



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 06:12 pm GMT

PDB ID : 3UBA
Title : Crystal structure of the complex of bovine lactoperoxidase with p-hydroxycinnamic acid at 2.6 Å resolution
Authors : Pandey, N.; Singh, A.K.; Singh, R.P.; Sinha, M.; Kaur, P.; Sharma, S.; Singh, T.P.
Deposited on : 2011-10-24
Resolution : 2.65 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (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

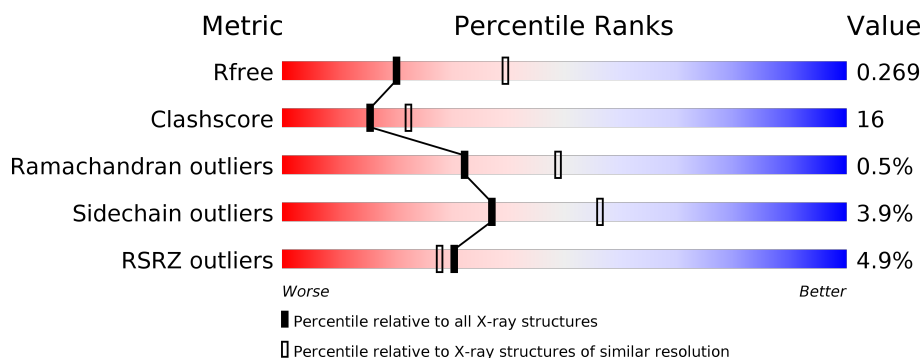
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	3491 (2.70-2.62)
Clashscore	112137	1026 (2.68-2.64)
Ramachandran outliers	110173	1010 (2.68-2.64)
Sidechain outliers	110143	1010 (2.68-2.64)
RSRZ outliers	101464	3511 (2.70-2.62)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	595	

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
10	GOL	A	621	-	-	X	-
8	HC4	A	700	-	-	X	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	PEG	A	603	-	-	-	X
9	PEG	A	619	-	-	-	X

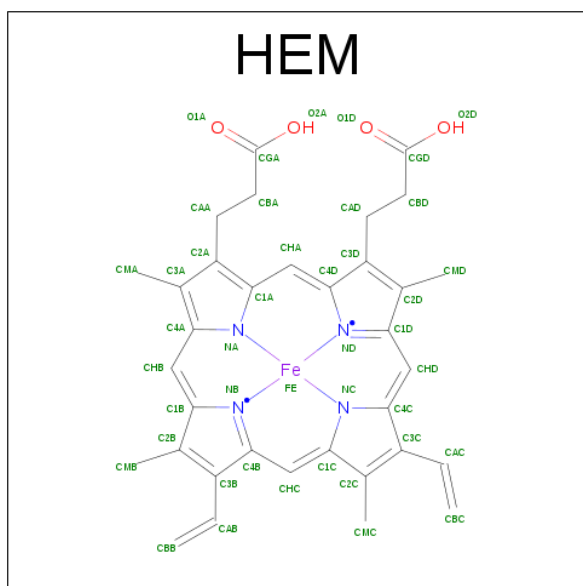
i

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 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $\text{C}_8\text{H}_{15}\text{NO}_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

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

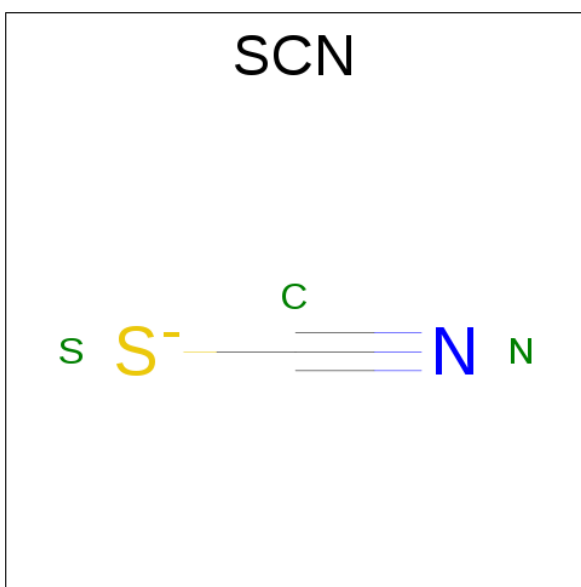
- Molecule 5 is IODIDE ION (three-letter code: IOD) (formula: I).

