Full wwPDB X-ray Structure Validation Report (i)

Dec 13, 2016 – 04:52 PM EST

PDB ID	:	3FAQ
Title	:	Crystal structure of lactoperoxidase complex with cyanide
Authors	:	Sheikh, I.A.; Singh, N.; Sharma, S.; Kaur, P.; Srinivasan, A.; Singh, T.P.
Deposited on	:	2008-11-18
Resolution	:	2.70 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:

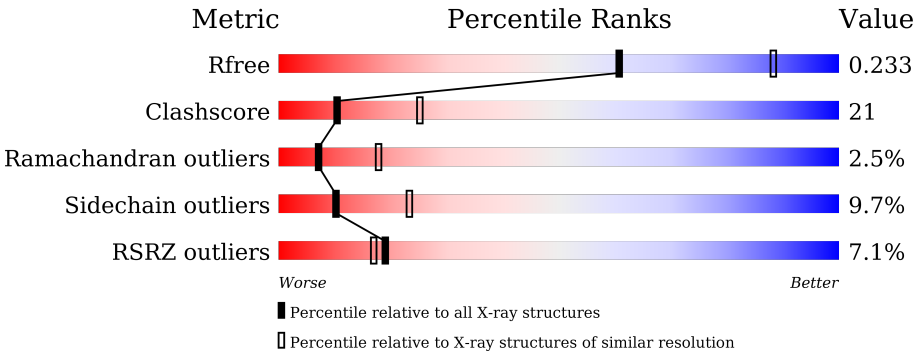
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

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 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	595	7% 60% 33% 6% •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	NAG	A	604	-	-	-	X
7	NAG	A	610	-	-	-	X

2 Entry composition

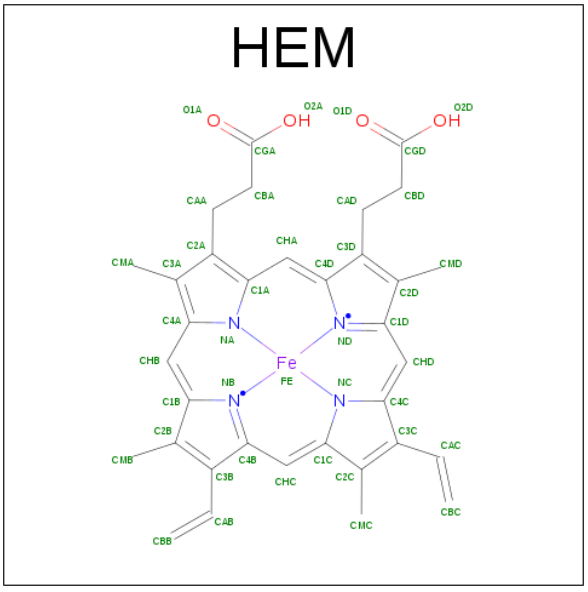
There are 10 unique types of molecules in this entry. The entry contains 5256 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

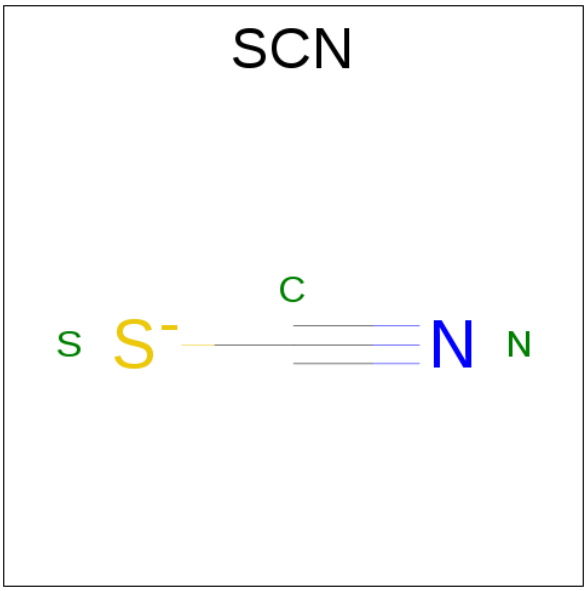
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	595	4778	3040	847	864	1	26	0	0	0

- 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
			Total	C	Fe	N	O		
2	A	1	43	34	1	4	4	0	0

- Molecule 3 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).

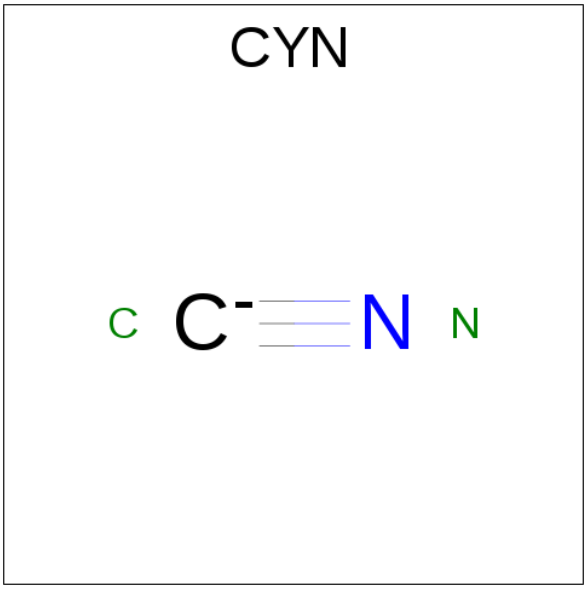


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N S 3 1 1 1	0	0
3	A	1	Total C N S 3 1 1 1	0	0

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

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

- Molecule 5 is CYANIDE ION (three-letter code: CYN) (formula: CN).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N 2 1 1	0	0

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

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

- Molecule 7 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 8 is a polymer of unknown type called SUGAR (3-MER).

