Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:43 AM GMT

PDB ID	:	3BXI
Title	:	Structure of the complex of bovine lactoperoxidase with its catalyzed product hypothiocyanate ion at 2.3A resolution
Authors	:	Singh, A.K.; Singh, N.; Sharma, S.; Shin, K.; Takase, M.; Kaur, P.; Srinivasan, A.; Singh, T.P.
Deposited on	:	2008-01-14
Resolution	:	2.30 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

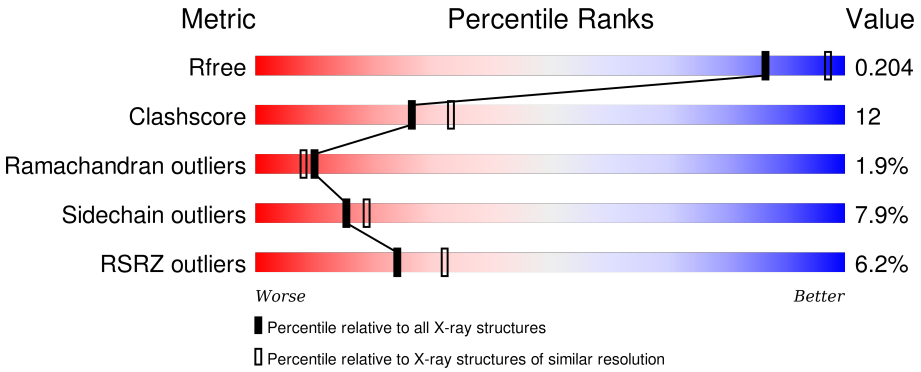
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	595	6% 73% 23%

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	NO3	A	608	-	X	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	NO3	A	609	-	X	-	X
7	NO3	A	610	-	X	-	X
7	NO3	A	611	-	X	-	-
7	NO3	A	612	-	X	-	X
9	OSM	A	614	-	-	X	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 5392 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 a polymer of unknown type called SUGAR (3-MER).

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

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

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

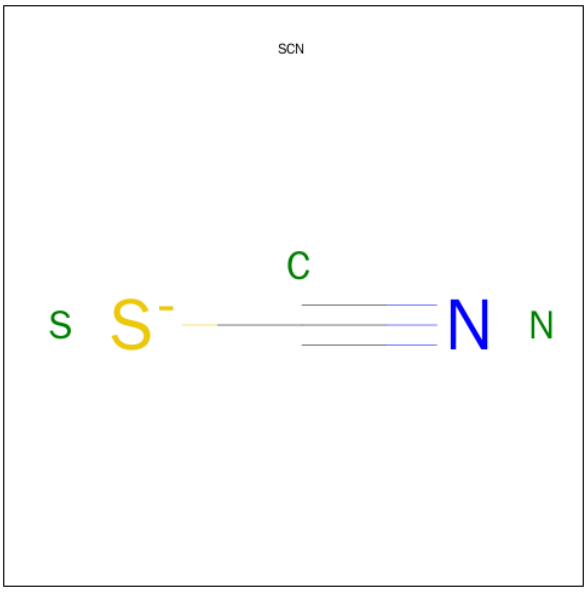
- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

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

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

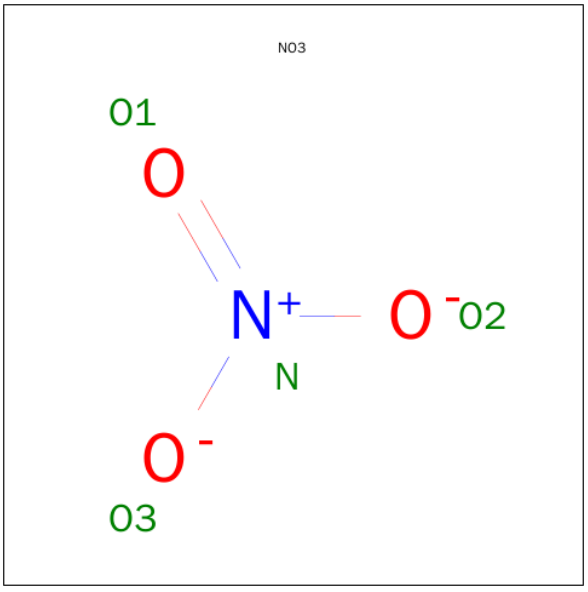
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Ca	0	0
			1	1		

- Molecule 6 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



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

- Molecule 7 is NITRATE ION (three-letter code: NO3) (formula: NO_3).



