



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 10:06 PM UTC

PDB ID : 9E15 / pdb_00009e15
Title : Alpha-Delta heterodimeric form of soluble hydrogenase I from *Pyrococcus furiosus*. Data processed and model refined in P1
Authors : Lanzilotta, W.N.; McTernan, P.M.; Adams, M.W.W.
Deposited on : 2024-10-21
Resolution : 2.60 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

<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

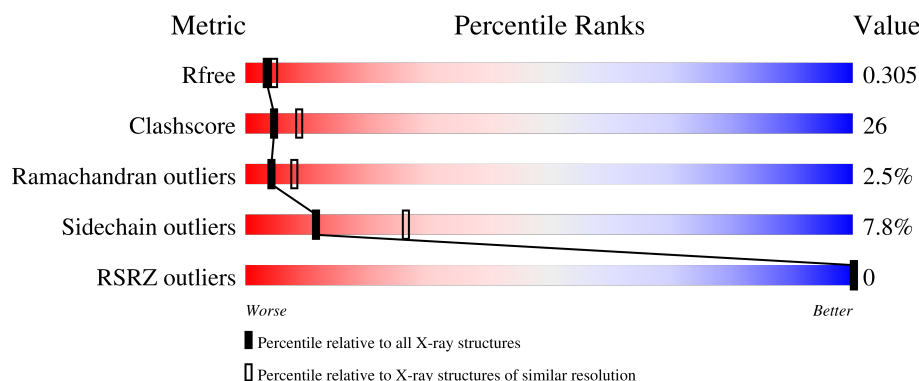
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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 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	266	<div> <div>50%</div> <div>40%</div> <div>5%</div> <div>.</div> <div>.</div> </div>
1	C	266	<div> <div>43%</div> <div>45%</div> <div>8%</div> <div>.</div> <div>.</div> </div>
1	E	266	<div> <div>47%</div> <div>44%</div> <div>5%</div> <div>.</div> </div>
1	G	266	<div> <div>55%</div> <div>39%</div> <div>.</div> <div>.</div> </div>
1	I	266	<div> <div>48%</div> <div>43%</div> <div>5%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	K	266	
1	M	266	
1	O	266	
2	B	424	
2	D	424	
2	F	424	
2	H	424	
2	J	424	
2	L	424	
2	N	424	
2	P	424	

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	SF4	A	501	-	-	X	-
3	SF4	C	501	-	-	X	-
3	SF4	C	502	-	-	X	-
3	SF4	C	503	-	-	X	-
3	SF4	E	501	-	-	X	-
3	SF4	E	503	-	-	X	-
3	SF4	G	501	-	-	X	-
3	SF4	G	503	-	-	X	-
3	SF4	I	501	-	-	X	-
3	SF4	K	501	-	-	X	-
3	SF4	K	502	-	-	X	-
3	SF4	K	503	-	-	X	-
3	SF4	M	502	-	-	X	-
3	SF4	M	503	-	-	X	-
3	SF4	O	501	-	-	X	-
4	FCO	B	501	-	-	X	-
4	FCO	D	501	-	-	X	-
4	FCO	F	501	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	FCO	H	501	-	-	X	-
4	FCO	J	501	-	-	X	-
4	FCO	L	501	-	-	X	-
4	FCO	N	501	-	-	X	-
4	FCO	P	501	-	-	X	-
5	NI	H	502	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 43445 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 Sulfhydrogenase 1 subunit delta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	256	Total	C	N	O	S	0	2	0
			2015	1296	328	371	20			
1	C	256	Total	C	N	O	S	0	1	0
			2008	1290	327	371	20			
1	E	256	Total	C	N	O	S	0	0	0
			2003	1287	327	369	20			
1	G	256	Total	C	N	O	S	0	0	0
			2003	1287	327	369	20			
1	I	256	Total	C	N	O	S	0	2	0
			2018	1298	330	370	20			
1	K	256	Total	C	N	O	S	0	0	0
			2003	1287	327	369	20			
1	M	256	Total	C	N	O	S	0	1	0
			2009	1292	328	369	20			
1	O	256	Total	C	N	O	S	0	1	0
			2009	1292	328	369	20			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	MET	-	initiating methionine	UNP E7FHU4
A	-8	HIS	-	expression tag	UNP E7FHU4
A	-7	HIS	-	expression tag	UNP E7FHU4
A	-6	HIS	-	expression tag	UNP E7FHU4
A	-5	HIS	-	expression tag	UNP E7FHU4
A	-4	HIS	-	expression tag	UNP E7FHU4
A	-3	HIS	-	expression tag	UNP E7FHU4
A	-2	HIS	-	expression tag	UNP E7FHU4
A	-1	HIS	-	expression tag	UNP E7FHU4
A	0	HIS	-	expression tag	UNP E7FHU4
C	-9	MET	-	initiating methionine	UNP E7FHU4
C	-8	HIS	-	expression tag	UNP E7FHU4
C	-7	HIS	-	expression tag	UNP E7FHU4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	HIS	-	expression tag	UNP E7FHU4
C	-5	HIS	-	expression tag	UNP E7FHU4
C	-4	HIS	-	expression tag	UNP E7FHU4
C	-3	HIS	-	expression tag	UNP E7FHU4
C	-2	HIS	-	expression tag	UNP E7FHU4
C	-1	HIS	-	expression tag	UNP E7FHU4
C	0	HIS	-	expression tag	UNP E7FHU4
E	-9	MET	-	initiating methionine	UNP E7FHU4
E	-8	HIS	-	expression tag	UNP E7FHU4
E	-7	HIS	-	expression tag	UNP E7FHU4
E	-6	HIS	-	expression tag	UNP E7FHU4
E	-5	HIS	-	expression tag	UNP E7FHU4
E	-4	HIS	-	expression tag	UNP E7FHU4
E	-3	HIS	-	expression tag	UNP E7FHU4
E	-2	HIS	-	expression tag	UNP E7FHU4
E	-1	HIS	-	expression tag	UNP E7FHU4
E	0	HIS	-	expression tag	UNP E7FHU4
G	-9	MET	-	initiating methionine	UNP E7FHU4
G	-8	HIS	-	expression tag	UNP E7FHU4
G	-7	HIS	-	expression tag	UNP E7FHU4
G	-6	HIS	-	expression tag	UNP E7FHU4
G	-5	HIS	-	expression tag	UNP E7FHU4
G	-4	HIS	-	expression tag	UNP E7FHU4
G	-3	HIS	-	expression tag	UNP E7FHU4
G	-2	HIS	-	expression tag	UNP E7FHU4
G	-1	HIS	-	expression tag	UNP E7FHU4
G	0	HIS	-	expression tag	UNP E7FHU4
I	-9	MET	-	initiating methionine	UNP E7FHU4
I	-8	HIS	-	expression tag	UNP E7FHU4
I	-7	HIS	-	expression tag	UNP E7FHU4
I	-6	HIS	-	expression tag	UNP E7FHU4
I	-5	HIS	-	expression tag	UNP E7FHU4
I	-4	HIS	-	expression tag	UNP E7FHU4
I	-3	HIS	-	expression tag	UNP E7FHU4
I	-2	HIS	-	expression tag	UNP E7FHU4
I	-1	HIS	-	expression tag	UNP E7FHU4
I	0	HIS	-	expression tag	UNP E7FHU4
K	-9	MET	-	initiating methionine	UNP E7FHU4
K	-8	HIS	-	expression tag	UNP E7FHU4
K	-7	HIS	-	expression tag	UNP E7FHU4
K	-6	HIS	-	expression tag	UNP E7FHU4
K	-5	HIS	-	expression tag	UNP E7FHU4

