



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 11:16 PM UTC

PDB ID : 4J15 / pdb_00004j15
Title : Crystal structure of human cytosolic aspartyl-tRNA synthetase, a component of multi-tRNA synthetase complex
Authors : Kim, K.R.; Park, S.H.; Kim, H.S.; Kim, B.-G.; Kim, D.G.; Rhee, K.H.; Park, M.S.; Kim, H.-J.; Kim, S.; Han, B.W.
Deposited on : 2013-02-01
Resolution : 2.24 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

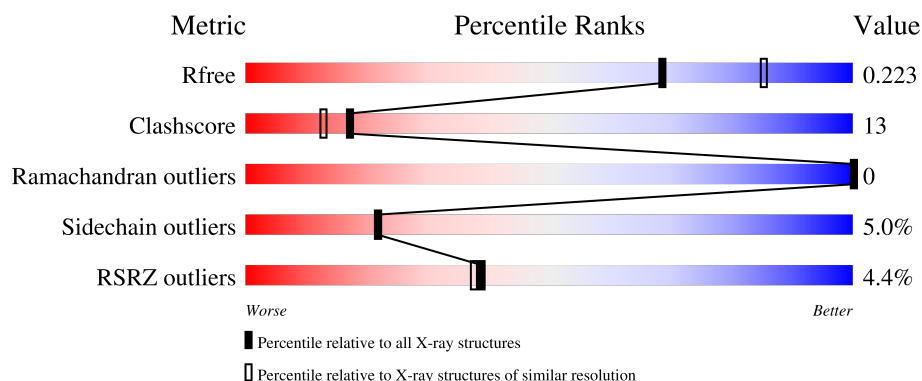
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.24 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	3416 (2.26-2.22)
Clashscore	190562	3556 (2.26-2.22)
Ramachandran outliers	187476	3500 (2.26-2.22)
Sidechain outliers	187428	3501 (2.26-2.22)
RSRZ outliers	180081	3415 (2.26-2.22)

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	521	
1	B	521	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7392 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 Aspartate-tRNA ligase, cytoplasmic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	431	Total	C	N	O	S	0	1	0
			3490	2213	612	645	20			
1	B	430	Total	C	N	O	S	0	3	0
			3500	2219	614	647	20			

There are 40 discrepancies between the modelled and reference sequences:

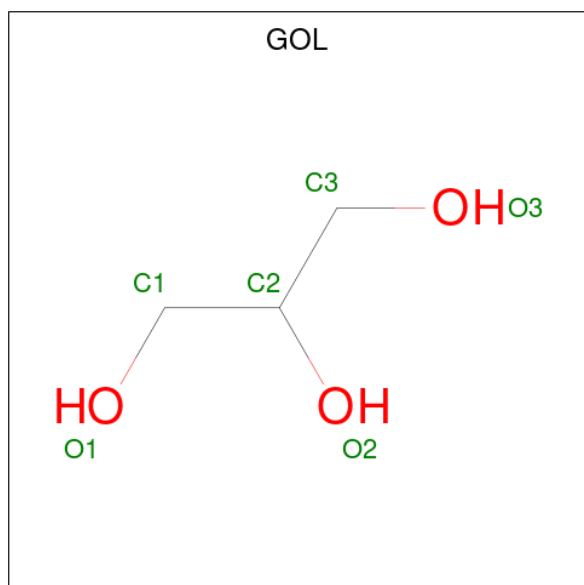
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP P14868
A	-18	GLY	-	expression tag	UNP P14868
A	-17	SER	-	expression tag	UNP P14868
A	-16	SER	-	expression tag	UNP P14868
A	-15	HIS	-	expression tag	UNP P14868
A	-14	HIS	-	expression tag	UNP P14868
A	-13	HIS	-	expression tag	UNP P14868
A	-12	HIS	-	expression tag	UNP P14868
A	-11	HIS	-	expression tag	UNP P14868
A	-10	HIS	-	expression tag	UNP P14868
A	-9	SER	-	expression tag	UNP P14868
A	-8	SER	-	expression tag	UNP P14868
A	-7	GLY	-	expression tag	UNP P14868
A	-6	LEU	-	expression tag	UNP P14868
A	-5	VAL	-	expression tag	UNP P14868
A	-4	PRO	-	expression tag	UNP P14868
A	-3	ARG	-	expression tag	UNP P14868
A	-2	GLY	-	expression tag	UNP P14868
A	-1	SER	-	expression tag	UNP P14868
A	0	HIS	-	expression tag	UNP P14868
B	-19	MET	-	expression tag	UNP P14868
B	-18	GLY	-	expression tag	UNP P14868
B	-17	SER	-	expression tag	UNP P14868
B	-16	SER	-	expression tag	UNP P14868
B	-15	HIS	-	expression tag	UNP P14868