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

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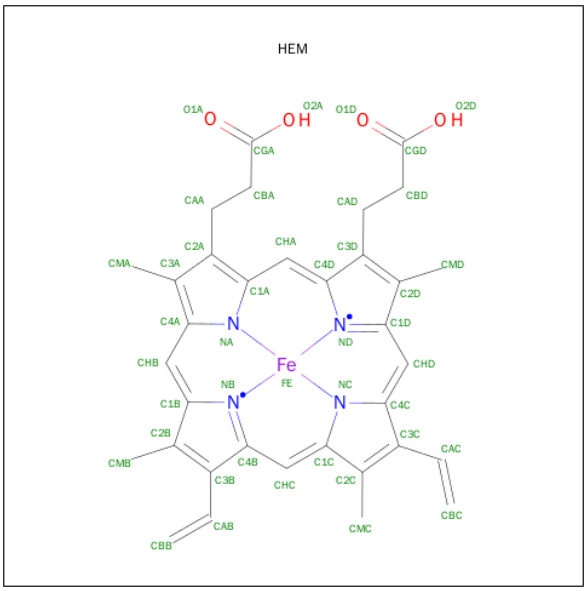
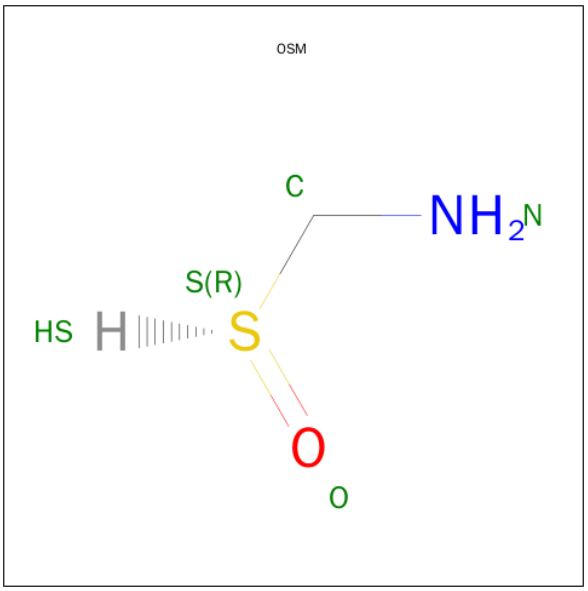
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total N O 4 1 3	0	0
7	A	1	Total N O 4 1 3	0	0

- Molecule 8 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 9 is 1-(OXIDOSULFANYL)METHANAMINE (three-letter code: OSM) (formula: CH_5NOS).



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

- Molecule 10 is water.

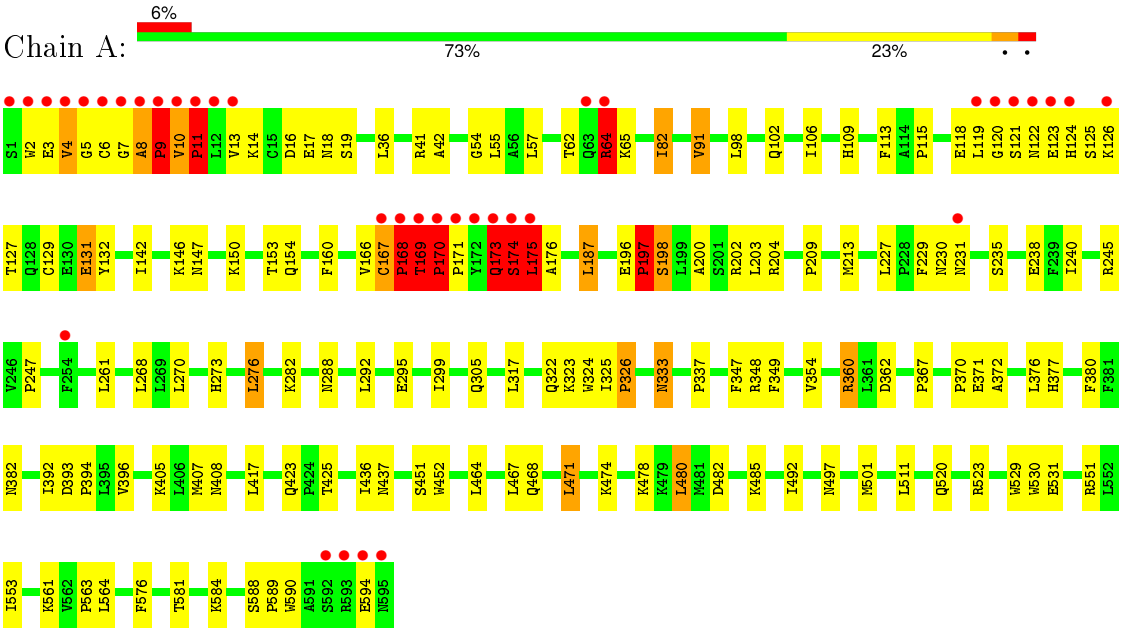
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	413	Total	O	0	0
			413	413		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Lactoperoxidase

