



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:02 PM GMT

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 : 2011-06-19
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 : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

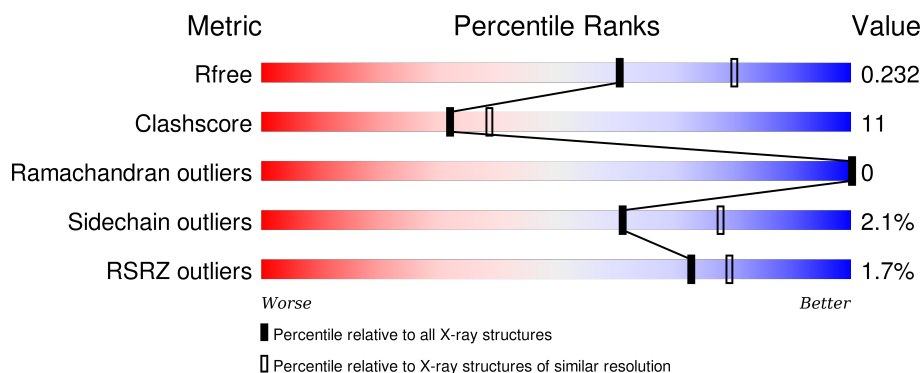
1 Overall quality at a glance

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}	91344	4425 (2.34-2.30)
Clashscore	102246	5057 (2.34-2.30)
Ramachandran outliers	100387	5008 (2.34-2.30)
Sidechain outliers	100360	5007 (2.34-2.30)
RSRZ outliers	91569	4432 (2.34-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	230	
1	B	230	
1	C	230	
1	D	230	
1	E	230	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	230	
1	G	230	
1	H	230	
1	I	230	
1	J	230	

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
2	NAG	A	225	-	-	X	-
3	MLK	E	260	-	-	-	X
3	MLK	J	260	-	-	-	X
6	MRD	B	250	-	-	-	X
6	MRD	C	250	-	-	-	X
6	MRD	D	250	-	-	-	X
6	MRD	D	251	-	-	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
8	MAN	E	230	-	-	-	X
8	MAN	J	230	-	-	-	X

2 Entry composition

There are 9 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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

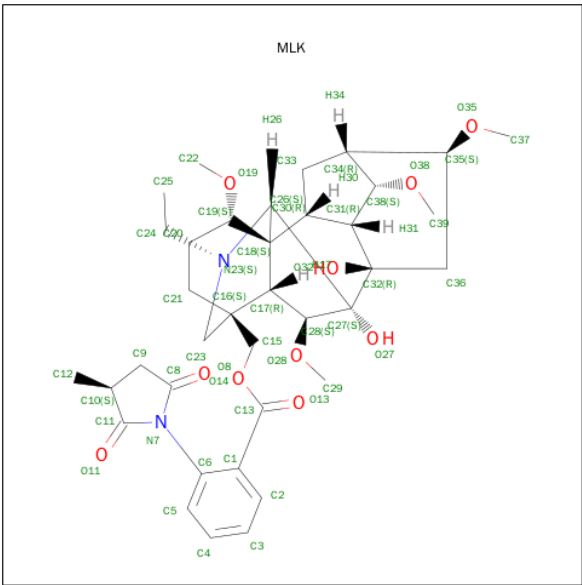
Chain	Residue	Modelled	Actual	Comment	Reference
J	-8	ASP	-	EXPRESSION TAG	UNP Q8WSF8
J	-7	TYR	-	EXPRESSION TAG	UNP Q8WSF8
J	-6	LYS	-	EXPRESSION TAG	UNP Q8WSF8
J	-5	ASP	-	EXPRESSION TAG	UNP Q8WSF8
J	-4	ASP	-	EXPRESSION TAG	UNP Q8WSF8
J	-3	ASP	-	EXPRESSION TAG	UNP Q8WSF8
J	-2	ASP	-	EXPRESSION TAG	UNP Q8WSF8
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 SUGAR (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	C	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	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		

- Molecule 3 is METHYLLYCACONITINE (three-letter code: MLK) (formula: C₃₇H₅₀N₂O₁₀).



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

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

Continued on next page...

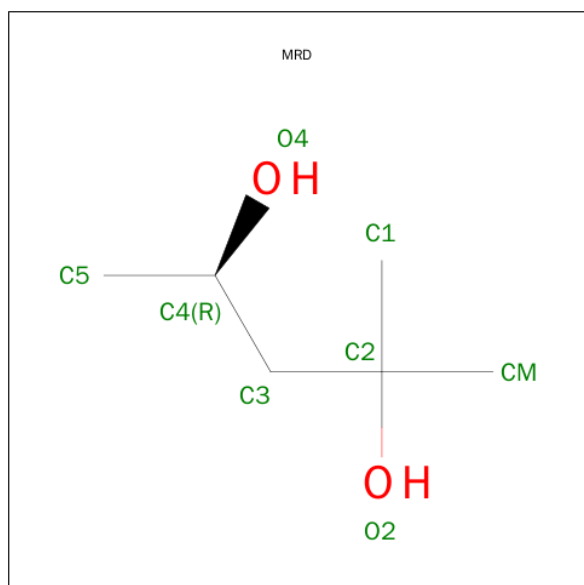
Continued from previous page...

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

- Molecule 5 is a polymer of unknown type called SUGAR (7-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	7	Total	C	N	O	0	0
			83	46	2	35		
5	G	7	Total	C	N	O	0	0
			83	46	2	35		

- Molecule 6 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: C₆H₁₄O₂).



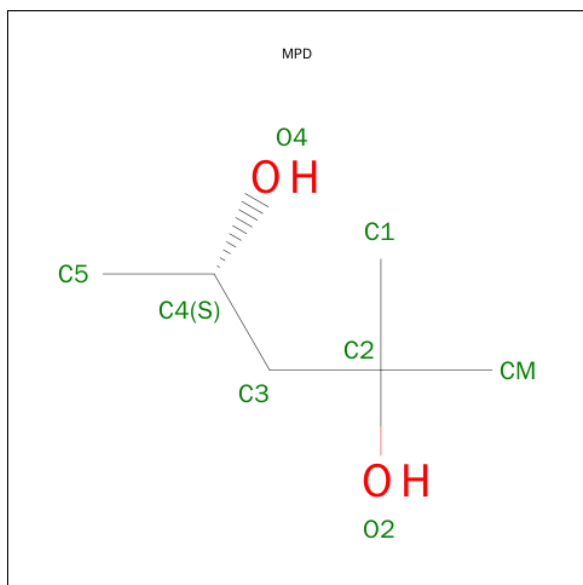
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			8	6	2		
6	C	1	Total	C	O	0	0
			8	6	2		
6	D	1	Total	C	O	0	0
			8	6	2		
6	D	1	Total	C	O	0	0
			8	6	2		
6	G	1	Total	C	O	0	0
			8	6	2		
6	H	1	Total	C	O	0	0
			8	6	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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 a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	E	6	Total	C	N	O	0	0
			72	40	2	30		
8	J	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	98	Total	O	0	0
			98	98		

Continued on next page...

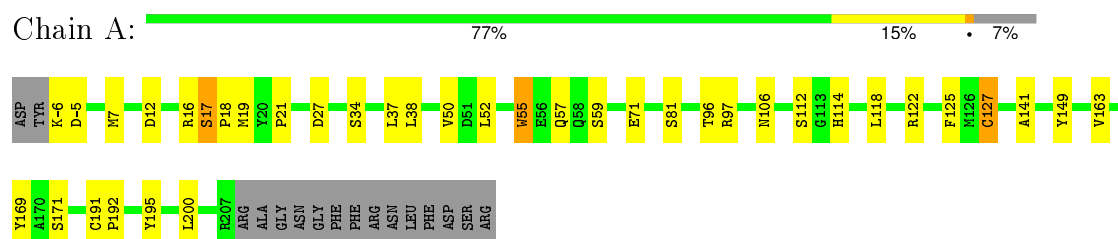
Continued from previous page...

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

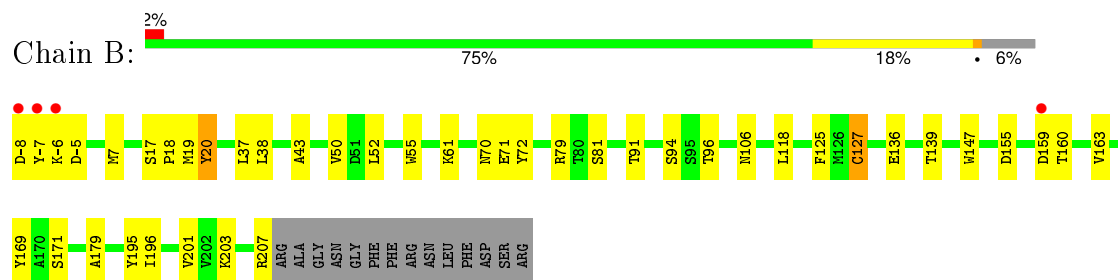
3 Residue-property plots

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.