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-4	HIS	-	expression tag	UNP E7FHU4
K	-3	HIS	-	expression tag	UNP E7FHU4
K	-2	HIS	-	expression tag	UNP E7FHU4
K	-1	HIS	-	expression tag	UNP E7FHU4
K	0	HIS	-	expression tag	UNP E7FHU4
M	-9	MET	-	initiating methionine	UNP E7FHU4
M	-8	HIS	-	expression tag	UNP E7FHU4
M	-7	HIS	-	expression tag	UNP E7FHU4
M	-6	HIS	-	expression tag	UNP E7FHU4
M	-5	HIS	-	expression tag	UNP E7FHU4
M	-4	HIS	-	expression tag	UNP E7FHU4
M	-3	HIS	-	expression tag	UNP E7FHU4
M	-2	HIS	-	expression tag	UNP E7FHU4
M	-1	HIS	-	expression tag	UNP E7FHU4
M	0	HIS	-	expression tag	UNP E7FHU4
O	-9	MET	-	initiating methionine	UNP E7FHU4
O	-8	HIS	-	expression tag	UNP E7FHU4
O	-7	HIS	-	expression tag	UNP E7FHU4
O	-6	HIS	-	expression tag	UNP E7FHU4
O	-5	HIS	-	expression tag	UNP E7FHU4
O	-4	HIS	-	expression tag	UNP E7FHU4
O	-3	HIS	-	expression tag	UNP E7FHU4
O	-2	HIS	-	expression tag	UNP E7FHU4
O	-1	HIS	-	expression tag	UNP E7FHU4
O	0	HIS	-	expression tag	UNP E7FHU4

- Molecule 2 is a protein called Sulfhydrogenase 1 subunit alpha.

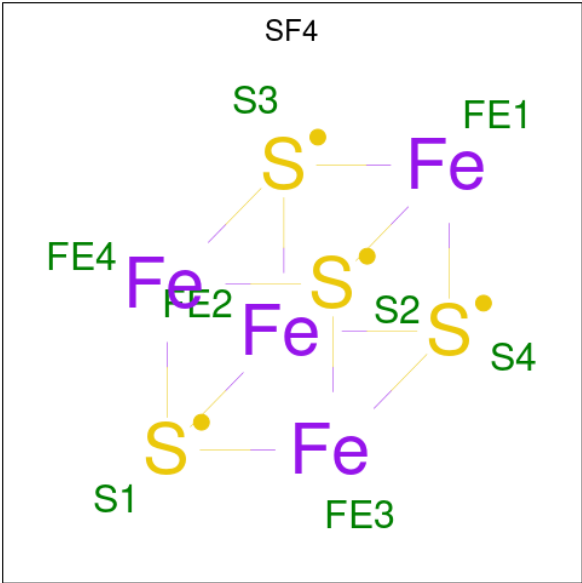
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	420	Total	C	N	O	S	0	3	0
			3349	2158	559	617	15			
2	D	419	Total	C	N	O	S	0	1	0
			3332	2145	556	616	15			
2	F	419	Total	C	N	O	S	0	3	0
			3343	2153	557	618	15			
2	H	420	Total	C	N	O	S	0	0	0
			3330	2143	555	617	15			
2	J	419	Total	C	N	O	S	0	1	0
			3331	2145	555	616	15			
2	L	421	Total	C	N	O	S	0	1	0
			3342	2151	558	618	15			
2	N	421	Total	C	N	O	S	0	1	0
			3342	2151	558	618	15			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	419	Total	C	N	O	S	0	0	0
			3325	2140	554	616	15			

- Molecule 3 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



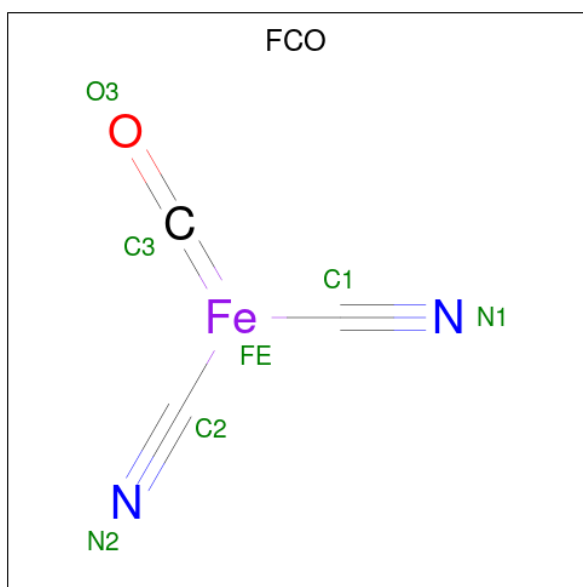
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		
3	E	1	Total	Fe	S	0	0
			8	4	4		
3	E	1	Total	Fe	S	0	0
			8	4	4		
3	E	1	Total	Fe	S	0	0
			8	4	4		
3	G	1	Total	Fe	S	0	0
			8	4	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	G	1	Total 8	Fe 4	S 4	0	0
3	G	1	Total 8	Fe 4	S 4	0	0
3	I	1	Total 8	Fe 4	S 4	0	0
3	I	1	Total 8	Fe 4	S 4	0	0
3	I	1	Total 8	Fe 4	S 4	0	0
3	K	1	Total 8	Fe 4	S 4	0	0
3	K	1	Total 8	Fe 4	S 4	0	0
3	K	1	Total 8	Fe 4	S 4	0	0
3	M	1	Total 8	Fe 4	S 4	0	0
3	M	1	Total 8	Fe 4	S 4	0	0
3	M	1	Total 8	Fe 4	S 4	0	0
3	O	1	Total 8	Fe 4	S 4	0	0
3	O	1	Total 8	Fe 4	S 4	0	0
3	O	1	Total 8	Fe 4	S 4	0	0

- Molecule 4 is CARBONMONOXIDE-(DICYANO) IRON (CCD ID: FCO) (formula: $\text{C}_3\text{FeN}_2\text{O}$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		
4	D	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		
4	F	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		
4	H	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		
4	J	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		
4	L	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		
4	N	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		
4	P	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		

- Molecule 5 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

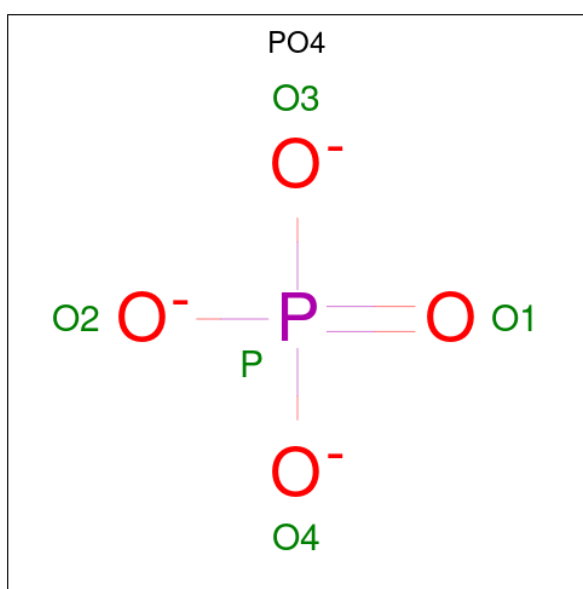
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Ni	0	0
			1	1		
5	D	1	Total	Ni	0	0
			1	1		
5	F	1	Total	Ni	0	0
			1	1		
5	H	1	Total	Ni	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	J	1	Total	Ni	0	0
			1	1		
5	L	1	Total	Ni	0	0
			1	1		
5	N	1	Total	Ni	0	0
			1	1		
5	P	1	Total	Ni	0	0
			1	1		

