



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:47 PM UTC

PDB ID : 5CNK / pdb_00005cnk
Title : mglur3 with glutamate
Authors : Monn, J.A.; Clawson, D.K.
Deposited on : 2015-07-17
Resolution : 3.15 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

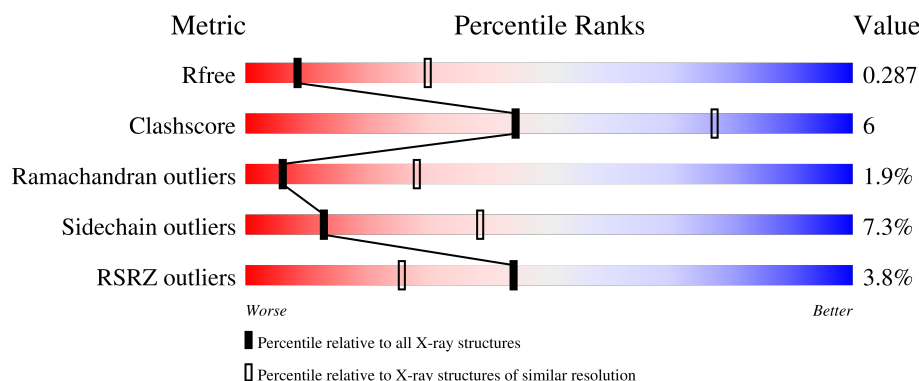
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)

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	517	 3% 70% 13% 14%
1	B	517	 3% 65% 15% 15%
1	C	517	 4% 65% 18% 13%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	IOD	A	604	-	-	X	-
3	IOD	B	602	-	-	X	-
3	IOD	C	603	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10563 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 Metabotropic glutamate receptor 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	444	Total	C	N	O	S	0	0	0
			3518	2237	608	659	14			
1	B	438	Total	C	N	O	S	0	0	0
			3478	2210	600	654	14			
1	C	448	Total	C	N	O	S	0	0	0
			3525	2234	607	670	14			

There are 36 discrepancies between the modelled and reference sequences:

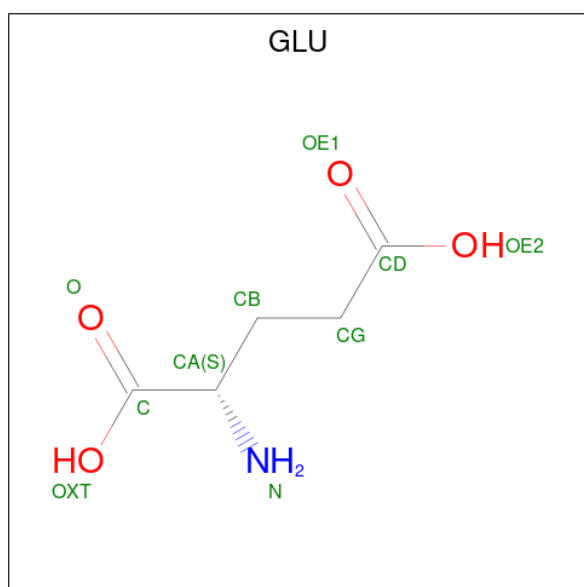
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP Q14832
A	0	ALA	-	expression tag	UNP Q14832
A	1	LEU	-	expression tag	UNP Q14832
A	240	SER	CYS	conflict	UNP Q14832
A	508	GLU	-	expression tag	UNP Q14832
A	509	GLY	-	expression tag	UNP Q14832
A	510	HIS	-	expression tag	UNP Q14832
A	511	HIS	-	expression tag	UNP Q14832
A	512	HIS	-	expression tag	UNP Q14832
A	513	HIS	-	expression tag	UNP Q14832
A	514	HIS	-	expression tag	UNP Q14832
A	515	HIS	-	expression tag	UNP Q14832
B	-1	MET	-	initiating methionine	UNP Q14832
B	0	ALA	-	expression tag	UNP Q14832
B	1	LEU	-	expression tag	UNP Q14832
B	240	SER	CYS	conflict	UNP Q14832
B	508	GLU	-	expression tag	UNP Q14832
B	509	GLY	-	expression tag	UNP Q14832
B	510	HIS	-	expression tag	UNP Q14832
B	511	HIS	-	expression tag	UNP Q14832
B	512	HIS	-	expression tag	UNP Q14832
B	513	HIS	-	expression tag	UNP Q14832
B	514	HIS	-	expression tag	UNP Q14832

