



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 06:06 pm GMT

PDB ID : 3GCK  
Title : Mode of ligand binding and assignment of subsites in mammalian peroxidases: crystal structure of lactoperoxidase complexes with acetyl salicylic acid, salicylhydroxamic acid and benzylhydroxamic acid  
Authors : Singh, A.K.; Singh, N.; Sinha, M.; Bhushan, A.; Kaur, P.; Srinivasan, A.; Sharma, S.; Singh, T.P.  
Deposited on : 2009-02-22  
Resolution : 2.90 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](mailto: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.

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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

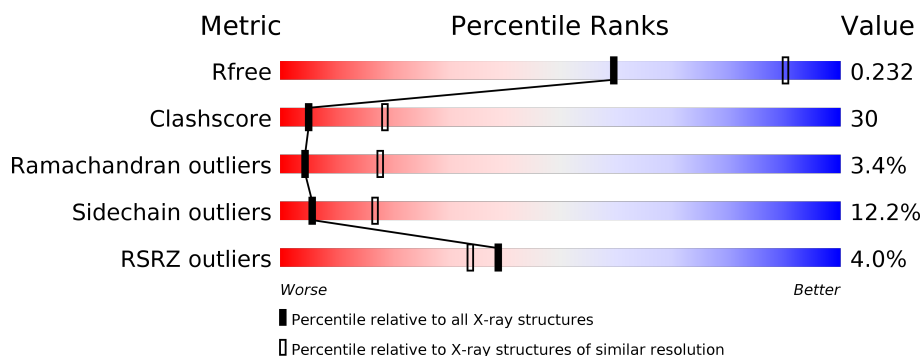
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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))
$R_{free}$	100719	1586 (2.90-2.90)
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RSRZ outliers	101464	1596 (2.90-2.90)

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  $\geq 3$ , 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>4%</div> <div>54%</div> <div>35%</div> <div>10%</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
7	IOD	A	615	-	-	X	-
8	SCN	A	616	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	BHO	A	800	-	X	X	X

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 5129 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
			4774	3037	847	863	1	26			

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



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

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

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

- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

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

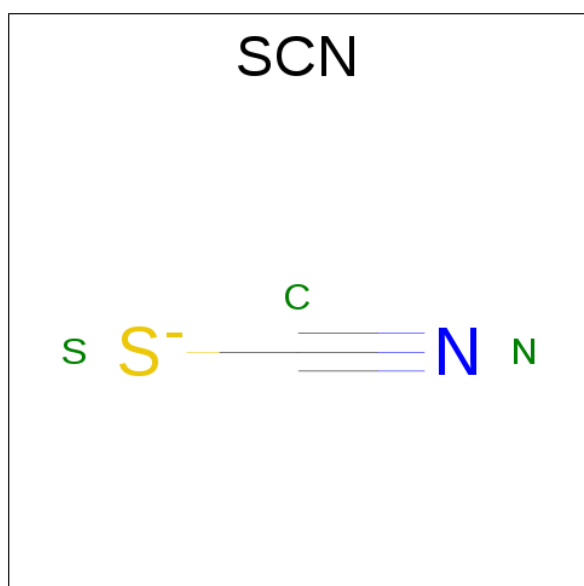
- Molecule 6 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 7 is IODIDE ION (three-letter code: IOD) (formula: I).

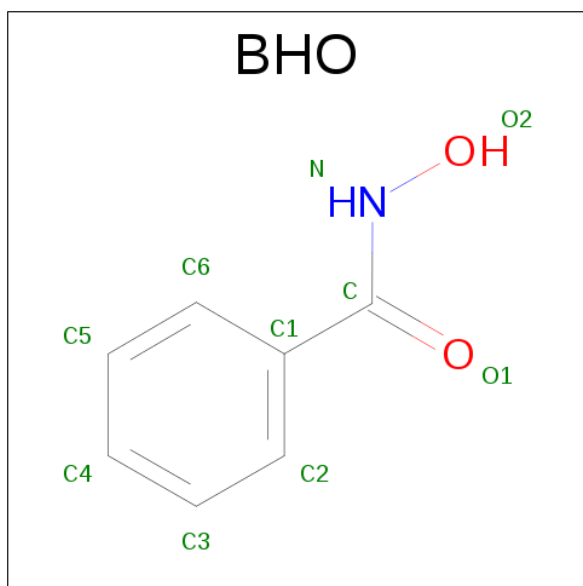
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	8	Total I 8 8	0	0

- Molecule 8 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	S	0	0
			3	1	1	1		

- Molecule 9 is BENZHYDROXAMIC ACID (three-letter code: BHO) (formula:  $C_7H_7NO_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	N	O	0	0
			10	7	1	2		