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP P14868
B	-13	HIS	-	expression tag	UNP P14868
B	-12	HIS	-	expression tag	UNP P14868
B	-11	HIS	-	expression tag	UNP P14868
B	-10	HIS	-	expression tag	UNP P14868
B	-9	SER	-	expression tag	UNP P14868
B	-8	SER	-	expression tag	UNP P14868
B	-7	GLY	-	expression tag	UNP P14868
B	-6	LEU	-	expression tag	UNP P14868
B	-5	VAL	-	expression tag	UNP P14868
B	-4	PRO	-	expression tag	UNP P14868
B	-3	ARG	-	expression tag	UNP P14868
B	-2	GLY	-	expression tag	UNP P14868
B	-1	SER	-	expression tag	UNP P14868
B	0	HIS	-	expression tag	UNP P14868

- 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	A	1	Total	C	O	0	0
			6	3	3		

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

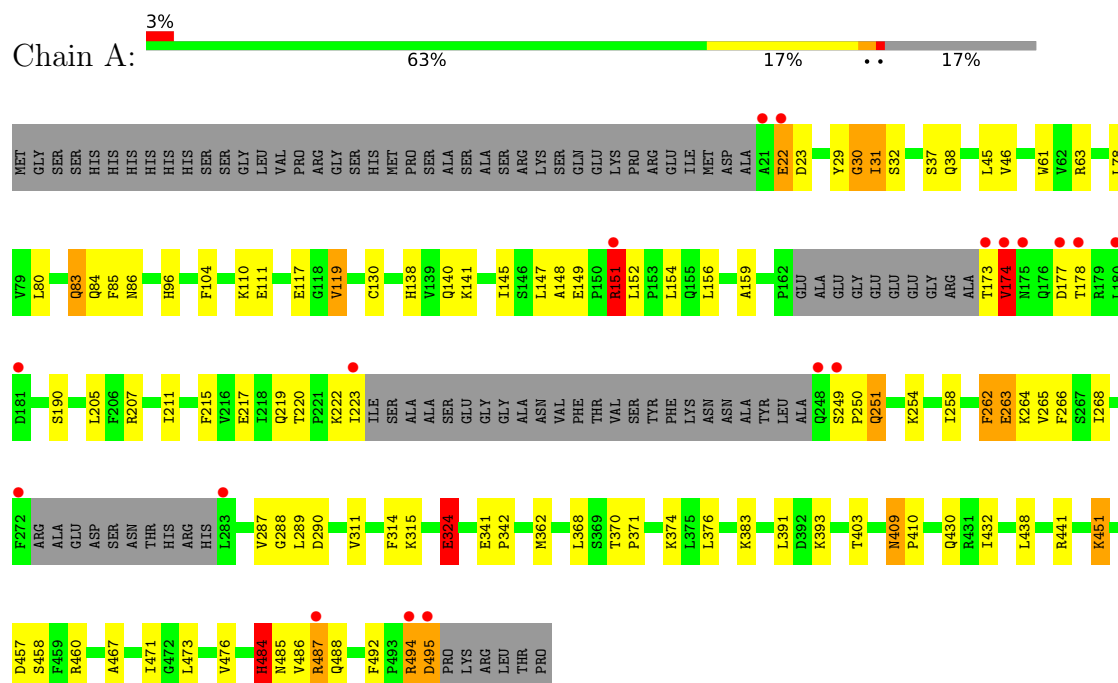
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	177	Total	O	0	0
			177	177		
3	B	177	Total	O	0	0
			177	177		

