Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 06:13 pm GMT

PDB ID	:	2PUM
Title	:	Crystal structure of bovine lactoperoxidase complex with catechol and iodide at 2.7 A resolution
Authors	:	Singh, A.K.; Singh, N.; Sharma, S.; Kaur, P.; Singh, T.P.
Deposited on	:	2007-05-09
Resolution	:	2.70 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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		0.198
Clashscore		15
Ramachandran outliers		2.0%
Sidechain outliers		11.0%
RSRZ outliers		5.2%

Worse *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
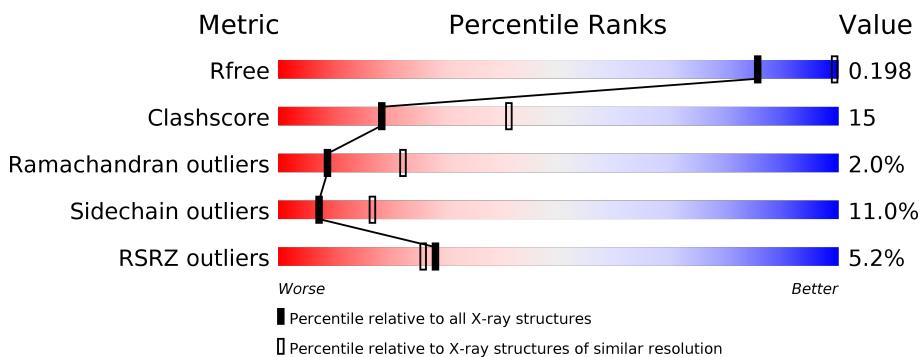
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (2.70-2.70)

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 <=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	5% ▐ 67% 25% 6% ·
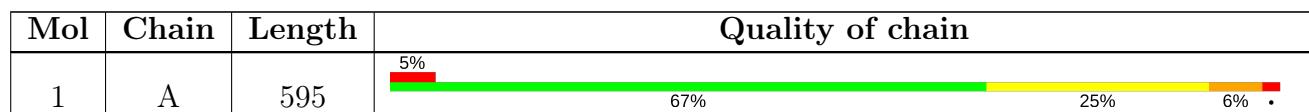
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	596	-	-	-	X
5	SCN	A	607	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	IOD	A	609	-	-	X	-
6	IOD	A	617	-	-	X	-

2 Entry composition ⓘ

There are 9 unique types of molecules in this entry. The entry contains 5260 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 4780	C 3041	N 847	O 865	P 1	S 26	0	1	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	198	SEP	SER	MODIFIED RESIDUE	UNP P80025

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

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

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

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

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

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

- Molecule 5 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).
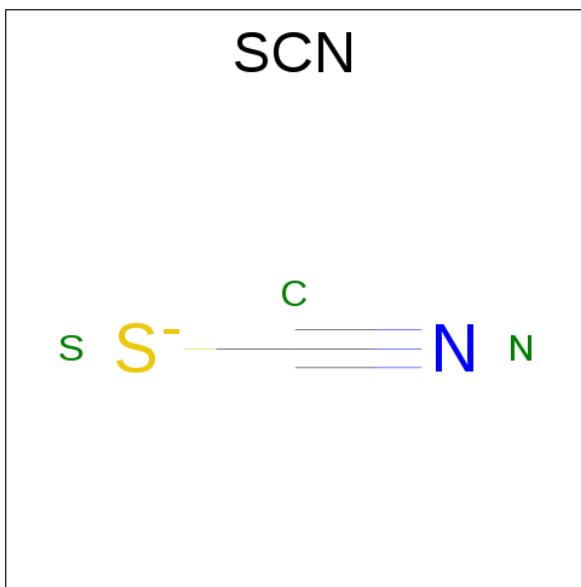
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	S		
5	A	1	3	1	1	1	0	0

- Molecule 6 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	I		
6	A	10	10	10	0	0

- Molecule 7 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).
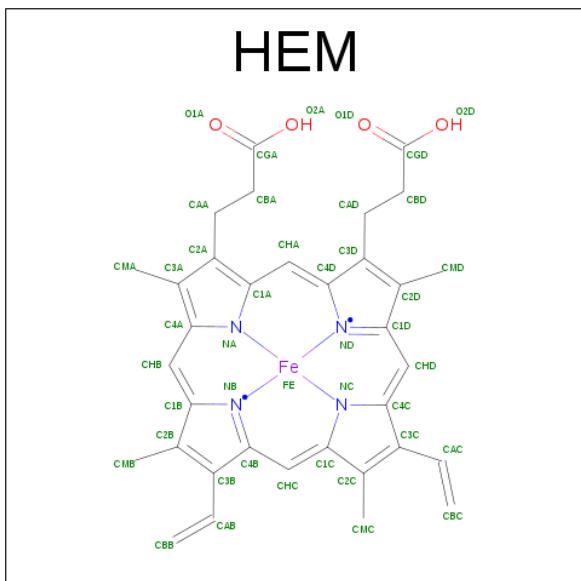
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
7	A	1	43	34	1	4	4	0	0

