



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 06:19 AM GMT

PDB ID : 2WME
Title : CRYSTALLOGRAPHIC STRUCTURE OF BETAIN ALDEHYDE DEHYDROGENASE FROM PSEUDOMONAS AERUGINOSA
Authors : Gonzalez-Segura, L.; Rudino-Pinera, E.; Munoz-Clares, R.A.; Horjales, E.
Deposited on : 2009-06-30
Resolution : 2.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

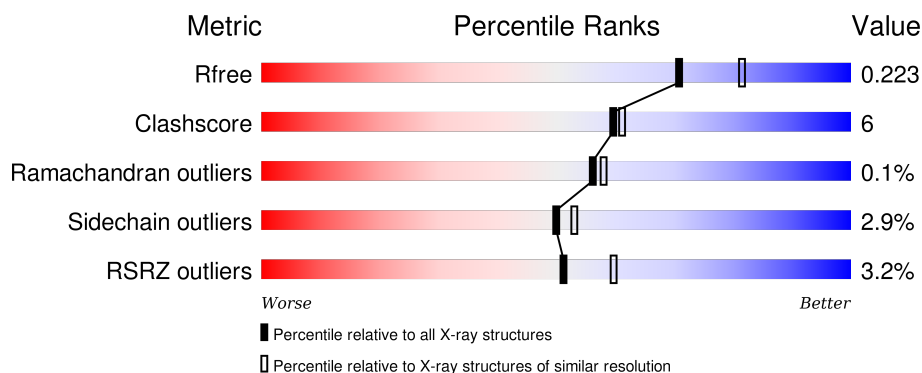
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	490	<div> <div>88%</div> <div>11%</div> </div>
1	B	490	<div> <div>91%</div> <div>8%</div> </div>
1	D	490	<div> <div>91%</div> <div>8%</div> </div>
1	F	490	<div> <div>3%</div> <div>85%</div> <div>13%</div> </div>
1	G	490	<div> <div>88%</div> <div>10%</div> </div>

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Mol	Chain	Length	Quality of chain
1	H	490	
2	C	490	
2	E	490	

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	GOL	A	1497	-	-	-	X
3	GOL	A	1498	-	-	-	X
3	GOL	A	1501	-	-	X	-
3	GOL	B	1497	-	-	-	X
3	GOL	C	1495	-	-	-	X
3	GOL	D	1496	-	-	X	-
3	GOL	E	1496	-	-	X	-
3	GOL	G	1495	-	-	X	-
3	GOL	G	1497	-	-	-	X
4	NAP	A	1491	-	-	-	X
4	NAP	D	1491	-	-	-	X
4	NAP	F	1491	-	-	-	X
4	NAP	G	1491	-	-	-	X
4	NAP	H	1491	-	-	-	X
5	BME	D	1492[A]	-	-	-	X
5	BME	D	1492[B]	-	-	-	X
5	BME	F	1492	-	-	-	X
5	BME	G	1492[A]	-	-	-	X
5	BME	G	1492[B]	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 33548 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 BETAINES ALDEHYDE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	489	Total	C	N	O	S	0	10	0
			3824	2398	673	739	14			
1	B	489	Total	C	N	O	S	0	7	0
			3800	2386	664	736	14			
1	D	489	Total	C	N	O	S	0	0	0
			3744	2351	657	722	14			
1	F	489	Total	C	N	O	S	0	5	0
			3789	2378	666	731	14			
1	G	489	Total	C	N	O	S	0	1	0
			3753	2356	658	725	14			
1	H	489	Total	C	N	O	S	0	1	0
			3753	2356	658	725	14			

- Molecule 2 is a protein called BETAINES ALDEHYDE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	489	Total	C	N	O	S	0	3	0
			3768	2364	660	729	15			
2	E	489	Total	C	N	O	S	0	3	0
			3767	2364	660	729	14			

