



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:00 AM GMT

PDB ID : 2Z5Z
Title : Crystal structure of the complex of buffalo Lactoperoxidase with fluoride ion at 3.5Å resolution
Authors : Sheikh, I.A.; Jain, R.; Singh, N.; Sharma, S.; Bhushan, A.; Kaur, P.; Srinivasan, A.; Singh, T.P.
Deposited on : 2007-07-20
Resolution : 3.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<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

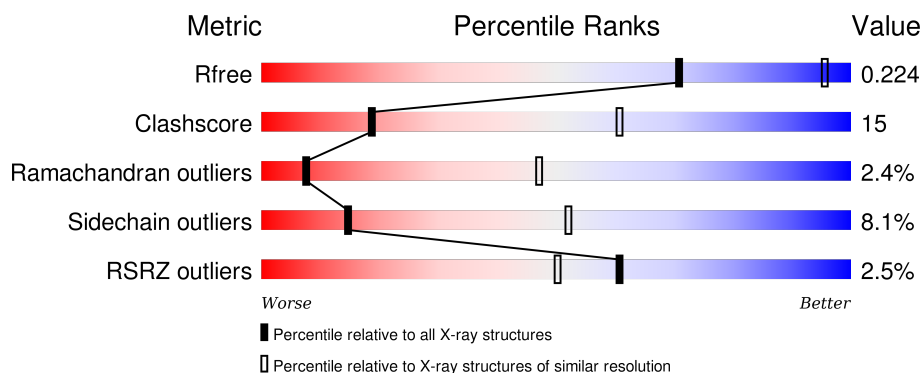
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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	595	<div> <div>3%</div> <div>72%</div> <div>23%</div> <div>• •</div> </div>

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
1	SEP	A	198	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	596	-	-	-	X
3	NAG	A	599	-	-	-	X
5	IOD	A	607	-	-	X	-
5	IOD	A	611	-	-	X	-
5	IOD	A	613	-	-	X	X
5	IOD	A	615	-	-	X	-
6	F	A	616	-	-	-	X
8	OSM	A	701	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 4990 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 Lactoperoxidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	595	Total	C	N	O	P	S	0	0	0
			4770	3032	845	865	1	27			

- Molecule 2 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	3	Total	C	N	O	0	0
			39	22	2	15		
2	A	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	N	O	0	0
			28	16	2	10		
3	A	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		

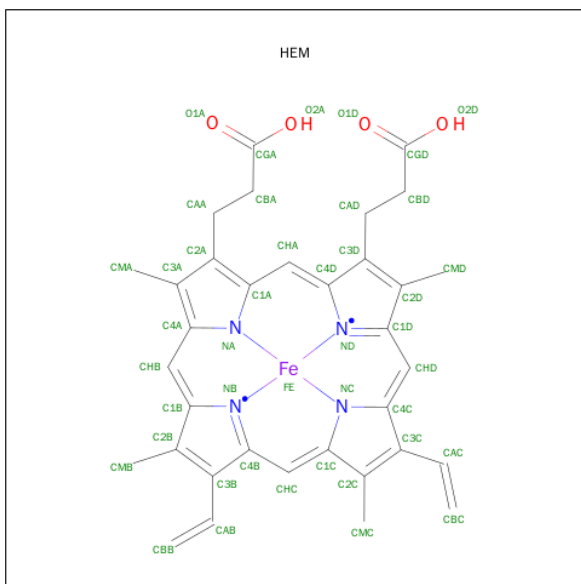
- Molecule 5 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	9	Total	I	0	0
			9	9		

- Molecule 6 is FLUORIDE ION (three-letter code: F) (formula: F).