- Molecule 8 is CATECHOL (three-letter code: CAQ) (formula: $C_6H_6O_2$).
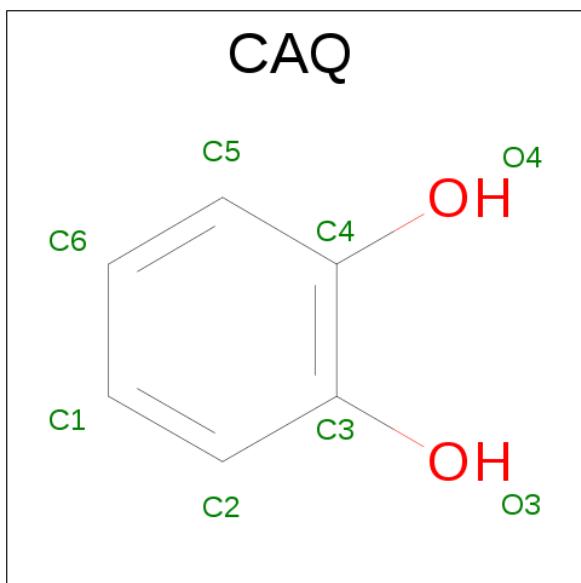
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
8	A	1	8	6	2	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	A	281	281	281	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: Lactoperoxidase
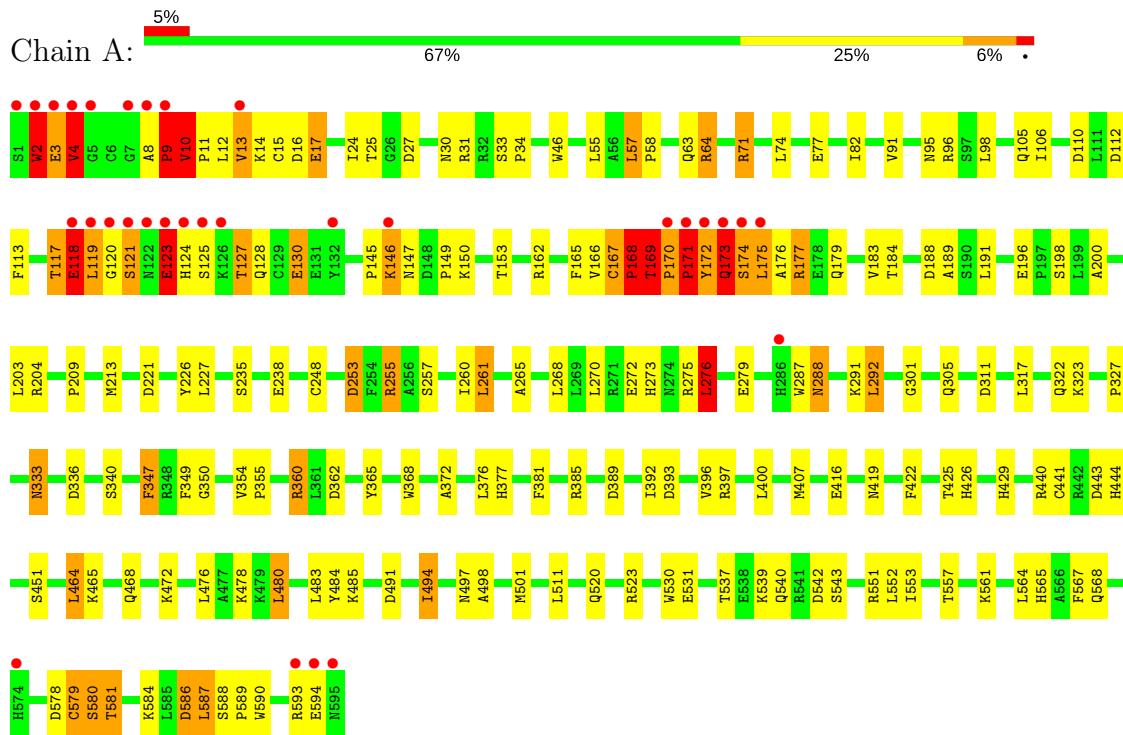
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	54.42Å 80.49Å 77.32Å 90.00° 102.60° 90.00°	Depositor
Resolution (Å)	24.93 – 2.70 24.93 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.2 (24.93-2.70) 99.4 (24.93-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.98 (at 2.72Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.165 , 0.203 0.168 , 0.198	Depositor DCC
R_{free} test set	912 reflections (5.38%)	DCC
Wilson B-factor (Å^2)	30.7	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 60.7	EDS
L-test for twinning [2]	$<|L|> = 0.50$, $<L^2> = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5260	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.39% 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: SCN, NAG, SEP, CAQ, HEM, IOD, CA, 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	0.77	2/4900 (0.0%)	1.06	31/6646 (0.5%)

