



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 19, 2020 – 08:22 pm BST

PDB ID : 3DWC
Title : Trypanosoma Cruzi Metallocoarboxypeptidase 1
Authors : Niemirowicz, G.; Fernandez, D.; Sola, M.; Cazzulo, J.J.; Aviles, F.X.; Gomis-Ruth, F.X.
Deposited on : 2008-07-22
Resolution : 2.10 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

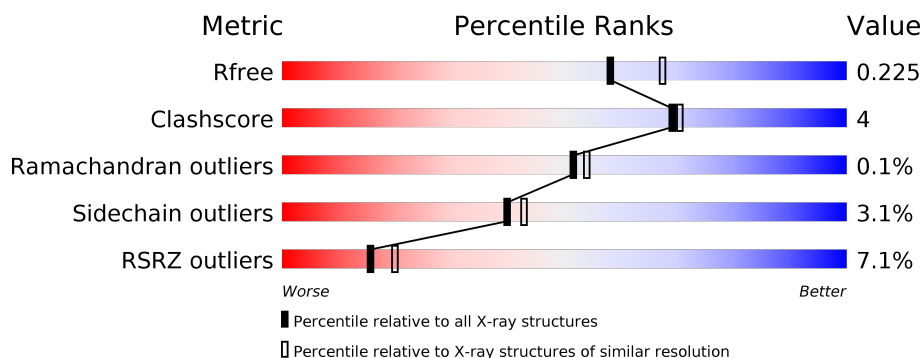
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	505	<div> <div>3%</div> <div> <div></div> <div>89%</div> <div>9%</div> <div></div> </div> </div>
1	B	505	<div> <div>9%</div> <div> <div></div> <div>89%</div> <div>10%</div> <div></div> </div> </div>
1	C	505	<div> <div>7%</div> <div> <div></div> <div>89%</div> <div>10%</div> <div></div> </div> </div>
1	D	505	<div> <div>9%</div> <div> <div></div> <div>84%</div> <div>11%</div> <div></div> </div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 17261 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 Metallocooxypeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	501	Total	C	N	O	S	0	0	0
			4035	2548	707	751	29			
1	B	504	Total	C	N	O	S	0	0	0
			4059	2560	713	757	29			
1	C	501	Total	C	N	O	S	0	0	0
			4035	2548	707	751	29			
1	D	483	Total	C	N	O	S	0	0	0
			3880	2449	678	725	28			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP Q6ZXC0
A	0	SER	-	EXPRESSION TAG	UNP Q6ZXC0
B	-1	GLY	-	EXPRESSION TAG	UNP Q6ZXC0
B	0	SER	-	EXPRESSION TAG	UNP Q6ZXC0
C	-1	GLY	-	EXPRESSION TAG	UNP Q6ZXC0
C	0	SER	-	EXPRESSION TAG	UNP Q6ZXC0
D	-1	GLY	-	EXPRESSION TAG	UNP Q6ZXC0
D	0	SER	-	EXPRESSION TAG	UNP Q6ZXC0

- Molecule 2 is COBALT (II) ION (three-letter code: CO) (formula: Co).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Co	0	0
			1	1		
2	A	1	Total	Co	0	0
			1	1		
2	D	1	Total	Co	0	0
			1	1		
2	C	1	Total	Co	0	0
			1	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



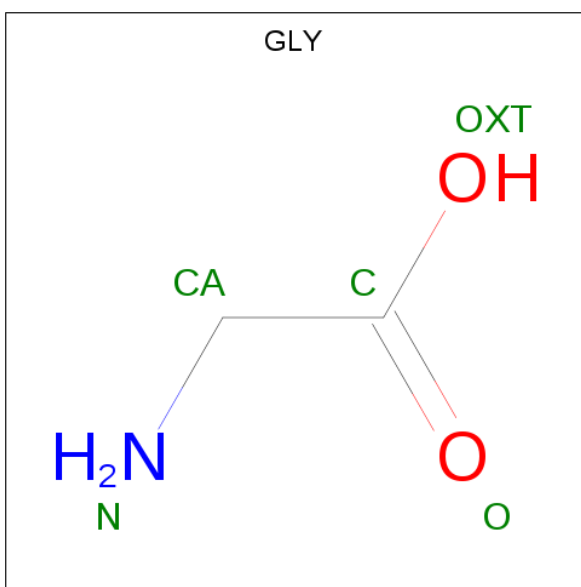
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



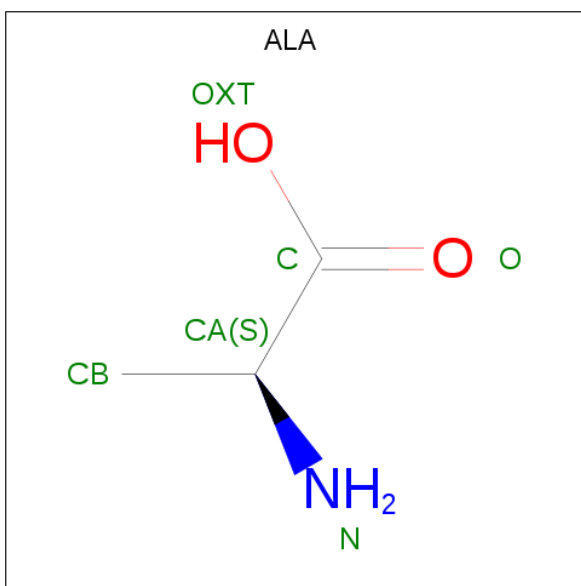
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is GLYCINE (three-letter code: GLY) (formula: $C_2H_5NO_2$).