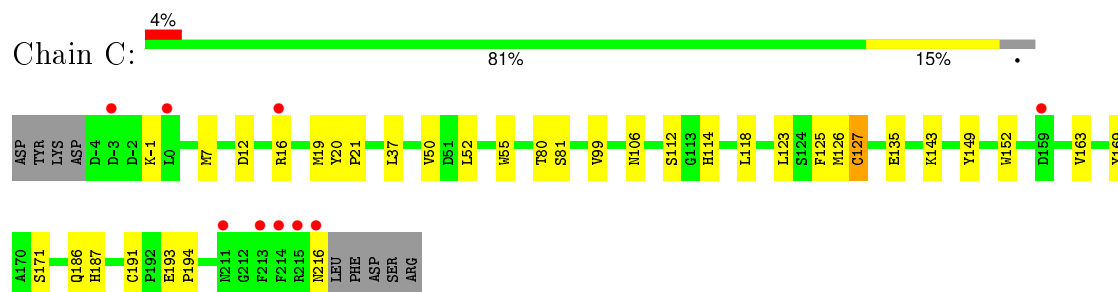
• Molecule 1: Soluble acetylcholine receptor



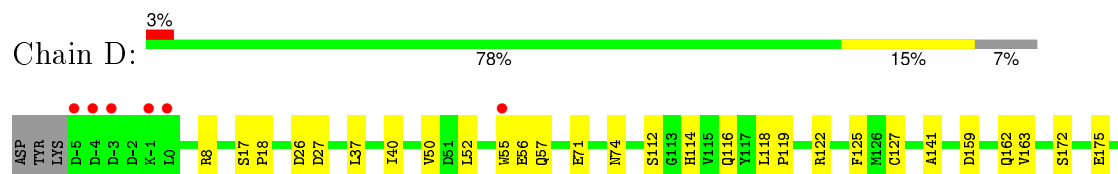
• Molecule 1: Soluble acetylcholine receptor



• Molecule 1: Soluble acetylcholine receptor



• Molecule 1: Soluble acetylcholine receptor





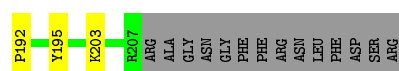
- Molecule 1: Soluble acetylcholine receptor

Chain E: 74% 20% 6%



- Molecule 1: Soluble acetylcholine receptor

Chain F: 79% 13% 7%



- Molecule 1: Soluble acetylcholine receptor

Chain G: 77% 16% 6%



- Molecule 1: Soluble acetylcholine receptor

Chain H: 77% 18% 4%



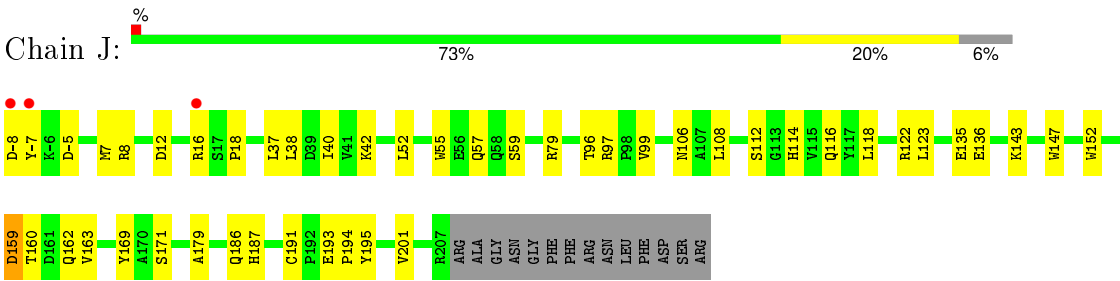
- Molecule 1: Soluble acetylcholine receptor

Chain I: 83% 10% 7%



PHE
PHE
ARG
ASN
LEU
PHE
ASP
SER
ARG

• Molecule 1: Soluble acetylcholine receptor



4 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	6291 reflections (5.32%)	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
Estimated twinning fraction	0.017 for k,h,-l 0.017 for -k,-h,-l 0.467 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 126426 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MPD, BMA, NAG, MLK, MRD, 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	0.47	0/1817	0.62	0/2476
1	B	0.63	4/1852 (0.2%)	0.66	0/2524
1	C	0.52	1/1888 (0.1%)	0.64	0/2573
1	D	0.40	0/1835	0.59	0/2501
1	E	0.41	0/1864	0.64	0/2540
1	F	0.49	2/1833 (0.1%)	0.65	0/2497
1	G	0.55	1/1871 (0.1%)	0.66	2/2550 (0.1%)
1	H	0.42	0/1877	0.65	0/2556
1	I	0.39	0/1818	0.62	0/2479
1	J	0.40	0/1874	0.63	0/2552
All	All	0.47	8/18529 (0.0%)	0.64	2/25248 (0.0%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	20	TYR	CD2-CE2	-5.86	1.30	1.39
1	B	72	TYR	CD2-CE2	-5.76	1.30	1.39
1	G	20	TYR	CD2-CE2	-5.44	1.31	1.39
1	B	72	TYR	CD1-CE1	-5.29	1.31	1.39
1	F	97[A]	ARG	CB-CG	-5.17	1.38	1.52
1	F	97[B]	ARG	CB-CG	-5.17	1.38	1.52
1	C	20	TYR	CD1-CE1	-5.16	1.31	1.39
1	B	20	TYR	CD1-CE1	-5.11	1.31	1.39

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	17	SER	CB-CA-C	5.24	120.06	110.10
1	G	14	PHE	CB-CA-C	-5.09	100.22	110.40

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	1752	0	1678	40	0
1	B	1781	0	1697	39	0
1	C	1815	0	1737	33	0
1	D	1764	0	1688	27	0
1	E	1789	0	1706	53	0
1	F	1762	0	1694	31	0
1	G	1793	0	1708	44	0
1	H	1810	0	1735	36	0
1	I	1753	0	1667	21	0
1	J	1796	0	1722	57	0
2	A	14	0	13	8	0
2	C	14	0	13	0	0
2	E	14	0	13	0	0
2	F	14	0	13	0	0
2	H	14	0	13	0	0
2	I	14	0	13	0	0
2	J	14	0	13	0	0
3	A	49	0	50	7	0
3	B	49	0	50	4	0
3	C	49	0	50	7	0
3	D	49	0	50	8	0
3	E	49	0	50	12	0
3	F	49	0	50	8	0
3	G	49	0	50	5	0
3	H	49	0	50	9	0
3	I	49	0	50	7	0
3	J	49	0	50	15	0
4	B	28	0	25	0	0
4	D	28	0	25	1	0
4	G	28	0	25	2	0
5	B	83	0	70	0	0
5	G	83	0	70	0	0
6	B	8	0	14	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	8	0	14	1	0
6	D	16	0	28	10	0
6	G	8	0	14	5	0
6	H	8	0	14	1	0
6	I	8	0	14	0	0
7	C	8	0	14	0	0
7	I	8	0	14	5	0
8	E	72	0	61	2	0
8	J	72	0	61	2	0
9	A	98	0	0	3	0
9	B	100	0	0	1	0
9	C	87	0	0	3	0
9	D	62	0	0	5	0
9	E	67	0	0	4	0
9	F	92	0	0	2	0
9	G	100	0	0	1	0
9	H	84	0	0	8	0
9	I	59	0	0	1	0
9	J	83	0	0	8	0
All	All	19701	0	18086	390	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 11.