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	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	10	VAL	N-CA	-5.62	1.35	1.46
1	A	9	PRO	C-N	-5.38	1.21	1.34

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	118[A]	GLU	O-C-N	-10.33	106.17	122.70
1	A	118[B]	GLU	O-C-N	-10.33	106.17	122.70
1	A	3	GLU	CA-C-N	-8.72	98.02	117.20
1	A	3	GLU	C-N-CA	8.00	141.69	121.70
1	A	253	ASP	CB-CG-OD2	7.65	125.19	118.30
1	A	3	GLU	N-CA-C	-6.92	92.32	111.00
1	A	3	GLU	N-CA-CB	6.82	122.88	110.60
1	A	27	ASP	CB-CG-OD2	6.71	124.33	118.30
1	A	336	ASP	CB-CG-OD2	6.66	124.30	118.30
1	A	170	PRO	CA-N-CD	-6.58	102.28	111.50
1	A	173	GLN	CA-C-N	6.21	130.86	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	171	PRO	CA-N-CD	-6.16	102.88	111.50
1	A	2	TRP	C-N-CA	6.08	136.90	121.70
1	A	3	GLU	O-C-N	5.93	132.19	122.70
1	A	172	TYR	CB-CG-CD1	5.81	124.48	121.00
1	A	173	GLN	C-N-CA	-5.78	107.25	121.70
1	A	112	ASP	CB-CG-OD2	5.77	123.49	118.30
1	A	311	ASP	CB-CG-OD2	5.76	123.49	118.30
1	A	542	ASP	CB-CG-OD2	5.74	123.47	118.30
1	A	168	PRO	C-N-CA	5.64	135.81	121.70
1	A	586	ASP	CB-CG-OD2	5.57	123.31	118.30
1	A	172	TYR	CB-CG-CD2	-5.55	117.67	121.00
1	A	276	LEU	CA-CB-CG	5.49	127.92	115.30
1	A	9	PRO	CA-C-N	-5.48	105.15	117.20
1	A	174	SER	N-CA-C	5.37	125.50	111.00
1	A	491	ASP	CB-CG-OD1	5.19	122.97	118.30
1	A	168	PRO	CA-C-N	-5.09	106.00	117.20
1	A	123	GLU	N-CA-C	5.09	124.75	111.00
1	A	443	ASP	CB-CG-OD2	5.08	122.87	118.30
1	A	594	GLU	CB-CA-C	-5.07	100.27	110.40
1	A	288	ASN	N-CA-CB	-5.03	101.55	110.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	118[A]	GLU	Mainchain
1	A	118[B]	GLU	Mainchain

