Full wwPDB X-ray Structure Validation Report (i)

May 26, 2020 – 11:40 am BST

PDB ID	:	2YAW
Title	:	HG INHIBITED SULFUR OXYGENASE REDUCTASE
Authors	:	Veith, A.; Urich, T.; Seyfarth, K.; Protze, J.; Frazao, C.; Kletzin, A.
Deposited on	:	2011-02-25
Resolution	:	2.50 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.50 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	Percentile Ranks	Value
Rfree		0.157
Clashscore		4
Ramachandran outliers		0
Sidechain outliers		2.1%
RSRZ outliers		0.3%

Worse ... *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
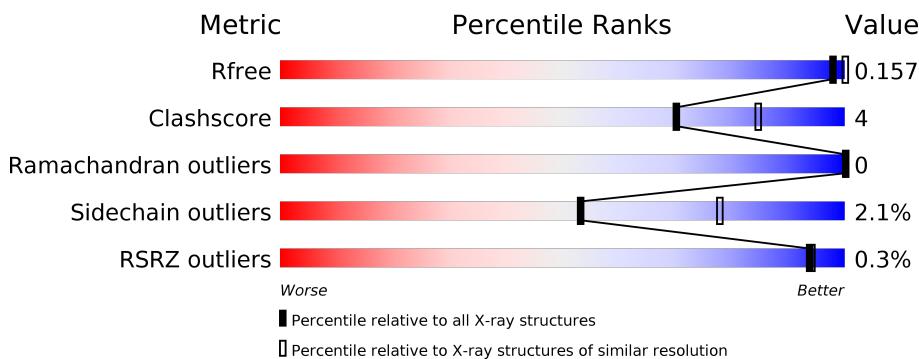
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 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 <=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	318	85% 11% •
1	B	318	85% 11% •
1	C	318	% 85% 11% • •
1	D	318	86% 11% •
1	E	318	85% 12% •
1	F	318	84% 12% • •

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 15539 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 SULFUR OXYGENASE/REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	307	Total 2499	C 1617	N 413	O 444	S 25	0	9	0
1	B	307	Total 2495	C 1613	N 413	O 446	S 23	0	9	0
1	C	307	Total 2492	C 1612	N 413	O 444	S 23	0	7	0
1	D	307	Total 2499	C 1617	N 411	O 447	S 24	0	9	0
1	E	307	Total 2495	C 1617	N 410	O 444	S 24	0	9	0
1	F	307	Total 2501	C 1619	N 413	O 445	S 24	0	10	0

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	309	ASN	-	expression tag	UNP P29082
A	310	ALA	-	expression tag	UNP P29082
A	311	TRP	-	expression tag	UNP P29082
A	312	ARG	-	expression tag	UNP P29082
A	313	HIS	-	expression tag	UNP P29082
A	314	PRO	-	expression tag	UNP P29082
A	315	GLN	-	expression tag	UNP P29082
A	316	PHE	-	expression tag	UNP P29082
A	317	GLY	-	expression tag	UNP P29082
A	318	GLY	-	expression tag	UNP P29082
B	309	ASN	-	expression tag	UNP P29082
B	310	ALA	-	expression tag	UNP P29082
B	311	TRP	-	expression tag	UNP P29082
B	312	ARG	-	expression tag	UNP P29082
B	313	HIS	-	expression tag	UNP P29082
B	314	PRO	-	expression tag	UNP P29082
B	315	GLN	-	expression tag	UNP P29082

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Chain	Residue	Modelled	Actual	Comment	Reference
B	316	PHE	-	expression tag	UNP P29082
B	317	GLY	-	expression tag	UNP P29082
B	318	GLY	-	expression tag	UNP P29082
C	309	ASN	-	expression tag	UNP P29082
C	310	ALA	-	expression tag	UNP P29082
C	311	TRP	-	expression tag	UNP P29082
C	312	ARG	-	expression tag	UNP P29082
C	313	HIS	-	expression tag	UNP P29082
C	314	PRO	-	expression tag	UNP P29082
C	315	GLN	-	expression tag	UNP P29082
C	316	PHE	-	expression tag	UNP P29082
C	317	GLY	-	expression tag	UNP P29082
C	318	GLY	-	expression tag	UNP P29082
D	309	ASN	-	expression tag	UNP P29082
D	310	ALA	-	expression tag	UNP P29082
D	311	TRP	-	expression tag	UNP P29082
D	312	ARG	-	expression tag	UNP P29082
D	313	HIS	-	expression tag	UNP P29082
D	314	PRO	-	expression tag	UNP P29082
D	315	GLN	-	expression tag	UNP P29082
D	316	PHE	-	expression tag	UNP P29082
D	317	GLY	-	expression tag	UNP P29082
D	318	GLY	-	expression tag	UNP P29082
E	309	ASN	-	expression tag	UNP P29082
E	310	ALA	-	expression tag	UNP P29082
E	311	TRP	-	expression tag	UNP P29082
E	312	ARG	-	expression tag	UNP P29082
E	313	HIS	-	expression tag	UNP P29082
E	314	PRO	-	expression tag	UNP P29082
E	315	GLN	-	expression tag	UNP P29082
E	316	PHE	-	expression tag	UNP P29082
E	317	GLY	-	expression tag	UNP P29082
E	318	GLY	-	expression tag	UNP P29082
F	309	ASN	-	expression tag	UNP P29082
F	310	ALA	-	expression tag	UNP P29082
F	311	TRP	-	expression tag	UNP P29082
F	312	ARG	-	expression tag	UNP P29082
F	313	HIS	-	expression tag	UNP P29082
F	314	PRO	-	expression tag	UNP P29082
F	315	GLN	-	expression tag	UNP P29082
F	316	PHE	-	expression tag	UNP P29082
F	317	GLY	-	expression tag	UNP P29082

