



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 30, 2017 – 06:42 PM EDT

PDB ID : 3SIO
Title : Ac-AChBP ligand binding domain (not including beta 9-10 linker) mutated to human alpha-7 nAChR
Authors : Nemecz, A.; Taylor, P.W.
Deposited on : unknown
Resolution : 2.32 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : **FAILED**
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

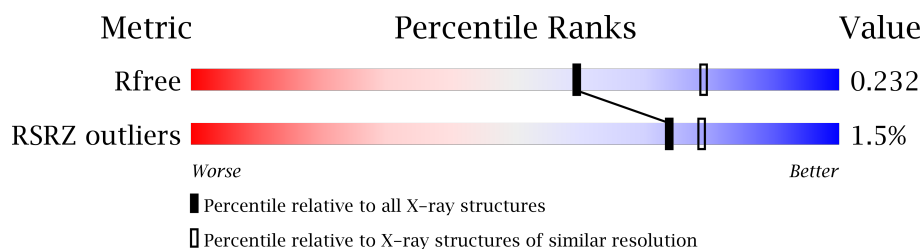
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.32 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	4787 (2.34-2.30)
RSRZ outliers	101464	4814 (2.34-2.30)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

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
3	MLK	E	260	-	-	-	X
3	MLK	J	260	-	-	-	X
5	MAN	E	230	-	-	-	X
5	MAN	J	230	-	-	-	X
6	MRD	B	250	-	-	-	X
6	MRD	C	250	-	-	-	X
6	MRD	D	250	-	-	-	X
6	MRD	G	250	-	-	-	X
6	MRD	H	250	-	-	-	X
6	MRD	I	222	-	-	-	X
7	MPD	C	222	-	-	-	X
7	MPD	I	250	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 19701 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 Soluble acetylcholine receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	7	0
			1752	1106	289	349	8			
1	B	216	Total	C	N	O	S	0	8	0
			1781	1124	289	360	8			
1	C	221	Total	C	N	O	S	0	9	0
			1815	1147	299	361	8			
1	D	214	Total	C	N	O	S	0	9	0
			1764	1113	288	355	8			
1	E	216	Total	C	N	O	S	0	9	0
			1789	1130	291	360	8			
1	F	214	Total	C	N	O	S	0	9	0
			1762	1112	292	350	8			
1	G	216	Total	C	N	O	S	0	10	0
			1793	1132	291	362	8			
1	H	221	Total	C	N	O	S	0	7	0
			1810	1143	302	357	8			
1	I	214	Total	C	N	O	S	0	6	0
			1753	1105	285	355	8			
1	J	216	Total	C	N	O	S	0	11	0
			1796	1135	294	358	9			

There are 290 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	ASP	-	EXPRESSION TAG	UNP Q8WSF8
A	-7	TYR	-	EXPRESSION TAG	UNP Q8WSF8
A	-6	LYS	-	EXPRESSION TAG	UNP Q8WSF8
A	-5	ASP	-	EXPRESSION TAG	UNP Q8WSF8
A	-4	ASP	-	EXPRESSION TAG	UNP Q8WSF8
A	-3	ASP	-	EXPRESSION TAG	UNP Q8WSF8
A	-2	ASP	-	EXPRESSION TAG	UNP Q8WSF8
A	-1	LYS	-	EXPRESSION TAG	UNP Q8WSF8
A	0	LEU	-	EXPRESSION TAG	UNP Q8WSF8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	32	TYR	THR	ENGINEERED MUTATION	UNP Q8WSF8
A	34	SER	GLY	ENGINEERED MUTATION	UNP Q8WSF8
A	36	SER	THR	ENGINEERED MUTATION	UNP Q8WSF8
A	38	LEU	GLN	ENGINEERED MUTATION	UNP Q8WSF8
A	55	TRP	TYR	ENGINEERED MUTATION	UNP Q8WSF8
A	59	SER	ARG	ENGINEERED MUTATION	UNP Q8WSF8
A	106	ASN	ILE	ENGINEERED MUTATION	UNP Q8WSF8
A	108	LEU	VAL	ENGINEERED MUTATION	UNP Q8WSF8
A	110	ASN	THR	ENGINEERED MUTATION	UNP Q8WSF8
A	111	SER	HIS	ENGINEERED MUTATION	UNP Q8WSF8
A	112	SER	ASP	ENGINEERED MUTATION	UNP Q8WSF8
A	114	HIS	SER	ENGINEERED MUTATION	UNP Q8WSF8
A	116	GLN	MET	ENGINEERED MUTATION	UNP Q8WSF8
A	117	TYR	PHE	ENGINEERED MUTATION	UNP Q8WSF8
A	118	LEU	ILE	ENGINEERED MUTATION	UNP Q8WSF8
A	148	SER	VAL	ENGINEERED MUTATION	UNP Q8WSF8
A	150	GLY	SER	ENGINEERED MUTATION	UNP Q8WSF8
A	152	TRP	PHE	ENGINEERED MUTATION	UNP Q8WSF8
A	220	SER	-	EXPRESSION TAG	UNP Q8WSF8
A	221	ARG	-	EXPRESSION TAG	UNP Q8WSF8
B	-8	ASP	-	EXPRESSION TAG	UNP Q8WSF8
B	-7	TYR	-	EXPRESSION TAG	UNP Q8WSF8
B	-6	LYS	-	EXPRESSION TAG	UNP Q8WSF8
B	-5	ASP	-	EXPRESSION TAG	UNP Q8WSF8
B	-4	ASP	-	EXPRESSION TAG	UNP Q8WSF8
B	-3	ASP	-	EXPRESSION TAG	UNP Q8WSF8
B	-2	ASP	-	EXPRESSION TAG	UNP Q8WSF8
B	-1	LYS	-	EXPRESSION TAG	UNP Q8WSF8
B	0	LEU	-	EXPRESSION TAG	UNP Q8WSF8
B	32	TYR	THR	ENGINEERED MUTATION	UNP Q8WSF8
B	34	SER	GLY	ENGINEERED MUTATION	UNP Q8WSF8
B	36	SER	THR	ENGINEERED MUTATION	UNP Q8WSF8
B	38	LEU	GLN	ENGINEERED MUTATION	UNP Q8WSF8
B	55	TRP	TYR	ENGINEERED MUTATION	UNP Q8WSF8
B	59	SER	ARG	ENGINEERED MUTATION	UNP Q8WSF8
B	106	ASN	ILE	ENGINEERED MUTATION	UNP Q8WSF8
B	108	LEU	VAL	ENGINEERED MUTATION	UNP Q8WSF8
B	110	ASN	THR	ENGINEERED MUTATION	UNP Q8WSF8
B	111	SER	HIS	ENGINEERED MUTATION	UNP Q8WSF8
B	112	SER	ASP	ENGINEERED MUTATION	UNP Q8WSF8
B	114	HIS	SER	ENGINEERED MUTATION	UNP Q8WSF8
B	116	GLN	MET	ENGINEERED MUTATION	UNP Q8WSF8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	117	TYR	PHE	ENGINEERED MUTATION	UNP Q8WSF8
B	118	LEU	ILE	ENGINEERED MUTATION	UNP Q8WSF8
B	148	SER	VAL	ENGINEERED MUTATION	UNP Q8WSF8
B	150	GLY	SER	ENGINEERED MUTATION	UNP Q8WSF8
B	152	TRP	PHE	ENGINEERED MUTATION	UNP Q8WSF8
B	220	SER	-	EXPRESSION TAG	UNP Q8WSF8
B	221	ARG	-	EXPRESSION TAG	UNP Q8WSF8
C	-8	ASP	-	EXPRESSION TAG	UNP Q8WSF8
C	-7	TYR	-	EXPRESSION TAG	UNP Q8WSF8
C	-6	LYS	-	EXPRESSION TAG	UNP Q8WSF8
C	-5	ASP	-	EXPRESSION TAG	UNP Q8WSF8
C	-4	ASP	-	EXPRESSION TAG	UNP Q8WSF8
C	-3	ASP	-	EXPRESSION TAG	UNP Q8WSF8
C	-2	ASP	-	EXPRESSION TAG	UNP Q8WSF8
C	-1	LYS	-	EXPRESSION TAG	UNP Q8WSF8
C	0	LEU	-	EXPRESSION TAG	UNP Q8WSF8
C	32	TYR	THR	ENGINEERED MUTATION	UNP Q8WSF8
C	34	SER	GLY	ENGINEERED MUTATION	UNP Q8WSF8
C	36	SER	THR	ENGINEERED MUTATION	UNP Q8WSF8
C	38	LEU	GLN	ENGINEERED MUTATION	UNP Q8WSF8
C	55	TRP	TYR	ENGINEERED MUTATION	UNP Q8WSF8
C	59	SER	ARG	ENGINEERED MUTATION	UNP Q8WSF8
C	106	ASN	ILE	ENGINEERED MUTATION	UNP Q8WSF8
C	108	LEU	VAL	ENGINEERED MUTATION	UNP Q8WSF8
C	110	ASN	THR	ENGINEERED MUTATION	UNP Q8WSF8
C	111	SER	HIS	ENGINEERED MUTATION	UNP Q8WSF8
C	112	SER	ASP	ENGINEERED MUTATION	UNP Q8WSF8
C	114	HIS	SER	ENGINEERED MUTATION	UNP Q8WSF8
C	116	GLN	MET	ENGINEERED MUTATION	UNP Q8WSF8
C	117	TYR	PHE	ENGINEERED MUTATION	UNP Q8WSF8
C	118	LEU	ILE	ENGINEERED MUTATION	UNP Q8WSF8
C	148	SER	VAL	ENGINEERED MUTATION	UNP Q8WSF8
C	150	GLY	SER	ENGINEERED MUTATION	UNP Q8WSF8
C	152	TRP	PHE	ENGINEERED MUTATION	UNP Q8WSF8
C	220	SER	-	EXPRESSION TAG	UNP Q8WSF8
C	221	ARG	-	EXPRESSION TAG	UNP Q8WSF8
D	-8	ASP	-	EXPRESSION TAG	UNP Q8WSF8
D	-7	TYR	-	EXPRESSION TAG	UNP Q8WSF8
D	-6	LYS	-	EXPRESSION TAG	UNP Q8WSF8
D	-5	ASP	-	EXPRESSION TAG	UNP Q8WSF8
D	-4	ASP	-	EXPRESSION TAG	UNP Q8WSF8
D	-3	ASP	-	EXPRESSION TAG	UNP Q8WSF8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	ASP	-	EXPRESSION TAG	UNP Q8WSF8
D	-1	LYS	-	EXPRESSION TAG	UNP Q8WSF8
D	0	LEU	-	EXPRESSION TAG	UNP Q8WSF8
D	32	TYR	THR	ENGINEERED MUTATION	UNP Q8WSF8
D	34	SER	GLY	ENGINEERED MUTATION	UNP Q8WSF8
D	36	SER	THR	ENGINEERED MUTATION	UNP Q8WSF8
D	38	LEU	GLN	ENGINEERED MUTATION	UNP Q8WSF8
D	55	TRP	TYR	ENGINEERED MUTATION	UNP Q8WSF8
D	59	SER	ARG	ENGINEERED MUTATION	UNP Q8WSF8
D	106	ASN	ILE	ENGINEERED MUTATION	UNP Q8WSF8
D	108	LEU	VAL	ENGINEERED MUTATION	UNP Q8WSF8
D	110	ASN	THR	ENGINEERED MUTATION	UNP Q8WSF8
D	111	SER	HIS	ENGINEERED MUTATION	UNP Q8WSF8
D	112	SER	ASP	ENGINEERED MUTATION	UNP Q8WSF8
D	114	HIS	SER	ENGINEERED MUTATION	UNP Q8WSF8
D	116	GLN	MET	ENGINEERED MUTATION	UNP Q8WSF8
D	117	TYR	PHE	ENGINEERED MUTATION	UNP Q8WSF8
D	118	LEU	ILE	ENGINEERED MUTATION	UNP Q8WSF8
D	148	SER	VAL	ENGINEERED MUTATION	UNP Q8WSF8
D	150	GLY	SER	ENGINEERED MUTATION	UNP Q8WSF8
D	152	TRP	PHE	ENGINEERED MUTATION	UNP Q8WSF8
D	220	SER	-	EXPRESSION TAG	UNP Q8WSF8
D	221	ARG	-	EXPRESSION TAG	UNP Q8WSF8
E	-8	ASP	-	EXPRESSION TAG	UNP Q8WSF8
E	-7	TYR	-	EXPRESSION TAG	UNP Q8WSF8
E	-6	LYS	-	EXPRESSION TAG	UNP Q8WSF8
E	-5	ASP	-	EXPRESSION TAG	UNP Q8WSF8
E	-4	ASP	-	EXPRESSION TAG	UNP Q8WSF8
E	-3	ASP	-	EXPRESSION TAG	UNP Q8WSF8
E	-2	ASP	-	EXPRESSION TAG	UNP Q8WSF8
E	-1	LYS	-	EXPRESSION TAG	UNP Q8WSF8
E	0	LEU	-	EXPRESSION TAG	UNP Q8WSF8
E	32	TYR	THR	ENGINEERED MUTATION	UNP Q8WSF8
E	34	SER	GLY	ENGINEERED MUTATION	UNP Q8WSF8
E	36	SER	THR	ENGINEERED MUTATION	UNP Q8WSF8
E	38	LEU	GLN	ENGINEERED MUTATION	UNP Q8WSF8
E	55	TRP	TYR	ENGINEERED MUTATION	UNP Q8WSF8
E	59	SER	ARG	ENGINEERED MUTATION	UNP Q8WSF8
E	106	ASN	ILE	ENGINEERED MUTATION	UNP Q8WSF8
E	108	LEU	VAL	ENGINEERED MUTATION	UNP Q8WSF8
E	110	ASN	THR	ENGINEERED MUTATION	UNP Q8WSF8
E	111	SER	HIS	ENGINEERED MUTATION	UNP Q8WSF8