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

- Molecule 9 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	4	Total C N O 50 28 2 20	0	0

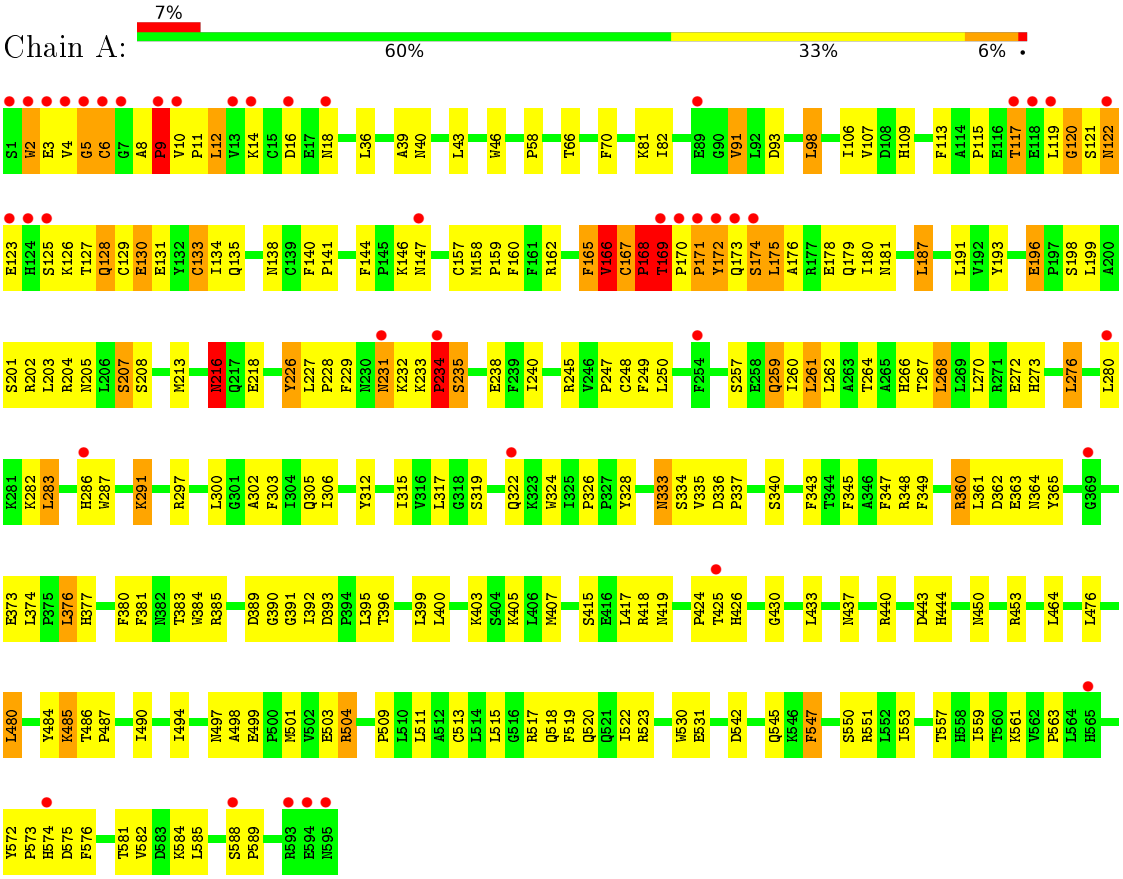
- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	274	Total O 274 274	0	0

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



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	54.45Å 80.67Å 77.80Å 90.00° 102.87° 90.00°	Depositor
Resolution (Å)	11.94 – 2.70 11.93 – 2.70	Depositor EDS
% Data completeness (in resolution range)	89.0 (11.94-2.70) 89.1 (11.93-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.45 (at 2.70Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.208 , 0.235 0.203 , 0.233	Depositor DCC
R_{free} test set	824 reflections (5.44%)	DCC
Wilson B-factor (Å^2)	33.2	Xtriage
Anisotropy	0.401	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 78.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5256	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.15% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SCN, NAG, SEP, CA, BMA, HEM, IOD, CYN, 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	0.51	3/4896 (0.1%)	0.96	22/6640 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	234	PRO	N-CD	6.71	1.57	1.47
1	A	234	PRO	CA-C	-6.24	1.40	1.52
1	A	234	PRO	C-N	-5.04	1.22	1.34

