



wwPDB X-ray Structure Validation Summary Report i

Feb 28, 2014 – 01:40 AM GMT

PDB ID : 3GWJ
Title : Crystal structure of Antheraea pernyi arylphorin
Authors : Ryu, K.S.; Lee, J.O.; Kwon, T.H.; Kim, S.
Deposited on : 2009-04-01
Resolution : 2.43 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

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

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

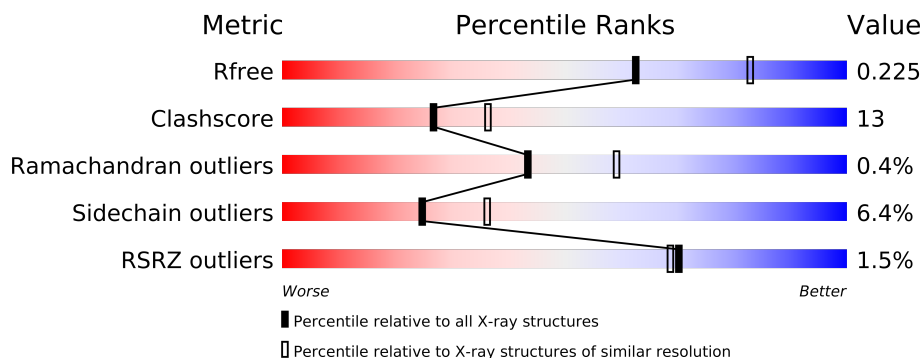
The following versions of software and data (see [references](#)) were used in the production of this report:

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

1 Overall quality at a glance



The reported resolution of this entry is 2.43 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	2989 (2.48-2.40)
Clashscore	79885	3698 (2.48-2.40)
Ramachandran outliers	78287	3639 (2.48-2.40)
Sidechain outliers	78261	3640 (2.48-2.40)
RSRZ outliers	66119	2993 (2.48-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	674	
1	B	674	
1	C	674	
1	D	674	
1	E	674	
1	F	674	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 36702 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Arylphorin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	674	Total	C	N	O	S	0	0	0
			5718	3752	906	1047	13			
1	B	674	Total	C	N	O	S	0	0	0
			5718	3752	906	1047	13			
1	C	674	Total	C	N	O	S	0	0	0
			5718	3752	906	1047	13			
1	D	674	Total	C	N	O	S	0	0	0
			5718	3752	906	1047	13			
1	E	674	Total	C	N	O	S	0	0	0
			5718	3752	906	1047	13			
1	F	674	Total	C	N	O	S	0	0	0
			5718	3752	906	1047	13			

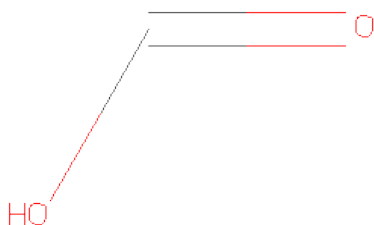
- Molecule 2 is a polymer of unknown type called SUGAR (12-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	12	Total	C	N	O	0	0
			138	76	2	60		
2	B	12	Total	C	N	O	0	0
			138	76	2	60		
2	C	12	Total	C	N	O	0	0
			138	76	2	60		
2	D	12	Total	C	N	O	0	0
			138	76	2	60		
2	E	12	Total	C	N	O	0	0
			138	76	2	60		
2	F	12	Total	C	N	O	0	0
			138	76	2	60		

- 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	B	2	Total	C	N	O	0	0
			28	16	2	10		
3	C	2	Total	C	N	O	0	0
			28	16	2	10		
3	D	2	Total	C	N	O	0	0
			28	16	2	10		
3	E	2	Total	C	N	O	0	0
			28	16	2	10		
3	F	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is FORMIC ACID (three-letter code: FMT) (formula: CH₂O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			3	1	2		
4	B	1	Total	C	O	0	0
			3	1	2		
4	C	1	Total	C	O	0	0
			3	1	2		
4	D	1	Total	C	O	0	0
			3	1	2		
4	E	1	Total	C	O	0	0
			3	1	2		
4	F	1	Total	C	O	0	0
			3	1	2		

- Molecule 5 is water.