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Chain	Residue	Modelled	Actual	Comment	Reference
B	515	HIS	-	expression tag	UNP Q14832
C	-1	MET	-	initiating methionine	UNP Q14832
C	0	ALA	-	expression tag	UNP Q14832
C	1	LEU	-	expression tag	UNP Q14832
C	240	SER	CYS	conflict	UNP Q14832
C	508	GLU	-	expression tag	UNP Q14832
C	509	GLY	-	expression tag	UNP Q14832
C	510	HIS	-	expression tag	UNP Q14832
C	511	HIS	-	expression tag	UNP Q14832
C	512	HIS	-	expression tag	UNP Q14832
C	513	HIS	-	expression tag	UNP Q14832
C	514	HIS	-	expression tag	UNP Q14832
C	515	HIS	-	expression tag	UNP Q14832

- Molecule 2 is GLUTAMIC ACID (CCD ID: GLU) (formula: C₅H₉NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	5	1	4		

- Molecule 3 is IODIDE ION (CCD ID: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	I	0	0
			4	4		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	3	Total I 3 3	0	0
3	C	3	Total I 3 3	0	0

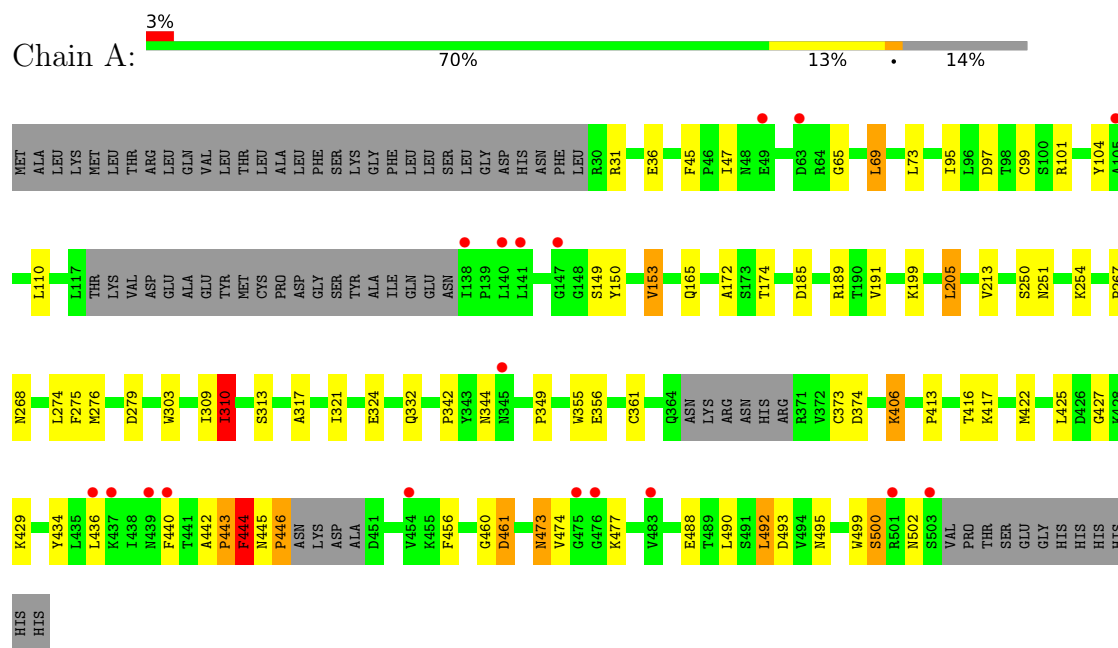
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	8	Total O 8 8	0	0
4	B	4	Total O 4 4	0	0
4	C	10	Total O 10 10	0	0