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Chain	Residue	Modelled	Actual	Comment	Reference
F	318	GLY	-	expression tag	UNP P29082

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total 1	Fe 1	0	0
2	E	1	Total 1	Fe 1	0	0
2	B	1	Total 1	Fe 1	0	0
2	C	1	Total 1	Fe 1	0	0
2	A	1	Total 1	Fe 1	0	0
2	F	1	Total 1	Fe 1	0	0

- Molecule 3 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	2	Total 2	Hg 2	0	0
3	E	2	Total 2	Hg 2	0	0
3	B	2	Total 2	Hg 2	0	0
3	C	2	Total 2	Hg 2	0	0
3	A	2	Total 2	Hg 2	0	0
3	F	2	Total 2	Hg 2	0	0

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).

ACT

OXT

O⁻

C

CH3

O

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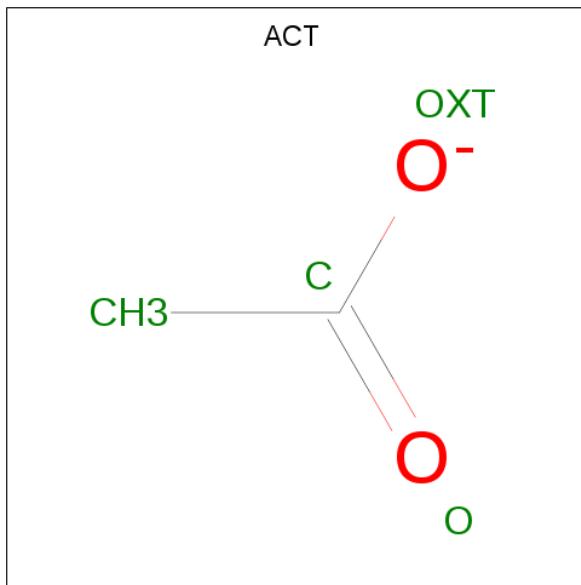
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0
4	C	1	Total 4	C 2	O 2	0	0
4	D	1	Total 4	C 2	O 2	0	0
4	E	1	Total 4	C 2	O 2	0	0
4	F	1	Total 4	C 2	O 2	0	0

- Molecule 5 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	81	Total 81	O 81	0	0
5	B	87	Total 87	O 87	0	0
5	C	88	Total 88	O 88	0	0
5	D	88	Total 88	O 88	0	0
5	E	80	Total 80	O 80	0	0
5	F	92	Total 92	O 92	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 the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: SULFUR OXYGENASE/REDUCTASE
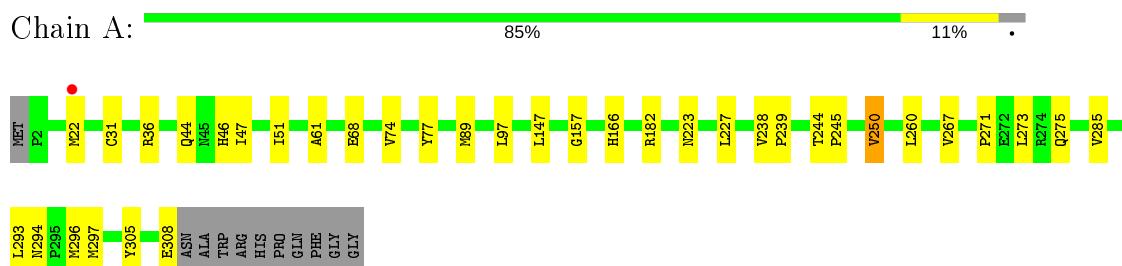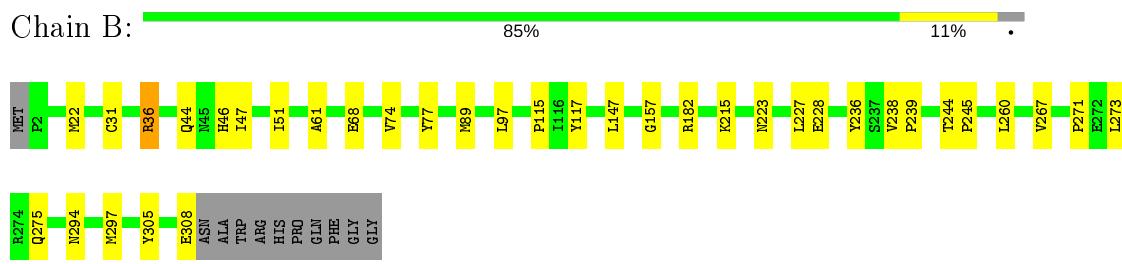
- Molecule 1: SULFUR OXYGENASE/REDUCTASE