- Molecule 6 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	O	P	0	0
			5	4	1		
6	B	1	Total	O	P	0	0
			5	4	1		
6	F	1	Total	O	P	0	0
			5	4	1		
6	F	1	Total	O	P	0	0
			5	4	1		
6	H	1	Total	O	P	0	0
			5	4	1		
6	I	1	Total	O	P	0	0
			5	4	1		
6	J	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	L	1	Total	O	P	0	0
			5	4	1		
6	P	1	Total	O	P	0	0
			5	4	1		
6	P	1	Total	O	P	0	0
			5	4	1		
6	P	1	Total	O	P	0	0
			5	4	1		

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	H	1	Total	Mg	0	0
			1	1		
7	P	1	Total	Mg	0	0
			1	1		

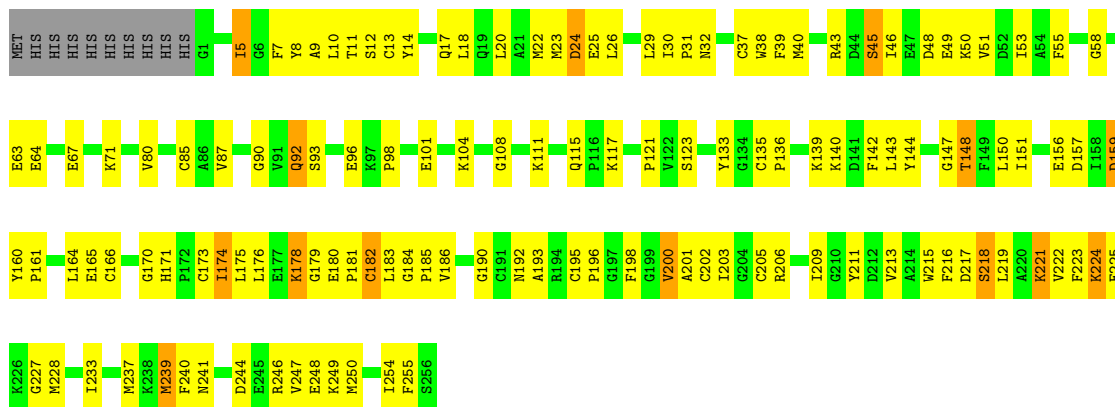
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	19	Total	O	0	0
			19	19		
8	B	37	Total	O	0	0
			37	37		
8	C	36	Total	O	0	0
			36	36		
8	D	27	Total	O	0	0
			27	27		
8	E	22	Total	O	0	0
			22	22		
8	F	29	Total	O	0	0
			29	29		
8	G	15	Total	O	0	0
			15	15		
8	H	40	Total	O	0	0
			40	40		
8	I	16	Total	O	0	0
			16	16		
8	J	25	Total	O	0	0
			25	25		
8	K	8	Total	O	0	0
			8	8		

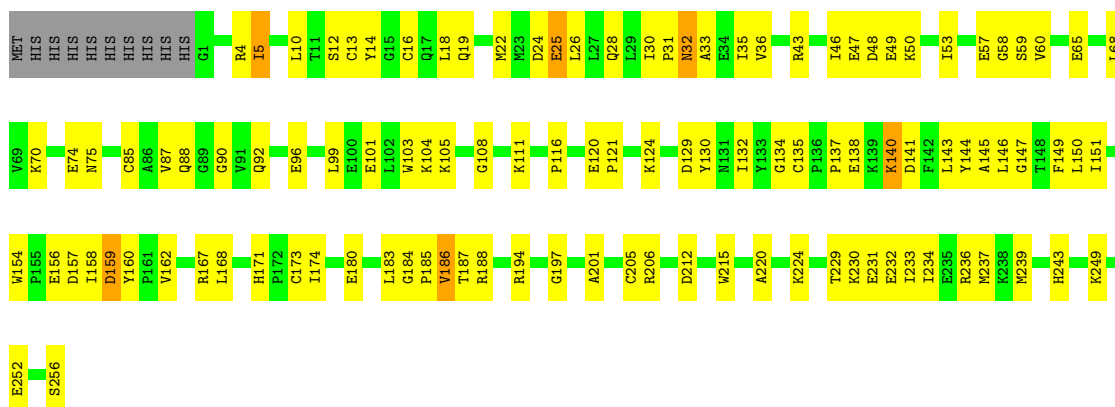
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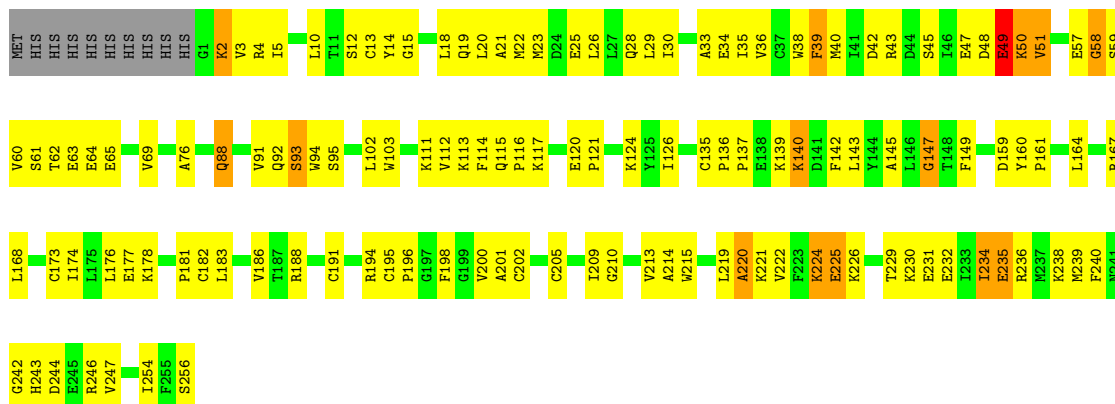
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	L	23	Total 23	O 23	0	0
8	M	11	Total 11	O 11	0	0
8	N	18	Total 18	O 18	0	0
8	O	13	Total 13	O 13	0	0
8	P	31	Total 31	O 31	0	0