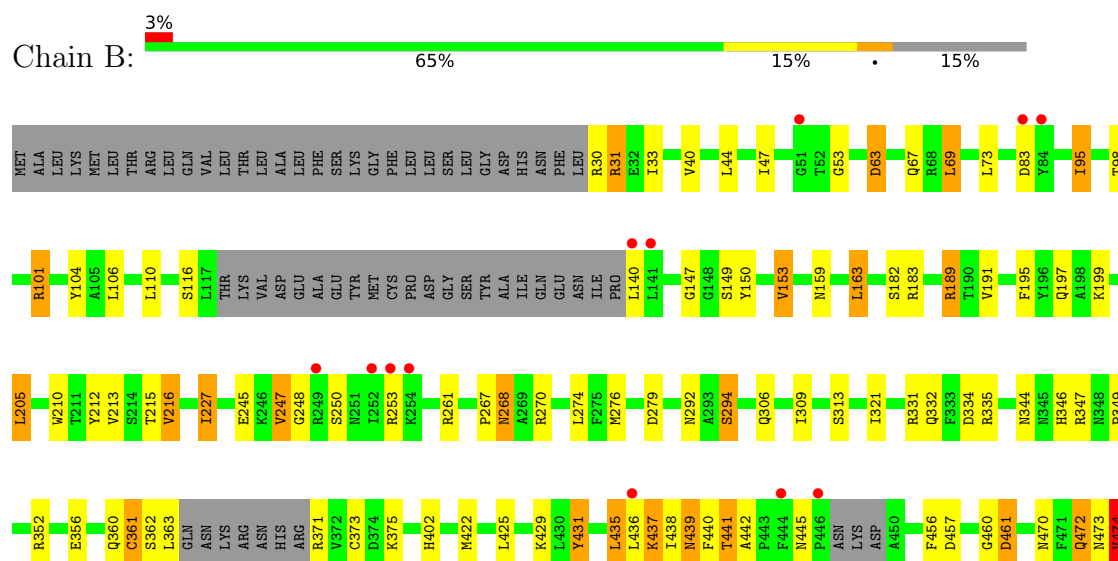
3 Residue-property plots

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: Metabotropic glutamate receptor 3

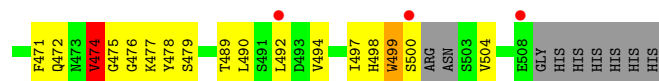
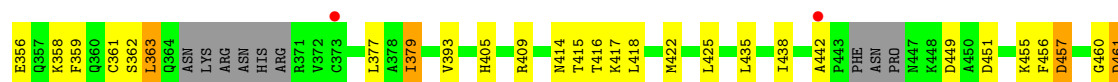
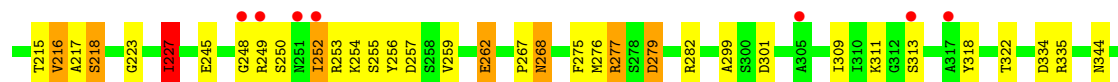
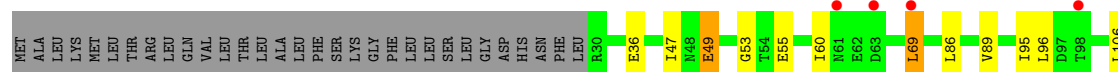


• Molecule 1: Metabotropic glutamate receptor 3





• Molecule 1: Metabotropic glutamate receptor 3



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	138.34Å 80.00Å 206.86Å 90.00° 130.73° 90.00°	Depositor
Resolution (Å)	78.38 – 3.15 78.38 – 3.15	Depositor EDS
% Data completeness (in resolution range)	97.8 (78.38-3.15) 97.8 (78.38-3.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 3.13Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.221 , 0.258 0.243 , 0.287	Depositor DCC
R_{free} test set	873 reflections (2.91%)	wwPDB-VP
Wilson B-factor (Å ²)	57.0	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 88.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.055 for $-1/2^*h+3/2^*k, 1/2^*h+1/2^*k, -1/2^*h-3/2^*k-l$ 0.059 for $-1/2^*h-3/2^*k, -1/2^*h+1/2^*k, -1/2^*h+3/2^*k-l$ 0.105 for $1/2^*h+3/2^*k, 1/2^*h-1/2^*k, -3/2^*h-3/2^*k-l$ 0.078 for $1/2^*h-3/2^*k, -1/2^*h-1/2^*k, -3/2^*h+3/2^*k-l$ 0.064 for $-h, -k, 2^*h+1$	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	10563	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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: IOD

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	0.86	2/3592 (0.1%)	1.35	21/4856 (0.4%)
1	B	0.87	0/3551	1.43	33/4800 (0.7%)
1	C	0.89	1/3596 (0.0%)	1.45	35/4866 (0.7%)
All	All	0.87	3/10739 (0.0%)	1.41	89/14522 (0.6%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	446	PRO	N-CD	14.95	1.68	1.47
1	A	473	ASN	CA-C	5.32	1.59	1.52
1	C	474	VAL	CA-C	5.16	1.59	1.52