All (390) 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:B:37[B]:LEU:HD11	1:B:52:LEU:HD11	1.18	1.11
1:J:160:THR:HG22	1:J:162:GLN:H	1.09	1.09
1:G:86:TRP:HE1	6:G:250:MRD:HMC1	1.18	1.08
2:A:225:NAG:H3	2:A:225:NAG:H83	1.43	1.00
1:G:52:LEU:HD22	1:G:54:TYR:HD2	1.26	0.96
1:B:37[B]:LEU:CD1	1:B:52:LEU:HD11	1.99	0.93
1:B:17:SER:HB3	1:B:18:PRO:HD2	1.47	0.93
1:A:-6:LYS:HG3	1:A:-5:ASP:H	1.38	0.89
1:G:52:LEU:HD22	1:G:54:TYR:CD2	2.07	0.88
1:B:17:SER:CB	1:B:18:PRO:HD2	2.04	0.88
1:J:37[A]:LEU:HD11	1:J:52:LEU:HD11	1.53	0.88
1:B:37[B]:LEU:HD11	1:B:52:LEU:CD1	2.03	0.87
1:J:160:THR:HG22	1:J:162:GLN:N	1.90	0.85
1:J:195:TYR:CZ	3:J:260:MLK:H331	2.12	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:37:LEU:HD13	1:F:163:VAL:HG11	1.60	0.82
7:I:250:MPD:HM2	7:I:250:MPD:H52	1.62	0.81
1:G:17:SER:OG	1:G:18:PRO:HD2	1.80	0.81
1:A:59:SER:HB2	1:A:114[B]:HIS:CE1	2.16	0.81
1:I:149:TYR:OH	7:I:250:MPD:HM3	1.81	0.80
1:A:17:SER:OG	1:A:18:PRO:CD	2.30	0.79
1:I:7:MET:SD	1:J:18:PRO:HG2	2.23	0.78
1:E:195:TYR:CZ	3:E:260:MLK:H331	2.19	0.78
1:A:12:ASP:HA	1:A:16:ARG:HG3	1.65	0.78
1:J:59:SER:HB2	1:J:114[B]:HIS:CE1	2.20	0.77
1:I:55:TRP:CH2	3:J:260:MLK:H292	2.19	0.77
1:H:81:SER:HA	1:H:106:ASN:HD22	1.50	0.76
1:G:149:TYR:OH	6:G:250:MRD:HMC3	1.84	0.76
1:D:55:TRP:CH2	3:E:260:MLK:H292	2.20	0.76
1:H:116:GLN:HE22	3:I:260:MLK:H373	1.49	0.76
1:E:152:TRP:CE3	1:E:193:GLU:HG3	2.22	0.75
1:B:81:SER:HA	1:B:106:ASN:HD22	1.52	0.74
1:J:160:THR:CG2	1:J:162:GLN:H	1.96	0.74
2:A:225:NAG:H3	2:A:225:NAG:C8	2.16	0.73
1:G:38:LEU:HD11	1:G:55:TRP:NE1	2.03	0.73
1:G:159[A]:ASP:OD1	1:G:160:THR:HG22	1.89	0.72
1:A:112:SER:OG	1:A:114[A]:HIS:HD2	1.72	0.71
1:D:162:GLN:HG3	9:D:358:HOH:O	1.89	0.71
1:D:141:ALA:HB3	6:D:251:MRD:H3C2	1.73	0.71
1:G:55:TRP:HE3	9:H:363:HOH:O	1.72	0.71
1:J:55:TRP:HE3	9:J:429:HOH:O	1.74	0.71
1:B:37[A]:LEU:HG	1:B:163:VAL:HG11	1.72	0.70
1:E:186:GLN:HG3	3:E:260:MLK:H3	1.73	0.70
1:H:52:LEU:HD13	1:H:125:PHE:HE2	1.55	0.70
9:A:386:HOH:O	1:E:55:TRP:HE3	1.74	0.70
1:C:135[B]:GLU:H	1:C:135[B]:GLU:CD	1.95	0.70
1:C:216:ASN:ND2	6:D:251:MRD:O4	2.25	0.69
1:G:86:TRP:NE1	6:G:250:MRD:HMC1	2.02	0.69
1:B:7:MET:HE2	1:C:21:PRO:HD3	1.73	0.69
1:G:81:SER:HA	1:G:106:ASN:HD22	1.58	0.69
3:J:260:MLK:H31	3:J:260:MLK:O28	1.94	0.68
1:B:-6:LYS:HG2	1:J:-7:TYR:CE1	2.27	0.68
1:A:52:LEU:HG	1:A:125:PHE:HE2	1.58	0.68
1:E:172:SER:O	1:E:207[A]:ARG:HD3	1.93	0.68
1:C:37[B]:LEU:HG	1:C:163:VAL:HG11	1.76	0.68
1:A:112:SER:OG	2:A:225:NAG:H82	1.93	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:55:TRP:CH2	3:G:260:MLK:H292	2.30	0.67
1:J:152:TRP:CE3	1:J:193:GLU:HG3	2.29	0.67
1:I:118:LEU:HD22	3:J:260:MLK:H242	1.76	0.67
1:C:81:SER:HA	1:C:106:ASN:HD22	1.60	0.67
1:A:17:SER:OG	1:A:18:PRO:HD3	1.94	0.66
1:F:112:SER:OG	1:F:114[A]:HIS:HD2	1.78	0.66
1:I:55:TRP:HH2	3:J:260:MLK:H292	1.62	0.65
1:A:37[B]:LEU:HG	1:A:163:VAL:HG11	1.77	0.65
1:I:37[B]:LEU:HG	1:I:163:VAL:HG11	1.79	0.64
1:E:195:TYR:CE2	3:E:260:MLK:H19	2.32	0.64
1:B:7:MET:CE	1:C:21:PRO:HD3	2.27	0.64
1:C:12:ASP:HA	1:C:16:ARG:HD3	1.79	0.64
1:D:172:SER:HB3	1:D:207[B]:ARG:HH22	1.62	0.64
1:F:7:MET:HG2	9:G:402:HOH:O	1.97	0.64
1:J:186:GLN:HG3	3:J:260:MLK:H3	1.79	0.64
1:C:55:TRP:CH2	3:D:260:MLK:H292	2.34	0.63
1:I:112:SER:OG	1:I:114:HIS:HD2	1.82	0.63
1:E:-7:TYR:OH	1:G:-6:LYS:HB2	1.99	0.63
1:E:195:TYR:CE2	3:E:260:MLK:H331	2.33	0.62
2:A:225:NAG:C3	2:A:225:NAG:H83	2.24	0.62
1:D:55:TRP:HH2	3:E:260:MLK:H292	1.62	0.62
1:F:-1:LYS:HE2	1:G:27:ASP:OD1	1.99	0.62
1:C:-1:LYS:HE2	1:D:27:ASP:OD1	2.00	0.62
1:G:37[B]:LEU:HG	1:G:163:VAL:HG11	1.81	0.61
1:E:195:TYR:CD2	3:E:260:MLK:H19	2.36	0.61
1:A:114[B]:HIS:CD2	2:A:225:NAG:O6	2.53	0.61
1:A:55:TRP:CH2	3:B:260:MLK:H292	2.35	0.61
1:C:55:TRP:CZ3	3:D:260:MLK:H292	2.36	0.61
1:G:116:GLN:HE22	3:H:260:MLK:C37	2.12	0.61
1:E:37[A]:LEU:HD11	1:E:52:LEU:HD11	1.81	0.61
1:G:37[A]:LEU:CD1	1:G:52:LEU:HD21	2.31	0.61
1:D:112:SER:OG	1:D:114:HIS:HD2	1.84	0.61
1:B:17:SER:CB	1:B:18:PRO:CD	2.77	0.60
1:F:136:GLU:HB2	9:F:342:HOH:O	2.01	0.60
1:A:17:SER:OG	1:A:18:PRO:HD2	2.00	0.60
1:D:37[B]:LEU:HG	1:D:163:VAL:HG11	1.83	0.60
1:F:12:ASP:O	1:F:16[B]:ARG:HB3	2.01	0.60
1:H:186[B]:GLN:HG3	3:H:260:MLK:H3	1.84	0.60
1:B:159[A]:ASP:OD1	1:B:160:THR:HG22	2.01	0.60
1:F:52[A]:LEU:HG	1:F:125:PHE:HE2	1.67	0.60
3:C:260:MLK:H31	3:C:260:MLK:O28	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:52:LEU:CD2	1:G:54:TYR:HD2	2.09	0.59
1:J:37[B]:LEU:HG	1:J:163:VAL:HG11	1.84	0.59
1:F:55:TRP:HH2	3:G:260:MLK:H292	1.67	0.59
3:E:260:MLK:H31	3:E:260:MLK:O28	2.03	0.59
1:J:152:TRP:CD2	1:J:193:GLU:HG3	2.38	0.59
1:G:37[A]:LEU:HD13	1:G:52:LEU:HD21	1.83	0.58
1:H:55:TRP:CH2	3:I:260:MLK:H292	2.37	0.58
1:H:213:PHE:HE1	1:H:215:ARG:HG3	1.68	0.58
1:J:195:TYR:CD2	3:J:260:MLK:H19	2.38	0.58
1:B:55:TRP:CH2	3:C:260:MLK:H292	2.39	0.58
1:A:-6:LYS:HG3	1:A:-5:ASP:N	2.13	0.58
1:F:37:LEU:HG	1:F:52[B]:LEU:HD11	1.86	0.58
1:G:195:TYR:CZ	3:G:260:MLK:H331	2.39	0.57
3:D:260:MLK:O28	3:D:260:MLK:H31	2.03	0.57
1:E:97[A]:ARG:NH2	9:E:367:HOH:O	2.37	0.57
1:E:16:ARG:NH2	1:H:16[A]:ARG:HH12	2.03	0.57
1:J:97[B]:ARG:NH2	9:J:405:HOH:O	2.37	0.57
1:B:17:SER:HB3	1:B:18:PRO:CD	2.29	0.57
1:J:37[A]:LEU:HD11	1:J:52:LEU:CD1	2.32	0.57
1:J:59:SER:HB2	1:J:114[B]:HIS:HE1	1.69	0.56
1:G:55:TRP:CE3	9:H:363:HOH:O	2.52	0.56
1:B:19:MET:HG3	1:B:20:TYR:O	2.05	0.56
1:J:160:THR:HG21	1:J:162:GLN:HB2	1.86	0.56
1:A:169:TYR:CZ	1:A:171:SER:HB2	2.41	0.56
1:G:17:SER:CB	1:G:18:PRO:HD2	2.35	0.56
1:J:38:LEU:HD21	1:J:55:TRP:CE2	2.40	0.56
1:B:195:TYR:CZ	3:B:260:MLK:H331	2.41	0.56
1:E:99:VAL:HG23	9:E:399:HOH:O	2.05	0.56
1:J:195:TYR:CE2	3:J:260:MLK:H19	2.40	0.56
1:H:16[A]:ARG:HH11	1:H:16[A]:ARG:HG3	1.71	0.56
1:B:-8:ASP:HB3	1:B:-5:ASP:CB	2.37	0.55
1:E:37[B]:LEU:HG	1:E:163:VAL:HG11	1.87	0.55
1:G:106:ASN:HD21	6:H:250:MRD:H5C3	1.71	0.55
1:A:21:PRO:HB2	1:E:6:LEU:HD23	1.87	0.55
1:C:216:ASN:HD21	6:D:251:MRD:C4	2.18	0.55
6:D:251:MRD:C5	9:D:437:HOH:O	2.54	0.55
1:F:50:VAL:HG21	1:F:127:CYS:SG	2.47	0.55
1:H:37[B]:LEU:HG	1:H:163:VAL:HG11	1.88	0.55
1:J:38:LEU:HD21	1:J:55:TRP:CZ2	2.42	0.55
1:D:172:SER:HB3	1:D:207[B]:ARG:NH2	2.21	0.55
1:A:112:SER:OG	1:A:114[A]:HIS:CD2	2.58	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:135:GLU:HA	1:H:205:ARG:HD2	1.90	0.54
1:G:38:LEU:HD11	1:G:55:TRP:HE1	1.71	0.54
1:C:7:MET:SD	1:D:18:PRO:HG2	2.47	0.54
1:E:152:TRP:CD2	1:E:193:GLU:HG3	2.41	0.54
1:A:34[B]:SER:OG	1:A:57:GLN:HB3	2.07	0.54
1:D:71:GLU:HA	1:I:71:GLU:HA	1.89	0.54
1:C:99:VAL:HG23	9:C:354:HOH:O	2.07	0.54
1:H:114:HIS:HB3	9:H:443:HOH:O	2.08	0.54
1:J:106:ASN:HB2	9:J:413:HOH:O	2.07	0.54
1:F:21:PRO:HD3	1:J:7[A]:MET:HE2	1.90	0.54
1:E:97[A]:ARG:NH1	9:E:352:HOH:O	2.41	0.53
1:E:112:SER:OG	1:E:114[A]:HIS:HD2	1.91	0.53
1:A:114[B]:HIS:NE2	2:A:225:NAG:O6	2.41	0.53
1:E:-8:ASP:HB3	1:E:-5:ASP:OD2	2.09	0.53
6:D:251:MRD:H5C3	6:D:251:MRD:HMC1	1.91	0.53
3:A:260:MLK:H292	1:E:55:TRP:CH2	2.44	0.53
1:G:114[B]:HIS:CE1	4:G:225:NAG:H62	2.44	0.53
3:F:260:MLK:H292	1:J:55:TRP:CH2	2.44	0.53
1:I:159[B]:ASP:OD1	1:I:160:THR:HG22	2.09	0.52
1:G:149:TYR:OH	6:G:250:MRD:CM	2.56	0.52
1:A:96:THR:O	1:E:122:ARG:HD2	2.10	0.52
1:J:135[B]:GLU:HG3	1:J:136:GLU:N	2.24	0.52
1:H:213:PHE:CE1	1:H:215:ARG:HG3	2.45	0.52
1:B:79:ARG:HG3	1:C:149:TYR:CE1	2.44	0.51
1:J:55:TRP:CE3	9:J:429:HOH:O	2.53	0.51
8:E:226:NAG:H81	9:E:439:HOH:O	2.10	0.51
2:A:225:NAG:C3	2:A:225:NAG:C8	2.88	0.51
3:I:260:MLK:H31	3:I:260:MLK:O28	2.10	0.51
1:D:178:SER:OG	1:D:203[B]:LYS:HD3	2.11	0.51
1:B:37[A]:LEU:HG	1:B:163:VAL:CG1	2.40	0.51
1:J:112:SER:OG	1:J:114[A]:HIS:HD2	1.93	0.51
6:D:251:MRD:H5C1	9:D:437:HOH:O	2.11	0.51
1:E:38:LEU:HD21	1:E:55:TRP:CZ2	2.46	0.51
1:G:55:TRP:CH2	3:H:260:MLK:H292	2.46	0.51
1:A:21:PRO:HD3	1:E:7:MET:HE2	1.93	0.51
1:C:50:VAL:HG21	1:C:127:CYS:SG	2.51	0.51
1:H:150:GLY:HA3	1:H:193:GLU:OE2	2.11	0.51
1:F:21:PRO:HB3	1:J:7[B]:MET:SD	2.52	0.50
1:A:21:PRO:HD3	1:E:7:MET:CE	2.41	0.50
1:C:112:SER:OG	1:C:114:HIS:HD2	1.93	0.50
1:H:159[B]:ASP:OD1	1:H:160:THR:HG22	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:169:TYR:CZ	1:G:171:SER:HB2	2.47	0.50
1:J:195:TYR:CE2	3:J:260:MLK:H331	2.47	0.50
1:C:216:ASN:ND2	6:D:251:MRD:C4	2.75	0.50
1:C:52[A]:LEU:HG	1:C:125:PHE:HE2	1.77	0.50
1:G:37[B]:LEU:HG	1:G:163:VAL:CG1	2.42	0.50
1:J:38:LEU:HD21	1:J:55:TRP:NE1	2.27	0.50
1:H:99:VAL:HG23	9:H:356:HOH:O	2.12	0.49
1:A:38:LEU:HD11	1:A:55:TRP:CZ2	2.47	0.49
1:D:57:GLN:HG2	9:D:404:HOH:O	2.11	0.49
1:C:186[B]:GLN:HG3	3:C:260:MLK:H3	1.92	0.49
3:F:260:MLK:H292	1:J:55:TRP:CZ3	2.47	0.49
3:A:260:MLK:H292	1:E:55:TRP:CZ3	2.48	0.49
7:I:250:MPD:HM2	7:I:250:MPD:C5	2.39	0.49
1:A:81:SER:HA	1:A:106[B]:ASN:OD1	2.12	0.49
1:F:114[B]:HIS:NE2	1:F:116:GLN:HG2	2.28	0.49
1:J:99:VAL:HG23	9:J:348:HOH:O	2.12	0.49
3:H:260:MLK:H242	3:H:260:MLK:O27	2.12	0.49
1:B:169:TYR:CZ	1:B:171:SER:HB2	2.48	0.49
1:G:7:MET:HE2	1:H:21:PRO:HD3	1.95	0.49
1:D:159[A]:ASP:OD1	9:D:403:HOH:O	2.20	0.49
1:E:38:LEU:HD21	1:E:55:TRP:CE2	2.48	0.48
1:B:-8:ASP:HB3	1:B:-5:ASP:HB2	1.95	0.48
1:G:122:ARG:HD2	1:H:96:THR:O	2.13	0.48
1:H:112:SER:OG	1:H:114:HIS:HD2	1.96	0.48
1:B:139:THR:OG1	1:B:203:LYS:HG3	2.13	0.48