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	4780	0	4692	140	0
2	A	78	0	68	2	0
3	A	56	0	50	0	0
4	A	1	0	0	0	0
5	A	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	10	0	0	6	0
7	A	43	0	30	7	0
8	A	8	0	4	0	0
9	A	281	0	0	16	0
All	All	5260	0	4844	146	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 (146) 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:578:ASP:OD1	1:A:580:SER:HB2	1.53	1.05
1:A:227:LEU:HD23	1:A:270:LEU:HD22	1.37	1.03
1:A:31:ARG:HD2	6:A:609:IOD:I	2.29	1.02
1:A:33:SER:HB2	9:A:896:HOH:O	1.62	1.00
1:A:118[A]:GLU:HG3	1:A:119:LEU:N	1.75	0.92
1:A:118[A]:GLU:HG3	1:A:119:LEU:H	1.09	0.88
1:A:106:ILE:HD11	1:A:265:ALA:HB1	1.59	0.84
7:A:618:HEM:HMB2	7:A:618:HEM:HBB2	1.60	0.81
1:A:167:CYS:CB	1:A:168:PRO:HD2	2.12	0.80
1:A:551:ARG:HD3	1:A:584:LYS:HA	1.62	0.80
7:A:618:HEM:CMB	7:A:618:HEM:HBB2	2.12	0.78
1:A:8:ALA:N	1:A:9:PRO:HD2	2.02	0.73
1:A:9:PRO:O	1:A:11:PRO:HD3	1.89	0.73
1:A:71:ARG:HG3	1:A:71:ARG:HH11	1.52	0.73
1:A:537:THR:OG1	1:A:540:GLN:HG3	1.89	0.72
1:A:167:CYS:CB	1:A:168:PRO:CD	2.67	0.72
1:A:196:GLU:HB3	1:A:198:SEP:O3P	1.88	0.72
1:A:167:CYS:HB3	1:A:168:PRO:HD2	1.72	0.72
6:A:609:IOD:I	9:A:723:HOH:O	2.78	0.71
1:A:275:ARG:NH1	9:A:800:HOH:O	2.26	0.69
1:A:130:GLU:CD	1:A:426:HIS:HD2	1.95	0.69
1:A:2:TRP:HA	1:A:4:VAL:HG13	1.75	0.69
1:A:327:PRO:HD2	9:A:799:HOH:O	1.93	0.68
7:A:618:HEM:HMB2	7:A:618:HEM:CBB	2.23	0.68
1:A:147:ASN:O	1:A:149:PRO:HD3	1.93	0.67
1:A:578:ASP:C	1:A:580:SER:H	1.98	0.67
1:A:167:CYS:HB3	1:A:168:PRO:CD	2.25	0.67
1:A:8:ALA:N	1:A:9:PRO:CD	2.58	0.67
1:A:464:LEU:O	1:A:468:GLN:HG3	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:ARG:NH1	1:A:372:ALA:HA	2.13	0.64
1:A:213:MET:HG2	1:A:273:HIS:CD2	2.33	0.63
1:A:71:ARG:HH11	1:A:71:ARG:CG	2.10	0.63
1:A:150:LYS:NZ	1:A:419:ASN:O	2.30	0.63
1:A:17:GLU:HG3	9:A:894:HOH:O	1.98	0.63
1:A:167:CYS:HB2	1:A:168:PRO:HD2	1.81	0.62
1:A:587:LEU:HD23	1:A:587:LEU:O	2.02	0.59
1:A:8:ALA:H	1:A:9:PRO:HD2	1.65	0.59
2:A:598:MAN:H2	9:A:861:HOH:O	2.02	0.59
1:A:121:SER:HB2	9:A:827:HOH:O	2.04	0.58
1:A:82:ILE:HG21	1:A:494:ILE:HD11	1.84	0.58
1:A:530:TRP:CE2	1:A:531:GLU:HG3	2.39	0.58
1:A:10:VAL:CG2	1:A:10:VAL:O	2.51	0.57
1:A:10:VAL:HG23	1:A:10:VAL:O	2.03	0.57
1:A:95:ASN:O	1:A:96:ARG:HD3	2.05	0.57
1:A:476:LEU:HD21	1:A:498:ALA:HB1	1.87	0.56
1:A:365:TYR:CE1	1:A:397:ARG:HB3	2.41	0.56
1:A:117:THR:OG1	1:A:162:ARG:O	2.23	0.55
1:A:191:LEU:H	1:A:191:LEU:HD23	1.71	0.55
1:A:272:GLU:O	1:A:276:LEU:HB2	2.06	0.55
1:A:71:ARG:NH1	1:A:71:ARG:CG	2.68	0.54
1:A:272:GLU:HG3	1:A:276:LEU:HD22	1.89	0.54
1:A:451:SER:HA	9:A:696:HOH:O	2.08	0.53
1:A:14:LYS:HG3	1:A:15:CYS:N	2.23	0.53
1:A:169:THR:OG1	1:A:170:PRO:CD	2.57	0.53
1:A:484:TYR:O	1:A:485:LYS:HB2	2.08	0.53
1:A:578:ASP:C	1:A:580:SER:N	2.61	0.53
1:A:422:PHE:HB2	1:A:429:HIS:CD2	2.44	0.53
1:A:400:LEU:HD11	1:A:553:ILE:HD13	1.91	0.52
1:A:288:ASN:O	1:A:292:LEU:HD23	2.10	0.52
1:A:567:PHE:HD2	6:A:617:IOD:I	2.63	0.52
1:A:64:ARG:C	1:A:64:ARG:HD3	2.30	0.52
1:A:127:THR:HA	1:A:130:GLU:HB2	1.91	0.52
1:A:123:GLU:HG2	1:A:125:SER:HB2	1.92	0.52
1:A:16:ASP:OD1	1:A:16:ASP:C	2.48	0.52
1:A:407:MET:HB3	1:A:501:MET:CE	2.40	0.52
1:A:16:ASP:HB2	9:A:816:HOH:O	2.09	0.51
1:A:33:SER:CB	9:A:896:HOH:O	2.36	0.51
1:A:110:ASP:OD2	1:A:189:ALA:N	2.43	0.51
1:A:9:PRO:HG3	9:A:708:HOH:O	2.11	0.51