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	255	SER	N-CA-C	-12.32	96.76	112.90
1	A	440	PHE	CA-CB-CG	10.79	124.59	113.80
1	A	310	ILE	N-CA-CB	-8.82	101.83	112.33
1	C	248	GLY	N-CA-C	8.59	125.19	114.37
1	B	439	ASN	CA-CB-CG	8.58	121.18	112.60
1	B	30	ARG	CA-C-N	7.91	136.64	121.54
1	B	30	ARG	C-N-CA	7.91	136.64	121.54
1	C	185	ASP	CA-CB-CG	7.57	120.17	112.60
1	C	249	ARG	CA-C-N	7.25	135.38	121.54
1	C	249	ARG	C-N-CA	7.25	135.38	121.54
1	A	185	ASP	CA-CB-CG	7.21	119.81	112.60
1	A	443	PRO	CA-C-N	7.01	132.52	121.72
1	A	443	PRO	C-N-CA	7.01	132.52	121.72
1	B	147	GLY	N-CA-C	6.95	122.70	111.38
1	B	267	PRO	CA-C-N	6.87	129.49	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	267	PRO	C-N-CA	6.87	129.49	120.28
1	C	393	VAL	CA-C-N	6.82	129.80	120.46
1	C	393	VAL	C-N-CA	6.82	129.80	120.46
1	C	267	PRO	CA-C-N	6.67	129.22	120.28
1	C	267	PRO	C-N-CA	6.67	129.22	120.28
1	A	267	PRO	CA-C-N	6.60	129.12	120.28
1	A	267	PRO	C-N-CA	6.60	129.12	120.28
1	C	223	GLY	CA-C-N	6.42	128.78	120.44
1	C	223	GLY	C-N-CA	6.42	128.78	120.44
1	B	361	CYS	CA-C-N	6.38	133.80	122.45
1	B	361	CYS	C-N-CA	6.38	133.80	122.45
1	A	461	ASP	CA-CB-CG	6.21	118.81	112.60
1	C	252	ILE	CA-C-N	6.00	133.01	121.54
1	C	252	ILE	C-N-CA	6.00	133.01	121.54
1	B	53	GLY	CA-C-N	5.95	129.05	120.79
1	B	53	GLY	C-N-CA	5.95	129.05	120.79
1	C	476	GLY	CA-C-N	5.89	132.09	122.07
1	C	476	GLY	C-N-CA	5.89	132.09	122.07
1	B	461	ASP	CA-CB-CG	5.87	118.47	112.60
1	C	461	ASP	CA-CB-CG	5.76	118.36	112.60
1	B	436	LEU	CA-C-N	5.74	131.51	122.21
1	B	436	LEU	C-N-CA	5.74	131.51	122.21
1	B	431	TYR	CA-C-N	5.72	127.88	120.44
1	B	431	TYR	C-N-CA	5.72	127.88	120.44
1	B	437	LYS	CA-C-N	5.71	130.41	122.93
1	B	437	LYS	C-N-CA	5.71	130.41	122.93
1	B	279	ASP	CA-CB-CG	5.69	118.29	112.60
1	B	440	PHE	CA-C-N	5.67	132.36	121.54
1	B	440	PHE	C-N-CA	5.67	132.36	121.54
1	C	279	ASP	CA-CB-CG	5.66	118.26	112.60
1	A	444	PHE	CA-CB-CG	5.65	119.45	113.80
1	B	101	ARG	CA-C-N	5.63	127.82	120.28
1	B	101	ARG	C-N-CA	5.63	127.82	120.28
1	A	279	ASP	CA-CB-CG	5.62	118.22	112.60
1	A	97	ASP	CA-CB-CG	5.58	118.18	112.60
1	C	262	GLU	CB-CG-CD	5.56	122.05	112.60
1	B	216	VAL	N-CA-CB	5.50	120.30	111.23
1	A	493	ASP	CA-C-N	5.45	127.92	120.46
1	A	493	ASP	C-N-CA	5.45	127.92	120.46
1	C	344	ASN	CA-CB-CG	5.38	117.98	112.60
1	B	182	SER	CA-C-N	5.35	127.39	120.44
1	B	182	SER	C-N-CA	5.35	127.39	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	176	ALA	CA-C-N	5.35	127.70	120.38
1	C	176	ALA	C-N-CA	5.35	127.70	120.38
1	C	106	LEU	CA-C-N	5.34	127.38	120.44
1	C	106	LEU	C-N-CA	5.34	127.38	120.44
1	C	49	GLU	CB-CG-CD	5.31	121.63	112.60
1	C	216	VAL	N-CA-CB	5.29	119.96	111.23
1	A	344	ASN	CA-CB-CG	5.26	117.86	112.60
1	B	344	ASN	CA-CB-CG	5.24	117.84	112.60
1	B	106	LEU	CA-C-N	5.22	127.22	120.44
1	B	106	LEU	C-N-CA	5.22	127.22	120.44
1	A	324	GLU	CB-CG-CD	5.20	121.43	112.60
1	C	334	ASP	CA-C-N	5.15	127.14	120.44
1	C	334	ASP	C-N-CA	5.15	127.14	120.44
1	C	335	ARG	CA-C-N	5.15	127.14	120.44
1	C	335	ARG	C-N-CA	5.15	127.14	120.44
1	A	493	ASP	CA-CB-CG	5.15	117.75	112.60
1	A	65	GLY	CA-C-N	5.14	127.04	120.56
1	A	65	GLY	C-N-CA	5.14	127.04	120.56
1	C	227	ILE	CA-C-N	5.13	127.47	120.54
1	C	227	ILE	C-N-CA	5.13	127.47	120.54
1	C	55	GLU	CA-C-N	5.13	129.27	120.71
1	C	55	GLU	C-N-CA	5.13	129.27	120.71
1	B	195	PHE	CA-C-N	5.11	127.39	120.44
1	B	195	PHE	C-N-CA	5.11	127.39	120.44
1	B	197	GLN	CA-C-N	5.07	127.33	120.38
1	B	197	GLN	C-N-CA	5.07	127.33	120.38
1	C	416	THR	N-CA-C	-5.07	107.14	113.38
1	A	413	PRO	CA-C-N	5.05	129.98	121.14
1	A	413	PRO	C-N-CA	5.05	129.98	121.14
1	C	457	ASP	CA-CB-CG	5.05	117.65	112.60
1	A	416	THR	N-CA-C	-5.02	107.20	113.38
1	B	474	VAL	N-CA-CB	5.00	119.48	111.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3518	0	3425	34	0
1	B	3478	0	3378	53	0
1	C	3525	0	3402	40	0
2	A	10	0	5	2	0
3	A	4	0	0	3	0
3	B	3	0	0	2	0
3	C	3	0	0	2	0
4	A	8	0	0	0	0
4	B	4	0	0	0	0
4	C	10	0	0	1	0
All	All	10563	0	10210	125	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 6.