- Molecule 1: SULFUR OXYGENASE/REDUCTASE

- Molecule 1: SULFUR OXYGENASE/REDUCTASE

Y305 L306 N307 E308 ASN ALA TRP ARG HIS PRO GLN PHE GLY GLY

• Molecule 1: SULFUR OXYGENASE/REDUCTASE

Chain E:

85%   12%   •

MET P2 M22 C31 R36 Q44 N45 H46 I47 I51 A61 E68 V74 Y77 M89 Q92 L97 G144 L147 G157 V160 V161 S167 N223 L227 E228 Y236 S237 P239 T244 P245 L260 P271 Q275

L281 V285 L293 N294 P295 M296 M297 Y305 E308 ASN ALA TRP ARG HIS PRO GLN PHE GLY GLY

• Molecule 1: SULFUR OXYGENASE/REDUCTASE

Chain F:

84%   12%   • •

MET P2 M22 C31 R36 Q44 N45 H46 I47 I51 A61 E68 V74 Y77 L97 L147 G157 V161 L194 V204 N223 L227 E228 N232 Y236 S237 V238 P239 T244 P245 W254 L260 P271 Q275 V276

L281 V285 L293 N294 M297 Y305 E308 ASN ALA TRP ARG HIS PRO GLN PHE GLY GLY
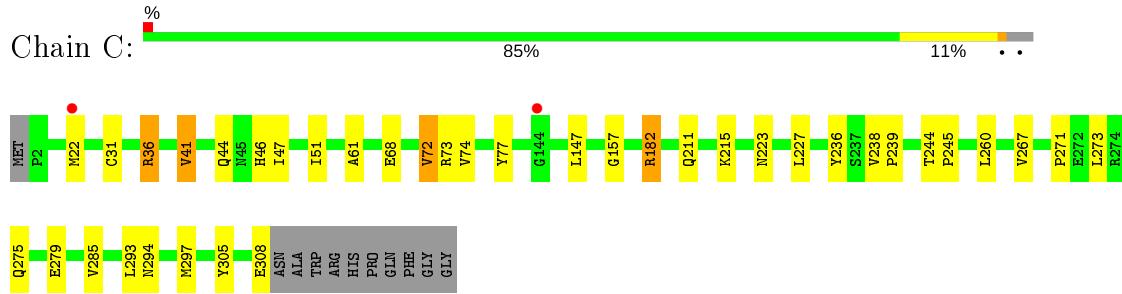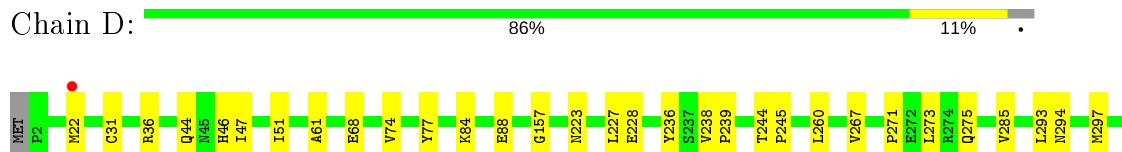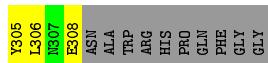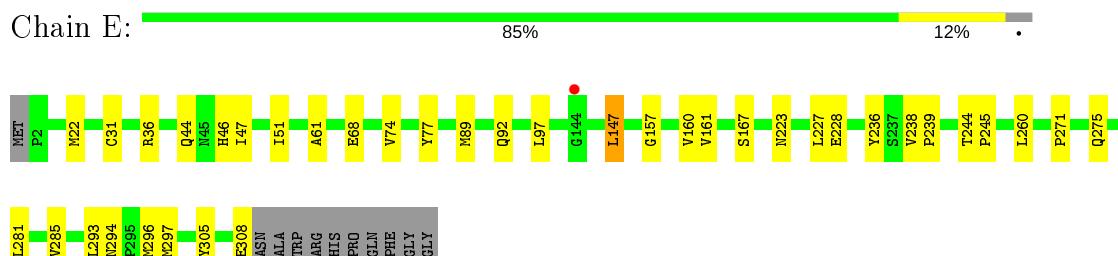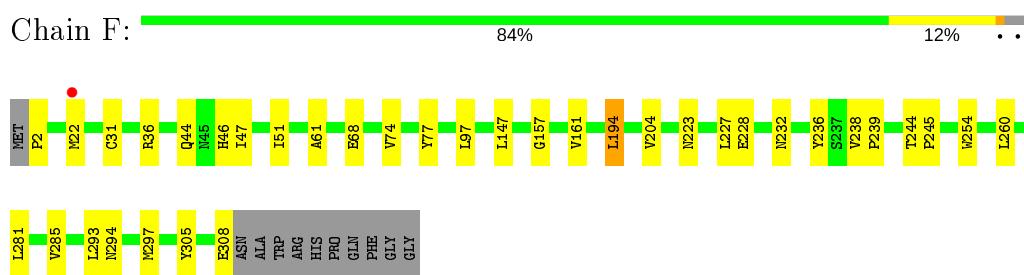
4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α, β, γ	161.88Å　161.88Å　154.37Å 90.00°　　90.00°　　90.00°	Depositor
Resolution (Å)	49.04　–　2.50 49.04　–　2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.04-2.50) 97.0 (49.04-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	3.98 (at 2.51Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.162　,　0.182 0.160　,　0.157	Depositor DCC
R_{free} test set	3333 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å^2)	29.7	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 47.3	EDS
L-test for twinning [2]	$<|L|>$ = 0.50, $<L^2>$ = 0.33	Xtriage
Estimated twinning fraction	0.000 for l,-k,h 0.001 for -l,-k,-h 0.009 for -h,-l,-k 0.000 for -h,l,k 0.017 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	15539	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<|L|>$, $<L^2>$ 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: ACT, HG, CSS, FE

