



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:15 AM UTC

PDB ID : 9XAU / pdb_00009xau
Title : Glyoxysomal Citrate Synthase 3 from Arabidopsis thaliana in complex with OAA
Authors : Nishio, K.; Takagi, K.; Mizushima, T.
Deposited on : 2025-10-23
Resolution : 1.95 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

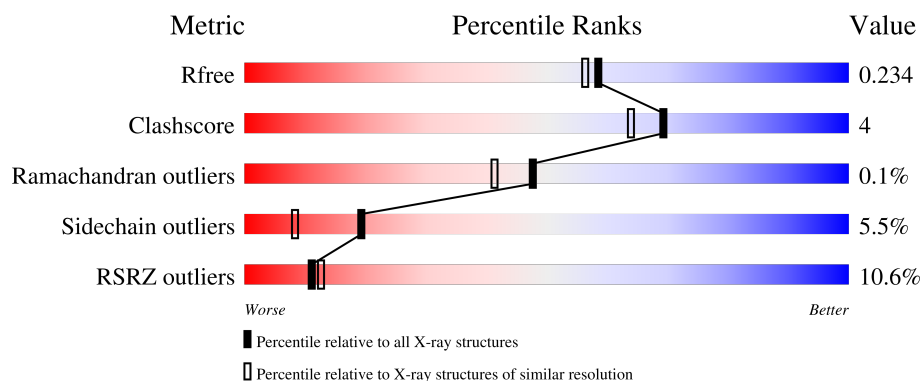
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	479	12% 81% 9% • 9%
1	B	479	11% 78% 12% • 9%
1	C	479	7% 81% 9% • 9%
1	D	479	9% 78% 11% • 9%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 14111 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.

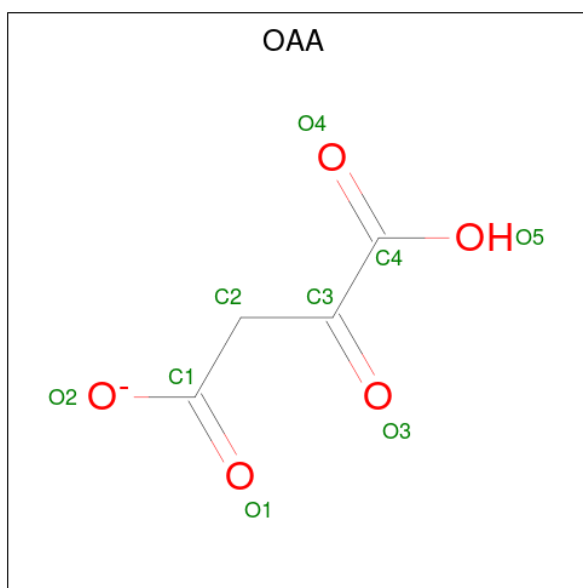
- Molecule 1 is a protein called Citrate synthase 3, peroxisomal.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	0	0	0
			3423	2194	585	630	14			
1	B	437	Total	C	N	O	S	0	0	0
			3413	2186	583	630	14			
1	C	436	Total	C	N	O	S	0	0	0
			3415	2188	584	629	14			
1	D	434	Total	C	N	O	S	0	0	0
			3392	2176	575	627	14			

There are 20 discrepancies between the modelled and reference sequences:

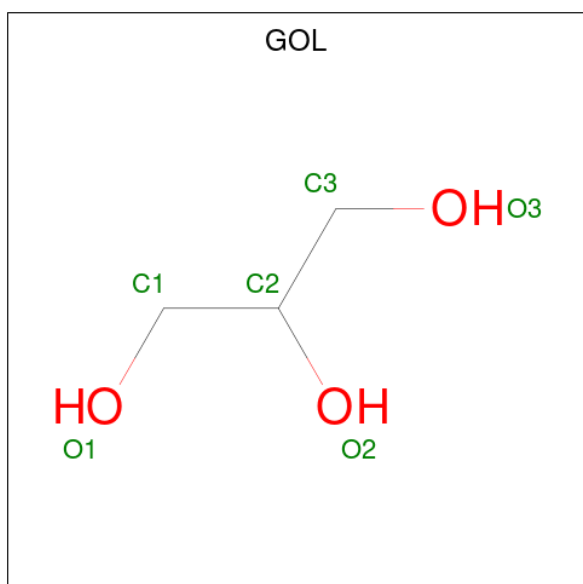
Chain	Residue	Modelled	Actual	Comment	Reference
A	31	GLY	-	expression tag	UNP Q9SJH7
A	32	PRO	-	expression tag	UNP Q9SJH7
A	33	LEU	-	expression tag	UNP Q9SJH7
A	34	GLY	-	expression tag	UNP Q9SJH7
A	35	SER	-	expression tag	UNP Q9SJH7
B	31	GLY	-	expression tag	UNP Q9SJH7
B	32	PRO	-	expression tag	UNP Q9SJH7
B	33	LEU	-	expression tag	UNP Q9SJH7
B	34	GLY	-	expression tag	UNP Q9SJH7
B	35	SER	-	expression tag	UNP Q9SJH7
C	31	GLY	-	expression tag	UNP Q9SJH7
C	32	PRO	-	expression tag	UNP Q9SJH7
C	33	LEU	-	expression tag	UNP Q9SJH7
C	34	GLY	-	expression tag	UNP Q9SJH7
C	35	SER	-	expression tag	UNP Q9SJH7
D	31	GLY	-	expression tag	UNP Q9SJH7
D	32	PRO	-	expression tag	UNP Q9SJH7
D	33	LEU	-	expression tag	UNP Q9SJH7
D	34	GLY	-	expression tag	UNP Q9SJH7
D	35	SER	-	expression tag	UNP Q9SJH7