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	234	PRO	CA-N-CD	-23.12	79.14	111.50
1	A	234	PRO	N-CA-CB	17.15	123.88	103.30
1	A	234	PRO	N-CD-CG	15.44	126.36	103.20
1	A	233	LYS	C-N-CA	12.60	174.93	122.00
1	A	233	LYS	C-N-CD	-11.27	95.82	120.60
1	A	234	PRO	C-N-CA	-8.61	100.19	121.70
1	A	166	VAL	N-CA-C	8.54	134.06	111.00
1	A	9	PRO	CA-N-CD	-8.12	100.13	111.50
1	A	216	ASN	CA-CB-CG	6.55	127.80	113.40
1	A	233	LYS	CA-C-N	-5.93	100.51	117.10
1	A	547	PHE	CB-CG-CD1	-5.92	116.66	120.80
1	A	121	SER	N-CA-C	-5.90	95.08	111.00
1	A	122	ASN	N-CA-CB	5.87	121.17	110.60
1	A	233	LYS	CB-CA-C	5.46	121.32	110.40
1	A	173	GLN	N-CA-C	5.33	125.38	111.00
1	A	233	LYS	O-C-N	5.30	131.17	121.10
1	A	196	GLU	C-N-CD	-5.18	109.20	120.60
1	A	122	ASN	N-CA-C	-5.16	97.08	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	231	ASN	CA-CB-CG	5.06	124.53	113.40
1	A	120	GLY	N-CA-C	5.04	125.71	113.10
1	A	390	GLY	N-CA-C	5.03	125.68	113.10
1	A	174	SER	N-CA-C	5.01	124.52	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	4778	0	4690	198	0
2	A	43	0	30	0	0
3	A	6	0	0	0	0
4	A	1	0	0	0	0
5	A	2	0	0	1	0
6	A	7	0	0	0	0
7	A	56	0	50	2	0
8	A	39	0	34	5	0
9	A	50	0	43	4	0
10	A	274	0	0	15	0
All	All	5256	0	4847	209	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 21.