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	54.63Å 80.67Å 77.68Å 90.00° 102.60° 90.00°	Depositor
Resolution (Å)	24.46 – 2.30 24.46 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.2 (24.46-2.30) 99.3 (24.46-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.41 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.168 , 0.218 0.169 , 0.204	Depositor DCC
R_{free} test set	932 reflections (3.31%)	DCC
Wilson B-factor (Å^2)	23.5	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 51.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 29120 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5392	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.39% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SCN, NAG, SEP, CA, OSM, HEM, NO3, 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	0.52	2/4891 (0.0%)	0.89	17/6634 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	168	PRO	N-CA	7.37	1.59	1.47
1	A	9	PRO	N-CA	5.66	1.56	1.47

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	10	VAL	C-N-CD	-20.49	75.53	120.60
1	A	10	VAL	N-CA-C	11.06	140.86	111.00
1	A	9	PRO	CA-N-CD	-8.55	99.53	111.50
1	A	168	PRO	CA-N-CD	-8.13	100.12	111.50
1	A	326	PRO	CA-N-CD	-7.62	100.83	111.50
1	A	167	CYS	CB-CA-C	7.22	124.84	110.40
1	A	170	PRO	CA-N-CD	-7.02	101.67	111.50
1	A	174	SER	N-CA-C	6.73	129.17	111.00
1	A	121	SER	N-CA-C	-5.85	95.21	111.00
1	A	167	CYS	CA-C-N	5.84	133.46	117.10
1	A	175	LEU	CA-CB-CG	5.72	128.46	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	7	GLY	N-CA-C	-5.65	98.97	113.10
1	A	11	PRO	CA-N-CD	-5.62	103.63	111.50
1	A	197	PRO	CA-N-CD	-5.59	103.68	111.50
1	A	2	TRP	CB-CA-C	-5.39	99.62	110.40
1	A	2	TRP	N-CA-C	-5.15	97.09	111.00
1	A	276	LEU	CA-CB-CG	5.10	127.03	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	197	PRO	Peptide
1	A	198	SEP	Mainchain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4774	0	4685	112	0
2	A	39	0	34	1	0
3	A	56	0	50	2	0
4	A	39	0	34	2	0
5	A	1	0	0	0	0
6	A	3	0	0	0	0
7	A	20	0	0	0	0
8	A	43	0	30	6	0
9	A	4	0	5	3	0
10	A	413	0	0	24	0
All	All	5392	0	4838	120	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 12.