- Molecule 2 is OXALOACETATE ION (CCD ID: OAA) (formula: $C_4H_3O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			9	4	5		
2	B	1	Total	C	O		
			9	4	5	0	0
2	C	1	Total	C	O	0	0
			9	4	5		
2	D	1	Total	C	O		
			9	4	5	0	0

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

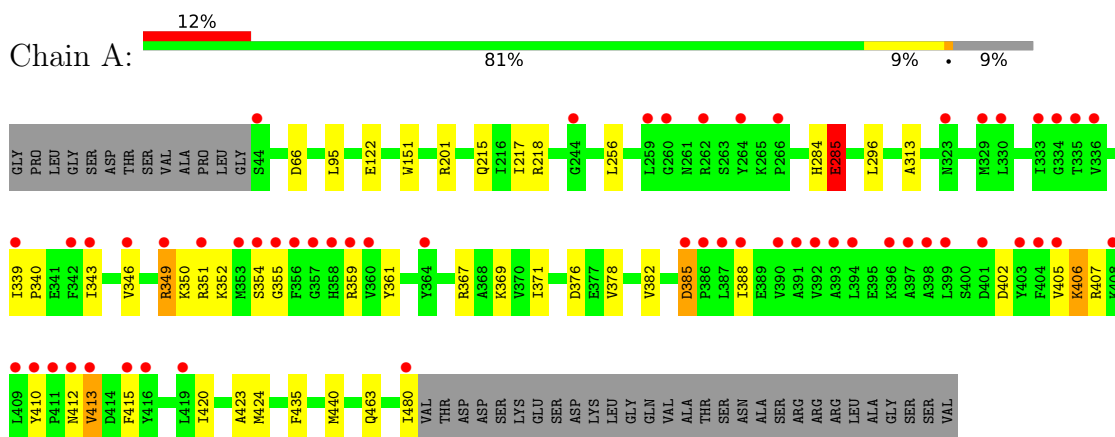
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	120	Total	O	0	0
			120	120		
4	B	92	Total	O	0	0
			92	92		
4	C	115	Total	O	0	0
			115	115		
4	D	99	Total	O	0	0
			99	99		

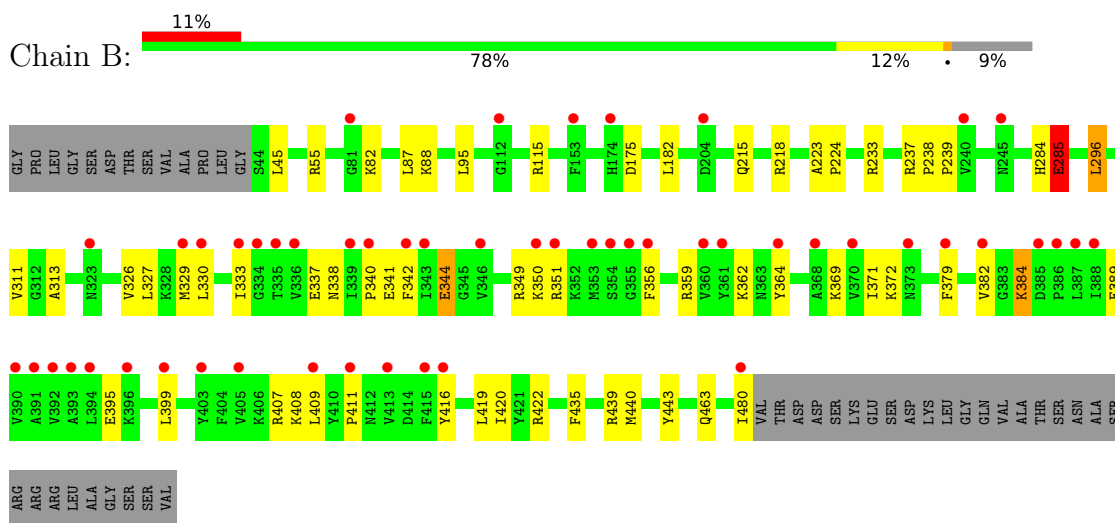
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