1:A:128:GLN:NE2	9:A:820:HOH:O	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:ARG:HH12	1:A:372:ALA:HA	1.76	0.51
1:A:106:ILE:HD11	1:A:265:ALA:CB	2.36	0.51
1:A:146:LYS:HE3	1:A:147:ASN:HD21	1.76	0.51
1:A:166:VAL:O	1:A:167:CYS:HB2	2.10	0.50
1:A:333:ASN:HD22	1:A:333:ASN:C	2.15	0.50
1:A:578:ASP:O	1:A:580:SER:N	2.45	0.50
1:A:106:ILE:HG23	1:A:191:LEU:HD11	1.93	0.50
1:A:9:PRO:O	1:A:11:PRO:CD	2.57	0.50
1:A:362:ASP:OD1	1:A:362:ASP:C	2.51	0.49
1:A:172:TYR:CD1	1:A:173:GLN:N	2.80	0.49
1:A:16:ASP:OD1	1:A:16:ASP:O	2.31	0.49
1:A:385:ARG:O	1:A:389:ASP:HB2	2.13	0.49
1:A:347:PHE:HB3	7:A:618:HEM:CMD	2.43	0.49
1:A:235:SER:HB3	1:A:238:GLU:HB2	1.94	0.48
1:A:565:HIS:HB3	6:A:617:IOD:I	2.83	0.48
1:A:118[A]:GLU:OE2	1:A:120:GLY:N	2.38	0.48
1:A:588:SER:C	1:A:590:TRP:H	2.16	0.48
1:A:268:LEU:CD1	1:A:392:ILE:HD12	2.42	0.48
1:A:580:SER:C	1:A:581:THR:HG1	2.17	0.48
1:A:165:PHE:CB	1:A:177:ARG:HD2	2.44	0.48
1:A:368:TRP:O	1:A:368:TRP:CE3	2.66	0.48
1:A:392:ILE:O	1:A:396:VAL:HG23	2.13	0.48
1:A:82:ILE:CG2	1:A:494:ILE:HD11	2.44	0.48
1:A:169:THR:OG1	1:A:170:PRO:HD3	2.14	0.48
1:A:257:SER:O	1:A:381:PHE:HA	2.14	0.47
1:A:188:ASP:O	1:A:189:ALA:HB3	2.14	0.47
1:A:165:PHE:CG	1:A:177:ARG:HD2	2.50	0.47
1:A:301:GLY:O	1:A:305:GLN:HG3	2.15	0.47
1:A:287:TRP:CE2	1:A:291:LYS:HD3	2.49	0.47
1:A:354:VAL:HA	1:A:355:PRO:HD3	1.79	0.47
1:A:255:ARG:HG2	6:A:608:IOD:I	2.85	0.47
1:A:567:PHE:HB2	6:A:617:IOD:I	2.85	0.47
1:A:30:ASN:O	1:A:34:PRO:HA	2.15	0.46
1:A:82:ILE:HD11	1:A:483:LEU:HD12	1.96	0.46
1:A:248:CYS:HB3	1:A:257:SER:OG	2.16	0.46
1:A:221:ASP:HB2	1:A:226:TYR:CZ	2.51	0.46
1:A:288:ASN:O	1:A:292:LEU:CD2	2.64	0.46
1:A:46:TRP:CE2	1:A:340:SER:HB3	2.51	0.45
1:A:58:PRO:HG3	1:A:162:ARG:NH2	2.31	0.45
1:A:105:GLN:NE2	7:A:618:HEM:C4B	2.84	0.45
1:A:543:SER:OG	1:A:586:ASP:O	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:578:ASP:O	1:A:581:THR:HB	2.17	0.45
2:A:602:NAG:H4	2:A:603:MAN:H2	1.61	0.45
1:A:200:ALA:O	1:A:204:ARG:HG3	2.18	0.44
1:A:440:ARG:O	1:A:440:ARG:HG3	2.18	0.44
1:A:349:PHE:CB	1:A:497:ASN:HD21	2.29	0.44
1:A:169:THR:HA	9:A:874:HOH:O	2.18	0.44
1:A:77:GLU:HB2	1:A:145:PRO:HG3	2.00	0.43
1:A:124:HIS:HA	1:A:127:THR:HB	1.99	0.43
1:A:468:GLN:O	1:A:472:LYS:N	2.51	0.43
1:A:63:GLN:HB2	9:A:805:HOH:O	2.18	0.43
1:A:57:LEU:HA	1:A:58:PRO:HD3	1.84	0.43
1:A:253:ASP:OD2	1:A:255:ARG:HD3	2.19	0.42
1:A:82:ILE:CD1	1:A:483:LEU:HD12	2.48	0.42
1:A:480:LEU:HA	1:A:480:LEU:HD12	1.76	0.42
1:A:276:LEU:HD12	1:A:587:LEU:HD11	2.01	0.42
1:A:393:ASP:OD1	1:A:557:THR:HB	2.20	0.42
1:A:113:PHE:HB3	1:A:183:VAL:HG13	2.02	0.42
1:A:292:LEU:HD13	1:A:292:LEU:HA	1.88	0.42
1:A:407:MET:HB3	1:A:501:MET:HE3	2.02	0.42
1:A:478:LYS:HE2	1:A:478:LYS:HB3	1.82	0.41
1:A:15:CYS:HA	9:A:684:HOH:O	2.21	0.41
1:A:441:CYS:HB3	9:A:672:HOH:O	2.19	0.41
1:A:63:GLN:O	1:A:71:ARG:NH1	2.53	0.41
1:A:425:THR:HB	1:A:426:HIS:ND1	2.35	0.41
1:A:25:THR:O	1:A:184:THR:HG22	2.21	0.41
1:A:377:HIS:HB3	1:A:416:GLU:OE2	2.21	0.41
1:A:179:GLN:HG2	1:A:444:HIS:CE1	2.56	0.41
1:A:350:GLY:HA3	7:A:618:HEM:CBC	2.50	0.41
1:A:347:PHE:HB3	7:A:618:HEM:HMD1	2.03	0.41
1:A:24:ILE:HA	1:A:24:ILE:HD13	1.83	0.41
1:A:260:ILE:HG23	1:A:261:LEU:N	2.36	0.41
1:A:261:LEU:HA	1:A:261:LEU:HD12	1.90	0.40
1:A:123:GLU:C	1:A:125:SER:N	2.75	0.40
1:A:12:LEU:O	1:A:13:VAL:HG13	2.22	0.40
1:A:287:TRP:CD2	1:A:291:LYS:HD3	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	593/595 (100%)	541 (91%)	40 (7%)	12 (2%)	9 22