All (120) 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:170:PRO:HD3	10:A:1010:HOH:O	1.56	1.02
1:A:55:LEU:HD23	10:A:1014:HOH:O	1.66	0.95
1:A:4:VAL:O	1:A:4:VAL:HG13	1.71	0.90
1:A:295:GLU:O	1:A:299:ILE:HD13	1.76	0.86
1:A:8:ALA:CB	1:A:9:PRO:HD2	2.08	0.83
1:A:360:ARG:NH1	1:A:372:ALA:HA	1.96	0.81
1:A:360:ARG:HH12	1:A:372:ALA:HA	1.45	0.80
1:A:8:ALA:HB3	1:A:9:PRO:HD2	1.64	0.80
1:A:240:ILE:HD11	1:A:382:ASN:HA	1.65	0.78
1:A:119:LEU:HD11	1:A:169:THR:CG2	2.12	0.78
1:A:227:LEU:HD23	1:A:270:LEU:HD22	1.64	0.78
3:A:605:NAG:H82	10:A:966:HOH:O	1.84	0.77
1:A:13:VAL:HA	10:A:1004:HOH:O	1.83	0.76
1:A:13:VAL:HG12	1:A:14:LYS:H	1.49	0.75
4:A:602:MAN:H61	10:A:699:HOH:O	1.87	0.75
1:A:196:GLU:HB3	1:A:198:SEP:O2P	1.88	0.73
1:A:8:ALA:CB	1:A:9:PRO:CD	2.65	0.73
1:A:150:LYS:HZ2	1:A:154:GLN:HE22	1.34	0.73
1:A:123:GLU:HB3	1:A:126:LYS:HE2	1.70	0.72
1:A:561:LYS:HG3	10:A:768:HOH:O	1.90	0.70
1:A:123:GLU:HG3	1:A:125:SER:H	1.57	0.70
1:A:82:ILE:HD12	1:A:480:LEU:HD13	1.71	0.69
1:A:13:VAL:HG12	1:A:14:LYS:N	2.09	0.68
1:A:235:SER:HB3	1:A:238:GLU:HG2	1.77	0.67
1:A:4:VAL:O	1:A:4:VAL:CG1	2.40	0.67
1:A:150:LYS:NZ	1:A:154:GLN:HE22	1.96	0.64
8:A:613:HEM:C1A	9:A:614:OSM:S	2.91	0.63
1:A:119:LEU:HD11	1:A:169:THR:HG22	1.82	0.60
1:A:530:TRP:CE2	1:A:531:GLU:HG3	2.37	0.59
1:A:333:ASN:HD22	1:A:333:ASN:C	2.04	0.59
1:A:119:LEU:HD11	1:A:169:THR:HG23	1.84	0.59
1:A:19:SER:HB3	10:A:1026:HOH:O	2.01	0.59
1:A:16:ASP:HB2	10:A:1002:HOH:O	2.02	0.58
1:A:102:GLN:O	1:A:106:ILE:HD13	2.03	0.58
1:A:323:LYS:HE3	1:A:324:TRP:CZ2	2.39	0.58
1:A:64:ARG:HH12	1:A:65:LYS:HE2	1.69	0.58
3:A:605:NAG:C1	10:A:818:HOH:O	2.53	0.57
1:A:322:GLN:HG3	10:A:798:HOH:O	2.05	0.57
1:A:408:ASN:HB2	10:A:784:HOH:O	2.04	0.57
1:A:169:THR:HG22	10:A:1010:HOH:O	2.03	0.57
1:A:467:LEU:HG	1:A:471:LEU:HD22	1.86	0.57
1:A:62:THR:O	1:A:64:ARG:N	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:ALA:HB1	1:A:9:PRO:CD	2.35	0.56
1:A:102:GLN:HE21	1:A:106:ILE:CD1	2.18	0.56
1:A:8:ALA:HB1	1:A:9:PRO:HD2	1.86	0.56
1:A:213:MET:HG2	1:A:273:HIS:CD2	2.41	0.55
1:A:396:VAL:HG11	1:A:553:ILE:HD12	1.88	0.54
8:A:613:HEM:NA	9:A:614:OSM:S	2.80	0.54
1:A:197:PRO:HB2	1:A:198:SEP:O3P	2.09	0.53
1:A:62:THR:HG22	1:A:64:ARG:HB3	1.91	0.53
1:A:142:ILE:CD1	1:A:436:ILE:HD13	2.40	0.52
1:A:425:THR:HB	10:A:1007:HOH:O	2.10	0.52
1:A:127:THR:O	1:A:131:GLU:HB2	2.10	0.51
1:A:362:ASP:OD1	1:A:362:ASP:C	2.48	0.50
1:A:17:GLU:HG3	10:A:1027:HOH:O	2.11	0.50
1:A:8:ALA:HB3	1:A:9:PRO:CD	2.37	0.50
1:A:142:ILE:HD11	1:A:436:ILE:HD13	1.93	0.50
1:A:588:SER:N	1:A:589:PRO:CD	2.75	0.50
1:A:19:SER:CB	10:A:1026:HOH:O	2.58	0.50
1:A:551:ARG:HD3	1:A:584:LYS:HA	1.94	0.49
1:A:118:GLU:HG2	1:A:120:GLY:H	1.77	0.49