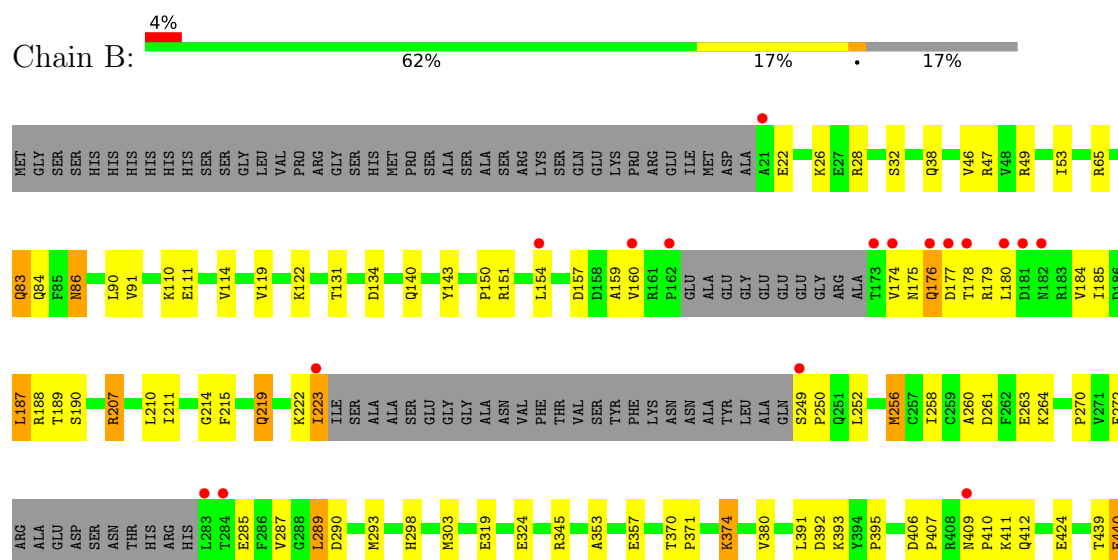
3 Residue-property plots

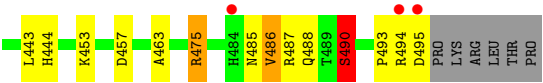
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Aspartate-tRNA ligase, cytoplasmic



- Molecule 1: Aspartate-tRNA ligase, cytoplasmic





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.88Å 141.92Å 68.50Å 90.00° 102.19° 90.00°	Depositor
Resolution (Å)	50.00 – 2.24 50.00 – 2.24	Depositor EDS
% Data completeness (in resolution range)	98.7 (50.00-2.24) 98.7 (50.00-2.24)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.77 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.197 , 0.228 0.199 , 0.223	Depositor DCC
R_{free} test set	2479 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	32.6	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 30.9	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	0.95	EDS
Total number of atoms	7392	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.87% 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

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	1.20	15/3556 (0.4%)	1.03	14/4796 (0.3%)
1	B	1.24	20/3567 (0.6%)	1.09	16/4811 (0.3%)
All	All	1.22	35/7123 (0.5%)	1.06	30/9607 (0.3%)

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	145	ILE	C-O	-8.61	1.15	1.24
1	A	30	GLY	C-O	-6.85	1.16	1.23
1	B	494	ARG	C-N	6.54	1.42	1.33
1	B	38	GLN	C-O	-6.53	1.15	1.24
1	B	439	THR	C-O	-6.52	1.16	1.24
1	B	475	ARG	C-O	-6.17	1.17	1.24
1	B	463	ALA	C-O	-6.15	1.16	1.24
1	B	207	ARG	C-O	-6.09	1.17	1.24
1	A	31	ILE	C-O	-6.00	1.17	1.24
1	B	490	SER	C-O	-5.94	1.17	1.24
1	B	391	LEU	C-O	-5.89	1.17	1.24
1	A	487	ARG	C-O	-5.81	1.16	1.24
1	B	289	LEU	C-O	-5.73	1.17	1.24
1	B	214	GLY	C-O	-5.61	1.16	1.24
1	A	147	LEU	C-O	-5.58	1.17	1.24
1	A	80	LEU	C-O	-5.52	1.17	1.24
1	B	83	GLN	C-O	-5.49	1.19	1.24
1	B	256	MET	C-O	-5.45	1.17	1.24
1	B	187	LEU	C-O	-5.42	1.17	1.24
1	B	374	LYS	C-O	-5.42	1.17	1.24
1	A	473	LEU	C-O	-5.41	1.17	1.24
1	A	78	LEU	C-O	-5.39	1.17	1.23
1	B	488	GLN	C-O	-5.36	1.17	1.24
1	A	148	ALA	C-O	-5.36	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	463	ALA	CA-CB	-5.32	1.44	1.53
1	A	376	LEU	C-O	-5.24	1.18	1.24
1	B	26	LYS	C-O	-5.21	1.18	1.24
1	B	486	VAL	C-O	-5.21	1.17	1.24
1	A	391	LEU	C-O	-5.18	1.17	1.24
1	A	265	VAL	C-O	-5.14	1.19	1.24
1	A	438	LEU	C-O	-5.10	1.18	1.24
1	B	444	HIS	C-O	-5.08	1.18	1.24
1	A	324	GLU	C-O	-5.08	1.17	1.24
1	A	151	ARG	C-O	-5.04	1.18	1.23
1	B	392	ASP	C-O	-5.01	1.17	1.23

