



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 26, 2014 – 03:04 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 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/ValidationPDFNotes.html>

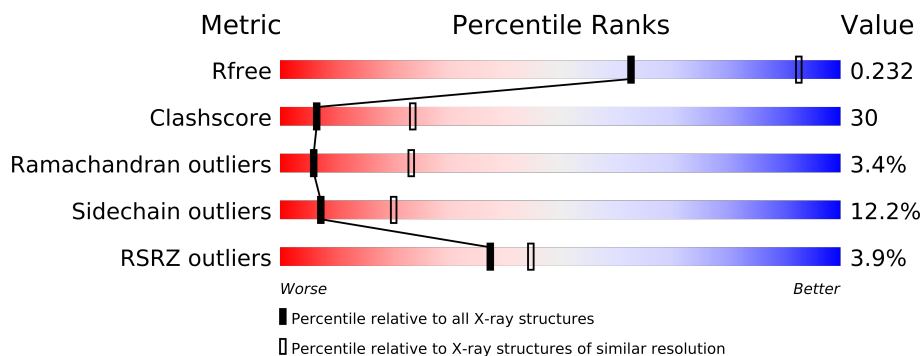
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	1053 (2.90-2.90)
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	595	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
8	SCN	A	616	X	-
9	BHO	A	800	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 hydrogen and 0 are deuterium.

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		

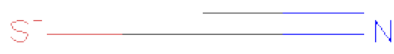
- Molecule 6 is a polymer of unknown type called SUGAR (2-MER).

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).

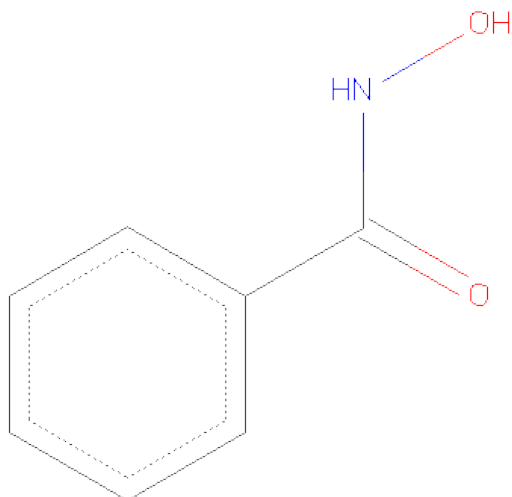
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	8	Total	I	0	0
			8	8		