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Chain	Residue	Modelled	Actual	Comment	Reference
E	112	SER	ASP	ENGINEERED MUTATION	UNP Q8WSF8
E	114	HIS	SER	ENGINEERED MUTATION	UNP Q8WSF8
E	116	GLN	MET	ENGINEERED MUTATION	UNP Q8WSF8
E	117	TYR	PHE	ENGINEERED MUTATION	UNP Q8WSF8
E	118	LEU	ILE	ENGINEERED MUTATION	UNP Q8WSF8
E	148	SER	VAL	ENGINEERED MUTATION	UNP Q8WSF8
E	150	GLY	SER	ENGINEERED MUTATION	UNP Q8WSF8
E	152	TRP	PHE	ENGINEERED MUTATION	UNP Q8WSF8
E	220	SER	-	EXPRESSION TAG	UNP Q8WSF8
E	221	ARG	-	EXPRESSION TAG	UNP Q8WSF8
F	-8	ASP	-	EXPRESSION TAG	UNP Q8WSF8
F	-7	TYR	-	EXPRESSION TAG	UNP Q8WSF8
F	-6	LYS	-	EXPRESSION TAG	UNP Q8WSF8
F	-5	ASP	-	EXPRESSION TAG	UNP Q8WSF8
F	-4	ASP	-	EXPRESSION TAG	UNP Q8WSF8
F	-3	ASP	-	EXPRESSION TAG	UNP Q8WSF8
F	-2	ASP	-	EXPRESSION TAG	UNP Q8WSF8
F	-1	LYS	-	EXPRESSION TAG	UNP Q8WSF8
F	0	LEU	-	EXPRESSION TAG	UNP Q8WSF8
F	32	TYR	THR	ENGINEERED MUTATION	UNP Q8WSF8
F	34	SER	GLY	ENGINEERED MUTATION	UNP Q8WSF8
F	36	SER	THR	ENGINEERED MUTATION	UNP Q8WSF8
F	38	LEU	GLN	ENGINEERED MUTATION	UNP Q8WSF8
F	55	TRP	TYR	ENGINEERED MUTATION	UNP Q8WSF8
F	59	SER	ARG	ENGINEERED MUTATION	UNP Q8WSF8
F	106	ASN	ILE	ENGINEERED MUTATION	UNP Q8WSF8
F	108	LEU	VAL	ENGINEERED MUTATION	UNP Q8WSF8
F	110	ASN	THR	ENGINEERED MUTATION	UNP Q8WSF8
F	111	SER	HIS	ENGINEERED MUTATION	UNP Q8WSF8
F	112	SER	ASP	ENGINEERED MUTATION	UNP Q8WSF8
F	114	HIS	SER	ENGINEERED MUTATION	UNP Q8WSF8
F	116	GLN	MET	ENGINEERED MUTATION	UNP Q8WSF8
F	117	TYR	PHE	ENGINEERED MUTATION	UNP Q8WSF8
F	118	LEU	ILE	ENGINEERED MUTATION	UNP Q8WSF8
F	148	SER	VAL	ENGINEERED MUTATION	UNP Q8WSF8
F	150	GLY	SER	ENGINEERED MUTATION	UNP Q8WSF8
F	152	TRP	PHE	ENGINEERED MUTATION	UNP Q8WSF8
F	220	SER	-	EXPRESSION TAG	UNP Q8WSF8
F	221	ARG	-	EXPRESSION TAG	UNP Q8WSF8
G	-8	ASP	-	EXPRESSION TAG	UNP Q8WSF8
G	-7	TYR	-	EXPRESSION TAG	UNP Q8WSF8
G	-6	LYS	-	EXPRESSION TAG	UNP Q8WSF8