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	494	ARG	O-C-N	16.55	144.32	123.14
1	B	177	ASP	N-CA-C	10.14	122.42	111.36
1	B	440[A]	GLU	CA-C-N	8.14	131.19	120.28
1	B	440[A]	GLU	C-N-CA	8.14	131.19	120.28
1	B	440[B]	GLU	CA-C-N	8.14	131.19	120.28
1	B	440[B]	GLU	C-N-CA	8.14	131.19	120.28
1	B	28[A]	ARG	CA-C-N	-7.91	107.38	122.09
1	B	28[A]	ARG	C-N-CA	-7.91	107.38	122.09
1	B	28[B]	ARG	CA-C-N	-7.91	107.38	122.09
1	B	28[B]	ARG	C-N-CA	-7.91	107.38	122.09
1	A	484	HIS	N-CA-C	7.75	119.80	111.36
1	B	494	ARG	CA-C-N	-7.59	108.03	121.70
1	B	494	ARG	C-N-CA	-7.59	108.03	121.70
1	A	83	GLN	CB-CA-C	-7.54	106.97	117.23
1	A	393	LYS	N-CA-C	7.09	120.85	111.28
1	B	174	VAL	N-CA-C	7.04	117.96	108.11
1	B	393	LYS	N-CA-C	7.03	120.77	111.28
1	A	151	ARG	N-CA-C	6.97	120.47	109.39
1	A	383	LYS	N-CA-C	6.60	118.56	111.36
1	A	174	VAL	O-C-N	-6.38	116.54	123.18
1	A	32	SER	CA-C-O	-6.26	113.94	121.89
1	B	176	GLN	N-CA-C	-6.22	104.56	111.71
1	A	22	GLU	N-CA-C	6.05	117.87	111.28
1	A	409	ASN	CA-C-N	6.00	126.11	119.87
1	A	409	ASN	C-N-CA	6.00	126.11	119.87
1	A	262	PHE	N-CA-C	5.77	117.65	111.36
1	B	150	PRO	N-CA-C	5.37	120.99	113.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	29	TYR	O-C-N	5.27	128.79	123.26
1	A	152	LEU	CA-C-N	5.08	124.87	119.28
1	A	152	LEU	C-N-CA	5.08	124.87	119.28

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	3490	0	3490	110	0
1	B	3500	0	3493	84	0
2	A	30	0	40	1	0
2	B	18	0	24	4	0
3	A	177	0	0	30	0
3	B	177	0	0	13	0
All	All	7392	0	7047	177	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 13.