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	VAL
1	A	167	CYS
1	A	168	PRO
1	A	176	ALA
1	A	169	THR
1	A	175	LEU
1	A	581	THR
1	A	3	GLU
1	A	589	PRO
1	A	579	CYS
1	A	209	PRO
1	A	171	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	518/517 (100%)	460 (89%)	58 (11%)	7 16

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	TRP
1	A	4	VAL
1	A	9	PRO
1	A	10	VAL
1	A	13	VAL
1	A	17	GLU
1	A	55	LEU
1	A	57	LEU
1	A	64	ARG
1	A	71	ARG
1	A	74	LEU
1	A	91	VAL
1	A	98	LEU
1	A	117	THR
1	A	118[A]	GLU
1	A	118[B]	GLU
1	A	119	LEU
1	A	121	SER
1	A	123	GLU
1	A	127	THR
1	A	130	GLU
1	A	146	LYS
1	A	153	THR
1	A	169	THR
1	A	171	PRO
1	A	173	GLN
1	A	174	SER
1	A	175	LEU
1	A	177	ARG
1	A	203	LEU
1	A	255	ARG
1	A	261	LEU
1	A	276	LEU
1	A	279	GLU
1	A	292	LEU
1	A	317	LEU
1	A	322	GLN
1	A	323	LYS
1	A	333	ASN
1	A	347	PHE
1	A	360	ARG
1	A	376	LEU
1	A	464	LEU

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Mol	Chain	Res	Type
1	A	465	LYS
1	A	480	LEU
1	A	494	ILE
1	A	511	LEU
1	A	520	GLN
1	A	523	ARG
1	A	539	LYS
1	A	552	LEU
1	A	561	LYS
1	A	564	LEU
1	A	568	GLN
1	A	579	CYS
1	A	580	SER
1	A	587	LEU
1	A	593	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	322	GLN
1	A	329	GLN
1	A	333	ASN
1	A	341	ASN
1	A	364	ASN
1	A	423	GLN
1	A	426	HIS
1	A	497	ASN
1	A	545	GLN
1	A	574	HIS