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-5	ASP	-	EXPRESSION TAG	UNP Q8WSF8
G	-4	ASP	-	EXPRESSION TAG	UNP Q8WSF8
G	-3	ASP	-	EXPRESSION TAG	UNP Q8WSF8
G	-2	ASP	-	EXPRESSION TAG	UNP Q8WSF8
G	-1	LYS	-	EXPRESSION TAG	UNP Q8WSF8
G	0	LEU	-	EXPRESSION TAG	UNP Q8WSF8
G	32	TYR	THR	ENGINEERED MUTATION	UNP Q8WSF8
G	34	SER	GLY	ENGINEERED MUTATION	UNP Q8WSF8
G	36	SER	THR	ENGINEERED MUTATION	UNP Q8WSF8
G	38	LEU	GLN	ENGINEERED MUTATION	UNP Q8WSF8
G	55	TRP	TYR	ENGINEERED MUTATION	UNP Q8WSF8
G	59	SER	ARG	ENGINEERED MUTATION	UNP Q8WSF8
G	106	ASN	ILE	ENGINEERED MUTATION	UNP Q8WSF8
G	108	LEU	VAL	ENGINEERED MUTATION	UNP Q8WSF8
G	110	ASN	THR	ENGINEERED MUTATION	UNP Q8WSF8
G	111	SER	HIS	ENGINEERED MUTATION	UNP Q8WSF8
G	112	SER	ASP	ENGINEERED MUTATION	UNP Q8WSF8
G	114	HIS	SER	ENGINEERED MUTATION	UNP Q8WSF8
G	116	GLN	MET	ENGINEERED MUTATION	UNP Q8WSF8
G	117	TYR	PHE	ENGINEERED MUTATION	UNP Q8WSF8
G	118	LEU	ILE	ENGINEERED MUTATION	UNP Q8WSF8
G	148	SER	VAL	ENGINEERED MUTATION	UNP Q8WSF8
G	150	GLY	SER	ENGINEERED MUTATION	UNP Q8WSF8
G	152	TRP	PHE	ENGINEERED MUTATION	UNP Q8WSF8
G	220	SER	-	EXPRESSION TAG	UNP Q8WSF8
G	221	ARG	-	EXPRESSION TAG	UNP Q8WSF8
H	-8	ASP	-	EXPRESSION TAG	UNP Q8WSF8
H	-7	TYR	-	EXPRESSION TAG	UNP Q8WSF8
H	-6	LYS	-	EXPRESSION TAG	UNP Q8WSF8
H	-5	ASP	-	EXPRESSION TAG	UNP Q8WSF8
H	-4	ASP	-	EXPRESSION TAG	UNP Q8WSF8
H	-3	ASP	-	EXPRESSION TAG	UNP Q8WSF8
H	-2	ASP	-	EXPRESSION TAG	UNP Q8WSF8
H	-1	LYS	-	EXPRESSION TAG	UNP Q8WSF8
H	0	LEU	-	EXPRESSION TAG	UNP Q8WSF8
H	32	TYR	THR	ENGINEERED MUTATION	UNP Q8WSF8
H	34	SER	GLY	ENGINEERED MUTATION	UNP Q8WSF8
H	36	SER	THR	ENGINEERED MUTATION	UNP Q8WSF8
H	38	LEU	GLN	ENGINEERED MUTATION	UNP Q8WSF8
H	55	TRP	TYR	ENGINEERED MUTATION	UNP Q8WSF8
H	59	SER	ARG	ENGINEERED MUTATION	UNP Q8WSF8
H	106	ASN	ILE	ENGINEERED MUTATION	UNP Q8WSF8

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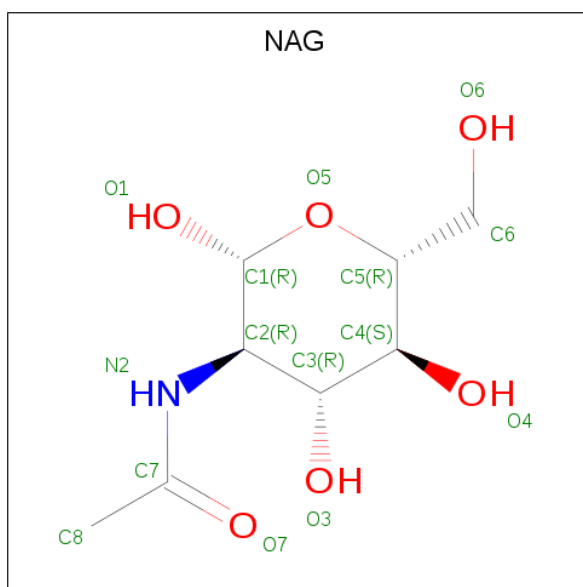
Chain	Residue	Modelled	Actual	Comment	Reference
H	108	LEU	VAL	ENGINEERED MUTATION	UNP Q8WSF8
H	110	ASN	THR	ENGINEERED MUTATION	UNP Q8WSF8
H	111	SER	HIS	ENGINEERED MUTATION	UNP Q8WSF8
H	112	SER	ASP	ENGINEERED MUTATION	UNP Q8WSF8
H	114	HIS	SER	ENGINEERED MUTATION	UNP Q8WSF8
H	116	GLN	MET	ENGINEERED MUTATION	UNP Q8WSF8
H	117	TYR	PHE	ENGINEERED MUTATION	UNP Q8WSF8
H	118	LEU	ILE	ENGINEERED MUTATION	UNP Q8WSF8
H	148	SER	VAL	ENGINEERED MUTATION	UNP Q8WSF8
H	150	GLY	SER	ENGINEERED MUTATION	UNP Q8WSF8
H	152	TRP	PHE	ENGINEERED MUTATION	UNP Q8WSF8
H	220	SER	-	EXPRESSION TAG	UNP Q8WSF8
H	221	ARG	-	EXPRESSION TAG	UNP Q8WSF8
I	-8	ASP	-	EXPRESSION TAG	UNP Q8WSF8
I	-7	TYR	-	EXPRESSION TAG	UNP Q8WSF8
I	-6	LYS	-	EXPRESSION TAG	UNP Q8WSF8
I	-5	ASP	-	EXPRESSION TAG	UNP Q8WSF8
I	-4	ASP	-	EXPRESSION TAG	UNP Q8WSF8
I	-3	ASP	-	EXPRESSION TAG	UNP Q8WSF8
I	-2	ASP	-	EXPRESSION TAG	UNP Q8WSF8
I	-1	LYS	-	EXPRESSION TAG	UNP Q8WSF8
I	0	LEU	-	EXPRESSION TAG	UNP Q8WSF8
I	32	TYR	THR	ENGINEERED MUTATION	UNP Q8WSF8
I	34	SER	GLY	ENGINEERED MUTATION	UNP Q8WSF8
I	36	SER	THR	ENGINEERED MUTATION	UNP Q8WSF8
I	38	LEU	GLN	ENGINEERED MUTATION	UNP Q8WSF8
I	55	TRP	TYR	ENGINEERED MUTATION	UNP Q8WSF8
I	59	SER	ARG	ENGINEERED MUTATION	UNP Q8WSF8
I	106	ASN	ILE	ENGINEERED MUTATION	UNP Q8WSF8
I	108	LEU	VAL	ENGINEERED MUTATION	UNP Q8WSF8
I	110	ASN	THR	ENGINEERED MUTATION	UNP Q8WSF8
I	111	SER	HIS	ENGINEERED MUTATION	UNP Q8WSF8
I	112	SER	ASP	ENGINEERED MUTATION	UNP Q8WSF8
I	114	HIS	SER	ENGINEERED MUTATION	UNP Q8WSF8
I	116	GLN	MET	ENGINEERED MUTATION	UNP Q8WSF8
I	117	TYR	PHE	ENGINEERED MUTATION	UNP Q8WSF8
I	118	LEU	ILE	ENGINEERED MUTATION	UNP Q8WSF8
I	148	SER	VAL	ENGINEERED MUTATION	UNP Q8WSF8
I	150	GLY	SER	ENGINEERED MUTATION	UNP Q8WSF8
I	152	TRP	PHE	ENGINEERED MUTATION	UNP Q8WSF8
I	220	SER	-	EXPRESSION TAG	UNP Q8WSF8
I	221	ARG	-	EXPRESSION TAG	UNP Q8WSF8