All (209) 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:547:PHE:HE2	1:A:585:LEU:HD22	1.33	0.93
1:A:175:LEU:CD2	1:A:176:ALA:H	1.88	0.86
1:A:196:GLU:HB3	1:A:198:SEP:O3P	1.74	0.85
1:A:551:ARG:HD3	1:A:584:LYS:HA	1.57	0.85
1:A:213:MET:HG2	1:A:273:HIS:CD2	2.15	0.82
1:A:169:THR:H	1:A:170:PRO:CD	1.95	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:THR:HB	1:A:426:HIS:CD2	2.19	0.78
1:A:123:GLU:HG3	1:A:125:SER:H	1.50	0.77
1:A:91:VAL:HG13	1:A:405:LYS:HG3	1.68	0.75
1:A:581:THR:HG22	1:A:581:THR:O	1.86	0.75
1:A:229:PHE:CD1	1:A:247:PRO:HG2	2.22	0.75
1:A:127:THR:HG23	1:A:131:GLU:HG3	1.68	0.74
1:A:302:ALA:O	1:A:306:ILE:HG13	1.90	0.72
1:A:123:GLU:HB3	1:A:126:LYS:NZ	2.05	0.71
1:A:588:SER:OG	1:A:589:PRO:HD3	1.91	0.70
1:A:10:VAL:HB	10:A:668:HOH:O	1.91	0.70
1:A:227:LEU:HD23	1:A:270:LEU:HD22	1.72	0.70
1:A:476:LEU:HD21	1:A:498:ALA:HB1	1.72	0.69
1:A:175:LEU:HD22	1:A:176:ALA:H	1.56	0.69
1:A:106:ILE:HG23	1:A:191:LEU:HD11	1.75	0.69
7:A:610:NAG:H61	10:A:775:HOH:O	1.92	0.69
1:A:503:GLU:O	1:A:504:ARG:HB2	1.90	0.68
1:A:175:LEU:HD23	1:A:176:ALA:H	1.58	0.68
1:A:123:GLU:HB3	1:A:126:LYS:CE	2.25	0.67
1:A:123:GLU:HB3	1:A:126:LYS:HE3	1.77	0.67
1:A:260:ILE:HD11	1:A:385:ARG:CB	2.25	0.67
1:A:187:LEU:HD13	1:A:305:GLN:HA	1.75	0.67
1:A:260:ILE:HD11	1:A:385:ARG:HB2	1.76	0.66
1:A:204:ARG:HD3	10:A:849:HOH:O	1.96	0.66
9:A:616:NAG:H2	10:A:843:HOH:O	1.94	0.66
1:A:146:LYS:O	1:A:147:ASN:HB2	1.94	0.66
1:A:130:GLU:HA	1:A:159:PRO:HG3	1.76	0.66
1:A:168:PRO:HB2	1:A:170:PRO:HD2	1.77	0.66
1:A:328:TYR:CD1	1:A:523:ARG:HD3	2.31	0.65
1:A:400:LEU:HD11	1:A:553:ILE:HD13	1.79	0.65
1:A:328:TYR:HD1	1:A:523:ARG:HD3	1.60	0.65
1:A:169:THR:N	1:A:170:PRO:CD	2.58	0.65
1:A:235:SER:HB3	1:A:238:GLU:HB2	1.80	0.64
1:A:547:PHE:CE2	1:A:585:LEU:HD22	2.24	0.63
1:A:126:LYS:NZ	1:A:126:LYS:HB2	2.13	0.63
1:A:165:PHE:CE2	1:A:172:TYR:HB2	2.34	0.63
1:A:179:GLN:HG2	1:A:444:HIS:CE1	2.33	0.63
1:A:81:LYS:HD2	10:A:763:HOH:O	1.98	0.62
1:A:226:TYR:OH	1:A:391:GLY:HA2	2.00	0.62
1:A:487:PRO:HA	1:A:490:ILE:HG13	1.80	0.62
1:A:348:ARG:HH11	1:A:437:ASN:HD22	1.47	0.61
1:A:168:PRO:HG3	1:A:172:TYR:CD1	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:615:NAG:H61	9:A:616:NAG:C7	2.31	0.60
1:A:287:TRP:CE2	1:A:291:LYS:HE3	2.36	0.60
8:A:613:NAG:H2	8:A:613:NAG:H61	1.84	0.60
1:A:381:PHE:CZ	1:A:424:PRO:HB3	2.36	0.60
1:A:324:TRP:O	1:A:326:PRO:HD2	2.03	0.59
1:A:165:PHE:HE2	1:A:172:TYR:HB2	1.65	0.59
1:A:393:ASP:HB2	10:A:652:HOH:O	2.03	0.59
1:A:574:HIS:HD2	1:A:575:ASP:OD1	1.86	0.59
1:A:205:ASN:OD1	1:A:207:SER:HB2	2.02	0.59
1:A:58:PRO:HD3	1:A:162:ARG:CZ	2.33	0.59
1:A:348:ARG:HD3	1:A:437:ASN:ND2	2.17	0.59
1:A:123:GLU:HB3	1:A:126:LYS:HZ2	1.67	0.59
1:A:166:VAL:CG2	1:A:178:GLU:HB2	2.32	0.58
1:A:168:PRO:HG2	1:A:169:THR:N	2.18	0.58
1:A:109:HIS:NE2	5:A:596:CYN:N	2.50	0.58
1:A:106:ILE:HG23	1:A:191:LEU:CD1	2.33	0.58
1:A:425:THR:HB	1:A:426:HIS:HD2	1.67	0.58
1:A:557:THR:OG1	1:A:559:ILE:HG12	2.04	0.58
1:A:82:ILE:HD13	1:A:480:LEU:HD13	1.86	0.58
1:A:126:LYS:HB2	1:A:126:LYS:HZ2	1.70	0.57
1:A:123:GLU:CB	1:A:126:LYS:HE3	2.34	0.57
1:A:333:ASN:HD22	1:A:333:ASN:N	2.03	0.57
1:A:417:LEU:HD22	1:A:433:LEU:HD22	1.86	0.57
1:A:348:ARG:HH11	1:A:437:ASN:ND2	2.04	0.56
1:A:169:THR:N	1:A:170:PRO:HD3	2.20	0.56
1:A:561:LYS:HE2	10:A:707:HOH:O	2.05	0.56
1:A:335:VAL:O	1:A:337:PRO:HD3	2.06	0.56
1:A:376:LEU:HD22	1:A:376:LEU:O	2.06	0.56
9:A:615:NAG:H61	9:A:616:NAG:O7	2.06	0.56
1:A:257:SER:O	1:A:381:PHE:HA	2.06	0.56
1:A:550:SER:HB2	1:A:582:VAL:HG11	1.86	0.56
1:A:129:CYS:HB2	10:A:811:HOH:O	2.07	0.55
1:A:175:LEU:HD22	1:A:176:ALA:N	2.21	0.55
1:A:130:GLU:CD	1:A:426:HIS:HD1	2.10	0.55
1:A:407:MET:HB3	1:A:501:MET:CE	2.37	0.55
9:A:616:NAG:O4	9:A:617:BMA:H61	2.06	0.55
1:A:165:PHE:O	1:A:180:ILE:HD11	2.06	0.54
1:A:3:GLU:HG2	1:A:5:GLY:H	1.72	0.54
1:A:513:CYS:O	1:A:517:ARG:HG3	2.07	0.54
1:A:166:VAL:HG22	1:A:178:GLU:O	2.09	0.53
1:A:2:TRP:CG	1:A:3:GLU:N	2.75	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:ASN:HB2	1:A:228:PRO:HA	1.89	0.53
1:A:123:GLU:HG3	1:A:125:SER:N	2.21	0.52
1:A:343:PHE:CD1	1:A:518:GLN:HG2	2.44	0.52
1:A:202:ARG:HD2	1:A:250:LEU:HD21	1.90	0.52
1:A:98:LEU:HD11	1:A:261:LEU:HD21	1.92	0.52
1:A:165:PHE:N	1:A:165:PHE:CD1	2.78	0.52
1:A:260:ILE:CD1	1:A:385:ARG:HB2	2.39	0.52
1:A:407:MET:HE2	10:A:874:HOH:O	2.09	0.51
1:A:530:TRP:CE2	1:A:531:GLU:HG3	2.45	0.51
1:A:175:LEU:CD2	1:A:176:ALA:N	2.66	0.51
1:A:426:HIS:CD2	1:A:426:HIS:N	2.78	0.51
1:A:117:THR:HG21	1:A:138:ASN:CG	2.31	0.51
1:A:324:TRP:HZ3	10:A:869:HOH:O	1.93	0.50
1:A:504:ARG:HG3	10:A:693:HOH:O	2.11	0.50
1:A:519:PHE:CD1	1:A:522:ILE:HD11	2.47	0.50
1:A:563:PRO:HD3	1:A:576:PHE:CE2	2.46	0.50