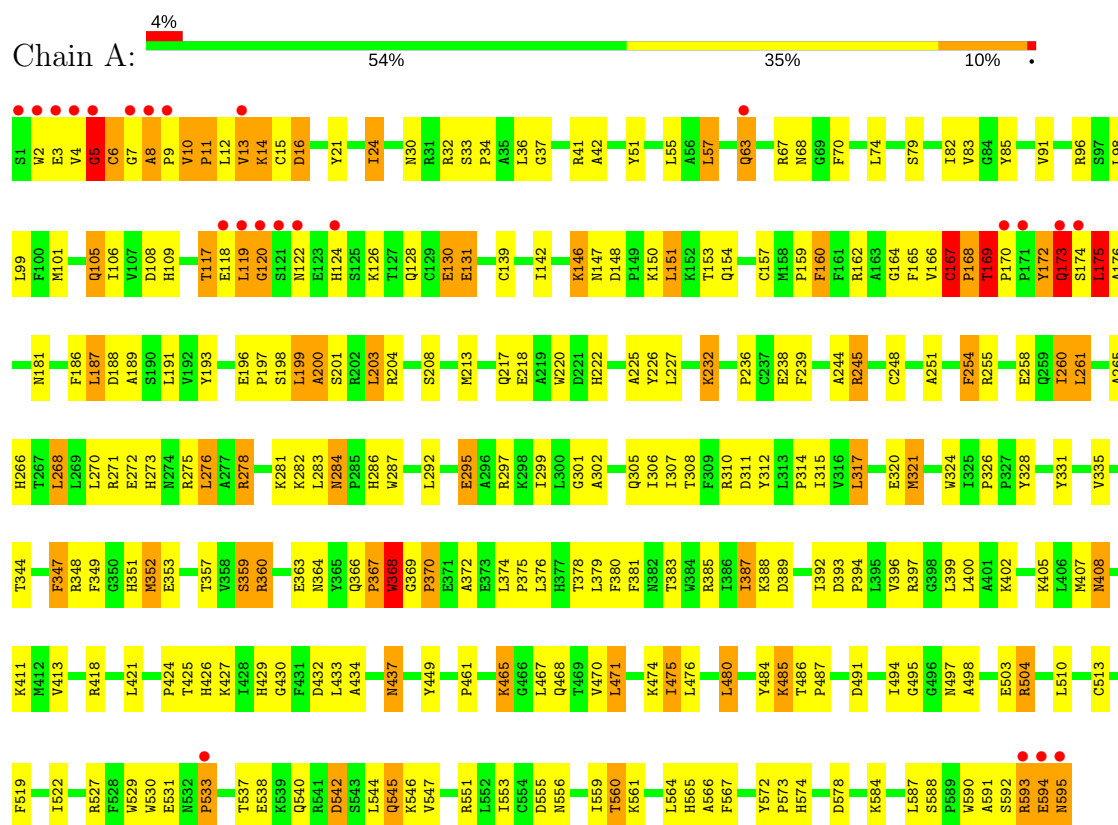
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	156	Total	O	0	0
			156	156		

### 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 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, $\alpha$ , $\beta$ , $\gamma$	54.52Å 80.11Å 68.57Å 90.00° 93.99° 90.00°	Depositor
Resolution (Å)	19.95 – 2.90 19.95 – 2.90	Depositor EDS
% Data completeness (in resolution range)	91.3 (19.95-2.90) 91.4 (19.95-2.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.67 (at 2.88Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, $R_{free}$	0.199 , 0.224 0.183 , 0.232	Depositor DCC
$R_{free}$ test set	599 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	42.1	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 56.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5129	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.44% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SCN, NAG, BHO, SEP, CA, NDG, 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	0.45	0/4891	0.84	10/6634 (0.2%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	167	CYS	CA-CB-SG	7.01	126.62	114.00
1	A	119	LEU	CA-CB-CG	6.92	131.23	115.30
1	A	173	GLN	N-CA-C	6.60	128.83	111.00
1	A	14	LYS	N-CA-C	6.16	127.63	111.00
1	A	593	ARG	N-CA-C	-5.99	94.84	111.00
1	A	5	GLY	N-CA-C	5.61	127.13	113.10
1	A	429	HIS	N-CA-C	-5.55	96.02	111.00
1	A	175	LEU	CA-CB-CG	5.42	127.76	115.30
1	A	181	ASN	N-CA-C	-5.27	96.78	111.00
1	A	169	THR	C-N-CD	-5.02	109.56	120.60

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	4774	0	4688	286	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	43	0	30	13	0
3	A	1	0	0	0	0
4	A	78	0	68	3	0
5	A	28	0	25	1	0
6	A	28	0	25	3	0
7	A	8	0	0	4	0
8	A	3	0	0	0	0
9	A	10	0	7	7	0
10	A	156	0	0	24	0
All	All	5129	0	4843	291	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 30.

