



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 02:43 PM GMT

PDB ID : 3UGX
Title : Crystal Structure of Visual Arrestin
Authors : Batra-Safferling, R.; Granzin, J.
Deposited on : 2011-11-03
Resolution : 2.65 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

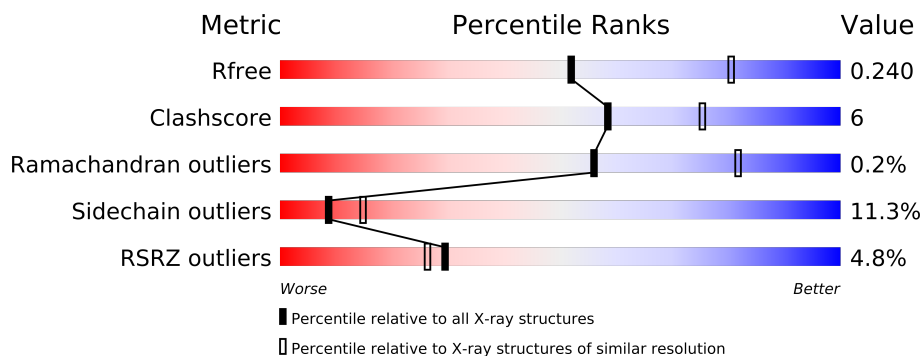
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.65 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}	66092	2393 (2.68-2.60)
Clashscore	79885	2915 (2.68-2.60)
Ramachandran outliers	78287	2865 (2.68-2.60)
Sidechain outliers	78261	2865 (2.68-2.60)
RSRZ outliers	66119	2393 (2.68-2.60)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	414	
1	B	414	
1	C	414	
1	D	414	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	PTD	A	405	-	X
2	PTD	A	406	-	X
2	PTD	A	407	-	X
2	PTD	A	408	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
2	PTD	A	410	-	X
2	PTD	A	411	-	X
2	PTD	A	412	-	X
2	PTD	B	406	-	X
2	PTD	B	407	-	X
2	PTD	C	405	-	X
2	PTD	C	406	-	X
2	PTD	C	407	-	X
2	PTD	D	407	-	X
3	NA	A	413	-	X
3	NA	B	408	-	X
4	EDO	A	415	-	X
4	EDO	B	409	-	X
4	EDO	C	409	-	X
4	EDO	D	408	-	X
5	IMD	D	405	-	X
6	K	C	408	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11230 atoms, of which 0 are hydrogen and 0 are deuterium.

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 S-arrestin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	369	Total	C	N	O	S	0	1	0
			2859	1832	474	544	9			
1	B	352	Total	C	N	O	S	0	0	0
			2662	1709	437	507	9			
1	C	358	Total	C	N	O	S	0	0	0
			2772	1783	461	520	8			
1	D	348	Total	C	N	O	S	0	0	0
			2608	1680	432	487	9			

There are 40 discrepancies between the modelled and reference sequences:

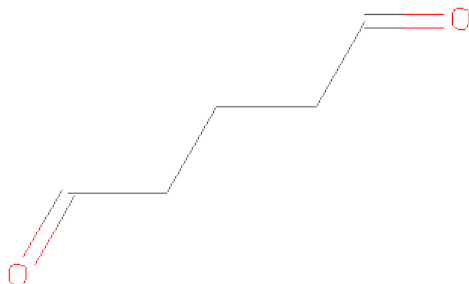
Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	ALA	-	EXPRESSION TAG	UNP P08168
A	-8	SER	-	EXPRESSION TAG	UNP P08168
A	-7	TRP	-	EXPRESSION TAG	UNP P08168
A	-6	SER	-	EXPRESSION TAG	UNP P08168
A	-5	HIS	-	EXPRESSION TAG	UNP P08168
A	-4	PRO	-	EXPRESSION TAG	UNP P08168
A	-3	GLN	-	EXPRESSION TAG	UNP P08168
A	-2	PHE	-	EXPRESSION TAG	UNP P08168
A	-1	GLU	-	EXPRESSION TAG	UNP P08168
A	0	LYS	-	EXPRESSION TAG	UNP P08168
B	-9	ALA	-	EXPRESSION TAG	UNP P08168
B	-8	SER	-	EXPRESSION TAG	UNP P08168
B	-7	TRP	-	EXPRESSION TAG	UNP P08168
B	-6	SER	-	EXPRESSION TAG	UNP P08168
B	-5	HIS	-	EXPRESSION TAG	UNP P08168
B	-4	PRO	-	EXPRESSION TAG	UNP P08168
B	-3	GLN	-	EXPRESSION TAG	UNP P08168
B	-2	PHE	-	EXPRESSION TAG	UNP P08168
B	-1	GLU	-	EXPRESSION TAG	UNP P08168
B	0	LYS	-	EXPRESSION TAG	UNP P08168
C	-9	ALA	-	EXPRESSION TAG	UNP P08168