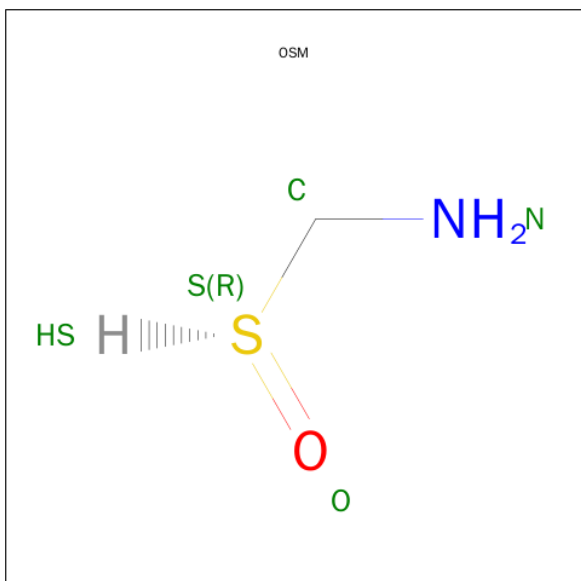
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	3	Total F 3 3	0	0

- Molecule 7 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C Fe N O 43 34 1 4 4	0	0

- Molecule 8 is 1-(OXIDOSULFANYL)METHANAMINE (three-letter code: OSM) (formula: CH_5NOS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	N	O	S	0	0
			4	1	1	1	1		

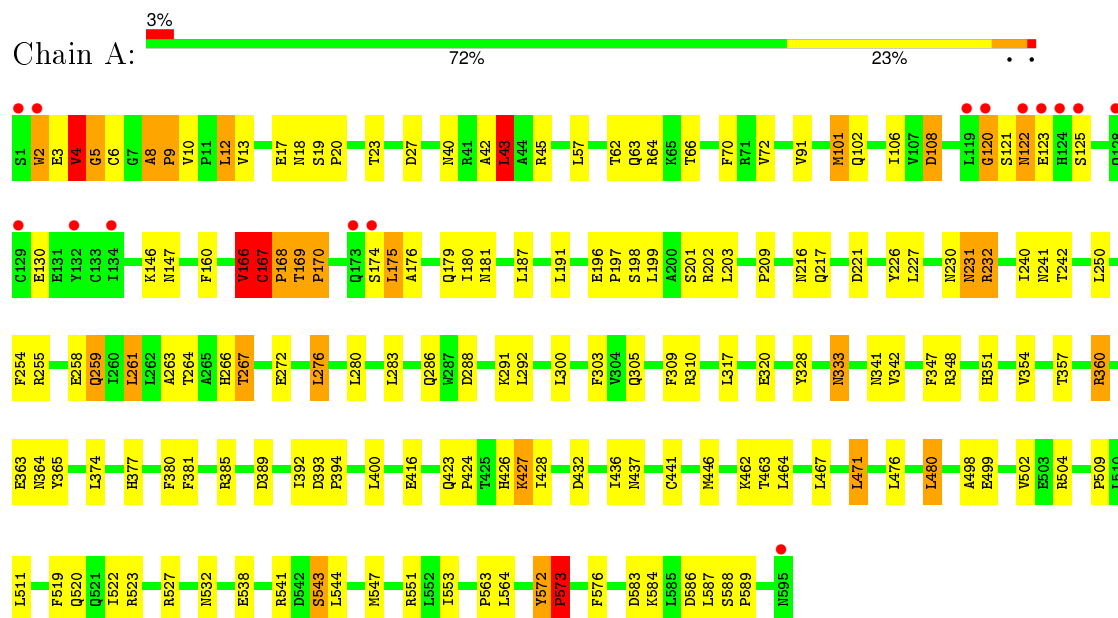
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	26	Total	O	0	0
			26	26		

3 Residue-property plots [i](#)

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: Lactoperoxidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.13Å 80.74Å 77.70Å 90.00° 102.94° 90.00°	Depositor
Resolution (Å)	75.81 – 3.50 44.16 – 3.50	Depositor EDS
% Data completeness (in resolution range)	83.2 (75.81-3.50) 83.2 (44.16-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.221 , 0.235 0.211 , 0.224	Depositor DCC
R_{free} test set	324 reflections (4.90%)	DCC
Wilson B-factor (Å ²)	45.7	Xtriage
Anisotropy	0.600	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 65.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 6966 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	4990	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.34% 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: NAG, F, CA, SEP, OSM, HEM, IOD, MAN

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	0.49	1/4886 (0.0%)	0.90	12/6627 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	573	PRO	N-CD	5.86	1.56	1.47