- Molecule 1: Sulfhydrogenase 1 subunit delta

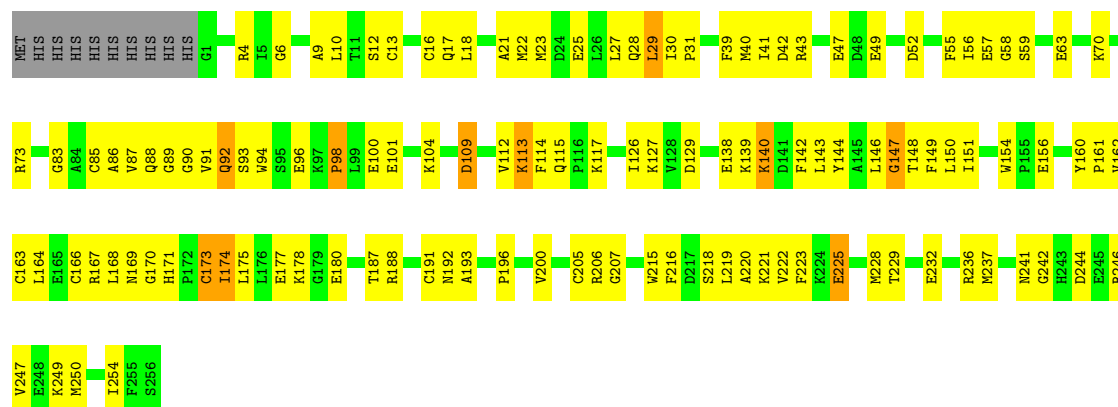


- Molecule 1: Sulfhydrogenase 1 subunit delta



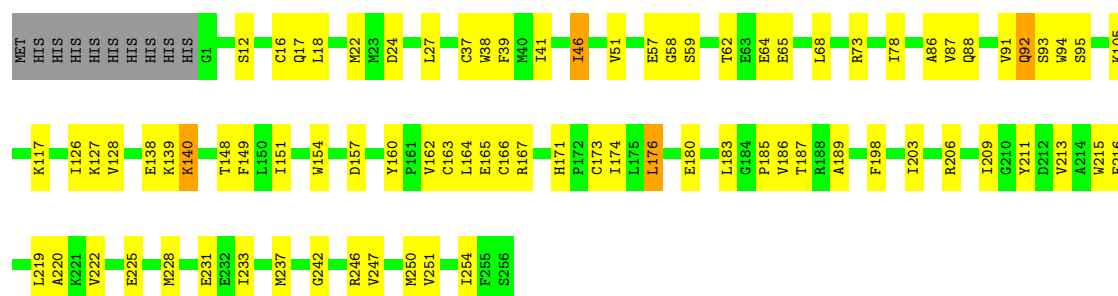
- Molecule 1: Sulfhydrogenase 1 subunit delta





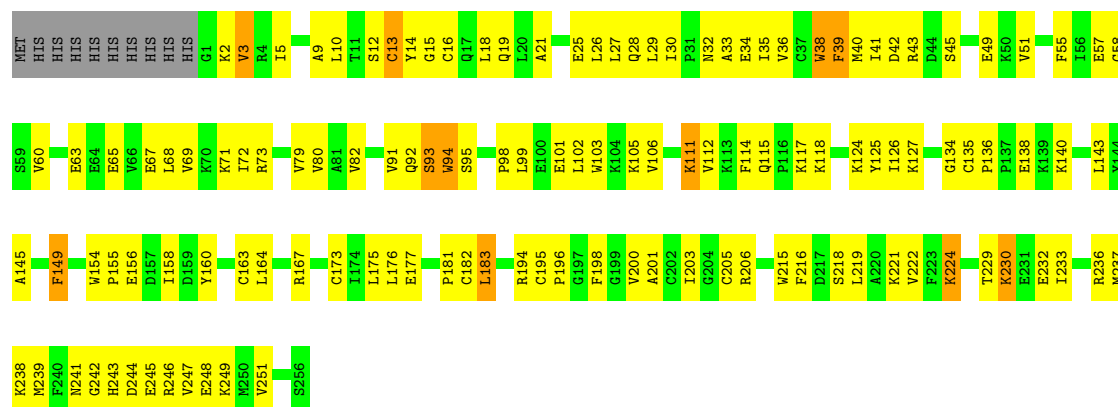
• Molecule 1: Sulfhydrylase 1 subunit delta

Chain M: 65% 29%



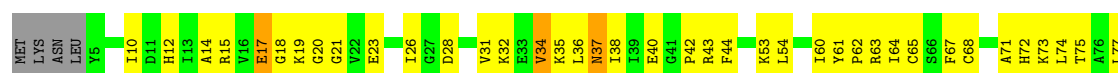
• Molecule 1: Sulfhydrylase 1 subunit delta