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

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

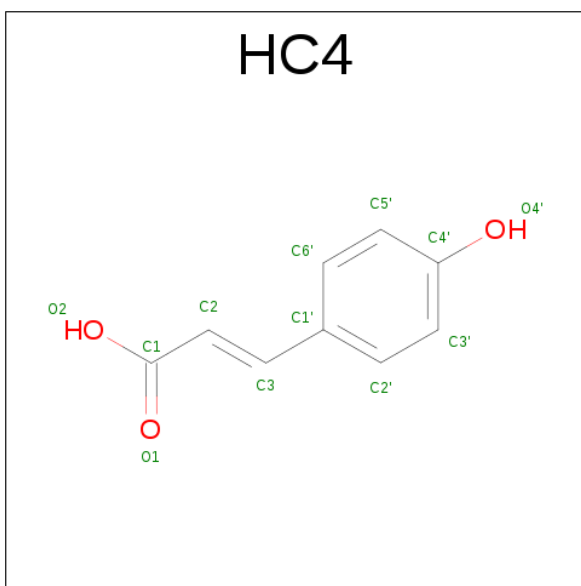
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Ca	0	0
			1	1		

- Molecule 7 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



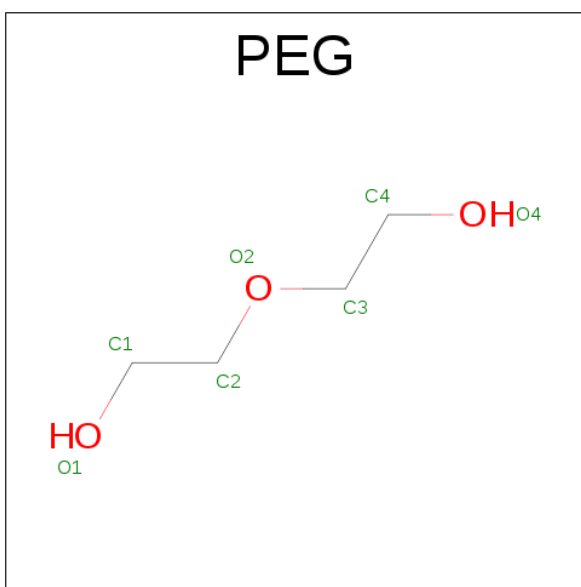
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	S	0	0
			3	1	1	1		

- Molecule 8 is 4'-HYDROXYCINNAMIC ACID (three-letter code: HC4) (formula: C₉H₈O₃).



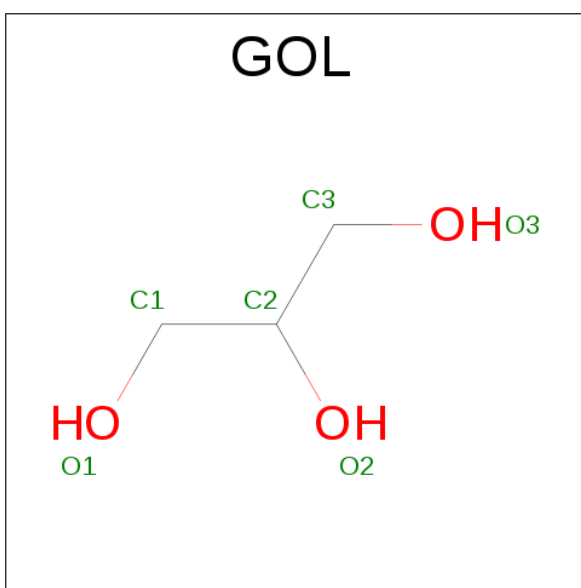
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			12	9	3		

- Molecule 9 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			7	4	3		
9	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 10 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 11 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	C	O	0	0
			4	2	2		
11	A	1	Total	C	O	0	0
			4	2	2		