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



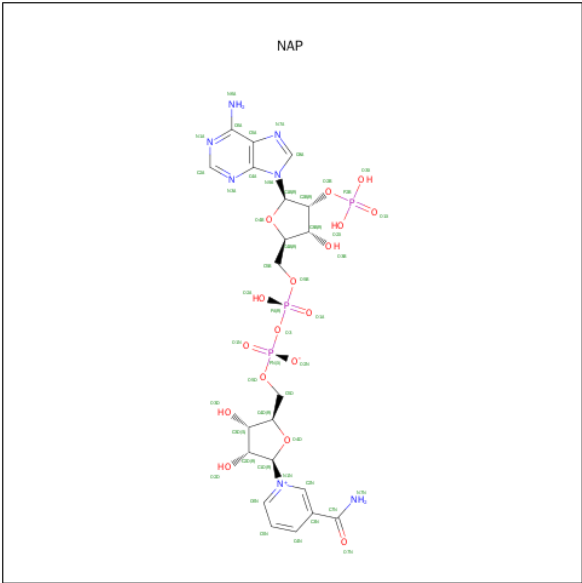
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	H	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	G	1	Total	C	O	0	0
			6	3	3		
3	G	1	Total	C	O	0	0
			6	3	3		
3	G	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



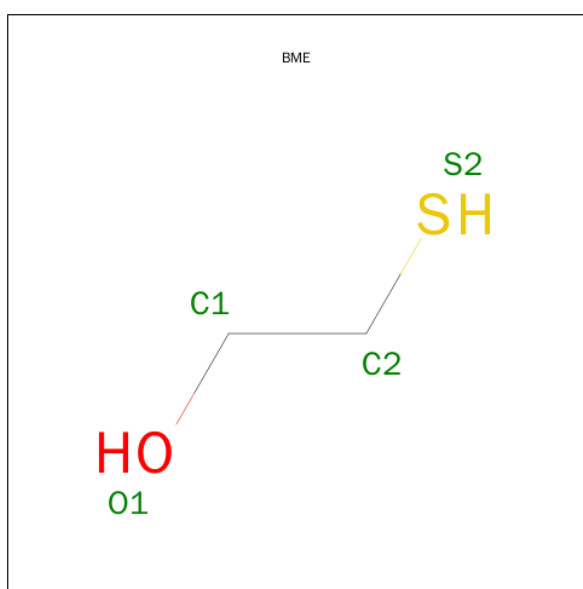
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	G	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	H	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 5 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	B	1	Total	C	O	S	0	0
			4	2	1	1		
5	D	1	Total	C	O	S	0	1
			8	4	2	2		
5	F	1	Total	C	O	S	0	0
			4	2	1	1		
5	G	1	Total	C	O	S	0	1
			8	4	2	2		

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	G	2	Total K 2 2	0	0
6	D	2	Total K 2 2	0	0
6	E	2	Total K 2 2	0	0
6	H	2	Total K 2 2	0	0
6	B	2	Total K 2 2	0	0
6	C	2	Total K 2 2	0	0
6	A	2	Total K 2 2	0	0
6	F	2	Total K 2 2	0	0

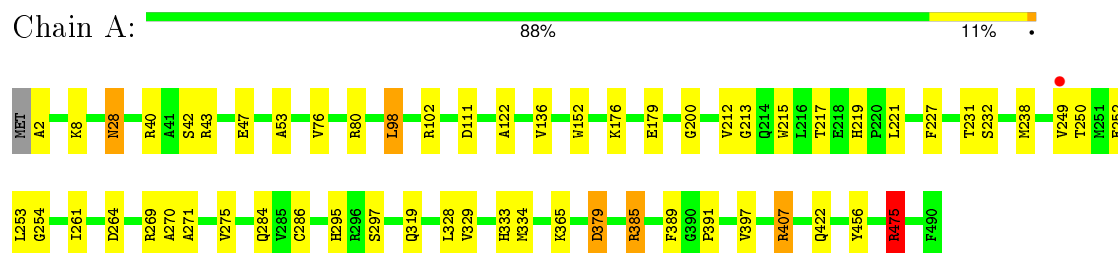
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	417	Total O 417 417	0	0
7	B	405	Total O 405 405	0	0
7	C	367	Total O 367 367	0	0
7	D	362	Total O 362 362	0	0
7	E	357	Total O 357 357	0	0
7	F	347	Total O 347 347	0	0
7	G	360	Total O 360 360	0	0
7	H	317	Total O 317 317	0	0

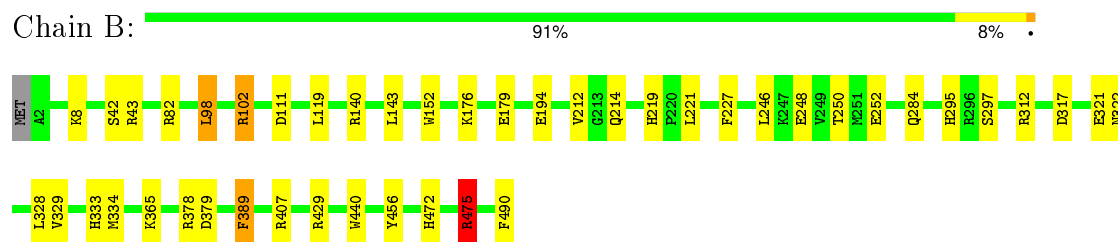
3 Residue-property plots

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.