All (177) 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:485:ASN:ND2	1:A:487:ARG:HG3	1.23	1.50
1:A:311:VAL:HA	3:A:860:HOH:O	1.42	1.18
1:A:494:ARG:HA	1:A:495:ASP:OD2	1.48	1.12
1:A:223:ILE:HD12	1:A:223:ILE:O	1.51	1.09
1:A:485:ASN:HD21	1:A:487:ARG:CG	1.67	1.08
1:A:485:ASN:ND2	1:A:487:ARG:CG	2.17	1.07
1:A:151:ARG:HG2	1:A:151:ARG:O	1.49	1.06
1:B:84:GLN:HG2	3:B:800:HOH:O	1.56	1.03
1:B:207:ARG:HD2	2:B:601:GOL:H31	1.37	1.00
1:B:249:SER:HB3	1:B:250:PRO:HD2	1.40	1.00
1:B:395:PRO:HA	3:B:849:HOH:O	1.63	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:VAL:HG21	1:B:219:GLN:HG2	1.44	0.97
1:A:190:SER:O	3:A:870:HOH:O	1.95	0.84
1:A:154:LEU:HD11	1:A:174:VAL:HG11	1.57	0.83
1:A:84:GLN:HG2	3:A:870:HOH:O	1.79	0.82
1:A:149:GLU:OE1	1:A:151:ARG:NH1	2.13	0.82
1:B:374:LYS:HE3	3:B:737:HOH:O	1.79	0.81
1:A:223:ILE:HG23	1:B:285:GLU:OE2	1.80	0.80
1:A:314:PHE:HB2	3:A:860:HOH:O	1.80	0.80
1:A:84:GLN:CG	3:A:870:HOH:O	2.29	0.80
1:A:207:ARG:HD2	2:B:601:GOL:H32	1.64	0.80
1:A:287:VAL:HG21	1:B:219:GLN:CG	2.12	0.79
1:B:84:GLN:CG	3:B:800:HOH:O	2.20	0.78
1:A:249:SER:OG	1:A:250:PRO:CD	2.34	0.76
1:B:249:SER:HB3	1:B:250:PRO:CD	2.16	0.76
1:B:47:ARG:NH2	1:B:49:ARG:HD3	2.01	0.75
1:A:154:LEU:CD1	1:A:174:VAL:HG11	2.15	0.75
3:A:850:HOH:O	1:B:263:GLU:HB2	1.86	0.74
1:A:219:GLN:CG	1:B:287:VAL:HG21	2.19	0.72
1:B:83:GLN:NE2	1:B:84:GLN:HB2	2.04	0.72
1:A:223:ILE:HD12	1:A:223:ILE:C	2.15	0.71
1:A:159:ALA:HA	1:A:174:VAL:HG21	1.72	0.71
1:A:314:PHE:CD2	3:A:860:HOH:O	2.44	0.71
1:B:303:MET:HE1	1:B:345:ARG:HD3	1.70	0.71
1:A:249:SER:OG	1:A:250:PRO:HD2	1.92	0.70
1:A:487:ARG:HH12	1:A:495:ASP:HA	1.55	0.69
1:A:219:GLN:OE1	3:A:837:HOH:O	2.10	0.67
1:A:38:GLN:HE21	1:B:407:PRO:HB2	1.59	0.67
1:A:494:ARG:HA	1:A:495:ASP:CG	2.19	0.67
1:B:176:GLN:HA	1:B:179:ARG:HD2	1.76	0.66
1:A:484:HIS:CE1	3:A:773:HOH:O	2.47	0.66
1:A:263:GLU:HG3	3:A:875:HOH:O	1.96	0.66
1:B:258:ILE:HD13	3:B:806:HOH:O	1.95	0.66
1:A:83:GLN:NE2	3:A:798:HOH:O	2.12	0.65
1:B:22:GLU:O	3:B:830:HOH:O	2.13	0.65
1:B:175:ASN:OD1	1:B:175:ASN:C	2.39	0.65
1:B:83:GLN:NE2	1:B:84:GLN:OE1	2.30	0.64
1:A:495:ASP:O	3:A:854:HOH:O	2.14	0.64
1:A:219:GLN:HG3	1:B:287:VAL:HG21	1.78	0.64
1:A:138:HIS:HB2	3:A:818:HOH:O	1.98	0.64
1:A:492:PHE:HE1	1:B:256:MET:HE2	1.64	0.63
1:B:190:SER:O	3:B:800:HOH:O	2.15	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:LYS:HD3	1:B:270:PRO:HG3	1.81	0.63
1:B:495:ASP:HB3	3:B:870:HOH:O	1.99	0.62
1:A:403:THR:O	1:A:441[A]:ARG:NH1	2.33	0.61
1:A:219:GLN:HG2	1:B:287:VAL:HG21	1.81	0.61
1:A:268:ILE:HG23	1:A:289:LEU:CD2	2.30	0.61
1:A:485:ASN:HD22	1:A:487:ARG:HG3	1.50	0.61
1:A:492:PHE:CE1	1:B:256:MET:HE2	2.36	0.60
1:B:176:GLN:HA	1:B:179:ARG:CD	2.31	0.60
3:A:847:HOH:O	1:B:65:ARG:NH2	2.35	0.59
1:A:223:ILE:CG2	1:B:285:GLU:OE2	2.51	0.59
1:A:487:ARG:HH12	1:A:495:ASP:CA	2.16	0.58
1:A:84:GLN:HB2	3:A:798:HOH:O	2.02	0.58
1:A:154:LEU:CD1	1:A:174:VAL:CG1	2.81	0.58
1:A:220:THR:HA	3:A:833:HOH:O	2.03	0.58
1:B:86:ASN:HD22	1:B:86:ASN:N	2.02	0.58
1:B:222:LYS:O	1:B:223:ILE:HG23	2.03	0.58
1:B:86:ASN:HD22	1:B:86:ASN:H	1.51	0.57
1:B:440[A]:GLU:O	1:B:443:LEU:HB2	2.04	0.57
1:B:485:ASN:HD21	1:B:487:ARG:HB2	1.71	0.56
1:B:485:ASN:ND2	1:B:487:ARG:HB2	2.20	0.56
1:B:412:GLN:HG2	3:B:849:HOH:O	2.04	0.56
1:A:96:HIS:HD2	3:A:725:HOH:O	1.87	0.56
1:A:485:ASN:HD21	1:A:487:ARG:HG3	0.74	0.55
1:B:86:ASN:ND2	1:B:131:THR:H	2.04	0.55
1:B:175:ASN:OD1	1:B:178:THR:N	2.29	0.55
1:B:440[B]:GLU:O	1:B:443:LEU:HB2	2.06	0.55
1:A:263:GLU:N	3:A:794:HOH:O	2.40	0.55
1:A:370:THR:HB	1:A:371:PRO:HD3	1.87	0.55
1:A:457:ASP:O	1:A:460:ARG:HG2	2.06	0.55
1:A:268:ILE:HG23	1:A:289:LEU:HD22	1.89	0.55
1:A:215:PHE:CD2	1:A:264:LYS:HB3	2.42	0.54
1:A:494:ARG:CA	1:A:495:ASP:OD2	2.39	0.54
1:A:494:ARG:O	1:A:494:ARG:HG2	2.08	0.54
1:B:83:GLN:NE2	1:B:84:GLN:CB	2.71	0.54
1:A:151:ARG:O	1:A:151:ARG:CG	2.30	0.53
2:A:603:GOL:H12	1:B:219:GLN:HB3	1.90	0.53
1:A:249:SER:O	1:A:250:PRO:C	2.51	0.53
1:A:494:ARG:HE	1:B:223:ILE:HD11	1.74	0.52
1:A:249:SER:O	1:A:251:GLN:N	2.43	0.52
1:A:374:LYS:HD2	3:A:858:HOH:O	2.09	0.52