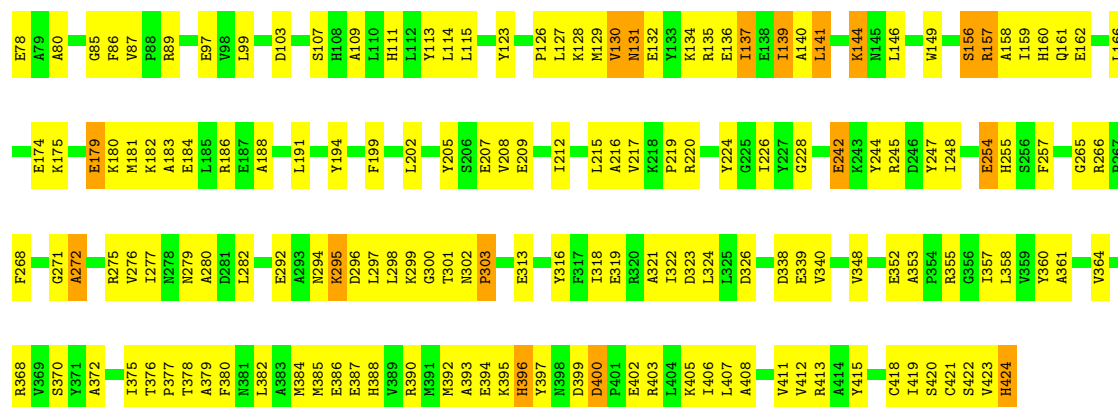
Chain O: 48% 44%



• Molecule 2: Sulfhydrylase 1 subunit alpha

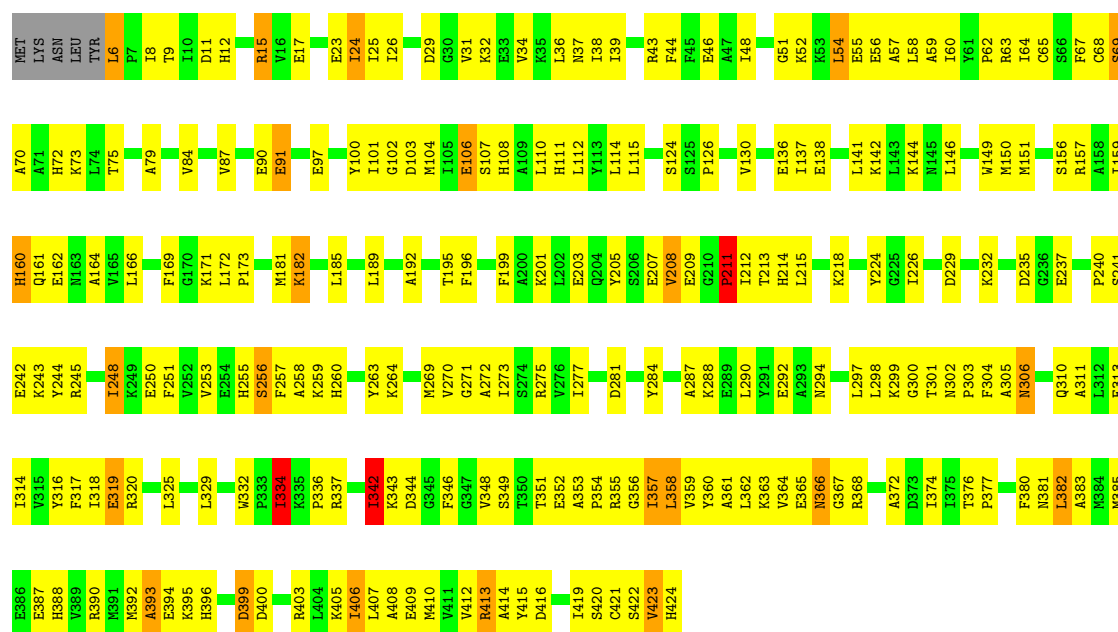
Chain B: 52% 42% 5%





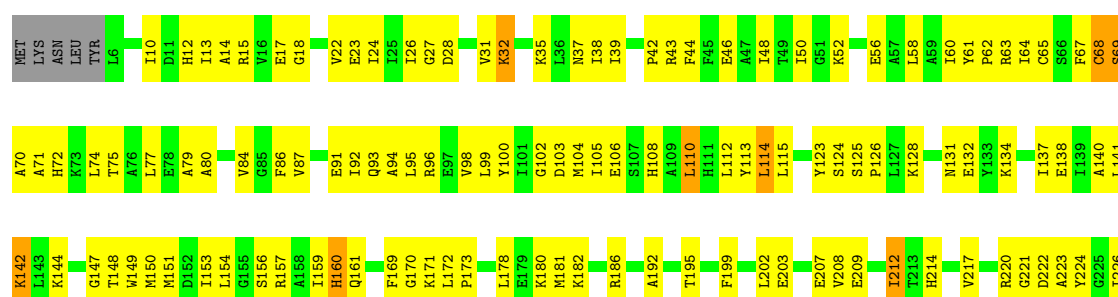
• Molecule 2: Sulfhydrylase 1 subunit alpha

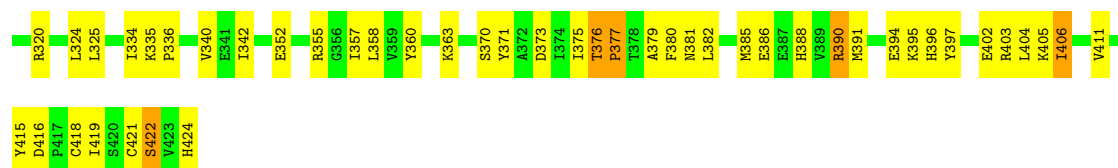
Chain D: 44% 48% 5% ..



• Molecule 2: Sulfhydrylase 1 subunit alpha

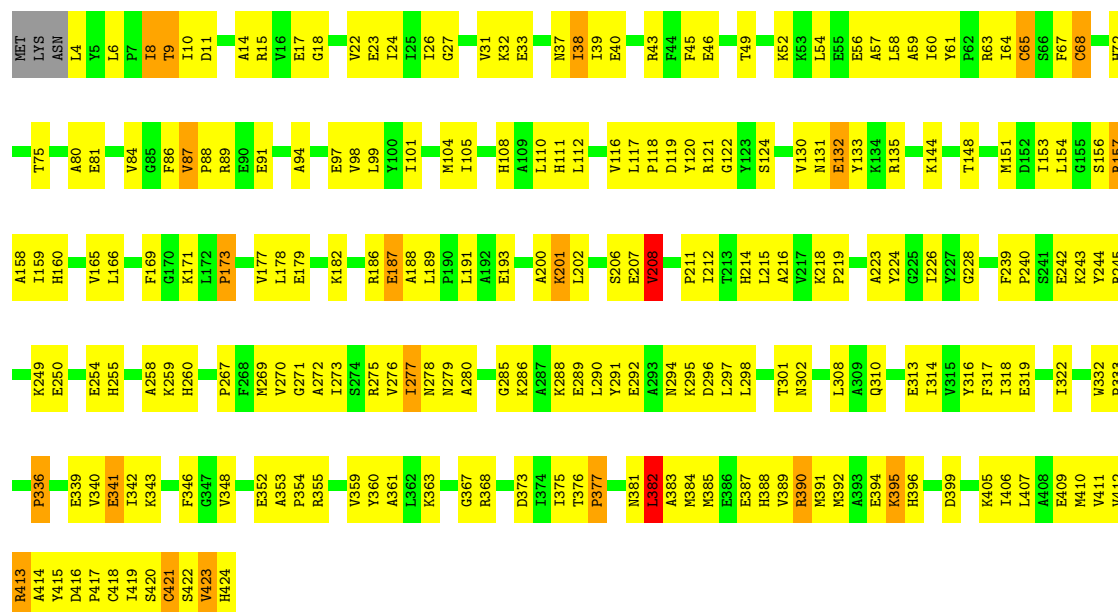
Chain F: 45% 50% ..





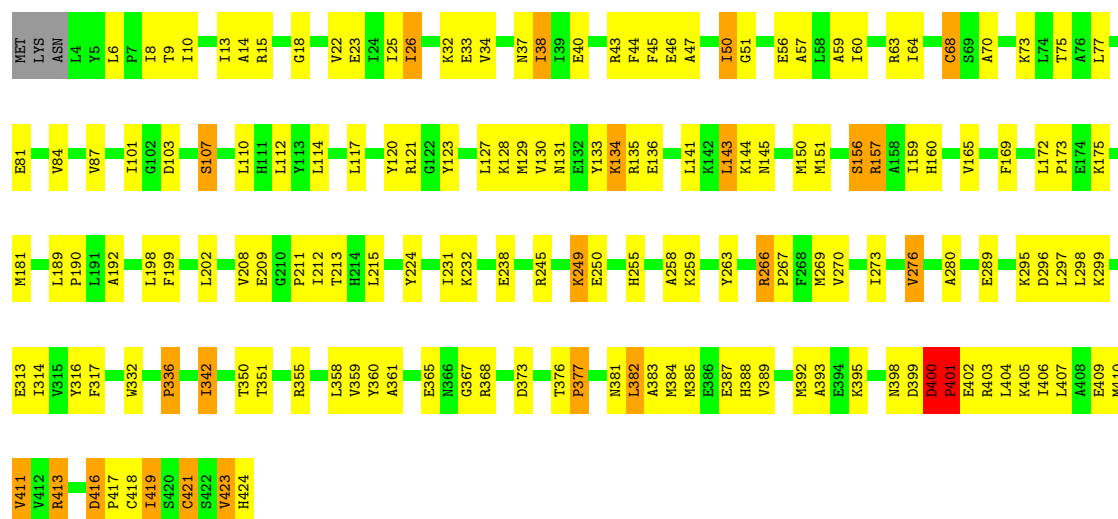
• Molecule 2: Sulfhydrogenase 1 subunit alpha