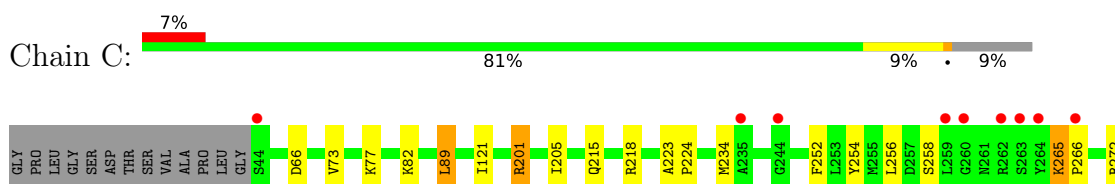
- Molecule 1: Citrate synthase 3, peroxisomal

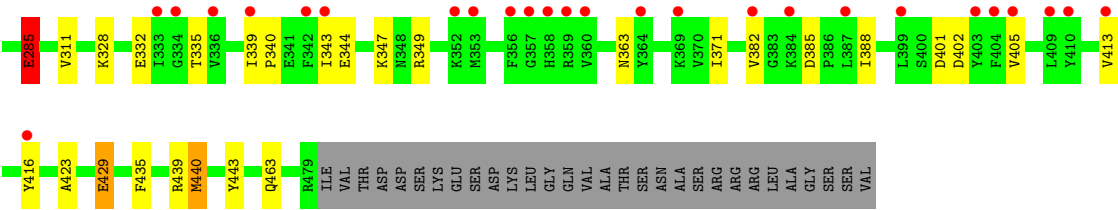


- Molecule 1: Citrate synthase 3, peroxisomal

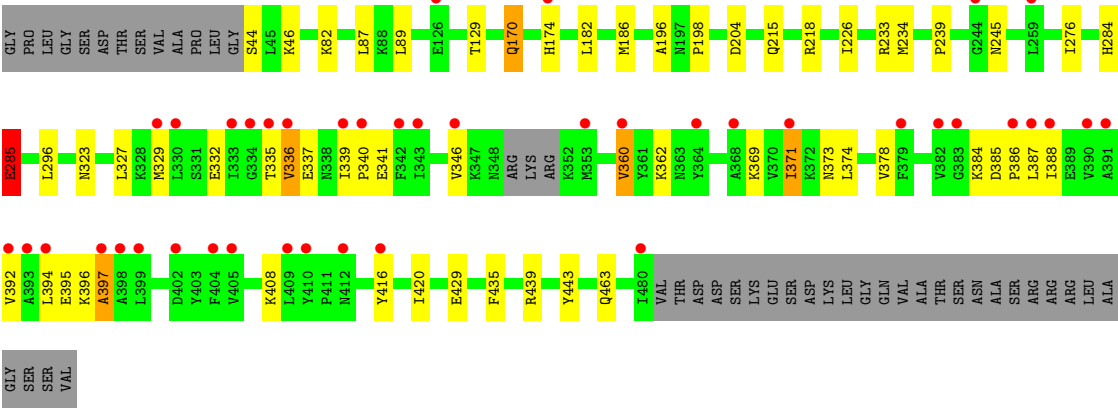
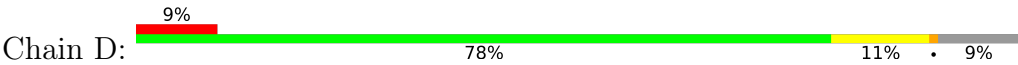


- Molecule 1: Citrate synthase 3, peroxisomal





● Molecule 1: Citrate synthase 3, peroxisomal



GLY
SER
SER
VAL

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	79.08Å 64.73Å 192.51Å 90.00° 92.62° 90.00°	Depositor
Resolution (Å)	48.10 – 1.95 48.10 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.10-1.95) 99.6 (48.10-1.95)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.186 , 0.225 0.195 , 0.234	Depositor DCC
R_{free} test set	7090 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	33.8	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 27.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.089 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14111	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% 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: GOL, OAA

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	0.64	0/3506	1.14	9/4757 (0.2%)
1	B	0.60	0/3496	1.11	6/4746 (0.1%)
1	C	0.64	0/3498	1.12	7/4746 (0.1%)
1	D	0.60	0/3474	1.09	7/4715 (0.1%)
All	All	0.62	0/13974	1.12	29/18964 (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	3
1	C	0	1
All	All	0	5