All (291) 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:167:CYS:HB3	1:A:168:PRO:HD3	1.28	1.11
1:A:167:CYS:SG	1:A:172:TYR:HE2	1.76	1.07
1:A:357:THR:HG22	1:A:375:PRO:HA	1.35	1.07
1:A:63:GLN:HE21	1:A:63:GLN:HA	1.13	1.06
1:A:167:CYS:HB3	1:A:168:PRO:CD	1.87	1.03
1:A:542:ASP:HA	1:A:545:GLN:HE21	1.22	1.02
1:A:108:ASP:HB2	1:A:347:PHE:CD2	1.94	1.01
1:A:167:CYS:SG	1:A:172:TYR:CE2	2.58	0.96
1:A:175:LEU:HD12	1:A:176:ALA:N	1.85	0.92
1:A:172:TYR:HD1	1:A:173:GLN:H	1.17	0.91
1:A:196:GLU:HB3	1:A:198:SEP:O2P	1.72	0.89
1:A:261:LEU:HG	1:A:399:LEU:HD21	1.55	0.88
1:A:169:THR:H	1:A:170:PRO:CD	1.85	0.86
1:A:63:GLN:NE2	1:A:63:GLN:HA	1.93	0.83
1:A:225:ALA:HB3	1:A:271:ARG:HG2	1.60	0.83
1:A:381:PHE:CZ	1:A:424:PRO:HG3	2.14	0.83
1:A:172:TYR:HD1	1:A:173:GLN:N	1.77	0.82
1:A:63:GLN:HE21	1:A:63:GLN:CA	1.92	0.81
1:A:175:LEU:HD12	1:A:176:ALA:H	1.47	0.79
1:A:166:VAL:O	1:A:167:CYS:HB2	1.82	0.78
1:A:169:THR:H	1:A:170:PRO:HD2	1.49	0.78
1:A:14:LYS:HG2	1:A:15:CYS:H	1.50	0.76
1:A:381:PHE:HZ	9:A:800:BHO:H3	1.49	0.76
1:A:278:ARG:HA	10:A:757:HOH:O	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:THR:HB	1:A:426:HIS:HD2	1.49	0.76
1:A:387:ILE:HG22	1:A:388:LYS:HG3	1.67	0.75
1:A:169:THR:N	1:A:170:PRO:CD	2.48	0.74
1:A:168:PRO:HB3	1:A:170:PRO:HD2	1.69	0.74
1:A:168:PRO:CB	1:A:170:PRO:HD2	2.17	0.74
1:A:284:ASN:N	1:A:284:ASN:HD22	1.85	0.74
1:A:564:LEU:HB3	1:A:565:HIS:HD2	1.53	0.74
1:A:139:CYS:HB2	10:A:629:HOH:O	1.87	0.74
1:A:542:ASP:HB2	10:A:754:HOH:O	1.88	0.74
1:A:302:ALA:O	1:A:306:ILE:HG13	1.89	0.73
1:A:287:TRP:HB3	1:A:292:LEU:HD13	1.70	0.73
1:A:381:PHE:CZ	9:A:800:BHO:H3	2.24	0.73
1:A:169:THR:CG2	1:A:170:PRO:HD3	2.20	0.72
1:A:227:LEU:HD11	1:A:266:HIS:HB3	1.69	0.72
1:A:105:GLN:HG3	2:A:605:HEM:C1C	2.25	0.72
1:A:593:ARG:O	1:A:594:GLU:HB2	1.88	0.71
1:A:282:LYS:HG2	1:A:283:LEU:HD23	1.73	0.71
1:A:314:PRO:HD3	1:A:321:MET:HE1	1.74	0.70
1:A:3:GLU:HG3	1:A:175:LEU:HD22	1.73	0.70
1:A:10:VAL:HG11	1:A:41:ARG:CZ	2.21	0.70
1:A:258:GLU:HB2	9:A:800:BHO:H2	1.73	0.69
1:A:542:ASP:HA	1:A:545:GLN:NE2	2.03	0.69
1:A:8:ALA:H	1:A:9:PRO:CD	2.04	0.69
1:A:150:LYS:HD3	1:A:154:GLN:NE2	2.07	0.69
1:A:108:ASP:HB2	1:A:347:PHE:HD2	1.55	0.68
1:A:260:ILE:HG21	1:A:379:LEU:HD13	1.73	0.68
1:A:258:GLU:O	1:A:380:PHE:HA	1.92	0.68
1:A:425:THR:HB	1:A:426:HIS:CD2	2.28	0.68
1:A:10:VAL:HG11	1:A:41:ARG:NH2	2.08	0.68
1:A:564:LEU:HB3	1:A:565:HIS:CD2	2.28	0.67
1:A:203:LEU:HB3	1:A:213:MET:HE1	1.75	0.67
1:A:120:GLY:HA2	10:A:698:HOH:O	1.94	0.67
1:A:213:MET:HG2	1:A:273:HIS:CD2	2.30	0.67
1:A:387:ILE:CG2	1:A:388:LYS:HG3	2.25	0.67
1:A:167:CYS:CB	1:A:168:PRO:CD	2.68	0.66
1:A:200:ALA:O	1:A:204:ARG:HG3	1.97	0.65
1:A:122:ASN:HB3	10:A:745:HOH:O	1.98	0.64
1:A:544:LEU:O	1:A:547:VAL:HG22	1.98	0.64
1:A:574:HIS:HB2	10:A:638:HOH:O	1.96	0.64
1:A:261:LEU:HG	1:A:399:LEU:CD2	2.27	0.64
1:A:203:LEU:HB3	1:A:213:MET:CE	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:565:HIS:HB3	7:A:615:IOD:I	2.67	0.64
1:A:146:LYS:O	1:A:147:ASN:HB2	1.96	0.64
1:A:588:SER:C	1:A:590:TRP:H	2.01	0.64
1:A:254:PHE:HD1	1:A:254:PHE:N	1.95	0.63
1:A:105:GLN:HG3	2:A:605:HEM:CHC	2.29	0.63
1:A:258:GLU:OE1	2:A:605:HEM:C2B	2.50	0.63
1:A:349:PHE:CB	1:A:497:ASN:HD21	2.11	0.62