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	573	PRO	CA-N-CD	-18.63	85.42	111.50
1	A	573	PRO	N-CA-CB	14.33	120.49	103.30
1	A	572	TYR	C-N-CD	-13.51	90.88	120.60
1	A	572	TYR	C-N-CA	12.77	175.62	122.00
1	A	573	PRO	N-CD-CG	11.71	120.77	103.20
1	A	572	TYR	O-C-N	7.29	134.94	121.10
1	A	108	ASP	CB-CG-OD2	-5.77	113.11	118.30
1	A	167	CYS	N-CA-C	-5.71	95.59	111.00
1	A	5	GLY	N-CA-C	5.36	126.50	113.10
1	A	427	LYS	N-CA-C	5.18	124.97	111.00
1	A	232	ARG	N-CA-C	5.03	124.57	111.00
1	A	43	LEU	CA-CB-CG	5.01	126.83	115.30

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	4770	0	4674	145	0
2	A	78	0	68	3	0
3	A	56	0	50	4	0
4	A	1	0	0	0	0
5	A	9	0	0	19	0
6	A	3	0	0	0	0
7	A	43	0	30	12	0
8	A	4	0	5	2	0
9	A	26	0	0	8	0
All	All	4990	0	4827	151	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 15.

All (151) 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:198:SEP:CB	1:A:198:SEP:CA	1.76	1.58
1:A:108:ASP:OD2	7:A:619:HEM:HMD1	1.24	1.34
1:A:167:CYS:HB3	1:A:168:PRO:HD2	1.23	1.18
1:A:198:SEP:OG	1:A:198:SEP:N	1.82	1.13
1:A:198:SEP:CB	1:A:198:SEP:N	2.12	1.12
1:A:258:GLU:OE2	7:A:619:HEM:HMB1	1.58	1.03
1:A:198:SEP:CB	1:A:198:SEP:C	2.35	1.03
1:A:258:GLU:OE2	7:A:619:HEM:CMB	2.08	1.01
1:A:217:GLN:HE21	3:A:599:NAG:H83	1.27	1.00
1:A:108:ASP:OD2	7:A:619:HEM:CMD	2.11	0.99
1:A:351:HIS:HD1	1:A:437:ASN:HD21	1.08	0.98
1:A:196:GLU:HB3	1:A:198:SEP:O3P	1.64	0.95
1:A:216:ASN:HA	5:A:611:IOD:I	2.36	0.94
5:A:615:IOD:I	9:A:724:HOH:O	2.54	0.94
1:A:8:ALA:HB1	1:A:9:PRO:HD2	1.47	0.92
1:A:341:ASN:HB3	5:A:607:IOD:I	2.40	0.91
1:A:169:THR:HB	1:A:170:PRO:HD2	1.52	0.89
1:A:8:ALA:HB1	1:A:9:PRO:CD	2.02	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:462:LYS:N	5:A:615:IOD:I	2.77	0.86
1:A:8:ALA:CB	1:A:9:PRO:HD2	2.05	0.84
1:A:263:ALA:O	1:A:267:THR:HG22	1.78	0.83
1:A:167:CYS:HB3	1:A:168:PRO:CD	2.06	0.83
1:A:12:LEU:HD23	9:A:712:HOH:O	1.81	0.81
1:A:120:GLY:C	1:A:122:ASN:H	1.84	0.81
1:A:169:THR:HB	1:A:170:PRO:CD	2.12	0.79
1:A:198:SEP:CB	1:A:199:LEU:N	2.47	0.78
1:A:63:GLN:HG2	9:A:720:HOH:O	1.86	0.76
1:A:8:ALA:O	1:A:10:VAL:HG22	1.87	0.75
1:A:2:TRP:HB2	1:A:4:VAL:HG22	1.69	0.75
1:A:463:THR:N	5:A:615:IOD:I	2.89	0.74
1:A:463:THR:OG1	5:A:615:IOD:I	2.72	0.73
1:A:2:TRP:CB	1:A:4:VAL:HG22	2.20	0.72
1:A:198:SEP:HB3	1:A:199:LEU:H	1.56	0.71
1:A:42:ALA:HB2	1:A:166:VAL:HG21	1.73	0.69
1:A:504:ARG:NH2	9:A:705:HOH:O	2.25	0.69
1:A:333:ASN:HD22	1:A:333:ASN:C	1.96	0.69
1:A:328:TYR:CD1	1:A:523:ARG:HD3	2.29	0.68