1:A:42:ALA:HB2	1:A:166:VAL:HG11	1.94	0.49
1:A:407:MET:HB3	1:A:501:MET:CE	2.43	0.48
1:A:150:LYS:NZ	1:A:154:GLN:NE2	2.60	0.48
1:A:16:ASP:HB3	10:A:1026:HOH:O	2.14	0.48
1:A:54:GLY:HA2	10:A:797:HOH:O	2.13	0.48
1:A:160:PHE:HD1	1:A:436:ILE:CD1	2.26	0.48
1:A:10:VAL:HG11	1:A:41:ARG:CZ	2.43	0.48
1:A:245:ARG:HD3	10:A:820:HOH:O	2.14	0.47
1:A:468:GLN:HG2	1:A:474:LYS:HA	1.96	0.47
1:A:417:LEU:HD21	8:A:613:HEM:HMB3	1.97	0.47
1:A:36:LEU:HG	1:A:337:PRO:HD2	1.97	0.47
1:A:348:ARG:HH11	1:A:437:ASN:ND2	2.13	0.46
1:A:282:LYS:HE3	1:A:282:LYS:HB2	1.56	0.46
8:A:613:HEM:HBC2	8:A:613:HEM:HMC2	1.98	0.45
1:A:131:GLU:HB3	1:A:132:TYR:CD1	2.51	0.45
4:A:603:NAG:H3	10:A:994:HOH:O	2.16	0.45
1:A:299:ILE:HD11	1:A:590:TRP:HE1	1.82	0.45
1:A:282:LYS:HD2	10:A:979:HOH:O	2.15	0.45
1:A:230:ASN:OD1	1:A:231:ASN:N	2.50	0.44
1:A:113:PHE:O	1:A:115:PRO:HD3	2.18	0.44
1:A:13:VAL:CG1	1:A:14:LYS:N	2.79	0.44
1:A:118:GLU:C	1:A:120:GLY:N	2.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:563:PRO:HD3	1:A:576:PHE:CE2	2.53	0.43
1:A:417:LEU:CD2	8:A:613:HEM:HMB3	2.48	0.43
1:A:478:LYS:HE2	1:A:478:LYS:HB2	1.41	0.43
1:A:131:GLU:HB3	1:A:132:TYR:CE1	2.53	0.43
1:A:146:LYS:O	1:A:147:ASN:HB2	2.18	0.43
1:A:354:VAL:HG11	8:A:613:HEM:CBB	2.48	0.43
1:A:229:PHE:CD1	1:A:247:PRO:HG2	2.54	0.43
1:A:109:HIS:NE2	9:A:614:OSM:S	2.89	0.42
1:A:523:ARG:HG3	1:A:529:TRP:CE2	2.53	0.42
1:A:91:VAL:HG13	1:A:405:LYS:HG3	2.01	0.42
1:A:423:GLN:HA	1:A:423:GLN:HE21	1.84	0.42
1:A:377:HIS:HA	1:A:380:PHE:CE2	2.55	0.42
1:A:392:ILE:HD12	1:A:393:ASP:N	2.34	0.42
1:A:299:ILE:HD11	1:A:590:TRP:NE1	2.35	0.42
1:A:187:LEU:HD13	1:A:305:GLN:HA	2.01	0.42
1:A:425:THR:CB	10:A:1007:HOH:O	2.67	0.42
2:A:597:NAG:H62	10:A:878:HOH:O	2.20	0.42
1:A:229:PHE:CG	1:A:247:PRO:HG2	2.55	0.42
1:A:348:ARG:HH11	1:A:437:ASN:HD22	1.68	0.42
1:A:200:ALA:O	1:A:204:ARG:HG3	2.19	0.42
1:A:392:ILE:HD12	1:A:392:ILE:C	2.40	0.41
1:A:349:PHE:HA	1:A:497:ASN:HD21	1.83	0.41
1:A:288:ASN:O	1:A:292:LEU:HD23	2.21	0.41
1:A:17:GLU:N	10:A:1026:HOH:O	2.52	0.41
1:A:175:LEU:CD2	1:A:176:ALA:H	2.34	0.41
1:A:370:PRO:HG2	1:A:371:GLU:HG3	2.03	0.41
1:A:452:TRP:CD1	1:A:492:ILE:HD13	2.55	0.41
1:A:173:GLN:CG	1:A:174:SER:H	2.34	0.41
1:A:3:GLU:C	1:A:5:GLY:H	2.22	0.41
1:A:10:VAL:HG21	1:A:41:ARG:NH2	2.36	0.40
1:A:581:THR:HG22	1:A:581:THR:O	2.21	0.40
1:A:393:ASP:HB2	1:A:394:PRO:HD3	2.02	0.40
1:A:129:CYS:HB2	10:A:900:HOH:O	2.21	0.40
1:A:202:ARG:NH2	1:A:231:ASN:HB2	2.36	0.40
1:A:160:PHE:HD1	1:A:436:ILE:HD12	1.87	0.40
1:A:482:ASP:O	1:A:485:LYS:NZ	2.47	0.40
1:A:173:GLN:HG2	1:A:174:SER:H	1.87	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%)	557 (94%)	24 (4%)	11 (2%)	10 8