1:A:16:ARG:NH2	9:A:381:HOH:O	2.43	0.48
1:G:116:GLN:HE22	3:H:260:MLK:H373	1.78	0.48
1:A:59:SER:CB	1:A:114[B]:HIS:CE1	2.93	0.48
1:E:114[B]:HIS:CE1	8:E:225:NAG:O6	2.66	0.48
1:D:50:VAL:HG21	1:D:127:CYS:SG	2.54	0.48
1:B:43:ALA:HA	1:B:50:VAL:HG22	1.96	0.47
1:E:93:TYR:CD2	3:E:260:MLK:C13	2.97	0.47
1:D:122:ARG:HD2	1:E:96:THR:O	2.14	0.47
1:G:86:TRP:HE1	6:G:250:MRD:CM	2.08	0.47
3:H:260:MLK:H31	3:H:260:MLK:O28	2.15	0.47
1:I:50:VAL:HG21	1:I:127:CYS:SG	2.55	0.47
1:E:135[C]:GLU:HG3	1:E:136:GLU:N	2.29	0.47
1:A:37[B]:LEU:HG	1:A:163:VAL:CG1	2.44	0.47
3:B:260:MLK:O28	3:B:260:MLK:H31	2.14	0.47
1:I:136[B]:GLU:CD	1:I:136[B]:GLU:H	2.18	0.47
1:J:187:HIS:NE2	1:J:194:PRO:HB3	2.30	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:19:MET:HG3	1:G:20:TYR:N	2.29	0.47
1:C:99:VAL:HG22	1:C:123:LEU:HD13	1.97	0.47
1:C:152:TRP:CE3	1:C:193:GLU:HB3	2.49	0.47
1:E:141:ALA:HA	1:E:200:LEU:O	2.15	0.46
1:J:12:ASP:HA	1:J:16[A]:ARG:HG2	1.96	0.46
1:H:79:ARG:HG3	1:I:149:TYR:CE1	2.51	0.46
1:G:52:LEU:HD23	1:G:53:VAL:N	2.30	0.46
1:J:97[B]:ARG:NH1	9:J:334:HOH:O	2.48	0.46
1:D:8:ARG:HD2	1:I:12:ASP:OD2	2.15	0.46
1:J:116[B]:GLN:NE2	8:J:225:NAG:O6	2.48	0.46
1:E:160:THR:HG22	1:E:162:GLN:H	1.81	0.46
1:H:97[B]:ARG:NH2	9:H:339:HOH:O	2.48	0.46
3:I:260:MLK:H242	3:I:260:MLK:O27	2.15	0.46
1:J:38:LEU:CD2	1:J:55:TRP:NE1	2.78	0.46
1:G:7:MET:CE	1:H:21:PRO:HD3	2.46	0.46
1:D:186[A]:GLN:HG3	1:D:187:HIS:N	2.30	0.46
1:C:193:GLU:HB2	1:C:194:PRO:HD2	1.97	0.46
1:F:159[A]:ASP:OD2	1:F:160:THR:HG22	2.16	0.46
1:J:-8:ASP:HA	1:J:-5:ASP:OD2	2.16	0.46
1:E:11:SER:OG	1:H:16[A]:ARG:NH2	2.49	0.46
1:J:99:VAL:HG22	1:J:123:LEU:HD13	1.98	0.46
3:F:260:MLK:O28	3:F:260:MLK:H31	2.16	0.45
1:H:215:ARG:NH2	9:H:444:HOH:O	2.49	0.45
1:B:-8:ASP:HB3	1:B:-5:ASP:HB3	1.97	0.45
1:B:70[B]:ASN:OD1	1:F:70[B]:ASN:ND2	2.49	0.45
1:F:96:THR:O	1:J:122:ARG:HD2	2.16	0.45
1:H:25[A]:LYS:HG2	9:H:383:HOH:O	2.17	0.45
1:A:191:CYS:HA	1:A:192:PRO:HD3	1.79	0.45
1:G:79:ARG:HG3	1:H:149:TYR:CE1	2.51	0.45
1:H:51:ASP:HA	1:H:123:LEU:O	2.16	0.45
3:I:260:MLK:H202	3:I:260:MLK:H223	1.73	0.45
1:G:38:LEU:HD11	1:G:55:TRP:CE2	2.51	0.45
1:H:55:TRP:HH2	3:I:260:MLK:H292	1.80	0.45
1:D:141:ALA:CB	6:D:251:MRD:H3C2	2.45	0.45
3:F:260:MLK:C29	3:F:260:MLK:H152	2.46	0.45
1:E:59:SER:HB2	1:E:114[B]:HIS:NE2	2.32	0.45
1:I:86:TRP:HE1	7:I:250:MPD:HM1	1.81	0.45
1:F:12:ASP:O	1:F:16[A]:ARG:HB3	2.17	0.45
1:F:169:TYR:CZ	1:F:171:SER:HB2	2.52	0.45
1:B:155:ASP:HA	1:B:196:ILE:HD12	1.98	0.45
1:A:-6:LYS:NZ	1:A:-5:ASP:HB2	2.32	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:37[B]:LEU:HG	1:J:163:VAL:CG1	2.47	0.45
1:A:19:MET:O	1:E:7:MET:HE2	2.17	0.45
6:C:250:MRD:H1C1	6:C:250:MRD:H4	1.84	0.45
6:D:250:MRD:H1C2	6:D:250:MRD:H4	1.78	0.45
1:D:40:ILE:HG12	1:D:52:LEU:CD2	2.47	0.45
1:F:50:VAL:CG2	1:F:127:CYS:SG	3.05	0.44
1:F:106:ASN:HB2	9:F:411:HOH:O	2.17	0.44
1:C:12:ASP:HA	1:C:16:ARG:CD	2.47	0.44
1:E:195:TYR:HE2	3:E:260:MLK:H222	1.81	0.44
1:E:16:ARG:HH21	1:H:16[A]:ARG:HH12	1.63	0.44
1:F:122:ARG:HD2	1:G:96:THR:O	2.18	0.44
1:J:79:ARG:HD3	1:J:108:LEU:HD13	1.99	0.44
1:H:143:LYS:HE2	9:H:418:HOH:O	2.17	0.44
1:A:27:ASP:OD1	1:E:-1:LYS:HG2	2.17	0.44
3:G:260:MLK:O28	3:G:260:MLK:H31	2.18	0.44
1:E:136:GLU:OE2	1:E:136:GLU:N	2.47	0.44
1:E:31:VAL:HB	1:E:156:LEU:HD23	2.00	0.44
1:F:37:LEU:HD13	1:F:163:VAL:CG1	2.41	0.44
1:C:114:HIS:HB3	9:C:447:HOH:O	2.17	0.44
1:J:99:VAL:HG22	1:J:123:LEU:CD1	2.47	0.44
1:J:147:TRP:O	3:J:260:MLK:H253	2.18	0.44
3:D:260:MLK:H26	3:D:260:MLK:H252	1.83	0.44
3:I:260:MLK:H152	3:I:260:MLK:H28	1.81	0.44
1:G:59:SER:HB3	1:G:114[B]:HIS:CE1	2.53	0.44
1:B:179:ALA:HA	1:B:201:VAL:O	2.18	0.43
3:B:260:MLK:N23	3:B:260:MLK:O19	2.51	0.43
1:B:38:LEU:HB3	1:C:126:MET:HE1	2.00	0.43
1:B:207[A]:ARG:NH2	9:B:398:HOH:O	2.50	0.43
3:D:260:MLK:H242	3:D:260:MLK:O27	2.18	0.43
1:F:21:PRO:HD3	1:J:7[A]:MET:CE	2.48	0.43
1:B:50:VAL:HG21	1:B:127:CYS:SG	2.59	0.43
1:A:71:GLU:HA	1:G:71:GLU:HA	2.00	0.43
1:B:7:MET:HE2	1:C:19:MET:O	2.19	0.43
1:F:136:GLU:CD	1:F:136:GLU:H	2.22	0.43
1:E:16:ARG:HD2	1:E:16:ARG:HA	1.71	0.43
1:G:79:ARG:HD3	1:G:108:LEU:HD13	2.01	0.43
1:B:71:GLU:HA	1:F:71:GLU:HA	2.00	0.43
1:D:186[B]:GLN:HG3	3:D:260:MLK:H3	1.99	0.43
1:A:59:SER:CB	1:A:114[B]:HIS:HE1	2.30	0.43
1:J:40:ILE:HG12	1:J:52:LEU:CD1	2.48	0.43
1:A:122:ARG:HD2	1:B:96:THR:O	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:260:MLK:O19	3:E:260:MLK:N23	2.50	0.43
3:A:260:MLK:H252	3:A:260:MLK:H26	1.85	0.43
1:E:37[A]:LEU:HD11	1:E:52:LEU:CD1	2.47	0.42
1:A:97[B]:ARG:NH1	9:A:409:HOH:O	2.52	0.42
1:I:155:ASP:HA	1:I:196:ILE:HD12	2.01	0.42
1:A:114[B]:HIS:CD2	2:A:225:NAG:HO6	2.35	0.42
1:I:122:ARG:HD2	1:J:96:THR:O	2.20	0.42
3:E:260:MLK:H362	3:E:260:MLK:H26	1.71	0.42
1:J:143:LYS:HE3	3:J:260:MLK:H5	2.01	0.42
1:J:143:LYS:HE3	3:J:260:MLK:C5	2.50	0.42
3:A:260:MLK:H152	3:A:260:MLK:H28	1.76	0.42
1:D:175:GLU:HB3	1:D:207[B]:ARG:HG2	2.01	0.42
3:D:260:MLK:H223	3:D:260:MLK:H202	1.84	0.42
3:C:260:MLK:H202	3:C:260:MLK:H223	1.73	0.42
1:E:59:SER:HB2	1:E:114[B]:HIS:CE1	2.54	0.42
1:D:56:GLU:O	1:D:119:PRO:HD2	2.20	0.42
7:I:250:MPD:CM	7:I:250:MPD:H52	2.43	0.42
1:J:57:GLN:HB2	9:J:444:HOH:O	2.19	0.42
3:H:260:MLK:H152	3:H:260:MLK:H28	1.74	0.42
3:D:260:MLK:H362	3:D:260:MLK:H26	1.80	0.42
1:G:175:GLU:HB3	1:G:207[B]:ARG:HG3	2.02	0.42
3:J:260:MLK:H223	3:J:260:MLK:H202	1.66	0.42
3:F:260:MLK:H252	3:F:260:MLK:H26	1.85	0.42
1:E:12:ASP:O	1:E:16:ARG:HB2	2.19	0.42
1:A:7:MET:SD	1:B:18:PRO:HG2	2.60	0.42
3:J:260:MLK:N23	3:J:260:MLK:O19	2.52	0.42
1:C:186[B]:GLN:HE21	1:C:186[B]:GLN:HB3	1.61	0.42
1:B:55:TRP:CZ3	3:C:260:MLK:H292	2.54	0.42
1:A:50:VAL:HG21	1:A:127:CYS:SG	2.60	0.42
3:A:260:MLK:H31	3:A:260:MLK:O28	2.20	0.42
1:C:12:ASP:OD1	1:J:8:ARG:HD2	2.19	0.42
1:A:149:TYR:CE1	1:E:79:ARG:HG3	2.54	0.42
1:C:169:TYR:CZ	1:C:171:SER:HB2	2.55	0.42
1:A:141:ALA:HA	1:A:200:LEU:O	2.20	0.42
1:I:37[B]:LEU:HG	1:I:163:VAL:CG1	2.49	0.42
4:D:225:NAG:H83	4:D:225:NAG:H2	1.73	0.42
1:I:38:LEU:HD21	1:I:55:TRP:NE1	2.34	0.41
1:E:79:ARG:HD3	1:E:108:LEU:HD13	2.00	0.41
1:F:203:LYS:NZ	1:F:203:LYS:HB3	2.35	0.41
1:B:91:THR:HG21	1:B:147:TRP:HB2	2.00	0.41
1:C:186[A]:GLN:HE21	1:C:187:HIS:H	1.67	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37[B]:LEU:HG	1:C:163:VAL:CG1	2.48	0.41
1:E:71[B]:GLU:OE1	1:H:8:ARG:NH2	2.53	0.41
1:F:203:LYS:HZ2	1:F:203:LYS:HB3	1.84	0.41
3:J:260:MLK:H26	3:J:260:MLK:H362	1.69	0.41
1:B:-8:ASP:OD1	1:B:-7:TYR:N	2.54	0.41
1:E:169:TYR:CZ	1:E:171:SER:HB2	2.55	0.41
1:H:81:SER:HA	1:H:106:ASN:ND2	2.28	0.41
1:E:38:LEU:HD21	1:E:55:TRP:NE1	2.36	0.41
3:G:260:MLK:N23	3:G:260:MLK:O19	2.53	0.41
3:C:260:MLK:H28	3:C:260:MLK:H152	1.72	0.41
1:F:47:THR:HG22	1:J:42:LYS:HB3	2.03	0.41
1:F:191:CYS:HA	1:F:192:PRO:HD2	1.85	0.41
3:H:260:MLK:N23	3:H:260:MLK:O19	2.54	0.41
1:G:43:ALA:HA	1:G:50:VAL:HG22	2.02	0.41
1:B:94:SER:O	1:B:125:PHE:HB2	2.20	0.41
3:H:260:MLK:H202	3:H:260:MLK:H223	1.81	0.41
1:E:40:ILE:HG12	1:E:52:LEU:CD1	2.50	0.41
1:H:16[A]:ARG:NH1	1:H:16[A]:ARG:HG3	2.35	0.41
1:D:17:SER:HB2	1:D:18:PRO:CD	2.51	0.41
1:D:52:LEU:HG	1:D:125:PHE:HE2	1.84	0.41
1:J:169:TYR:CZ	1:J:171:SER:HB2	2.55	0.41
1:G:114[A]:HIS:HE1	4:G:226:NAG:H83	1.86	0.41
1:H:3:GLN:HG2	9:I:341:HOH:O	2.21	0.41
6:B:250:MRD:H1C2	6:B:250:MRD:H4	1.60	0.41
1:E:38:LEU:CD2	1:E:55:TRP:NE1	2.84	0.40
1:D:163:VAL:HG21	1:D:200:LEU:CD1	2.51	0.40
1:G:50:VAL:HG21	1:G:127:CYS:SG	2.61	0.40
1:H:128:ASP:HA	1:H:129:PRO:HD3	1.78	0.40
1:F:195:TYR:CZ	3:F:260:MLK:H331	2.56	0.40
3:F:260:MLK:H28	3:F:260:MLK:H152	1.79	0.40
1:B:55:TRP:HH2	3:C:260:MLK:H292	1.86	0.40
8:J:225:NAG:H83	9:J:390:HOH:O	2.20	0.40
1:H:50:VAL:HG21	1:H:127:CYS:SG	2.60	0.40
1:H:122:ARG:HD2	1:I:96:THR:O	2.21	0.40
1:J:179:ALA:HA	1:J:201:VAL:O	2.21	0.40
1:D:141:ALA:H	6:D:251:MRD:H5C2	1.87	0.40
3:F:260:MLK:O19	3:F:260:MLK:N23	2.54	0.40
1:A:195:TYR:CZ	3:A:260:MLK:H331	2.56	0.40
3:A:260:MLK:C29	3:A:260:MLK:H152	2.51	0.40
1:I:163:VAL:HG21	1:I:200:LEU:CD1	2.52	0.40
1:E:50:VAL:HG21	1:E:127:CYS:SG	2.61	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:LYS:HE3	9:C:320:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	218/230 (95%)	217 (100%)	1 (0%)	0	100	100
1	B	222/230 (96%)	220 (99%)	2 (1%)	0	100	100
1	C	228/230 (99%)	226 (99%)	2 (1%)	0	100	100
1	D	221/230 (96%)	218 (99%)	3 (1%)	0	100	100
1	E	223/230 (97%)	220 (99%)	3 (1%)	0	100	100
1	F	220/230 (96%)	216 (98%)	4 (2%)	0	100	100
1	G	224/230 (97%)	223 (100%)	1 (0%)	0	100	100
1	H	226/230 (98%)	224 (99%)	2 (1%)	0	100	100
1	I	219/230 (95%)	216 (99%)	3 (1%)	0	100	100
1	J	224/230 (97%)	220 (98%)	4 (2%)	0	100	100
All	All	2225/2300 (97%)	2200 (99%)	25 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	202/208 (97%)	198 (98%)	4 (2%)	63	79
1	B	206/208 (99%)	200 (97%)	6 (3%)	50	66
1	C	208/208 (100%)	204 (98%)	4 (2%)	65	80
1	D	204/208 (98%)	199 (98%)	5 (2%)	55	72
1	E	207/208 (100%)	206 (100%)	1 (0%)	92	97
1	F	204/208 (98%)	198 (97%)	6 (3%)	50	66
1	G	208/208 (100%)	202 (97%)	6 (3%)	50	66
1	H	206/208 (99%)	197 (96%)	9 (4%)	35	47
1	I	202/208 (97%)	199 (98%)	3 (2%)	72	85
1	J	208/208 (100%)	204 (98%)	4 (2%)	65	80
All	All	2055/2080 (99%)	2007 (98%)	48 (2%)	61	75