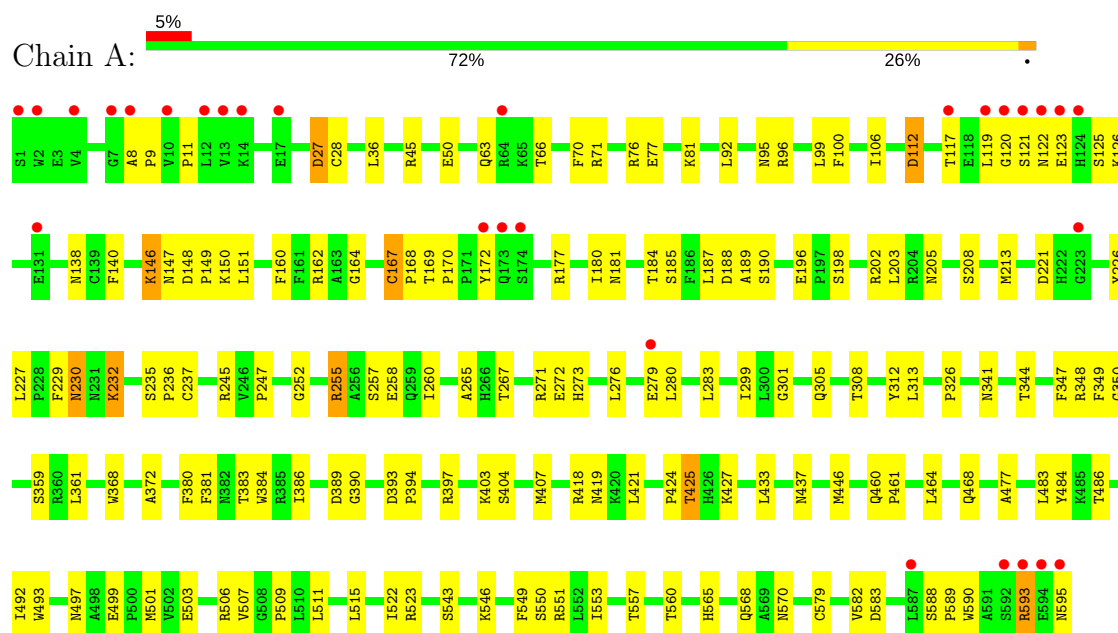
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	114	Total	O	0	0
			114	114		

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, α , β , γ	54.05Å 80.23Å 76.10Å 90.00° 103.33° 90.00°	Depositor
Resolution (Å)	43.99 – 2.65 43.99 – 2.65	Depositor EDS
% Data completeness (in resolution range)	97.9 (43.99-2.65) 98.0 (43.99-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.05 (at 2.65Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.219 , 0.238 0.214 , 0.269	Depositor DCC
R_{free} test set	921 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	44.9	Xtriage
Anisotropy	0.953	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 43.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5054	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.20% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 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: GOL, SCN, NAG, HC4, SEP, CA, EDO, HEM, PEG, IOD

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	0.71	2/6634 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	390	GLY	N-CA-C	5.26	126.24	113.10
1	A	484	TYR	N-CA-C	-5.18	97.02	111.00

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	4684	151	0
2	A	43	0	30	10	0
3	A	42	0	39	5	0
4	A	28	0	25	1	0
5	A	9	0	0	3	0
6	A	1	0	0	0	0
7	A	3	0	0	0	0
8	A	12	0	7	7	0
9	A	14	0	20	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	A	6	0	8	5	0
11	A	8	0	12	0	0
12	A	114	0	0	9	0
All	All	5054	0	4825	161	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 16.

