptide
1	D	204	HIS	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	2754	0	2690	27	0
1	B	2781	0	2732	37	0
1	C	2700	0	2640	25	0
1	D	2768	0	2727	35	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
2	C	5	0	0	0	0
3	A	1	0	0	0	0
4	A	6	0	8	0	0
4	B	6	0	8	0	0
5	D	4	0	6	1	0
6	A	371	0	0	1	0
6	B	382	0	0	5	0
6	C	315	0	0	2	0
6	D	372	0	0	3	0
All	All	12485	0	10811	118	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 5.

All (118) 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:197:LEU:HD12	1:C:197:LEU:N	1.88	0.88
1:D:160[B]:LEU:HD13	6:D:974:HOH:O	1.76	0.85
1:D:301[A]:ARG:HG3	1:D:301[A]:ARG:NH1	2.01	0.76
1:B:10:ARG:N	1:B:21:SER:HG	1.85	0.74
1:D:301[A]:ARG:HG3	1:D:301[A]:ARG:HH11	1.61	0.65
1:C:197:LEU:CD1	1:C:197:LEU:N	2.59	0.65
1:D:325:CYS:HB3	1:D:333:LEU:HD13	1.82	0.62
1:A:339:SER:OG	1:A:341:GLU:OE2	2.16	0.61
1:B:276:LEU:HD13	1:B:312:VAL:HG11	1.81	0.61
1:A:276:LEU:HD13	1:A:312:VAL:HG11	1.83	0.61
1:C:193:GLN:O	1:C:197:LEU:HD13	2.01	0.61
1:C:345:GLU:OE1	1:C:368:ARG:NH2	2.34	0.60
1:A:203:LEU:HD23	1:A:204:HIS:N	2.16	0.60
1:A:191:LEU:HD11	1:A:262[B]:MET:CG	2.32	0.59
1:B:111:TYR:CE1	6:B:1248:HOH:O	2.52	0.59
1:C:189:PRO:HD2	1:C:258:LEU:HD21	1.85	0.59
1:C:276:LEU:HD13	1:C:312:VAL:HG11	1.85	0.58
1:D:267:GLU:HG3	6:D:948:HOH:O	2.02	0.58
1:A:203:LEU:C	1:A:203:LEU:HD23	2.23	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:347:PRO:HG2	1:C:366:LEU:HD22	1.86	0.58
1:C:37:TYR:CD2	1:C:62:PRO:HB2	2.40	0.57
1:B:344:ILE:HG13	1:B:369:LEU:HD23	1.85	0.57
1:C:331:PHE:CD1	1:C:342:SER:HB3	2.40	0.57
1:D:216:VAL:HG23	1:D:247:ASP:HB3	1.85	0.57
1:D:258:LEU:O	1:D:262[B]:MET:HG2	2.05	0.57
1:D:325:CYS:HB3	1:D:333:LEU:CD1	2.35	0.57
1:A:19:ILE:HG22	1:A:20:HIS:CD2	2.40	0.56
1:C:17:ARG:CZ	6:C:1726:HOH:O	2.54	0.55
1:D:141[B]:ARG:HH21	1:D:141[B]:ARG:HB2	1.72	0.55
1:C:196:SER:C	1:C:197:LEU:HD12	2.27	0.54
1:B:24:ARG:NE	6:B:2011:HOH:O	2.33	0.54
1:B:141[B]:ARG:NH1	6:B:759:HOH:O	2.41	0.53
1:A:203:LEU:HD23	1:A:204:HIS:CA	2.39	0.53
1:B:12:ALA:HB3	1:D:378:ASP:OD1	2.09	0.52
1:A:47:VAL:HG13	1:B:350:MET:SD	2.49	0.52
1:D:160[A]:LEU:HD13	6:D:1741:HOH:O	2.09	0.52
1:B:159:PRO:HD2	1:B:160[A]:LEU:HD23	1.91	0.52
1:C:264[A]:ARG:NH1	1:C:264[A]:ARG:HB2	2.25	0.52
1:A:191:LEU:HG	1:A:262[B]:MET:HG2	1.91	0.51
1:B:132[B]:VAL:HG12	1:B:133:ALA:N	2.25	0.51
1:D:191:LEU:HD11	1:D:262[A]:MET:HE2	1.92	0.51
1:A:170:ALA:HA	1:A:180:VAL:HG21	1.93	0.51
1:B:189:PRO:HD3	1:B:204:HIS:CE1	2.45	0.51
1:B:191:LEU:HD11	1:B:262[B]:MET:CG	2.41	0.50
1:B:304:ARG:CZ	1:B:304:ARG:HB3	2.40	0.50
1:B:325:CYS:HB3	1:B:333:LEU:HD13	1.93	0.50
1:D:276:LEU:HD13	1:D:312:VAL:HG11	1.93	0.50
1:A:209:TYR:CE1	1:A:338:GLY:HA2	2.48	0.49
1:B:298:VAL:HG22	1:B:301:ARG:HH12	1.77	0.49
1:C:209:TYR:CD1	1:C:262[A]:MET:SD	3.06	0.49
1:C:208:LLP:O3	1:C:208:LLP:NZ	2.46	0.49
1:C:196:SER:OG	1:C:197:LEU:HD12	2.12	0.48
1:B:209:TYR:CD1	1:B:262[A]:MET:SD	3.07	0.48
1:C:194:PRO:HB2	1:C:202:VAL:HG22	1.96	0.48
1:A:330:ILE:HD12	1:A:382:ASP:HB2	1.96	0.48
1:A:331:PHE:CD1	1:A:342:SER:HB3	2.49	0.48
1:D:301[A]:ARG:HH11	1:D:301[A]:ARG:CG	2.26	0.48