All (125) 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:446:PRO:N	1:A:446:PRO:CD	1.68	1.43
1:B:216:VAL:HG22	1:B:245:GLU:HB2	1.38	1.03
1:C:216:VAL:HG22	1:C:245:GLU:HB2	1.42	0.98
1:C:438:ILE:HG22	1:C:455:LYS:HB3	1.50	0.92
1:B:247:VAL:HG23	1:B:248:GLY:H	1.38	0.89
1:A:321:ILE:HD11	1:A:499:TRP:HZ3	1.42	0.81
1:A:442:ALA:O	1:A:444:PHE:N	2.13	0.81
1:B:83:ASP:O	1:B:83:ASP:OD1	2.02	0.78
1:B:474:VAL:HG23	1:B:475:GLY:H	1.51	0.74
1:A:321:ILE:HD11	1:A:499:TRP:CZ3	2.25	0.70
1:A:101:ARG:HE	1:A:104:TYR:HB2	1.58	0.68
1:B:494:VAL:HA	1:B:497:ILE:HD12	1.76	0.68
1:C:149:SER:HB3	3:C:603:IOD:I	2.65	0.67
1:C:494:VAL:HA	1:C:497:ILE:HD12	1.76	0.65
1:C:414:ASN:ND2	4:C:701:HOH:O	2.24	0.65
1:B:470:ASN:ND2	1:B:497:ILE:HG23	2.14	0.63
1:B:149:SER:HB3	3:B:602:IOD:I	2.69	0.63
1:C:217:ALA:HB2	1:C:227:ILE:HG13	1.81	0.61
1:C:475:GLY:C	1:C:477:LYS:H	2.08	0.61
1:B:356:GLU:HA	1:B:361:CYS:HB2	1.82	0.61
1:C:356:GLU:HA	1:C:361:CYS:HB2	1.83	0.61
1:A:174:THR:HG1	2:A:601:GLU:N	2.00	0.60
1:C:299:ALA:HB3	1:C:322:THR:HG22	1.84	0.60
1:B:402:HIS:HB3	1:B:437:LYS:CE	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:360:GLN:HB2	1:B:371:ARG:HH22	1.67	0.58
1:B:438:ILE:HG23	1:B:438:ILE:O	2.04	0.57
1:A:303:TRP:HA	1:A:309:ILE:CD1	2.36	0.56
1:A:189:ARG:HG3	1:A:191:VAL:O	2.04	0.56
1:B:189:ARG:HG3	1:B:191:VAL:O	2.07	0.55
1:C:471:PHE:CZ	1:C:478:TYR:HB3	2.42	0.55
1:B:153:VAL:HG21	3:B:602:IOD:I	2.77	0.55
1:B:474:VAL:HG23	1:B:475:GLY:N	2.22	0.54
1:C:47:ILE:HD12	1:C:69:LEU:HD12	1.88	0.54
1:A:374:ASP:OD1	1:C:199:LYS:HE2	2.07	0.54
1:B:470:ASN:HD22	1:B:497:ILE:HG23	1.71	0.54
1:C:189:ARG:HG3	1:C:191:VAL:O	2.07	0.54
1:B:274:LEU:HD22	1:B:276:MET:HE2	1.90	0.54
1:A:251:ASN:HA	1:B:375:LYS:HG3	1.89	0.54
1:B:63:ASP:O	1:B:67:GLN:HB2	2.08	0.54
1:B:306:GLN:HB2	1:B:309:ILE:HD12	1.91	0.53
1:B:402:HIS:HB3	1:B:437:LYS:HE2	1.91	0.52
1:C:256:TYR:HA	1:C:259:VAL:HG22	1.92	0.52
1:A:205:LEU:HD13	1:A:213:VAL:HG11	1.91	0.52
1:B:44:LEU:HD22	1:B:98:THR:HG22	1.91	0.52
1:A:47:ILE:HD12	1:A:69:LEU:HD12	1.91	0.52
1:A:473:ASN:O	1:A:477:LYS:O	2.27	0.52
1:A:189:ARG:HD3	1:A:461:ASP:OD1	2.10	0.51
1:B:402:HIS:HB3	1:B:437:LYS:CD	2.41	0.51
1:C:218:SER:HB2	1:C:276:MET:HA	1.92	0.51
1:C:359:PHE:CD1	1:C:377:LEU:HD22	2.46	0.50
1:A:149:SER:HB2	3:A:604:IOD:I	2.82	0.50
1:A:172:ALA:HB1	2:A:601:GLU:HG3	1.93	0.50
1:A:499:TRP:O	1:A:500:SER:C	2.53	0.50
1:C:472:GLN:HG2	1:C:498:HIS:HB2	1.93	0.50
1:B:205:LEU:HD23	1:B:210:TRP:HE3	1.77	0.50
1:B:247:VAL:HG23	1:B:248:GLY:N	2.17	0.50
1:C:414:ASN:OD1	1:C:415:THR:HG23	2.13	0.49
1:B:189:ARG:HD3	1:B:461:ASP:OD1	2.12	0.49
1:C:489:THR:HG22	1:C:490:LEU:N	2.28	0.49
1:C:189:ARG:HD3	1:C:461:ASP:OD1	2.13	0.49
1:B:457:ASP:HB2	1:B:461:ASP:H	1.78	0.48
1:B:402:HIS:HB3	1:B:437:LYS:HD3	1.95	0.48
1:C:457:ASP:HB2	1:C:461:ASP:H	1.79	0.48
1:B:472:GLN:HG3	1:B:498:HIS:HB2	1.96	0.48