Chain L: 47% 47% 5%



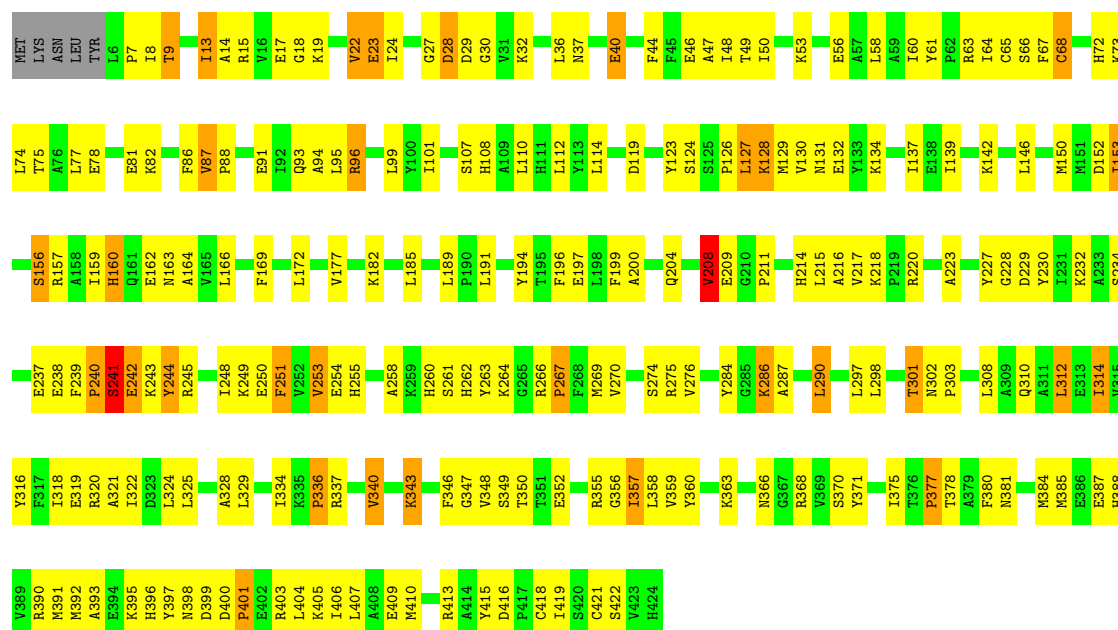
• Molecule 2: Sulfhydrogenase 1 subunit alpha

Chain N: 61% 33% 5%



• Molecule 2: Sulfhydrogenase 1 subunit alpha

Category	Percentage
Very bad	46%
Bad	45%
Good	7%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	94.23Å 111.15Å 141.09Å 90.06° 90.02° 90.00°	Depositor
Resolution (Å)	35.84 – 2.60 35.84 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.5 (35.84-2.60) 90.2 (35.84-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.05 (at 2.61Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.267 , 0.305 0.267 , 0.305	Depositor DCC
R_{free} test set	2007 reflections (1.16%)	wwPDB-VP
Wilson B-factor (Å ²)	37.1	Xtriage
Anisotropy	0.812	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 13.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.417 for h,-k,-l 0.438 for -h,k,-l 0.407 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	43445	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 27.18 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.3037e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: FCO, NI, SF4, MG, PO4

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	0.88	7/2064 (0.3%)	1.14	11/2781 (0.4%)
1	C	0.61	1/2054 (0.0%)	0.97	8/2769 (0.3%)
1	E	0.56	0/2046	0.82	0/2758
1	G	0.51	0/2046	0.77	0/2758
1	I	0.46	0/2064	0.78	1/2780 (0.0%)
1	K	0.51	0/2046	0.76	1/2758 (0.0%)
1	M	0.48	0/2055	0.67	0/2769
1	O	0.46	0/2055	0.77	0/2769
2	B	0.52	0/3429	0.81	0/4628
2	D	0.55	0/3406	0.86	4/4599 (0.1%)
2	F	0.64	3/3423 (0.1%)	0.95	6/4621 (0.1%)
2	H	0.55	0/3400	0.82	2/4591 (0.0%)
2	J	0.53	0/3404	0.78	4/4595 (0.1%)
2	L	0.52	0/3416	0.85	3/4613 (0.1%)
2	N	0.71	8/3416 (0.2%)	1.02	17/4613 (0.4%)
2	P	0.51	0/3395	0.80	1/4584 (0.0%)
All	All	0.57	19/43719 (0.0%)	0.86	58/58986 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	2
2	D	0	1
2	H	0	1
2	N	0	1
All	All	0	6

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	196	PRO	CB-CG	19.97	2.49	1.49
2	N	400	ASP	C-N	-17.92	1.10	1.33
1	A	196	PRO	N-CD	13.14	1.66	1.47
2	N	267	PRO	CB-CG	-11.84	0.90	1.49
2	F	240	PRO	CB-CG	10.37	2.01	1.49

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	401	PRO	N-CD-CG	-22.60	69.30	103.20
1	A	196	PRO	N-CD-CG	-20.87	71.90	103.20
1	A	196	PRO	CB-CG-CD	-19.80	42.75	106.10
2	N	267	PRO	CA-CB-CG	-19.58	67.30	104.50
2	N	267	PRO	N-CD-CG	-18.67	75.19	103.20

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	23	MET	Peptide
1	C	120	GLU	Mainchain
1	C	121	PRO	Mainchain
2	D	15	ARG	Peptide
2	H	186	ARG	Peptide

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	2015	0	2013	103	0
1	C	2008	0	2000	148	1
1	E	2003	0	1995	123	0
1	G	2003	0	1994	89	0
1	I	2018	0	2019	114	1
1	K	2003	0	1997	107	1
1	M	2009	0	2006	71	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	O	2009	0	2007	110	1
2	B	3349	0	3387	174	1
2	D	3332	0	3359	213	1
2	F	3343	0	3376	220	1
2	H	3330	0	3355	163	0
2	J	3331	0	3365	187	1
2	L	3342	0	3363	206	0
2	N	3342	0	3363	145	0
2	P	3325	0	3352	205	0
3	A	24	0	0	6	0
3	C	24	0	0	13	0
3	E	24	0	0	9	0
3	G	24	0	0	6	0
3	I	24	0	0	3	0
3	K	24	0	0	17	0
3	M	24	0	0	6	0
3	O	24	0	0	3	0
4	B	7	0	0	5	0
4	D	7	0	0	8	0
4	F	7	0	0	7	0
4	H	7	0	0	5	0
4	J	7	0	0	5	0
4	L	7	0	0	16	0
4	N	7	0	0	19	0
4	P	7	0	0	5	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
5	F	1	0	0	0	0
5	H	1	0	0	2	0
5	J	1	0	0	0	0
5	L	1	0	0	0	0
5	N	1	0	0	0	0
5	P	1	0	0	1	0
6	B	10	0	0	0	0
6	F	10	0	0	0	0
6	H	5	0	0	0	0
6	I	5	0	0	1	0
6	J	5	0	0	0	0
6	L	5	0	0	1	0
6	P	15	0	0	1	0
7	H	1	0	0	0	0
7	P	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	19	0	0	5	0
8	B	37	0	0	2	0
8	C	36	0	0	4	0
8	D	27	0	0	9	0
8	E	22	0	0	2	0
8	F	29	0	0	7	0
8	G	15	0	0	2	0
8	H	40	0	0	7	0
8	I	16	0	0	2	0
8	J	25	0	0	2	0
8	K	8	0	0	0	0
8	L	23	0	0	8	0
8	M	11	0	0	0	0
8	N	18	0	0	4	0
8	O	13	0	0	4	0
8	P	31	0	0	10	0
All	All	43445	0	42951	2217	4

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 26.