1:A:284:ASN:HD21	1:A:591:ALA:HA	1.64	0.62
1:A:295:GLU:O	1:A:299:ILE:HG13	2.00	0.62
1:A:63:GLN:NE2	1:A:63:GLN:CA	2.55	0.62
1:A:254:PHE:CD1	1:A:254:PHE:N	2.67	0.62
1:A:160:PHE:C	1:A:160:PHE:CD2	2.73	0.61
1:A:193:TYR:OH	1:A:297:ARG:HA	2.00	0.61
1:A:150:LYS:HD3	1:A:154:GLN:HE22	1.64	0.61
1:A:108:ASP:CB	1:A:347:PHE:CD2	2.79	0.61
1:A:551:ARG:HD3	1:A:584:LYS:HG2	1.80	0.61
4:A:598:MAN:H2	10:A:708:HOH:O	2.01	0.61
1:A:530:TRP:CE2	1:A:531:GLU:HG3	2.38	0.59
1:A:503:GLU:HB2	10:A:695:HOH:O	2.02	0.59
1:A:468:GLN:OE1	1:A:474:LYS:HG3	2.03	0.59
1:A:287:TRP:HB3	1:A:292:LEU:CD1	2.33	0.59
1:A:8:ALA:H	1:A:9:PRO:HD3	1.67	0.59
1:A:283:LEU:C	1:A:284:ASN:HD22	2.06	0.58
1:A:310:ARG:NH2	1:A:547:VAL:O	2.33	0.58
1:A:37:GLY:HA3	1:A:186:PHE:CZ	2.38	0.58
1:A:281:LYS:HG3	10:A:685:HOH:O	2.03	0.58
1:A:351:HIS:CE1	1:A:433:LEU:HD21	2.39	0.58
1:A:148:ASP:O	1:A:151:LEU:HB2	2.03	0.57
1:A:387:ILE:HG22	1:A:388:LYS:N	2.19	0.57
1:A:385:ARG:O	1:A:389:ASP:HB3	2.03	0.57
1:A:587:LEU:O	1:A:590:TRP:HB2	2.04	0.57
1:A:2:TRP:CG	1:A:3:GLU:N	2.73	0.57
1:A:108:ASP:OD1	2:A:605:HEM:C2D	2.57	0.57
1:A:588:SER:C	1:A:590:TRP:N	2.58	0.57
1:A:197:PRO:O	1:A:198:SEP:C	2.48	0.57
1:A:402:LYS:HD2	10:A:748:HOH:O	2.04	0.57
1:A:349:PHE:HB2	1:A:497:ASN:HD21	1.68	0.56
1:A:8:ALA:N	1:A:9:PRO:CD	2.68	0.56
1:A:106:ILE:HG23	1:A:191:LEU:HD11	1.87	0.56
1:A:475:ILE:HB	10:A:756:HOH:O	2.05	0.56
1:A:546:LYS:HA	10:A:760:HOH:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:LEU:HG	1:A:203:LEU:CD2	2.36	0.56
1:A:360:ARG:NH1	1:A:372:ALA:HA	2.21	0.56
1:A:124:HIS:O	1:A:128:GLN:HB2	2.05	0.55
1:A:106:ILE:HD11	1:A:265:ALA:CB	2.35	0.55
1:A:276:LEU:HD12	1:A:587:LEU:HD21	1.88	0.55
1:A:150:LYS:NZ	1:A:154:GLN:HE22	2.05	0.55
1:A:531:GLU:O	1:A:533:PRO:HD3	2.06	0.55
1:A:159:PRO:HG3	1:A:426:HIS:CE1	2.42	0.55
1:A:328:TYR:HE2	1:A:531:GLU:O	1.91	0.55
1:A:170:PRO:HA	10:A:650:HOH:O	2.07	0.54
1:A:108:ASP:CB	1:A:347:PHE:HD2	2.19	0.54
1:A:426:HIS:CD2	1:A:426:HIS:N	2.74	0.54
1:A:172:TYR:CD1	1:A:173:GLN:N	2.67	0.54
1:A:519:PHE:HA	1:A:522:ILE:HG12	1.88	0.54
1:A:169:THR:HG22	1:A:170:PRO:HD3	1.90	0.54
1:A:16:ASP:OD1	1:A:16:ASP:C	2.46	0.54
1:A:567:PHE:HB2	7:A:615:IOD:I	2.78	0.54
1:A:301:GLY:O	1:A:305:GLN:HG3	2.08	0.53
1:A:168:PRO:HB2	1:A:170:PRO:HD2	1.89	0.53
1:A:314:PRO:HB3	1:A:321:MET:CE	2.38	0.53
1:A:8:ALA:HB3	1:A:167:CYS:O	2.08	0.53
1:A:564:LEU:C	1:A:565:HIS:HD2	2.11	0.53
1:A:504:ARG:NH2	7:A:610:IOD:I	3.12	0.53
1:A:217:GLN:NE2	5:A:599:NDG:O7	2.41	0.53
1:A:131:GLU:HG3	10:A:682:HOH:O	2.07	0.53
1:A:284:ASN:N	1:A:284:ASN:ND2	2.53	0.53
1:A:465:LYS:HA	1:A:468:GLN:HE21	1.74	0.53
1:A:239:PHE:CZ	1:A:427:LYS:HB2	2.43	0.53
1:A:393:ASP:N	1:A:394:PRO:HD2	2.24	0.53
1:A:407:MET:HG3	10:A:655:HOH:O	2.09	0.52
1:A:565:HIS:N	1:A:565:HIS:CD2	2.77	0.52
1:A:540:GLN:HG2	1:A:590:TRP:CE3	2.44	0.52
1:A:165:PHE:HZ	1:A:170:PRO:O	1.93	0.52
1:A:348:ARG:CZ	2:A:605:HEM:HAD2	2.40	0.52
1:A:408:ASN:C	1:A:408:ASN:OD1	2.48	0.52
1:A:588:SER:O	1:A:590:TRP:N	2.42	0.52
1:A:559:ILE:HA	7:A:613:IOD:I	2.80	0.52
1:A:74:LEU:HG	10:A:641:HOH:O	2.09	0.52
1:A:12:LEU:HD22	10:A:700:HOH:O	2.09	0.52
1:A:227:LEU:HD23	1:A:270:LEU:HD22	1.91	0.52