1:A:349:PHE:HB2	1:A:497:ASN:HD21	1.77	0.49
1:A:6:CYS:HB3	1:A:167:CYS:SG	2.53	0.49
1:A:8:ALA:N	1:A:9:PRO:CD	2.76	0.49
1:A:98:LEU:CD1	1:A:261:LEU:HD21	2.43	0.49
1:A:377:HIS:HA	1:A:380:PHE:CE2	2.47	0.49
1:A:499:GLU:OE1	1:A:509:PRO:HD2	2.13	0.49
1:A:43:LEU:CD2	1:A:181:ASN:HB2	2.43	0.49
1:A:46:TRP:CE2	1:A:340:SER:HB3	2.48	0.48
1:A:572:TYR:CE2	1:A:573:PRO:HB3	2.48	0.48
1:A:260:ILE:HD11	1:A:385:ARG:HB3	1.93	0.48
1:A:484:TYR:O	1:A:486:THR:N	2.44	0.48
1:A:126:LYS:HB3	10:A:867:HOH:O	2.14	0.48
1:A:581:THR:CG2	1:A:581:THR:O	2.56	0.47
1:A:187:LEU:CD1	1:A:305:GLN:HA	2.44	0.47
1:A:240:ILE:HD11	1:A:384:TRP:HD1	1.79	0.47
1:A:286:HIS:HB2	10:A:780:HOH:O	2.13	0.47
1:A:453:ARG:NH1	1:A:499:GLU:OE2	2.45	0.47
1:A:16:ASP:OD1	1:A:16:ASP:O	2.32	0.47
1:A:272:GLU:HG3	1:A:276:LEU:HD22	1.94	0.47
1:A:360:ARG:NH2	1:A:389:ASP:OD2	2.47	0.47
1:A:245:ARG:HH21	1:A:245:ARG:HG3	1.79	0.47
1:A:503:GLU:O	1:A:504:ARG:CB	2.57	0.47
1:A:272:GLU:O	1:A:276:LEU:HD22	2.15	0.46
1:A:166:VAL:HG21	1:A:178:GLU:HB2	1.96	0.46
1:A:168:PRO:CG	1:A:169:THR:N	2.75	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:PHE:HE2	1:A:158:MET:CE	2.29	0.46
1:A:187:LEU:HB3	1:A:305:GLN:HG2	1.96	0.46
1:A:162:ARG:HA	1:A:443:ASP:OD2	2.15	0.46
1:A:287:TRP:NE1	1:A:291:LYS:HE3	2.32	0.45
1:A:362:ASP:C	1:A:362:ASP:OD1	2.55	0.45
1:A:262:LEU:O	1:A:266:HIS:HD2	2.00	0.45
1:A:166:VAL:CG2	1:A:178:GLU:O	2.64	0.45
1:A:484:TYR:C	1:A:486:THR:H	2.18	0.45
8:A:613:NAG:C2	8:A:613:NAG:H61	2.46	0.45
1:A:127:THR:HG23	1:A:131:GLU:CG	2.42	0.45
1:A:400:LEU:HD11	1:A:553:ILE:CD1	2.44	0.45
8:A:613:NAG:H2	8:A:613:NAG:C6	2.46	0.45
8:A:613:NAG:H4	8:A:614:MAN:H2	1.71	0.45
1:A:70:PHE:CD1	1:A:485:LYS:HB2	2.52	0.45
1:A:120:GLY:HA2	1:A:123:GLU:OE1	2.17	0.45
1:A:349:PHE:CB	1:A:497:ASN:HD21	2.30	0.45
1:A:419:ASN:O	1:A:430:GLY:HA2	2.16	0.44
1:A:333:ASN:ND2	1:A:333:ASN:N	2.65	0.44
1:A:407:MET:HB3	1:A:501:MET:HE2	1.98	0.44
1:A:450:ASN:HD21	1:A:487:PRO:HB2	1.81	0.44
1:A:333:ASN:H	1:A:333:ASN:ND2	2.15	0.44
1:A:133:CYS:SG	1:A:157:CYS:CB	3.06	0.44
1:A:227:LEU:HD22	10:A:623:HOH:O	2.16	0.44
1:A:193:TYR:CE2	1:A:297:ARG:HG3	2.52	0.44
1:A:319:SER:OG	1:A:503:GLU:HB3	2.18	0.44
1:A:572:TYR:HA	1:A:573:PRO:HA	1.70	0.44
1:A:82:ILE:HG21	1:A:494:ILE:HD11	1.99	0.44
1:A:199:LEU:C	1:A:201:SER:H	2.21	0.44
1:A:300:LEU:O	1:A:303:PHE:HB3	2.18	0.44
1:A:547:PHE:CE2	1:A:585:LEU:HD13	2.52	0.44
1:A:58:PRO:HD3	1:A:162:ARG:NH1	2.32	0.44
1:A:268:LEU:HD11	1:A:392:ILE:CD1	2.48	0.44
1:A:345:PHE:HZ	1:A:440:ARG:HG3	1.83	0.43
1:A:135:GLN:HB2	1:A:141:PRO:HD2	2.00	0.43
1:A:312:TYR:O	1:A:315:ILE:HG12	2.19	0.43
1:A:249:PHE:CE2	1:A:383:THR:HG22	2.52	0.43
1:A:282:LYS:HB2	1:A:282:LYS:HE3	1.67	0.43
1:A:264:THR:O	1:A:267:THR:HB	2.19	0.43
1:A:8:ALA:N	1:A:9:PRO:HD2	2.33	0.43
1:A:268:LEU:HD11	1:A:392:ILE:HD11	2.01	0.43
8:A:613:NAG:C2	8:A:613:NAG:C6	2.96	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:VAL:HG23	1:A:4:VAL:O	2.18	0.43
1:A:364:ASN:O	1:A:365:TYR:HB2	2.19	0.42
1:A:264:THR:HG23	1:A:392:ILE:HB	2.01	0.42
1:A:36:LEU:HD12	1:A:36:LEU:HA	1.71	0.42
1:A:93:ASP:O	1:A:403:LYS:HD3	2.19	0.42
7:A:604:NAG:C6	7:A:606:NAG:C1	2.97	0.42
1:A:202:ARG:HD3	10:A:669:HOH:O	2.19	0.42
1:A:283:LEU:HD22	1:A:283:LEU:O	2.19	0.42
1:A:333:ASN:HD22	1:A:334:SER:N	2.16	0.42
1:A:199:LEU:C	1:A:201:SER:N	2.73	0.41
1:A:240:ILE:C	1:A:240:ILE:HD12	2.40	0.41
1:A:3:GLU:OE1	1:A:6:CYS:SG	2.76	0.41
1:A:130:GLU:HG2	1:A:426:HIS:CE1	2.55	0.41
1:A:248:CYS:HA	1:A:383:THR:HG21	2.02	0.41
1:A:202:ARG:CD	1:A:250:LEU:HD21	2.49	0.41
1:A:360:ARG:O	1:A:361:LEU:HD23	2.20	0.41
1:A:113:PHE:O	1:A:115:PRO:HD3	2.20	0.41
1:A:376:LEU:HD13	1:A:380:PHE:CZ	2.55	0.41
1:A:396:THR:O	1:A:399:LEU:HB2	2.19	0.41
1:A:345:PHE:CZ	1:A:440:ARG:HG3	2.55	0.41
1:A:276:LEU:O	1:A:280:LEU:HG	2.21	0.41
1:A:336:ASP:HA	1:A:337:PRO:HD2	1.96	0.41
1:A:373:GLU:O	1:A:374:LEU:HD23	2.20	0.41
1:A:395:LEU:HD23	1:A:395:LEU:HA	1.93	0.41
1:A:240:ILE:HD11	1:A:384:TRP:CD1	2.56	0.41
1:A:125:SER:HA	1:A:128:GLN:HB3	2.02	0.41
1:A:160:PHE:CD1	1:A:160:PHE:C	2.94	0.41
1:A:235:SER:CB	1:A:238:GLU:HB2	2.50	0.41
1:A:39:ALA:O	1:A:40:ASN:HB2	2.21	0.41
1:A:66:THR:HB	1:A:70:PHE:N	2.36	0.41
1:A:324:TRP:CZ2	1:A:513:CYS:HB2	2.56	0.40
1:A:106:ILE:O	1:A:107:VAL:C	2.59	0.40
1:A:12:LEU:H	1:A:12:LEU:HG	1.57	0.40
1:A:345:PHE:HE2	1:A:440:ARG:HB3	1.86	0.40
1:A:515:LEU:HA	1:A:515:LEU:HD23	1.92	0.40
1:A:343:PHE:CG	1:A:518:GLN:HG2	2.56	0.40
1:A:144:PHE:HE2	1:A:158:MET:HE3	1.85	0.40
1:A:140:PHE:O	1:A:160:PHE:HB3	2.22	0.40
1:A:259:GLN:O	1:A:260:ILE:C	2.60	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%)	537 (91%)	40 (7%)	15 (2%)	7 18