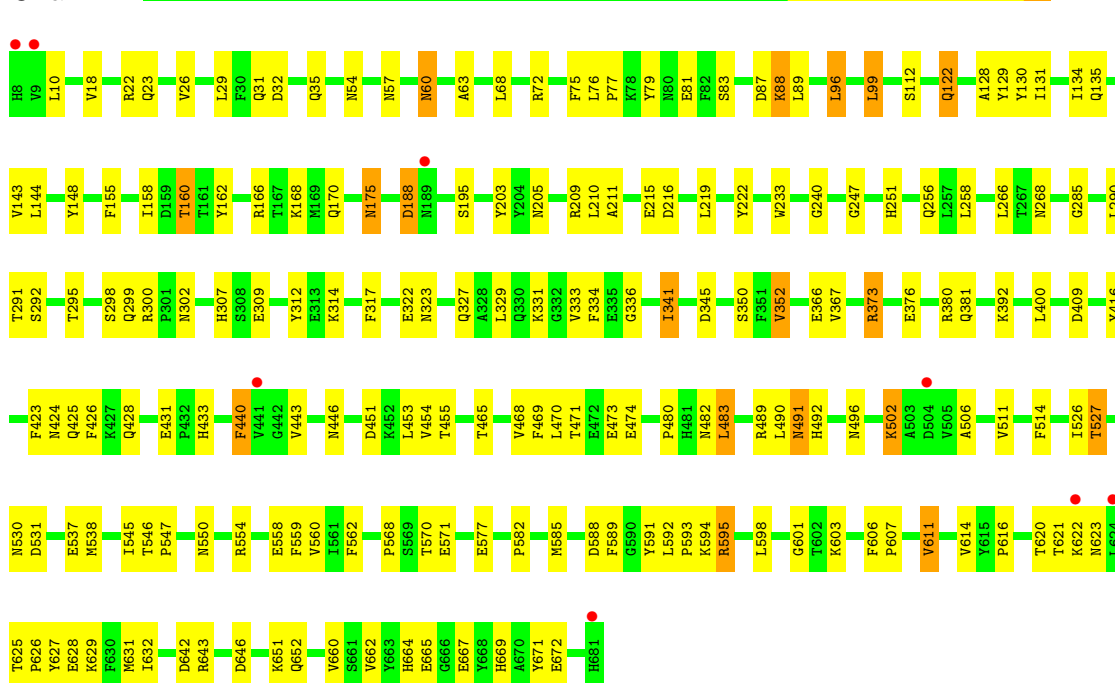
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	225	Total 225	O 225	0	0
5	B	241	Total 241	O 241	0	0
5	C	200	Total 200	O 200	0	0
5	D	243	Total 243	O 243	0	0
5	E	218	Total 218	O 218	0	0
5	F	253	Total 253	O 253	0	0

3 Residue-property plots

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

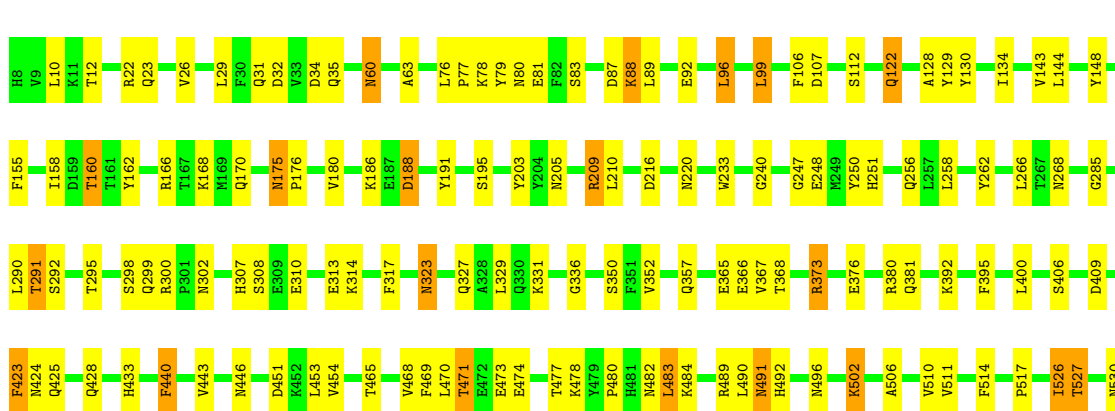
• Molecule 1: Arylphorin

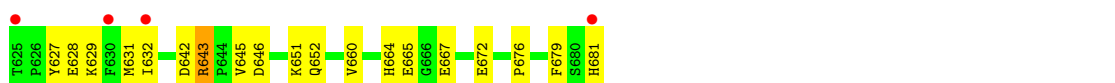
Chain A:



• Molecule 1: Arylphorin

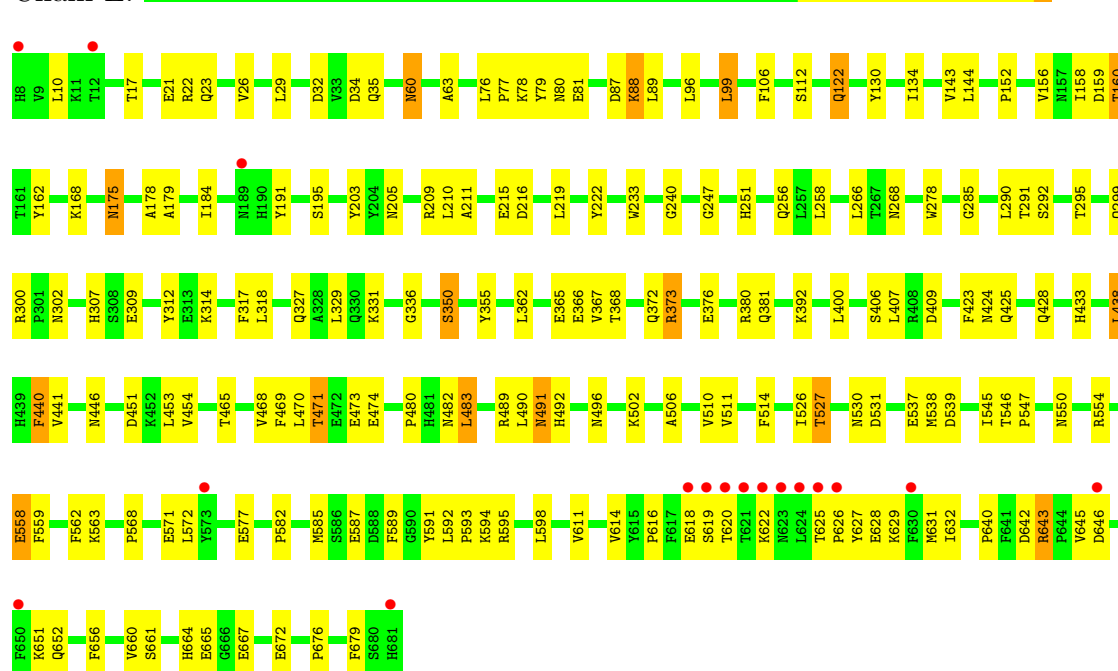
Chain B:





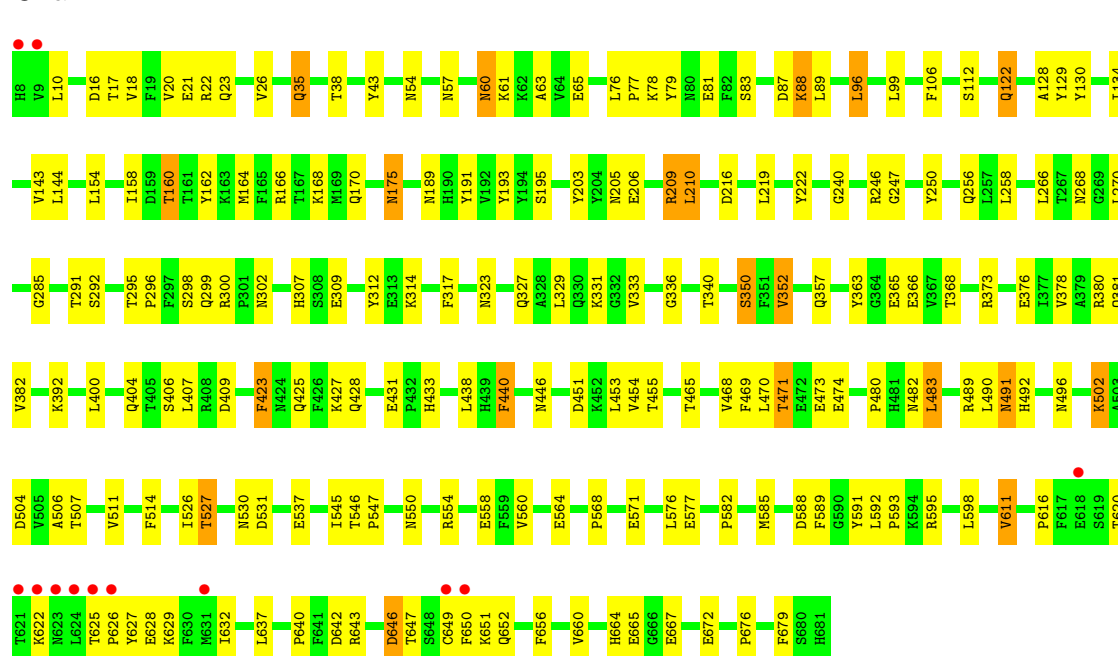
- Molecule 1: Arylphorin

Chain E:



- Molecule 1: Arylphorin

Chain F:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	121.20Å 119.47Å 319.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.80 – 2.43 48.80 – 2.43	Depositor EDS
% Data completeness (in resolution range)	95.7 (48.80-2.43) 95.8 (48.80-2.43)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.10 (at 2.42Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.182 , 0.229 0.182 , 0.225	Depositor DCC
R_{free} test set	8410 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	32.3	Xtriage
Anisotropy	0.276	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 13.2	EDS
Estimated twinning fraction	0.023 for k,h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 168292 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	36702	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.12% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GLC, FMT, BMA, NAG, 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	0.40	0/5907	0.58	0/8017
1	B	0.40	0/5907	0.59	0/8017
1	C	0.41	0/5907	0.59	0/8017
1	D	0.40	0/5907	0.58	0/8017
1	E	0.40	0/5907	0.58	0/8017
1	F	0.41	0/5907	0.59	1/8017 (0.0%)
All	All	0.40	0/35442	0.59	1/48102 (0.0%)

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	D	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	649	CYS	CA-CB-SG	-6.93	101.53	114.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	342	TYR	Sidechain

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5718	0	5424	151	0
1	B	5718	0	5424	157	0
1	C	5718	0	5424	150	0
1	D	5718	0	5424	159	0
1	E	5718	0	5424	159	0
1	F	5718	0	5424	162	0
2	A	138	0	115	0	0
2	B	138	0	115	1	0
2	C	138	0	115	1	0
2	D	138	0	115	0	0
2	E	138	0	115	0	0
2	F	138	0	115	2	0
3	A	28	0	25	0	0
3	B	28	0	25	0	0
3	C	28	0	25	0	0
3	D	28	0	25	0	0
3	E	28	0	25	0	0
3	F	28	0	25	0	0
4	A	3	0	1	1	0
4	B	3	0	1	2	0
4	C	3	0	1	1	0
4	D	3	0	1	1	0
4	E	3	0	1	1	0
4	F	3	0	1	1	0
5	A	225	0	0	7	0
5	B	241	0	0	11	0
5	C	200	0	0	12	0
5	D	243	0	0	11	0
5	E	218	0	0	14	0
5	F	253	0	0	11	0
All	All	36702	0	33390	899	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 13.