1:A:150:TYR:HB2	1:A:153:VAL:HG13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:431:TYR:HA	1:B:435:LEU:HB2	1.94	0.48
3:A:605:IOD:I	1:B:346:HIS:NE2	3.16	0.47
1:B:216:VAL:CG2	1:B:245:GLU:HB2	2.27	0.47
1:C:277:ARG:HD3	1:C:279:ASP:OD1	2.14	0.47
1:C:358:LYS:HE2	1:C:379:ILE:HG23	1.96	0.47
1:B:101:ARG:HE	1:B:104:TYR:HB2	1.79	0.47
1:C:282:ARG:HD3	1:C:309:ILE:HA	1.97	0.46
1:A:31:ARG:HD2	1:A:349:PRO:HB2	1.98	0.46
1:B:31:ARG:HD2	1:B:349:PRO:HB2	1.98	0.46
1:A:310:ILE:HD11	1:A:317:ALA:HB1	1.98	0.45
1:B:159:ASN:O	1:B:163:LEU:HD13	2.16	0.45
1:C:215:THR:HB	1:C:227:ILE:HD11	1.98	0.45
1:B:101:ARG:HH21	1:B:104:TYR:HB2	1.81	0.45
1:B:362:SER:O	1:B:363:LEU:HD22	2.16	0.45
1:A:99:CYS:SG	1:A:104:TYR:CE2	3.10	0.45
1:A:356:GLU:HA	1:A:361:CYS:HB2	1.99	0.45
1:C:499:TRP:CZ2	1:C:504:VAL:HG22	2.51	0.45
1:C:456:PHE:HB3	1:C:460:GLY:HA2	1.99	0.45
1:C:149:SER:HA	1:C:172:ALA:HB3	2.00	0.44
1:C:362:SER:O	1:C:363:LEU:HD22	2.17	0.44
1:A:406:LYS:HD3	1:A:434:TYR:HD1	1.83	0.44
1:A:69:LEU:C	1:A:69:LEU:HD23	2.41	0.44
1:C:318:TYR:CE2	1:C:500:SER:HB3	2.53	0.44
1:B:73:LEU:HD23	1:B:347:ARG:HD2	2.00	0.44
1:C:212:TYR:HE2	1:C:268:ASN:HD22	1.65	0.43
1:B:456:PHE:HB3	1:B:460:GLY:HA2	2.00	0.43
1:A:274:LEU:HB3	1:A:276:MET:HE2	1.99	0.43
1:A:73:LEU:HD11	1:A:95:ILE:HD12	2.01	0.43
1:A:165:GLN:O	1:A:427:GLY:HA3	2.19	0.43
1:C:150:TYR:HB2	1:C:153:VAL:HG13	2.01	0.43
1:C:254:LYS:HA	1:C:257:ASP:H	1.84	0.43
1:B:69:LEU:C	1:B:69:LEU:HD23	2.44	0.42
1:B:331:ARG:HA	1:B:334:ASP:OD2	2.19	0.42
1:B:40:VAL:HG21	1:B:140:LEU:HD22	2.02	0.42
1:C:405:HIS:CE1	1:C:409:ARG:HD2	2.54	0.42
1:A:73:LEU:CD1	1:A:95:ILE:HD12	2.50	0.42
1:B:33:ILE:HB	1:B:95:ILE:HB	2.02	0.42
1:B:205:LEU:HD22	1:B:213:VAL:HG11	2.02	0.42
1:B:402:HIS:O	1:B:437:LYS:NZ	2.53	0.42
1:A:456:PHE:HB3	1:A:460:GLY:HA2	2.02	0.42
1:B:47:ILE:CD1	1:B:69:LEU:HD12	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:356:GLU:HG2	1:B:361:CYS:HB2	2.02	0.42
1:C:474:VAL:HG21	1:C:479:SER:OG	2.20	0.42
1:B:321:ILE:HD11	1:B:499:TRP:CZ3	2.55	0.41
1:B:150:TYR:HB2	1:B:153:VAL:HG13	2.01	0.41
1:B:473:ASN:O	1:B:474:VAL:HG22	2.20	0.41
1:B:270:ARG:HH21	1:B:294:SER:N	2.18	0.41
1:A:153:VAL:HG21	3:A:604:IOD:I	2.90	0.41
1:C:86:LEU:HD22	1:C:89:VAL:HB	2.02	0.41
1:A:45:PHE:HB2	1:A:47:ILE:HD11	2.03	0.41
1:B:215:THR:HB	1:B:227:ILE:HD11	2.01	0.41
1:A:490:LEU:HG	1:A:492:LEU:HD22	2.02	0.41
1:A:342:PRO:HD3	1:A:355:TRP:CD2	2.55	0.41
1:B:212:TYR:CE2	1:B:268:ASN:HB2	2.56	0.40
1:C:96:LEU:HD13	1:C:108:GLN:HB3	2.03	0.40
1:C:153:VAL:HG21	3:C:603:IOD:I	2.92	0.40
1:C:69:LEU:C	1:C:69:LEU:HD23	2.46	0.40
1:C:148:GLY:HA3	1:C:154:SER:OG	2.21	0.40
1:A:149:SER:HA	1:A:172:ALA:HB3	2.03	0.40
1:B:332:GLN:OE1	1:B:335:ARG:NH2	2.54	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	436/517 (84%)	413 (95%)	17 (4%)	6 (1%)	9	34
1	B	430/517 (83%)	390 (91%)	30 (7%)	10 (2%)	5	24
1	C	438/517 (85%)	394 (90%)	35 (8%)	9 (2%)	5	26
All	All	1304/1551 (84%)	1197 (92%)	82 (6%)	25 (2%)	6	28