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-8	ASP	-	EXPRESSION TAG	UNP Q8WSF8
J	-7	TYR	-	EXPRESSION TAG	UNP Q8WSF8
J	-6	LYS	-	EXPRESSION TAG	UNP Q8WSF8
J	-5	ASP	-	EXPRESSION TAG	UNP Q8WSF8
J	-4	ASP	-	EXPRESSION TAG	UNP Q8WSF8
J	-3	ASP	-	EXPRESSION TAG	UNP Q8WSF8
J	-2	ASP	-	EXPRESSION TAG	UNP Q8WSF8
J	-1	LYS	-	EXPRESSION TAG	UNP Q8WSF8
J	0	LEU	-	EXPRESSION TAG	UNP Q8WSF8
J	32	TYR	THR	ENGINEERED MUTATION	UNP Q8WSF8
J	34	SER	GLY	ENGINEERED MUTATION	UNP Q8WSF8
J	36	SER	THR	ENGINEERED MUTATION	UNP Q8WSF8
J	38	LEU	GLN	ENGINEERED MUTATION	UNP Q8WSF8
J	55	TRP	TYR	ENGINEERED MUTATION	UNP Q8WSF8
J	59	SER	ARG	ENGINEERED MUTATION	UNP Q8WSF8
J	106	ASN	ILE	ENGINEERED MUTATION	UNP Q8WSF8
J	108	LEU	VAL	ENGINEERED MUTATION	UNP Q8WSF8
J	110	ASN	THR	ENGINEERED MUTATION	UNP Q8WSF8
J	111	SER	HIS	ENGINEERED MUTATION	UNP Q8WSF8
J	112	SER	ASP	ENGINEERED MUTATION	UNP Q8WSF8
J	114	HIS	SER	ENGINEERED MUTATION	UNP Q8WSF8
J	116	GLN	MET	ENGINEERED MUTATION	UNP Q8WSF8
J	117	TYR	PHE	ENGINEERED MUTATION	UNP Q8WSF8
J	118	LEU	ILE	ENGINEERED MUTATION	UNP Q8WSF8
J	148	SER	VAL	ENGINEERED MUTATION	UNP Q8WSF8
J	150	GLY	SER	ENGINEERED MUTATION	UNP Q8WSF8
J	152	TRP	PHE	ENGINEERED MUTATION	UNP Q8WSF8
J	220	SER	-	EXPRESSION TAG	UNP Q8WSF8
J	221	ARG	-	EXPRESSION TAG	UNP Q8WSF8

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



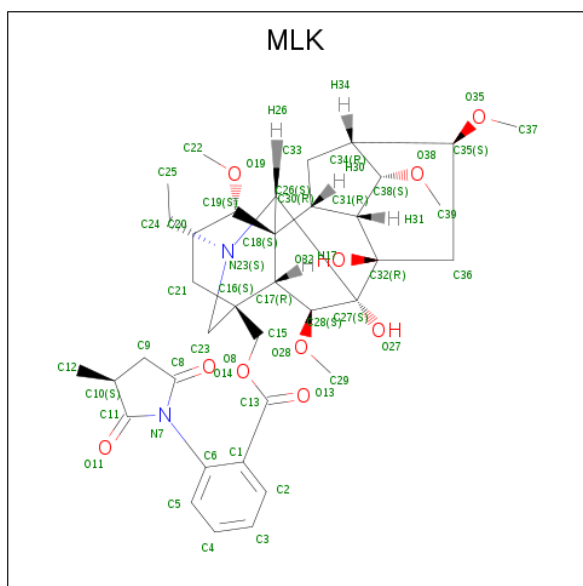
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	E	1	Total	C	N	O	0	0
			14	8	1	5		
2	E	1	Total	C	N	O	0	0
			14	8	1	5		
2	E	1	Total	C	N	O	0	0
			14	8	1	5		
2	F	1	Total	C	N	O	0	0
			14	8	1	5		
2	G	1	Total	C	N	O	0	0
			14	8	1	5		
2	G	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	G	1	Total	C	N	O	0	0
			14	8	1	5		
2	G	1	Total	C	N	O	0	0
			14	8	1	5		
2	H	1	Total	C	N	O	0	0
			14	8	1	5		
2	I	1	Total	C	N	O	0	0
			14	8	1	5		
2	J	1	Total	C	N	O	0	0
			14	8	1	5		
2	J	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is METHYLLYCACONITINE (three-letter code: MLK) (formula: $C_{37}H_{50}N_2O_{10}$).



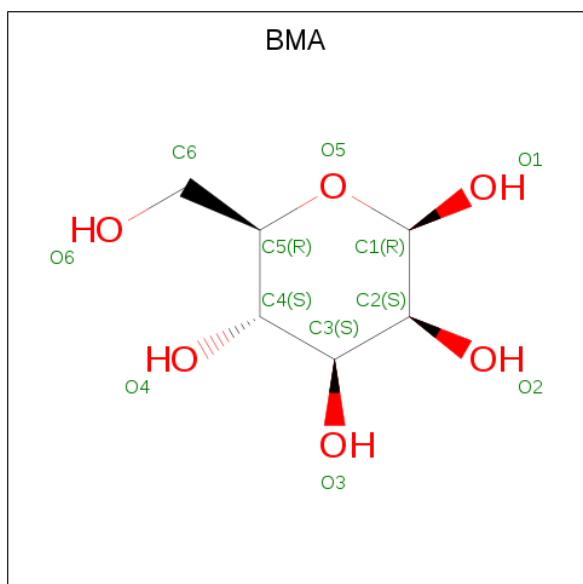
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			49	37	2	10		
3	B	1	Total	C	N	O	0	0
			49	37	2	10		
3	C	1	Total	C	N	O	0	0
			49	37	2	10		
3	D	1	Total	C	N	O	0	0
			49	37	2	10		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	E	1	Total	C	N	O	0	0
			49	37	2	10		
3	F	1	Total	C	N	O	0	0
			49	37	2	10		
3	G	1	Total	C	N	O	0	0
			49	37	2	10		
3	H	1	Total	C	N	O	0	0
			49	37	2	10		
3	I	1	Total	C	N	O	0	0
			49	37	2	10		
3	J	1	Total	C	N	O	0	0
			49	37	2	10		

- Molecule 4 is BETA-D-MANNOSE (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



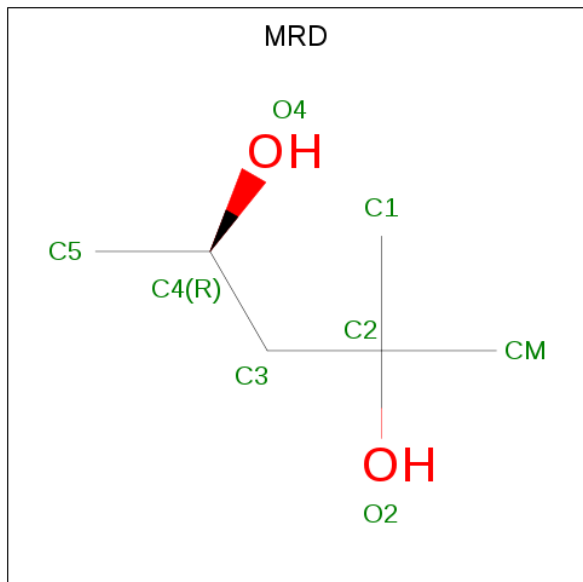
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			11	6	5		
4	E	1	Total	C	O	0	0
			11	6	5		
4	G	1	Total	C	O	0	0
			11	6	5		
4	J	1	Total	C	O	0	0
			11	6	5		

- Molecule 5 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



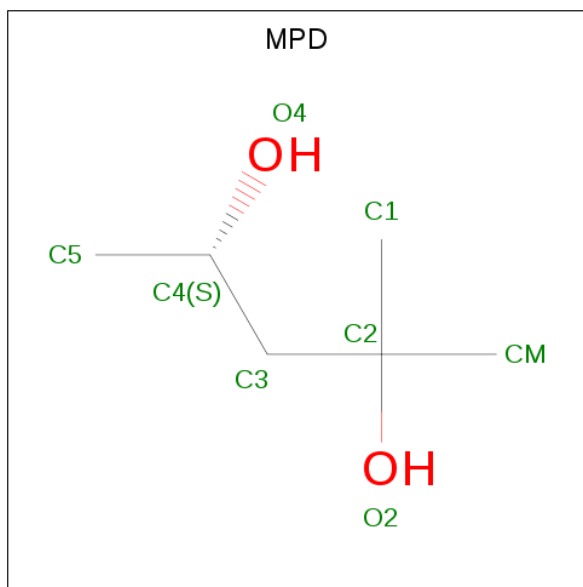
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			11	6	5		
5	B	1	Total	C	O	0	0
			11	6	5		
5	B	1	Total	C	O	0	0
			11	6	5		
5	B	1	Total	C	O	0	0
			11	6	5		
5	E	1	Total	C	O	0	0
			11	6	5		
5	E	1	Total	C	O	0	0
			11	6	5		
5	E	1	Total	C	O	0	0
			11	6	5		
5	G	1	Total	C	O	0	0
			11	6	5		
5	G	1	Total	C	O	0	0
			11	6	5		
5	G	1	Total	C	O	0	0
			11	6	5		
5	G	1	Total	C	O	0	0
			11	6	5		
5	J	1	Total	C	O	0	0
			11	6	5		
5	J	1	Total	C	O	0	0
			11	6	5		
5	J	1	Total	C	O	0	0
			11	6	5		