1:A:198:SEP:HB3	1:A:199:LEU:N	2.08	0.66
1:A:198:SEP:CB	1:A:198:SEP:H	1.91	0.66
1:A:354:VAL:HG11	7:A:619:HEM:CBB	2.27	0.64
1:A:288:ASP:HB2	1:A:291:LYS:CB	2.28	0.64
1:A:258:GLU:OE2	7:A:619:HEM:HMB2	1.96	0.64
1:A:221:ASP:HB2	1:A:226:TYR:CZ	2.32	0.64
1:A:202:ARG:HD3	1:A:250:LEU:HD21	1.81	0.63
1:A:146:LYS:O	1:A:147:ASN:HB2	1.99	0.62
1:A:563:PRO:HD3	1:A:576:PHE:CE2	2.34	0.62
1:A:169:THR:O	1:A:170:PRO:O	2.18	0.62
1:A:354:VAL:HG11	7:A:619:HEM:HBB1	1.82	0.61
1:A:351:HIS:HD1	1:A:437:ASN:ND2	1.88	0.61
1:A:276:LEU:HD12	1:A:587:LEU:HD11	1.83	0.61
1:A:446:MET:CE	5:A:607:IOD:I	3.19	0.60
1:A:328:TYR:HD1	1:A:523:ARG:HD3	1.66	0.60
1:A:393:ASP:HB2	1:A:394:PRO:HD3	1.83	0.60
1:A:62:THR:HG22	1:A:64:ARG:HG2	1.83	0.60
1:A:106:ILE:HG23	1:A:191:LEU:HD11	1.83	0.59
1:A:120:GLY:C	1:A:122:ASN:N	2.55	0.59
1:A:167:CYS:CB	1:A:168:PRO:HD2	2.13	0.59
1:A:216:ASN:CG	5:A:611:IOD:I	3.11	0.59
1:A:544:LEU:HD23	1:A:547:MET:HE3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:538:GLU:HG3	1:A:541:ARG:NH2	2.19	0.58
1:A:169:THR:CB	1:A:170:PRO:CD	2.82	0.57
1:A:197:PRO:O	1:A:198:SEP:C	2.31	0.57
1:A:232:ARG:O	1:A:232:ARG:HG3	2.04	0.57
1:A:385:ARG:O	1:A:389:ASP:HB3	2.05	0.57
1:A:108:ASP:CG	7:A:619:HEM:HMD1	2.16	0.56
1:A:175:LEU:HD23	1:A:176:ALA:H	1.71	0.56
3:A:599:NAG:O6	3:A:600:NAG:H82	2.05	0.56
1:A:446:MET:HE1	5:A:607:IOD:I	2.77	0.55
1:A:544:LEU:HD23	1:A:547:MET:CE	2.37	0.55
1:A:216:ASN:CA	5:A:611:IOD:I	3.21	0.54
1:A:381:PHE:CZ	1:A:424:PRO:HB3	2.43	0.54
1:A:476:LEU:HD21	1:A:498:ALA:HB1	1.90	0.53
1:A:288:ASP:HB2	1:A:291:LYS:HB2	1.90	0.53
1:A:2:TRP:HB3	1:A:4:VAL:HG22	1.91	0.53
1:A:363:GLU:O	5:A:614:IOD:I	2.97	0.53
1:A:499:GLU:OE1	1:A:509:PRO:HD2	2.09	0.52
1:A:45:ARG:NE	9:A:727:HOH:O	2.41	0.52
1:A:572:TYR:CD2	1:A:573:PRO:HD3	2.44	0.52
1:A:288:ASP:HB2	1:A:291:LYS:HB3	1.92	0.52
1:A:198:SEP:OG	1:A:198:SEP:CA	2.36	0.52
2:A:602:NAG:H2	2:A:602:NAG:H61	1.93	0.51
1:A:101:MET:CE	1:A:102:GLN:HA	2.41	0.51
1:A:423:GLN:HE21	1:A:423:GLN:HA	1.77	0.50
1:A:217:GLN:NE2	3:A:599:NAG:H83	2.10	0.50
1:A:527:ARG:O	1:A:532:ASN:ND2	2.44	0.50
1:A:3:GLU:O	1:A:5:GLY:N	2.44	0.50
1:A:63:GLN:CG	9:A:720:HOH:O	2.53	0.50
1:A:288:ASP:O	1:A:292:LEU:HD23	2.12	0.50
1:A:241:ASN:ND2	2:A:601:NAG:C7	2.74	0.50
1:A:259:GLN:HE22	1:A:261:LEU:HB2	1.76	0.49
1:A:272:GLU:HA	1:A:272:GLU:OE1	2.11	0.49
1:A:446:MET:HE3	5:A:607:IOD:I	2.81	0.49
1:A:400:LEU:HD13	1:A:563:PRO:HD2	1.93	0.49
1:A:333:ASN:ND2	1:A:333:ASN:C	2.62	0.49