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	250	SER
1	A	443	PRO
1	A	500	SER
1	B	253	ARG
1	B	441	THR
1	C	250	SER
1	C	253	ARG
1	B	247	VAL
1	C	53	GLY
1	C	252	ILE
1	C	435	LEU
1	B	250	SER
1	B	292	ASN
1	B	474	VAL
1	C	449	ASP
1	C	451	ASP
1	A	502	ASN
1	B	31	ARG
1	B	488	GLU
1	C	474	VAL
1	A	474	VAL
1	A	488	GLU
1	B	294	SER
1	B	442	ALA
1	C	442	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	373/445 (84%)	350 (94%)	23 (6%)	16	44
1	B	368/445 (83%)	341 (93%)	27 (7%)	13	38
1	C	372/445 (84%)	341 (92%)	31 (8%)	10	34
All	All	1113/1335 (83%)	1032 (93%)	81 (7%)	13	38

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	GLU
1	A	69	LEU
1	A	110	LEU
1	A	153	VAL
1	A	199	LYS
1	A	205	LEU
1	A	254	LYS
1	A	268	ASN
1	A	275	PHE
1	A	310	ILE
1	A	313	SER
1	A	332	GLN
1	A	373	CYS
1	A	406	LYS
1	A	417	LYS
1	A	422	MET
1	A	425	LEU
1	A	429	LYS
1	A	436	LEU
1	A	444	PHE
1	A	445	ASN
1	A	492	LEU
1	A	495	ASN
1	B	63	ASP
1	B	69	LEU
1	B	95	ILE
1	B	110	LEU
1	B	116	SER
1	B	153	VAL
1	B	163	LEU
1	B	183	ARG
1	B	189	ARG
1	B	199	LYS
1	B	205	LEU
1	B	227	ILE
1	B	261	ARG
1	B	268	ASN
1	B	313	SER
1	B	352	ARG
1	B	373	CYS
1	B	422	MET
1	B	425	LEU
1	B	429	LYS