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	ALA
1	A	11	PRO
1	A	167	CYS
1	A	168	PRO
1	A	169	THR
1	A	174	SER
1	A	122	ASN
1	A	170	PRO
1	A	173	GLN
1	A	64	ARG
1	A	171	PRO

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	517/517 (100%)	476 (92%)	41 (8%)	15 19

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	VAL
1	A	6	CYS
1	A	9	PRO
1	A	11	PRO
1	A	18	ASN
1	A	57	LEU
1	A	64	ARG
1	A	82	ILE
1	A	91	VAL
1	A	98	LEU
1	A	124	HIS
1	A	131	GLU
1	A	153	THR
1	A	168	PRO
1	A	169	THR
1	A	170	PRO
1	A	173	GLN
1	A	174	SER
1	A	175	LEU
1	A	187	LEU
1	A	203	LEU
1	A	209	PRO
1	A	261	LEU
1	A	268	LEU
1	A	276	LEU
1	A	317	LEU
1	A	325	ILE
1	A	326	PRO
1	A	333	ASN
1	A	347	PHE
1	A	360	ARG
1	A	367	PRO
1	A	376	LEU
1	A	451	SER
1	A	464	LEU
1	A	471	LEU
1	A	480	LEU
1	A	511	LEU
1	A	520	GLN
1	A	564	LEU
1	A	594	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	122	ASN
1	A	147	ASN
1	A	154	GLN
1	A	333	ASN
1	A	364	ASN
1	A	423	GLN
1	A	437	ASN
1	A	497	ASN
1	A	520	GLN
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	8,9,10	1.56	2 (25%)	8,12,14	1.97	2 (25%)

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	P-O3P	2.03	1.62	1.54
1	A	198	SEP	P-O1P	3.12	1.61	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	198	SEP	O2P-P-OG	-2.91	98.19	106.56
1	A	198	SEP	OG-P-O1P	4.43	118.41	107.14

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 (i)

10 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	A	596	1,2	14,14,15	0.80	0	15,19,21	1.29	3 (20%)
2	NAG	A	597	2	14,14,15	1.00	1 (7%)	15,19,21	1.15	1 (6%)
2	MAN	A	598	2	11,11,12	0.69	0	14,15,17	1.23	1 (7%)
3	NAG	A	599	1,3	14,14,15	0.67	0	15,19,21	0.81	0
3	NAG	A	600	3	14,14,15	0.65	0	15,19,21	1.52	3 (20%)
4	NAG	A	601	1,4	14,14,15	0.61	0	15,19,21	0.93	0
4	MAN	A	602	4	11,11,12	0.82	0	14,15,17	1.10	2 (14%)
4	NAG	A	603	4	14,14,15	1.08	2 (14%)	15,19,21	1.68	3 (20%)
3	NAG	A	604	1,3	14,14,15	1.06	2 (14%)	15,19,21	1.43	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	A	605	3	14,14,15	0.72	1 (7%)	15,19,21	2.13	3 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	596	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	597	2	-	0/6/23/26	0/1/1/1
2	MAN	A	598	2	-	0/2/19/22	0/1/1/1
3	NAG	A	599	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	600	3	-	0/6/23/26	0/1/1/1
4	NAG	A	601	1,4	-	0/6/23/26	0/1/1/1
4	MAN	A	602	4	-	0/2/19/22	1/1/1/1
4	NAG	A	603	4	-	0/6/23/26	0/1/1/1
3	NAG	A	604	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	605	3	-	0/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	603	NAG	O5-C1	2.01	1.47	1.43
3	A	604	NAG	C1-C2	2.10	1.55	1.52
3	A	605	NAG	C1-C2	2.15	1.55	1.52
3	A	604	NAG	C3-C2	2.22	1.57	1.52
2	A	597	NAG	C1-C2	2.54	1.56	1.52
4	A	603	NAG	O5-C5	2.65	1.49	1.43