1:A:244:GLY:HA3	1:B:247[A]:ASP:OD2	2.14	0.48
1:D:103:HIS:ND1	1:D:148:THR:OG1	2.40	0.47
1:B:12:ALA:HB3	1:D:378:ASP:CG	2.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141[B]:ARG:HB2	1:B:141[B]:ARG:HE	1.28	0.47
1:B:190:ALA:O	1:B:304:ARG:NH1	2.48	0.47
1:D:208:LLP:O3	1:D:208:LLP:NZ	2.47	0.46
1:D:37:TYR:CD2	1:D:62:PRO:HB2	2.50	0.46
1:A:141:ARG:HA	1:A:144:ILE:HD12	1.96	0.46
1:C:296:HIS:CE1	6:C:2006:HOH:O	2.68	0.46
1:D:209:TYR:CD1	1:D:262[B]:MET:SD	3.09	0.46
1:B:191:LEU:HD11	1:B:262[B]:MET:SD	2.55	0.46
1:B:106:ILE:HB	1:B:107:PRO:CD	2.46	0.46
1:C:214:SER:HG	1:C:339[B]:SER:HB3	1.80	0.45
1:B:132[B]:VAL:CG1	1:B:133:ALA:N	2.80	0.45
1:B:191:LEU:HD21	1:B:262[B]:MET:HG3	1.99	0.45
1:D:331:PHE:CD1	1:D:342:SER:HB3	2.52	0.45
1:D:79:PHE:CZ	1:D:226[B]:GLU:HG3	2.51	0.45
1:B:111:TYR:CD1	6:B:1248:HOH:O	2.69	0.45
1:B:208:LLP:HG2	1:B:337:LEU:HG	1.98	0.45
1:A:184:ASN:HB3	1:A:204:HIS:CE1	2.52	0.45
1:C:344:ILE:HG13	1:C:369:LEU:HD23	1.98	0.44
1:A:208:LLP:O3	1:A:208:LLP:NZ	2.51	0.44
1:C:132[B]:VAL:HG11	1:C:143:ALA:CB	2.47	0.44
1:D:209:TYR:CE1	1:D:338:GLY:HA2	2.53	0.44
1:C:209:TYR:CE1	1:C:338:GLY:HA2	2.52	0.44
1:D:160[B]:LEU:HA	1:D:286:LEU:HD13	1.99	0.44
1:A:132[A]:VAL:HG11	1:A:143:ALA:HB2	2.00	0.43
1:B:225:ASP:HB3	1:B:228:LEU:HB2	1.99	0.43
1:D:160[A]:LEU:HA	1:D:286:LEU:HD13	2.00	0.43
1:D:197:LEU:CD1	1:D:302:GLN:HB2	2.48	0.43
1:B:304:ARG:NH1	6:B:958:HOH:O	2.52	0.43
1:B:35:PRO:HB2	1:B:37:TYR:CE2	2.54	0.43
1:C:191:LEU:HG	1:C:262[B]:MET:HG2	2.01	0.43
1:A:208:LLP:HG2	1:A:337:LEU:HG	2.01	0.42
1:D:197:LEU:HD11	1:D:302:GLN:HB2	2.01	0.42
1:D:335:GLU:O	1:D:336:SER:CB	2.67	0.42
1:A:158:ASN:HA	1:A:159:PRO:HA	1.81	0.42
1:C:111:TYR:CE2	1:C:113:GLY:HA3	2.55	0.42
1:A:75:GLU:HG3	1:A:222:VAL:HG21	2.01	0.42
1:B:246:PHE:HE1	1:C:246:PHE:HD1	1.66	0.42
1:A:132[A]:VAL:HG11	1:A:143:ALA:CB	2.49	0.42
1:A:208:LLP:N	1:A:208:LLP:CD	2.82	0.42
1:B:10:ARG:HA	1:B:11:PHE:CB	2.50	0.41
1:D:25:PRO:HD3	5:D:389:EDO:H11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:LEU:O	1:B:121:VAL:HB	2.20	0.41
1:D:323:GLN:O	1:D:327:LYS:HG3	2.20	0.41
1:A:195:LEU:HB2	6:A:1226:HOH:O	2.20	0.41
1:B:226[A]:GLU:O	1:B:226[A]:GLU:OE2	2.39	0.41
1:D:190:ALA:HB3	1:D:262[B]:MET:HG3	2.02	0.41
1:A:209:TYR:CD1	1:A:262[A]:MET:SD	3.14	0.41
1:B:190:ALA:O	1:B:191:LEU:HD23	2.20	0.41
1:B:341:GLU:HB3	1:D:19:ILE:CG2	2.51	0.41
1:D:189:PRO:HD3	1:D:204:HIS:CE1	2.56	0.41
1:B:166:ILE:HD13	1:B:194:PRO:HB3	2.03	0.41
1:C:264[A]:ARG:HD3	1:C:264[A]:ARG:HA	1.77	0.41
1:A:106:ILE:HB	1:A:107:PRO:CD	2.51	0.41
1:D:345:GLU:HG2	1:D:346:HIS:N	2.36	0.41
1:A:30:GLY:O	1:A:31:ALA:C	2.59	0.40
1:B:158:ASN:HA	1:B:159:PRO:HA	1.83	0.40
1:D:159:PRO:HG2	1:D:160[B]:LEU:HD12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	376/392 (96%)	366 (97%)	9 (2%)	1 (0%)	41	31
1	B	380/392 (97%)	368 (97%)	11 (3%)	1 (0%)	41	31
1	C	369/392 (94%)	357 (97%)	12 (3%)	0	100	100
1	D	375/392 (96%)	366 (98%)	9 (2%)	0	100	100
All	All	1500/1568 (96%)	1457 (97%)	41 (3%)	2 (0%)	51	42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	11	PHE
1	A	188	SER