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	0.30	0/2601	0.58	5/3521 (0.1%)
1	B	0.30	0/2597	0.59	7/3517 (0.2%)
1	C	0.31	0/2585	0.84	11/3501 (0.3%)
1	D	0.29	0/2600	0.57	3/3521 (0.1%)
1	E	0.30	0/2596	0.57	3/3517 (0.1%)
1	F	0.30	0/2606	0.61	5/3529 (0.1%)
All	All	0.30	0/15585	0.63	34/21106 (0.2%)

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	182[A]	ARG	NE-CZ-NH2	-17.32	111.64	120.30
1	C	182[B]	ARG	NE-CZ-NH2	-17.32	111.64	120.30
1	C	182[A]	ARG	NE-CZ-NH1	16.82	128.71	120.30
1	C	182[B]	ARG	NE-CZ-NH1	16.82	128.71	120.30
1	E	36	ARG	NE-CZ-NH1	12.34	126.47	120.30
1	D	36	ARG	NE-CZ-NH1	12.08	126.34	120.30
1	E	36	ARG	NE-CZ-NH2	-11.83	114.39	120.30
1	B	36	ARG	NE-CZ-NH1	11.80	126.20	120.30
1	D	36	ARG	NE-CZ-NH2	-11.55	114.52	120.30
1	B	36	ARG	NE-CZ-NH2	-11.42	114.59	120.30
1	A	36	ARG	NE-CZ-NH2	-9.98	115.31	120.30
1	A	36	ARG	NE-CZ-NH1	9.95	125.27	120.30
1	C	36	ARG	NE-CZ-NH1	9.81	125.20	120.30
1	C	36	ARG	NE-CZ-NH2	-9.64	115.48	120.30
1	F	36	ARG	NE-CZ-NH2	-9.33	115.64	120.30
1	F	36	ARG	NE-CZ-NH1	9.29	124.95	120.30
1	C	182[A]	ARG	CD-NE-CZ	7.55	134.18	123.60
1	C	182[B]	ARG	CD-NE-CZ	7.55	134.18	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	72	VAL	CB-CA-C	-7.53	97.10	111.40
1	B	182[A]	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	B	182[B]	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	C	41	VAL	CG1-CB-CG2	5.98	120.47	110.90
1	E	36	ARG	CD-NE-CZ	5.76	131.67	123.60
1	B	36	ARG	CD-NE-CZ	5.76	131.66	123.60
1	C	72	VAL	CG1-CB-CG2	5.74	120.08	110.90
1	D	36	ARG	CD-NE-CZ	5.70	131.58	123.60
1	F	276	VAL	CG1-CB-CG2	5.61	119.88	110.90
1	A	250	VAL	CG1-CB-CG2	5.32	119.41	110.90
1	B	182[A]	ARG	NE-CZ-NH1	5.27	122.93	120.30
1	B	182[B]	ARG	NE-CZ-NH1	5.27	122.93	120.30
1	A	182[A]	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	A	182[B]	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	F	161	VAL	CG1-CB-CG2	5.09	119.05	110.90
1	F	204	VAL	CG1-CB-CG2	5.02	118.93	110.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2499	0	2460	18	0
1	B	2495	0	2448	19	1
1	C	2492	0	2450	20	1
1	D	2499	0	2452	18	0
1	E	2495	0	2456	20	1
1	F	2501	0	2461	17	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	2	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	2	0	0	1	0
3	C	2	0	0	1	0
3	D	2	0	0	1	0
3	E	2	0	0	1	0
3	F	2	0	0	1	0
4	A	4	0	3	1	0
4	B	4	0	3	1	0
4	C	4	0	3	1	0
4	D	4	0	3	1	0
4	E	4	0	3	1	0
4	F	4	0	3	1	0
5	A	81	0	0	0	0
5	B	87	0	0	2	0
5	C	88	0	0	3	0
5	D	88	0	0	0	0
5	E	80	0	0	0	0
5	F	92	0	0	0	0
All	All	15539	0	14745	107	2