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Mol	Chain	Res	Type
1	B	435	LEU
1	B	439	ASN
1	B	441	THR
1	B	445	ASN
1	B	472	GLN
1	B	492	LEU
1	B	499	TRP
1	C	36	GLU
1	C	49	GLU
1	C	60	ILE
1	C	69	LEU
1	C	95	ILE
1	C	110	LEU
1	C	111	GLU
1	C	153	VAL
1	C	183	ARG
1	C	189	ARG
1	C	199	LYS
1	C	205	LEU
1	C	211	THR
1	C	218	SER
1	C	227	ILE
1	C	262	GLU
1	C	268	ASN
1	C	275	PHE
1	C	277	ARG
1	C	301	ASP
1	C	311	LYS
1	C	313	SER
1	C	363	LEU
1	C	379	ILE
1	C	417	LYS
1	C	418	LEU
1	C	422	MET
1	C	425	LEU
1	C	474	VAL
1	C	492	LEU
1	C	499	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	268	ASN
1	A	360	GLN
1	B	165	GLN
1	B	360	GLN
1	B	445	ASN
1	B	470	ASN
1	C	48	ASN
1	C	165	GLN
1	C	360	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 10 are monoatomic - leaving 1 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	GLU	A	601	-	8,9,9	2.08	2 (25%)	8,11,11	1.53	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	GLU	A	601	-	-	2/9/9/9	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	GLU	O-C	5.04	1.37	1.22
2	A	601	GLU	OXT-C	-2.50	1.22	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	GLU	CG-CB-CA	-2.42	108.31	113.86
2	A	601	GLU	OE2-CD-OE1	-2.16	117.77	123.33

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	GLU	N-CA-CB-CG
2	A	601	GLU	CA-CB-CG-CD

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	GLU	2	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	444/517 (85%)	0.61	18 (4%) 41 24	25, 55, 87, 119	0
1	B	438/517 (84%)	0.49	13 (2%) 52 32	17, 52, 80, 103	0
1	C	448/517 (86%)	0.60	20 (4%) 38 22	22, 53, 85, 101	0
All	All	1330/1551 (85%)	0.57	51 (3%) 44 26	17, 54, 85, 119	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	251	ASN	5.5
1	A	476	GLY	3.9
1	A	501	ARG	3.7
1	A	503	SER	3.6
1	A	147	GLY	3.3
1	C	305	ALA	3.3
1	C	248	GLY	3.2
1	A	475	GLY	3.2
1	B	84	TYR	3.2
1	C	317	ALA	3.2
1	B	446	PRO	3.0
1	A	140	LEU	2.9
1	A	141	LEU	2.9
1	A	436	LEU	2.8
1	B	140	LEU	2.8
1	C	249	ARG	2.8
1	C	138	ILE	2.7
1	B	254	LYS	2.6
1	A	138	ILE	2.6
1	A	105	ALA	2.6
1	C	313	SER	2.6
1	B	83	ASP	2.6
1	A	345	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	252	ILE	2.5
1	A	63	ASP	2.5
1	C	61	ASN	2.5
1	C	63	ASP	2.5
1	A	437	LYS	2.5
1	A	439	ASN	2.4
1	A	440	PHE	2.4
1	C	180	ASP	2.4
1	B	252	ILE	2.3
1	C	98	THR	2.3
1	C	492	LEU	2.2
1	A	454	VAL	2.2
1	C	159	ASN	2.2
1	C	373	CYS	2.2
1	C	508	GLU	2.2
1	A	483	VAL	2.2
1	C	500	SER	2.2
1	C	442	ALA	2.2
1	B	51	GLY	2.2
1	B	249	ARG	2.2
1	B	141	LEU	2.1
1	B	436	LEU	2.1
1	C	69	LEU	2.1
1	A	49	GLU	2.1
1	B	444	PHE	2.1
1	C	195	PHE	2.1
1	B	499	TRP	2.0
1	B	253	ARG	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	GLU	A	601	10/10	0.96	0.08	33,39,40,41	0
3	IOD	A	605	1/1	0.97	0.08	92,92,92,92	0
3	IOD	C	603	1/1	0.98	0.11	78,78,78,78	0
3	IOD	A	602	1/1	0.99	0.02	53,53,53,53	0
3	IOD	B	602	1/1	0.99	0.05	84,84,84,84	0
3	IOD	B	603	1/1	0.99	0.03	51,51,51,51	0
3	IOD	C	601	1/1	0.99	0.04	62,62,62,62	0
3	IOD	A	604	1/1	0.99	0.04	69,69,69,69	0
3	IOD	A	603	1/1	1.00	0.01	45,45,45,45	0
3	IOD	C	602	1/1	1.00	0.01	42,42,42,42	0
3	IOD	B	601	1/1	1.00	0.02	57,57,57,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.