All (161) 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:HB2	1:A:168:PRO:HD3	1.37	1.06
2:A:605:HEM:HMC2	2:A:605:HEM:HBC2	1.39	1.04
1:A:95:ASN:HD22	10:A:621:GOL:H12	1.23	1.03
2:A:605:HEM:HBB2	2:A:605:HEM:HMB1	1.40	0.98
1:A:146:LYS:HE3	1:A:147:ASN:ND2	1.79	0.98
1:A:150:LYS:HE2	1:A:419:ASN:HD22	1.29	0.98
3:A:596:NAG:O7	10:A:621:GOL:H11	1.65	0.96
1:A:196:GLU:HB3	1:A:198:SEP:O3P	1.66	0.93
1:A:213:MET:HG2	1:A:273:HIS:CD2	2.03	0.93
1:A:168:PRO:HG2	1:A:172:TYR:HB2	1.52	0.91
1:A:167:CYS:CB	1:A:168:PRO:HD3	2.00	0.90
1:A:169:THR:HG23	12:A:725:HOH:O	1.73	0.89
1:A:167:CYS:HB2	1:A:168:PRO:CD	2.02	0.88
1:A:117:THR:HG22	1:A:164:GLY:HA2	1.57	0.85
1:A:551:ARG:HD3	1:A:583:ASP:O	1.78	0.83
2:A:605:HEM:CMC	2:A:605:HEM:HBC2	2.09	0.81
2:A:605:HEM:HBB2	2:A:605:HEM:CMB	2.10	0.81
1:A:150:LYS:CE	1:A:419:ASN:HD22	1.94	0.78
1:A:279:GLU:O	1:A:283:LEU:HD12	1.83	0.78
1:A:213:MET:CG	1:A:273:HIS:CD2	2.68	0.77
1:A:150:LYS:HE2	1:A:419:ASN:ND2	2.01	0.74
1:A:258:GLU:HB2	8:A:700:HC4:H6'	1.69	0.73
1:A:425:THR:HG23	1:A:425:THR:O	1.90	0.72
1:A:196:GLU:CB	1:A:198:SEP:O3P	2.38	0.72
1:A:95:ASN:ND2	10:A:621:GOL:H12	2.02	0.71
1:A:425:THR:CG2	1:A:425:THR:O	2.38	0.71
1:A:146:LYS:HG3	1:A:147:ASN:N	2.04	0.70
1:A:258:GLU:CB	8:A:700:HC4:H6'	2.22	0.69
1:A:230:ASN:C	1:A:230:ASN:OD1	2.30	0.69
1:A:258:GLU:HG3	8:A:700:HC4:H6'	1.75	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:THR:HG22	12:A:725:HOH:O	1.92	0.68
1:A:348:ARG:HH11	1:A:437:ASN:ND2	1.91	0.68
1:A:205:ASN:C	1:A:205:ASN:OD1	2.33	0.67
1:A:326:PRO:O	1:A:523:ARG:NH2	2.23	0.67
1:A:418:ARG:HH22	9:A:603:PEG:H42	1.60	0.67
1:A:188:ASP:O	1:A:189:ALA:HB3	1.95	0.66
1:A:27:ASP:O	1:A:28:CYS:HB2	1.96	0.65
1:A:99:LEU:HD21	1:A:549:PHE:CD2	2.33	0.64
1:A:593:ARG:HG3	1:A:593:ARG:O	1.96	0.64
1:A:76:ARG:HH22	1:A:419:ASN:HD21	1.45	0.64
1:A:117:THR:CG2	1:A:164:GLY:HA2	2.27	0.63
1:A:272:GLU:HA	1:A:272:GLU:OE1	1.99	0.62
1:A:301:GLY:O	1:A:305:GLN:HG3	1.99	0.62
1:A:184:THR:OG1	1:A:188:ASP:OD2	2.17	0.62
1:A:258:GLU:CG	8:A:700:HC4:H6'	2.30	0.62
1:A:582:VAL:HA	12:A:625:HOH:O	2.00	0.61
1:A:348:ARG:NH2	2:A:605:HEM:HAD1	2.15	0.61
2:A:605:HEM:CBB	2:A:605:HEM:HMB1	2.25	0.61
1:A:255:ARG:HB3	8:A:700:HC4:H2	1.82	0.61
2:A:605:HEM:HMC2	2:A:605:HEM:CBC	2.24	0.61
1:A:237:CYS:HB3	12:A:732:HOH:O	2.01	0.60
1:A:348:ARG:HH11	1:A:437:ASN:HD22	1.49	0.60
1:A:123:GLU:HG3	1:A:125:SER:H	1.66	0.60