- Molecule 6 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			8	6	2		
6	C	1	Total	C	O	0	0
			8	6	2		
6	D	1	Total	C	O	0	0
			8	6	2		
6	D	1	Total	C	O	0	0
			8	6	2		
6	G	1	Total	C	O	0	0
			8	6	2		
6	H	1	Total	C	O	0	0
			8	6	2		
6	I	1	Total	C	O	0	0
			8	6	2		

- Molecule 7 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			8	6	2		
7	I	1	Total	C	O	0	0
			8	6	2		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	98	Total	O	0	0
			98	98		
8	B	100	Total	O	0	0
			100	100		
8	C	87	Total	O	0	0
			87	87		
8	D	62	Total	O	0	0
			62	62		
8	E	67	Total	O	0	0
			67	67		
8	F	92	Total	O	0	0
			92	92		
8	G	100	Total	O	0	0
			100	100		
8	H	84	Total	O	0	0
			84	84		
8	I	59	Total	O	0	0
			59	59		
8	J	83	Total	O	0	0
			83	83		

MolProbity failed to run properly - this section is therefore empty.

3 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	143.22Å 142.37Å 144.48Å 90.00° 90.02° 90.00°	Depositor
Resolution (Å)	48.16 – 2.32 48.16 – 2.29	Depositor EDS
% Data completeness (in resolution range)	95.9 (48.16-2.32) 97.7 (48.16-2.29)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.63 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.182 , 0.230 0.184 , 0.232	Depositor DCC
R_{free} test set	6289 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	36.7	Xtriage
Anisotropy	0.355	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 23.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.017 for k,h,-l 0.017 for -k,-h,-l 0.467 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	19701	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

4.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

4.6 Ligand geometry [i](#)

58 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	$\# Z > 2$
2	NAG	A	225	1	14,14,15	0.55	0	15,19,21	1.85	4 (26%)
3	MLK	A	260	-	55,56,56	1.10	3 (5%)	77,92,92	1.47	11 (14%)
2	NAG	B	225	1,2	14,14,15	0.64	0	15,19,21	1.56	2 (13%)
2	NAG	B	226	2	14,14,15	0.60	0	15,19,21	1.20	2 (13%)
2	NAG	B	240	1,2	14,14,15	0.54	0	15,19,21	0.84	1 (6%)
2	NAG	B	241	2,4	14,14,15	0.44	0	15,19,21	1.82	5 (33%)
4	BMA	B	242	2,5	11,11,12	0.36	0	13,15,17	1.04	1 (7%)
5	MAN	B	243	5,4	11,11,12	0.73	0	13,15,17	0.84	0
5	MAN	B	244	5	11,11,12	0.47	0	13,15,17	0.87	1 (7%)
5	MAN	B	245	5	11,11,12	0.53	0	13,15,17	0.83	0
5	MAN	B	246	4	11,11,12	0.66	0	13,15,17	0.91	0
6	MRD	B	250	-	7,7,7	0.33	0	9,10,10	0.47	0
3	MLK	B	260	-	55,56,56	1.06	4 (7%)	77,92,92	1.52	12 (15%)
7	MPD	C	222	-	7,7,7	0.32	0	9,10,10	0.35	0
2	NAG	C	225	1	14,14,15	0.46	0	15,19,21	1.04	1 (6%)
6	MRD	C	250	-	7,7,7	0.28	0	9,10,10	0.16	0
3	MLK	C	260	-	55,56,56	1.12	3 (5%)	77,92,92	1.49	10 (12%)
2	NAG	D	225	1,2	14,14,15	0.37	0	15,19,21	1.72	2 (13%)
2	NAG	D	226	2	14,14,15	0.59	0	15,19,21	1.79	4 (26%)
6	MRD	D	250	-	7,7,7	0.36	0	9,10,10	0.36	0
6	MRD	D	251	-	7,7,7	0.30	0	9,10,10	0.44	0
3	MLK	D	260	-	55,56,56	1.04	4 (7%)	77,92,92	1.46	16 (20%)
2	NAG	E	225	1,2	14,14,15	0.44	0	15,19,21	1.27	1 (6%)
2	NAG	E	226	2,4	14,14,15	0.50	0	15,19,21	0.74	0
4	BMA	E	227	2,5	11,11,12	0.26	0	13,15,17	0.59	0
5	MAN	E	228	5,4	11,11,12	0.80	1 (9%)	13,15,17	1.81	2 (15%)
5	MAN	E	230	5	11,11,12	0.46	0	13,15,17	1.44	1 (7%)
5	MAN	E	231	4	11,11,12	0.58	0	13,15,17	0.66	0
2	NAG	E	240	1	14,14,15	0.48	0	15,19,21	1.05	1 (6%)
3	MLK	E	260	-	55,56,56	1.07	3 (5%)	77,92,92	1.56	16 (20%)
2	NAG	F	225	1	14,14,15	0.41	0	15,19,21	1.10	1 (6%)
3	MLK	F	260	-	55,56,56	1.08	3 (5%)	77,92,92	1.47	10 (12%)
2	NAG	G	225	1,2	14,14,15	0.57	0	15,19,21	1.34	3 (20%)
2	NAG	G	226	2	14,14,15	0.51	0	15,19,21	1.27	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	G	240	1,2	14,14,15	0.60	0	15,19,21	0.73	0
2	NAG	G	241	2,4	14,14,15	0.56	0	15,19,21	1.00	1 (6%)
4	BMA	G	242	2,5	11,11,12	0.43	0	13,15,17	0.67	0
5	MAN	G	243	5,4	11,11,12	0.73	0	13,15,17	0.98	1 (7%)
5	MAN	G	244	5	11,11,12	0.61	0	13,15,17	0.58	0
5	MAN	G	245	5	11,11,12	0.69	0	13,15,17	1.29	1 (7%)
5	MAN	G	246	4	11,11,12	0.56	0	13,15,17	0.92	0
6	MRD	G	250	-	7,7,7	0.36	0	9,10,10	0.30	0
3	MLK	G	260	-	55,56,56	1.10	2 (3%)	77,92,92	1.57	13 (16%)
2	NAG	H	225	1	14,14,15	0.52	0	15,19,21	0.69	0
6	MRD	H	250	-	7,7,7	0.28	0	9,10,10	0.23	0
3	MLK	H	260	-	55,56,56	1.09	4 (7%)	77,92,92	1.48	12 (15%)
6	MRD	I	222	-	7,7,7	0.40	0	9,10,10	0.56	0
2	NAG	I	225	1	14,14,15	0.39	0	15,19,21	1.38	1 (6%)
7	MPD	I	250	-	7,7,7	0.24	0	9,10,10	0.39	0
3	MLK	I	260	-	55,56,56	1.03	3 (5%)	77,92,92	1.51	13 (16%)
2	NAG	J	225	1,2	14,14,15	0.45	0	15,19,21	1.45	2 (13%)
2	NAG	J	226	2,4	14,14,15	0.54	0	15,19,21	0.63	0
4	BMA	J	227	2,5	11,11,12	0.41	0	13,15,17	0.73	0
5	MAN	J	228	5,4	11,11,12	0.48	0	13,15,17	1.65	1 (7%)
5	MAN	J	230	5	11,11,12	0.65	0	13,15,17	1.23	1 (7%)
5	MAN	J	231	4	11,11,12	0.64	0	13,15,17	1.13	1 (7%)
2	NAG	J	240	1	14,14,15	0.50	0	15,19,21	0.90	1 (6%)
3	MLK	J	260	-	55,56,56	1.08	3 (5%)	77,92,92	1.52	15 (19%)