1:B:119:VAL:CG2	1:B:140:GLN:NE2	2.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:ALA:CA	1:A:174:VAL:HG21	2.40	0.51
1:A:249:SER:OG	1:A:250:PRO:HD3	2.08	0.51
1:B:264:LYS:HE2	1:B:293:MET:HE3	1.92	0.51
1:B:490:SER:O	1:B:493:PRO:HD3	2.11	0.50
1:A:258:ILE:HA	3:A:794:HOH:O	2.10	0.50
1:A:223:ILE:C	1:A:223:ILE:CD1	2.82	0.50
1:A:494:ARG:HH21	1:B:223:ILE:HD12	1.76	0.50
1:B:175:ASN:OD1	1:B:175:ASN:O	2.29	0.50
1:B:406:ASP:HB3	1:B:409:ASN:O	2.11	0.50
1:A:262:PHE:HB2	3:A:794:HOH:O	2.12	0.49
1:A:37:SER:HB3	1:B:298:HIS:CG	2.48	0.48
1:B:53:ILE:HD11	1:B:122:LYS:HG3	1.96	0.48
1:B:303:MET:HE1	1:B:345:ARG:CD	2.42	0.48
1:A:63:ARG:HD2	2:B:602:GOL:H12	1.94	0.48
1:A:254:LYS:HD3	1:A:290:ASP:HB3	1.95	0.48
1:A:471:ILE:HD12	1:A:476:VAL:HG21	1.95	0.47
1:B:410:PRO:HD3	3:B:837:HOH:O	2.15	0.47
1:A:30:GLY:HA2	1:A:104:PHE:CZ	2.50	0.47
1:A:138:HIS:CB	3:A:818:HOH:O	2.62	0.47
1:A:314:PHE:CB	3:A:860:HOH:O	2.52	0.47
1:B:154:LEU:HD21	1:B:159:ALA:HB2	1.95	0.46
1:A:154:LEU:HD13	1:A:174:VAL:CG1	2.46	0.46
1:A:311:VAL:CA	3:A:860:HOH:O	2.26	0.45
1:B:83:GLN:HE21	1:B:84:GLN:CG	2.29	0.45
1:A:207:ARG:CZ	1:A:268:ILE:HD12	2.47	0.45
1:A:223:ILE:HD11	3:B:864:HOH:O	2.17	0.45
1:A:324:GLU:H	1:A:324:GLU:CD	2.24	0.45
1:B:83:GLN:CD	1:B:84:GLN:H	2.24	0.45
1:B:453:LYS:NZ	1:B:457:ASP:OD1	2.50	0.45
1:A:250:PRO:HB3	3:A:816:HOH:O	2.17	0.45
1:A:494:ARG:HE	1:B:223:ILE:CD1	2.28	0.45
1:B:151:ARG:HH11	1:B:151:ARG:HG3	1.81	0.44
1:B:114:VAL:HA	1:B:143:TYR:O	2.17	0.44
1:B:215:PHE:CG	1:B:264:LYS:HB3	2.52	0.44
1:A:263:GLU:HG2	1:A:264:LYS:N	2.32	0.44
1:A:484:HIS:N	1:A:488:GLN:OE1	2.50	0.44
1:B:475:ARG:HD2	3:B:752:HOH:O	2.18	0.44
1:B:83:GLN:NE2	1:B:84:GLN:CG	2.81	0.44
1:B:110:LYS:O	1:B:111:GLU:HB2	2.18	0.43
1:B:151:ARG:HG3	1:B:151:ARG:NH1	2.34	0.43
1:B:157:ASP:HB2	3:B:805:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:LYS:O	1:A:111:GLU:HB2	2.18	0.43
1:A:262:PHE:O	1:A:263:GLU:CD	2.62	0.43
1:B:119:VAL:CG2	1:B:140:GLN:HE21	2.31	0.43
1:A:22:GLU:HG2	1:A:23:ASP:N	2.32	0.43
1:B:83:GLN:HE21	1:B:84:GLN:HG3	1.83	0.43
1:A:85:PHE:CD2	1:A:85:PHE:N	2.87	0.43
1:A:222:LYS:HB2	3:A:820:HOH:O	2.18	0.43
1:B:353:ALA:O	1:B:357:GLU:HG3	2.19	0.43
1:B:83:GLN:CG	1:B:84:GLN:H	2.31	0.43
1:A:266:PHE:HA	1:A:290:ASP:O	2.17	0.43
1:A:37:SER:HB3	1:B:298:HIS:CD2	2.54	0.42
1:A:223:ILE:O	1:A:223:ILE:CD1	2.43	0.42
1:B:260:ALA:O	1:B:261:ASP:HB2	2.18	0.42
1:A:86:ASN:OD1	1:A:130:CYS:HA	2.18	0.42
3:A:820:HOH:O	1:B:272:PHE:HZ	2.01	0.42
1:A:119:VAL:HG23	3:A:818:HOH:O	2.18	0.42
1:A:362:MET:HE1	1:A:368:LEU:HD23	2.02	0.42
1:A:45:LEU:HD23	1:A:61:TRP:HB3	2.00	0.42
1:A:159:ALA:N	1:A:174:VAL:HG21	2.34	0.42
1:A:262:PHE:O	1:A:263:GLU:OE2	2.38	0.42
1:A:458:SER:HB2	1:B:184:VAL:HG21	2.00	0.42
1:A:311:VAL:C	3:A:860:HOH:O	2.60	0.42
1:A:205:LEU:HA	3:A:836:HOH:O	2.20	0.42
1:A:432:ILE:CD1	1:A:441[A]:ARG:HG3	2.50	0.42
1:B:185:ILE:O	1:B:188:ARG:HB2	2.20	0.42
1:B:176:GLN:O	1:B:179:ARG:HG2	2.20	0.41
1:B:187:LEU:HD23	1:B:187:LEU:HA	1.94	0.41
1:B:370:THR:HB	1:B:371:PRO:HD3	2.02	0.41
1:A:117:GLU:HB3	1:A:141:LYS:HB2	2.00	0.41
1:B:160:VAL:CG1	1:B:189:THR:HB	2.50	0.41
1:B:184:VAL:O	1:B:188:ARG:HG3	2.20	0.41
1:A:215:PHE:CG	1:A:264:LYS:HB3	2.56	0.41
1:B:207:ARG:HD2	2:B:601:GOL:C3	2.27	0.41
1:A:341:GLU:HA	1:A:342:PRO:HA	1.90	0.41
1:A:430:GLN:HA	1:A:467:ALA:HB2	2.03	0.41
1:A:494:ARG:O	1:A:494:ARG:CG	2.66	0.41
1:A:96:HIS:CD2	1:A:140:GLN:HG2	2.56	0.40
1:A:217:GLU:HB2	1:A:266:PHE:CZ	2.56	0.40
1:B:53:ILE:HD13	1:B:134:ASP:HB3	2.03	0.40
1:B:210:LEU:HD23	1:B:210:LEU:HA	1.93	0.40
1:A:288:GLY:HA2	1:A:471:ILE:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:LYS:HE3	1:A:451:LYS:HB3	1.69	0.40
1:A:409:ASN:HA	1:A:410:PRO:HD2	1.87	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	424/521 (81%)	410 (97%)	14 (3%)	0	100	100
1	B	425/521 (82%)	414 (97%)	11 (3%)	0	100	100
All	All	849/1042 (82%)	824 (97%)	25 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	385/456 (84%)	366 (95%)	19 (5%)	22	23
1	B	386/456 (85%)	367 (95%)	19 (5%)	22	23
All	All	771/912 (84%)	733 (95%)	38 (5%)	22	23