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

- Molecule 6 is ALANINE (three-letter code: ALA) (formula: C₃H₇NO₂).



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

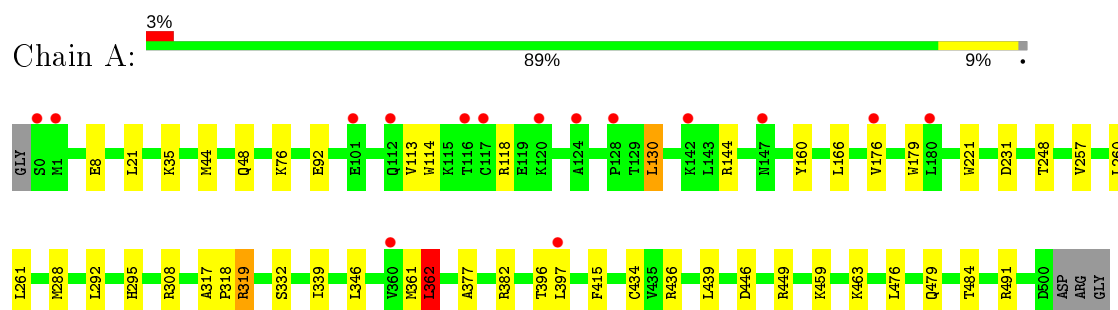
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	307	Total 307	O 307	0	0
7	B	284	Total 284	O 284	0	0
7	C	284	Total 284	O 284	0	0
7	D	245	Total 245	O 245	0	0

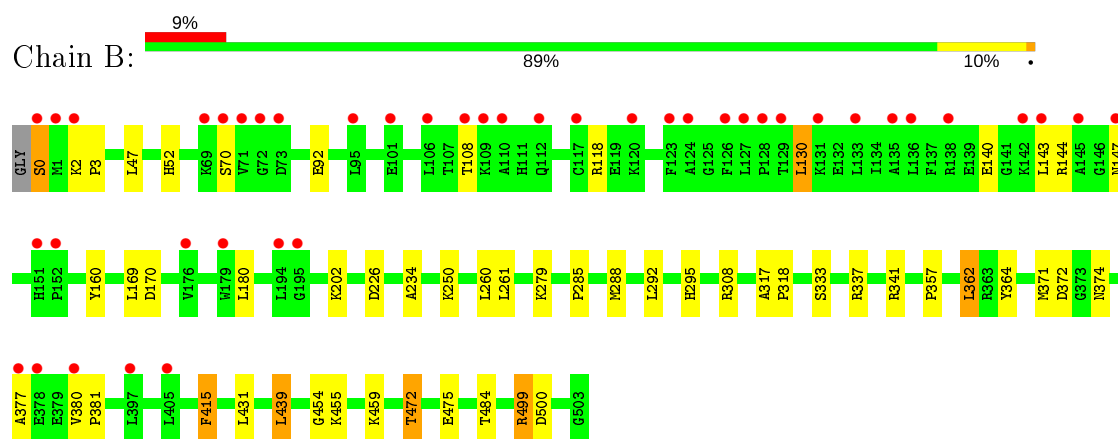
3 Residue-property plots [i](#)

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.