- 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		

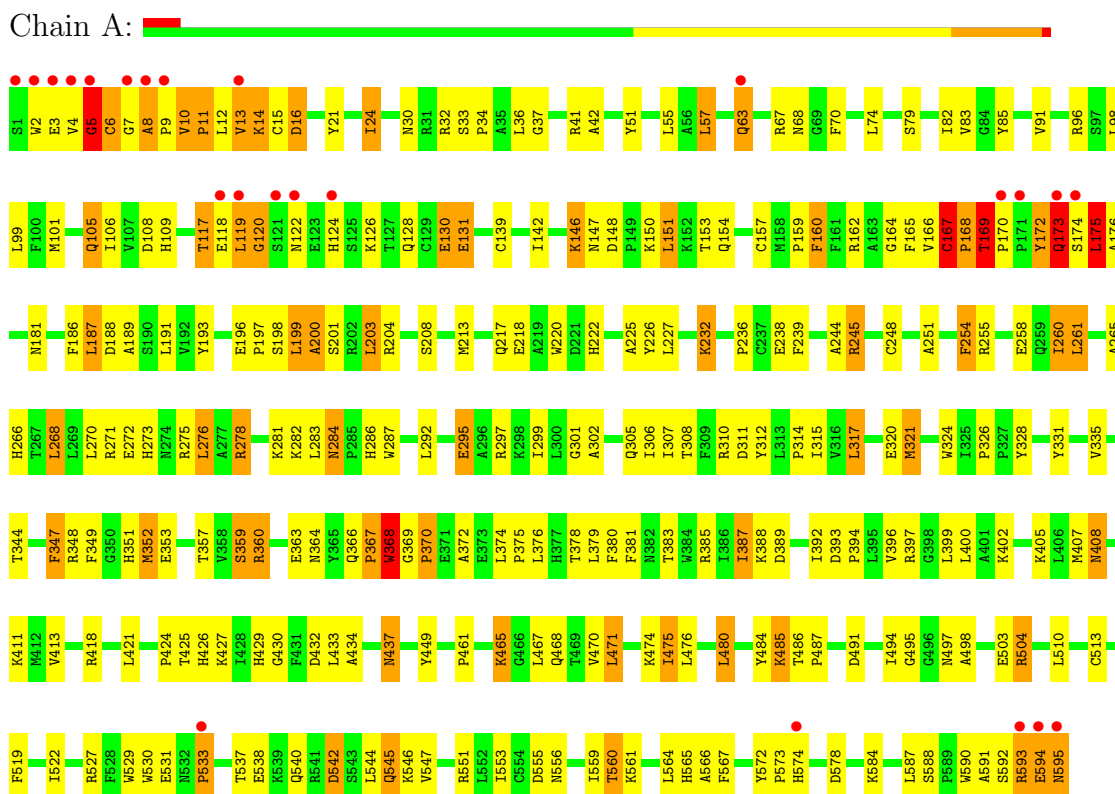
- Molecule 10 is water.

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

3 Residue-property plots

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	54.52Å 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
$\langle I/\sigma(I) \rangle$ ¹	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 (5.25%)	DCC
Wilson B-factor (Å ²)	42.1	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 23.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 11998 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5129	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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, 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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4774	0	4688	286	0
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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 30.