1:A:565:HIS:HB3	5:A:612:IOD:I	2.73	0.59
1:A:418:ARG:NH2	9:A:603:PEG:H42	2.17	0.58
3:A:596:NAG:O7	10:A:621:GOL:C1	2.47	0.58
1:A:368:TRP:CZ3	1:A:389:ASP:OD1	2.56	0.58
1:A:227:LEU:HD21	1:A:267:THR:HA	1.85	0.58
1:A:203:LEU:HD11	1:A:252:GLY:HA2	1.86	0.57
1:A:258:GLU:HG3	8:A:700:HC4:C6'	2.34	0.57
1:A:8:ALA:HB3	1:A:9:PRO:HD3	1.86	0.57
1:A:368:TRP:HZ3	1:A:389:ASP:OD1	1.88	0.57
1:A:424:PRO:O	1:A:425:THR:HB	2.04	0.56
1:A:66:THR:HB	1:A:70:PHE:O	2.04	0.56
1:A:168:PRO:HB2	1:A:170:PRO:O	2.06	0.55
1:A:350:GLY:HA3	2:A:605:HEM:CBC	2.36	0.55
1:A:499:GLU:OE1	1:A:509:PRO:HD2	2.06	0.55
1:A:383:THR:HB	12:A:732:HOH:O	2.06	0.55
1:A:169:THR:N	1:A:170:PRO:HD2	2.22	0.54
1:A:546:LYS:HE3	1:A:583:ASP:OD1	2.07	0.54
1:A:140:PHE:O	1:A:160:PHE:HB3	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:MET:CG	1:A:273:HIS:HD2	2.21	0.54
1:A:407:MET:HB3	1:A:501:MET:CE	2.38	0.54
1:A:120:GLY:HA3	1:A:126:LYS:HE2	1.89	0.53
1:A:95:ASN:O	1:A:96:ARG:NH1	2.36	0.53
1:A:276:LEU:O	1:A:280:LEU:HG	2.08	0.52
1:A:208:SER:HB3	3:A:599:NAG:H62	1.92	0.52
1:A:393:ASP:HB2	1:A:394:PRO:HD3	1.90	0.52
1:A:230:ASN:OD1	1:A:232:LYS:N	2.44	0.51
1:A:77:GLU:OE2	1:A:81:LYS:NZ	2.44	0.51
1:A:169:THR:N	1:A:170:PRO:CD	2.73	0.51
1:A:177:ARG:HA	12:A:670:HOH:O	2.10	0.51
1:A:255:ARG:CB	8:A:700:HC4:H2	2.41	0.50
1:A:106:ILE:HD11	1:A:265:ALA:HB3	1.93	0.50
1:A:568:GLN:HE21	1:A:570:ASN:HD21	1.59	0.50
1:A:221:ASP:HB2	1:A:226:TYR:CZ	2.46	0.49
1:A:257:SER:O	1:A:381:PHE:HA	2.12	0.49
1:A:9:PRO:CD	1:A:167:CYS:HA	2.43	0.49
1:A:549:PHE:CE2	1:A:553:ILE:HD11	2.48	0.49
1:A:146:LYS:CE	1:A:147:ASN:ND2	2.64	0.49
1:A:267:THR:O	1:A:271:ARG:HG3	2.13	0.48
1:A:188:ASP:O	1:A:189:ALA:CB	2.61	0.48
1:A:63:GLN:HA	12:A:719:HOH:O	2.12	0.48
1:A:258:GLU:O	1:A:380:PHE:HA	2.13	0.48
1:A:189:ALA:O	1:A:190:SER:C	2.52	0.48
1:A:213:MET:HG2	1:A:273:HIS:HD2	1.71	0.48
1:A:349:PHE:CB	1:A:497:ASN:HD21	2.26	0.48
1:A:553:ILE:O	1:A:557:THR:OG1	2.28	0.47
1:A:213:MET:HG2	1:A:273:HIS:NE2	2.29	0.47
1:A:361:LEU:O	1:A:397:ARG:HD2	2.14	0.47
1:A:92:LEU:HD13	1:A:403:LYS:HB2	1.96	0.47
1:A:380:PHE:CE2	1:A:421:LEU:HA	2.48	0.47
1:A:299:ILE:HD11	1:A:590:TRP:NE1	2.30	0.47
1:A:468:GLN:HG2	1:A:477:ALA:HB3	1.96	0.47
1:A:76:ARG:HH22	1:A:419:ASN:ND2	2.13	0.47
1:A:121:SER:O	1:A:122:ASN:CB	2.63	0.47
1:A:260:ILE:HD11	1:A:386:ILE:HG13	1.95	0.46
1:A:112:ASP:CG	1:A:344:THR:HG22	2.35	0.46
1:A:146:LYS:HE3	1:A:147:ASN:HD21	1.75	0.46