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 4.

All (107) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:MET:HG2	4:A:405:ACT:H3	1.55	0.88
1:C:297:MET:HG2	4:C:405:ACT:H3	1.55	0.87
1:B:297:MET:HG2	4:B:405:ACT:H3	1.55	0.86
1:D:297:MET:HG2	4:D:405:ACT:H3	1.60	0.82
1:F:297:MET:HG2	4:F:405:ACT:H3	1.64	0.80
1:C:31:CSS:SG	3:C:404:HG:HG	2.01	0.77
1:A:31:CSS:SG	3:A:404:HG:HG	2.02	0.77
1:C:36:ARG:HD3	5:C:2004:HOH:O	1.84	0.76
1:B:31:CSS:SG	3:B:404:HG:HG	2.09	0.71
1:F:31:CSS:SG	3:F:404:HG:HG	2.10	0.69
1:E:31:CSS:SG	3:E:404:HG:HG	2.12	0.67
1:D:31:CSS:SG	3:D:404:HG:HG	2.16	0.63
1:B:36:ARG:CZ	5:B:2004:HOH:O	2.45	0.63
1:F:194:LEU:HD22	1:F:254:TRP:C	2.25	0.56
1:F:223:ASN:ND2	1:F:227:LEU:O	2.38	0.55
1:F:238:VAL:HB	1:F:239:PRO:HD3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:238:VAL:HB	1:D:239:PRO:HD3	1.90	0.53
1:C:73:ARG:NH1	5:C:2017:HOH:O	2.42	0.53
1:C:223:ASN:ND2	1:C:227:LEU:O	2.40	0.52
1:B:223:ASN:ND2	1:B:227:LEU:O	2.39	0.52
1:B:238:VAL:HB	1:B:239:PRO:HD3	1.92	0.51
1:E:238:VAL:HB	1:E:239:PRO:HD3	1.91	0.51
1:A:238:VAL:HB	1:A:239:PRO:HD3	1.93	0.50
1:A:305:TYR:O	1:A:308:GLU:HG2	2.11	0.50
1:E:305:TYR:O	1:E:308:GLU:HG2	2.12	0.50
1:B:305:TYR:O	1:B:308:GLU:HG2	2.12	0.49
1:D:223:ASN:ND2	1:D:227:LEU:O	2.41	0.49
1:C:238:VAL:HB	1:C:239:PRO:HD3	1.93	0.49
1:A:223:ASN:ND2	1:A:227:LEU:O	2.40	0.49
1:F:305:TYR:O	1:F:308:GLU:HG2	2.13	0.49
1:D:84:LYS:O	1:D:88[B]:GLU:HG3	2.13	0.48
1:E:297:MET:HG2	4:E:405:ACT:H3	1.95	0.48
1:C:305:TYR:O	1:C:308:GLU:HG2	2.13	0.48
1:E:223:ASN:ND2	1:E:227:LEU:O	2.39	0.48
1:A:166:HIS:CE1	1:A:250:VAL:HG13	2.49	0.48
1:D:305:TYR:O	1:D:308:GLU:HG2	2.14	0.48
1:E:296:MET:HB2	1:E:297:MET:SD	2.55	0.47
1:E:160[B]:VAL:HG22	1:E:161:VAL:N	2.29	0.47
1:C:260:LEU:HD23	1:C:260:LEU:C	2.36	0.46
1:C:182[A]:ARG:NH2	1:C:279:GLU:OE2	2.49	0.46
1:B:36:ARG:NH1	5:B:2004:HOH:O	2.47	0.46
1:D:244:THR:HA	1:D:245:PRO:C	2.37	0.45
1:A:244:THR:HA	1:A:245:PRO:C	2.37	0.45
1:C:285:VAL:HA	1:E:236:TYR:CE1	2.52	0.45
1:F:260:LEU:HD23	1:F:260:LEU:C	2.38	0.44
1:C:244:THR:HA	1:C:245:PRO:C	2.39	0.44
1:B:244:THR:HA	1:B:245:PRO:C	2.39	0.43
1:C:271:PRO:O	1:C:275:GLN:HG2	2.18	0.43
1:C:236:TYR:CE1	1:E:285:VAL:HA	2.54	0.43
1:E:244:THR:HA	1:E:245:PRO:C	2.38	0.43
1:C:44:GLN:HG2	1:C:46:HIS:CE1	2.53	0.43