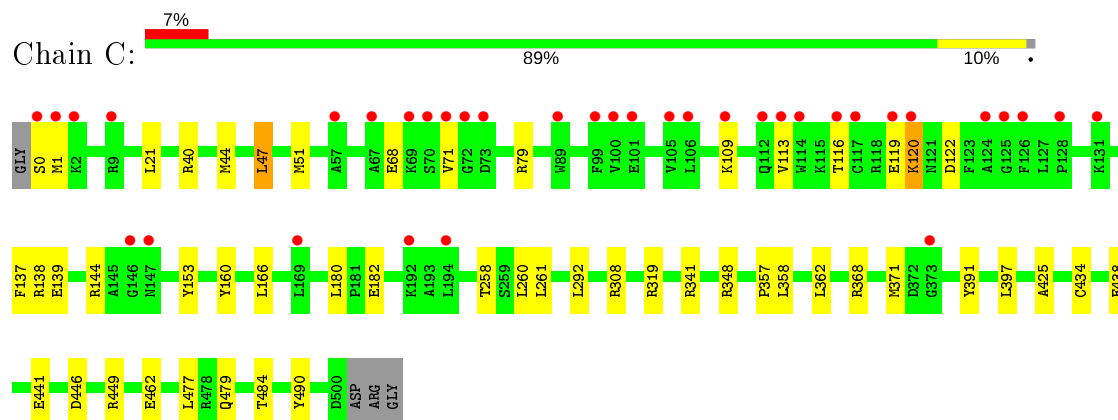
• Molecule 1: Metallocoarboxypeptidase



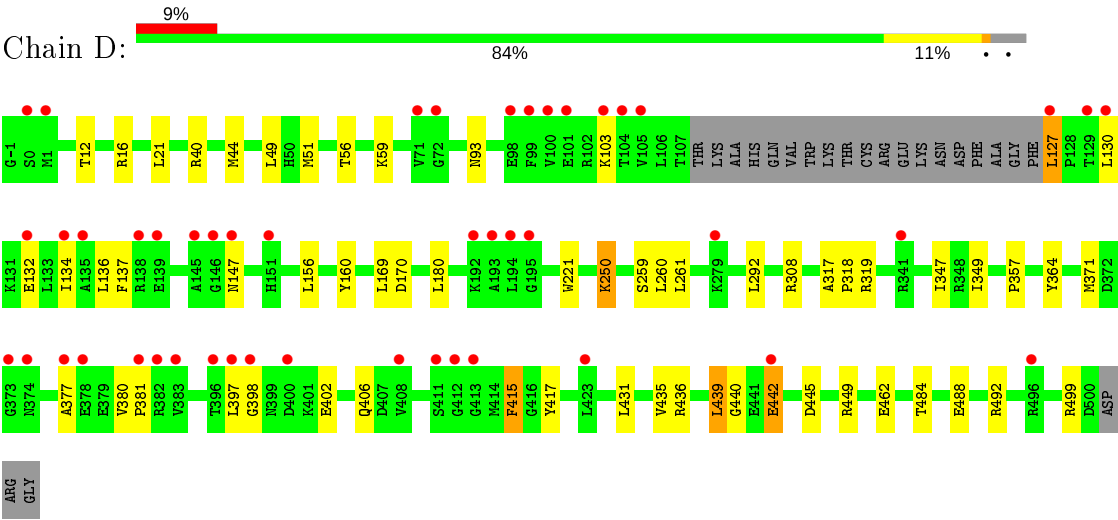
• Molecule 1: Metallocoarboxypeptidase



• Molecule 1: Metallocoarboxypeptidase



● Molecule 1: Metallocoarboxypeptidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	89.40Å 136.25Å 117.86Å 90.00° 103.06° 90.00°	Depositor
Resolution (Å)	46.23 – 2.10 46.21 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.23-2.10) 100.0 (46.21-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.57 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.179 , 0.221 0.187 , 0.225	Depositor DCC
R_{free} test set	3915 reflections (2.45%)	wwPDB-VP
Wilson B-factor (Å ²)	29.3	Xtriage
Anisotropy	0.439	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 63.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17261	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.11% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CO, CSX, 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	0.82	1/4114 (0.0%)	0.81	4/5540 (0.1%)
1	B	0.75	0/4138	0.78	5/5570 (0.1%)
1	C	0.77	2/4114 (0.0%)	0.76	3/5540 (0.1%)
1	D	0.74	2/3953 (0.1%)	0.75	3/5322 (0.1%)
All	All	0.77	5/16319 (0.0%)	0.77	15/21972 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	132	GLU	CD-OE1	7.24	1.33	1.25
1	C	182	GLU	CG-CD	6.01	1.60	1.51
1	A	434	CYS	CB-SG	-5.80	1.72	1.81
1	C	462	GLU	CG-CD	5.03	1.59	1.51
1	D	132	GLU	CD-OE2	5.02	1.31	1.25