The worst 5 of 2217 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:F:240:PRO:CG	2:F:240:PRO:CD	1.82	1.57
2:N:377:PRO:HD2	4:N:501:FCO:C1	1.25	1.56
2:L:377:PRO:HD2	4:L:501:FCO:C1	1.40	1.48
2:L:377:PRO:HD2	4:L:501:FCO:N1	1.24	1.45
2:N:377:PRO:CD	4:N:501:FCO:N1	1.78	1.42

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:390:ARG:NH1	1:I:225:GLU:OE2[1_455]	2.07	0.13
2:F:387:GLU:OE2	1:O:221:LYS:NZ[1_656]	2.11	0.09
2:B:395:LYS:NZ	1:K:225:GLU:O[1_556]	2.12	0.08
1:C:225:GLU:OE1	2:J:390:ARG:NH1[1_456]	2.12	0.08

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	256/266 (96%)	228 (89%)	25 (10%)	3 (1%)	10	23
1	C	255/266 (96%)	224 (88%)	24 (9%)	7 (3%)	4	7
1	E	254/266 (96%)	226 (89%)	23 (9%)	5 (2%)	6	12
1	G	254/266 (96%)	218 (86%)	34 (13%)	2 (1%)	16	34
1	I	256/266 (96%)	224 (88%)	26 (10%)	6 (2%)	5	9
1	K	254/266 (96%)	215 (85%)	32 (13%)	7 (3%)	4	6
1	M	255/266 (96%)	239 (94%)	14 (6%)	2 (1%)	16	34
1	O	255/266 (96%)	230 (90%)	21 (8%)	4 (2%)	7	16
2	B	421/424 (99%)	358 (85%)	54 (13%)	9 (2%)	5	11
2	D	418/424 (99%)	362 (87%)	34 (8%)	22 (5%)	1	1
2	F	420/424 (99%)	366 (87%)	44 (10%)	10 (2%)	4	9
2	H	418/424 (99%)	371 (89%)	38 (9%)	9 (2%)	5	10
2	J	418/424 (99%)	360 (86%)	48 (12%)	10 (2%)	4	9
2	L	420/424 (99%)	356 (85%)	49 (12%)	15 (4%)	2	4
2	N	420/424 (99%)	384 (91%)	28 (7%)	8 (2%)	6	13
2	P	417/424 (98%)	354 (85%)	45 (11%)	18 (4%)	2	2
All	All	5391/5520 (98%)	4715 (88%)	539 (10%)	137 (2%)	4	8

5 of 137 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	214	ALA
2	D	382	LEU
2	F	69	SER
2	F	382	LEU
2	F	401	PRO

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	217/227 (96%)	193 (89%)	24 (11%)	6	12
1	C	216/227 (95%)	189 (88%)	27 (12%)	4	9
1	E	215/227 (95%)	196 (91%)	19 (9%)	9	21
1	G	215/227 (95%)	204 (95%)	11 (5%)	21	45
1	I	217/227 (96%)	197 (91%)	20 (9%)	8	19
1	K	215/227 (95%)	199 (93%)	16 (7%)	13	29
1	M	216/227 (95%)	207 (96%)	9 (4%)	26	52
1	O	216/227 (95%)	198 (92%)	18 (8%)	10	23
2	B	353/355 (99%)	324 (92%)	29 (8%)	10	24
2	D	351/355 (99%)	324 (92%)	27 (8%)	12	27
2	F	353/355 (99%)	324 (92%)	29 (8%)	10	24
2	H	350/355 (99%)	327 (93%)	23 (7%)	15	34
2	J	351/355 (99%)	321 (92%)	30 (8%)	10	22
2	L	351/355 (99%)	323 (92%)	28 (8%)	11	25
2	N	351/355 (99%)	332 (95%)	19 (5%)	20	42
2	P	350/355 (99%)	318 (91%)	32 (9%)	9	19
All	All	4537/4656 (97%)	4176 (92%)	361 (8%)	11	25

5 of 361 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	J	342	ILE
1	M	95	SER
2	J	411	VAL
2	L	68	CYS
2	N	157	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	75	ASN
2	N	278	ASN
2	L	72	HIS
1	M	19	GLN
2	P	204	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 53 ligands modelled in this entry, 10 are monoatomic - leaving 43 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	$\# Z > 2$
3	SF4	G	503	1	0,12,12	-	-	-		
3	SF4	K	501	1	0,12,12	-	-	-		
6	PO4	P	503	-	4,4,4	0.83	0	6,6,6	0.86	0
3	SF4	K	502	1	0,12,12	-	-	-		
3	SF4	O	503	1	0,12,12	-	-	-		
6	PO4	J	503	-	4,4,4	0.92	0	6,6,6	0.79	0
3	SF4	I	502	1	0,12,12	-	-	-		
4	FCO	F	501	2	0,6,6	-	-	-		
4	FCO	H	501	2	0,6,6	-	-	-		
4	FCO	N	501	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SF4	O	502	1	0,12,12	-	-	-		
3	SF4	E	503	1	0,12,12	-	-	-		
3	SF4	C	501	1	0,12,12	-	-	-		
3	SF4	M	503	1	0,12,12	-	-	-		
4	FCO	J	501	2	0,6,6	-	-	-		
4	FCO	B	501	2	0,6,6	-	-	-		
3	SF4	O	501	1,2	0,12,12	-	-	-		
6	PO4	P	505	-	4,4,4	0.67	0	6,6,6	0.75	0
3	SF4	C	502	1	0,12,12	-	-	-		
3	SF4	G	501	1	0,12,12	-	-	-		
3	SF4	M	502	1	0,12,12	-	-	-		
6	PO4	I	504	-	4,4,4	0.98	0	6,6,6	0.89	0
4	FCO	L	501	2	0,6,6	-	-	-		
3	SF4	E	501	1,2	0,12,12	-	-	-		
3	SF4	M	501	1	0,12,12	-	-	-		
3	SF4	A	503	1	0,12,12	-	-	-		
3	SF4	I	503	1	0,12,12	-	-	-		
3	SF4	K	503	1	0,12,12	-	-	-		
3	SF4	A	501	1	0,12,12	-	-	-		
6	PO4	F	504	-	4,4,4	0.86	0	6,6,6	0.43	0
6	PO4	L	503	-	4,4,4	0.81	0	6,6,6	0.67	0
3	SF4	A	502	1	0,12,12	-	-	-		
4	FCO	D	501	2	0,6,6	-	-	-		
6	PO4	B	504	-	4,4,4	0.68	0	6,6,6	0.58	0
4	FCO	P	501	2	0,6,6	-	-	-		
3	SF4	C	503	1	0,12,12	-	-	-		
6	PO4	B	503	-	4,4,4	0.68	0	6,6,6	1.11	0
3	SF4	G	502	1	0,12,12	-	-	-		
3	SF4	E	502	1	0,12,12	-	-	-		
3	SF4	I	501	1	0,12,12	-	-	-		
6	PO4	H	503	-	4,4,4	1.05	0	6,6,6	1.01	0
6	PO4	F	503	-	4,4,4	0.86	0	6,6,6	0.62	0
6	PO4	P	504	-	4,4,4	0.82	0	6,6,6	1.02	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
3	SF4	G	503	1	-	-	0/6/5/5
3	SF4	K	501	1	-	-	0/6/5/5
3	SF4	K	502	1	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SF4	O	503	1	-	-	0/6/5/5
3	SF4	I	502	1	-	-	0/6/5/5
3	SF4	O	502	1	-	-	0/6/5/5
3	SF4	E	503	1	-	-	0/6/5/5
3	SF4	C	501	1	-	-	0/6/5/5
3	SF4	M	503	1	-	-	0/6/5/5
3	SF4	O	501	1,2	-	-	0/6/5/5
3	SF4	C	502	1	-	-	0/6/5/5
3	SF4	G	501	1	-	-	0/6/5/5
3	SF4	M	502	1	-	-	0/6/5/5
3	SF4	E	501	1,2	-	-	0/6/5/5
3	SF4	M	501	1	-	-	0/6/5/5
3	SF4	A	503	1	-	-	0/6/5/5
3	SF4	I	503	1	-	-	0/6/5/5
3	SF4	K	503	1	-	-	0/6/5/5
3	SF4	A	501	1	-	-	0/6/5/5
3	SF4	A	502	1	-	-	0/6/5/5
3	SF4	C	503	1	-	-	0/6/5/5
3	SF4	G	502	1	-	-	0/6/5/5
3	SF4	E	502	1	-	-	0/6/5/5
3	SF4	I	501	1	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