1:A:8:ALA:CB	1:A:9:PRO:CD	2.67	0.49
1:A:187:LEU:HD13	1:A:305:GLN:HA	1.95	0.49
1:A:467:LEU:HG	1:A:471:LEU:HD22	1.94	0.48
1:A:101:MET:HE3	1:A:102:GLN:HA	1.94	0.48
1:A:309:PHE:HB3	5:A:613:IOD:I	2.83	0.48
1:A:360:ARG:HA	1:A:394:PRO:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:PHE:HE2	1:A:436:ILE:HG23	1.80	0.47
1:A:377:HIS:HA	1:A:380:PHE:CE2	2.50	0.47
1:A:9:PRO:O	1:A:10:VAL:HG13	2.15	0.47
1:A:258:GLU:HG3	8:A:701:OSM:HN1	1.79	0.46
1:A:320:GLU:HG3	1:A:502:VAL:HG11	1.96	0.46
1:A:342:VAL:HB	5:A:607:IOD:I	2.85	0.46
1:A:551:ARG:HD3	1:A:584:LYS:HA	1.97	0.46
1:A:23:THR:OG1	1:A:27:ASP:O	2.33	0.46
1:A:2:TRP:O	1:A:3:GLU:HB2	2.16	0.45
1:A:432:ASP:C	1:A:432:ASP:OD1	2.55	0.45
1:A:300:LEU:O	1:A:303:PHE:HB3	2.17	0.45
1:A:254:PHE:HE2	9:A:706:HOH:O	1.99	0.45
1:A:43:LEU:HD23	1:A:179:GLN:HB2	1.98	0.45
1:A:217:GLN:HE21	3:A:599:NAG:C8	2.12	0.45
1:A:167:CYS:O	1:A:168:PRO:O	2.35	0.45
1:A:10:VAL:HG12	1:A:40:ASN:O	2.17	0.45
1:A:255:ARG:HG2	8:A:701:OSM:H2	1.99	0.44
1:A:259:GLN:HB2	1:A:259:GLN:HE21	1.54	0.44
1:A:123:GLU:HG3	1:A:125:SER:H	1.82	0.44
5:A:609:IOD:I	9:A:705:HOH:O	2.92	0.44
1:A:230:ASN:OD1	1:A:231:ASN:N	2.50	0.44
1:A:351:HIS:CD2	7:A:619:HEM:NC	2.86	0.44
1:A:8:ALA:O	1:A:9:PRO:C	2.56	0.44
1:A:66:THR:HB	1:A:70:PHE:N	2.32	0.44
1:A:480:LEU:HD12	1:A:480:LEU:HA	1.85	0.43
7:A:619:HEM:HMC2	7:A:619:HEM:HBC2	2.01	0.43
1:A:166:VAL:C	1:A:167:CYS:O	2.52	0.43
1:A:543:SER:OG	1:A:586:ASP:O	2.36	0.43
1:A:342:VAL:N	5:A:607:IOD:I	3.22	0.43
1:A:227:LEU:HD11	1:A:266:HIS:HB3	2.00	0.43
1:A:588:SER:N	1:A:589:PRO:CD	2.82	0.42
1:A:310:ARG:HB2	5:A:613:IOD:I	2.89	0.42
1:A:198:SEP:O	1:A:199:LEU:C	2.57	0.42
1:A:424:PRO:O	5:A:612:IOD:I	3.07	0.42
1:A:130:GLU:OE2	1:A:426:HIS:HB3	2.20	0.42
1:A:519:PHE:HA	1:A:522:ILE:HG12	2.02	0.42
1:A:364:ASN:O	1:A:365:TYR:HB2	2.20	0.41
1:A:19:SER:HA	1:A:20:PRO:HD3	1.85	0.41
1:A:348:ARG:HG2	7:A:619:HEM:C2D	2.55	0.41
1:A:166:VAL:HG13	1:A:180:ILE:HG12	2.03	0.41
1:A:377:HIS:HB3	1:A:416:GLU:OE1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:GLN:H	1:A:63:GLN:HG2	1.58	0.41
2:A:602:NAG:H4	2:A:603:MAN:H2	1.75	0.41
1:A:180:ILE:HG22	1:A:181:ASN:N	2.36	0.40
1:A:462:LYS:HB2	5:A:615:IOD:I	2.92	0.40
1:A:146:LYS:O	1:A:147:ASN:CB	2.69	0.40
1:A:354:VAL:HG21	7:A:619:HEM:CBB	2.52	0.40
1:A:357:THR:HA	1:A:374:LEU:O	2.21	0.40
1:A:221:ASP:HB2	1:A:226:TYR:CE2	2.55	0.40
1:A:264:THR:HG23	1:A:392:ILE:HD12	2.02	0.40
1:A:400:LEU:HD11	1:A:553:ILE:HD13	2.02	0.40