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	337	ARG	NE-CZ-NH1	7.09	123.84	120.30
1	B	499	ARG	NE-CZ-NH1	6.75	123.67	120.30
1	D	499	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	C	144	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	A	362	LEU	CA-CB-CG	5.40	127.72	115.30
1	A	382	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	D	319	ARG	NE-CZ-NH2	5.27	122.94	120.30
1	B	362	LEU	CA-CB-CG	5.26	127.40	115.30
1	B	341	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	A	144	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	C	319	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	C	319	ARG	CG-CD-NE	-5.14	101.01	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	319	ARG	NE-CZ-NH1	-5.14	117.73	120.30
1	B	337	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	A	319	ARG	NE-CZ-NH2	-5.09	117.76	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4035	0	3988	28	0
1	B	4059	0	4008	32	0
1	C	4035	0	3988	27	0
1	D	3880	0	3838	33	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	15	0	0	0	0
3	B	25	0	0	1	0
3	C	15	0	0	0	0
3	D	10	0	0	0	0
4	A	36	0	48	2	0
4	B	18	0	24	1	0
5	B	4	0	2	1	0
6	B	5	0	5	1	0
7	A	307	0	0	1	0
7	B	284	0	0	1	0
7	C	284	0	0	2	0
7	D	245	0	0	0	0
All	All	17261	0	15901	119	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (119) 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:B:0:SER:N	1:B:70:SER:OG	2.00	0.93
1:C:261:LEU:HD13	1:C:308:ARG:CZ	2.02	0.89
1:C:261:LEU:HD13	1:C:308:ARG:NH1	1.93	0.84
1:C:68:GLU:O	1:C:71:VAL:HG23	1.82	0.78
1:B:472:THR:HG21	7:B:1331:HOH:O	1.82	0.77
1:C:160:TYR:HB3	1:C:292:LEU:HD12	1.69	0.74
1:D:137:PHE:HB3	1:D:371:MET:HE1	1.70	0.74
1:A:176:VAL:CG1	1:A:361:MET:HE1	2.18	0.74
1:C:166:LEU:HD21	1:C:368:ARG:CZ	2.18	0.73
1:B:472:THR:HG22	1:B:475:GLU:H	1.54	0.71
1:C:166:LEU:HD21	1:C:368:ARG:NH2	2.06	0.71
1:A:346:LEU:HD22	1:A:396:THR:HG22	1.73	0.70
1:B:372:ASP:HB3	1:B:374:ASN:HD22	1.55	0.70
1:D:137:PHE:HB3	1:D:371:MET:CE	2.23	0.69
1:A:160:TYR:HB3	1:A:292:LEU:HD12	1.75	0.69
1:A:44:MET:O	1:A:48:GLN:HG3	1.95	0.67
1:A:439:LEU:CD1	1:A:459:LYS:HE3	2.25	0.66
1:D:127:LEU:HD12	1:D:127:LEU:C	2.15	0.66
1:A:176:VAL:HG11	1:A:361:MET:HE1	1.76	0.66
1:B:180:LEU:HD21	1:B:357:PRO:HG2	1.78	0.64
1:D:160:TYR:HB3	1:D:292:LEU:HD12	1.80	0.64
1:D:261:LEU:HD13	1:D:308:ARG:CZ	2.28	0.63
1:A:439:LEU:HD11	1:A:459:LYS:HE3	1.80	0.62
1:B:454:GLY:H	5:B:701:GLY:N	1.98	0.62
1:B:484:THR:HG22	3:B:606:SO4:O3	2.00	0.61
1:D:180:LEU:HD21	1:D:357:PRO:HG2	1.83	0.61
1:C:21:LEU:HG	1:C:47:LEU:HD13	1.83	0.60
1:D:435:VAL:HG13	1:D:439:LEU:HD22	1.82	0.59
1:C:446:ASP:OD1	1:C:449:ARG:NH1	2.35	0.59
1:C:180:LEU:HD21	1:C:357:PRO:HG2	1.85	0.59
1:B:455:LYS:HG3	6:B:702:ALA:HB3	1.85	0.58
1:D:317:ALA:HB3	1:D:318:PRO:HD3	1.84	0.58
1:B:130:LEU:HD13	1:B:377:ALA:HB1	1.85	0.57
1:B:52:HIS:ND1	1:B:92:GLU:OE2	2.34	0.57
1:D:397:LEU:HD12	1:D:398:GLY:N	2.20	0.56
1:A:176:VAL:HG12	1:A:361:MET:HE1	1.88	0.56
1:A:446:ASP:OD1	1:A:449:ARG:NH2	2.39	0.56
1:D:292:LEU:HD11	1:D:417:TYR:CE2	2.41	0.55
1:A:317:ALA:HB3	1:A:318:PRO:HD3	1.88	0.55
1:D:347:ILE:HD11	1:D:402:GLU:HG2	1.88	0.55
1:C:71:VAL:HG12	1:C:79:ARG:HD3	1.88	0.54
1:C:153:TYR:HB2	1:C:371:MET:HG2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:435:VAL:CG1	1:D:439:LEU:HD22	2.38	0.53
1:C:21:LEU:HD12	1:C:51:MET:SD	2.48	0.53
1:D:130:LEU:HD12	1:D:377:ALA:HB1	1.92	0.52
1:B:234:ALA:O	1:B:250:LYS:HE2	2.10	0.52