1:D:260:LEU:HD23	1:D:260:LEU:C	2.37	0.43
1:A:260:LEU:C	1:A:260:LEU:HD23	2.39	0.43
1:D:285:VAL:HA	1:F:236:TYR:CE1	2.54	0.43
1:E:260:LEU:C	1:E:260:LEU:HD23	2.39	0.43
1:B:267:VAL:HA	1:B:273:LEU:HG	2.01	0.43
1:F:244:THR:HA	1:F:245:PRO:C	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:260:LEU:C	1:B:260:LEU:HD23	2.38	0.42
1:D:46:HIS:HB3	1:D:293:LEU:HB3	2.00	0.42
1:C:46:HIS:HB3	1:C:293:LEU:HB3	2.01	0.42
1:A:271:PRO:O	1:A:275:GLN:HG2	2.19	0.42
1:B:157:GLY:HA2	1:B:294:ASN:OD1	2.20	0.42
1:F:157:GLY:HA2	1:F:294:ASN:OD1	2.19	0.42
1:B:44:GLN:HG2	1:B:46:HIS:CE1	2.54	0.42
1:E:51:ILE:HB	1:E:61:ALA:HB1	2.02	0.42
1:E:271:PRO:O	1:E:275:GLN:HG2	2.20	0.42
1:E:47:ILE:HD13	1:E:74:VAL:HG12	2.02	0.42
1:A:157:GLY:HA2	1:A:294:ASN:OD1	2.20	0.42
1:A:51:ILE:HB	1:A:61:ALA:HB1	2.02	0.42
1:A:46:HIS:HB3	1:A:293:LEU:HB3	2.01	0.42
1:A:44:GLN:HG2	1:A:46:HIS:CE1	2.55	0.42
1:D:236:TYR:CE2	1:F:285:VAL:HA	2.55	0.42
1:E:157:GLY:HA2	1:E:294:ASN:OD1	2.20	0.42
1:B:47:ILE:HD13	1:B:74:VAL:HG12	2.01	0.41
1:A:285:VAL:HA	1:B:236:TYR:CE1	2.54	0.41
1:B:51:ILE:HB	1:B:61:ALA:HB1	2.02	0.41
1:F:271:PRO:O	1:F:275:GLN:HG2	2.20	0.41
1:F:51:ILE:HB	1:F:61:ALA:HB1	2.03	0.41
1:A:267:VAL:HA	1:A:273:LEU:HG	2.03	0.41
1:C:211:GLN:HB3	5:C:2051:HOH:O	2.19	0.41
1:E:46:HIS:HB3	1:E:293:LEU:HB3	2.01	0.41
1:F:46:HIS:HB3	1:F:293:LEU:HB3	2.02	0.41
1:D:44:GLN:HG2	1:D:46:HIS:CE1	2.56	0.41
1:A:47:ILE:HD13	1:A:74:VAL:HG12	2.03	0.41
1:B:271:PRO:O	1:B:275:GLN:HG2	2.20	0.41
1:C:51:ILE:HB	1:C:61:ALA:HB1	2.03	0.41
1:C:47:ILE:HD13	1:C:74:VAL:HG12	2.02	0.41
1:D:157:GLY:HA2	1:D:294:ASN:OD1	2.20	0.41
1:C:157:GLY:HA2	1:C:294:ASN:OD1	2.20	0.41
1:B:89:MET:SD	1:B:97:LEU:HD11	2.60	0.41
1:E:147:LEU:HD12	1:E:147:LEU:HA	1.97	0.41
1:F:44:GLN:HG2	1:F:46:HIS:CE1	2.56	0.41
1:C:267:VAL:HA	1:C:273:LEU:HG	2.02	0.41
1:D:51:ILE:HB	1:D:61:ALA:HB1	2.02	0.41
1:A:296[A]:MET:HB2	1:A:297:MET:SD	2.61	0.41
1:A:89:MET:SD	1:A:97:LEU:HD11	2.60	0.41
1:D:267:VAL:HA	1:D:273:LEU:HG	2.02	0.41
1:B:115:PRO:HB2	1:B:117:TYR:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:47:ILE:HD13	1:D:74:VAL:HG12	2.03	0.40
1:E:44:GLN:HG2	1:E:46:HIS:CE1	2.55	0.40
1:F:47:ILE:HD13	1:F:74:VAL:HG12	2.03	0.40
1:D:271:PRO:O	1:D:275:GLN:HG2	2.21	0.40
1:E:89:MET:SD	1:E:97:LEU:HD11	2.62	0.40