31 monomers are involved in 136 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	503	SF4	3	0
3	K	501	SF4	8	0
3	K	502	SF4	2	0
3	I	502	SF4	1	0
4	F	501	FCO	7	0
4	H	501	FCO	5	0
4	N	501	FCO	19	0
3	E	503	SF4	5	0
3	C	501	SF4	5	0
3	M	503	SF4	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	J	501	FCO	5	0
4	B	501	FCO	5	0
3	O	501	SF4	3	0
3	C	502	SF4	2	0
3	G	501	SF4	3	0
3	M	502	SF4	2	0
6	I	504	PO4	1	0
4	L	501	FCO	16	0
3	E	501	SF4	3	0
3	M	501	SF4	1	0
3	A	503	SF4	1	0
3	K	503	SF4	7	0
3	A	501	SF4	4	0
6	L	503	PO4	1	0
3	A	502	SF4	1	0
4	D	501	FCO	8	0
4	P	501	FCO	5	0
3	C	503	SF4	6	0
3	E	502	SF4	1	0
3	I	501	SF4	2	0
6	P	504	PO4	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
2	N	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	N	400:ASP	C	401:PRO	N	1.11

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	256/266 (96%)	-1.32	0 100 100	31, 46, 60, 68	2 (0%)
1	C	256/266 (96%)	-1.26	0 100 100	30, 48, 58, 69	1 (0%)
1	E	256/266 (96%)	-1.33	0 100 100	31, 46, 57, 63	0
1	G	256/266 (96%)	-1.36	0 100 100	28, 46, 58, 68	0
1	I	256/266 (96%)	-1.27	0 100 100	25, 51, 65, 78	2 (0%)
1	K	256/266 (96%)	-1.31	0 100 100	24, 50, 65, 80	0
1	M	256/266 (96%)	-1.30	0 100 100	25, 50, 63, 75	1 (0%)
1	O	256/266 (96%)	-1.29	0 100 100	30, 50, 63, 73	1 (0%)
2	B	420/424 (99%)	-1.34	0 100 100	24, 44, 56, 64	3 (0%)
2	D	419/424 (98%)	-1.35	0 100 100	29, 45, 58, 73	1 (0%)
2	F	419/424 (98%)	-1.33	0 100 100	27, 44, 58, 68	3 (0%)
2	H	420/424 (99%)	-1.35	0 100 100	29, 43, 57, 76	0
2	J	419/424 (98%)	-1.31	0 100 100	33, 47, 61, 72	1 (0%)
2	L	421/424 (99%)	-1.31	0 100 100	28, 46, 61, 78	1 (0%)
2	N	421/424 (99%)	-1.33	0 100 100	29, 46, 60, 75	1 (0%)
2	P	419/424 (98%)	-1.32	0 100 100	32, 47, 61, 71	0
All	All	5406/5520 (97%)	-1.32	0 100 100	24, 46, 61, 80	17 (0%)

There are no RSRZ outliers to report.

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 oligosaccharides 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. 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
6	PO4	F	503	5/5	0.95	0.08	52,56,63,76	0
6	PO4	H	503	5/5	0.96	0.08	30,40,52,61	0
6	PO4	B	503	5/5	0.97	0.06	39,49,57,64	0
6	PO4	F	504	5/5	0.97	0.07	59,68,84,86	0
6	PO4	B	504	5/5	0.97	0.06	41,51,65,71	0
6	PO4	I	504	5/5	0.97	0.08	36,47,57,60	0
6	PO4	J	503	5/5	0.97	0.07	50,55,67,71	0
6	PO4	L	503	5/5	0.97	0.05	55,65,71,75	0
6	PO4	P	503	5/5	0.97	0.05	45,51,58,63	0
6	PO4	P	504	5/5	0.97	0.07	37,48,59,61	0
6	PO4	P	505	5/5	0.97	0.06	51,58,66,78	0
7	MG	H	504	1/1	0.97	0.03	18,18,18,18	0
3	SF4	M	502	8/8	0.99	0.03	33,43,47,62	0
3	SF4	O	501	8/8	0.99	0.03	24,37,41,55	0
5	NI	J	502	1/1	0.99	0.04	76,76,76,76	0
5	NI	P	502	1/1	0.99	0.02	72,72,72,72	0
3	SF4	C	501	8/8	0.99	0.02	18,28,39,41	0
3	SF4	C	502	8/8	0.99	0.04	33,45,59,70	0
3	SF4	E	502	8/8	0.99	0.03	31,42,54,59	0
3	SF4	I	501	8/8	0.99	0.02	23,30,35,35	0
7	MG	P	506	1/1	0.99	0.02	26,26,26,26	0
3	SF4	C	503	8/8	1.00	0.02	56,59,68,69	0
3	SF4	O	502	8/8	1.00	0.02	31,52,60,63	0
3	SF4	O	503	8/8	1.00	0.02	36,43,48,56	0
4	FCO	B	501	7/7	1.00	0.03	37,42,53,57	0
4	FCO	D	501	7/7	1.00	0.04	49,51,59,60	0
4	FCO	F	501	7/7	1.00	0.04	43,45,48,53	0
4	FCO	H	501	7/7	1.00	0.04	45,46,53,63	0
4	FCO	J	501	7/7	1.00	0.04	39,43,62,67	0
4	FCO	L	501	7/7	1.00	0.03	40,45,57,88	0
4	FCO	N	501	7/7	1.00	0.03	43,50,65,149	0
4	FCO	P	501	7/7	1.00	0.05	44,47,49,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	NI	B	502	1/1	1.00	0.03	71,71,71,71	0
5	NI	D	502	1/1	1.00	0.01	69,69,69,69	0
5	NI	F	502	1/1	1.00	0.02	51,51,51,51	0
5	NI	H	502	1/1	1.00	0.02	83,83,83,83	0
3	SF4	E	501	8/8	1.00	0.02	24,29,39,41	0
5	NI	L	502	1/1	1.00	0.01	87,87,87,87	0
5	NI	N	502	1/1	1.00	0.01	69,69,69,69	0
3	SF4	A	503	8/8	1.00	0.03	36,41,47,61	0
3	SF4	E	503	8/8	1.00	0.02	41,55,57,58	0
3	SF4	G	501	8/8	1.00	0.02	26,35,42,44	0
3	SF4	G	502	8/8	1.00	0.02	24,31,41,46	0
3	SF4	G	503	8/8	1.00	0.03	30,43,52,54	0
3	SF4	A	501	8/8	1.00	0.01	34,39,46,46	0
3	SF4	I	502	8/8	1.00	0.02	40,50,57,65	0
3	SF4	I	503	8/8	1.00	0.03	30,43,48,54	0
3	SF4	K	501	8/8	1.00	0.02	26,43,46,62	0
3	SF4	K	502	8/8	1.00	0.02	34,40,49,52	0
3	SF4	K	503	8/8	1.00	0.02	35,58,66,80	0
3	SF4	M	501	8/8	1.00	0.02	28,36,41,43	0
3	SF4	A	502	8/8	1.00	0.02	31,40,46,47	0
3	SF4	M	503	8/8	1.00	0.02	45,55,71,72	0

6.5 Other polymers [i](#)

There are no such residues in this entry.