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	592/595 (100%)	538 (91%)	40 (7%)	14 (2%)	7 47

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	VAL
1	A	6	CYS
1	A	8	ALA
1	A	9	PRO
1	A	17	GLU
1	A	122	ASN
1	A	168	PRO
1	A	169	THR
1	A	170	PRO
1	A	174	SER
1	A	573	PRO

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Mol	Chain	Res	Type
1	A	167	CYS
1	A	120	GLY
1	A	166	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	516/516 (100%)	474 (92%)	42 (8%)	15	52

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	TRP
1	A	4	VAL
1	A	12	LEU
1	A	13	VAL
1	A	18	ASN
1	A	43	LEU
1	A	57	LEU
1	A	72	VAL
1	A	91	VAL
1	A	101	MET
1	A	121	SER
1	A	166	VAL
1	A	175	LEU
1	A	201	SER
1	A	203	LEU
1	A	209	PRO
1	A	231	ASN
1	A	240	ILE
1	A	242	THR
1	A	259	GLN
1	A	261	LEU
1	A	267	THR
1	A	276	LEU

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Mol	Chain	Res	Type
1	A	280	LEU
1	A	283	LEU
1	A	286	GLN
1	A	317	LEU
1	A	333	ASN
1	A	347	PHE
1	A	360	ARG
1	A	427	LYS
1	A	428	ILE
1	A	441	CYS
1	A	464	LEU
1	A	471	LEU
1	A	480	LEU
1	A	511	LEU
1	A	520	GLN
1	A	543	SER
1	A	564	LEU
1	A	573	PRO
1	A	583	ASP

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

Mol	Chain	Res	Type
1	A	217	GLN
1	A	259	GLN
1	A	322	GLN
1	A	333	ASN
1	A	364	ASN
1	A	423	GLN
1	A	468	GLN
1	A	497	ASN
1	A	570	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	SEP	A	198	1	8,9,10	3.99	3 (37%)	8,12,14	7.36	5 (62%)

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	SEP	A	198	1	-	0/6/8/10	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	SEP	CA-N	-4.16	1.34	1.47
1	A	198	SEP	O-C	6.30	1.48	1.19
1	A	198	SEP	CB-CA	7.97	1.76	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	SEP	OG-CB-CA	-18.26	92.70	108.27
1	A	198	SEP	O3P-P-O1P	-3.96	97.84	110.58
1	A	198	SEP	O2P-P-OG	3.77	117.42	106.56
1	A	198	SEP	O-C-CA	4.89	138.21	125.49
1	A	198	SEP	OG-P-O1P	6.40	123.43	107.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	198	SEP	12	0