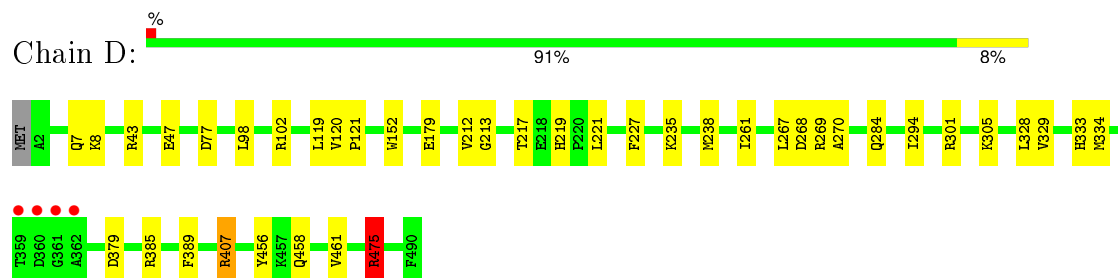
- Molecule 1: BETAINE ALDEHYDE DEHYDROGENASE



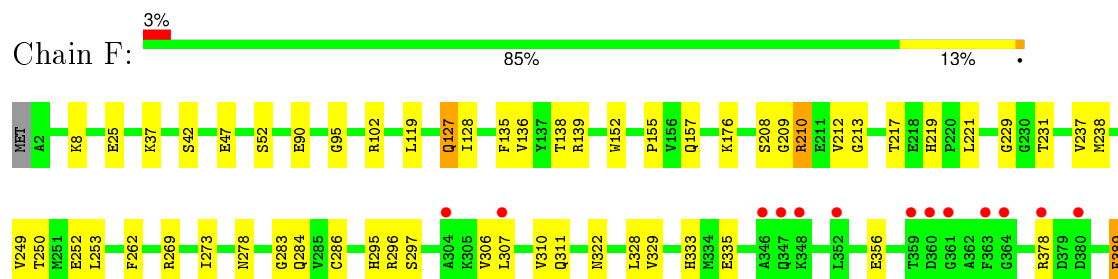
- Molecule 1: BETAINE ALDEHYDE DEHYDROGENASE



- Molecule 1: BETAINE ALDEHYDE DEHYDROGENASE

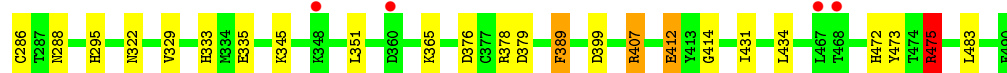
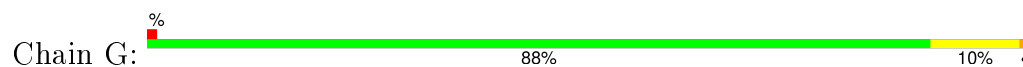


- Molecule 1: BETAINE ALDEHYDE DEHYDROGENASE

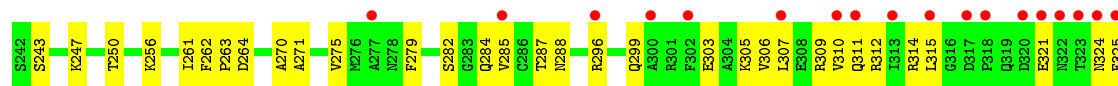
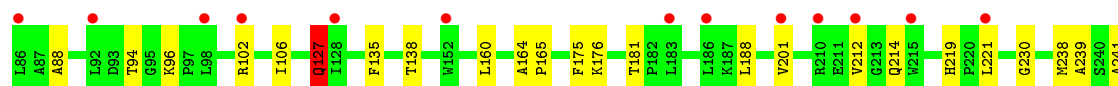
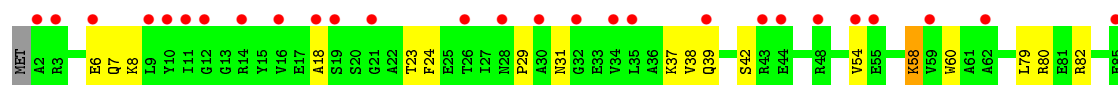
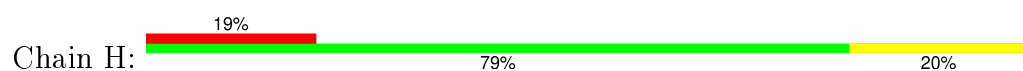