1:A:130:LEU:HD13	1:A:377:ALA:HB1	1.91	0.51
1:B:371:MET:CE	1:B:415:PHE:CE2	2.94	0.51
1:C:166:LEU:HD21	1:C:368:ARG:NE	2.25	0.51
1:D:170:ASP:OD2	1:D:364:TYR:OH	2.19	0.51
1:B:371:MET:HE3	1:B:415:PHE:CE2	2.46	0.51
1:C:434:CYS:O	1:C:438:GLU:HG3	2.11	0.50
1:D:261:LEU:HD13	1:D:308:ARG:NH1	2.25	0.50
1:D:103:LYS:HD2	1:D:136:LEU:HD21	1.94	0.49
1:B:170:ASP:OD2	1:B:364:TYR:OH	2.18	0.49
1:C:137:PHE:O	1:C:371:MET:HE1	2.12	0.49
1:B:439:LEU:HD13	1:B:459:LYS:HE3	1.94	0.49
1:D:347:ILE:HG22	1:D:349:ILE:HG12	1.95	0.49
1:A:439:LEU:HD11	1:A:459:LYS:CE	2.41	0.49
1:D:371:MET:HE3	1:D:415:PHE:CD2	2.47	0.49
1:A:76:LYS:H	4:A:703:GOL:H11	1.78	0.49
1:D:380:VAL:N	1:D:381:PRO:HD2	2.27	0.48
1:B:499:ARG:HD2	1:B:500:ASP:OD1	2.13	0.48
1:C:109:LYS:O	1:C:113:VAL:HG23	2.13	0.48
1:C:477:LEU:HD12	7:C:1191:HOH:O	2.13	0.48
1:D:250:LYS:O	1:D:259:SER:OG	2.21	0.48
1:B:130:LEU:HD13	1:B:377:ALA:CB	2.44	0.47
1:B:317:ALA:HB3	1:B:318:PRO:HD3	1.96	0.47
1:D:127:LEU:CD1	1:D:127:LEU:C	2.82	0.47
1:C:116:THR:HA	1:C:119:GLU:HG2	1.95	0.47
1:B:140:GLU:O	1:B:144:ARG:HG3	2.15	0.47
1:D:440:GLY:HA3	1:D:442:GLU:OE2	2.15	0.47
1:D:12:THR:O	1:D:16:ARG:HG2	2.16	0.46
1:A:179:TRP:CD1	1:A:491:ARG:HD2	2.51	0.46
1:A:436:ARG:HD2	7:A:1865:HOH:O	2.15	0.46
1:C:138:ARG:HA	1:C:371:MET:HE3	1.97	0.46
1:A:231:ASP:O	1:A:248:THR:HA	2.16	0.46
1:C:0:SER:OG	1:C:1:MET:N	2.47	0.46
1:A:476:LEU:O	1:A:479:GLN:HG3	2.16	0.46
1:A:362:LEU:C	1:A:362:LEU:HD12	2.36	0.45
1:B:130:LEU:CD1	1:B:377:ALA:HB1	2.46	0.45
1:C:358:LEU:HD22	1:C:391:TYR:HB3	1.98	0.45
1:C:166:LEU:CD2	1:C:368:ARG:NH2	2.77	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:436:ARG:NH2	1:D:445:ASP:OD1	2.45	0.45
1:B:261:LEU:HD23	1:B:308:ARG:CZ	2.47	0.45
1:D:371:MET:HE3	1:D:415:PHE:HD2	1.82	0.45
1:B:2:LYS:HB3	1:B:3:PRO:CD	2.47	0.44
1:B:169:LEU:HD13	1:B:364:TYR:CE2	2.53	0.44
1:C:425:ALA:HB1	1:C:490:TYR:CE1	2.52	0.44
1:A:261:LEU:HD13	1:A:308:ARG:CZ	2.48	0.44
1:A:261:LEU:HD11	1:A:339:ILE:HD12	1.98	0.44
1:D:371:MET:CE	1:D:415:PHE:CD2	3.01	0.44
1:B:371:MET:HE3	1:B:415:PHE:HE2	1.83	0.43
1:D:169:LEU:HD23	1:D:169:LEU:HA	1.88	0.43
1:B:333:SER:OG	4:B:707:GOL:H32	2.19	0.43
1:D:21:LEU:HD12	1:D:51:MET:SD	2.58	0.43
1:A:257:VAL:HG12	1:A:261:LEU:HD12	2.01	0.43
1:A:114:TRP:CZ2	1:A:118:ARG:HD3	2.54	0.43
1:A:439:LEU:N	1:A:439:LEU:HD12	2.33	0.42
1:D:488:GLU:HG3	1:D:492:ARG:HD2	2.01	0.42
1:D:134:ILE:HA	1:D:134:ILE:HD13	1.86	0.42
1:A:21:LEU:HD11	1:A:48:GLN:HG2	2.00	0.42
1:B:261:LEU:HD23	1:B:308:ARG:NH2	2.34	0.42
1:B:472:THR:HB	1:B:475:GLU:OE1	2.19	0.42
1:A:8:GLU:OE2	4:A:705:GOL:H11	2.21	0.41
1:A:35:LYS:HB2	1:B:226:ASP:O	2.20	0.41
1:C:261:LEU:CD1	1:C:308:ARG:CZ	2.88	0.41
1:D:56:THR:HG22	1:D:93:ASN:HD22	1.85	0.41
1:B:2:LYS:HB3	1:B:3:PRO:HD3	2.02	0.41
1:D:156:LEU:CD1	1:D:371:MET:CE	2.99	0.41
1:A:463:LYS:O	1:A:479:GLN:NE2	2.45	0.41
1:B:285:PRO:O	1:B:288:MET:HG3	2.20	0.41
1:A:318:PRO:HB2	1:A:319:ARG:NH1	2.36	0.40
1:B:380:VAL:HB	1:B:381:PRO:HD3	2.02	0.40
1:C:258:THR:HB	7:C:1208:HOH:O	2.22	0.40
1:D:40:ARG:O	1:D:44:MET:HG3	2.20	0.40
1:C:120:LYS:HG3	1:C:122:ASP:HB2	2.03	0.40
1:B:160:TYR:HB3	1:B:292:LEU:HD22	2.04	0.40
1:C:40:ARG:O	1:C:44:MET: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	498/505 (99%)	488 (98%)	10 (2%)	0	100	100
1	B	501/505 (99%)	491 (98%)	10 (2%)	0	100	100
1	C	498/505 (99%)	491 (99%)	7 (1%)	0	100	100
1	D	478/505 (95%)	470 (98%)	6 (1%)	2 (0%)	34	32
All	All	1975/2020 (98%)	1940 (98%)	33 (2%)	2 (0%)	51	54