5.5 Carbohydrates ⓘ

10 carbohydrates 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	NAG	A	596	1,2	14,14,15	0.66	0	15,19,21	1.84	6 (40%)
2	NAG	A	597	2	14,14,15	0.88	0	15,19,21	1.34	2 (13%)
2	MAN	A	598	2	11,11,12	0.87	0	14,15,17	0.69	0
3	NAG	A	599	1,3	14,14,15	1.49	2 (14%)	15,19,21	2.46	3 (20%)
3	NAG	A	600	3	14,14,15	0.79	0	15,19,21	2.40	3 (20%)
2	NAG	A	601	1,2	14,14,15	0.60	0	15,19,21	1.07	1 (6%)
2	NAG	A	602	2	14,14,15	0.97	1 (7%)	15,19,21	2.53	4 (26%)
2	MAN	A	603	2	11,11,12	0.86	1 (9%)	14,15,17	0.45	0
3	NAG	A	604	1,3	14,14,15	0.70	0	15,19,21	1.61	3 (20%)
3	NAG	A	605	3	14,14,15	0.54	0	15,19,21	1.11	1 (6%)

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	NAG	A	596	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	597	2	-	0/6/23/26	0/1/1/1
2	MAN	A	598	2	-	0/2/19/22	0/1/1/1
3	NAG	A	599	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	600	3	-	0/6/23/26	0/1/1/1
2	NAG	A	601	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	602	2	-	0/6/23/26	0/1/1/1
2	MAN	A	603	2	-	0/2/19/22	0/1/1/1
3	NAG	A	604	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	605	3	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	603	MAN	C2-C3	2.03	1.55	1.52
2	A	602	NAG	O5-C5	2.56	1.49	1.43
3	A	599	NAG	O5-C1	2.57	1.48	1.43
3	A	599	NAG	O5-C5	3.66	1.51	1.43

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	602	NAG	C4-C3-C2	-7.43	99.68	111.23
3	A	599	NAG	C2-N2-C7	-5.89	115.48	123.04
3	A	600	NAG	C2-N2-C7	-3.95	117.96	123.04
2	A	602	NAG	C2-N2-C7	-3.49	118.56	123.04
2	A	596	NAG	C2-N2-C7	-3.37	118.71	123.04
2	A	597	NAG	C2-N2-C7	-3.25	118.86	123.04
3	A	605	NAG	C2-N2-C7	-2.71	119.55	123.04
3	A	604	NAG	C2-N2-C7	-2.60	119.70	123.04
2	A	596	NAG	C6-C5-C4	-2.46	106.94	113.02
2	A	596	NAG	O5-C5-C6	-2.22	102.54	107.35
2	A	596	NAG	C3-C4-C5	2.31	114.23	110.20
2	A	601	NAG	C3-C4-C5	2.41	114.40	110.20
2	A	596	NAG	C4-C3-C2	2.44	115.02	111.23
2	A	602	NAG	C3-C2-N2	2.53	116.63	110.56
2	A	596	NAG	C1-O5-C5	2.77	115.77	112.25
3	A	599	NAG	C3-C4-C5	2.82	115.11	110.20
2	A	597	NAG	C4-C3-C2	2.87	115.69	111.23
3	A	600	NAG	C3-C4-C5	2.90	115.25	110.20
3	A	604	NAG	C3-C4-C5	3.10	115.60	110.20
2	A	602	NAG	C1-O5-C5	3.18	116.28	112.25
3	A	604	NAG	C4-C3-C2	4.16	117.69	111.23
3	A	599	NAG	C1-O5-C5	6.18	120.10	112.25
3	A	600	NAG	C1-O5-C5	7.61	121.91	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	599	NAG	4	0
3	A	600	NAG	1	0
2	A	601	NAG	1	0
2	A	602	NAG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	603	MAN	1	0

5.6 Ligand geometry

Of 15 ligands modelled in this entry, 13 are monoatomic - leaving 2 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
7	HEM	A	619	1	30,50,50	3.12	8 (26%)	24,82,82	2.42	10 (41%)
8	OSM	A	701	-	1,3,3	0.67	0	0,2,2	0.00	-