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	9,9,10	2.02	1 (11%)	9,12,14	1.89	2 (22%)

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	-	0/5/8/10	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	SEP	CA-C	5.23	1.57	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	SEP	OG-CB-CA	2.08	110.22	108.17
1	A	198	SEP	P-OG-CB	3.29	127.37	118.30

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	198	SEP	1	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	0.56	0	15,19,21	1.89	4 (26%)
2	NAG	A	597	2	14,14,15	0.62	0	15,19,21	1.43	2 (13%)
2	MAN	A	598	2	11,11,12	0.57	0	13,15,17	1.34	1 (7%)
3	NAG	A	599	1,3	14,14,15	0.66	0	15,19,21	1.47	3 (20%)
3	NAG	A	600	3	14,14,15	0.63	0	15,19,21	1.87	3 (20%)
2	NAG	A	601	1,2	14,14,15	0.67	0	15,19,21	1.71	3 (20%)
2	NAG	A	602	2	14,14,15	0.59	0	15,19,21	1.61	1 (6%)
2	MAN	A	603	2	11,11,12	0.50	0	13,15,17	2.11	5 (38%)
3	NAG	A	604	1,3	14,14,15	0.83	0	15,19,21	2.09	5 (33%)
3	NAG	A	605	3	14,14,15	0.64	0	15,19,21	1.57	2 (13%)

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	1/1/1/1
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

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	596	NAG	O5-C1-C2	-4.41	105.33	111.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	NAG	O5-C1-C2	-4.20	105.63	111.47
3	A	605	NAG	O5-C1-C2	-4.01	105.89	111.47
3	A	604	NAG	O5-C1-C2	-3.42	106.71	111.47
2	A	596	NAG	C3-C4-C5	-3.42	104.19	110.22
3	A	599	NAG	O5-C1-C2	-3.32	106.86	111.47
3	A	600	NAG	C2-N2-C7	-3.22	118.24	122.94
2	A	601	NAG	O4-C4-C3	-3.07	103.68	110.36
3	A	605	NAG	C1-O5-C5	-3.03	107.99	112.17
2	A	603	MAN	C3-C4-C5	-2.37	106.05	110.22
2	A	601	NAG	C2-N2-C7	-2.34	119.53	122.94
2	A	603	MAN	C2-C3-C4	-2.03	107.34	110.88
3	A	604	NAG	O3-C3-C2	-2.02	105.07	109.39
2	A	596	NAG	C1-O5-C5	2.04	114.98	112.17
3	A	604	NAG	O4-C4-C3	2.11	114.95	110.36
3	A	599	NAG	C1-O5-C5	2.13	115.11	112.17
2	A	603	MAN	C1-C2-C3	2.47	112.79	109.65
2	A	603	MAN	O5-C1-C2	2.56	114.81	110.79
3	A	599	NAG	C4-C3-C2	2.64	114.89	111.02
3	A	604	NAG	C1-O5-C5	2.76	115.97	112.17
2	A	596	NAG	O4-C4-C5	2.76	116.23	109.28
2	A	597	NAG	C1-O5-C5	2.92	116.19	112.17
2	A	597	NAG	C4-C3-C2	3.29	115.84	111.02
3	A	600	NAG	C1-O5-C5	3.54	117.04	112.17
3	A	600	NAG	O5-C1-C2	3.56	116.43	111.47
2	A	598	MAN	C1-O5-C5	3.72	117.29	112.17
3	A	604	NAG	C4-C3-C2	5.25	118.72	111.02
2	A	603	MAN	C1-O5-C5	5.57	119.84	112.17
2	A	602	NAG	C1-O5-C5	5.69	120.00	112.17

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	598	MAN	C1-C2-C3-C4-C5-O5

3 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	598	MAN	1	0
2	A	602	NAG	1	0

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

5.6 Ligand geometry ⓘ

Of 14 ligands modelled in this entry, 11 are monoatomic - leaving 3 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	$\#|Z| > 2$
5	SCN	A	607	-	1,2,2	0.20	0	0,1,1	0.00	-
7	HEM	A	618	1,9	28,50,50	2.24	6 (21%)	17,82,82	1.41	3 (17%)
8	CAQ	A	619	-	8,8,8	2.23	1 (12%)	10,10,10	2.21	4 (40%)