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-8	SER	-	EXPRESSION TAG	UNP P08168
C	-7	TRP	-	EXPRESSION TAG	UNP P08168
C	-6	SER	-	EXPRESSION TAG	UNP P08168
C	-5	HIS	-	EXPRESSION TAG	UNP P08168
C	-4	PRO	-	EXPRESSION TAG	UNP P08168
C	-3	GLN	-	EXPRESSION TAG	UNP P08168
C	-2	PHE	-	EXPRESSION TAG	UNP P08168
C	-1	GLU	-	EXPRESSION TAG	UNP P08168
C	0	LYS	-	EXPRESSION TAG	UNP P08168
D	-9	ALA	-	EXPRESSION TAG	UNP P08168
D	-8	SER	-	EXPRESSION TAG	UNP P08168
D	-7	TRP	-	EXPRESSION TAG	UNP P08168
D	-6	SER	-	EXPRESSION TAG	UNP P08168
D	-5	HIS	-	EXPRESSION TAG	UNP P08168
D	-4	PRO	-	EXPRESSION TAG	UNP P08168
D	-3	GLN	-	EXPRESSION TAG	UNP P08168
D	-2	PHE	-	EXPRESSION TAG	UNP P08168
D	-1	GLU	-	EXPRESSION TAG	UNP P08168
D	0	LYS	-	EXPRESSION TAG	UNP P08168

- Molecule 2 is PENTANEDIAL (three-letter code: PTD) (formula: C₅H₈O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			7	5	2		
2	A	1	Total	C	O	0	0
			7	5	2		

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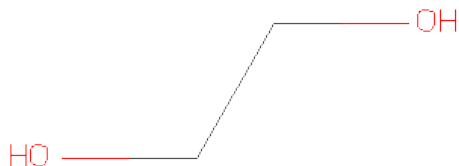
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 7 5 2	0	0
2	A	1	Total C O 7 5 2	0	0
2	A	1	Total C O 7 5 2	0	0
2	A	1	Total C O 7 5 2	0	0
2	A	1	Total C O 7 5 2	0	0
2	A	1	Total C O 7 5 2	0	0
2	B	1	Total C O 7 5 2	0	0
2	B	1	Total C O 7 5 2	0	0
2	C	1	Total C O 7 5 2	0	0
2	C	1	Total C O 7 5 2	0	0
2	C	1	Total C O 7 5 2	0	0
2	D	1	Total C O 7 5 2	0	0

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

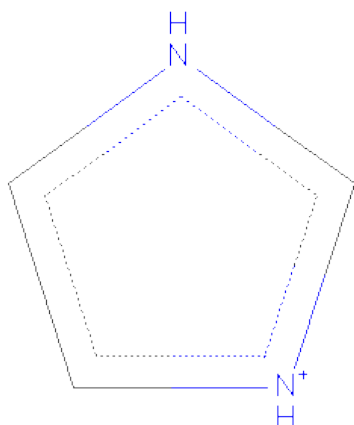
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Na 1 1	0	0
3	A	1	Total Na 1 1	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

- Molecule 5 is IMIDAZOLE (three-letter code: IMD) (formula: C₃H₅N₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	N	0	0
			5	3	2		
5	D	1	Total	C	N	0	0
			5	3	2		
5	D	1	Total	C	N	0	0
			5	3	2		

- Molecule 6 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	1	Total	K	0	0
			1	1		

- Molecule 7 is water.

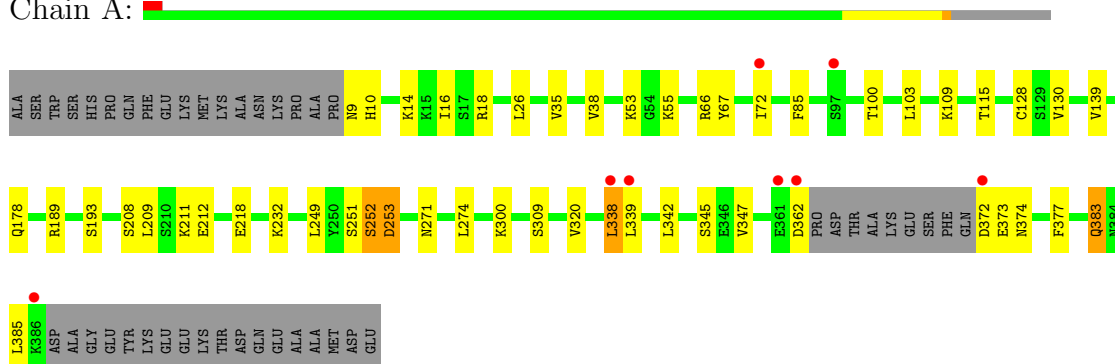
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	68	Total	O	0	0
			68	68		
7	B	31	Total	O	0	0
			31	31		
7	C	45	Total	O	0	0
			45	45		
7	D	41	Total	O	0	0
			41	41		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