The worst 5 of 899 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:134:ILE:HD11	1:D:144:LEU:HD11	1.38	1.06
1:C:134:ILE:HD11	1:C:144:LEU:HD11	1.41	1.02
1:C:23:GLN:HE22	1:C:143:VAL:H	1.06	1.00
1:B:134:ILE:HD11	1:B:144:LEU:HD11	1.48	0.96
1:B:35:GLN:HE22	1:B:470:LEU:H	1.12	0.96

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	672/674 (100%)	649 (97%)	20 (3%)	3 (0%)	43	59
1	B	672/674 (100%)	649 (97%)	21 (3%)	2 (0%)	50	66
1	C	672/674 (100%)	653 (97%)	17 (2%)	2 (0%)	50	66
1	D	672/674 (100%)	655 (98%)	13 (2%)	4 (1%)	33	46
1	E	672/674 (100%)	651 (97%)	18 (3%)	3 (0%)	43	59
1	F	672/674 (100%)	649 (97%)	20 (3%)	3 (0%)	43	59
All	All	4032/4044 (100%)	3906 (97%)	109 (3%)	17 (0%)	43	59

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	87	ASP
1	C	646	ASP
1	E	240	GLY
1	F	240	GLY
1	F	646	ASP

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	613/613 (100%)	574 (94%)	39 (6%)	25	36
1	B	613/613 (100%)	570 (93%)	43 (7%)	21	32
1	C	613/613 (100%)	574 (94%)	39 (6%)	25	36
1	D	613/613 (100%)	573 (94%)	40 (6%)	24	35
1	E	613/613 (100%)	575 (94%)	38 (6%)	26	38
1	F	613/613 (100%)	576 (94%)	37 (6%)	27	40
All	All	3678/3678 (100%)	3442 (94%)	236 (6%)	25	36

5 of 236 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	453	LEU
1	D	203	TYR
1	F	423	PHE
1	C	491	ASN
1	C	614	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 183 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	381	GLN
1	D	175	ASN
1	F	323	ASN
1	C	446	ASN
1	D	23	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