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	275/292 (94%)	273 (99%)	2 (1%)	84	83
1	B	279/292 (96%)	274 (98%)	5 (2%)	59	53
1	C	271/292 (93%)	266 (98%)	5 (2%)	59	53
1	D	276/292 (94%)	273 (99%)	3 (1%)	73	72
All	All	1101/1168 (94%)	1086 (99%)	15 (1%)	73	63

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	337	LEU
1	A	345	GLU
1	B	100	PRO
1	B	226[A]	GLU
1	B	226[B]	GLU
1	B	337	LEU
1	B	345	GLU
1	C	188	SER
1	C	264[A]	ARG
1	C	264[B]	ARG
1	C	339[A]	SER
1	C	339[B]	SER
1	D	336	SER
1	D	339	SER
1	D	351	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	D	208	1	23,24,25	2.24	8 (34%)	25,32,34	2.31	11 (44%)
1	LLP	C	208	1	23,24,25	1.49	5 (21%)	25,32,34	1.98	6 (24%)
1	LLP	B	208	1	23,24,25	2.57	9 (39%)	25,32,34	2.38	9 (36%)
1	LLP	A	208	1	23,24,25	2.17	6 (26%)	25,32,34	2.05	10 (40%)

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	D	208	1	-	4/16/17/19	0/1/1/1
1	LLP	C	208	1	-	2/16/17/19	0/1/1/1
1	LLP	B	208	1	-	3/16/17/19	0/1/1/1
1	LLP	A	208	1	-	4/16/17/19	0/1/1/1