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	285	GLU	N-CA-CB	-12.47	89.42	110.49
1	D	285	GLU	N-CA-CB	-12.19	89.89	110.49
1	D	285	GLU	CB-CA-C	10.15	130.62	110.42
1	A	285	GLU	CB-CA-C	9.99	128.03	116.54
1	C	285	GLU	N-CA-CB	-9.35	94.69	110.49
1	B	285	GLU	CB-CA-C	9.28	128.89	110.42
1	C	285	GLU	CB-CA-C	8.83	128.00	110.42
1	A	285	GLU	N-CA-CB	-7.23	92.96	111.04
1	A	361	TYR	N-CA-CB	6.91	120.99	109.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	435	PHE	CA-CB-CG	6.74	120.54	113.80
1	A	413	VAL	N-CA-CB	6.63	118.31	110.55
1	D	435	PHE	CA-CB-CG	6.40	120.20	113.80
1	B	88	LYS	N-CA-CB	-6.12	100.62	111.08
1	A	66	ASP	CA-CB-CG	6.04	118.64	112.60
1	C	285	GLU	CB-CG-CD	6.01	122.82	112.60
1	C	66	ASP	CA-CB-CG	6.00	118.60	112.60
1	D	129	THR	CA-CB-OG1	-5.99	100.61	109.60
1	C	435	PHE	CA-CB-CG	5.80	119.60	113.80
1	A	122	GLU	CB-CG-CD	5.72	122.33	112.60
1	D	170	GLN	CB-CA-C	5.58	121.05	109.95
1	B	45	LEU	N-CA-CB	-5.42	102.34	110.73
1	B	435	PHE	CA-CB-CG	5.34	119.14	113.80
1	A	440	MET	CB-CA-C	-5.23	101.78	110.68
1	C	440	MET	CB-CA-C	-5.21	101.82	110.68
1	A	376	ASP	CA-CB-CG	5.21	117.81	112.60
1	C	285	GLU	CG-CD-OE2	-5.17	106.50	118.40
1	B	356	PHE	CA-CB-CG	5.12	118.92	113.80
1	D	360	VAL	CB-CA-C	5.08	115.57	111.05
1	D	435	PHE	N-CA-CB	-5.01	102.74	110.20

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	201	ARG	Sidechain
1	B	115	ARG	Sidechain
1	B	237	ARG	Sidechain
1	B	55	ARG	Sidechain
1	C	201	ARG	Sidechain