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	605	NAG	C3-C2-N2	-4.72	99.25	110.56
2	A	596	NAG	C2-N2-C7	-2.55	119.76	123.04
3	A	600	NAG	C2-N2-C7	-2.21	120.19	123.04
4	A	603	NAG	C3-C2-N2	-2.16	105.38	110.56
2	A	596	NAG	C3-C4-C5	-2.01	106.69	110.20
4	A	602	MAN	C1-C2-C3	2.10	112.02	109.54
2	A	596	NAG	C1-O5-C5	2.17	115.00	112.25
4	A	603	NAG	C3-C4-C5	2.33	114.27	110.20
3	A	600	NAG	C3-C4-C5	2.39	114.36	110.20
4	A	602	MAN	C1-O5-C5	2.81	115.81	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	605	NAG	C3-C4-C5	2.99	115.41	110.20
2	A	597	NAG	C4-C3-C2	3.01	115.91	111.23
2	A	598	MAN	C3-C4-C5	3.23	115.83	110.20
3	A	600	NAG	C4-C3-C2	3.83	117.18	111.23
3	A	604	NAG	C4-C3-C2	4.26	117.86	111.23
4	A	603	NAG	C1-O5-C5	5.13	118.75	112.25
3	A	605	NAG	C4-C3-C2	5.33	119.51	111.23

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	602	MAN	C1-C2-C3-C4-C5-O5

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	597	NAG	1	0
4	A	602	MAN	1	0
4	A	603	NAG	1	0
3	A	605	NAG	2	0

5.6 Ligand geometry

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 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	$\#\|Z\| > 2$
6	SCN	A	607	-	2,2,2	2.59	1 (50%)	1,1,1	0.04	0
7	NO3	A	608	-	3,3,3	3.00	3 (100%)	3,3,3	0.18	0
7	NO3	A	609	-	3,3,3	3.30	3 (100%)	3,3,3	0.22	0
7	NO3	A	610	-	3,3,3	3.27	3 (100%)	3,3,3	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	NO3	A	611	-	3,3,3	3.28	3 (100%)	3,3,3	0.27	0
7	NO3	A	612	-	3,3,3	3.26	3 (100%)	3,3,3	0.17	0
8	HEM	A	613	1	30,50,50	2.99	14 (46%)	24,82,82	2.17	6 (25%)
9	OSM	A	614	-	1,3,3	0.48	0	0,2,2	0.00	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	SCN	A	607	-	-	0/0/0/0	0/0/0/0
7	NO3	A	608	-	-	0/0/0/0	0/0/0/0
7	NO3	A	609	-	-	0/0/0/0	0/0/0/0
7	NO3	A	610	-	-	0/0/0/0	0/0/0/0
7	NO3	A	611	-	-	0/0/0/0	0/0/0/0
7	NO3	A	612	-	-	0/0/0/0	0/0/0/0
8	HEM	A	613	1	-	0/10/54/54	0/0/8/8
9	OSM	A	614	-	-	0/0/1/1	0/0/0/0