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	484	THR
1	D	406	GLN

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	431/433 (100%)	418 (97%)	13 (3%)	41	44
1	B	433/433 (100%)	417 (96%)	16 (4%)	34	35
1	C	431/433 (100%)	420 (97%)	11 (3%)	46	50
1	D	415/433 (96%)	402 (97%)	13 (3%)	40	43
All	All	1710/1732 (99%)	1657 (97%)	53 (3%)	40	43

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	GLU
1	A	113	VAL
1	A	130	LEU
1	A	166	LEU
1	A	221	TRP
1	A	260	LEU
1	A	288	MET
1	A	295	HIS
1	A	332	SER
1	A	362	LEU
1	A	397	LEU
1	A	415	PHE
1	A	484	THR
1	B	0	SER
1	B	47	LEU
1	B	108	THR
1	B	118	ARG
1	B	130	LEU
1	B	143	LEU
1	B	147	ASN
1	B	202	LYS
1	B	260	LEU
1	B	279	LYS
1	B	295	HIS
1	B	362	LEU
1	B	415	PHE
1	B	431	LEU
1	B	439	LEU
1	B	472	THR
1	C	47	LEU
1	C	120	LYS
1	C	139	GLU
1	C	260	LEU
1	C	341	ARG
1	C	348	ARG
1	C	362	LEU
1	C	397	LEU
1	C	441	GLU
1	C	479	GLN
1	C	484	THR
1	D	49	LEU
1	D	59	LYS
1	D	127	LEU

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Mol	Chain	Res	Type
1	D	147	ASN
1	D	221	TRP
1	D	250	LYS
1	D	260	LEU
1	D	415	PHE
1	D	431	LEU
1	D	439	LEU
1	D	442	GLU
1	D	449	ARG
1	D	462	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	167	GLN
1	A	305	GLN
1	A	461	ASN
1	B	147	ASN
1	B	191	GLN
1	B	305	GLN
1	B	374	ASN
1	C	48	GLN
1	C	93	ASN
1	C	188	GLN
1	C	305	GLN
1	D	93	ASN
1	D	147	ASN
1	D	191	GLN
1	D	359	HIS
1	D	374	ASN
1	D	479	GLN

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	CSX	B	34	1	3,6,7	0.87	0	1,6,8	0.22	0
1	CSX	A	34	1	3,6,7	0.81	0	1,6,8	0.37	0
1	CSX	D	34	1	3,6,7	0.51	0	1,6,8	1.10	0
1	CSX	C	34	1	3,6,7	0.69	0	1,6,8	1.31	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
1	CSX	B	34	1	-	0/1/5/7	-
1	CSX	A	34	1	-	0/1/5/7	-
1	CSX	D	34	1	-	0/1/5/7	-
1	CSX	C	34	1	-	0/1/5/7	-