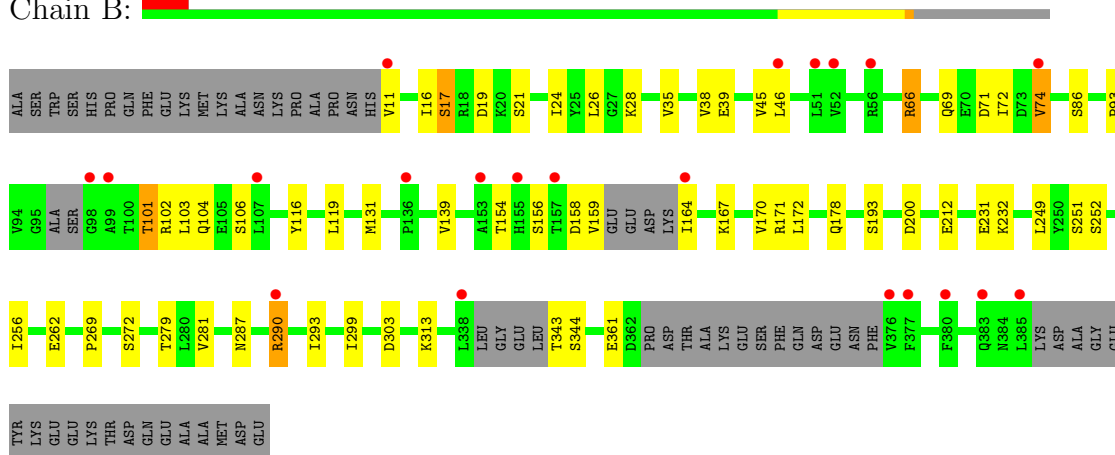
• Molecule 1: S-arrestin

Chain A:



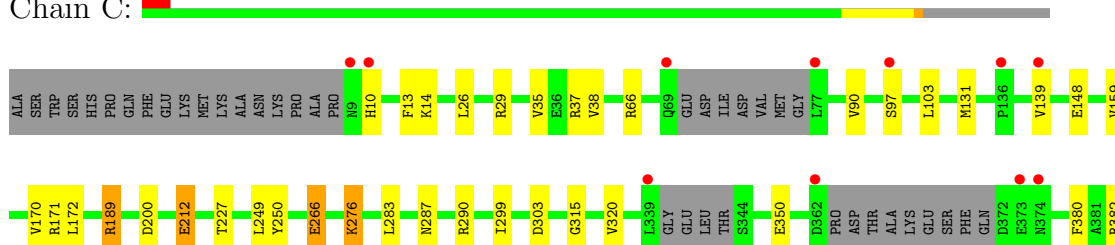
• Molecule 1: S-arrestin

Chain B:



• Molecule 1: S-arrestin

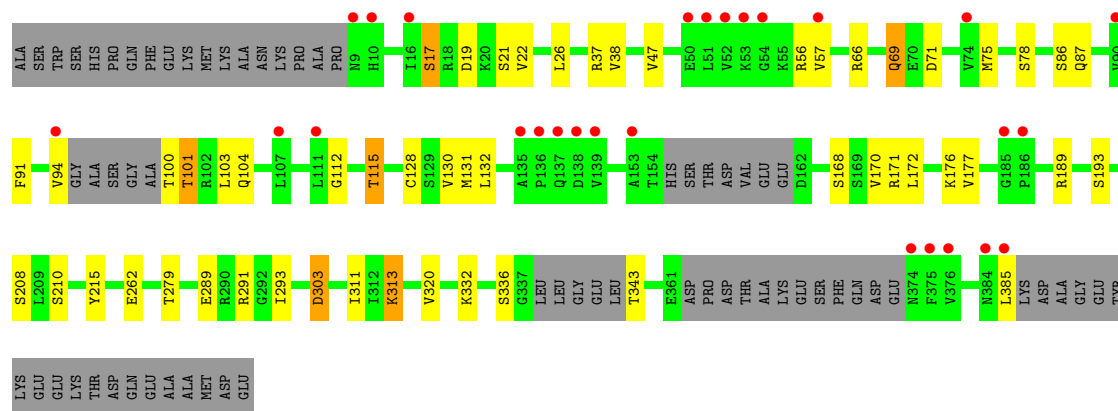
Chain C:





- Molecule 1: S-arrestin

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	168.36Å 184.33Å 90.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.89 – 2.65 32.89 – 2.65	Depositor EDS
% Data completeness (in resolution range)	98.6 (32.89-2.65) 98.4 (32.89-2.65)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 2.65Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.209 , 0.253 0.195 , 0.240	Depositor DCC
R_{free} test set	4062 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	49.8	Xtriage
Anisotropy	0.428	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 38.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 81359 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11230	wwPDB-VP
Average B, all atoms (Å ²)	57.0	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.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, K, PTD, IMD, EDO

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	0.42	0/2919	0.62	0/3969
1	B	0.38	0/2712	0.58	0/3698
1	C	0.40	0/2827	0.59	0/3841
1	D	0.42	0/2660	0.60	0/3632
All	All	0.40	0/11118	0.60	0/15140

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2859	0	0	20	0
1	B	2662	0	0	15	0
1	C	2772	0	0	15	0
1	D	2608	0	0	18	0
2	A	56	0	64	10	0
2	B	14	0	16	0	0
2	C	21	0	24	6	0
2	D	7	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	8	0	12	2	0
4	B	4	0	6	0	0
4	C	12	0	18	0	0
4	D	4	0	6	2	0
5	B	5	0	5	2	0
5	D	10	0	10	2	0
6	C	1	0	0	0	0
7	A	68	0	0	2	0
7	B	31	0	0	3	0
7	C	45	0	0	4	0
7	D	41	0	0	4	0
All	All	11230	0	169	70	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (70) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:128:CYS:N	5:D:406:IMD:H5	1.94	0.82
1:B:290:ARG:NH1	1:B:299:ILE:O	2.21	0.73
1:D:189:ARG:NH1	1:D:208:SER:OG	2.22	0.72
1:C:266:GLU:OE2	1:C:276:LYS:NZ	2.23	0.71
1:C:290:ARG:NH1	1:C:299:ILE:O	2.22	0.71
1:C:303:ASP:OD2	1:C:382:ARG:NH1	2.23	0.71
1:C:148:GLU:OE2	1:C:171:ARG:NE	2.24	0.71
1:D:87:GLN:N	7:D:435:HOH:O	2.27	0.67
1:B:93:PRO:CG	1:B:116:TYR:CD2	2.78	0.67
1:A:55:LYS:CE	2:A:405:PTD:HC31	2.26	0.66
1:D:215:TYR:CZ	4:D:408:EDO:H21	2.33	0.64
2:C:407:PTD:HC1	7:C:412:HOH:O	1.99	0.61
1:A:377:PHE:CD2	2:A:409:PTD:HC5	2.36	0.61
1:D:303:ASP:OD1	1:D:303:ASP:N	2.34	0.60
1:B:313:LYS:NZ	7:B:436:HOH:O	2.36	0.59
4:A:415:EDO:O2	1:B:200:ASP:OD1	2.21	0.58
1:A:252:SER:OG	2:A:407:PTD:HC5	2.04	0.58
1:D:100:THR:CG2	1:D:101:THR:N	2.67	0.58
1:D:57:VAL:N	1:D:91:PHE:O	2.37	0.58
1:D:313:LYS:N	7:D:442:HOH:O	2.38	0.57
1:B:74:VAL:O	2:C:406:PTD:O1	2.22	0.57
1:A:252:SER:CB	2:A:407:PTD:HC5	2.35	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:178:GLN:OE1	2:A:410:PTD:HC5	2.05	0.56
1:A:338:LEU:O	1:A:342:LEU:N	2.40	0.55
1:A:85:PHE:N	4:A:414:EDO:HO1	2.05	0.55
1:B:93:PRO:CG	1:B:116:TYR:CE2	2.91	0.54
1:B:101:THR:N	1:B:104:GLN:OE1	2.41	0.53
1:C:189:ARG:O	2:C:406:PTD:HC31	2.09	0.53
1:A:252:SER:OG	2:A:407:PTD:HC1	2.10	0.52
1:B:17:SER:OG	1:B:167:LYS:O	2.28	0.52
1:B:28:LYS:NZ	1:B:39:GLU:OE2	2.43	0.52
5:B:405:IMD:N1	7:B:435:HOH:O	2.28	0.51
1:C:283:LEU:O	1:C:287:ASN:ND2	2.44	0.50
1:A:383:GLN:OE1	1:A:383:GLN:N	2.45	0.50
1:A:9:ASN:OD1	1:A:374:ASN:ND2	2.45	0.50
1:B:158:ASP:N	1:B:159:VAL:CA	2.75	0.49
1:B:178:GLN:N	7:B:413:HOH:O	2.46	0.49
1:B:102:ARG:O	1:B:106:SER:OG	2.31	0.49
1:A:271:ASN:O	7:A:453:HOH:O	2.20	0.48
1:A:211:LYS:NZ	1:A:218:GLU:OE2	2.46	0.48
1:D:112:GLY:O	1:D:115:THR:OG1	2.32	0.48
1:A:18:ARG:NH2	7:A:483:HOH:O	2.47	0.47
1:C:139:VAL:O	7:C:427:HOH:O	2.20	0.47
1:D:17:SER:OG	1:D:22:VAL:O	2.33	0.47
1:D:313:LYS:CG	7:D:442:HOH:O	2.63	0.47
1:D:176:LYS:NZ	7:D:446:HOH:O	2.48	0.47
1:D:311:ILE:O	1:D:313:LYS:CE	2.63	0.46
1:D:128:CYS:N	5:D:406:IMD:C5	2.73	0.46
1:B:269:PRO:O	1:B:272:SER:OG	2.34	0.46
1:C:315:GLY:N	7:C:444:HOH:O	2.48	0.46
1:A:309:SER:O	2:A:410:PTD:HC42	2.15	0.46
1:D:101:THR:N	1:D:104:GLN:OE1	2.48	0.46
1:B:19:ASP:OD1	1:B:21:SER:N	2.50	0.45
1:C:148:GLU:OE1	7:C:413:HOH:O	2.21	0.45
1:D:215:TYR:CE2	4:D:408:EDO:H21	2.51	0.45
1:A:128:CYS:CB	2:A:410:PTD:HC31	2.47	0.45
1:C:13:PHE:CE1	1:C:29:ARG:CZ	3.00	0.44
1:A:67:TYR:OH	1:A:253:ASP:OD2	2.36	0.44
1:A:130:VAL:CG2	2:A:410:PTD:HC21	2.47	0.44
1:C:29:ARG:NE	1:C:380:PHE:O	2.51	0.44
1:D:66:ARG:NH1	1:D:69:GLN:OE1	2.52	0.42
1:D:289:GLU:OE2	1:D:291:ARG:NE	2.53	0.42
1:A:14:LYS:NZ	2:A:409:PTD:HC41	2.35	0.42
1:A:253:ASP:OD1	1:A:253:ASP:N	2.54	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:250:TYR:O	2:C:405:PTD:HC31	2.19	0.41
1:A:300:LYS:O	1:A:385:LEU:N	2.53	0.41
1:C:212:GLU:OE1	2:C:407:PTD:O5	2.38	0.41
1:C:13:PHE:CE1	1:C:29:ARG:NH1	2.89	0.41
1:B:66:ARG:CG	5:B:405:IMD:H2	2.51	0.40
1:C:350:GLU:O	2:C:406:PTD:HC5	2.22	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	366/414 (88%)	358 (98%)	7 (2%)	1 (0%)	50	77
1	B	342/414 (83%)	332 (97%)	9 (3%)	1 (0%)	50	77
1	C	350/414 (84%)	344 (98%)	5 (1%)	1 (0%)	50	77
1	D	338/414 (82%)	332 (98%)	6 (2%)	0	100	100
All	All	1396/1656 (84%)	1366 (98%)	27 (2%)	3 (0%)	56	82