All (291) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:425:THR:HB	1:A:426:HIS:HD2	1.49	0.76
1:A:278:ARG:HA	10:A:757:HOH:O	1.85	0.76
1:A:387:ILE:HG22	1:A:388:LYS:HG3	1.67	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:542:ASP:HA	1:A:545:GLN:NE2	2.03	0.69
1:A:258:GLU:HB2	9:A:800:BHO:H2	1.73	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
1:A:565:HIS:HB3	7:A:615:IOD:I	2.67	0.64
1:A:588:SER:C	1:A:590:TRP:H	2.01	0.64
1:A:146:LYS:O	1:A:147:ASN:HB2	1.96	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:254:PHE:N	1:A:254:PHE:HD1	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:284:ASN:HD21	1:A:591:ALA:HA	1.64	0.62
1:A:349:PHE:CB	1:A:497:ASN:HD21	2.11	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
4:A:598:MAN:H2	10:A:708:HOH:O	2.01	0.61
1:A:551:ARG:HD3	1:A:584:LYS:HG2	1.80	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:387:ILE:HG22	1:A:388:LYS:N	2.19	0.57
1:A:148:ASP:O	1:A:151:LEU:HB2	2.03	0.57
1:A:587:LEU:O	1:A:590:TRP:HB2	2.04	0.57
1:A:385:ARG:O	1:A:389:ASP:HB3	2.03	0.57
1:A:108:ASP:OD1	2:A:605:HEM:C2D	2.57	0.57
1:A:2:TRP:CG	1:A:3:GLU:N	2.73	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:8:ALA:N	1:A:9:PRO:CD	2.68	0.56
1:A:349:PHE:HB2	1:A:497:ASN:HD21	1.68	0.56
1:A:475:ILE:HB	10:A:756:HOH:O	2.05	0.56
1:A:106:ILE:HG23	1:A:191:LEU:HD11	1.87	0.56
1:A:546:LYS:HA	10:A:760:HOH:O	2.05	0.56
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:106:ILE:HD11	1:A:265:ALA:CB	2.35	0.55
1:A:124:HIS:O	1:A:128:GLN:HB2	2.05	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:8:ALA:HB3	1:A:167:CYS:O	2.08	0.53
1:A:314:PRO:HB3	1:A:321:MET:CE	2.38	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:540:GLN:HG2	1:A:590:TRP:CE3	2.44	0.52
1:A:565:HIS:N	1:A:565:HIS:CD2	2.77	0.52
1:A:407:MET:HG3	10:A:655:HOH:O	2.09	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:588:SER:O	1:A:590:TRP:N	2.42	0.52
1:A:408:ASN:C	1:A:408:ASN:OD1	2.48	0.52
1:A:74:LEU:HG	10:A:641:HOH:O	2.09	0.52
1:A:559:ILE:HA	7:A:613:IOD:I	2.80	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:108:ASP:CG	2:A:605:HEM:CHD	2.79	0.51
1:A:560:THR:O	1:A:578:ASP:HA	2.10	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
2:A:605:HEM:HMB1	2:A:605:HEM:HBB2	1.93	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
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:593:ARG:O	1:A:594:GLU:CB	2.59	0.49
1:A:106:ILE:HD11	1:A:265:ALA:HB1	1.95	0.49
1:A:348:ARG:HH11	1:A:437:ASN:ND2	2.10	0.49
1:A:407:MET:SD	1:A:408:ASN:N	2.86	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:357:THR:HB	1:A:374:LEU:O	2.14	0.48
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: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: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:352:MET:CB	1:A:407:MET:HG2	2.44	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:175:LEU:HD13	10:A:725:HOH:O	2.13	0.47
1:A:117:THR:HG23	1:A:164:GLY:HA2	1.96	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:13:VAL:CG1	1:A:14:LYS:N	2.78	0.47
1:A:564:LEU:C	1:A:565:HIS:CD2	2.88	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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: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:21:TYR:OH	1:A:295:GLU:OE1	2.33	0.45
1:A:236:PRO:HB3	10:A:640:HOH:O	2.14	0.45
1:A:108:ASP:CG	2:A:605:HEM:HHD	2.37	0.45
1:A:475:ILE:HD11	10:A:689:HOH:O	2.16	0.45
1:A:432:ASP:C	1:A:432:ASP:OD1	2.55	0.45
1:A:367:PRO:O	1:A:369:GLY:N	2.46	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
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:424:PRO:CG	9:A:800:BHO:H4	2.49	0.43
1:A:491:ASP:O	1:A:494:ILE:HG22	2.19	0.43
1:A:286:HIS:NE2	1:A:595:ASN:HB3	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:118:GLU:CG	1:A:118:GLU:O	2.67	0.43
1:A:510:LEU:O	1:A:513:CYS:HB3	2.18	0.43
1:A:424:PRO:HG2	9:A:800:BHO:H4	2.00	0.43
1:A:10:VAL:CG1	1:A:41:ARG:NE	2.82	0.43
1:A:331:TYR:CD1	1:A:527:ARG:HA	2.54	0.43
1:A:268:LEU:HD12	1:A:268:LEU:HA	1.54	0.43
1:A:449:TYR:CD1	1:A:495:GLY:HA3	2.54	0.43
1:A:227:LEU:HD13	1:A:251:ALA:HB2	1.99	0.43
1:A:109:HIS:CD2	1:A:255:ARG:CZ	3.02	0.43
1:A:387:ILE:CG2	1:A:388:LYS:N	2.81	0.42
1:A:199:LEU:C	1:A:201:SER:N	2.72	0.42
1:A:484:TYR:O	1:A:486:THR:N	2.52	0.42
1:A:187:LEU:HA	1:A:187:LEU:HD23	1.83	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: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:275:ARG:CD	1:A:555:ASP:HB3	2.50	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
1:A:99:LEU:HD23	1:A:566:ALA:HB1	2.02	0.42
4:A:597:NAG:O7	4:A:597:NAG:H3	2.19	0.42
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:286:HIS:HD1	1:A:286:HIS:H	1.68	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
1:A:11:PRO:HB2	1:A:12:LEU:H	1.71	0.41
6:A:607:NAG:H5	6:A:607:NAG:N2	2.35	0.41
1:A:317:LEU:O	1:A:320:GLU:HB2	2.21	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:308:THR:O	1:A:312:TYR:HB3	2.20	0.41
1:A:475:ILE:CG1	1:A:476:LEU:N	2.84	0.41
1:A:360:ARG:NH1	1:A:372:ALA:CA	2.83	0.41
1:A:588:SER:O	1:A:591:ALA:N	2.54	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:101:MET:SD	1:A:101:MET:C	3.00	0.40
1:A:348:ARG:CZ	2:A:605:HEM:CAD	2.99	0.40
1:A:292:LEU:HD12	1:A:292:LEU:HA	1.85	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:561:LYS:NZ	1:A:578:ASP:OD2	2.54	0.40
1:A:486:THR:HA	1:A:487:PRO:HD3	1.96	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	592/595 (100%)	513 (87%)	59 (10%)	20 (3%)	6 23