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	PRO
1	A	12	LEU
1	A	168	PRO
1	A	169	THR
1	A	171	PRO
1	A	174	SER
1	A	234	PRO
1	A	14	LYS
1	A	485	LYS
1	A	2	TRP
1	A	122	ASN
1	A	9	PRO
1	A	18	ASN
1	A	133	CYS
1	A	5	GLY

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%)	467 (90%)	50 (10%)	10 23

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	CYS
1	A	9	PRO
1	A	91	VAL
1	A	98	LEU
1	A	117	THR
1	A	119	LEU
1	A	128	GLN
1	A	130	GLU
1	A	134	ILE
1	A	165	PHE
1	A	166	VAL
1	A	167	CYS
1	A	168	PRO
1	A	169	THR
1	A	171	PRO
1	A	172	TYR
1	A	175	LEU
1	A	187	LEU
1	A	203	LEU
1	A	207	SER
1	A	208	SER
1	A	216	ASN
1	A	218	GLU
1	A	226	TYR
1	A	231	ASN
1	A	232	LYS
1	A	234	PRO
1	A	235	SER
1	A	259	GLN
1	A	261	LEU
1	A	268	LEU
1	A	276	LEU
1	A	283	LEU
1	A	291	LYS
1	A	317	LEU
1	A	322	GLN
1	A	333	ASN
1	A	347	PHE
1	A	360	ARG
1	A	363	GLU
1	A	376	LEU
1	A	415	SER