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	3423	0	3430	28	0
1	B	3413	0	3401	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3415	0	3419	26	0
1	D	3392	0	3390	25	0
2	A	9	0	2	0	0
2	B	9	0	2	0	0
2	C	9	0	2	0	0
2	D	9	0	2	0	0
3	B	6	0	8	0	0
4	A	120	0	0	1	0
4	B	92	0	0	0	0
4	C	115	0	0	0	0
4	D	99	0	0	1	0
All	All	14111	0	13656	96	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 (96) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:ARG:NH2	4:A:701:HOH:O	1.75	1.19
1:B:395:GLU:O	1:B:399:LEU:HG	1.79	0.83
1:C:272:ARG:HH21	1:C:272:ARG:HG3	1.45	0.81
1:C:463:GLN:NE2	1:D:285:GLU:HG3	1.97	0.79
1:A:285:GLU:HG3	1:B:463:GLN:NE2	1.99	0.77
1:A:355:GLY:O	1:A:412:ASN:HB3	1.86	0.76
1:C:285:GLU:HG3	1:D:463:GLN:NE2	2.04	0.72
1:C:382:VAL:HG21	1:C:423:ALA:HB1	1.71	0.72
1:D:215:GLN:HE22	1:D:218:ARG:HH11	1.41	0.67
1:B:395:GLU:OE1	1:B:416:TYR:OH	2.11	0.67
1:C:285:GLU:HG3	1:D:463:GLN:CD	2.19	0.67
1:D:378:VAL:HG21	1:D:420:ILE:HG23	1.77	0.65
1:A:215:GLN:HE22	1:A:218:ARG:HH11	1.44	0.65
1:A:367:ARG:HB2	1:A:413:VAL:HG11	1.79	0.64
1:A:367:ARG:HB2	1:A:413:VAL:CG1	2.27	0.64
1:C:311:VAL:CG1	1:C:440:MET:HE1	2.28	0.64
1:C:215:GLN:HE22	1:C:218:ARG:HH11	1.45	0.63
1:B:364:TYR:OH	1:B:399:LEU:HD13	1.98	0.63
1:A:402:ASP:HA	1:A:405:VAL:HB	1.80	0.62
1:B:351:ARG:HH21	1:B:351:ARG:HG3	1.65	0.61
1:A:339:ILE:HB	1:A:340:PRO:HD3	1.83	0.60
1:D:336:VAL:O	1:D:339:ILE:HG12	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:272:ARG:HG3	1:C:272:ARG:NH2	2.14	0.58
1:A:385:ASP:OD1	1:A:388:ILE:HG12	2.04	0.58
1:B:215:GLN:HE22	1:B:218:ARG:HH11	1.51	0.57
1:C:385:ASP:HB3	1:C:388:ILE:HG12	1.86	0.57
1:B:95:LEU:HD12	1:B:359:ARG:NH1	2.20	0.57
1:A:151:TRP:CZ3	1:A:217:ILE:HD11	2.41	0.56
1:C:340:PRO:O	1:C:343:ILE:HG13	2.07	0.55
1:A:346:VAL:O	1:A:349:ARG:NH1	2.39	0.54
1:A:285:GLU:HG3	1:B:463:GLN:CD	2.33	0.54
1:D:385:ASP:OD1	1:D:386:PRO:HD2	2.06	0.54
1:A:296:LEU:HD22	1:B:313:ALA:HB2	1.90	0.53
1:C:89:LEU:HD22	1:D:89:LEU:HG	1.90	0.53
1:C:463:GLN:NE2	1:D:285:GLU:CG	2.72	0.52
1:B:311:VAL:CG1	1:B:440:MET:HE1	2.41	0.51
1:C:371:ILE:HG22	1:C:416:TYR:HB2	1.93	0.51
1:C:311:VAL:HG13	1:C:440:MET:HE1	1.92	0.51
1:D:339:ILE:HB	1:D:340:PRO:HD3	1.93	0.51
1:B:362:LYS:HB3	1:B:408:LYS:HG2	1.92	0.50
1:A:463:GLN:NE2	1:B:285:GLU:HG3	2.25	0.50
1:B:329:MET:O	1:B:333:ILE:HG13	2.11	0.50
1:A:151:TRP:CE3	1:A:217:ILE:HD11	2.47	0.50
1:A:463:GLN:CD	1:B:285:GLU:HG2	2.36	0.49
1:D:362:LYS:HB3	1:D:408:LYS:HD3	1.93	0.49
1:B:395:GLU:OE2	1:B:399:LEU:HD11	2.13	0.49
1:B:223:ALA:HB3	1:B:224:PRO:HD3	1.95	0.48
1:C:463:GLN:CD	1:D:285:GLU:HG2	2.39	0.47
1:A:378:VAL:HG21	1:A:420:ILE:HG23	1.97	0.47
1:C:254:TYR:O	1:C:258:SER:HB2	2.14	0.47
1:D:186:MET:HE3	4:D:734:HOH:O	2.14	0.47
1:C:234:MET:HE1	1:C:429:GLU:OE1	2.15	0.47
1:D:371:ILE:HG21	1:D:416:TYR:HB2	1.98	0.46
1:D:385:ASP:OD1	1:D:387:LEU:HD23	2.15	0.46
1:D:392:VAL:O	1:D:396:LYS:HG2	2.14	0.46
1:A:313:ALA:HB2	1:B:296:LEU:HD22	1.98	0.46
1:D:170:GLN:OE1	1:D:239:PRO:HB3	2.16	0.46
1:D:396:LYS:O	1:D:397:ALA:HB2	2.16	0.46
1:B:175:ASP:OD1	1:B:175:ASP:N	2.46	0.46
1:B:326:VAL:O	1:B:330:LEU:HG	2.17	0.45
1:B:379:PHE:HB3	1:B:384:LYS:HB3	1.98	0.45
1:C:347:LYS:NZ	1:C:401:ASP:OD2	2.49	0.45
1:A:413:VAL:C	1:A:415:PHE:H	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:395:GLU:HG3	1:B:411:PRO:CG	2.47	0.45
1:A:340:PRO:HA	1:A:343:ILE:CG1	2.47	0.44
1:B:338:ASN:O	1:B:342:PHE:N	2.46	0.44
1:B:223:ALA:N	1:B:224:PRO:CD	2.79	0.44
1:C:463:GLN:CD	1:D:285:GLU:CG	2.91	0.44
1:A:412:ASN:CG	1:A:413:VAL:N	2.76	0.44
1:C:252:PHE:CZ	1:C:256:LEU:HD11	2.53	0.43
1:C:339:ILE:HB	1:C:340:PRO:HD3	2.01	0.43
1:A:412:ASN:CG	1:A:413:VAL:H	2.26	0.43
1:A:285:GLU:CG	1:B:463:GLN:CD	2.91	0.42
1:D:276:ILE:CG2	1:D:374:LEU:HD11	2.49	0.42
1:C:223:ALA:N	1:C:224:PRO:CD	2.82	0.42
1:C:439:ARG:HG3	1:C:443:TYR:CZ	2.55	0.42
1:B:182:LEU:C	1:B:182:LEU:HD13	2.45	0.42
1:C:265:LYS:HA	1:C:266:PRO:HD3	1.94	0.41
1:A:382:VAL:HG21	1:A:423:ALA:HB1	2.02	0.41
1:D:44:SER:OG	1:D:46:LYS:HB3	2.20	0.41
1:B:395:GLU:HG3	1:B:411:PRO:HG2	2.01	0.41
1:B:238:PRO:HA	1:B:239:PRO:HD3	1.91	0.41
1:B:340:PRO:O	1:B:344:GLU:HB3	2.21	0.41
1:C:121:ILE:HD12	1:C:121:ILE:HA	1.94	0.41
1:A:420:ILE:O	1:A:424:MET:HG3	2.21	0.41
1:A:402:ASP:O	1:A:406:LYS:HG3	2.21	0.41
1:C:201:ARG:HB3	1:C:205:ILE:HD13	2.03	0.41
1:D:395:GLU:OE1	1:D:416:TYR:OH	2.34	0.41
1:D:439:ARG:HG3	1:D:443:TYR:CZ	2.55	0.41
1:D:182:LEU:HD23	1:D:226:ILE:HG22	2.03	0.41
1:B:371:ILE:HG23	1:B:420:ILE:CD1	2.51	0.40
1:A:340:PRO:HA	1:A:343:ILE:HG13	2.02	0.40
1:A:463:GLN:NE2	1:B:285:GLU:CG	2.83	0.40
1:B:416:TYR:HA	1:B:419:LEU:HD12	2.02	0.40
1:B:439:ARG:HG3	1:B:443:TYR:CZ	2.56	0.40
1:D:196:ALA:O	1:D:198:PRO:HD3	2.21	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	435/479 (91%)	425 (98%)	10 (2%)	0	100	100
1	B	435/479 (91%)	422 (97%)	13 (3%)	0	100	100
1	C	434/479 (91%)	425 (98%)	9 (2%)	0	100	100
1	D	430/479 (90%)	422 (98%)	7 (2%)	1 (0%)	43	36
All	All	1734/1916 (90%)	1694 (98%)	39 (2%)	1 (0%)	48	41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	397	ALA