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	ILE
1	A	46	VAL
1	A	119	VAL
1	A	151	ARG
1	A	156	LEU
1	A	173	THR
1	A	174	VAL
1	A	177	ASP
1	A	178	THR
1	A	211	ILE
1	A	251	GLN
1	A	263	GLU
1	A	315	LYS
1	A	324	GLU
1	A	451	LYS
1	A	484	HIS
1	A	486	VAL
1	A	494	ARG
1	A	495	ASP
1	B	32	SER
1	B	46	VAL
1	B	86	ASN
1	B	90	LEU
1	B	91	VAL
1	B	180	LEU
1	B	211	ILE
1	B	219	GLN
1	B	223	ILE
1	B	252	LEU
1	B	289	LEU
1	B	290	ASP
1	B	319	GLU
1	B	324	GLU
1	B	380	VAL
1	B	411	LYS
1	B	424	GLU
1	B	486	VAL
1	B	490	SER

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	38	GLN

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Mol	Chain	Res	Type
1	A	54	GLN
1	A	83	GLN
1	A	88	GLN
1	A	96	HIS
1	A	132	GLN
1	A	204	HIS
1	A	219	GLN
1	A	326	GLN
1	A	372	ASN
1	A	414	ASN
1	A	430	GLN
1	A	444	HIS
1	A	485	ASN
1	B	83	GLN
1	B	84	GLN
1	B	86	ASN
1	B	125	GLN
1	B	132	GLN
1	B	140	GLN
1	B	182	ASN
1	B	204	HIS
1	B	312	GLN
1	B	318	GLN
1	B	378	HIS
1	B	414	ASN
1	B	430	GLN
1	B	485	ASN