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.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 4 are monoatomic - leaving 24 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	$\# Z > 2$
4	GOL	A	705	-	5,5,5	0.53	0	5,5,5	0.92	0
3	SO4	C	603	-	4,4,4	0.32	0	6,6,6	0.42	0
4	GOL	A	708	-	5,5,5	0.45	0	5,5,5	0.66	0
4	GOL	A	703	-	5,5,5	0.41	0	5,5,5	0.56	0
4	GOL	B	706	-	5,5,5	0.42	0	5,5,5	0.62	0
3	SO4	C	605	-	4,4,4	0.20	0	6,6,6	0.37	0
3	SO4	B	602	-	4,4,4	0.18	0	6,6,6	0.24	0
4	GOL	A	711	-	5,5,5	0.34	0	5,5,5	0.47	0
3	SO4	B	606	-	4,4,4	0.16	0	6,6,6	0.49	0
3	SO4	D	608	-	4,4,4	0.19	0	6,6,6	0.43	0
3	SO4	C	613	-	4,4,4	0.19	0	6,6,6	0.28	0
4	GOL	A	704	-	5,5,5	0.44	0	5,5,5	0.55	0
3	SO4	B	611	-	4,4,4	0.20	0	6,6,6	0.20	0
3	SO4	A	604	-	4,4,4	0.36	0	6,6,6	0.59	0
3	SO4	A	609	-	4,4,4	0.14	0	6,6,6	0.39	0
4	GOL	B	709	-	5,5,5	0.46	0	5,5,5	0.68	0
3	SO4	B	607	-	4,4,4	0.13	0	6,6,6	0.36	0
4	GOL	A	710	-	5,5,5	0.28	0	5,5,5	0.61	0
4	GOL	B	707	-	5,5,5	0.40	0	5,5,5	0.26	0
3	SO4	A	610	-	4,4,4	0.22	0	6,6,6	0.76	0
3	SO4	B	612	-	4,4,4	0.19	0	6,6,6	0.43	0
3	SO4	D	601	-	4,4,4	0.15	0	6,6,6	0.18	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	705	-	-	0/4/4/4	-
4	GOL	A	711	-	-	4/4/4/4	-
4	GOL	B	707	-	-	2/4/4/4	-
4	GOL	A	708	-	-	2/4/4/4	-
4	GOL	A	703	-	-	2/4/4/4	-
4	GOL	A	704	-	-	4/4/4/4	-
4	GOL	B	706	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	B	709	-	-	2/4/4/4	-
4	GOL	A	710	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	706	GOL	C1-C2-C3-O3
4	B	706	GOL	O2-C2-C3-O3
4	A	711	GOL	O1-C1-C2-C3
4	A	711	GOL	C1-C2-C3-O3
4	A	704	GOL	C1-C2-C3-O3
4	A	704	GOL	O2-C2-C3-O3
4	A	708	GOL	O1-C1-C2-C3
4	A	703	GOL	C1-C2-C3-O3
4	A	704	GOL	O1-C1-C2-C3
4	B	709	GOL	C1-C2-C3-O3
4	B	707	GOL	C1-C2-C3-O3
4	A	711	GOL	O2-C2-C3-O3
4	A	704	GOL	O1-C1-C2-O2
4	B	709	GOL	O2-C2-C3-O3
4	A	708	GOL	O1-C1-C2-O2
4	A	703	GOL	O2-C2-C3-O3
4	A	711	GOL	O1-C1-C2-O2
4	B	707	GOL	O2-C2-C3-O3

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	705	GOL	1	0
4	A	703	GOL	1	0
3	B	606	SO4	1	0
4	B	707	GOL	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	500/505 (99%)	0.32	15 (3%)	50	56	30, 37, 48, 56	0
1	B	503/505 (99%)	0.45	43 (8%)	10	13	24, 35, 52, 54	0
1	C	500/505 (99%)	0.40	36 (7%)	15	19	28, 37, 52, 56	0
1	D	482/505 (95%)	0.48	47 (9%)	7	10	28, 37, 55, 60	0
All	All	1985/2020 (98%)	0.41	141 (7%)	16	20	24, 37, 52, 60	0