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	366/399 (92%)	350 (96%)	16 (4%)	25	15
1	B	363/399 (91%)	342 (94%)	21 (6%)	18	7
1	C	365/399 (92%)	349 (96%)	16 (4%)	25	15
1	D	363/399 (91%)	336 (93%)	27 (7%)	13	4
All	All	1457/1596 (91%)	1377 (94%)	80 (6%)	19	8

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	LEU
1	A	256	LEU
1	A	284	HIS
1	A	285	GLU
1	A	349	ARG
1	A	350	LYS
1	A	351	ARG
1	A	352	LYS
1	A	354	SER
1	A	369	LYS
1	A	371	ILE
1	A	385	ASP
1	A	406	LYS
1	A	407	ARG
1	A	410	TYR
1	A	480	ILE
1	B	82	LYS
1	B	87	LEU
1	B	233	ARG
1	B	284	HIS
1	B	285	GLU
1	B	296	LEU
1	B	327	LEU
1	B	337	GLU
1	B	341	GLU
1	B	344	GLU
1	B	349	ARG
1	B	350	LYS
1	B	369	LYS
1	B	372	LYS
1	B	382	VAL
1	B	384	LYS
1	B	389	GLU
1	B	407	ARG
1	B	409	LEU
1	B	422	ARG
1	B	480	ILE
1	C	73	VAL
1	C	77	LYS
1	C	82	LYS
1	C	89	LEU
1	C	265	LYS
1	C	285	GLU

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Mol	Chain	Res	Type
1	C	328	LYS
1	C	332	GLU
1	C	335	THR
1	C	344	GLU
1	C	349	ARG
1	C	363	ASN
1	C	402	ASP
1	C	405	VAL
1	C	413	VAL
1	C	429	GLU
1	D	82	LYS
1	D	87	LEU
1	D	174	HIS
1	D	204	ASP
1	D	233	ARG
1	D	234	MET
1	D	245	ASN
1	D	284	HIS
1	D	285	GLU
1	D	296	LEU
1	D	323	ASN
1	D	327	LEU
1	D	329	MET
1	D	332	GLU
1	D	335	THR
1	D	336	VAL
1	D	337	GLU
1	D	341	GLU
1	D	346	VAL
1	D	360	VAL
1	D	369	LYS
1	D	371	ILE
1	D	373	ASN
1	D	384	LYS
1	D	388	ILE
1	D	394	LEU
1	D	429	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	215	GLN

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Mol	Chain	Res	Type
1	A	338	ASN
1	B	127	ASN
1	B	203	GLN
1	B	215	GLN
1	B	373	ASN
1	B	462	GLN
1	C	174	HIS
1	C	215	GLN
1	C	348	ASN
1	C	363	ASN
1	D	59	ASN
1	D	163	GLN
1	D	215	GLN
1	D	323	ASN
1	D	463	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