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
7	HEM	A	619	1	-	0/10/54/54	0/0/8/8
8	OSM	A	701	-	-	0/0/1/1	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	619	HEM	C3B-C4B	-12.58	1.40	1.51
7	A	619	HEM	C3D-C4D	-7.05	1.42	1.51
7	A	619	HEM	C2C-C1C	-5.32	1.42	1.52
7	A	619	HEM	C2B-C1B	-2.85	1.42	1.51
7	A	619	HEM	C2D-C1D	-2.62	1.43	1.51
7	A	619	HEM	C1A-CHA	-2.34	1.33	1.39
7	A	619	HEM	FE-ND	-2.09	1.86	1.97
7	A	619	HEM	C3C-CAC	2.59	1.56	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	619	HEM	CAA-C2A-C1A	-2.90	123.85	127.01
7	A	619	HEM	C3B-CAB-CBB	-2.90	120.00	124.46
7	A	619	HEM	CMA-C3A-C4A	-2.01	125.04	128.36
7	A	619	HEM	CMD-C2D-C3D	2.27	124.41	114.35
7	A	619	HEM	C2C-C1C-CHC	2.51	127.50	123.68
7	A	619	HEM	C3C-CAC-CBC	2.96	129.00	124.46
7	A	619	HEM	CMB-C2B-C3B	3.15	124.39	116.53
7	A	619	HEM	CAD-C3D-C2D	4.53	126.23	113.22
7	A	619	HEM	CAD-C3D-C4D	5.18	130.75	112.47
7	A	619	HEM	CMC-C2C-C3C	5.33	129.83	116.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	619	HEM	12	0
8	A	701	OSM	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	594/595 (99%)	-0.39	15 (2%)	61 50	2, 20, 73, 126	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	125	SER	3.6
1	A	129	CYS	3.4
1	A	2	TRP	3.1
1	A	1	SER	3.0
1	A	119	LEU	2.9
1	A	122	ASN	2.9
1	A	123	GLU	2.9
1	A	174	SER	2.6
1	A	128	GLN	2.6
1	A	132	TYR	2.6
1	A	173	GLN	2.5
1	A	120	GLY	2.5
1	A	595	ASN	2.5
1	A	124	HIS	2.4
1	A	134	ILE	2.3

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
1	SEP	A	198	10/11	0.85	0.27	-	43,55,57,61	0

6.3 Carbohydrates [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	NAG	A	599	14/15	0.81	0.38	2.64	3,7,9,9	14
2	NAG	A	596	14/15	0.83	0.37	2.63	2,2,2,2	14
2	NAG	A	601	14/15	0.91	0.24	0.58	2,2,2,2	14
3	NAG	A	605	14/15	0.72	0.38	-	39,40,41,41	14
2	MAN	A	598	11/12	0.74	0.42	-	30,32,32,32	11
3	NAG	A	604	14/15	0.74	0.39	-	55,59,61,61	14
2	NAG	A	597	14/15	0.86	0.33	-	15,16,18,18	14
2	NAG	A	602	14/15	0.70	0.37	-	4,6,8,9	14
2	MAN	A	603	11/12	0.74	0.37	-	65,66,67,68	11
3	NAG	A	600	14/15	0.78	0.41	-	16,17,18,18	14

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
6	F	A	616	1/1	0.52	0.66	6.06	25,25,25,25	1
5	IOD	A	613	1/1	0.92	0.25	3.32	21,21,21,21	1
7	HEM	A	619	43/43	0.95	0.18	0.01	4,4,7,31	0
5	IOD	A	614	1/1	0.67	0.24	-0.25	41,41,41,41	1
5	IOD	A	611	1/1	0.81	0.21	-0.36	25,25,25,25	1
5	IOD	A	607	1/1	0.94	0.14	-0.43	14,14,14,14	1
5	IOD	A	608	1/1	0.96	0.10	-1.28	40,40,40,40	1
4	CA	A	606	1/1	0.96	0.07	-3.45	5,5,5,5	0
5	IOD	A	615	1/1	0.88	0.16	-	35,35,35,35	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	IOD	A	612	1/1	0.86	0.14	-	37,37,37,37	1
6	F	A	618	1/1	0.83	0.91	-	25,25,25,25	1
5	IOD	A	609	1/1	0.76	0.17	-	57,57,57,57	1
8	OSM	A	701	4/4	0.95	0.27	-	18,18,18,18	0
5	IOD	A	610	1/1	0.77	0.13	-	42,42,42,42	1
6	F	A	617	1/1	0.80	0.92	-	25,25,25,25	1

6.5 Other polymers [i](#)

There are no such residues in this entry.