84 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	801	1,2	12,14,15	0.56	0	15,19,21	0.75	0
2	NAG	A	802	2	12,14,15	0.58	0	15,19,21	0.93	0
2	BMA	A	803	2	10,11,12	0.43	0	11,15,17	0.46	0
2	MAN	A	804	2	10,11,12	0.31	0	11,15,17	0.46	0
2	MAN	A	805	2	10,11,12	0.43	0	11,15,17	0.32	0
2	MAN	A	806	2	10,11,12	0.46	0	11,15,17	0.41	0
2	GLC	A	807	2	10,11,12	0.33	0	11,15,17	0.81	0
2	MAN	A	808	2	10,11,12	0.45	0	11,15,17	0.56	0
2	MAN	A	809	2	10,11,12	0.53	0	11,15,17	0.58	0
2	MAN	A	810	2	10,11,12	0.46	0	11,15,17	0.29	0
2	MAN	A	811	2	10,11,12	0.47	0	11,15,17	0.21	0
2	MAN	A	812	2	10,11,12	0.44	0	11,15,17	0.30	0
3	NAG	A	901	1,3	12,14,15	0.46	0	15,19,21	0.75	0
3	NAG	A	902	3	12,14,15	0.42	0	15,19,21	0.63	0
2	NAG	B	801	1,2	12,14,15	0.49	0	15,19,21	0.73	0
2	NAG	B	802	2	12,14,15	0.47	0	15,19,21	0.89	0
2	BMA	B	803	2	10,11,12	0.43	0	11,15,17	0.33	0
2	MAN	B	804	2	10,11,12	0.39	0	11,15,17	0.35	0
2	MAN	B	805	2	10,11,12	0.43	0	11,15,17	0.42	0
2	MAN	B	806	2	10,11,12	0.42	0	11,15,17	0.28	0
2	GLC	B	807	2	10,11,12	0.42	0	11,15,17	0.28	0
2	MAN	B	808	2	10,11,12	0.49	0	11,15,17	0.36	0
2	MAN	B	809	2	10,11,12	0.50	0	11,15,17	1.10	1 (9%)
2	MAN	B	810	2	10,11,12	0.63	0	11,15,17	0.65	0
2	MAN	B	811	2	10,11,12	0.50	0	11,15,17	0.22	0
2	MAN	B	812	2	10,11,12	0.46	0	11,15,17	0.77	0
3	NAG	B	901	1,3	12,14,15	0.45	0	15,19,21	0.69	0
3	NAG	B	902	3	12,14,15	0.47	0	15,19,21	0.67	0
2	NAG	C	801	1,2	12,14,15	0.51	0	15,19,21	0.91	1 (6%)
2	NAG	C	802	2	12,14,15	0.53	0	15,19,21	0.88	0
2	BMA	C	803	2	10,11,12	0.51	0	11,15,17	0.39	0
2	MAN	C	804	2	10,11,12	0.37	0	11,15,17	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MAN	C	805	2	10,11,12	0.37	0	11,15,17	0.46	0
2	MAN	C	806	2	10,11,12	0.43	0	11,15,17	0.46	0
2	GLC	C	807	2	10,11,12	0.37	0	11,15,17	0.40	0
2	MAN	C	808	2	10,11,12	0.45	0	11,15,17	0.48	0
2	MAN	C	809	2	10,11,12	0.54	0	11,15,17	0.66	0
2	MAN	C	810	2	10,11,12	0.47	0	11,15,17	0.27	0
2	MAN	C	811	2	10,11,12	0.40	0	11,15,17	0.35	0
2	MAN	C	812	2	10,11,12	0.46	0	11,15,17	0.28	0
3	NAG	C	901	1,3	12,14,15	0.59	0	15,19,21	0.85	1 (6%)
3	NAG	C	902	3	12,14,15	0.43	0	15,19,21	0.67	0
2	NAG	D	801	1,2	12,14,15	0.51	0	15,19,21	0.80	1 (6%)
2	NAG	D	802	2	12,14,15	0.54	0	15,19,21	0.85	0
2	BMA	D	803	2	10,11,12	0.48	0	11,15,17	0.45	0
2	MAN	D	804	2	10,11,12	0.34	0	11,15,17	0.56	0
2	MAN	D	805	2	10,11,12	0.37	0	11,15,17	0.44	0
2	MAN	D	806	2	10,11,12	0.43	0	11,15,17	0.40	0
2	GLC	D	807	2	10,11,12	0.37	0	11,15,17	0.43	0
2	MAN	D	808	2	10,11,12	0.44	0	11,15,17	0.44	0
2	MAN	D	809	2	10,11,12	0.58	0	11,15,17	1.04	1 (9%)
2	MAN	D	810	2	10,11,12	0.40	0	11,15,17	0.74	0
2	MAN	D	811	2	10,11,12	0.53	0	11,15,17	0.18	0
2	MAN	D	812	2	10,11,12	0.47	0	11,15,17	0.75	0
3	NAG	D	901	1,3	12,14,15	0.55	0	15,19,21	0.66	0
3	NAG	D	902	3	12,14,15	0.49	0	15,19,21	0.67	0
2	NAG	E	801	1,2	12,14,15	0.43	0	15,19,21	0.78	1 (6%)
2	NAG	E	802	2	12,14,15	0.50	0	15,19,21	0.89	0
2	BMA	E	803	2	10,11,12	0.52	0	11,15,17	0.54	0
2	MAN	E	804	2	10,11,12	0.35	0	11,15,17	0.58	0
2	MAN	E	805	2	10,11,12	0.42	0	11,15,17	0.38	0
2	MAN	E	806	2	10,11,12	0.49	0	11,15,17	0.46	0
2	GLC	E	807	2	10,11,12	0.38	0	11,15,17	0.77	0
2	MAN	E	808	2	10,11,12	0.47	0	11,15,17	0.43	0
2	MAN	E	809	2	10,11,12	0.60	0	11,15,17	0.88	1 (9%)
2	MAN	E	810	2	10,11,12	0.42	0	11,15,17	0.68	0
2	MAN	E	811	2	10,11,12	0.41	0	11,15,17	0.23	0
2	MAN	E	812	2	10,11,12	0.47	0	11,15,17	0.30	0
3	NAG	E	901	1,3	12,14,15	0.47	0	15,19,21	0.73	0
3	NAG	E	902	3	12,14,15	0.47	0	15,19,21	0.71	0
2	NAG	F	801	1,2	12,14,15	0.46	0	15,19,21	0.77	0
2	NAG	F	802	2	12,14,15	0.57	0	15,19,21	1.06	0
2	BMA	F	803	2	10,11,12	0.48	0	11,15,17	0.33	0
2	MAN	F	804	2	10,11,12	0.46	0	11,15,17	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MAN	F	805	2	10,11,12	0.36	0	11,15,17	0.53	0
2	MAN	F	806	2	10,11,12	0.39	0	11,15,17	0.42	0
2	GLC	F	807	2	10,11,12	0.37	0	11,15,17	0.22	0