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	SER
1	A	55	TRP
1	A	118	LEU
1	A	127	CYS
1	B	61	LYS
1	B	118	LEU
1	B	127	CYS
1	B	136[A]	GLU
1	B	136[B]	GLU
1	B	136[C]	GLU
1	C	80	THR
1	C	118	LEU
1	C	127	CYS
1	C	191	CYS
1	D	26	ASP
1	D	74	ASN
1	D	116	GLN
1	D	118	LEU
1	D	191	CYS
1	E	91	THR
1	F	16[A]	ARG
1	F	16[B]	ARG
1	F	25	LYS
1	F	118	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	127	CYS
1	F	160	THR
1	G	17	SER
1	G	118	LEU
1	G	135[A]	GLU
1	G	135[B]	GLU
1	G	159[A]	ASP
1	G	159[B]	ASP
1	H	-3	ASP
1	H	18	PRO
1	H	25[A]	LYS
1	H	25[B]	LYS
1	H	80	THR
1	H	118	LEU
1	H	127	CYS
1	H	191	CYS
1	H	216	ASN
1	I	-5	ASP
1	I	118	LEU
1	I	191	CYS
1	J	118	LEU
1	J	159[A]	ASP
1	J	159[B]	ASP
1	J	191	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	15	ASN
1	A	57	GLN
1	A	162	GLN
1	A	199	ASN
1	B	3	GLN
1	B	106	ASN
1	B	114	HIS
1	C	106	ASN
1	C	114	HIS
1	C	216	ASN
1	D	3	GLN
1	D	57	GLN
1	D	114	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	116	GLN
1	D	184	GLN
1	F	15	ASN
1	F	57	GLN
1	G	3	GLN
1	G	106	ASN
1	G	116	GLN
1	H	15	ASN
1	H	106	ASN
1	H	114	HIS
1	H	116	GLN
1	H	216	ASN
1	I	3	GLN
1	I	57	GLN
1	I	114	HIS
1	I	162	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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 ⓘ