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
5	SCN	A	607	-	-	0/0/0/0	0/0/0/0
7	HEM	A	618	1,9	-	0/6/54/54	0/0/8/8
8	CAQ	A	619	-	-	0/0/0/0	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	618	HEM	C3B-C2B	-6.31	1.32	1.40
7	A	618	HEM	C3C-C2C	-3.41	1.35	1.40
7	A	618	HEM	CAA-C2A	2.69	1.56	1.52
7	A	618	HEM	C3B-CAB	3.18	1.54	1.47
7	A	618	HEM	C3C-CAC	3.92	1.55	1.47
7	A	618	HEM	C3D-C2D	4.99	1.52	1.37
8	A	619	CAQ	C4-C3	6.08	1.50	1.40

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	619	CAQ	C5-C4-C3	-4.28	114.87	119.66
7	A	618	HEM	C1D-C2D-C3D	-2.52	105.24	107.00
8	A	619	CAQ	C6-C1-C2	-2.24	117.13	120.21
7	A	618	HEM	CMA-C3A-C4A	-2.07	125.28	128.46
8	A	619	CAQ	O3-C3-C4	2.11	124.00	118.51
7	A	618	HEM	C4A-C3A-C2A	2.70	108.88	107.00
8	A	619	CAQ	C1-C6-C5	3.35	124.81	120.21

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	618	HEM	7	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	594/595 (99%)	-0.31	31 (5%)	28	26	12, 27, 69, 106	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	TRP	10.3
1	A	174	SER	8.3
1	A	120	GLY	7.4
1	A	121	SER	7.0
1	A	1	SER	6.2
1	A	8	ALA	5.8
1	A	595	ASN	5.4
1	A	170	PRO	5.1
1	A	173	GLN	4.9
1	A	171	PRO	4.9
1	A	122	ASN	4.7
1	A	172	TYR	4.5
1	A	124	HIS	4.1
1	A	9	PRO	4.1
1	A	593	ARG	3.8
1	A	4	VAL	3.7
1	A	119	LEU	3.6
1	A	7	GLY	3.5
1	A	123	GLU	3.5
1	A	3	GLU	3.4
1	A	126	LYS	3.4
1	A	594	GLU	3.2
1	A	175	LEU	3.2
1	A	574	HIS	3.1
1	A	13	VAL	2.5
1	A	125	SER	2.4
1	A	132	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	5	GLY	2.4
1	A	146	LYS	2.2
1	A	286	HIS	2.1
1	A	118[A]	GLU	2.0

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. 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($Å^2$)	Q<0.9
1	SEP	A	198	10/11	0.92	0.17	-	20,27,28,30	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($Å^2$)	Q<0.9
2	NAG	A	596	14/15	0.86	0.27	2.43	47,53,61,68	0
3	NAG	A	599	14/15	0.95	0.19	1.55	42,44,47,49	0
2	NAG	A	601	14/15	0.97	0.14	-0.31	44,47,54,59	0
3	NAG	A	604	14/15	0.83	0.27	-	51,60,63,67	0
2	MAN	A	598	11/12	0.47	0.50	-	91,92,93,94	0
2	MAN	A	603	11/12	0.75	0.36	-	86,89,91,92	0
3	NAG	A	600	14/15	0.80	0.32	-	53,58,61,61	0
3	NAG	A	605	14/15	0.78	0.50	-	70,73,75,77	0
2	NAG	A	602	14/15	0.83	0.29	-	67,73,76,82	0
2	NAG	A	597	14/15	0.85	0.45	-	76,82,84,87	0

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	SCN	A	607	3/3	0.97	0.19	3.71	18,18,18,20	0
7	HEM	A	618	43/43	0.97	0.11	-0.36	8,16,18,25	0
6	IOD	A	611	1/1	0.98	0.07	-1.19	86,86,86,86	0
4	CA	A	606	1/1	0.98	0.08	-1.81	17,17,17,17	0
6	IOD	A	610	1/1	1.00	0.07	-1.95	21,21,21,21	0
6	IOD	A	613	1/1	0.98	0.04	-2.65	59,59,59,59	0
6	IOD	A	614	1/1	0.98	0.04	-3.59	77,77,77,77	0
6	IOD	A	615	1/1	0.99	0.03	-4.54	58,58,58,58	0
6	IOD	A	616	1/1	0.99	0.05	-	54,54,54,54	0
6	IOD	A	609	1/1	0.81	0.18	-	98,98,98,98	0
6	IOD	A	608	1/1	0.99	0.07	-	65,65,65,65	0
6	IOD	A	612	1/1	0.96	0.07	-	99,99,99,99	0
8	CAQ	A	619	8/8	0.83	0.41	-	36,37,39,41	0
6	IOD	A	617	1/1	0.96	0.16	-	99,99,99,99	0

6.5 Other polymers ⓘ

There are no such residues in this entry.