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	208	LLP	C4-C4'	5.86	1.57	1.46
1	A	208	LLP	O3-C3	-5.38	1.24	1.37
1	B	208	LLP	O3-C3	-4.96	1.25	1.37
1	A	208	LLP	C4-C4'	4.72	1.55	1.46
1	A	208	LLP	C2-N1	4.56	1.42	1.33
1	D	208	LLP	O3-C3	-4.49	1.26	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	208	LLP	C2-N1	4.28	1.41	1.33
1	D	208	LLP	C4-C4'	3.99	1.54	1.46
1	D	208	LLP	CD-CE	3.95	1.65	1.51
1	B	208	LLP	CE-NZ	3.95	1.55	1.46
1	D	208	LLP	C2'-C2	3.78	1.56	1.50
1	B	208	LLP	C4'-NZ	3.63	1.39	1.27
1	A	208	LLP	C4'-NZ	3.33	1.38	1.27
1	B	208	LLP	C6-N1	3.29	1.41	1.34
1	D	208	LLP	C4-C5	-3.17	1.38	1.42
1	C	208	LLP	O3-C3	-3.13	1.29	1.37
1	C	208	LLP	CB-CA	2.86	1.57	1.53
1	C	208	LLP	CD-CE	2.75	1.61	1.51
1	B	208	LLP	P-OP3	-2.71	1.44	1.54
1	D	208	LLP	C4'-NZ	2.68	1.36	1.27
1	D	208	LLP	P-OP3	-2.67	1.44	1.54
1	B	208	LLP	C4-C5	-2.59	1.38	1.42
1	C	208	LLP	C4'-NZ	2.43	1.35	1.27
1	B	208	LLP	C2'-C2	2.42	1.54	1.50
1	A	208	LLP	CE-NZ	2.27	1.51	1.46
1	C	208	LLP	C2'-C2	2.23	1.54	1.50
1	A	208	LLP	C6-N1	2.22	1.39	1.34
1	D	208	LLP	CG-CB	2.20	1.61	1.52

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	208	LLP	OP2-P-OP4	-6.21	90.21	106.73
1	B	208	LLP	OP4-C5'-C5	5.30	119.44	109.35
1	C	208	LLP	C4-C3-C2	-5.02	117.08	120.19
1	B	208	LLP	C4-C3-C2	4.55	123.01	120.19
1	B	208	LLP	OP2-P-OP4	-4.34	95.19	106.73
1	D	208	LLP	OP4-C5'-C5	4.24	117.43	109.35
1	A	208	LLP	OP4-C5'-C5	3.84	116.67	109.35
1	C	208	LLP	OP4-C5'-C5	3.70	116.41	109.35
1	B	208	LLP	C3-C2-N1	-3.59	116.13	120.77
1	C	208	LLP	C3-C4-C5	3.47	120.92	118.26
1	A	208	LLP	CD-CE-NZ	3.45	119.39	110.93
1	C	208	LLP	CG-CD-CE	-3.42	101.67	113.57
1	A	208	LLP	OP2-P-OP4	-3.39	97.70	106.73
1	B	208	LLP	C4-C4'-NZ	-3.26	109.33	124.31
1	B	208	LLP	C2'-C2-N1	3.21	123.95	117.67
1	B	208	LLP	CD-CE-NZ	3.15	118.65	110.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	208	LLP	C5'-C5-C6	-3.13	114.22	119.37
1	D	208	LLP	C3-C2-N1	-3.12	116.74	120.77
1	A	208	LLP	C2'-C2-C3	-3.03	117.15	120.89
1	D	208	LLP	C5'-C5-C6	-2.87	114.66	119.37
1	D	208	LLP	CD-CE-NZ	2.80	117.80	110.93
1	A	208	LLP	C4-C4'-NZ	-2.80	111.45	124.31
1	A	208	LLP	C2'-C2-N1	2.71	122.96	117.67
1	B	208	LLP	OP3-P-OP2	2.69	117.92	107.64
1	A	208	LLP	C4-C3-C2	2.65	121.83	120.19
1	C	208	LLP	OP2-P-OP4	-2.61	99.80	106.73
1	D	208	LLP	C2'-C2-C3	2.59	124.09	120.89
1	B	208	LLP	OP4-P-OP1	-2.57	99.27	106.47
1	D	208	LLP	C5-C6-N1	-2.54	119.59	123.82
1	D	208	LLP	OP2-P-OP1	2.52	120.56	110.68
1	D	208	LLP	C4-C4'-NZ	-2.47	112.99	124.31
1	A	208	LLP	OP3-P-OP2	2.39	116.78	107.64
1	D	208	LLP	C4-C3-C2	2.20	121.55	120.19
1	A	208	LLP	C5-C4-C4'	2.18	125.14	121.56
1	C	208	LLP	CD-CG-CB	2.13	121.16	113.62
1	D	208	LLP	C6-N1-C2	2.05	122.97	119.17