2	MAN	F	808	2	10,11,12	0.44	0	11,15,17	0.39	0
2	MAN	F	809	2	10,11,12	0.56	0	11,15,17	0.63	0
2	MAN	F	810	2	10,11,12	0.41	0	11,15,17	0.26	0
2	MAN	F	811	2	10,11,12	0.39	0	11,15,17	0.20	0
2	MAN	F	812	2	10,11,12	0.48	0	11,15,17	0.27	0
3	NAG	F	901	1,3	12,14,15	0.45	0	15,19,21	0.76	0
3	NAG	F	902	3	12,14,15	0.49	0	15,19,21	0.76	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
2	NAG	A	801	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	802	2	-	0/6/23/26	0/1/1/1
2	BMA	A	803	2	-	0/2/19/22	0/1/1/1
2	MAN	A	804	2	-	0/2/19/22	0/1/1/1
2	MAN	A	805	2	-	0/2/19/22	0/1/1/1
2	MAN	A	806	2	-	0/2/19/22	0/1/1/1
2	GLC	A	807	2	-	0/2/19/22	0/1/1/1
2	MAN	A	808	2	-	0/2/19/22	0/1/1/1
2	MAN	A	809	2	-	0/2/19/22	0/1/1/1
2	MAN	A	810	2	-	0/2/19/22	0/1/1/1
2	MAN	A	811	2	-	0/2/19/22	0/1/1/1
2	MAN	A	812	2	-	0/2/19/22	0/1/1/1
3	NAG	A	901	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	902	3	-	0/6/23/26	0/1/1/1
2	NAG	B	801	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	802	2	-	0/6/23/26	0/1/1/1
2	BMA	B	803	2	-	0/2/19/22	0/1/1/1
2	MAN	B	804	2	-	0/2/19/22	0/1/1/1
2	MAN	B	805	2	-	0/2/19/22	0/1/1/1
2	MAN	B	806	2	-	0/2/19/22	0/1/1/1
2	GLC	B	807	2	-	0/2/19/22	0/1/1/1
2	MAN	B	808	2	-	0/2/19/22	0/1/1/1
2	MAN	B	809	2	-	0/2/19/22	0/1/1/1
2	MAN	B	810	2	-	0/2/19/22	0/1/1/1
2	MAN	B	811	2	-	0/2/19/22	0/1/1/1
2	MAN	B	812	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	901	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	902	3	-	0/6/23/26	0/1/1/1
2	NAG	C	801	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	802	2	-	0/6/23/26	0/1/1/1
2	BMA	C	803	2	-	0/2/19/22	0/1/1/1
2	MAN	C	804	2	-	0/2/19/22	0/1/1/1
2	MAN	C	805	2	-	0/2/19/22	0/1/1/1
2	MAN	C	806	2	-	0/2/19/22	0/1/1/1
2	GLC	C	807	2	-	0/2/19/22	0/1/1/1
2	MAN	C	808	2	-	0/2/19/22	0/1/1/1
2	MAN	C	809	2	-	0/2/19/22	0/1/1/1
2	MAN	C	810	2	-	0/2/19/22	0/1/1/1
2	MAN	C	811	2	-	0/2/19/22	0/1/1/1
2	MAN	C	812	2	-	0/2/19/22	0/1/1/1
3	NAG	C	901	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	902	3	-	0/6/23/26	0/1/1/1
2	NAG	D	801	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	802	2	-	0/6/23/26	0/1/1/1
2	BMA	D	803	2	-	0/2/19/22	0/1/1/1
2	MAN	D	804	2	-	0/2/19/22	0/1/1/1
2	MAN	D	805	2	-	0/2/19/22	0/1/1/1
2	MAN	D	806	2	-	0/2/19/22	0/1/1/1
2	GLC	D	807	2	-	0/2/19/22	0/1/1/1
2	MAN	D	808	2	-	0/2/19/22	0/1/1/1
2	MAN	D	809	2	-	0/2/19/22	0/1/1/1
2	MAN	D	810	2	-	0/2/19/22	0/1/1/1
2	MAN	D	811	2	-	0/2/19/22	0/1/1/1
2	MAN	D	812	2	-	0/2/19/22	0/1/1/1
3	NAG	D	901	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	902	3	-	0/6/23/26	0/1/1/1
2	NAG	E	801	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	802	2	-	0/6/23/26	0/1/1/1
2	BMA	E	803	2	-	0/2/19/22	0/1/1/1
2	MAN	E	804	2	-	0/2/19/22	0/1/1/1
2	MAN	E	805	2	-	0/2/19/22	0/1/1/1
2	MAN	E	806	2	-	0/2/19/22	0/1/1/1
2	GLC	E	807	2	-	0/2/19/22	0/1/1/1
2	MAN	E	808	2	-	0/2/19/22	0/1/1/1
2	MAN	E	809	2	-	0/2/19/22	0/1/1/1
2	MAN	E	810	2	-	0/2/19/22	0/1/1/1
2	MAN	E	811	2	-	0/2/19/22	0/1/1/1
2	MAN	E	812	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	901	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	902	3	-	0/6/23/26	0/1/1/1
2	NAG	F	801	1,2	-	0/6/23/26	0/1/1/1
2	NAG	F	802	2	-	0/6/23/26	0/1/1/1
2	BMA	F	803	2	-	0/2/19/22	0/1/1/1
2	MAN	F	804	2	-	0/2/19/22	0/1/1/1
2	MAN	F	805	2	-	0/2/19/22	0/1/1/1
2	MAN	F	806	2	-	0/2/19/22	0/1/1/1
2	GLC	F	807	2	-	0/2/19/22	0/1/1/1
2	MAN	F	808	2	-	0/2/19/22	0/1/1/1
2	MAN	F	809	2	-	0/2/19/22	0/1/1/1
2	MAN	F	810	2	-	0/2/19/22	0/1/1/1
2	MAN	F	811	2	-	0/2/19/22	0/1/1/1
2	MAN	F	812	2	-	0/2/19/22	0/1/1/1
3	NAG	F	901	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	902	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	809	MAN	C4-C3-C2	2.89	114.39	110.50
2	B	809	MAN	C4-C3-C2	-2.88	106.63	110.50
2	E	809	MAN	C4-C3-C2	2.41	113.74	110.50
2	C	801	NAG	C2-N2-C7	-2.40	119.06	123.09
3	C	901	NAG	C3-C2-N2	-2.40	108.11	111.76