32 carbohydrates are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	B	225	1,4	14,14,15	0.63	0	15,19,21	1.49	2 (13%)
4	NAG	B	226	4	14,14,15	0.58	0	15,19,21	1.23	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	B	240	1,5	14,14,15	0.53	0	15,19,21	0.88	1 (6%)
5	NAG	B	241	5	14,14,15	0.43	0	15,19,21	1.74	3 (20%)
5	BMA	B	242	5	11,11,12	0.36	0	14,15,17	1.03	1 (7%)
5	MAN	B	243	5	11,11,12	0.71	0	14,15,17	0.87	0
5	MAN	B	244	5	11,11,12	0.45	0	14,15,17	0.89	1 (7%)
5	MAN	B	245	5	11,11,12	0.52	0	14,15,17	0.86	0
5	MAN	B	246	5	11,11,12	0.64	0	14,15,17	0.91	0
4	NAG	D	225	1,4	14,14,15	0.36	0	15,19,21	1.75	2 (13%)
4	NAG	D	226	4	14,14,15	0.57	0	15,19,21	1.66	3 (20%)
8	NAG	E	225	1,8	14,14,15	0.43	0	15,19,21	1.33	1 (6%)
8	NAG	E	226	8	14,14,15	0.49	0	15,19,21	0.79	0
8	BMA	E	227	8	11,11,12	0.25	0	14,15,17	0.70	0
8	MAN	E	228	8	11,11,12	0.78	0	14,15,17	1.74	2 (14%)
8	MAN	E	230	8	11,11,12	0.44	0	14,15,17	1.48	1 (7%)
8	MAN	E	231	8	11,11,12	0.57	0	14,15,17	0.68	0
4	NAG	G	225	1,4	14,14,15	0.56	0	15,19,21	1.27	1 (6%)
4	NAG	G	226	4	14,14,15	0.49	0	15,19,21	1.08	0
5	NAG	G	240	1,5	14,14,15	0.58	0	15,19,21	0.70	0
5	NAG	G	241	5	14,14,15	0.55	0	15,19,21	0.80	0
5	BMA	G	242	5	11,11,12	0.42	0	14,15,17	0.73	0
5	MAN	G	243	5	11,11,12	0.71	0	14,15,17	0.98	1 (7%)
5	MAN	G	244	5	11,11,12	0.59	0	14,15,17	0.70	0
5	MAN	G	245	5	11,11,12	0.67	0	14,15,17	1.32	1 (7%)
5	MAN	G	246	5	11,11,12	0.55	0	14,15,17	0.92	0
8	NAG	J	225	1,8	14,14,15	0.44	0	15,19,21	1.42	1 (6%)
8	NAG	J	226	8	14,14,15	0.52	0	15,19,21	0.67	0
8	BMA	J	227	8	11,11,12	0.40	0	14,15,17	0.83	0
8	MAN	J	228	8	11,11,12	0.47	0	14,15,17	1.79	2 (14%)
8	MAN	J	230	8	11,11,12	0.63	0	14,15,17	1.18	1 (7%)
8	MAN	J	231	8	11,11,12	0.62	0	14,15,17	1.17	2 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	225	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	226	4	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	B	240	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	241	5	-	0/6/23/26	0/1/1/1
5	BMA	B	242	5	-	0/2/19/22	0/1/1/1
5	MAN	B	243	5	-	0/2/19/22	0/1/1/1
5	MAN	B	244	5	-	0/2/19/22	0/1/1/1
5	MAN	B	245	5	-	0/2/19/22	0/1/1/1
5	MAN	B	246	5	-	0/2/19/22	0/1/1/1
4	NAG	D	225	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	226	4	-	0/6/23/26	0/1/1/1
8	NAG	E	225	1,8	-	0/6/23/26	0/1/1/1
8	NAG	E	226	8	-	0/6/23/26	0/1/1/1
8	BMA	E	227	8	-	0/2/19/22	0/1/1/1
8	MAN	E	228	8	-	0/2/19/22	0/1/1/1
8	MAN	E	230	8	-	0/2/19/22	0/1/1/1
8	MAN	E	231	8	-	0/2/19/22	0/1/1/1
4	NAG	G	225	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	226	4	-	0/6/23/26	0/1/1/1
5	NAG	G	240	1,5	-	0/6/23/26	0/1/1/1
5	NAG	G	241	5	-	0/6/23/26	0/1/1/1
5	BMA	G	242	5	-	0/2/19/22	0/1/1/1
5	MAN	G	243	5	-	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	5	-	0/2/19/22	0/1/1/1
8	NAG	J	225	1,8	-	0/6/23/26	0/1/1/1
8	NAG	J	226	8	-	0/6/23/26	0/1/1/1
8	BMA	J	227	8	-	0/2/19/22	0/1/1/1
8	MAN	J	228	8	-	0/2/19/22	1/1/1/1
8	MAN	J	230	8	-	0/2/19/22	0/1/1/1
8	MAN	J	231	8	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	E	228	MAN	O5-C1-C2	-4.42	103.68	110.86
4	D	225	NAG	C2-N2-C7	-3.63	118.37	123.04
4	D	226	NAG	C1-O5-C5	-3.52	107.78	112.25
4	B	226	NAG	C2-N2-C7	-3.42	118.65	123.04
8	J	230	MAN	O5-C1-C2	-3.23	105.62	110.86
5	B	241	NAG	C4-C3-C2	-3.19	106.26	111.23
8	J	231	MAN	O5-C1-C2	-2.37	107.02	110.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	J	231	MAN	C1-O5-C5	-2.07	109.61	112.25
4	B	226	NAG	C4-C3-C2	2.18	114.62	111.23
5	B	241	NAG	C2-N2-C7	2.28	125.97	123.04
5	G	243	MAN	C1-C2-C3	2.29	112.25	109.54
5	B	242	BMA	C1-C2-C3	2.30	112.27	109.54
8	J	228	MAN	O5-C5-C6	2.36	112.46	107.35
5	B	240	NAG	C1-O5-C5	2.48	115.40	112.25
4	D	226	NAG	C4-C3-C2	2.52	115.15	111.23
4	B	225	NAG	C3-C4-C5	2.52	114.59	110.20
5	B	244	MAN	C1-O5-C5	2.62	115.57	112.25
4	G	225	NAG	C1-O5-C5	3.47	116.65	112.25
4	B	225	NAG	C4-C3-C2	3.72	117.02	111.23
5	G	245	MAN	C1-C2-C3	3.79	114.03	109.54
8	E	228	MAN	C3-C4-C5	3.88	116.96	110.20
4	D	226	NAG	C3-C4-C5	3.90	117.00	110.20
5	B	241	NAG	C1-O5-C5	3.95	117.26	112.25
8	E	225	NAG	C1-O5-C5	4.14	117.50	112.25
8	E	230	MAN	C1-O5-C5	4.55	118.02	112.25
8	J	225	NAG	C1-O5-C5	4.69	118.20	112.25
4	D	225	NAG	C1-O5-C5	4.85	118.41	112.25
8	J	228	MAN	C1-O5-C5	5.36	119.06	112.25