1:A:245:ARG:HD3	12:A:597:HOH:O	2.15	0.46
1:A:468:GLN:HG2	1:A:477:ALA:CB	2.46	0.46
1:A:393:ASP:CB	1:A:394:PRO:HD3	2.46	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ARG:HA	5:A:615:IOD:I	2.86	0.46
1:A:393:ASP:N	1:A:394:PRO:CD	2.79	0.45
1:A:464:LEU:O	1:A:468:GLN:HG3	2.16	0.45
1:A:460:GLN:HA	1:A:461:PRO:HD2	1.70	0.45
1:A:208:SER:CB	3:A:599:NAG:H62	2.47	0.45
1:A:167:CYS:CB	1:A:168:PRO:CD	2.66	0.44
1:A:341:ASN:HB3	1:A:446:MET:HE3	1.99	0.44
1:A:359:SER:HA	1:A:372:ALA:O	2.16	0.44
1:A:279:GLU:O	1:A:283:LEU:CD1	2.62	0.44
1:A:522:ILE:HA	1:A:522:ILE:HD13	1.65	0.44
1:A:96:ARG:HD2	1:A:100:PHE:CD2	2.52	0.44
1:A:384:TRP:CH2	4:A:601:NAG:H2	2.53	0.44
1:A:350:GLY:HA3	2:A:605:HEM:CAC	2.47	0.44
1:A:349:PHE:HB2	1:A:497:ASN:HD21	1.82	0.44
1:A:196:GLU:CG	1:A:198:SEP:O3P	2.65	0.44
1:A:308:THR:O	1:A:312:TYR:HB3	2.17	0.44
1:A:148:ASP:OD1	1:A:150:LYS:HB2	2.18	0.43
1:A:213:MET:HG3	1:A:273:HIS:CD2	2.50	0.43
1:A:138:ASN:O	1:A:162:ARG:HG3	2.18	0.43
1:A:63:GLN:CG	1:A:71:ARG:HH12	2.31	0.43
1:A:348:ARG:NH1	1:A:437:ASN:HD22	2.15	0.43
1:A:313:LEU:HA	1:A:313:LEU:HD23	1.80	0.43
1:A:237:CYS:HA	1:A:381:PHE:O	2.19	0.43
1:A:433:LEU:HD12	1:A:433:LEU:HA	1.65	0.43
1:A:492:ILE:HG23	1:A:493:TRP:N	2.33	0.43
1:A:63:GLN:CG	1:A:71:ARG:NH1	2.82	0.42
1:A:187:LEU:HD12	1:A:187:LEU:HA	1.88	0.42
1:A:235:SER:HA	1:A:236:PRO:HD3	1.89	0.42
1:A:202:ARG:NH1	5:A:617:IOD:I	3.23	0.42
1:A:36:LEU:HD11	9:A:619:PEG:H12	2.02	0.42
1:A:588:SER:N	1:A:589:PRO:CD	2.83	0.41
1:A:63:GLN:HG3	1:A:71:ARG:NH1	2.35	0.41
1:A:8:ALA:HB3	1:A:9:PRO:CD	2.49	0.41
1:A:169:THR:H	1:A:170:PRO:HD2	1.83	0.41
1:A:229:PHE:CG	1:A:247:PRO:HG2	2.55	0.41
1:A:229:PHE:HB3	1:A:247:PRO:HG2	2.02	0.41
1:A:205:ASN:O	1:A:205:ASN:OD1	2.37	0.41
2:A:605:HEM:CMC	2:A:605:HEM:CBC	2.86	0.41
1:A:511:LEU:O	1:A:515:LEU:HG	2.21	0.41
1:A:560:THR:HA	1:A:579:CYS:SG	2.60	0.41
1:A:407:MET:HB3	1:A:501:MET:HE1	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:596:NAG:H2	10:A:621:GOL:H31	2.02	0.41
1:A:149:PRO:HG2	9:A:603:PEG:H21	2.02	0.41
1:A:180:ILE:CG2	1:A:181:ASN:N	2.82	0.41
1:A:185:SER:O	1:A:522:ILE:HD12	2.20	0.41
1:A:501:MET:HG2	1:A:506:ARG:HA	2.03	0.41
1:A:568:GLN:HG3	1:A:570:ASN:HD21	1.86	0.41
1:A:170:PRO:HA	12:A:675:HOH:O	2.21	0.40
1:A:299:ILE:HD11	1:A:590:TRP:HE1	1.85	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%)	555 (94%)	34 (6%)	3 (0%)	32	49