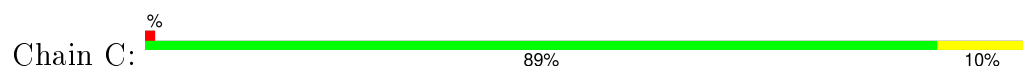
• Molecule 1: BETAINNE ALDEHYDE DEHYDROGENASE



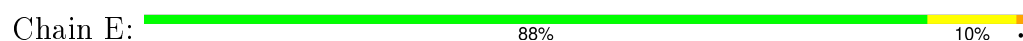
• Molecule 1: BETAINNE ALDEHYDE DEHYDROGENASE

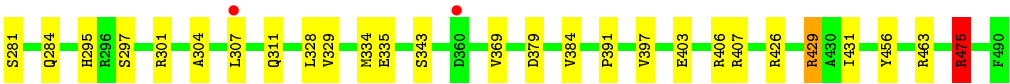


• Molecule 2: BETAINNE ALDEHYDE DEHYDROGENASE



• Molecule 2: BETAINNE ALDEHYDE DEHYDROGENASE





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	334.95Å 133.01Å 101.81Å 90.00° 94.94° 90.00°	Depositor
Resolution (Å)	42.68 – 2.10 42.66 – 2.10	Depositor EDS
% Data completeness (in resolution range)	95.2 (42.68-2.10) 95.1 (42.66-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.20 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.166 , 0.211 0.167 , 0.223	Depositor DCC
R_{free} test set	12459 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	21.7	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 245989 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	33548	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, CSO, K, NAP, BME

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	1.04	0/3892	0.91	11/5273 (0.2%)
1	B	1.00	2/3868 (0.1%)	0.87	9/5242 (0.2%)
1	D	0.98	0/3812	0.82	5/5166 (0.1%)
1	F	0.92	0/3857	0.79	4/5225 (0.1%)
1	G	0.95	3/3821 (0.1%)	0.82	3/5178 (0.1%)
1	H	0.85	1/3821 (0.0%)	0.79	2/5178 (0.0%)
2	C	0.95	1/3821 (0.0%)	0.84	8/5177 (0.2%)
2	E	0.95	1/3827 (0.0%)	0.87	12/5185 (0.2%)
All	All	0.96	8/30719 (0.0%)	0.84	54/41624 (0.1%)

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	248	GLU	CB-CG	6.22	1.64	1.52
1	G	412	GLU	CG-CD	6.12	1.61	1.51
1	H	127	GLN	CB-CG	5.33	1.67	1.52
2	E	44	GLU	CG-CD	5.31	1.59	1.51
1	B	440	TRP	CB-CG	5.28	1.59	1.50

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	475	ARG	NE-CZ-NH1	12.35	126.47	120.30
1	B	475	ARG	NE-CZ-NH1	11.50	126.05	120.30
1	A	475	ARG	NE-CZ-NH2	-10.35	115.12	120.30
2	E	3	ARG	NE-CZ-NH1	10.27	125.43	120.30
1	A	407	ARG	NE-CZ-NH1	10.27	125.43	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3824	0	3787	46	0
1	B	3800	0	3761	29	0
1	D	3744	0	3714	27	0
1	F	3789	0	3758	53	0
1	G	3753	0	3720	40	0
1	H	3753	0	3720	70	0
2	C	3768	0	3732	31	0
2	E	3767	0	3732	41	0
3	A	36	0	48	6	0
3	B	18	0	24	3	0
3	C	18	0	24	2	0
3	D	12	0	16	7	0
3	E	12	0	16	6	0
3	F	6	0	8	1	0
3	G	18	0	24	4	0
3	H	6	0	8	1	0
4	A	31	0	11	9	0
4	B	31	0	11	4	0
4	C	31	0	11	0	0
4	D	31	0	11	7	0
4	E	31	0	11	2	0
4	F	31	0	11	3	0
4	G	31	0	11	1	0
4	H	31	0	11	2	0
5	A	4	0	6	3	0
5	B	4	0	5	1	0
5	D	8	0	11	0	0
5	F	4	0	6	2	0
5	G	8	0	12	3	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
6	C	2	0	0	0	0
6	D	2	0	0	0	0
6	E	2	0	0	0	0
6	F	2	0	0	0	0
6	G	2	0	0	0	0
6	H	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	417	0	0	2	0
7	B	405	0	0	6	0
7	C	367	0	0	9	0
7	D	362	0	0	10	0
7	E	357	0	0	8	0
7	F	347	0	0	8	0
7	G	360	0	0	6	0
7	H	317	0	0	17	0
All	All	33548	0	30220	348	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.