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Mol	Chain	Res	Type
1	A	418	ARG
1	A	464	LEU
1	A	480	LEU
1	A	504	ARG
1	A	511	LEU
1	A	520	GLN
1	A	542	ASP
1	A	545	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	217	GLN
1	A	284	ASN
1	A	322	GLN
1	A	333	ASN
1	A	341	ASN
1	A	423	GLN
1	A	437	ASN
1	A	497	ASN
1	A	574	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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	7,9,10	1.16	0	8,12,14	3.64	4 (50%)

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

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	198	SEP	O3P-P-O1P	-3.14	100.36	110.63
1	A	198	SEP	O3P-P-O2P	2.85	117.90	107.44
1	A	198	SEP	O2P-P-OG	3.52	116.99	106.72
1	A	198	SEP	OG-CB-CA	8.34	115.52	108.26

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.5 Carbohydrates (i)

11 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	$\#\|Z\| > 2$
7	NAG	A	604	1,7	14,14,15	0.57	0	15,19,21	1.50	3 (20%)
7	NAG	A	606	7	14,14,15	0.67	0	15,19,21	1.38	2 (13%)
7	NAG	A	610	1,7	14,14,15	0.62	0	15,19,21	0.88	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	NAG	A	611	7	14,14,15	0.71	0	15,19,21	2.09	5 (33%)
8	NAG	A	612	1,8	14,14,15	0.76	0	15,19,21	0.95	1 (6%)
8	NAG	A	613	8	14,14,15	1.04	1 (7%)	15,19,21	0.95	1 (6%)
8	MAN	A	614	8	11,11,12	0.77	1 (9%)	15,15,17	2.13	3 (20%)
9	NAG	A	615	1,9	14,14,15	0.92	0	15,19,21	1.42	2 (13%)
9	NAG	A	616	9	14,14,15	1.41	3 (21%)	15,19,21	1.60	1 (6%)
9	BMA	A	617	9	11,11,12	0.81	0	15,15,17	0.63	0
9	MAN	A	618	9	11,11,12	0.57	0	15,15,17	0.54	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	A	604	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	606	7	-	0/6/23/26	0/1/1/1
7	NAG	A	610	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	611	7	-	0/6/23/26	0/1/1/1
8	NAG	A	612	1,8	-	0/6/23/26	0/1/1/1
8	NAG	A	613	8	-	0/6/23/26	0/1/1/1
8	MAN	A	614	8	-	0/2/19/22	0/1/1/1
9	NAG	A	615	1,9	-	0/6/23/26	0/1/1/1
9	NAG	A	616	9	-	0/6/23/26	0/1/1/1
9	BMA	A	617	9	-	0/2/19/22	1/1/1/1
9	MAN	A	618	9	-	0/2/19/22	1/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	614	MAN	C2-C3	2.01	1.55	1.52
9	A	616	NAG	O5-C5	2.06	1.48	1.43
9	A	616	NAG	O5-C1	2.22	1.47	1.43
9	A	616	NAG	C1-C2	2.51	1.56	1.52
8	A	613	NAG	C1-C2	2.57	1.56	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	604	NAG	C4-C3-C2	-3.80	105.44	111.34
7	A	611	NAG	C2-N2-C7	-3.24	118.89	123.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	604	NAG	C2-N2-C7	-3.09	119.09	123.11
7	A	606	NAG	C2-N2-C7	-2.67	119.64	123.11
8	A	612	NAG	C2-N2-C7	-2.47	119.89	123.11
7	A	604	NAG	C3-C4-C5	-2.33	106.07	110.23
7	A	610	NAG	C2-N2-C7	-2.22	120.22	123.11
9	A	615	NAG	C2-N2-C7	-2.19	120.25	123.11
8	A	613	NAG	C1-O5-C5	2.11	115.24	112.14
7	A	611	NAG	C3-C4-C5	2.49	114.67	110.23
7	A	611	NAG	O5-C5-C4	2.50	114.27	110.13
8	A	614	MAN	O5-C1-C2	2.51	114.90	110.89
8	A	614	MAN	C2-C3-C4	2.55	115.50	111.05
7	A	611	NAG	C6-C5-C4	3.03	120.57	112.99
7	A	606	NAG	C4-C3-C2	3.64	116.99	111.34
9	A	616	NAG	C1-O5-C5	3.84	117.78	112.14
9	A	615	NAG	C4-C3-C2	4.24	117.91	111.34
7	A	611	NAG	C1-O5-C5	5.34	119.99	112.14
8	A	614	MAN	C1-C2-C3	7.05	118.09	109.55

There are no chirality outliers.

There are no torsion outliers.