1:A:560:THR:O	1:A:578:ASP:HA	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ASP:CG	2:A:605:HEM:CHD	2.79	0.51
1:A:188:ASP:O	1:A:189:ALA:HB3	2.09	0.51
1:A:324:TRP:C	1:A:326:PRO:HD3	2.31	0.51
1:A:284:ASN:OD1	1:A:592:SER:HB3	2.10	0.51
1:A:314:PRO:HB3	1:A:321:MET:HE2	1.93	0.51
1:A:232:LYS:HG2	10:A:677:HOH:O	2.09	0.50
1:A:357:THR:HG22	1:A:375:PRO:CA	2.25	0.50
1:A:271:ARG:NH1	1:A:392:ILE:HD11	2.27	0.50
1:A:426:HIS:CE1	10:A:648:HOH:O	2.65	0.50
2:A:605:HEM:HMB1	2:A:605:HEM:HBB2	1.93	0.50
1:A:191:LEU:H	1:A:191:LEU:HD23	1.76	0.50
1:A:260:ILE:CD1	1:A:385:ARG:HB2	2.42	0.50
1:A:51:TYR:HB3	1:A:57:LEU:O	2.12	0.50
1:A:260:ILE:CG2	1:A:379:LEU:HD13	2.41	0.50
1:A:220:TRP:HD1	10:A:739:HOH:O	1.95	0.49
1:A:360:ARG:O	1:A:368:TRP:HB2	2.11	0.49
1:A:484:TYR:C	1:A:486:THR:H	2.16	0.49
1:A:106:ILE:HD11	1:A:265:ALA:HB1	1.95	0.49
1:A:593:ARG:O	1:A:594:GLU:CB	2.59	0.49
1:A:407:MET:SD	1:A:408:ASN:N	2.86	0.49
1:A:348:ARG:HH11	1:A:437:ASN:ND2	2.10	0.49
1:A:595:ASN:C	1:A:595:ASN:HD22	2.16	0.49
6:A:604:NAG:O3	6:A:607:NAG:C1	2.60	0.49
1:A:258:GLU:OE2	2:A:605:HEM:HHB	2.14	0.48
1:A:282:LYS:HB2	1:A:282:LYS:NZ	2.29	0.48
1:A:357:THR:HB	1:A:374:LEU:O	2.14	0.48
1:A:544:LEU:C	1:A:546:LYS:H	2.16	0.48
1:A:130:GLU:HA	1:A:159:PRO:HB3	1.95	0.48
1:A:352:MET:CB	1:A:407:MET:HG2	2.44	0.48
1:A:387:ILE:HG22	1:A:388:LYS:CG	2.39	0.48
1:A:564:LEU:CB	1:A:565:HIS:HD2	2.25	0.48
1:A:67:ARG:O	1:A:68:ASN:HB2	2.13	0.47
1:A:394:PRO:HA	1:A:397:ARG:NH1	2.29	0.47
1:A:117:THR:HG23	1:A:164:GLY:HA2	1.96	0.47
1:A:175:LEU:HD13	10:A:725:HOH:O	2.13	0.47
1:A:353:GLU:HA	1:A:405:LYS:O	2.13	0.47
1:A:83:VAL:HG12	1:A:413:VAL:HB	1.97	0.47
1:A:244:ALA:HB2	4:A:601:NAG:O6	2.15	0.47
1:A:169:THR:N	1:A:170:PRO:HD3	2.29	0.47
1:A:360:ARG:NH1	1:A:372:ALA:C	2.67	0.47
1:A:564:LEU:C	1:A:565:HIS:CD2	2.88	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:VAL:CG1	1:A:14:LYS:N	2.78	0.47
1:A:461:PRO:HG3	1:A:470:VAL:HG21	1.96	0.47
1:A:10:VAL:HG11	1:A:41:ARG:NE	2.28	0.47
1:A:476:LEU:HD21	1:A:498:ALA:HB1	1.97	0.47
1:A:108:ASP:HB2	1:A:347:PHE:CE2	2.46	0.46
1:A:238:GLU:HB3	1:A:245:ARG:HA	1.96	0.46
1:A:248:CYS:HA	1:A:383:THR:HG21	1.97	0.46
1:A:310:ARG:NE	1:A:311:ASP:OD1	2.43	0.46
1:A:3:GLU:C	1:A:5:GLY:H	2.17	0.46
1:A:400:LEU:HD11	1:A:553:ILE:CD1	2.46	0.46
1:A:314:PRO:CD	1:A:321:MET:HE1	2.41	0.46
1:A:276:LEU:CD1	1:A:587:LEU:HD21	2.46	0.46
1:A:381:PHE:HZ	9:A:800:BHO:C3	2.23	0.46
1:A:424:PRO:CD	9:A:800:BHO:H4	2.46	0.46
1:A:236:PRO:HB3	10:A:640:HOH:O	2.14	0.45
1:A:21:TYR:OH	1:A:295:GLU:OE1	2.33	0.45
1:A:2:TRP:O	1:A:4:VAL:N	2.42	0.45
1:A:159:PRO:CG	1:A:426:HIS:CE1	2.99	0.45
1:A:367:PRO:O	1:A:369:GLY:N	2.46	0.45
1:A:432:ASP:C	1:A:432:ASP:OD1	2.55	0.45
1:A:475:ILE:HD11	10:A:689:HOH:O	2.16	0.45
1:A:108:ASP:CG	2:A:605:HEM:HHD	2.37	0.45
1:A:480:LEU:HD12	1:A:480:LEU:HA	1.79	0.45
1:A:530:TRP:CZ2	1:A:531:GLU:HG3	2.52	0.45
1:A:335:VAL:CG2	6:A:604:NAG:H61	2.47	0.45
1:A:108:ASP:OD1	2:A:605:HEM:C1D	2.70	0.44
1:A:108:ASP:OD2	1:A:347:PHE:HB3	2.17	0.44
1:A:142:ILE:O	1:A:157:CYS:HB2	2.17	0.44
1:A:331:TYR:HA	10:A:628:HOH:O	2.17	0.44
1:A:258:GLU:OE1	2:A:605:HEM:C1B	2.71	0.44
1:A:299:ILE:O	1:A:302:ALA:N	2.50	0.44
1:A:465:LYS:HA	1:A:468:GLN:NE2	2.32	0.44