The worst 5 of 348 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)
2:C:297:SER:HB3	7:C:2223:HOH:O	1.32	1.25
1:G:73:ARG:HD2	7:G:2072:HOH:O	1.34	1.25
1:G:43:ARG:HH11	1:G:43:ARG:HG2	1.07	1.09
1:A:286:CYS:SG	5:A:1492:BME:S2	2.46	1.07
1:G:335:GLU:HG2	7:G:2256:HOH:O	1.55	1.05

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	497/490 (101%)	480 (97%)	17 (3%)	0	100	100
1	B	494/490 (101%)	480 (97%)	14 (3%)	0	100	100
1	D	487/490 (99%)	470 (96%)	17 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	492/490 (100%)	481 (98%)	11 (2%)	0	100	100
1	G	488/490 (100%)	474 (97%)	13 (3%)	1 (0%)	52	53
1	H	488/490 (100%)	462 (95%)	25 (5%)	1 (0%)	52	53
2	C	488/490 (100%)	473 (97%)	14 (3%)	1 (0%)	52	53
2	E	489/490 (100%)	468 (96%)	21 (4%)	0	100	100
All	All	3923/3920 (100%)	3788 (97%)	132 (3%)	3 (0%)	56	58

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	363	PHE
2	C	414	GLY
1	G	414	GLY

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	400/391 (102%)	390 (98%)	10 (2%)	55	59
1	B	397/391 (102%)	385 (97%)	12 (3%)	48	51
1	D	390/391 (100%)	383 (98%)	7 (2%)	66	72
1	F	395/391 (101%)	382 (97%)	13 (3%)	45	47
1	G	391/391 (100%)	381 (97%)	10 (3%)	54	58
1	H	391/391 (100%)	375 (96%)	16 (4%)	37	36
2	C	391/390 (100%)	380 (97%)	11 (3%)	51	55
2	E	392/390 (100%)	379 (97%)	13 (3%)	45	47
All	All	3147/3126 (101%)	3055 (97%)	92 (3%)	50	53