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	35	VAL
1	B	35	VAL
1	C	35	VAL

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	315/368 (86%)	283 (90%)	32 (10%)	11	19
1	B	287/368 (78%)	244 (85%)	43 (15%)	4	7
1	C	304/368 (83%)	282 (93%)	22 (7%)	21	38
1	D	276/368 (75%)	239 (87%)	37 (13%)	6	9
All	All	1182/1472 (80%)	1048 (89%)	134 (11%)	9	15

All (134) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	HIS
1	A	16	ILE
1	A	26	LEU
1	A	38	VAL
1	A	53	LYS
1	A	66	ARG
1	A	72	ILE
1	A	100	THR
1	A	103	LEU
1	A	109	LYS
1	A	115	THR
1	A	139	VAL
1	A	189	ARG
1	A	193	SER
1	A	208	SER
1	A	209	LEU
1	A	212	GLU
1	A	232	LYS
1	A	249	LEU
1	A	251	SER
1	A	252	SER
1	A	253	ASP
1	A	274	LEU
1	A	320	VAL
1	A	338	LEU
1	A	339	LEU
1	A	345	SER
1	A	347	VAL
1	A	362	ASP
1	A	372	ASP
1	A	373	GLU
1	A	383	GLN
1	B	11	VAL

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Mol	Chain	Res	Type
1	B	16	ILE
1	B	17	SER
1	B	24	ILE
1	B	26	LEU
1	B	38	VAL
1	B	45	VAL
1	B	46	LEU
1	B	66	ARG
1	B	69	GLN
1	B	71	ASP
1	B	72	ILE
1	B	74	VAL
1	B	86	SER
1	B	101	THR
1	B	103	LEU
1	B	119	LEU
1	B	131	MET
1	B	139	VAL
1	B	154	THR
1	B	156	SER
1	B	164	ILE
1	B	170	VAL
1	B	171	ARG
1	B	172	LEU
1	B	193	SER
1	B	212	GLU
1	B	231	GLU
1	B	232	LYS
1	B	249	LEU
1	B	251	SER
1	B	252	SER
1	B	256	ILE
1	B	262	GLU
1	B	279	THR
1	B	281	VAL
1	B	287	ASN
1	B	290	ARG
1	B	293	ILE
1	B	303	ASP
1	B	343	THR
1	B	344	SER
1	B	361	GLU

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Mol	Chain	Res	Type
1	C	10	HIS
1	C	14	LYS
1	C	26	LEU
1	C	37	ARG
1	C	38	VAL
1	C	66	ARG
1	C	90	VAL
1	C	97	SER
1	C	103	LEU
1	C	131	MET
1	C	159	VAL
1	C	170	VAL
1	C	172	LEU
1	C	189	ARG
1	C	200	ASP
1	C	212	GLU
1	C	227	THR
1	C	249	LEU
1	C	266	GLU
1	C	276	LYS
1	C	320	VAL
1	C	385	LEU
1	D	17	SER
1	D	19	ASP
1	D	21	SER
1	D	26	LEU
1	D	37	ARG
1	D	38	VAL
1	D	47	VAL
1	D	56	ARG
1	D	69	GLN
1	D	71	ASP
1	D	75	MET
1	D	78	SER
1	D	86	SER
1	D	94	VAL
1	D	101	THR
1	D	103	LEU
1	D	115	THR
1	D	130	VAL
1	D	131	MET
1	D	132	LEU

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Mol	Chain	Res	Type
1	D	168	SER
1	D	170	VAL
1	D	171	ARG
1	D	172	LEU
1	D	177	VAL
1	D	193	SER
1	D	210	SER
1	D	262	GLU
1	D	279	THR
1	D	293	ILE
1	D	303	ASP
1	D	313	LYS
1	D	320	VAL
1	D	332	LYS