All (141) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	124	ALA	6.6
1	D	105	VAL	5.9
1	B	1	MET	5.8
1	D	397	LEU	5.7
1	B	71	VAL	5.6
1	D	130	LEU	5.4
1	C	147	ASN	5.4
1	D	195	GLY	5.0
1	B	70	SER	4.9
1	C	0	SER	4.9
1	D	193	ALA	4.8
1	B	0	SER	4.8
1	D	373	GLY	4.7
1	B	69	LYS	4.5
1	B	128	PRO	4.3
1	A	112	GLN	4.2
1	C	117	CYS	4.1
1	C	70	SER	4.1
1	C	116	THR	4.1
1	B	145	ALA	4.0
1	C	99	PHE	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	112	GLN	4.0
1	D	146	GLY	4.0
1	B	73	ASP	4.0
1	A	0	SER	3.9
1	D	147	ASN	3.8
1	C	2	LYS	3.8
1	C	126	PHE	3.7
1	B	142	LYS	3.6
1	C	67	ALA	3.6
1	B	126	PHE	3.5
1	B	2	LYS	3.4
1	D	127	LEU	3.4
1	C	71	VAL	3.4
1	C	105	VAL	3.4
1	B	112	GLN	3.4
1	D	71	VAL	3.4
1	D	129	THR	3.4
1	D	103	LYS	3.4
1	A	147	ASN	3.4
1	C	1	MET	3.4
1	A	120	LYS	3.3
1	D	0	SER	3.3
1	C	69	LYS	3.2
1	C	89	TRP	3.2
1	D	104	THR	3.2
1	B	110	ALA	3.2
1	B	147	ASN	3.1
1	C	120	LYS	3.1
1	B	129	THR	3.1
1	B	397	LEU	3.1
1	D	99	PHE	3.1
1	D	396	THR	3.0
1	B	377	ALA	3.0
1	C	124	ALA	3.0
1	C	114	TRP	3.0
1	A	1	MET	3.0
1	B	151	HIS	3.0
1	D	135	ALA	2.9
1	C	73	ASP	2.9
1	C	194	LEU	2.9
1	C	192	LYS	2.9
1	C	9	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	128	PRO	2.8
1	B	117	CYS	2.8
1	B	108	THR	2.8
1	C	125	GLY	2.8
1	D	194	LEU	2.8
1	B	152	PRO	2.8
1	C	113	VAL	2.7
1	D	151	HIS	2.7
1	D	374	ASN	2.7
1	B	138	ARG	2.7
1	D	381	PRO	2.7
1	D	382	ARG	2.7
1	B	127	LEU	2.7
1	D	412	GLY	2.7
1	C	119	GLU	2.6
1	D	101	GLU	2.6
1	B	194	LEU	2.6
1	D	378	GLU	2.6
1	D	134	ILE	2.6
1	D	423	LEU	2.6
1	D	139	GLU	2.5
1	A	124	ALA	2.5
1	B	143	LEU	2.5
1	C	373	GLY	2.5
1	B	101	GLU	2.5
1	D	192	LYS	2.5
1	B	95	LEU	2.4
1	C	106	LEU	2.4
1	B	120	LYS	2.4
1	B	109	LYS	2.4
1	D	413	GLY	2.4
1	A	128	PRO	2.4
1	B	380	VAL	2.4
1	D	279	LYS	2.4
1	D	72	GLY	2.4
1	D	100	VAL	2.4
1	D	377	ALA	2.4
1	D	408	VAL	2.3
1	D	442	GLU	2.3
1	B	131	LYS	2.3
1	B	135	ALA	2.3
1	B	136	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	398	GLY	2.3
1	A	142	LYS	2.3
1	D	400	ASP	2.3
1	B	133	LEU	2.3
1	A	101	GLU	2.3
1	B	405	LEU	2.2
1	A	180	LEU	2.2
1	A	117	CYS	2.2
1	D	138	ARG	2.2
1	C	100	VAL	2.2
1	B	179	TRP	2.2
1	A	397	LEU	2.2
1	B	195	GLY	2.2
1	B	123	PHE	2.2
1	D	132	GLU	2.2
1	C	72	GLY	2.2
1	A	176	VAL	2.1
1	A	116	THR	2.1
1	C	101	GLU	2.1
1	C	109	LYS	2.1
1	B	106	LEU	2.1
1	D	411	SER	2.1
1	D	383	VAL	2.1
1	B	72	GLY	2.1
1	C	131	LYS	2.1
1	B	378	GLU	2.1
1	D	98	GLU	2.0
1	D	496	ARG	2.0
1	D	1	MET	2.0
1	D	145	ALA	2.0
1	A	360	VAL	2.0
1	B	176	VAL	2.0
1	C	146	GLY	2.0
1	C	57	ALA	2.0
1	C	169	LEU	2.0
1	D	341	ARG	2.0

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(\AA^2)	Q<0.9
1	CSX	C	34	7/8	0.90	0.19	32,33,38,42	0
1	CSX	B	34	7/8	0.92	0.12	29,30,38,40	0
1	CSX	D	34	7/8	0.93	0.16	31,32,38,38	0
1	CSX	A	34	7/8	0.95	0.09	34,35,40,44	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	A	708	6/6	0.56	0.27	51,52,53,54	0
5	GLY	B	701	4/5	0.60	0.27	38,40,40,40	0
6	ALA	B	702	5/6	0.70	0.19	41,41,42,42	0
4	GOL	A	705	6/6	0.74	0.16	40,42,42,42	0
4	GOL	A	703	6/6	0.78	0.19	45,46,47,47	0
4	GOL	B	709	6/6	0.79	0.20	45,47,47,47	0
3	SO4	B	602	5/5	0.79	0.30	81,81,82,82	0
4	GOL	A	710	6/6	0.82	0.17	49,50,51,51	0
4	GOL	A	711	6/6	0.82	0.23	50,52,54,55	0
3	SO4	B	612	5/5	0.87	0.20	54,57,58,59	0
4	GOL	B	707	6/6	0.89	0.13	56,56,57,57	0
4	GOL	A	704	6/6	0.89	0.17	28,34,36,40	0
3	SO4	B	611	5/5	0.90	0.30	70,70,71,71	0
3	SO4	C	605	5/5	0.91	0.23	47,49,50,50	0
4	GOL	B	706	6/6	0.93	0.15	31,34,36,39	0
3	SO4	B	606	5/5	0.93	0.18	49,51,53,54	0
3	SO4	C	613	5/5	0.93	0.15	63,63,65,65	0
3	SO4	B	607	5/5	0.93	0.31	64,66,66,66	0
3	SO4	A	609	5/5	0.94	0.20	57,57,58,59	0
3	SO4	D	608	5/5	0.95	0.13	40,40,43,43	0
3	SO4	D	601	5/5	0.96	0.19	59,60,61,61	0
3	SO4	A	604	5/5	0.97	0.24	39,41,45,46	0
3	SO4	A	610	5/5	0.98	0.12	35,35,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	CO	D	999	1/1	0.98	0.08	45,45,45,45	0
3	SO4	C	603	5/5	0.98	0.14	31,33,34,36	0
2	CO	B	999	1/1	0.99	0.08	40,40,40,40	0
2	CO	A	999	1/1	0.99	0.09	43,43,43,43	0
2	CO	C	999	1/1	0.99	0.08	44,44,44,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.