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	618	MAN	C1-C2-C3-C4-C5-O5
9	A	617	BMA	C1-C2-C3-C4-C5-O5

8 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	604	NAG	1	0
7	A	606	NAG	1	0
7	A	610	NAG	1	0
8	A	613	NAG	5	0
8	A	614	MAN	1	0
9	A	615	NAG	2	0
9	A	616	NAG	4	0
9	A	617	BMA	1	0

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	CYN	A	596	-	0,1,1	0.00	-	0,0,0	0.00	-
2	HEM	A	605	1	24,50,50	2.26	8 (33%)	16,82,82	2.19	2 (12%)
3	SCN	A	607	-	2,2,2	1.64	1 (50%)	1,1,1	0.25	0
3	SCN	A	608	-	2,2,2	1.62	1 (50%)	1,1,1	0.22	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CYN	A	596	-	-	0/0/0/0	0/0/0/0
2	HEM	A	605	1	-	0/6/54/54	0/0/8/8
3	SCN	A	607	-	-	0/0/0/0	0/0/0/0
3	SCN	A	608	-	-	0/0/0/0	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	605	HEM	C3B-C2B	-5.49	1.33	1.40
2	A	605	HEM	C3C-C2C	-3.30	1.36	1.40
3	A	608	SCN	C-S	2.29	1.77	1.63
3	A	607	SCN	C-S	2.32	1.77	1.63
2	A	605	HEM	CAA-C2A	2.46	1.56	1.52
2	A	605	HEM	C3C-CAC	2.64	1.53	1.47
2	A	605	HEM	C3B-CAB	2.73	1.53	1.47
2	A	605	HEM	C1B-NB	2.94	1.40	1.36
2	A	605	HEM	CAD-C3D	4.03	1.57	1.52
2	A	605	HEM	C3D-C2D	4.50	1.51	1.37

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	605	HEM	C3B-CAB-CBB	-6.86	112.61	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	605	HEM	CMA-C3A-C4A	-3.09	123.05	128.31

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
5	A	596	CYN	1	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%)	0.14	42 (7%)	19	17	10, 28, 72, 100	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	SER	7.6
1	A	122	ASN	7.3
1	A	174	SER	7.2
1	A	13	VAL	5.9
1	A	123	GLU	5.9
1	A	7	GLY	5.6
1	A	593	ARG	5.6
1	A	171	PRO	5.6
1	A	173	GLN	5.1
1	A	170	PRO	5.0
1	A	595	ASN	5.0
1	A	118	GLU	4.1
1	A	124	HIS	4.0
1	A	2	TRP	3.9
1	A	5	GLY	3.9
1	A	594	GLU	3.7
1	A	6	CYS	3.7
1	A	425	THR	3.5
1	A	172	TYR	3.4
1	A	588	SER	3.2
1	A	231	ASN	3.1
1	A	234	PRO	3.0
1	A	169	THR	3.0
1	A	9	PRO	2.9
1	A	147	ASN	2.8
1	A	119	LEU	2.8
1	A	125	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	89	GLU	2.6
1	A	565	HIS	2.4
1	A	117	THR	2.3
1	A	286	HIS	2.3
1	A	4	VAL	2.3
1	A	14	LYS	2.2
1	A	574	HIS	2.2
1	A	10	VAL	2.2
1	A	16	ASP	2.2
1	A	254	PHE	2.2
1	A	3	GLU	2.1
1	A	18	ASN	2.1
1	A	369	GLY	2.1
1	A	322	GLN	2.0
1	A	280	LEU	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	0.95	0.17	-	31,40,42,43	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
7	NAG	A	604	14/15	0.77	0.34	3.46	57,63,66,70	0
7	NAG	A	610	14/15	0.82	0.22	2.05	48,50,55,57	0
8	NAG	A	612	14/15	0.85	0.19	0.46	51,53,55,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
9	MAN	A	618	11/12	0.75	0.61	-	77,79,79,79	0
8	NAG	A	613	14/15	0.84	0.39	-	68,72,75,76	0
9	NAG	A	615	14/15	0.76	0.39	-	58,64,67,69	0
7	NAG	A	606	14/15	0.82	0.40	-	73,75,77,77	0
8	MAN	A	614	11/12	0.70	0.54	-	79,81,81,81	0
9	BMA	A	617	11/12	0.71	0.44	-	79,80,80,80	0
9	NAG	A	616	14/15	0.50	0.69	-	74,77,79,80	0
7	NAG	A	611	14/15	0.72	0.46	-	59,62,63,63	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, 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	HEM	A	605	43/43	0.90	0.18	0.26	18,26,30,35	0
3	SCN	A	607	3/3	0.96	0.18	0.13	16,16,16,19	0
6	IOD	A	597	1/1	0.99	0.15	-0.76	52,52,52,52	1
6	IOD	A	603	1/1	0.99	0.04	-2.15	61,61,61,61	0
6	IOD	A	600	1/1	0.98	0.06	-2.19	90,90,90,90	0
6	IOD	A	602	1/1	1.00	0.04	-3.04	21,21,21,21	0
4	CA	A	609	1/1	0.98	0.05	-3.36	17,17,17,17	0
6	IOD	A	601	1/1	0.99	0.04	-4.20	66,66,66,66	0
6	IOD	A	599	1/1	0.97	0.05	-4.21	79,79,79,79	0
3	SCN	A	608	3/3	0.91	0.14	-	32,32,36,37	0
6	IOD	A	598	1/1	0.97	0.12	-	56,56,56,56	1
5	CYN	A	596	2/2	0.97	0.13	-	35,35,35,38	0

6.5 Other polymers

There are no such residues in this entry.