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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 ⓘ

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%)	7 20

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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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 chains 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	7.72	2 (22%)	10,12,14	4.34	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
1	SEP	A	198	1	-	0/6/8/10	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	SEP	O-C	22.88	1.27	1.11
1	A	198	SEP	P-O1P	2.45	1.59	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	SEP	C-CA-N	-12.26	101.58	113.83
1	A	198	SEP	P-OG-CB	3.99	129.73	118.19
1	A	198	SEP	OG-CB-CA	2.54	112.28	108.69
1	A	198	SEP	O2P-P-OG	-2.53	99.66	106.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	12,14,15	0.66	0	15,19,21	1.21	3 (20%)
4	NAG	A	597	4	12,14,15	1.06	1 (8%)	15,19,21	1.05	1 (6%)
4	MAN	A	598	4	10,11,12	0.57	0	11,15,17	1.43	2 (18%)
5	NDG	A	599	1,5	12,14,15	0.65	0	15,19,21	0.76	1 (6%)
5	NAG	A	600	5	12,14,15	0.50	0	15,19,21	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	601	1,4	12,14,15	0.62	0	15,19,21	0.99	1 (6%)
4	NAG	A	602	4	12,14,15	0.44	0	15,19,21	1.06	0
4	MAN	A	603	4	10,11,12	0.54	0	11,15,17	1.00	1 (9%)
6	NAG	A	604	1,6	12,14,15	0.44	0	15,19,21	1.03	1 (6%)
6	NAG	A	607	6	12,14,15	0.71	0	15,19,21	0.89	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
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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	597	NAG	C3-C2	2.78	1.58	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	604	NAG	C3-C2-N2	-3.22	106.85	111.76
4	A	598	MAN	C4-C3-C2	3.07	114.63	110.50
4	A	598	MAN	C3-C4-C5	2.62	114.88	110.20
4	A	601	NAG	C3-C2-N2	-2.57	107.84	111.76
4	A	596	NAG	C3-C2-N2	-2.43	108.06	111.76
4	A	603	MAN	C3-C4-C5	-2.15	106.36	110.20
4	A	597	NAG	C6-C5-C4	2.10	118.06	113.00
4	A	596	NAG	C2-N2-C7	-2.03	119.69	123.09
4	A	596	NAG	O5-C5-C6	-2.03	104.86	106.98
6	A	607	NAG	O5-C5-C4	-2.02	108.09	110.65