1	D	336	SER
1	D	343	THR
1	D	385	LEU

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

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 27 ligands modelled in this entry, 3 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
2	PTD	A	405	-	6,6,6	1.64	2 (33%)	5,5,5	1.42	0
2	PTD	A	406	-	6,6,6	1.66	2 (33%)	5,5,5	1.63	1 (20%)
2	PTD	A	407	-	6,6,6	1.62	2 (33%)	5,5,5	1.30	0
2	PTD	A	408	-	6,6,6	1.62	2 (33%)	5,5,5	1.30	0
2	PTD	A	409	-	6,6,6	1.65	2 (33%)	5,5,5	1.42	0
2	PTD	A	410	-	6,6,6	1.70	2 (33%)	5,5,5	1.45	1 (20%)
2	PTD	A	411	-	6,6,6	1.60	2 (33%)	5,5,5	1.45	0
2	PTD	A	412	-	6,6,6	1.63	2 (33%)	5,5,5	1.36	0
4	EDO	A	414	-	3,3,3	0.52	0	2,2,2	0.24	0
4	EDO	A	415	-	3,3,3	0.56	0	2,2,2	0.35	0
5	IMD	B	405	-	5,5,5	1.39	2 (40%)	5,5,5	0.17	0
2	PTD	B	406	-	6,6,6	1.64	2 (33%)	5,5,5	1.39	0
2	PTD	B	407	-	6,6,6	1.63	2 (33%)	5,5,5	1.39	0
4	EDO	B	409	-	3,3,3	0.51	0	2,2,2	0.46	0
2	PTD	C	405	-	6,6,6	1.64	2 (33%)	5,5,5	1.26	0
2	PTD	C	406	-	6,6,6	1.62	2 (33%)	5,5,5	1.32	0
2	PTD	C	407	-	6,6,6	1.65	2 (33%)	5,5,5	1.17	0
4	EDO	C	409	-	3,3,3	0.54	0	2,2,2	0.44	0
4	EDO	C	410	-	3,3,3	0.61	0	2,2,2	0.31	0
4	EDO	C	411	-	3,3,3	0.56	0	2,2,2	0.30	0
5	IMD	D	405	-	5,5,5	1.39	2 (40%)	5,5,5	0.15	0
5	IMD	D	406	-	5,5,5	1.37	1 (20%)	5,5,5	0.19	0
2	PTD	D	407	-	6,6,6	1.63	2 (33%)	5,5,5	1.55	0
4	EDO	D	408	-	3,3,3	0.59	0	2,2,2	0.11	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	PTD	A	405	-	-	0/4/4/4	0/0/0/0
2	PTD	A	406	-	-	0/4/4/4	0/0/0/0
2	PTD	A	407	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PTD	A	408	-	-	0/4/4/4	0/0/0/0
2	PTD	A	409	-	-	0/4/4/4	0/0/0/0
2	PTD	A	410	-	-	0/4/4/4	0/0/0/0
2	PTD	A	411	-	-	0/4/4/4	0/0/0/0
2	PTD	A	412	-	-	0/4/4/4	0/0/0/0
4	EDO	A	414	-	-	0/1/1/1	0/0/0/0
4	EDO	A	415	-	-	0/1/1/1	0/0/0/0
5	IMD	B	405	-	-	0/0/0/0	0/1/1/1
2	PTD	B	406	-	-	0/4/4/4	0/0/0/0
2	PTD	B	407	-	-	0/4/4/4	0/0/0/0
4	EDO	B	409	-	-	0/1/1/1	0/0/0/0
2	PTD	C	405	-	-	0/4/4/4	0/0/0/0
2	PTD	C	406	-	-	0/4/4/4	0/0/0/0
2	PTD	C	407	-	-	0/4/4/4	0/0/0/0
4	EDO	C	409	-	-	0/1/1/1	0/0/0/0
4	EDO	C	410	-	-	0/1/1/1	0/0/0/0
4	EDO	C	411	-	-	0/1/1/1	0/0/0/0
5	IMD	D	405	-	-	0/0/0/0	0/1/1/1
5	IMD	D	406	-	-	0/0/0/0	0/1/1/1
2	PTD	D	407	-	-	0/4/4/4	0/0/0/0
4	EDO	D	408	-	-	0/1/1/1	0/0/0/0