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

8 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	601	-	5,5,5	0.36	0	5,5,5	0.37	0
2	GOL	B	603	-	5,5,5	0.39	0	5,5,5	0.46	0
2	GOL	B	602	-	5,5,5	0.44	0	5,5,5	0.62	0
2	GOL	A	602	-	5,5,5	0.35	0	5,5,5	0.44	0
2	GOL	A	603	-	5,5,5	0.40	0	5,5,5	0.45	0
2	GOL	A	601	-	5,5,5	0.41	0	5,5,5	0.37	0
2	GOL	A	604	-	5,5,5	0.29	0	5,5,5	0.40	0
2	GOL	A	605	-	5,5,5	0.36	0	5,5,5	0.14	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	601	-	-	0/4/4/4	-
2	GOL	B	603	-	-	0/4/4/4	-
2	GOL	B	602	-	-	2/4/4/4	-
2	GOL	A	602	-	-	0/4/4/4	-
2	GOL	A	603	-	-	4/4/4/4	-
2	GOL	A	601	-	-	2/4/4/4	-
2	GOL	A	604	-	-	2/4/4/4	-
2	GOL	A	605	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	GOL	O1-C1-C2-O2
2	A	601	GOL	O1-C1-C2-C3
2	A	603	GOL	C1-C2-C3-O3
2	A	603	GOL	O2-C2-C3-O3
2	A	605	GOL	C1-C2-C3-O3
2	B	602	GOL	O1-C1-C2-C3
2	A	603	GOL	O1-C1-C2-O2
2	A	604	GOL	O1-C1-C2-O2
2	A	603	GOL	O1-C1-C2-C3
2	A	604	GOL	O1-C1-C2-C3
2	B	602	GOL	O1-C1-C2-O2
2	A	605	GOL	O2-C2-C3-O3

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	GOL	3	0
2	B	602	GOL	1	0
2	A	603	GOL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	439:THR	C	440[B]:GLU	N	1.20

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	431/521 (82%)	0.03	18 (4%) 40 39	14, 32, 49, 76	1 (0%)
1	B	430/521 (82%)	-0.02	20 (4%) 36 35	15, 30, 56, 84	3 (0%)
All	All	861/1042 (82%)	0.00	38 (4%) 39 37	14, 31, 51, 84	4 (0%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	180	LEU	5.8
1	A	173	THR	4.4
1	A	22	GLU	3.9
1	B	283	LEU	3.9
1	B	249	SER	3.8
1	B	181	ASP	3.7
1	B	174	VAL	3.6
1	B	173	THR	3.5
1	A	249	SER	3.5
1	B	21	ALA	3.4
1	B	284	THR	3.3
1	B	495	ASP	3.2
1	A	21	ALA	3.2
1	A	223	ILE	3.2
1	B	178	THR	3.0
1	A	181	ASP	2.9
1	B	162	PRO	2.8
1	B	223	ILE	2.7
1	A	248	GLN	2.6
1	B	176	GLN	2.6
1	B	177	ASP	2.6
1	A	487	ARG	2.4
1	B	160	VAL	2.4
1	B	409	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	178	THR	2.3
1	B	494	ARG	2.3
1	A	272	PHE	2.3
1	A	177	ASP	2.3
1	A	283	LEU	2.2
1	A	174	VAL	2.2
1	A	175	ASN	2.2
1	B	154	LEU	2.1
1	B	484[A]	HIS	2.1
1	A	151	ARG	2.1
1	A	180	LEU	2.1
1	A	495	ASP	2.1
1	A	494	ARG	2.1
1	B	182	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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(Å ²)	Q<0.9
2	GOL	A	603	6/6	0.71	0.20	59,60,61,61	0
2	GOL	A	604	6/6	0.79	0.17	56,56,57,58	0
2	GOL	B	601	6/6	0.83	0.15	53,54,54,54	0
2	GOL	B	602	6/6	0.83	0.18	39,41,42,42	0
2	GOL	A	605	6/6	0.84	0.17	64,64,64,65	0
2	GOL	B	603	6/6	0.89	0.12	46,49,50,50	0
2	GOL	A	601	6/6	0.90	0.12	46,49,49,50	0
2	GOL	A	602	6/6	0.92	0.15	41,43,44,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.