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry ⓘ

6 ligands 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	FMT	A	2003	-	2,2,2	0.58	0	1,1,1	0.08	0
4	FMT	B	2002	-	2,2,2	0.63	0	1,1,1	0.10	0
4	FMT	C	2004	-	2,2,2	0.62	0	1,1,1	0.11	0
4	FMT	D	2001	-	2,2,2	0.62	0	1,1,1	0.08	0
4	FMT	E	2005	-	2,2,2	0.63	0	1,1,1	0.10	0
4	FMT	F	2006	-	2,2,2	0.59	0	1,1,1	0.08	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FMT	A	2003	-	-	0/0/0/0	0/0/0/0
4	FMT	B	2002	-	-	0/0/0/0	0/0/0/0
4	FMT	C	2004	-	-	0/0/0/0	0/0/0/0
4	FMT	D	2001	-	-	0/0/0/0	0/0/0/0
4	FMT	E	2005	-	-	0/0/0/0	0/0/0/0
4	FMT	F	2006	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	674/674 (100%)	-0.44	8 (1%) 75 75	18, 33, 64, 96	0
1	B	674/674 (100%)	-0.43	2 (0%) 91 93	16, 32, 63, 94	0
1	C	674/674 (100%)	-0.38	9 (1%) 74 73	17, 34, 65, 97	0
1	D	674/674 (100%)	-0.35	13 (1%) 64 61	17, 33, 63, 96	0
1	E	674/674 (100%)	-0.33	17 (2%) 54 52	17, 34, 65, 97	0
1	F	674/674 (100%)	-0.42	12 (1%) 65 63	17, 33, 66, 96	0
All	All	4044/4044 (100%)	-0.39	61 (1%) 70 69	16, 33, 65, 97	0

The worst 5 of 61 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	8	HIS	5.8
1	F	621	THR	5.4
1	D	681	HIS	4.7
1	B	650	PHE	4.6
1	F	8	HIS	4.6