All (2) 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)
1:B:215:LYS:NZ	1:E:92:GLN:NE2[6_564]	1.98	0.22
1:C:215:LYS:NZ	1:F:232:ASN:OD1[6_564]	2.17	0.03

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	313/318 (98%)	307 (98%)	6 (2%)	0	100	100
1	B	313/318 (98%)	307 (98%)	6 (2%)	0	100	100
1	C	311/318 (98%)	305 (98%)	6 (2%)	0	100	100
1	D	313/318 (98%)	307 (98%)	6 (2%)	0	100	100
1	E	313/318 (98%)	307 (98%)	6 (2%)	0	100	100
1	F	314/318 (99%)	308 (98%)	6 (2%)	0	100	100
All	All	1877/1908 (98%)	1841 (98%)	36 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	273/272 (100%)	268 (98%)	5 (2%)	59	81
1	B	273/272 (100%)	268 (98%)	5 (2%)	59	81
1	C	271/272 (100%)	264 (97%)	7 (3%)	46	72
1	D	273/272 (100%)	268 (98%)	5 (2%)	59	81
1	E	273/272 (100%)	266 (97%)	7 (3%)	46	72
1	F	274/272 (101%)	264 (96%)	10 (4%)	35	61
All	All	1637/1632 (100%)	1598 (98%)	39 (2%)	53	74

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22[A]	MET
1	A	22[B]	MET
1	A	68	GLU
1	A	77	TYR
1	A	147	LEU
1	B	22[A]	MET
1	B	22[B]	MET
1	B	68	GLU
1	B	77	TYR
1	B	147	LEU
1	C	22[A]	MET
1	C	22[B]	MET
1	C	41	VAL
1	C	68	GLU
1	C	72	VAL
1	C	77	TYR
1	C	147	LEU
1	D	22[A]	MET
1	D	22[B]	MET
1	D	68	GLU
1	D	77	TYR
1	D	306	LEU

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Mol	Chain	Res	Type
1	E	22[A]	MET
1	E	22[B]	MET
1	E	68	GLU
1	E	77	TYR
1	E	147	LEU
1	E	167	SER
1	E	281	LEU
1	F	2	PRO
1	F	22[A]	MET
1	F	22[B]	MET
1	F	68	GLU
1	F	77	TYR
1	F	97	LEU
1	F	147	LEU
1	F	194	LEU
1	F	276	VAL
1	F	281	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	GLN
1	A	127	ASN
1	A	247	GLN
1	B	76	GLN
1	B	127	ASN
1	B	247	GLN
1	C	76	GLN
1	C	127	ASN
1	C	247	GLN
1	D	127	ASN
1	D	247	GLN
1	E	76	GLN
1	E	127	ASN
1	E	247	GLN
1	F	76	GLN
1	F	127	ASN
1	F	247	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)

6 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	$\#|Z| > 2$
1	CSS	F	31	1	4,6,7	1.18	0	1,6,8	0.36	0
1	CSS	D	31	1	4,6,7	1.16	0	1,6,8	0.27	0
1	CSS	B	31	1	4,6,7	1.29	0	1,6,8	0.68	0
1	CSS	E	31	1	4,6,7	1.26	0	1,6,8	0.75	0
1	CSS	C	31	1	4,6,7	1.24	0	1,6,8	0.57	0
1	CSS	A	31	1	4,6,7	1.13	0	1,6,8	0.18	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
1	CSS	F	31	1	-	0/1/5/7	-
1	CSS	D	31	1	-	0/1/5/7	-
1	CSS	B	31	1	-	0/1/5/7	-
1	CSS	E	31	1	-	0/1/5/7	-
1	CSS	C	31	1	-	0/1/5/7	-
1	CSS	A	31	1	-	0/1/5/7	-