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	410	PTD	O5-C5	2.97	1.40	1.19
2	A	410	PTD	O1-C1	2.83	1.39	1.19
2	A	409	PTD	O5-C5	2.81	1.39	1.19
2	C	407	PTD	O1-C1	2.79	1.39	1.19
2	A	406	PTD	O1-C1	2.79	1.39	1.19
2	B	406	PTD	O1-C1	2.79	1.39	1.19
2	C	405	PTD	O5-C5	2.77	1.39	1.19
2	A	406	PTD	O5-C5	2.77	1.39	1.19
2	C	405	PTD	O1-C1	2.77	1.39	1.19
2	D	407	PTD	O5-C5	2.76	1.39	1.19
2	A	405	PTD	O5-C5	2.75	1.39	1.19
2	D	407	PTD	O1-C1	2.75	1.39	1.19
2	A	405	PTD	O1-C1	2.75	1.38	1.19
2	A	409	PTD	O1-C1	2.74	1.38	1.19
2	B	407	PTD	O1-C1	2.74	1.38	1.19
2	A	407	PTD	O5-C5	2.74	1.38	1.19
2	A	408	PTD	O1-C1	2.73	1.38	1.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	406	PTD	O5-C5	2.73	1.38	1.19
2	A	408	PTD	O5-C5	2.73	1.38	1.19
2	B	407	PTD	O5-C5	2.72	1.38	1.19
2	A	412	PTD	O5-C5	2.72	1.38	1.19
2	C	407	PTD	O5-C5	2.72	1.38	1.19
2	A	411	PTD	O5-C5	2.72	1.38	1.19
2	C	406	PTD	O5-C5	2.72	1.38	1.19
2	A	412	PTD	O1-C1	2.72	1.38	1.19
2	A	407	PTD	O1-C1	2.70	1.38	1.19
2	C	406	PTD	O1-C1	2.69	1.38	1.19
2	A	411	PTD	O1-C1	2.65	1.38	1.19
5	D	405	IMD	C2-N3	2.13	1.35	1.31
5	B	405	IMD	C2-N1	2.13	1.35	1.31
5	D	406	IMD	C2-N3	2.11	1.35	1.31
5	B	405	IMD	C2-N3	2.10	1.35	1.31
5	D	405	IMD	C2-N1	2.05	1.35	1.31

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	410	PTD	C3-C4-C5	2.20	121.05	112.45
2	A	406	PTD	C3-C4-C5	2.02	120.32	112.45