1:A:10:VAL:HA	1:A:11:PRO:HD3	1.78	0.44
1:A:494:ILE:HA	1:A:494:ILE:HD12	1.81	0.44
1:A:119:LEU:HD23	1:A:169:THR:HG23	2.00	0.44
1:A:169:THR:HG23	1:A:170:PRO:HD3	1.95	0.44
1:A:392:ILE:O	1:A:396:VAL:HG23	2.16	0.44
1:A:118:GLU:HG2	1:A:118:GLU:O	2.17	0.44
1:A:79:SER:OG	1:A:418:ARG:HD2	2.18	0.44
1:A:364:ASN:O	1:A:366:GLN:HG2	2.17	0.43
1:A:146:LYS:O	1:A:147:ASN:CB	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:ILE:HA	1:A:24:ILE:HD13	1.69	0.43
1:A:378:THR:C	1:A:379:LEU:HD23	2.39	0.43
1:A:328:TYR:CZ	1:A:529:TRP:HD1	2.36	0.43
1:A:32:ARG:HE	1:A:32:ARG:HB3	1.62	0.43
1:A:491:ASP:O	1:A:494:ILE:HG22	2.19	0.43
1:A:424:PRO:CG	9:A:800:BHO:H4	2.49	0.43
1:A:118:GLU:CG	1:A:118:GLU:O	2.67	0.43
1:A:286:HIS:NE2	1:A:595:ASN:HB3	2.33	0.43
1:A:510:LEU:O	1:A:513:CYS:HB3	2.18	0.43
1:A:10:VAL:CG1	1:A:41:ARG:NE	2.82	0.43
1:A:268:LEU:HA	1:A:268:LEU:HD12	1.54	0.43
1:A:331:TYR:CD1	1:A:527:ARG:HA	2.54	0.43
1:A:424:PRO:HG2	9:A:800:BHO:H4	2.00	0.43
1:A:449:TYR:CD1	1:A:495:GLY:HA3	2.54	0.43
1:A:109:HIS:CD2	1:A:255:ARG:CZ	3.02	0.43
1:A:227:LEU:HD13	1:A:251:ALA:HB2	1.99	0.43
1:A:187:LEU:HA	1:A:187:LEU:HD23	1.83	0.42
1:A:199:LEU:C	1:A:201:SER:N	2.72	0.42
1:A:387:ILE:CG2	1:A:388:LYS:N	2.81	0.42
1:A:484:TYR:O	1:A:486:THR:N	2.52	0.42
1:A:366:GLN:O	1:A:367:PRO:C	2.58	0.42
1:A:42:ALA:HB2	1:A:166:VAL:HG21	2.01	0.42
1:A:425:THR:CB	1:A:426:HIS:HD2	2.26	0.42
1:A:272:GLU:HB2	1:A:556:ASN:HD21	1.85	0.42
1:A:359:SER:CB	1:A:402:LYS:HE3	2.49	0.42
1:A:432:ASP:OD1	1:A:434:ALA:N	2.52	0.42
1:A:572:TYR:HA	1:A:573:PRO:HA	1.80	0.42
1:A:275:ARG:CD	1:A:555:ASP:HB3	2.50	0.42
1:A:283:LEU:C	1:A:284:ASN:ND2	2.72	0.42
1:A:82:ILE:HD13	1:A:480:LEU:CD1	2.50	0.42
1:A:70:PHE:CD1	1:A:485:LYS:HB3	2.55	0.42
1:A:349:PHE:CD1	1:A:349:PHE:C	2.92	0.42
1:A:467:LEU:HG	1:A:471:LEU:HD22	2.02	0.42
4:A:597:NAG:H3	4:A:597:NAG:O7	2.19	0.42
1:A:99:LEU:HD23	1:A:566:ALA:HB1	2.02	0.42
1:A:286:HIS:HD1	1:A:286:HIS:H	1.68	0.41
1:A:348:ARG:HG2	2:A:605:HEM:HMD3	2.01	0.41
1:A:305:GLN:HB3	1:A:529:TRP:CZ3	2.55	0.41
1:A:96:ARG:NH2	1:A:315:ILE:HB	2.35	0.41
1:A:324:TRP:O	1:A:326:PRO:HD3	2.21	0.41
1:A:30:ASN:HB3	1:A:33:SER:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:PRO:HB2	1:A:12:LEU:H	1.71	0.41
1:A:317:LEU:O	1:A:320:GLU:HB2	2.21	0.41
6:A:607:NAG:H5	6:A:607:NAG:N2	2.35	0.41
1:A:537:THR:N	1:A:540:GLN:OE1	2.41	0.41
1:A:7:GLY:C	1:A:10:VAL:HG23	2.41	0.41
1:A:360:ARG:C	1:A:368:TRP:HB2	2.41	0.41
1:A:85:TYR:CD1	1:A:411:LYS:HG2	2.54	0.41
1:A:380:PHE:CE2	1:A:421:LEU:HA	2.55	0.41
1:A:308:THR:O	1:A:312:TYR:HB3	2.20	0.41
1:A:360:ARG:NH1	1:A:372:ALA:CA	2.83	0.41
1:A:475:ILE:CG1	1:A:476:LEU:N	2.84	0.41
1:A:588:SER:O	1:A:591:ALA:N	2.54	0.40
1:A:101:MET:SD	1:A:101:MET:C	3.00	0.40
1:A:349:PHE:HB2	1:A:497:ASN:ND2	2.33	0.40
1:A:272:GLU:HB2	1:A:556:ASN:ND2	2.37	0.40
1:A:292:LEU:HD12	1:A:292:LEU:HA	1.85	0.40
1:A:348:ARG:CZ	2:A:605:HEM:CAD	2.99	0.40
1:A:117:THR:OG1	1:A:162:ARG:O	2.38	0.40
1:A:394:PRO:HA	1:A:397:ARG:HH11	1.85	0.40
1:A:486:THR:HA	1:A:487:PRO:HD3	1.96	0.40
1:A:561:LYS:NZ	1:A:578:ASP:OD2	2.54	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%)	513 (87%)	59 (10%)	20 (3%)	<b>4</b> <b>18</b>