5 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	OAA	B	601	-	8,8,8	4.32	1 (12%)	8,10,10	1.58	2 (25%)
2	OAA	A	601	-	8,8,8	4.12	3 (37%)	8,10,10	1.44	1 (12%)
3	GOL	B	602	-	5,5,5	0.18	0	5,5,5	0.48	0
2	OAA	D	601	-	8,8,8	4.56	3 (37%)	8,10,10	1.15	0
2	OAA	C	601	-	8,8,8	4.50	2 (25%)	8,10,10	1.60	2 (25%)

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	OAA	B	601	-	-	0/8/8/8	-
2	OAA	A	601	-	-	0/8/8/8	-
3	GOL	B	602	-	-	4/4/4/4	-
2	OAA	D	601	-	-	0/8/8/8	-
2	OAA	C	601	-	-	0/8/8/8	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	OAA	C3-C4	-12.28	1.35	1.53
2	D	601	OAA	C3-C4	-12.19	1.35	1.53
2	B	601	OAA	C3-C4	-11.78	1.35	1.53
2	A	601	OAA	C3-C4	-10.89	1.37	1.53
2	A	601	OAA	O5-C4	-3.04	1.22	1.30
2	C	601	OAA	O5-C4	-2.37	1.24	1.30
2	D	601	OAA	O2-C1	-2.29	1.23	1.30
2	D	601	OAA	O5-C4	-2.13	1.24	1.30
2	A	601	OAA	O2-C1	-2.05	1.24	1.30

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	OAA	O5-C4-C3	2.36	120.14	113.59
2	B	601	OAA	O4-C4-C3	-2.36	118.87	121.81
2	B	601	OAA	O5-C4-C3	2.35	120.12	113.59
2	C	601	OAA	O5-C4-C3	2.16	119.59	113.59
2	C	601	OAA	O4-C4-C3	-2.00	119.32	121.81

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	602	GOL	O1-C1-C2-C3
3	B	602	GOL	C1-C2-C3-O3
3	B	602	GOL	O2-C2-C3-O3
3	B	602	GOL	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

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	437/479 (91%)	0.49	56 (12%) 7 9	21, 34, 95, 128	0
1	B	437/479 (91%)	0.59	52 (11%) 9 10	23, 40, 118, 151	0
1	C	436/479 (91%)	0.36	35 (8%) 18 21	22, 34, 80, 103	0
1	D	434/479 (90%)	0.54	42 (9%) 13 15	23, 40, 108, 137	0
All	All	1744/1916 (91%)	0.49	185 (10%) 11 13	21, 37, 100, 151	0