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	225	1	-	0/6/23/26	0/1/1/1
3	MLK	A	260	-	-	0/24/141/141	0/2/8/8
2	NAG	B	225	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	226	2	-	0/6/23/26	0/1/1/1
2	NAG	B	240	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	241	2,4	-	0/6/23/26	0/1/1/1
4	BMA	B	242	2,5	-	0/2/19/22	0/1/1/1
5	MAN	B	243	5,4	-	0/2/19/22	0/1/1/1
5	MAN	B	244	5	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MAN	B	245	5	-	0/2/19/22	0/1/1/1
5	MAN	B	246	4	-	0/2/19/22	0/1/1/1
6	MRD	B	250	-	-	0/5/5/5	0/0/0/0
3	MLK	B	260	-	-	0/24/141/141	0/2/8/8
7	MPD	C	222	-	-	0/5/5/5	0/0/0/0
2	NAG	C	225	1	-	0/6/23/26	0/1/1/1
6	MRD	C	250	-	-	0/5/5/5	0/0/0/0
3	MLK	C	260	-	-	0/24/141/141	0/2/8/8
2	NAG	D	225	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	226	2	-	0/6/23/26	0/1/1/1
6	MRD	D	250	-	-	0/5/5/5	0/0/0/0
6	MRD	D	251	-	-	0/5/5/5	0/0/0/0
3	MLK	D	260	-	-	0/24/141/141	0/2/8/8
2	NAG	E	225	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	226	2,4	-	0/6/23/26	0/1/1/1
4	BMA	E	227	2,5	-	0/2/19/22	0/1/1/1
5	MAN	E	228	5,4	-	0/2/19/22	0/1/1/1
5	MAN	E	230	5	-	0/2/19/22	0/1/1/1
5	MAN	E	231	4	-	0/2/19/22	0/1/1/1
2	NAG	E	240	1	-	0/6/23/26	0/1/1/1
3	MLK	E	260	-	-	0/24/141/141	0/2/8/8
2	NAG	F	225	1	-	0/6/23/26	0/1/1/1
3	MLK	F	260	-	-	0/24/141/141	0/2/8/8
2	NAG	G	225	1,2	-	0/6/23/26	0/1/1/1
2	NAG	G	226	2	-	0/6/23/26	0/1/1/1
2	NAG	G	240	1,2	-	0/6/23/26	0/1/1/1
2	NAG	G	241	2,4	-	0/6/23/26	0/1/1/1
4	BMA	G	242	2,5	-	0/2/19/22	0/1/1/1
5	MAN	G	243	5,4	-	0/2/19/22	0/1/1/1
5	MAN	G	244	5	-	0/2/19/22	0/1/1/1
5	MAN	G	245	5	-	0/2/19/22	0/1/1/1
5	MAN	G	246	4	-	0/2/19/22	0/1/1/1
6	MRD	G	250	-	-	0/5/5/5	0/0/0/0
3	MLK	G	260	-	-	0/24/141/141	0/2/8/8
2	NAG	H	225	1	-	0/6/23/26	0/1/1/1
6	MRD	H	250	-	-	0/5/5/5	0/0/0/0
3	MLK	H	260	-	-	0/24/141/141	0/2/8/8
6	MRD	I	222	-	-	0/5/5/5	0/0/0/0
2	NAG	I	225	1	-	0/6/23/26	0/1/1/1
7	MPD	I	250	-	-	0/5/5/5	0/0/0/0
3	MLK	I	260	-	-	0/24/141/141	0/2/8/8
2	NAG	J	225	1,2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	J	226	2,4	-	0/6/23/26	0/1/1/1
4	BMA	J	227	2,5	-	0/2/19/22	0/1/1/1
5	MAN	J	228	5,4	-	0/2/19/22	1/1/1/1
5	MAN	J	230	5	-	0/2/19/22	0/1/1/1
5	MAN	J	231	4	-	0/2/19/22	0/1/1/1
2	NAG	J	240	1	-	0/6/23/26	0/1/1/1
3	MLK	J	260	-	-	0/24/141/141	0/2/8/8

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	260	MLK	C8-N7	-4.63	1.34	1.40
3	C	260	MLK	C8-N7	-4.39	1.34	1.40
3	G	260	MLK	C8-N7	-4.38	1.34	1.40
3	F	260	MLK	C8-N7	-4.29	1.34	1.40
3	H	260	MLK	C8-N7	-4.26	1.34	1.40
3	B	260	MLK	C8-N7	-4.13	1.34	1.40
3	E	260	MLK	C8-N7	-4.09	1.35	1.40
3	J	260	MLK	C8-N7	-4.09	1.35	1.40
3	I	260	MLK	C8-N7	-3.88	1.35	1.40
3	G	260	MLK	C11-N7	-3.87	1.34	1.40
3	D	260	MLK	C8-N7	-3.64	1.35	1.40
3	F	260	MLK	C11-N7	-3.63	1.35	1.40
3	A	260	MLK	C11-N7	-3.54	1.35	1.40
3	C	260	MLK	C11-N7	-3.51	1.35	1.40
3	B	260	MLK	C11-N7	-3.50	1.35	1.40
3	E	260	MLK	C11-N7	-3.43	1.35	1.40
3	J	260	MLK	C11-N7	-3.43	1.35	1.40
3	D	260	MLK	C11-N7	-3.37	1.35	1.40
3	I	260	MLK	C11-N7	-3.33	1.35	1.40
3	H	260	MLK	C11-N7	-3.33	1.35	1.40
3	A	260	MLK	C6-N7	-2.59	1.41	1.44
3	F	260	MLK	C6-N7	-2.35	1.41	1.44
3	C	260	MLK	C6-N7	-2.31	1.41	1.44
3	E	260	MLK	C6-N7	-2.26	1.41	1.44
3	D	260	MLK	C6-N7	-2.22	1.41	1.44
3	J	260	MLK	C6-N7	-2.15	1.41	1.44
3	H	260	MLK	C6-N7	-2.10	1.41	1.44
3	H	260	MLK	C18-C19	-2.08	1.51	1.55
3	B	260	MLK	C18-C19	-2.03	1.51	1.55
3	D	260	MLK	C18-C19	-2.02	1.51	1.55
3	I	260	MLK	C6-N7	-2.02	1.41	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	228	MAN	O5-C1	-2.02	1.40	1.43
3	B	260	MLK	C31-C38	2.04	1.57	1.53