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	CYS
1	A	167	CYS
1	A	169	THR
1	A	368	TRP
1	A	5	GLY
1	A	11	PRO
1	A	168	PRO
1	A	200	ALA
1	A	485	LYS
1	A	260	ILE
1	A	533	PRO
1	A	222	HIS
1	A	232	LYS
1	A	120	GLY
1	A	8	ALA
1	A	430	GLY
1	A	594	GLU
1	A	370	PRO
1	A	34	PRO
1	A	367	PRO

### 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	517/517 (100%)	454 (88%)	63 (12%)	<b>6</b> <b>17</b>

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	CYS
1	A	10	VAL
1	A	13	VAL
1	A	16	ASP
1	A	24	ILE
1	A	36	LEU
1	A	55	LEU

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Mol	Chain	Res	Type
1	A	57	LEU
1	A	63	GLN
1	A	91	VAL
1	A	98	LEU
1	A	105	GLN
1	A	117	THR
1	A	126	LYS
1	A	130	GLU
1	A	131	GLU
1	A	146	LYS
1	A	151	LEU
1	A	153	THR
1	A	160	PHE
1	A	172	TYR
1	A	173	GLN
1	A	174	SER
1	A	175	LEU
1	A	187	LEU
1	A	199	LEU
1	A	203	LEU
1	A	208	SER
1	A	218	GLU
1	A	226	TYR
1	A	245	ARG
1	A	254	PHE
1	A	261	LEU
1	A	268	LEU
1	A	276	LEU
1	A	278	ARG
1	A	284	ASN
1	A	295	GLU
1	A	307	ILE
1	A	317	LEU
1	A	321	MET
1	A	344	THR
1	A	347	PHE
1	A	352	MET
1	A	359	SER
1	A	360	ARG
1	A	363	GLU
1	A	368	TRP
1	A	370	PRO

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Mol	Chain	Res	Type
1	A	376	LEU
1	A	387	ILE
1	A	408	ASN
1	A	437	ASN
1	A	465	LYS
1	A	471	LEU
1	A	475	ILE
1	A	480	LEU
1	A	504	ARG
1	A	538	GLU
1	A	542	ASP
1	A	545	GLN
1	A	560	THR
1	A	595	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	GLN
1	A	154	GLN
1	A	426	HIS
1	A	437	ASN
1	A	497	ASN
1	A	545	GLN
1	A	556	ASN
1	A	558	HIS
1	A	565	HIS
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	9,9,10	1.31	1 (11%)	9,12,14	2.35	3 (33%)

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	P-O1P	2.55	1.59	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	SEP	O2P-P-OG	-2.66	99.66	106.73
1	A	198	SEP	P-OG-CB	4.15	129.73	118.30
1	A	198	SEP	OG-CB-CA	4.17	112.28	108.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	198	SEP	2	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	$\# Z  > 2$
4	NAG	A	596	1,4	14,14,15	0.70	0	15,19,21	1.18	2 (13%)
4	NAG	A	597	4	14,14,15	1.12	2 (14%)	15,19,21	1.46	4 (26%)
4	MAN	A	598	4	11,11,12	0.77	0	13,15,17	1.57	3 (23%)
5	NDG	A	599	1,5	14,14,15	0.75	0	15,19,21	0.76	1 (6%)
5	NAG	A	600	5	14,14,15	0.64	0	15,19,21	0.74	0
4	NAG	A	601	1,4	14,14,15	0.61	0	15,19,21	0.88	1 (6%)
4	NAG	A	602	4	14,14,15	0.64	0	15,19,21	1.18	1 (6%)
4	MAN	A	603	4	11,11,12	0.97	0	13,15,17	2.21	3 (23%)
6	NAG	A	604	1,6	14,14,15	0.51	0	15,19,21	0.95	1 (6%)
6	NAG	A	607	6	14,14,15	0.55	0	15,19,21	1.06	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	596	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	597	4	-	0/6/23/26	0/1/1/1
4	MAN	A	598	4	-	0/2/19/22	0/1/1/1
5	NDG	A	599	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	600	5	-	0/6/23/26	0/1/1/1
4	NAG	A	601	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	602	4	-	0/6/23/26	0/1/1/1
4	MAN	A	603	4	-	0/2/19/22	0/1/1/1
6	NAG	A	604	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	607	6	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	597	NAG	C1-C2	2.30	1.55	1.52
4	A	597	NAG	C3-C2	2.66	1.58	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	597	NAG	C1-C2-N2	-2.51	106.19	110.49
4	A	596	NAG	C2-N2-C7	-2.23	119.69	122.94
5	A	599	NDG	C2-N2-C7	-2.21	119.72	122.94
4	A	603	MAN	C3-C4-C5	-2.19	106.36	110.22
4	A	597	NAG	C1-O5-C5	-2.06	109.33	112.17
4	A	598	MAN	C2-C3-C4	2.15	114.63	110.88
4	A	597	NAG	C6-C5-C4	2.16	118.06	113.00
4	A	596	NAG	C1-O5-C5	2.20	115.20	112.17
4	A	601	NAG	C4-C3-C2	2.21	114.26	111.02
6	A	604	NAG	C1-C2-N2	2.62	114.97	110.49
4	A	598	MAN	C3-C4-C5	2.65	114.88	110.22
4	A	602	NAG	C1-O5-C5	2.79	116.02	112.17
4	A	597	NAG	C4-C3-C2	3.47	116.10	111.02
4	A	598	MAN	C1-C2-C3	3.74	114.39	109.65
4	A	603	MAN	O5-C1-C2	3.88	116.87	110.79
4	A	603	MAN	C1-C2-C3	6.22	117.54	109.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	597	NAG	1	0
4	A	598	MAN	1	0
5	A	599	NDG	1	0
4	A	601	NAG	1	0
6	A	604	NAG	2	0
6	A	607	NAG	2	0

## 5.6 Ligand geometry

Of 12 ligands modelled in this entry, 9 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
2	HEM	A	605	1	28,50,50	2.94	14 (50%)	17,82,82	3.64	7 (41%)
8	SCN	A	616	-	1,2,2	5.16	1 (100%)	0,1,1	0.00	-
9	BHO	A	800	-	10,10,10	3.54	6 (60%)	12,12,12	4.71	7 (58%)