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	167	CYS
1	A	11	PRO
1	A	119	LEU

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%)	497 (96%)	20 (4%)	37	56

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ASP
1	A	50	GLU
1	A	112	ASP
1	A	146	LYS
1	A	151	LEU
1	A	230	ASN
1	A	232	LYS
1	A	255	ARG
1	A	347	PHE
1	A	404	SER
1	A	425	THR
1	A	427	LYS
1	A	483	LEU
1	A	486	THR
1	A	503	GLU
1	A	507	VAL
1	A	543	SER
1	A	550	SER
1	A	593	ARG
1	A	595	ASN

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	122	ASN
1	A	138	ASN
1	A	147	ASN
1	A	217	GLN
1	A	273	HIS
1	A	419	ASN
1	A	437	ASN
1	A	468	GLN
1	A	497	ASN
1	A	521	GLN
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	1.55	1 (11%)	9,12,14	1.29	1 (11%)

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	3.70	1.55	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	SEP	OG-CB-CA	2.20	110.33	108.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	198	SEP	3	0

5.5 Carbohydrates [i](#)

2 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	601	1,4	14,14,15	2.25	4 (28%)	15,19,21	2.02	5 (33%)
4	NAG	A	602	4	14,14,15	1.07	2 (14%)	15,19,21	2.27	4 (26%)

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	601	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	602	4	-	0/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	601	NAG	O4-C4	-6.09	1.28	1.43
4	A	601	NAG	O5-C5	-3.95	1.35	1.43
4	A	601	NAG	C4-C5	-2.65	1.47	1.53
4	A	601	NAG	C3-C2	-2.29	1.47	1.52
4	A	602	NAG	C3-C2	-2.20	1.47	1.52
4	A	602	NAG	C1-C2	-2.18	1.49	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	602	NAG	C4-C3-C2	-6.17	101.97	111.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	NAG	O4-C4-C5	-3.95	99.33	109.28
4	A	601	NAG	C1-O5-C5	-3.01	108.02	112.17
4	A	601	NAG	O4-C4-C3	-2.53	104.84	110.36
4	A	601	NAG	C4-C3-C2	-2.10	107.93	111.02
4	A	602	NAG	O5-C1-C2	2.20	114.53	111.47
4	A	602	NAG	C3-C4-C5	3.12	115.72	110.22
4	A	601	NAG	C3-C4-C5	3.61	116.57	110.22
4	A	602	NAG	C1-O5-C5	3.99	117.66	112.17

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
4	A	601	NAG	1	0

5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 10 are monoatomic - leaving 11 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	$\# Z > 2$
3	NAG	A	596	1	14,14,15	1.15	2 (14%)	15,19,21	1.12	1 (6%)
3	NAG	A	599	1	14,14,15	1.11	2 (14%)	15,19,21	1.06	1 (6%)
9	PEG	A	603	-	6,6,6	1.31	1 (16%)	5,5,5	0.95	0
3	NAG	A	604	1	14,14,15	1.08	2 (14%)	15,19,21	1.04	1 (6%)
2	HEM	A	605	1	28,50,50	2.27	8 (28%)	17,82,82	1.44	3 (17%)
9	PEG	A	619	-	6,6,6	1.24	1 (16%)	5,5,5	0.98	0
7	SCN	A	620	-	1,2,2	1.73	0	0,1,1	0.00	-
10	GOL	A	621	-	5,5,5	0.28	0	5,5,5	0.30	0
11	EDO	A	623	-	3,3,3	0.64	0	2,2,2	1.04	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	EDO	A	624	-	3,3,3	0.68	0	2,2,2	0.97	0
8	HC4	A	700	-	9,12,12	1.32	1 (11%)	11,15,15	1.37	2 (18%)

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
3	NAG	A	596	1	-	0/6/23/26	0/1/1/1
3	NAG	A	599	1	-	0/6/23/26	0/1/1/1
9	PEG	A	603	-	-	0/4/4/4	0/0/0/0
3	NAG	A	604	1	-	0/6/23/26	0/1/1/1
2	HEM	A	605	1	-	0/6/54/54	0/0/8/8
9	PEG	A	619	-	-	0/4/4/4	0/0/0/0
7	SCN	A	620	-	-	0/0/0/0	0/0/0/0
10	GOL	A	621	-	-	0/4/4/4	0/0/0/0
11	EDO	A	623	-	-	0/1/1/1	0/0/0/0
11	EDO	A	624	-	-	0/1/1/1	0/0/0/0
8	HC4	A	700	-	-	0/3/5/5	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	605	HEM	C3B-C2B	-4.98	1.33	1.40
2	A	605	HEM	C3C-C2C	-4.77	1.34	1.40
3	A	599	NAG	O5-C5	-2.68	1.37	1.43
9	A	603	PEG	C2-C1	-2.57	1.36	1.49
3	A	604	NAG	O5-C5	-2.55	1.38	1.43
3	A	596	NAG	O5-C5	-2.52	1.38	1.43
9	A	619	PEG	C2-C1	-2.51	1.36	1.49
3	A	596	NAG	O5-C1	-2.46	1.39	1.43
3	A	604	NAG	O5-C1	-2.43	1.39	1.43
3	A	599	NAG	O5-C1	-2.16	1.40	1.43
2	A	605	HEM	CMC-C2C	2.04	1.55	1.51
2	A	605	HEM	C4D-ND	2.06	1.39	1.36
2	A	605	HEM	C1D-ND	2.24	1.40	1.36
2	A	605	HEM	C3C-CAC	3.20	1.54	1.47
8	A	700	HC4	C3-C2	3.82	1.51	1.31
2	A	605	HEM	C3B-CAB	4.25	1.56	1.47
2	A	605	HEM	C3D-C2D	5.33	1.53	1.37