All (171) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	260	MLK	C21-C16-C23	-4.60	107.26	111.47
5	E	228	MAN	O5-C1-C2	-4.54	103.68	110.79
3	A	260	MLK	C16-C17-C28	-4.18	102.17	112.16
3	F	260	MLK	C16-C17-C28	-4.10	102.35	112.16
3	J	260	MLK	C33-C34-C35	-3.86	105.04	111.75
3	C	260	MLK	C21-C16-C23	-3.86	107.94	111.47
3	E	260	MLK	C16-C17-C28	-3.77	103.15	112.16
3	H	260	MLK	C16-C17-C28	-3.74	103.23	112.16
3	E	260	MLK	C33-C34-C35	-3.72	105.29	111.75
3	B	260	MLK	C33-C34-C35	-3.70	105.32	111.75
3	C	260	MLK	C33-C34-C35	-3.69	105.35	111.75
3	H	260	MLK	C33-C34-C35	-3.66	105.40	111.75
3	C	260	MLK	C16-C17-C28	-3.51	103.77	112.16
3	B	260	MLK	C16-C17-C28	-3.48	103.84	112.16
3	G	260	MLK	C16-C17-C28	-3.44	103.94	112.16
3	J	260	MLK	C16-C17-C28	-3.38	104.07	112.16
3	H	260	MLK	C21-C16-C23	-3.35	108.40	111.47
3	A	260	MLK	C33-C34-C35	-3.30	106.02	111.75
5	J	230	MAN	O5-C1-C2	-3.30	105.62	110.79
3	F	260	MLK	C33-C34-C35	-3.28	106.05	111.75
2	B	241	NAG	C4-C3-C2	-3.24	106.26	111.02
2	D	226	NAG	C1-O5-C5	-3.18	107.78	112.17
2	D	226	NAG	O5-C1-C2	-3.15	107.09	111.47
3	I	260	MLK	C33-C34-C35	-3.15	106.29	111.75
3	B	260	MLK	C21-C16-C23	-3.14	108.59	111.47
2	D	225	NAG	C2-N2-C7	-3.14	118.37	122.94
3	G	260	MLK	C33-C34-C35	-3.12	106.34	111.75
3	A	260	MLK	C37-O35-C35	-3.08	105.39	114.02
3	F	260	MLK	C29-O28-C28	-3.08	108.60	114.29
3	D	260	MLK	C21-C16-C23	-3.06	108.67	111.47
3	I	260	MLK	C16-C17-C28	-3.04	104.88	112.16
3	H	260	MLK	C37-O35-C35	-3.00	105.61	114.02
3	F	260	MLK	C37-O35-C35	-2.99	105.63	114.02
3	D	260	MLK	C37-O35-C35	-2.98	105.68	114.02
3	E	260	MLK	C29-O28-C28	-2.97	108.80	114.29
3	I	260	MLK	C37-O35-C35	-2.96	105.73	114.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	226	NAG	C2-N2-C7	-2.94	118.65	122.94
3	A	260	MLK	C21-C16-C23	-2.94	108.78	111.47
2	G	226	NAG	O5-C1-C2	-2.93	107.39	111.47
3	C	260	MLK	C37-O35-C35	-2.91	105.87	114.02
3	J	260	MLK	C21-C16-C23	-2.89	108.83	111.47
3	G	260	MLK	C39-O38-C38	-2.88	106.68	114.54
3	D	260	MLK	C16-C17-C28	-2.83	105.39	112.16
3	A	260	MLK	C29-O28-C28	-2.80	109.11	114.29
3	D	260	MLK	C33-C34-C35	-2.78	106.92	111.75
3	I	260	MLK	C29-O28-C28	-2.77	109.17	114.29
3	J	260	MLK	C29-O28-C28	-2.77	109.17	114.29
3	J	260	MLK	C37-O35-C35	-2.70	106.45	114.02
3	E	260	MLK	C21-C16-C23	-2.65	109.05	111.47
3	E	260	MLK	C37-O35-C35	-2.64	106.61	114.02
3	G	260	MLK	C24-N23-C26	-2.62	111.22	114.63
3	G	260	MLK	C37-O35-C35	-2.60	106.73	114.02
3	G	260	MLK	C38-C34-C35	-2.59	108.17	111.73
3	B	260	MLK	C37-O35-C35	-2.56	106.86	114.02
3	I	260	MLK	C39-O38-C38	-2.55	107.56	114.54
3	E	260	MLK	C18-C30-C31	-2.52	114.28	117.17
3	I	260	MLK	C22-O19-C19	-2.52	107.03	113.64
3	D	260	MLK	C39-O38-C38	-2.51	107.67	114.54
3	H	260	MLK	C24-N23-C26	-2.49	111.39	114.63
3	D	260	MLK	C38-C34-C35	-2.47	108.33	111.73
3	C	260	MLK	C18-C30-C31	-2.46	114.36	117.17
3	D	260	MLK	C18-C30-C31	-2.45	114.36	117.17
2	B	241	NAG	O5-C1-C2	-2.45	108.07	111.47
3	E	260	MLK	O14-C13-O13	-2.44	118.66	123.64
3	E	260	MLK	C24-N23-C26	-2.43	111.46	114.63
3	C	260	MLK	C39-O38-C38	-2.43	107.90	114.54
5	J	231	MAN	O5-C1-C2	-2.41	107.02	110.79
3	G	260	MLK	C15-C16-C17	-2.39	108.36	112.22
3	B	260	MLK	C39-O38-C38	-2.37	108.05	114.54
3	D	260	MLK	C24-N23-C26	-2.35	111.56	114.63
3	J	260	MLK	C24-N23-C26	-2.33	111.59	114.63
3	J	260	MLK	C18-C30-C31	-2.33	114.50	117.17
3	F	260	MLK	C21-C16-C23	-2.33	109.34	111.47
2	A	225	NAG	O7-C7-C8	-2.28	117.92	122.06
3	I	260	MLK	C18-C30-C31	-2.27	114.57	117.17
2	G	241	NAG	O5-C1-C2	-2.25	108.34	111.47
3	D	260	MLK	C22-O19-C19	-2.25	107.74	113.64
3	B	260	MLK	C29-O28-C28	-2.25	110.14	114.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	260	MLK	C39-O38-C38	-2.19	108.55	114.54
3	H	260	MLK	C39-O38-C38	-2.18	108.58	114.54
3	I	260	MLK	C38-C34-C35	-2.16	108.76	111.73
3	B	260	MLK	C24-N23-C26	-2.15	111.82	114.63
3	E	260	MLK	C39-O38-C38	-2.15	108.67	114.54
3	I	260	MLK	C24-N23-C26	-2.15	111.83	114.63
2	J	225	NAG	O5-C1-C2	-2.14	108.50	111.47
3	H	260	MLK	C27-C26-N23	-2.13	114.96	117.52
2	G	225	NAG	O5-C1-C2	-2.13	108.51	111.47
3	D	260	MLK	C27-C26-N23	-2.12	114.97	117.52
3	J	260	MLK	C22-O19-C19	-2.12	108.07	113.64
3	I	260	MLK	C21-C16-C23	-2.12	109.53	111.47
3	G	260	MLK	C27-C26-N23	-2.10	115.00	117.52
3	D	260	MLK	C29-O28-C28	-2.07	110.47	114.29
3	A	260	MLK	C22-O19-C19	-2.04	108.30	113.64
3	J	260	MLK	O14-C13-O13	-2.04	119.48	123.64
3	E	260	MLK	C38-C34-C35	-2.01	108.97	111.73
3	B	260	MLK	C22-O19-C19	-2.01	108.37	113.64
3	B	260	MLK	C9-C8-N7	2.01	109.54	108.03
3	B	260	MLK	C10-C11-N7	2.04	109.48	108.28
3	G	260	MLK	C21-C16-C17	2.04	112.50	110.00
5	G	243	MAN	C1-C2-C3	2.05	112.25	109.65
4	B	242	BMA	C1-C2-C3	2.06	112.27	109.65
3	J	260	MLK	O19-C19-C18	2.07	112.29	108.36
2	B	241	NAG	C2-N2-C7	2.07	125.97	122.94
3	A	260	MLK	C9-C8-N7	2.09	109.60	108.03
3	E	260	MLK	O8-C8-N7	2.12	125.97	123.98
3	F	260	MLK	O19-C19-C18	2.15	112.44	108.36
2	B	241	NAG	C1-C2-N2	2.15	114.16	110.49
3	D	260	MLK	O11-C11-N7	2.15	126.43	124.29
2	G	225	NAG	C4-C3-C2	2.16	114.18	111.02
3	D	260	MLK	O8-C8-N7	2.16	126.01	123.98
3	D	260	MLK	C10-C11-N7	2.18	109.57	108.28
3	H	260	MLK	C9-C8-N7	2.20	109.68	108.03
3	I	260	MLK	C9-C8-N7	2.25	109.72	108.03
2	E	240	NAG	C1-O5-C5	2.28	115.31	112.17
3	E	260	MLK	C10-C11-N7	2.30	109.64	108.28
3	C	260	MLK	O14-C13-C1	2.32	116.92	112.20
3	H	260	MLK	O14-C13-C1	2.32	116.92	112.20
2	B	240	NAG	C1-O5-C5	2.34	115.40	112.17
3	A	260	MLK	C10-C11-N7	2.37	109.68	108.28
3	C	260	MLK	C10-C11-N7	2.39	109.69	108.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	260	MLK	C1-C6-N7	2.44	123.14	121.05
2	B	226	NAG	C4-C3-C2	2.46	114.62	111.02
5	B	244	MAN	C1-O5-C5	2.47	115.57	112.17
2	B	225	NAG	C3-C4-C5	2.48	114.59	110.22
3	A	260	MLK	O19-C19-C18	2.49	113.08	108.36
2	J	240	NAG	C1-O5-C5	2.49	115.60	112.17
3	J	260	MLK	C10-C11-N7	2.55	109.78	108.28
3	F	260	MLK	C9-C8-N7	2.57	109.96	108.03
3	G	260	MLK	C10-C11-N7	2.59	109.81	108.28
2	A	225	NAG	C8-C7-N2	2.64	120.88	116.11
3	E	260	MLK	O14-C15-C16	2.66	111.97	108.29
3	H	260	MLK	C15-O14-C13	2.68	122.11	116.52
3	F	260	MLK	C10-C11-N7	2.77	109.92	108.28
2	D	226	NAG	C4-C3-C2	2.82	115.15	111.02
3	C	260	MLK	C15-O14-C13	2.84	122.44	116.52
3	H	260	MLK	C10-C11-N7	2.88	109.98	108.28
3	B	260	MLK	O14-C13-C1	2.90	118.09	112.20
3	J	260	MLK	O14-C13-C1	2.93	118.16	112.20
2	C	225	NAG	C1-O5-C5	3.04	116.36	112.17
3	G	260	MLK	O14-C13-C1	3.15	118.60	112.20
2	F	225	NAG	C1-O5-C5	3.24	116.63	112.17
2	G	225	NAG	C1-O5-C5	3.25	116.65	112.17
3	J	260	MLK	C1-C6-N7	3.29	123.87	121.05
3	A	260	MLK	O14-C13-C1	3.34	119.00	112.20
3	I	260	MLK	O14-C13-C1	3.42	119.15	112.20
3	F	260	MLK	C23-C16-C17	3.45	111.06	108.19
5	G	245	MAN	C1-C2-C3	3.45	114.03	109.65
3	D	260	MLK	O14-C13-C1	3.57	119.47	112.20
3	E	260	MLK	O14-C13-C1	3.66	119.64	112.20
2	A	225	NAG	C2-N2-C7	3.66	128.28	122.94
3	F	260	MLK	O14-C13-C1	3.68	119.68	112.20
2	B	241	NAG	C1-O5-C5	3.70	117.26	112.17
5	E	228	MAN	C3-C4-C5	3.83	116.96	110.22
3	D	260	MLK	C23-C16-C17	3.84	111.39	108.19
2	D	226	NAG	C3-C4-C5	3.85	117.00	110.22
2	E	225	NAG	C1-O5-C5	3.87	117.50	112.17
3	J	260	MLK	C23-C16-C17	4.04	111.56	108.19
3	E	260	MLK	C23-C16-C17	4.05	111.56	108.19
2	B	225	NAG	C4-C3-C2	4.09	117.02	111.02
2	A	225	NAG	C1-O5-C5	4.24	118.01	112.17
5	E	230	MAN	C1-O5-C5	4.25	118.02	112.17
2	J	225	NAG	C1-O5-C5	4.38	118.20	112.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	260	MLK	C23-C16-C17	4.43	111.88	108.19
2	D	225	NAG	C1-O5-C5	4.53	118.41	112.17
2	I	225	NAG	C1-O5-C5	4.58	118.48	112.17
3	A	260	MLK	C23-C16-C17	4.76	112.16	108.19
3	I	260	MLK	C23-C16-C17	4.88	112.25	108.19
3	G	260	MLK	C23-C16-C17	4.91	112.28	108.19
5	J	228	MAN	C1-O5-C5	5.00	119.06	112.17
3	C	260	MLK	C23-C16-C17	5.60	112.86	108.19
3	B	260	MLK	C23-C16-C17	5.72	112.96	108.19