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	599	NDG	C2-N2-C7	-2.01	119.72	123.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	49,50,50	6.83	26 (53%)	46,82,82	2.67	20 (43%)
8	SCN	A	616	-	2,2,2	3.01	2 (100%)	1,1,1	0.13	0
9	BHO	A	800	-	10,10,10	3.25	6 (60%)	12,12,12	4.54	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	-	0/14/114/114	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 (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	605	HEM	C2B-C1B	31.26	1.52	1.44
2	A	605	HEM	C3D-C4D	23.17	1.50	1.44
2	A	605	HEM	C2D-C1D	17.58	1.48	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	605	HEM	C4A-C3A	9.13	1.51	1.40
2	A	605	HEM	C3B-CAB	6.84	1.62	1.40
9	A	800	BHO	O2-N	6.61	1.51	1.39
2	A	605	HEM	C3D-C2D	6.59	1.55	1.43
2	A	605	HEM	FE-NC	6.22	2.21	1.97
2	A	605	HEM	FE-NB	5.91	2.19	1.97
2	A	605	HEM	CHB-C1B	5.82	1.44	1.35
2	A	605	HEM	CAA-C2A	4.78	1.60	1.52
2	A	605	HEM	CMC-C2C	4.71	1.62	1.47
2	A	605	HEM	C3C-CAC	4.66	1.55	1.40
9	A	800	BHO	C3-C2	4.27	1.48	1.39
9	A	800	BHO	C6-C1	3.66	1.45	1.39
8	A	616	SCN	C-S	3.43	1.85	1.63
2	A	605	HEM	CMB-C2B	3.30	1.57	1.47
9	A	800	BHO	O1-C	3.08	1.29	1.23
9	A	800	BHO	C4-C3	3.03	1.46	1.37
2	A	605	HEM	C4A-NA	-2.84	1.31	1.36
2	A	605	HEM	C1C-NC	2.84	1.42	1.38
2	A	605	HEM	CBA-CGA	-2.77	1.43	1.50
2	A	605	HEM	C4D-ND	-2.72	1.34	1.39
8	A	616	SCN	C-N	2.52	1.33	1.15
2	A	605	HEM	FE-NA	2.46	2.02	1.92
2	A	605	HEM	CHC-C4B	-2.36	1.33	1.39
9	A	800	BHO	C5-C6	2.31	1.44	1.39
2	A	605	HEM	CMA-C3A	-2.18	1.47	1.51
2	A	605	HEM	C1B-NB	-2.17	1.35	1.39
2	A	605	HEM	CHC-C1C	2.12	1.40	1.36
2	A	605	HEM	C3B-C2B	-2.11	1.40	1.43
2	A	605	HEM	CAA-CBA	2.11	1.64	1.53
2	A	605	HEM	CAD-C3D	2.08	1.59	1.51
2	A	605	HEM	C1A-C2A	2.07	1.47	1.43