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

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

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	225	NAG	1	0
8	E	225	NAG	1	0
8	E	226	NAG	1	0
4	G	225	NAG	1	0
4	G	226	NAG	1	0
8	J	225	NAG	2	0

5.6 Ligand geometry ⓘ

26 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	0.54	0	15,19,21	1.93	4 (26%)
3	MLK	A	260	-	55,56,56	1.09	3 (5%)	74,92,92	1.52	11 (14%)
6	MRD	B	250	-	6,7,7	0.37	0	7,10,10	0.57	0
3	MLK	B	260	-	55,56,56	1.05	3 (5%)	74,92,92	1.53	11 (14%)
7	MPD	C	222	-	6,7,7	0.36	0	7,10,10	0.51	0
2	NAG	C	225	1	14,14,15	0.45	0	15,19,21	1.14	1 (6%)
6	MRD	C	250	-	6,7,7	0.32	0	7,10,10	0.42	0
3	MLK	C	260	-	55,56,56	1.10	4 (7%)	74,92,92	1.52	10 (13%)
6	MRD	D	250	-	6,7,7	0.39	0	7,10,10	0.41	0
6	MRD	D	251	-	6,7,7	0.30	0	7,10,10	0.37	0
3	MLK	D	260	-	55,56,56	1.03	4 (7%)	74,92,92	1.48	15 (20%)
2	NAG	E	240	1	14,14,15	0.47	0	15,19,21	1.09	1 (6%)
3	MLK	E	260	-	55,56,56	1.06	4 (7%)	74,92,92	1.62	15 (20%)
2	NAG	F	225	1	14,14,15	0.40	0	15,19,21	1.19	2 (13%)
3	MLK	F	260	-	55,56,56	1.07	3 (5%)	74,92,92	1.55	11 (14%)
6	MRD	G	250	-	6,7,7	0.40	0	7,10,10	0.49	0
3	MLK	G	260	-	55,56,56	1.09	3 (5%)	74,92,92	1.56	11 (14%)
2	NAG	H	225	1	14,14,15	0.51	0	15,19,21	0.78	0
6	MRD	H	250	-	6,7,7	0.29	0	7,10,10	0.50	0
3	MLK	H	260	-	55,56,56	1.08	4 (7%)	74,92,92	1.50	10 (13%)
6	MRD	I	222	-	6,7,7	0.42	0	7,10,10	0.40	0
2	NAG	I	225	1	14,14,15	0.38	0	15,19,21	1.47	1 (6%)
7	MPD	I	250	-	6,7,7	0.28	0	7,10,10	0.28	0
3	MLK	I	260	-	55,56,56	1.02	3 (5%)	74,92,92	1.53	14 (18%)
2	NAG	J	240	1	14,14,15	0.48	0	15,19,21	0.96	1 (6%)
3	MLK	J	260	-	55,56,56	1.07	4 (7%)	74,92,92	1.56	12 (16%)

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
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
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	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
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	240	1	-	0/6/23/26	0/1/1/1
3	MLK	J	260	-	-	0/24/141/141	0/2/8/8

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	260	MLK	C8-N7	-4.59	1.34	1.40
3	C	260	MLK	C8-N7	-4.35	1.34	1.40
3	G	260	MLK	C8-N7	-4.34	1.34	1.40
3	F	260	MLK	C8-N7	-4.25	1.34	1.40
3	H	260	MLK	C8-N7	-4.22	1.34	1.40
3	B	260	MLK	C8-N7	-4.09	1.34	1.40
3	E	260	MLK	C8-N7	-4.05	1.35	1.40
3	J	260	MLK	C8-N7	-4.05	1.35	1.40
3	I	260	MLK	C8-N7	-3.84	1.35	1.40
3	G	260	MLK	C11-N7	-3.63	1.34	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	260	MLK	C8-N7	-3.61	1.35	1.40
3	F	260	MLK	C11-N7	-3.40	1.35	1.39
3	A	260	MLK	C11-N7	-3.31	1.35	1.39
3	C	260	MLK	C11-N7	-3.29	1.35	1.39
3	B	260	MLK	C11-N7	-3.28	1.35	1.39
3	E	260	MLK	C11-N7	-3.22	1.35	1.39
3	J	260	MLK	C11-N7	-3.21	1.35	1.39
3	D	260	MLK	C11-N7	-3.15	1.35	1.39
3	I	260	MLK	C11-N7	-3.12	1.35	1.39
3	H	260	MLK	C11-N7	-3.12	1.35	1.39
3	A	260	MLK	C6-N7	-2.57	1.41	1.44
3	F	260	MLK	C6-N7	-2.32	1.41	1.44
3	H	260	MLK	C18-C19	-2.31	1.51	1.55
3	C	260	MLK	C6-N7	-2.29	1.41	1.44
3	B	260	MLK	C18-C19	-2.26	1.51	1.55
3	D	260	MLK	C18-C19	-2.25	1.51	1.55
3	E	260	MLK	C6-N7	-2.24	1.41	1.44
3	D	260	MLK	C6-N7	-2.20	1.41	1.44
3	C	260	MLK	C18-C19	-2.19	1.51	1.55
3	J	260	MLK	C18-C19	-2.18	1.51	1.55
3	G	260	MLK	C18-C19	-2.14	1.51	1.55
3	J	260	MLK	C6-N7	-2.13	1.41	1.44
3	E	260	MLK	C18-C19	-2.11	1.52	1.55
3	H	260	MLK	C6-N7	-2.08	1.41	1.44
3	I	260	MLK	C18-C19	-2.05	1.52	1.55

All (130) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	260	MLK	C16-C17-C28	-5.05	102.17	112.70
3	F	260	MLK	C16-C17-C28	-4.97	102.35	112.70
3	E	260	MLK	C16-C17-C28	-4.58	103.15	112.70
3	H	260	MLK	C16-C17-C28	-4.54	103.23	112.70
3	C	260	MLK	C16-C17-C28	-4.28	103.77	112.70
3	B	260	MLK	C16-C17-C28	-4.25	103.84	112.70
3	G	260	MLK	C16-C17-C28	-4.20	103.94	112.70
3	G	260	MLK	C21-C16-C23	-4.14	107.26	111.47
3	J	260	MLK	C16-C17-C28	-4.14	104.07	112.70
3	J	260	MLK	C33-C34-C35	-3.94	105.04	112.03
3	E	260	MLK	C33-C34-C35	-3.80	105.29	112.03
3	B	260	MLK	C33-C34-C35	-3.79	105.32	112.03
3	C	260	MLK	C33-C34-C35	-3.77	105.35	112.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	260	MLK	C16-C17-C28	-3.75	104.88	112.70
3	H	260	MLK	C33-C34-C35	-3.74	105.40	112.03
3	D	260	MLK	C16-C17-C28	-3.51	105.39	112.70
3	C	260	MLK	C21-C16-C23	-3.47	107.94	111.47
3	A	260	MLK	C33-C34-C35	-3.39	106.02	112.03
3	F	260	MLK	C33-C34-C35	-3.37	106.05	112.03
3	I	260	MLK	C33-C34-C35	-3.24	106.29	112.03
3	G	260	MLK	C33-C34-C35	-3.21	106.34	112.03
3	A	260	MLK	C37-O35-C35	-3.20	105.39	114.09
3	H	260	MLK	C37-O35-C35	-3.12	105.61	114.09
3	F	260	MLK	C37-O35-C35	-3.12	105.63	114.09
3	D	260	MLK	C37-O35-C35	-3.09	105.68	114.09
3	I	260	MLK	C37-O35-C35	-3.08	105.73	114.09
3	C	260	MLK	C37-O35-C35	-3.03	105.87	114.09
3	F	260	MLK	C29-O28-C28	-3.03	108.60	114.39
3	H	260	MLK	C21-C16-C23	-3.02	108.40	111.47
3	E	260	MLK	C29-O28-C28	-2.92	108.80	114.39
3	D	260	MLK	C33-C34-C35	-2.88	106.92	112.03
3	B	260	MLK	C21-C16-C23	-2.83	108.59	111.47
3	J	260	MLK	C37-O35-C35	-2.81	106.45	114.09
3	G	260	MLK	C39-O38-C38	-2.80	106.68	114.59
3	A	260	MLK	C29-O28-C28	-2.76	109.11	114.39
3	E	260	MLK	C37-O35-C35	-2.75	106.61	114.09
3	D	260	MLK	C21-C16-C23	-2.75	108.67	111.47
3	I	260	MLK	C29-O28-C28	-2.73	109.17	114.39
3	G	260	MLK	C38-C34-C35	-2.73	108.17	111.86
3	J	260	MLK	C29-O28-C28	-2.73	109.17	114.39
3	E	260	MLK	O14-C13-O13	-2.72	118.66	123.66
3	G	260	MLK	C37-O35-C35	-2.71	106.73	114.09
3	B	260	MLK	C37-O35-C35	-2.66	106.86	114.09
3	A	260	MLK	C21-C16-C23	-2.64	108.78	111.47
3	D	260	MLK	C38-C34-C35	-2.60	108.33	111.86
3	J	260	MLK	C21-C16-C23	-2.60	108.83	111.47
3	I	260	MLK	C39-O38-C38	-2.49	107.56	114.59
3	E	260	MLK	C18-C30-C31	-2.47	114.28	117.24
3	D	260	MLK	C39-O38-C38	-2.45	107.67	114.59
3	C	260	MLK	C18-C30-C31	-2.41	114.36	117.24
3	D	260	MLK	C18-C30-C31	-2.40	114.36	117.24
3	E	260	MLK	C21-C16-C23	-2.38	109.05	111.47
3	C	260	MLK	C39-O38-C38	-2.37	107.90	114.59
3	B	260	MLK	C39-O38-C38	-2.31	108.05	114.59
3	G	260	MLK	C15-C16-C17	-2.31	108.36	112.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	260	MLK	C38-C34-C35	-2.29	108.76	111.86
3	J	260	MLK	C18-C30-C31	-2.28	114.50	117.24
3	J	260	MLK	O14-C13-O13	-2.28	119.48	123.66
3	I	260	MLK	C22-O19-C19	-2.28	107.03	113.63
2	A	225	NAG	O7-C7-C8	-2.26	117.92	122.06
3	I	260	MLK	C18-C30-C31	-2.23	114.57	117.24
3	B	260	MLK	C29-O28-C28	-2.22	110.14	114.39
3	F	260	MLK	O14-C13-O13	-2.21	119.60	123.66
3	A	260	MLK	O14-C13-O13	-2.19	119.63	123.66
3	J	260	MLK	C39-O38-C38	-2.14	108.55	114.59
3	E	260	MLK	C38-C34-C35	-2.13	108.97	111.86
3	H	260	MLK	C39-O38-C38	-2.13	108.58	114.59
3	B	260	MLK	O14-C15-C16	-2.11	105.74	108.31
3	I	260	MLK	O14-C13-O13	-2.11	119.79	123.66
2	F	225	NAG	C2-N2-C7	-2.10	120.34	123.04
3	E	260	MLK	C39-O38-C38	-2.10	108.67	114.59
3	F	260	MLK	C21-C16-C23	-2.09	109.34	111.47
3	I	260	MLK	O8-C8-C9	-2.09	124.60	127.41
3	A	260	MLK	C38-C34-C35	-2.07	109.06	111.86
3	D	260	MLK	C29-O28-C28	-2.05	110.47	114.39
3	B	260	MLK	C38-C34-C35	-2.04	109.09	111.86
3	F	260	MLK	C38-C34-C35	-2.03	109.11	111.86
3	G	260	MLK	O14-C13-O13	-2.03	119.92	123.66
3	D	260	MLK	C22-O19-C19	-2.03	107.74	113.63
3	D	260	MLK	O8-C8-C9	-2.02	124.70	127.41
3	I	260	MLK	C9-C8-N7	2.03	109.72	108.07
3	D	260	MLK	O11-C11-N7	2.05	126.43	124.33
3	H	260	MLK	C18-C17-C28	2.05	105.80	102.98
3	E	260	MLK	O8-C8-N7	2.12	125.97	123.94
3	D	260	MLK	O8-C8-N7	2.16	126.01	123.94
3	A	260	MLK	O19-C19-C18	2.17	113.08	108.46
3	F	260	MLK	C9-C8-N7	2.33	109.96	108.07
3	E	260	MLK	C1-C6-N7	2.41	123.14	121.07
2	E	240	NAG	C1-O5-C5	2.41	115.31	112.25
2	A	225	NAG	C8-C7-N2	2.49	120.88	116.11
3	H	260	MLK	C15-O14-C13	2.53	122.11	116.64
3	I	260	MLK	C10-C11-N7	2.53	109.45	108.06
3	B	260	MLK	C10-C11-N7	2.59	109.48	108.06
3	C	260	MLK	O14-C13-C1	2.61	116.92	112.16
3	H	260	MLK	O14-C13-C1	2.62	116.92	112.16
2	J	240	NAG	C1-O5-C5	2.64	115.60	112.25
3	C	260	MLK	C15-O14-C13	2.68	122.44	116.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	260	MLK	C10-C11-N7	2.74	109.57	108.06
3	E	260	MLK	C10-C11-N7	2.86	109.64	108.06
3	A	260	MLK	C10-C11-N7	2.94	109.68	108.06
3	C	260	MLK	C10-C11-N7	2.96	109.69	108.06
3	E	260	MLK	O14-C15-C16	3.01	111.97	108.31
3	F	260	MLK	C23-C16-C17	3.09	111.06	108.22
3	J	260	MLK	C10-C11-N7	3.13	109.78	108.06
3	G	260	MLK	C10-C11-N7	3.17	109.81	108.06
2	C	225	NAG	C1-O5-C5	3.24	116.36	112.25
3	J	260	MLK	C1-C6-N7	3.26	123.87	121.07
3	B	260	MLK	O14-C13-C1	3.26	118.09	112.16
3	J	260	MLK	O14-C13-C1	3.29	118.16	112.16
3	F	260	MLK	C10-C11-N7	3.37	109.92	108.06
3	D	260	MLK	C23-C16-C17	3.45	111.39	108.22
2	F	225	NAG	C1-O5-C5	3.45	116.63	112.25
3	H	260	MLK	C10-C11-N7	3.49	109.98	108.06
3	G	260	MLK	O14-C13-C1	3.54	118.60	112.16
3	J	260	MLK	C23-C16-C17	3.62	111.56	108.22
3	E	260	MLK	C23-C16-C17	3.63	111.56	108.22
3	A	260	MLK	O14-C13-C1	3.76	119.00	112.16
3	I	260	MLK	O14-C13-C1	3.84	119.15	112.16
3	H	260	MLK	C23-C16-C17	3.98	111.88	108.22
3	D	260	MLK	O14-C13-C1	4.01	119.47	112.16
2	A	225	NAG	C2-N2-C7	4.08	128.28	123.04
3	E	260	MLK	O14-C13-C1	4.11	119.64	112.16
3	F	260	MLK	O14-C13-C1	4.13	119.68	112.16
3	A	260	MLK	C23-C16-C17	4.28	112.16	108.22
3	I	260	MLK	C23-C16-C17	4.38	112.25	108.22
3	G	260	MLK	C23-C16-C17	4.41	112.28	108.22
2	A	225	NAG	C1-O5-C5	4.54	118.01	112.25
2	I	225	NAG	C1-O5-C5	4.91	118.48	112.25
3	C	260	MLK	C23-C16-C17	5.04	112.86	108.22
3	B	260	MLK	C23-C16-C17	5.15	112.96	108.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