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	613	HEM	C3B-C4B	-11.38	1.41	1.51
8	A	613	HEM	C2D-C3D	-3.81	1.43	1.54
8	A	613	HEM	C3D-C4D	-3.11	1.47	1.51
8	A	613	HEM	C1A-CHA	-2.70	1.32	1.39
8	A	613	HEM	CHC-C4B	-2.43	1.32	1.38
8	A	613	HEM	C2D-C1D	-2.30	1.44	1.51
8	A	613	HEM	C2B-C1B	-2.11	1.45	1.51
8	A	613	HEM	FE-NB	2.06	2.08	1.97
8	A	613	HEM	CAD-CBD	2.13	1.63	1.52
7	A	608	NO3	O2-N	2.55	1.38	1.25
8	A	613	HEM	CAD-C3D	2.55	1.59	1.54
7	A	608	NO3	O3-N	2.73	1.39	1.25
8	A	613	HEM	C4C-NC	2.84	1.39	1.36
7	A	612	NO3	O2-N	2.86	1.40	1.25
7	A	612	NO3	O3-N	2.92	1.40	1.25
7	A	609	NO3	O2-N	2.99	1.40	1.25
7	A	609	NO3	O3-N	2.99	1.40	1.25
7	A	610	NO3	O2-N	3.01	1.40	1.25
7	A	611	NO3	O2-N	3.01	1.40	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	610	NO3	O3-N	3.02	1.41	1.25
7	A	611	NO3	O3-N	3.03	1.41	1.25
8	A	613	HEM	CMC-C2C	3.18	1.60	1.53
6	A	607	SCN	C-S	3.55	1.86	1.63
7	A	608	NO3	O1-N	3.61	1.39	1.24
7	A	610	NO3	O1-N	3.73	1.39	1.24
7	A	611	NO3	O1-N	3.74	1.39	1.24
7	A	609	NO3	O1-N	3.84	1.40	1.24
7	A	612	NO3	O1-N	3.90	1.40	1.24
8	A	613	HEM	C3B-CAB	4.05	1.58	1.51
8	A	613	HEM	C3C-CAC	4.38	1.59	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	613	HEM	CAD-C3D-C2D	2.06	119.14	113.22
8	A	613	HEM	CAA-CBA-CGA	2.13	116.65	112.75
8	A	613	HEM	C3C-CAC-CBC	3.04	129.12	124.46
8	A	613	HEM	CMC-C2C-C3C	3.26	124.67	116.53
8	A	613	HEM	CMB-C2B-C3B	3.99	126.50	116.53
8	A	613	HEM	CAD-C3D-C4D	7.23	137.95	112.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	613	HEM	6	0
9	A	614	OSM	3	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^{th} 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%)	-0.01	37 (6%) 24 32	9, 24, 59, 82	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	TRP	14.5
1	A	1	SER	12.3
1	A	4	VAL	10.3
1	A	121	SER	8.9
1	A	595	ASN	8.8
1	A	7	GLY	8.6
1	A	10	VAL	8.0
1	A	122	ASN	7.5
1	A	9	PRO	7.5
1	A	174	SER	7.4
1	A	8	ALA	7.3
1	A	5	GLY	6.6
1	A	3	GLU	6.6
1	A	170	PRO	6.5
1	A	173	GLN	5.9
1	A	594	GLU	5.6
1	A	593	ARG	5.5
1	A	11	PRO	5.5
1	A	172	TYR	5.5
1	A	6	CYS	5.4
1	A	171	PRO	5.3
1	A	12	LEU	4.5
1	A	119	LEU	4.2
1	A	120	GLY	3.8
1	A	126	LYS	3.8
1	A	13	VAL	3.7
1	A	175	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	167	CYS	3.3
1	A	123	GLU	3.3
1	A	169	THR	3.3
1	A	124	HIS	3.2
1	A	168	PRO	3.2
1	A	63	GLN	3.0
1	A	64	ARG	2.8
1	A	254	PHE	2.4
1	A	592	SER	2.1
1	A	231	ASN	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^{th} 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	0.75	0.20	-	27,30,51,51	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^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	NAG	A	596	14/15	0.77	0.25	1.90	51,56,61,69	0
3	NAG	A	599	14/15	0.94	0.13	0.23	33,44,49,54	0
4	NAG	A	601	14/15	0.94	0.12	-0.21	42,44,51,56	0
4	NAG	A	603	14/15	0.80	0.28	-	63,68,71,76	0
3	NAG	A	600	14/15	0.82	0.25	-	60,63,66,68	0
3	NAG	A	605	14/15	0.71	0.47	-	74,77,78,78	0
3	NAG	A	604	14/15	0.81	0.21	-	55,62,64,70	0
4	MAN	A	602	11/12	0.78	0.39	-	79,82,82,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	NAG	A	597	14/15	0.70	0.52	-	77,82,84,88	0
2	MAN	A	598	11/12	0.49	0.47	-	92,94,94,95	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^{th} 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
7	NO3	A	612	4/4	0.86	0.36	13.08	53,54,54,54	0
9	OSM	A	614	4/4	0.68	0.27	7.29	40,40,41,48	0
7	NO3	A	609	4/4	0.95	0.28	6.70	59,59,59,59	0
7	NO3	A	610	4/4	0.87	0.20	3.21	43,44,44,45	0
7	NO3	A	608	4/4	0.98	0.15	2.79	15,17,20,21	0
6	SCN	A	607	3/3	0.90	0.15	0.78	61,61,62,62	0
8	HEM	A	613	43/43	0.96	0.12	0.69	8,11,15,17	0
5	CA	A	606	1/1	0.99	0.08	-1.04	12,12,12,12	0
7	NO3	A	611	4/4	0.89	0.16	-	43,44,44,45	0

6.5 Other polymers (i)

There are no such residues in this entry.