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.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	F	31	CSS	1	0
1	D	31	CSS	1	0
1	B	31	CSS	1	0
1	E	31	CSS	1	0
1	C	31	CSS	1	0
1	A	31	CSS	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 24 ligands modelled in this entry, 18 are monoatomic - leaving 6 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	ACT	E	405	3	1,3,3	1.38	0	0,3,3	0.00	-
4	ACT	B	405	3	1,3,3	1.59	0	0,3,3	0.00	-
4	ACT	C	405	3	1,3,3	1.52	0	0,3,3	0.00	-
4	ACT	A	405	3	1,3,3	1.58	0	0,3,3	0.00	-
4	ACT	F	405	3	1,3,3	1.60	0	0,3,3	0.00	-
4	ACT	D	405	3	1,3,3	1.69	0	0,3,3	0.00	-

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.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	405	ACT	1	0
4	B	405	ACT	1	0
4	C	405	ACT	1	0
4	A	405	ACT	1	0
4	F	405	ACT	1	0
4	D	405	ACT	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 (i)

6.1 Protein, DNA and RNA chains (i)

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	306/318 (96%)	-0.72	1 (0%)	94	94	15, 24, 50, 80	0
1	B	306/318 (96%)	-0.70	0	100	100	16, 25, 51, 80	0
1	C	306/318 (96%)	-0.77	2 (0%)	87	89	16, 24, 50, 80	0
1	D	306/318 (96%)	-0.71	1 (0%)	94	94	16, 25, 51, 80	0
1	E	306/318 (96%)	-0.68	1 (0%)	94	94	17, 25, 51, 80	0
1	F	306/318 (96%)	-0.73	1 (0%)	94	94	16, 24, 50, 80	0
All	All	1836/1908 (96%)	-0.72	6 (0%)	94	94	15, 25, 51, 80	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	22[A]	MET	2.8
1	D	22[A]	MET	2.6
1	A	22[A]	MET	2.2
1	F	22[A]	MET	2.1
1	E	144	GLY	2.1
1	C	144	GLY	2.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	CSS	F	31	7/8	0.97	0.10	28,31,36,89	0
1	CSS	E	31	7/8	0.97	0.09	20,30,48,93	0
1	CSS	B	31	7/8	0.98	0.09	23,26,41,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	CSS	D	31	7/8	0.98	0.09	21,23,40,94	0
1	CSS	C	31	7/8	0.98	0.08	20,29,39,80	0
1	CSS	A	31	7/8	0.98	0.08	25,28,34,106	0

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. 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
3	HG	E	406	1/1	0.88	0.15	73,73,73,73	1
3	HG	A	406	1/1	0.94	0.11	65,65,65,65	1
3	HG	D	406	1/1	0.94	0.08	65,65,65,65	1
4	ACT	D	405	4/4	0.95	0.33	10,19,20,24	4
4	ACT	C	405	4/4	0.95	0.41	7,14,22,28	4
3	HG	C	406	1/1	0.96	0.11	59,59,59,59	1
3	HG	B	406	1/1	0.96	0.09	61,61,61,61	1
4	ACT	F	405	4/4	0.97	0.22	13,15,23,25	4
3	HG	F	406	1/1	0.97	0.12	66,66,66,66	1
4	ACT	A	405	4/4	0.97	0.27	15,19,27,30	4
2	FE	C	401	1/1	0.98	0.04	39,39,39,39	0
4	ACT	B	405	4/4	0.98	0.24	6,27,28,28	4
4	ACT	E	405	4/4	0.99	0.25	9,20,21,29	4
2	FE	A	401	1/1	0.99	0.07	38,38,38,38	0
3	HG	B	404	1/1	0.99	0.07	37,37,37,37	1
2	FE	B	401	1/1	0.99	0.02	37,37,37,37	0
3	HG	F	404	1/1	0.99	0.05	37,37,37,37	1
3	HG	A	404	1/1	0.99	0.04	35,35,35,35	1
3	HG	D	404	1/1	0.99	0.05	36,36,36,36	1
3	HG	C	404	1/1	0.99	0.07	40,40,40,40	1
2	FE	F	401	1/1	1.00	0.04	35,35,35,35	0
2	FE	D	401	1/1	1.00	0.05	39,39,39,39	0
3	HG	E	404	1/1	1.00	0.06	37,37,37,37	1
2	FE	E	401	1/1	1.00	0.03	39,39,39,39	0

6.5 Other polymers (i)

There are no such residues in this entry.