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	208	LLP	O-C-CA-CB
1	C	208	LLP	C4-C4'-NZ-CE
1	C	208	LLP	O-C-CA-CB
1	B	208	LLP	O-C-CA-CB
1	A	208	LLP	O-C-CA-CB
1	A	208	LLP	C4-C4'-NZ-CE
1	B	208	LLP	C4-C4'-NZ-CE
1	D	208	LLP	CG-CD-CE-NZ
1	B	208	LLP	CA-CB-CG-CD
1	A	208	LLP	CA-CB-CG-CD
1	D	208	LLP	CA-CB-CG-CD
1	D	208	LLP	C4-C4'-NZ-CE
1	A	208	LLP	CG-CD-CE-NZ

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	208	LLP	1	0
1	C	208	LLP	1	0
1	B	208	LLP	1	0
1	A	208	LLP	3	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 for Mogul analysis.

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	B	389	-	4,4,4	0.18	0	6,6,6	0.41	0
2	SO4	A	389	-	4,4,4	0.49	0	6,6,6	0.67	0
2	SO4	C	389	-	4,4,4	0.52	0	6,6,6	0.41	0
4	GOL	A	392	-	5,5,5	0.69	0	5,5,5	0.47	0
2	SO4	A	390	-	4,4,4	0.17	0	6,6,6	0.44	0
4	GOL	B	391	-	5,5,5	0.72	0	5,5,5	0.97	0
2	SO4	B	390	-	4,4,4	0.63	0	6,6,6	0.13	0
5	EDO	D	389	-	3,3,3	0.36	0	2,2,2	0.99	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
5	EDO	D	389	-	-	1/1/1/1	-
4	GOL	A	392	-	-	2/4/4/4	-
4	GOL	B	391	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	391	GOL	O1-C1-C2-O2
4	B	391	GOL	O1-C1-C2-C3
4	A	392	GOL	C1-C2-C3-O3
4	B	391	GOL	C1-C2-C3-O3
4	A	392	GOL	O2-C2-C3-O3
5	D	389	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	389	EDO	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, 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	374/392 (95%)	-0.56	0 100 100	8, 14, 23, 30	1 (0%)
1	B	373/392 (95%)	-0.46	6 (1%) 72 74	7, 14, 23, 34	0
1	C	365/392 (93%)	-0.50	3 (0%) 86 87	9, 15, 24, 33	0
1	D	372/392 (94%)	-0.50	1 (0%) 94 94	7, 15, 24, 38	0
All	All	1484/1568 (94%)	-0.51	10 (0%) 87 89	7, 15, 24, 38	1 (0%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	11	PHE	6.1
1	D	11	PHE	5.8
1	B	10	ARG	4.3
1	B	357	GLY	3.6
1	C	48	GLY	3.3
1	B	358	SER	3.1
1	B	351	THR	2.9
1	C	46	GLY	2.7
1	C	47	VAL	2.2
1	B	360	LEU	2.2

6.2 Non-standard residues in protein, DNA, RNA chains

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	B	208	24/25	0.96	0.08	7,13,19,21	0
1	LLP	A	208	24/25	0.96	0.09	6,13,20,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	LLP	C	208	24/25	0.97	0.07	9,14,20,22	0
1	LLP	D	208	24/25	0.98	0.07	8,12,17,19	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. 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(\AA^2)	Q<0.9
4	GOL	B	391	6/6	0.57	0.17	38,43,44,45	0
5	EDO	D	389	4/4	0.83	0.21	25,31,32,36	0
4	GOL	A	392	6/6	0.85	0.26	22,28,31,37	0
2	SO4	C	389	5/5	0.91	0.16	29,31,32,35	5
2	SO4	B	390	5/5	0.94	0.14	18,24,28,29	5
2	SO4	B	389	5/5	0.96	0.14	54,54,55,56	0
2	SO4	A	389	5/5	0.97	0.09	18,22,29,36	0
2	SO4	A	390	5/5	0.98	0.12	13,15,17,21	5
3	NA	A	391	1/1	0.98	0.04	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.