18 monomers are involved in 113 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	225	NAG	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	260	MLK	7	0
6	B	250	MRD	1	0
3	B	260	MLK	4	0
6	C	250	MRD	1	0
3	C	260	MLK	7	0
6	D	250	MRD	1	0
6	D	251	MRD	9	0
3	D	260	MLK	8	0
3	E	260	MLK	12	0
3	F	260	MLK	8	0
6	G	250	MRD	5	0
3	G	260	MLK	5	0
6	H	250	MRD	1	0
3	H	260	MLK	9	0
7	I	250	MPD	5	0
3	I	260	MLK	7	0
3	J	260	MLK	15	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	214/230 (93%)	-0.41	0 100 100	21, 32, 63, 93	0
1	B	216/230 (93%)	-0.36	4 (1%) 70 77	20, 32, 65, 97	0
1	C	221/230 (96%)	-0.20	9 (4%) 41 49	20, 32, 78, 109	0
1	D	214/230 (93%)	-0.30	6 (2%) 56 66	21, 35, 76, 107	0
1	E	216/230 (93%)	-0.33	0 100 100	21, 32, 64, 98	0
1	F	214/230 (93%)	-0.39	0 100 100	21, 32, 61, 90	0
1	G	216/230 (93%)	-0.39	3 (1%) 78 83	21, 32, 62, 97	0
1	H	221/230 (96%)	-0.22	9 (4%) 41 49	20, 32, 78, 114	0
1	I	214/230 (93%)	-0.27	3 (1%) 78 83	22, 35, 78, 119	0
1	J	216/230 (93%)	-0.37	3 (1%) 78 83	20, 32, 63, 98	0
All	All	2162/2300 (94%)	-0.32	37 (1%) 73 79	20, 33, 70, 119	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	213	PHE	5.4
1	H	212	GLY	5.2
1	C	213	PHE	5.1
1	H	215	ARG	4.8
1	C	-3	ASP	4.1
1	C	0	LEU	4.0
1	B	-8	ASP	3.8
1	H	159[A]	ASP	3.7
1	I	-3	ASP	3.6
1	B	159[A]	ASP	3.6
1	C	159[A]	ASP	3.4
1	H	0	LEU	3.4
1	D	-1	LYS	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	159[A]	ASP	3.1
1	C	211	ASN	3.1
1	H	-3	ASP	2.9
1	C	215	ARG	2.9
1	H	211	ASN	2.7
1	D	-5	ASP	2.7
1	G	-7	TYR	2.6
1	B	-7	TYR	2.6
1	H	15	ASN	2.5
1	J	16[A]	ARG	2.5
1	J	-8	ASP	2.4
1	C	214	PHE	2.4
1	J	-7	TYR	2.4
1	D	55	TRP	2.4
1	H	214	PHE	2.3
1	D	-4	ASP	2.3
1	C	216	ASN	2.3
1	C	16	ARG	2.2
1	D	-3	ASP	2.2
1	I	1	HIS	2.1
1	B	-6	LYS	2.1
1	I	189	SER	2.1
1	G	-8	ASP	2.1
1	D	0	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
8	MAN	E	230	11/12	0.94	0.15	5.11	60,73,83,83	0
8	MAN	J	230	11/12	0.87	0.17	4.38	61,70,91,91	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
8	MAN	J	231	11/12	0.77	0.28	1.59	82,102,114,115	0
4	NAG	D	225	14/15	0.92	0.15	1.56	68,74,86,97	0
4	NAG	B	225	14/15	0.90	0.13	1.15	57,65,78,79	0
8	MAN	E	231	11/12	0.91	0.22	0.97	65,78,90,94	0
5	MAN	B	244	11/12	0.94	0.17	0.84	70,76,84,87	0
5	BMA	G	242	11/12	0.81	0.16	0.35	61,77,87,91	0
4	NAG	G	225	14/15	0.91	0.11	0.05	54,68,79,82	0
8	NAG	J	225	14/15	0.91	0.13	-0.32	45,54,69,74	0
8	NAG	E	225	14/15	0.93	0.11	-0.35	42,50,70,73	0
8	MAN	J	228	11/12	0.72	0.26	-	100,103,109,115	0
5	BMA	B	242	11/12	0.86	0.15	-	63,81,88,95	0
8	BMA	J	227	11/12	0.83	0.23	-	95,101,112,114	0
5	MAN	B	245	11/12	0.83	0.12	-	87,92,99,101	0
8	MAN	E	228	11/12	0.80	0.24	-	91,102,109,112	0
5	NAG	B	241	14/15	0.84	0.17	-	73,90,96,97	0
5	NAG	B	240	14/15	0.91	0.17	-	69,75,82,91	0
8	BMA	E	227	11/12	0.90	0.13	-	81,87,99,100	0
4	NAG	D	226	14/15	0.82	0.26	-	98,102,109,110	0
4	NAG	G	226	14/15	0.73	0.28	-	70,93,104,105	0
5	MAN	B	243	11/12	0.91	0.17	-	70,73,84,94	0
4	NAG	B	226	14/15	0.84	0.27	-	84,91,102,104	0
8	NAG	J	226	14/15	0.89	0.11	-	66,73,80,91	0
5	MAN	G	244	11/12	0.96	0.19	-	73,85,89,92	0
5	NAG	G	240	14/15	0.90	0.19	-	68,76,83,95	0
5	MAN	B	246	11/12	0.90	0.23	-	65,76,87,88	0
5	NAG	G	241	14/15	0.88	0.23	-	79,90,95,99	0
5	MAN	G	245	11/12	0.74	0.19	-	80,97,109,111	0
5	MAN	G	243	11/12	0.92	0.15	-	71,79,84,99	0
8	NAG	E	226	14/15	0.90	0.09	-	57,71,82,85	0
5	MAN	G	246	11/12	0.91	0.29	-	61,76,87,88	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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
7	MPD	C	222	8/8	0.84	0.31	14.65	43,61,73,87	0

Continued on next page...

Continued from previous page...

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
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
2	NAG	I	225	14/15	0.87	0.18	1.59	58,71,77,78	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
2	NAG	J	240	14/15	0.77	0.20	0.66	67,78,87,87	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	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
3	MLK	B	260	49/49	0.93	0.11	-0.35	31,42,52,63	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	H	225	14/15	0.88	0.13	-	61,68,77,84	0
2	NAG	C	225	14/15	0.91	0.14	-	60,67,76,84	0

6.5 Other polymers [i](#)

There are no such residues in this entry.