All (185) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	409	LEU	7.6
1	A	415	PHE	6.3
1	A	404	PHE	6.2
1	B	394	LEU	5.5
1	C	266	PRO	5.3
1	A	411	PRO	5.2
1	D	399	LEU	4.9
1	A	410	TYR	4.9
1	B	391	ALA	4.7
1	B	368	ALA	4.6
1	B	392	VAL	4.5
1	D	364	TYR	4.5
1	B	364	TYR	4.4
1	A	403	TYR	4.4
1	D	391	ALA	4.4
1	C	364	TYR	4.4
1	D	343	ILE	4.4
1	C	358	HIS	4.4
1	A	360	VAL	4.3
1	B	386	PRO	4.3
1	D	405	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	330	LEU	4.2
1	D	388	ILE	4.1
1	D	394	LEU	4.1
1	C	357	GLY	4.0
1	B	388	ILE	4.0
1	C	410	TYR	3.9
1	A	354	SER	3.9
1	A	266	PRO	3.9
1	A	356	PHE	3.9
1	A	399	LEU	3.9
1	A	355	GLY	3.9
1	A	336	VAL	3.8
1	A	343	ILE	3.7
1	A	353	MET	3.7
1	A	359	ARG	3.7
1	C	260	GLY	3.7
1	A	416	TYR	3.6
1	D	336	VAL	3.6
1	C	409	LEU	3.6
1	D	387	LEU	3.6
1	C	353	MET	3.5
1	B	342	PHE	3.5
1	A	394	LEU	3.5
1	B	343	ILE	3.5
1	A	412	ASN	3.5
1	D	342	PHE	3.5
1	C	264	TYR	3.4
1	A	413	VAL	3.4
1	C	399	LEU	3.4
1	A	264	TYR	3.4
1	C	416	TYR	3.4
1	D	333	ILE	3.4
1	D	390	VAL	3.4
1	D	386	PRO	3.3
1	A	398	ALA	3.3
1	B	399	LEU	3.3
1	C	359	ARG	3.3
1	A	346	VAL	3.2
1	B	387	LEU	3.2
1	A	480	ILE	3.2
1	B	393	ALA	3.2
1	A	405	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	330	LEU	3.2
1	B	333	ILE	3.2
1	D	174	HIS	3.2
1	A	335	THR	3.1
1	A	397	ALA	3.1
1	B	336	VAL	3.1
1	B	480	ILE	3.1
1	B	382	VAL	3.1
1	A	244	GLY	3.0
1	D	334	GLY	3.0
1	D	339	ILE	3.0
1	B	405	VAL	3.0
1	B	174	HIS	3.0
1	B	335	THR	3.0
1	D	392	VAL	2.9
1	C	356	PHE	2.9
1	A	391	ALA	2.9
1	D	330	LEU	2.9
1	A	408	LYS	2.9
1	B	354	SER	2.9
1	A	260	GLY	2.9
1	D	409	LEU	2.9
1	C	336	VAL	2.8
1	A	393	ALA	2.8
1	D	402	ASP	2.8
1	A	390	VAL	2.8
1	B	153	PHE	2.8
1	D	259	LEU	2.8
1	B	411	PRO	2.8
1	C	44	SER	2.8
1	B	396	LYS	2.8
1	B	346	VAL	2.8
1	B	390	VAL	2.8
1	B	413	VAL	2.8
1	C	352	LYS	2.7
1	C	244	GLY	2.7
1	A	387	LEU	2.7
1	B	323	ASN	2.7
1	D	398	ALA	2.7
1	B	416	TYR	2.7
1	A	329	MET	2.7
1	B	409	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	396	LYS	2.7
1	B	373	ASN	2.7
1	B	370	VAL	2.7
1	D	416	TYR	2.6
1	A	358	HIS	2.6
1	D	371	ILE	2.6
1	A	349	ARG	2.6
1	A	342	PHE	2.6
1	B	355	GLY	2.6
1	D	335	THR	2.6
1	D	346	VAL	2.6
1	D	412	ASN	2.6
1	A	388	ILE	2.5
1	C	333	ILE	2.5
1	C	334	GLY	2.5
1	A	392	VAL	2.5
1	C	384	LYS	2.5
1	B	334	GLY	2.5
1	C	360	VAL	2.5
1	C	404	PHE	2.5
1	D	244	GLY	2.5
1	A	333	ILE	2.5
1	A	339	ILE	2.5
1	B	379	PHE	2.4
1	C	262	ARG	2.4
1	B	353	MET	2.4
1	D	360	VAL	2.4
1	A	259	LEU	2.4
1	B	360	VAL	2.4
1	D	329	MET	2.4
1	C	263	SER	2.4
1	B	350	LYS	2.4
1	D	397	ALA	2.3
1	D	353	MET	2.3
1	B	351	ARG	2.3
1	B	385	ASP	2.3
1	B	356	PHE	2.3
1	B	340	PRO	2.3
1	D	480	ILE	2.3
1	A	262	ARG	2.2
1	A	386	PRO	2.2
1	B	361	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	368	ALA	2.2
1	D	383	GLY	2.2
1	C	387	LEU	2.2
1	A	44	SER	2.2
1	C	235	ALA	2.2
1	D	393	ALA	2.2
1	C	405	VAL	2.2
1	C	403	TYR	2.2
1	D	404	PHE	2.2
1	C	343	ILE	2.2
1	C	413	VAL	2.2
1	A	401	ASP	2.2
1	B	112	GLY	2.2
1	D	126	GLU	2.1
1	A	385	ASP	2.1
1	B	204	ASP	2.1
1	A	357	GLY	2.1
1	B	81	GLY	2.1
1	C	259	LEU	2.1
1	C	342	PHE	2.1
1	D	379	PHE	2.1
1	B	339	ILE	2.1
1	B	403	TYR	2.1
1	D	382	VAL	2.1
1	C	369	LYS	2.1
1	B	329	MET	2.1
1	D	340	PRO	2.1
1	B	415	PHE	2.1
1	C	339	ILE	2.1
1	D	410	TYR	2.1
1	A	351	ARG	2.1
1	A	323	ASN	2.1
1	A	364	TYR	2.0
1	B	240	VAL	2.0
1	A	419	LEU	2.0
1	A	334	GLY	2.0
1	B	245	ASN	2.0
1	C	382	VAL	2.0

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

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

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($\text{\AA}^2$)	Q<0.9
3	GOL	B	602	6/6	0.89	0.10	49,59,63,67	0
2	OAA	B	601	9/9	0.90	0.10	37,39,48,49	0
2	OAA	D	601	9/9	0.91	0.10	34,39,46,49	0
2	OAA	C	601	9/9	0.93	0.08	34,38,46,47	0
2	OAA	A	601	9/9	0.95	0.07	29,34,39,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.