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	800	BHO	C1-C-N	9.43	132.24	116.34
9	A	800	BHO	O1-C-C1	-8.93	105.35	121.01
2	A	605	HEM	CBD-CAD-C3D	-8.00	96.90	114.37
2	A	605	HEM	C4D-ND-C1D	7.16	112.49	105.16
9	A	800	BHO	C5-C6-C1	5.83	127.89	120.32
2	A	605	HEM	C1A-C2A-C3A	-4.80	101.95	106.92
2	A	605	HEM	CHD-C1D-ND	4.78	128.55	124.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	605	HEM	CAD-CBD-CGD	4.14	126.41	113.48
2	A	605	HEM	C1B-NB-C4B	3.97	109.22	105.16
2	A	605	HEM	CHA-C4D-ND	3.96	129.75	124.31
9	A	800	BHO	C3-C2-C1	-3.86	115.31	120.32
2	A	605	HEM	C2D-C1D-ND	-3.81	108.43	112.93
2	A	605	HEM	CAA-CBA-CGA	3.27	123.99	113.47
2	A	605	HEM	CMC-C2C-C3C	3.20	133.71	126.16
9	A	800	BHO	C4-C5-C6	-3.09	115.02	120.17
9	A	800	BHO	O2-N-C	3.03	127.94	119.64
2	A	605	HEM	C3B-C4B-NB	-2.95	111.89	114.00
2	A	605	HEM	C4C-NC-C1C	2.85	108.50	105.53
2	A	605	HEM	C2A-C1A-NA	2.81	113.63	109.73
9	A	800	BHO	C4-C3-C2	2.53	124.38	120.17
2	A	605	HEM	C3A-C4A-CHB	2.35	130.47	126.00
2	A	605	HEM	CHC-C1C-NC	2.33	126.76	124.73
2	A	605	HEM	CAD-C3D-C4D	2.23	128.54	124.53
2	A	605	HEM	C4A-CHB-C1B	2.16	130.32	127.47
2	A	605	HEM	C2A-C1A-CHA	-2.09	122.03	126.00
2	A	605	HEM	CHB-C4A-NA	-2.07	121.12	124.58
2	A	605	HEM	C4A-C3A-C2A	2.04	108.41	107.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	595/595 (100%)	-0.41	24 (4%)	36 43	8, 30, 73, 100	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	594	GLU	8.1
1	A	595	ASN	7.3
1	A	1	SER	6.1
1	A	2	TRP	5.6
1	A	8	ALA	5.6
1	A	122	ASN	5.1
1	A	4	VAL	4.9
1	A	121	SER	4.1
1	A	119	LEU	4.0
1	A	174	SER	3.6
1	A	170	PRO	3.2
1	A	3	GLU	2.5
1	A	593	ARG	2.4
1	A	63	GLN	2.4
1	A	173	GLN	2.3
1	A	5	GLY	2.3
1	A	118	GLU	2.3
1	A	7	GLY	2.3
1	A	124	HIS	2.3
1	A	574	HIS	2.2
1	A	533	PRO	2.2
1	A	9	PRO	2.2
1	A	171	PRO	2.1
1	A	13	VAL	2.1

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	SEP	A	198	10/11	0.12	-0.73	24,31,36,38	0

6.3 Carbohydrates ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
6	NAG	A	604	14/15	0.28	2.10	66,70,72,73	0
4	NAG	A	596	14/15	0.23	1.21	62,66,69,74	0
4	NAG	A	601	14/15	0.22	1.03	59,61,64,70	0
5	NDG	A	599	14/15	0.17	0.31	52,55,55,56	0
4	MAN	A	603	11/12	0.39	-1.13	87,89,90,90	0
4	MAN	A	598	11/12	0.33	-	85,85,86,87	0
5	NAG	A	600	14/15	0.25	-	58,59,61,61	0
6	NAG	A	607	14/15	0.38	-	77,79,82,82	0
4	NAG	A	602	14/15	0.35	-	75,77,80,84	0
4	NAG	A	597	14/15	0.41	-	78,81,83,83	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	RSR	LLDF	B-factors(Å ²)	Q<0.9
9	BHO	A	800	10/10	0.30	4.75	35,36,37,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	HEM	A	605	43/43	0.15	0.16	7,10,16,22	0
8	SCN	A	616	3/3	0.17	-0.09	15,15,16,23	0
7	IOD	A	610	1/1	0.10	-1.43	76,76,76,76	1
7	IOD	A	609	1/1	0.06	-1.76	96,96,96,96	0
7	IOD	A	615	1/1	0.10	-1.87	64,64,64,64	1
3	CA	A	606	1/1	0.10	-2.25	14,14,14,14	0
7	IOD	A	614	1/1	0.04	-2.34	69,69,69,69	0
7	IOD	A	613	1/1	0.03	-2.55	100,100,100,100	0
7	IOD	A	608	1/1	0.06	-2.92	32,32,32,32	0
7	IOD	A	612	1/1	0.04	-2.98	87,87,87,87	0
7	IOD	A	611	1/1	0.02	-3.75	65,65,65,65	0

6.5 Other polymers ⓘ

There are no such residues in this entry.