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	369/414 (89%)	-0.26	8 (2%) 59 56	23, 42, 90, 133	0
1	B	352/414 (85%)	0.06	21 (5%) 21 18	29, 58, 120, 140	0
1	C	358/414 (86%)	-0.19	13 (3%) 41 38	25, 47, 90, 162	0
1	D	348/414 (84%)	0.01	27 (7%) 13 10	26, 52, 117, 141	0
All	All	1427/1656 (86%)	-0.10	69 (4%) 29 26	23, 48, 114, 162	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	98	GLY	4.9
1	B	377	PHE	4.7
1	D	385	LEU	4.5
1	D	375	PHE	4.5
1	B	99	ALA	4.4
1	B	376	VAL	4.3
1	D	51	LEU	4.3
1	D	139	VAL	4.2
1	B	338	LEU	3.9
1	C	339	LEU	3.8
1	C	373	GLU	3.8
1	B	385	LEU	3.8
1	D	376	VAL	3.7
1	A	97	SER	3.6
1	D	94	VAL	3.6
1	D	186	PRO	3.5
1	D	74	VAL	3.5
1	D	153	ALA	3.5
1	A	72	ILE	3.5
1	C	386	LYS	3.4
1	B	157	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	90	VAL	3.3
1	D	52	VAL	3.3
1	B	380	PHE	3.3
1	B	51	LEU	3.3
1	C	9	ASN	3.2
1	B	153	ALA	3.2
1	D	9	ASN	3.1
1	B	11	VAL	3.1
1	C	139	VAL	3.1
1	A	362	ASP	3.1
1	D	16	ILE	2.9
1	D	10	HIS	2.8
1	C	362	ASP	2.8
1	D	135	ALA	2.8
1	D	57	VAL	2.7
1	A	386	LYS	2.7
1	B	52	VAL	2.7
1	D	384	ASN	2.7
1	C	77	LEU	2.7
1	C	385	LEU	2.6
1	B	290	ARG	2.6
1	A	339	LEU	2.6
1	B	46	LEU	2.6
1	C	69	GLN	2.5
1	D	50	GLU	2.5
1	C	97	SER	2.5
1	C	136	PRO	2.4
1	A	372	ASP	2.4
1	D	107	LEU	2.4
1	B	107	LEU	2.4
1	A	338	LEU	2.3
1	D	185	GLY	2.3
1	C	10	HIS	2.3
1	B	136	PRO	2.3
1	D	137	GLN	2.2
1	D	111	LEU	2.2
1	D	54	GLY	2.2
1	A	361	GLU	2.2
1	D	136	PRO	2.2
1	D	53	LYS	2.2
1	B	383	GLN	2.2
1	B	164	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	74	VAL	2.1
1	C	374	ASN	2.1
1	B	56	ARG	2.1
1	D	374	ASN	2.1
1	B	155	HIS	2.0
1	D	138	ASP	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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	NA	B	408	1/1	0.39	20.08	45,45,45,45	0
2	PTD	C	407	7/7	0.30	11.36	57,64,71,76	0
4	EDO	B	409	4/4	0.28	9.01	55,60,61,70	0
4	EDO	A	415	4/4	0.22	6.58	59,63,64,68	0
2	PTD	A	411	7/7	0.27	6.09	65,71,75,77	0
2	PTD	A	408	7/7	0.22	4.99	68,70,72,72	0
2	PTD	B	407	7/7	0.25	4.77	62,65,71,74	0
2	PTD	A	412	7/7	0.27	4.55	59,63,72,72	0
6	K	C	408	1/1	0.25	4.29	88,88,88,88	0
2	PTD	C	405	7/7	0.36	4.02	69,72,76,77	0
2	PTD	A	410	7/7	0.27	3.96	55,56,62,63	0
2	PTD	A	406	7/7	0.24	3.82	27,35,36,38	0
2	PTD	D	407	7/7	0.21	3.50	52,61,69,69	0
4	EDO	C	409	4/4	0.21	3.18	58,59,63,65	0
2	PTD	A	407	7/7	0.29	2.87	62,70,78,82	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	PTD	B	406	7/7	0.21	2.43	69,73,81,83	0
4	EDO	D	408	4/4	0.36	2.40	62,63,63,63	0
3	NA	A	413	1/1	0.15	2.34	34,34,34,34	0
2	PTD	C	406	7/7	0.30	2.29	60,63,84,92	0
2	PTD	A	405	7/7	0.24	2.07	42,48,72,75	0
5	IMD	D	405	5/5	0.18	2.04	72,73,74,75	0
5	IMD	B	405	5/5	0.21	1.79	86,89,89,89	0
5	IMD	D	406	5/5	0.21	1.57	80,81,88,91	0
4	EDO	C	411	4/4	0.18	1.52	60,65,78,85	0
4	EDO	A	414	4/4	0.20	1.50	36,39,41,49	0
2	PTD	A	409	7/7	0.22	0.89	45,54,76,77	0
4	EDO	C	410	4/4	0.15	-0.67	26,30,37,38	0

6.5 Other polymers ⓘ

There are no such residues in this entry.