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	HEM	A	605	1	-	0/6/54/54	0/0/8/8
8	SCN	A	616	-	-	0/0/0/0	0/0/0/0
9	BHO	A	800	-	-	0/6/6/6	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	605	HEM	C4B-CHC	-2.41	1.33	1.40
2	A	605	HEM	C4D-ND	-2.36	1.34	1.36
2	A	605	HEM	C4A-NA	-2.31	1.31	1.36
2	A	605	HEM	CMA-C3A	-2.22	1.47	1.51
2	A	605	HEM	C1D-ND	2.24	1.40	1.36
2	A	605	HEM	CMB-C2B	2.85	1.57	1.51
9	A	800	BHO	C5-C6	2.86	1.44	1.38
9	A	800	BHO	O1-C	2.91	1.29	1.23
2	A	605	HEM	C3C-C2C	3.09	1.44	1.40
2	A	605	HEM	CAD-C3D	3.56	1.59	1.52
9	A	800	BHO	C4-C3	3.56	1.46	1.38
2	A	605	HEM	C3C-CAC	3.69	1.55	1.47
9	A	800	BHO	C6-C1	3.83	1.45	1.39
2	A	605	HEM	C1C-NC	4.47	1.42	1.36
2	A	605	HEM	CAA-C2A	4.93	1.60	1.52
2	A	605	HEM	CMC-C2C	4.93	1.62	1.51
8	A	616	SCN	C-N	5.16	1.33	1.15
9	A	800	BHO	C3-C2	5.24	1.48	1.38
2	A	605	HEM	C3D-C2D	5.94	1.55	1.37
9	A	800	BHO	O2-N	6.90	1.51	1.39
2	A	605	HEM	C3B-CAB	7.15	1.62	1.47

All (14) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	800	BHO	O1-C-C1	-8.79	105.35	120.94
2	A	605	HEM	CBD-CAD-C3D	-8.16	96.90	112.47
9	A	800	BHO	C3-C2-C1	-4.28	115.31	120.35
9	A	800	BHO	C4-C5-C6	-3.77	115.02	120.21
2	A	605	HEM	C1D-C2D-C3D	-2.99	104.92	107.00
2	A	605	HEM	C4A-C3A-C2A	2.04	108.41	107.00
2	A	605	HEM	C3B-C4B-NB	2.07	111.89	109.21
9	A	800	BHO	C4-C3-C2	3.04	124.38	120.21
9	A	800	BHO	O2-N-C	3.17	127.94	119.67
2	A	605	HEM	CMC-C2C-C3C	4.75	133.71	124.89
9	A	800	BHO	C5-C6-C1	6.42	127.89	120.35
2	A	605	HEM	CAA-CBA-CGA	6.63	123.99	112.66
2	A	605	HEM	CAD-CBD-CGD	8.05	126.41	112.66
9	A	800	BHO	C1-C-N	9.57	132.24	116.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	605	HEM	13	0
9	A	800	BHO	7	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	594/595 (99%)	-0.42	24 (4%) 39 34	8, 30, 73, 100	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	594	GLU	7.9
1	A	595	ASN	6.5
1	A	1	SER	5.7
1	A	2	TRP	5.2
1	A	122	ASN	4.9
1	A	8	ALA	4.8
1	A	4	VAL	4.6
1	A	121	SER	4.3
1	A	119	LEU	4.2
1	A	174	SER	3.9
1	A	170	PRO	3.4
1	A	593	ARG	2.5
1	A	13	VAL	2.4
1	A	7	GLY	2.4
1	A	118	GLU	2.4
1	A	124	HIS	2.3
1	A	3	GLU	2.3
1	A	173	GLN	2.3
1	A	63	GLN	2.2
1	A	120	GLY	2.2
1	A	171	PRO	2.2
1	A	5	GLY	2.1
1	A	9	PRO	2.1
1	A	533	PRO	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	SEP	A	198	10/11	0.97	0.12	-	24,31,36,38	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	NAG	A	596	14/15	0.87	0.24	1.43	62,66,69,74	0
4	NAG	A	601	14/15	0.90	0.21	1.01	59,61,64,70	0
5	NDG	A	599	14/15	0.92	0.17	0.49	52,55,55,56	0
5	NAG	A	600	14/15	0.92	0.26	-	58,59,61,61	0
6	NAG	A	607	14/15	0.83	0.39	-	77,79,82,82	0
4	MAN	A	598	11/12	0.64	0.35	-	85,85,86,87	0
6	NAG	A	604	14/15	0.92	0.27	-	66,70,72,73	0
4	MAN	A	603	11/12	0.63	0.40	-	87,89,90,90	0
4	NAG	A	602	14/15	0.76	0.35	-	75,77,80,84	0
4	NAG	A	597	14/15	0.80	0.43	-	78,81,83,83	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
9	BHO	A	800	10/10	0.84	0.31	5.22	35,36,37,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	HEM	A	605	43/43	0.96	0.15	0.18	7,10,16,22	0
8	SCN	A	616	3/3	0.88	0.16	-0.21	15,15,16,23	0
7	IOD	A	609	1/1	0.98	0.06	-1.73	96,96,96,96	0
3	CA	A	606	1/1	0.98	0.12	-2.00	14,14,14,14	0
7	IOD	A	612	1/1	0.98	0.05	-2.70	87,87,87,87	0
7	IOD	A	608	1/1	1.00	0.06	-2.77	32,32,32,32	0
7	IOD	A	613	1/1	0.99	0.03	-2.78	100,100,100,100	0
7	IOD	A	611	1/1	0.99	0.03	-3.66	65,65,65,65	0
7	IOD	A	610	1/1	0.95	0.09	-	76,76,76,76	1
7	IOD	A	614	1/1	0.98	0.04	-	69,69,69,69	0
7	IOD	A	615	1/1	0.97	0.13	-	64,64,64,64	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.