5 of 92 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	8	LYS
2	E	431	ILE
1	H	385	ARG
2	E	37	LYS
2	E	176	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	219	HIS
2	E	127	GLN
1	H	127	GLN
1	D	295	HIS
2	E	219	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	CSO	C	286[A]	2	3,6,7	0.75	0	1,6,8	2.32	1 (100%)
2	CSO	C	286[B]	2	3,6,7	0.67	0	1,6,8	1.74	0
2	CSO	E	286	2	3,6,7	0.82	0	1,6,8	1.74	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	CSO	C	286[A]	2	-	0/1/5/7	0/0/0/0
2	CSO	C	286[B]	2	-	0/1/5/7	0/0/0/0
2	CSO	E	286	2	-	0/1/5/7	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	286[A]	CSO	O-C-CA	-2.32	119.43	125.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	286[B]	CSO	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 52 ligands modelled in this entry, 16 are monoatomic - leaving 36 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAP	A	1491	-	27,33,52	0.97	1 (3%)	34,52,80	2.39	6 (17%)
5	BME	A	1492	-	3,3,3	0.30	0	2,2,2	0.70	0
3	GOL	A	1496	-	5,5,5	0.70	0	5,5,5	0.95	0
3	GOL	A	1497	-	5,5,5	0.43	0	5,5,5	0.38	0
3	GOL	A	1498	-	5,5,5	0.50	0	5,5,5	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	A	1499	-	5,5,5	0.22	0	5,5,5	0.81	0
3	GOL	A	1500	-	5,5,5	0.87	0	5,5,5	1.37	1 (20%)
3	GOL	A	1501	-	5,5,5	0.52	0	5,5,5	0.65	0
4	NAP	B	1491	-	27,33,52	1.04	1 (3%)	34,52,80	1.92	4 (11%)
5	BME	B	1492	-	3,3,3	0.54	0	2,2,2	0.44	0
3	GOL	B	1495	-	5,5,5	0.59	0	5,5,5	0.60	0
3	GOL	B	1496	-	5,5,5	1.04	0	5,5,5	1.41	1 (20%)
3	GOL	B	1497	-	5,5,5	0.38	0	5,5,5	0.76	0
4	NAP	C	1491	-	27,33,52	1.13	2 (7%)	34,52,80	2.32	7 (20%)
3	GOL	C	1495	-	5,5,5	0.59	0	5,5,5	0.58	0
3	GOL	C	1496	-	5,5,5	0.73	0	5,5,5	0.56	0
3	GOL	C	1497	-	5,5,5	0.45	0	5,5,5	0.73	0
4	NAP	D	1491	-	27,33,52	0.93	1 (3%)	34,52,80	2.27	5 (14%)
5	BME	D	1492[A]	-	3,3,3	0.22	0	2,2,2	0.80	0
5	BME	D	1492[B]	-	3,3,3	0.63	0	2,2,2	0.27	0
3	GOL	D	1495	-	5,5,5	0.26	0	5,5,5	0.20	0
3	GOL	D	1496	-	5,5,5	0.66	0	5,5,5	0.48	0
4	NAP	E	1491	-	27,33,52	1.22	2 (7%)	34,52,80	2.23	5 (14%)
3	GOL	E	1495	-	5,5,5	0.31	0	5,5,5	0.41	0
3	GOL	E	1496	-	5,5,5	0.40	0	5,5,5	0.76	0
4	NAP	F	1491	-	27,33,52	1.04	2 (7%)	34,52,80	2.38	8 (23%)
5	BME	F	1492	-	3,3,3	0.79	0	2,2,2	0.43	0
3	GOL	F	1495	-	5,5,5	0.35	0	5,5,5	0.56	0
4	NAP	G	1491	-	27,33,52	0.93	1 (3%)	34,52,80	2.27	5 (14%)
5	BME	G	1492[A]	-	3,3,3	0.51	0	2,2,2	0.39	0
5	BME	G	1492[B]	-	3,3,3	0.51	0	2,2,2	0.33	0
3	GOL	G	1495	-	5,5,5	0.45	0	5,5,5	0.78	0
3	GOL	G	1496	-	5,5,5	0.39	0	5,5,5	0.70	0
3	GOL	G	1497	-	5,5,5	0.52	0	5,5,5	0.42	0
4	NAP	H	1491	-	27,33,52	0.81	0	34,52,80	2.06	2 (5%)
3	GOL	H	1495	-	5,5,5	0.56	0	5,5,5	0.64	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAP	A	1491	-	-	0/17/37/67	0/3/3/5
5	BME	A	1492	-	-	0/1/1/1	0/0/0/0
3	GOL	A	1496	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	1497	-	-	0/4/4/4	0/0/0/0
3	GOL	A	1498	-	-	0/4/4/4	0/0/0/0
3	GOL	A	1499	-	-	0/4/4/4	0/0/0/0
3	GOL	A	1500	-	-	0/4/4/4	0/0/0/0
3	GOL	A	1501	-	-	0/4/4/4	0/0/0/0
4	NAP	B	1491	-	-	0/17/37/67	0/3/3/5
5	BME	B	1492	-	-	0/1/1/1	0/0/0/0
3	GOL	B	1495	-	-	0/4/4/4	0/0/0/0
3	GOL	B	1496	-	-	0/4/4/4	0/0/0/0
3	GOL	B	1497	-	-	0/4/4/4	0/0/0/0
4	NAP	C	1491	-	-	0/17/37/67	0/3/3/5
3	GOL	C	1495	-	-	0/4/4/4	0/0/0/0
3	GOL	C	1496	-	-	0/4/4/4	0/0/0/0
3	GOL	C	1497	-	-	0/4/4/4	0/0/0/0
4	NAP	D	1491	-	-	0/17/37/67	0/3/3/5
5	BME	D	1492[A]	-	-	0/1/1/1	0/0/0/0
5	BME	D	1492[B]	-	-	0/1/1/1	0/0/0/0
3	GOL	D	1495	-	-	0/4/4/4	0/0/0/0
3	GOL	D	1496	-	-	0/4/4/4	0/0/0/0
4	NAP	E	1491	-	-	0/17/37/67	0/3/3/5
3	GOL	E	1495	-	-	0/4/4/4	0/0/0/0
3	GOL	E	1496	-	-	0/4/4/4	0/0/0/0
4	NAP	F	1491	-	-	0/17/37/67	0/3/3/5
5	BME	F	1492	-	-	0/1/1/1	0/0/0/0
3	GOL	F	1495	-	-	0/4/4/4	0/0/0/0
4	NAP	G	1491	-	-	0/17/37/67	0/3/3/5
5	BME	G	1492[A]	-	-	0/1/1/1	0/0/0/0
5	BME	G	1492[B]	-	-	0/1/1/1	0/0/0/0
3	GOL	G	1495	-	-	0/4/4/4	0/0/0/0
3	GOL	G	1496	-	-	0/4/4/4	0/0/0/0
3	GOL	G	1497	-	-	0/4/4/4	0/0/0/0
4	NAP	H	1491	-	-	0/17/37/67	0/3/3/5
3	GOL	H	1495	-	-	0/4/4/4	0/0/0/0