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	J	228	MAN	C1-C2-C3-C4-C5-O5

No monomer is involved in short contacts.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 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	214/230 (93%)	-0.45	0 100 100	21, 32, 63, 93	0
1	B	216/230 (93%)	-0.41	4 (1%) 67 73	20, 32, 65, 97	0
1	C	221/230 (96%)	-0.25	9 (4%) 38 45	20, 32, 78, 109	0
1	D	214/230 (93%)	-0.34	5 (2%) 61 67	21, 35, 76, 107	0
1	E	216/230 (93%)	-0.38	0 100 100	21, 32, 64, 98	0
1	F	214/230 (93%)	-0.44	0 100 100	21, 32, 61, 90	0
1	G	216/230 (93%)	-0.44	2 (0%) 84 87	21, 32, 62, 97	0
1	H	221/230 (96%)	-0.27	9 (4%) 38 45	20, 32, 78, 114	0
1	I	214/230 (93%)	-0.31	1 (0%) 90 93	22, 35, 78, 119	0
1	J	216/230 (93%)	-0.41	3 (1%) 75 80	20, 32, 63, 98	0
All	All	2162/2300 (94%)	-0.37	33 (1%) 74 79	20, 33, 70, 119	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	213	PHE	5.2
1	H	212	GLY	5.0
1	C	213	PHE	4.9
1	H	215	ARG	4.6
1	C	-3	ASP	3.9
1	C	0	LEU	3.8
1	B	-8	ASP	3.6
1	H	159[A]	ASP	3.6
1	I	-3	ASP	3.5
1	B	159[A]	ASP	3.5
1	C	159[A]	ASP	3.3
1	H	0	LEU	3.3
1	D	-1	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	G	159[A]	ASP	3.0
1	C	211	ASN	3.0
1	C	215	ARG	2.9
1	H	-3	ASP	2.8
1	H	211	ASN	2.6
1	D	-5	ASP	2.6
1	G	-7	TYR	2.5
1	B	-7	TYR	2.5
1	J	16[A]	ARG	2.4
1	H	15	ASN	2.4
1	J	-8	ASP	2.3
1	C	214	PHE	2.3
1	J	-7	TYR	2.3
1	D	55	TRP	2.3
1	D	-4	ASP	2.2
1	H	214	PHE	2.2
1	C	216	ASN	2.2
1	C	16	ARG	2.2
1	D	-3	ASP	2.1
1	B	-6	LYS	2.0

5.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
7	MPD	C	222	8/8	0.84	0.31	14.65	43,61,73,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
7	MPD	I	250	8/8	0.89	0.39	13.92	44,57,65,72	0
6	MRD	I	222	8/8	0.76	0.25	10.91	51,61,73,74	0
3	MLK	J	260	49/49	0.85	0.38	9.15	46,66,81,92	0
6	MRD	C	250	8/8	0.92	0.28	8.43	40,53,61,71	0
6	MRD	H	250	8/8	0.94	0.21	6.59	42,54,62,73	0
3	MLK	E	260	49/49	0.82	0.34	6.59	40,64,84,91	0
6	MRD	D	250	8/8	0.88	0.24	5.62	48,58,73,73	0
5	MAN	E	230	11/12	0.94	0.15	5.11	60,73,83,83	0
5	MAN	J	230	11/12	0.87	0.17	4.38	61,70,91,91	0
6	MRD	G	250	8/8	0.88	0.12	2.65	31,47,57,58	0
6	MRD	B	250	8/8	0.90	0.17	2.10	37,50,67,68	0
5	MAN	J	231	11/12	0.77	0.28	1.59	82,102,114,115	0
2	NAG	I	225	14/15	0.87	0.18	1.59	58,71,77,78	0
2	NAG	D	225	14/15	0.92	0.15	1.56	68,74,86,97	0
2	NAG	B	225	14/15	0.90	0.13	1.15	57,65,78,79	0
5	MAN	E	231	11/12	0.91	0.22	0.97	65,78,90,94	0
2	NAG	E	240	14/15	0.83	0.23	0.95	69,81,89,98	0
2	NAG	F	225	14/15	0.86	0.17	0.92	56,70,79,83	0
5	MAN	B	244	11/12	0.94	0.17	0.84	70,76,84,87	0
2	NAG	J	240	14/15	0.77	0.20	0.66	67,78,87,87	0
4	BMA	G	242	11/12	0.81	0.16	0.35	61,77,87,91	0
3	MLK	G	260	49/49	0.93	0.12	0.33	31,42,51,60	0
6	MRD	D	251	8/8	0.72	0.21	0.10	52,63,71,74	0
2	NAG	G	225	14/15	0.91	0.11	0.05	54,68,79,82	0
2	NAG	A	225	14/15	0.91	0.13	-0.04	59,66,78,80	0
3	MLK	A	260	49/49	0.93	0.12	-0.06	29,42,52,69	0
3	MLK	D	260	49/49	0.94	0.12	-0.08	35,46,55,62	0
3	MLK	C	260	49/49	0.94	0.11	-0.16	31,43,52,62	0
3	MLK	I	260	49/49	0.94	0.12	-0.20	35,45,52,58	0
2	NAG	J	225	14/15	0.91	0.13	-0.32	45,54,69,74	0
3	MLK	B	260	49/49	0.93	0.11	-0.35	31,42,52,63	0
2	NAG	E	225	14/15	0.93	0.11	-0.35	42,50,70,73	0
3	MLK	H	260	49/49	0.94	0.10	-0.60	31,42,52,61	0
3	MLK	F	260	49/49	0.94	0.10	-0.74	33,42,54,70	0
2	NAG	D	226	14/15	0.82	0.26	-	98,102,109,110	0
5	MAN	G	246	11/12	0.91	0.29	-	61,76,87,88	0
2	NAG	G	226	14/15	0.73	0.28	-	70,93,104,105	0
5	MAN	J	228	11/12	0.72	0.26	-	100,103,109,115	0
4	BMA	B	242	11/12	0.86	0.15	-	63,81,88,95	0
5	MAN	B	246	11/12	0.90	0.23	-	65,76,87,88	0
5	MAN	B	245	11/12	0.83	0.12	-	87,92,99,101	0
5	MAN	B	243	11/12	0.91	0.17	-	70,73,84,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	NAG	H	225	14/15	0.88	0.13	-	61,68,77,84	0
2	NAG	G	241	14/15	0.88	0.23	-	79,90,95,99	0
2	NAG	B	226	14/15	0.84	0.27	-	84,91,102,104	0
2	NAG	C	225	14/15	0.91	0.14	-	60,67,76,84	0
2	NAG	E	226	14/15	0.90	0.09	-	57,71,82,85	0
5	MAN	E	228	11/12	0.80	0.24	-	91,102,109,112	0
2	NAG	G	240	14/15	0.90	0.19	-	68,76,83,95	0
2	NAG	B	241	14/15	0.84	0.17	-	73,90,96,97	0
5	MAN	G	243	11/12	0.92	0.15	-	71,79,84,99	0
5	MAN	G	244	11/12	0.96	0.19	-	73,85,89,92	0
5	MAN	G	245	11/12	0.74	0.19	-	80,97,109,111	0
2	NAG	J	226	14/15	0.89	0.11	-	66,73,80,91	0
2	NAG	B	240	14/15	0.91	0.17	-	69,75,82,91	0
4	BMA	J	227	11/12	0.83	0.23	-	95,101,112,114	0
4	BMA	E	227	11/12	0.90	0.13	-	81,87,99,100	0

5.5 Other polymers ⓘ

There are no such residues in this entry.