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	700	HC4	C1'-C3-C2	-3.23	113.19	125.88
3	A	596	NAG	C4-C3-C2	-2.96	106.69	111.02
2	A	605	HEM	C1D-C2D-C3D	-2.46	105.29	107.00
3	A	604	NAG	C2-N2-C7	-2.20	119.73	122.94
8	A	700	HC4	C3'-C2'-C1'	-2.07	118.56	121.28
2	A	605	HEM	CMA-C3A-C4A	-2.07	125.29	128.46
3	A	599	NAG	O5-C1-C2	2.47	114.91	111.47
2	A	605	HEM	C4A-C3A-C2A	2.53	108.76	107.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	596	NAG	3	0
3	A	599	NAG	2	0
9	A	603	PEG	3	0
2	A	605	HEM	10	0
9	A	619	PEG	1	0
10	A	621	GOL	5	0
8	A	700	HC4	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, 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%)	-0.09	29 (4%) 30 28	26, 48, 94, 140	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	TRP	15.3
1	A	173	GLN	9.0
1	A	121	SER	7.6
1	A	12	LEU	7.5
1	A	122	ASN	7.0
1	A	7	GLY	6.6
1	A	174	SER	6.2
1	A	8	ALA	5.9
1	A	4	VAL	5.8
1	A	1	SER	5.3
1	A	595	ASN	5.0
1	A	120	GLY	4.4
1	A	594	GLU	4.1
1	A	13	VAL	4.1
1	A	124	HIS	3.8
1	A	587	LEU	3.8
1	A	593	ARG	3.4
1	A	172	TYR	3.0
1	A	117	THR	2.9
1	A	119	LEU	2.6
1	A	223	GLY	2.6
1	A	123	GLU	2.5
1	A	64	ARG	2.5
1	A	17	GLU	2.3
1	A	592	SER	2.2
1	A	131	GLU	2.2
1	A	10	VAL	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	14	LYS	2.0
1	A	279	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	0.90	0.21	-	34,44,45,45	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
4	NAG	A	601	14/15	0.85	0.20	0.68	43,47,54,55	0
4	NAG	A	602	14/15	0.84	0.26	-	59,66,73,73	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, 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
9	PEG	A	603	7/7	0.84	0.33	9.26	66,70,72,74	0
8	HC4	A	700	12/12	0.81	0.36	6.08	33,34,34,35	12
9	PEG	A	619	7/7	0.85	0.23	2.27	74,75,75,75	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
11	EDO	A	623	4/4	0.81	0.27	1.25	81,86,88,91	0
7	SCN	A	620	3/3	0.94	0.17	1.06	53,53,54,55	0
5	IOD	A	610	1/1	0.93	0.19	0.47	98,98,98,98	0
3	NAG	A	599	14/15	0.84	0.16	0.39	41,51,53,54	0
2	HEM	A	605	43/43	0.93	0.18	0.24	14,18,22,24	0
10	GOL	A	621	6/6	0.86	0.16	0.24	46,47,48,51	0
6	CA	A	606	1/1	0.97	0.17	-0.50	39,39,39,39	0
5	IOD	A	615	1/1	1.00	0.10	-1.80	48,48,48,48	0
5	IOD	A	616	1/1	0.99	0.07	-2.18	65,65,65,65	0
5	IOD	A	609	1/1	0.99	0.06	-2.44	69,69,69,69	0
5	IOD	A	608	1/1	0.99	0.06	-2.48	77,77,77,77	0
5	IOD	A	607	1/1	0.97	0.05	-2.54	86,86,86,86	0
3	NAG	A	604	14/15	0.81	0.23	-	49,59,63,64	0
5	IOD	A	611	1/1	0.97	0.15	-	98,98,98,98	0
5	IOD	A	617	1/1	0.97	0.04	-	86,86,86,86	0
11	EDO	A	624	4/4	0.81	0.22	-	43,46,48,51	0
5	IOD	A	612	1/1	0.95	0.08	-	93,93,93,93	1
3	NAG	A	596	14/15	0.77	0.37	-	53,67,77,86	0

6.5 Other polymers [i](#)

There are no such residues in this entry.