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	NAG	B	902	14/15	0.26	53.80	88,90,91,91	0
3	NAG	D	902	14/15	0.49	14.54	98,102,104,105	0
3	NAG	C	901	14/15	0.22	14.17	63,68,72,76	0
2	MAN	E	810	11/12	0.36	10.93	87,89,91,92	0
3	NAG	F	902	14/15	0.38	10.23	86,89,92,92	0
2	MAN	B	811	11/12	0.27	6.69	83,87,90,94	0
2	MAN	C	810	11/12	0.45	6.57	86,91,92,92	0
2	MAN	A	810	11/12	0.32	5.74	86,90,92,93	0
2	MAN	B	810	11/12	0.29	5.67	88,89,91,91	0
3	NAG	D	901	14/15	0.25	5.62	79,86,90,95	0
3	NAG	C	902	14/15	0.32	5.07	79,82,84,85	0
3	NAG	B	901	14/15	0.20	4.94	67,72,77,81	0
2	MAN	D	810	11/12	0.34	4.83	87,91,93,93	0
3	NAG	A	902	14/15	0.18	3.59	63,68,70,71	0
2	MAN	F	810	11/12	0.24	3.54	85,90,91,91	0
3	NAG	E	901	14/15	0.17	2.49	60,65,68,70	0
2	GLC	B	807	11/12	0.20	2.41	56,57,59,61	0
2	MAN	F	811	11/12	0.31	1.44	86,87,90,94	0
3	NAG	F	901	14/15	0.17	1.42	67,74,79,81	0
2	GLC	C	807	11/12	0.22	1.25	53,55,58,58	0
2	MAN	A	811	11/12	0.38	1.24	84,88,90,94	0
2	GLC	A	807	11/12	0.18	1.03	53,57,59,60	0
2	MAN	E	804	11/12	0.11	0.65	34,36,39,41	0
2	MAN	D	811	11/12	0.32	0.32	88,90,91,96	0
2	GLC	F	807	11/12	0.17	0.30	50,53,55,58	0
2	NAG	E	802	14/15	0.10	0.27	29,32,34,37	0
2	GLC	D	807	11/12	0.15	0.09	51,55,59,60	0
2	MAN	E	811	11/12	0.23	0.08	86,88,90,95	0
2	MAN	A	805	11/12	0.10	0.06	33,35,39,42	0
2	NAG	D	802	14/15	0.10	0.03	24,32,39,40	0
2	MAN	F	809	11/12	0.21	0.01	79,80,82,84	0
2	NAG	F	802	14/15	0.10	0.01	29,31,33,39	0
3	NAG	A	901	14/15	0.11	-0.06	39,49,52,56	0
2	NAG	A	802	14/15	0.09	-0.14	29,33,37,43	0
2	GLC	E	807	11/12	0.13	-0.35	57,60,62,62	0
2	MAN	A	809	11/12	0.21	-0.41	79,82,83,86	0
2	MAN	E	806	11/12	0.12	-0.59	44,45,50,54	0
2	MAN	A	806	11/12	0.09	-0.60	40,42,45,49	0
2	MAN	C	804	11/12	0.10	-0.62	32,32,34,35	0
2	NAG	E	801	14/15	0.08	-0.64	24,27,29,29	0
2	MAN	A	804	11/12	0.09	-0.65	36,37,39,40	0
2	MAN	D	809	11/12	0.21	-0.68	81,83,85,87	0
2	NAG	A	801	14/15	0.09	-0.74	20,26,31,31	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	NAG	C	801	14/15	0.08	-0.76	20,25,28,30	0
2	NAG	B	801	14/15	0.10	-0.78	22,24,29,32	0
2	MAN	C	806	11/12	0.10	-0.82	40,41,43,50	0
2	MAN	F	806	11/12	0.10	-0.87	40,40,43,46	0
2	MAN	C	811	11/12	0.22	-0.88	85,87,89,94	0
2	NAG	D	801	14/15	0.08	-0.93	22,24,29,30	0
2	MAN	D	806	11/12	0.10	-1.03	39,43,45,49	0
2	MAN	F	805	11/12	0.09	-1.08	28,32,36,37	0
2	MAN	B	806	11/12	0.09	-1.09	40,42,46,50	0
2	NAG	F	801	14/15	0.09	-1.10	21,24,26,27	0
2	NAG	C	802	14/15	0.09	-1.17	25,31,37,40	0
2	MAN	D	804	11/12	0.09	-1.26	34,36,39,40	0
2	NAG	B	802	14/15	0.09	-1.31	28,32,37,38	0
2	MAN	C	805	11/12	0.09	-1.42	32,33,36,38	0
2	MAN	B	805	11/12	0.09	-1.71	32,35,38,41	0
2	MAN	D	805	11/12	0.09	-1.85	33,35,36,40	0
2	MAN	E	805	11/12	0.09	-2.35	29,34,38,44	0
2	MAN	B	804	11/12	0.08	-2.87	34,36,37,38	0
2	MAN	F	804	11/12	0.07	-4.69	34,35,37,38	0
2	BMA	A	803	11/12	0.10	-	36,39,48,59	0
2	MAN	C	812	11/12	0.47	-	97,99,101,101	0
2	MAN	A	812	11/12	0.36	-	96,98,100,100	0
2	MAN	B	812	11/12	0.51	-	95,99,101,103	0
2	MAN	B	809	11/12	0.14	-	78,79,81,86	0
2	MAN	E	808	11/12	0.11	-	61,65,75,84	0
2	MAN	D	812	11/12	0.64	-	97,100,101,102	0
2	MAN	F	812	11/12	0.46	-	97,99,100,100	0
2	BMA	E	803	11/12	0.08	-	31,39,44,55	0
2	MAN	C	809	11/12	0.24	-	79,80,83,86	0
2	BMA	D	803	11/12	0.09	-	35,38,47,56	0
2	MAN	E	809	11/12	0.18	-	78,81,82,85	0
2	MAN	B	808	11/12	0.14	-	63,69,77,84	0
2	MAN	A	808	11/12	0.20	-	66,70,77,85	0
2	MAN	E	812	11/12	0.43	-	96,99,100,101	0
3	NAG	E	902	14/15	0.20	-	72,74,76,76	0
2	BMA	C	803	11/12	0.08	-	32,37,46,55	0
2	BMA	B	803	11/12	0.08	-	36,39,48,57	0
2	MAN	D	808	11/12	0.09	-	63,70,76,83	0
2	MAN	C	808	11/12	0.14	-	62,66,75,83	0
2	MAN	F	808	11/12	0.14	-	63,67,76,84	0
2	BMA	F	803	11/12	0.08	-	33,35,42,53	0

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	FMT	B	2002	3/3	0.10	0.23	21,21,22,23	0
4	FMT	F	2006	3/3	0.08	-0.32	23,23,26,26	0
4	FMT	C	2004	3/3	0.07	-1.08	23,23,25,28	0
4	FMT	E	2005	3/3	0.07	-1.19	12,12,16,18	0
4	FMT	A	2003	3/3	0.06	-1.30	22,22,29,31	0
4	FMT	D	2001	3/3	0.06	-2.14	30,30,31,33	0

6.5 Other polymers ⓘ

There are no such residues in this entry.