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1491	NAP	C2A-N3A	2.03	1.35	1.32
4	C	1491	NAP	C2A-N3A	2.22	1.36	1.32
4	B	1491	NAP	O4B-C1B	2.40	1.44	1.41
4	F	1491	NAP	C4A-N3A	2.50	1.39	1.35
4	F	1491	NAP	O4B-C1B	2.50	1.44	1.41

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1491	NAP	N3A-C2A-N1A	-11.72	119.92	128.89
4	D	1491	NAP	N3A-C2A-N1A	-11.57	120.03	128.89
4	F	1491	NAP	N3A-C2A-N1A	-11.03	120.45	128.89
4	G	1491	NAP	N3A-C2A-N1A	-10.82	120.61	128.89
4	C	1491	NAP	N3A-C2A-N1A	-10.36	120.96	128.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

25 monomers are involved in 61 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1491	NAP	9	0
5	A	1492	BME	3	0
3	A	1501	GOL	6	0
4	B	1491	NAP	4	0
5	B	1492	BME	1	0
3	B	1495	GOL	3	0
3	B	1496	GOL	1	0
3	C	1496	GOL	1	0
3	C	1497	GOL	1	0
4	D	1491	NAP	7	0
3	D	1495	GOL	1	0
3	D	1496	GOL	6	0
4	E	1491	NAP	2	0
3	E	1495	GOL	1	0
3	E	1496	GOL	5	0
4	F	1491	NAP	3	0
5	F	1492	BME	2	0
3	F	1495	GOL	1	0
4	G	1491	NAP	1	0
5	G	1492[A]	BME	1	0
5	G	1492[B]	BME	2	0
3	G	1495	GOL	4	0
3	G	1496	GOL	1	0
4	H	1491	NAP	2	0
3	H	1495	GOL	1	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	489/490 (99%)	-0.16	1 (0%) 95 96	9, 20, 25, 36	0
1	B	489/490 (99%)	-0.12	0 100 100	10, 20, 26, 36	0
1	D	489/490 (99%)	-0.06	4 (0%) 87 90	10, 20, 27, 33	0
1	F	489/490 (99%)	0.13	13 (2%) 58 65	12, 21, 28, 34	0
1	G	489/490 (99%)	-0.09	4 (0%) 87 90	12, 20, 27, 35	0
1	H	489/490 (99%)	1.04	93 (19%) 2 2	15, 23, 31, 37	0
2	C	488/490 (99%)	-0.03	7 (1%) 78 82	11, 20, 27, 36	0
2	E	488/490 (99%)	-0.13	2 (0%) 93 94	10, 20, 26, 33	0
All	All	3910/3920 (99%)	0.07	124 (3%) 51 60	9, 20, 28, 37	0

The worst 5 of 124 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	362	ALA	6.1
1	H	363	PHE	5.8
1	H	359	THR	5.8
1	H	98	LEU	4.8
1	H	382	THR	4.7

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	CSO	C	286[B]	7/8	0.91	0.21	-	22,23,25,26	7
2	CSO	E	286	7/8	0.93	0.12	-	19,22,26,30	0
2	CSO	C	286[A]	7/8	0.91	0.21	-	15,22,23,25	7

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	GOL	A	1498	6/6	0.92	0.24	9.75	35,36,37,37	0
3	GOL	B	1497	6/6	0.89	0.22	6.21	27,38,42,44	0
5	BME	D	1492[B]	4/4	0.84	0.25	5.69	18,19,20,21	4
5	BME	D	1492[A]	4/4	0.84	0.25	5.68	28,29,30,34	4
4	NAP	F	1491	31/48	0.90	0.29	4.94	26,37,48,51	0
5	BME	G	1492[B]	4/4	0.85	0.27	4.68	37,38,39,41	4
3	GOL	A	1497	6/6	0.92	0.18	4.22	23,28,32,32	0
5	BME	F	1492	4/4	0.89	0.18	4.19	39,42,44,48	0
4	NAP	G	1491	31/48	0.90	0.21	3.83	26,31,44,48	31
5	BME	G	1492[A]	4/4	0.85	0.27	3.65	21,23,23,24	4
3	GOL	C	1495	6/6	0.86	0.19	3.55	42,47,48,50	0
4	NAP	A	1491	31/48	0.89	0.20	3.02	21,28,45,46	31
3	GOL	G	1497	6/6	0.82	0.21	2.96	33,34,35,36	0
4	NAP	D	1491	31/48	0.90	0.19	2.72	24,28,44,46	31
4	NAP	H	1491	31/48	0.79	0.28	2.20	24,33,43,44	31
3	GOL	E	1495	6/6	0.91	0.15	1.89	45,46,46,47	0
3	GOL	A	1500	6/6	0.82	0.17	1.85	25,29,30,33	0
3	GOL	D	1495	6/6	0.93	0.18	1.85	36,42,43,45	0
3	GOL	H	1495	6/6	0.79	0.22	1.55	41,46,46,47	0
3	GOL	C	1497	6/6	0.79	0.18	1.52	31,34,35,41	0
3	GOL	A	1496	6/6	0.89	0.17	1.36	21,27,28,30	0
3	GOL	D	1496	6/6	0.85	0.16	1.28	27,30,30,33	0
4	NAP	E	1491	31/48	0.93	0.14	1.09	13,19,42,44	31

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	GOL	B	1496	6/6	0.86	0.15	1.02	30,31,32,33	0
5	BME	A	1492	4/4	0.94	0.16	0.68	26,26,28,33	0
4	NAP	B	1491	31/48	0.93	0.15	0.58	19,23,39,41	31
3	GOL	G	1496	6/6	0.92	0.13	0.41	35,36,38,39	0
4	NAP	C	1491	31/48	0.93	0.14	0.38	19,25,46,50	0
3	GOL	B	1495	6/6	0.90	0.14	0.08	37,38,40,42	0
3	GOL	G	1495	6/6	0.92	0.13	0.03	35,39,39,40	0
5	BME	B	1492	4/4	0.94	0.14	-0.01	31,35,35,36	0
3	GOL	F	1495	6/6	0.94	0.11	-0.12	26,27,31,33	0
6	K	F	1494	1/1	0.99	0.10	-0.26	21,21,21,21	0
6	K	H	1494	1/1	0.95	0.13	-0.51	32,32,32,32	0
6	K	G	1494	1/1	0.99	0.10	-0.52	23,23,23,23	0
6	K	H	1493	1/1	0.97	0.17	-0.68	32,32,32,32	0
6	K	E	1494	1/1	0.99	0.07	-1.16	21,21,21,21	0
6	K	C	1494	1/1	0.99	0.05	-1.74	20,20,20,20	0
6	K	F	1493	1/1	0.99	0.09	-1.82	26,26,26,26	0
6	K	B	1494	1/1	0.99	0.03	-1.91	16,16,16,16	0
6	K	D	1493	1/1	0.99	0.08	-2.03	23,23,23,23	0
6	K	A	1494	1/1	0.99	0.03	-2.45	17,17,17,17	0
6	K	G	1493	1/1	0.99	0.08	-2.79	17,17,17,17	0
6	K	D	1494	1/1	0.98	0.04	-2.99	18,18,18,18	0
6	K	B	1493	1/1	0.99	0.07	-3.47	17,17,17,17	0
6	K	A	1493	1/1	0.99	0.06	-3.88	20,20,20,20	0
6	K	C	1493	1/1	0.99	0.06	-5.10	22,22,22,22	0
6	K	E	1493	1/1	0.99	0.05	-5.61	19,19,19,19	0
3	GOL	E	1496	6/6	0.79	0.46	-	41,45,46,47	0
3	GOL	A	1501	6/6	0.89	0.19	-	34,41,43,43	0
3	GOL	A	1499	6/6	0.84	0.19	-	33,35,38,41	0
3	GOL	C	1496	6/6	0.77	0.20	-	37,38,40,42	0

6.5 Other polymers ⓘ

There are no such residues in this entry.