



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:02 PM GMT

PDB ID : 3SH1
Title : Ac-AChBP ligand binding domain mutated to human alpha-7 nAChR
Authors : Nemecz, A.; Taylor, P.W.
Deposited on : 2011-06-15
Resolution : 2.90 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

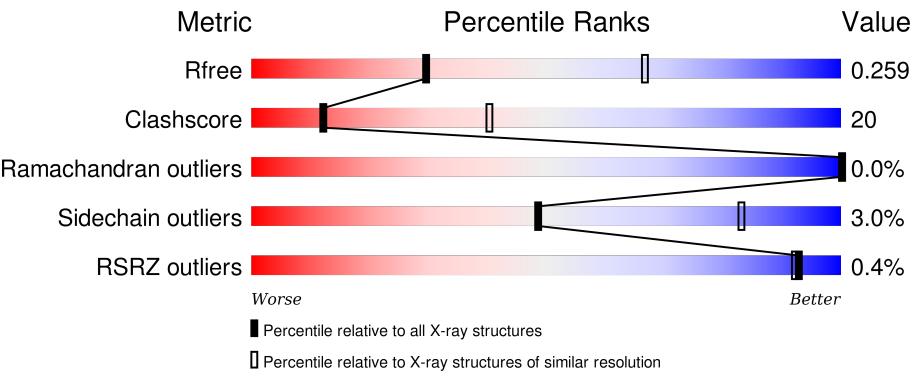
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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	<div><div></div><div>67%25%7%</div></div>
1	B	230	<div><div></div><div>67%27%7%</div></div>
1	C	230	<div><div>%</div><div>63%30%6%</div></div>
1	D	230	<div><div></div><div>67%25%7%</div></div>
1	E	230	<div><div></div><div>68%24%7%</div></div>

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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
3	NAG	D	250	-	-	-	X
5	MRD	B	305	-	-	-	X
5	MRD	D	305	-	-	-	X
5	MRD	E	305	-	-	-	X
6	MPD	A	223	-	-	-	X
6	MPD	G	222	-	-	-	X
6	MPD	G	305	-	-	-	X
6	MPD	J	305	-	-	-	X
7	NAG	B	275[A]	-	-	-	X
7	NAG	C	250	-	-	-	X
7	NAG	E	275[A]	-	-	-	X
7	NAG	E	275[B]	-	-	-	X
7	NAG	I	275[A]	-	-	-	X
7	NAG	I	275[B]	X	-	-	X
9	NAG	J	250	-	-	X	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 18393 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	22	2	0
			1734	1092	286	348	8			
1	B	215	Total	C	N	O	S	10	3	0
			1743	1097	285	353	8			
1	C	216	Total	C	N	O	S	8	5	0
			1764	1111	292	353	8			
1	D	214	Total	C	N	O	S	3	3	0
			1733	1092	283	350	8			
1	E	215	Total	C	N	O	S	12	3	0
			1751	1101	292	350	8			
1	F	214	Total	C	N	O	S	0	2	0
			1733	1092	285	348	8			
1	G	214	Total	C	N	O	S	4	0	0
			1716	1081	280	347	8			
1	H	215	Total	C	N	O	S	0	2	0
			1741	1096	287	350	8			
1	I	214	Total	C	N	O	S	0	2	0
			1728	1087	283	350	8			
1	J	215	Total	C	N	O	S	8	4	0
			1754	1103	292	351	8			

There are 360 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	184	SER	GLN	ENGINEERED MUTATION	UNP Q8WSF8
A	185	GLU	VAL	ENGINEERED MUTATION	UNP Q8WSF8
A	186	ARG	GLN	ENGINEERED MUTATION	UNP Q8WSF8
A	187	PHE	HIS	ENGINEERED MUTATION	UNP Q8WSF8
A	189	GLU	SER	ENGINEERED MUTATION	UNP Q8WSF8
A	192	LYS	PRO	ENGINEERED MUTATION	UNP Q8WSF8
A	196	PRO	ILE	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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	184	SER	GLN	ENGINEERED MUTATION	UNP Q8WSF8
B	185	GLU	VAL	ENGINEERED MUTATION	UNP Q8WSF8
B	186	ARG	GLN	ENGINEERED MUTATION	UNP Q8WSF8
B	187	PHE	HIS	ENGINEERED MUTATION	UNP Q8WSF8
B	189	GLU	SER	ENGINEERED MUTATION	UNP Q8WSF8
B	192	LYS	PRO	ENGINEERED MUTATION	UNP Q8WSF8
B	196	PRO	ILE	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	184	SER	GLN	ENGINEERED MUTATION	UNP Q8WSF8
C	185	GLU	VAL	ENGINEERED MUTATION	UNP Q8WSF8
C	186	ARG	GLN	ENGINEERED MUTATION	UNP Q8WSF8
C	187	PHE	HIS	ENGINEERED MUTATION	UNP Q8WSF8
C	189	GLU	SER	ENGINEERED MUTATION	UNP Q8WSF8
C	192	LYS	PRO	ENGINEERED MUTATION	UNP Q8WSF8
C	196	PRO	ILE	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
D	184	SER	GLN	ENGINEERED MUTATION	UNP Q8WSF8
D	185	GLU	VAL	ENGINEERED MUTATION	UNP Q8WSF8
D	186	ARG	GLN	ENGINEERED MUTATION	UNP Q8WSF8
D	187	PHE	HIS	ENGINEERED MUTATION	UNP Q8WSF8
D	189	GLU	SER	ENGINEERED MUTATION	UNP Q8WSF8
D	192	LYS	PRO	ENGINEERED MUTATION	UNP Q8WSF8
D	196	PRO	ILE	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
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	184	SER	GLN	ENGINEERED MUTATION	UNP Q8WSF8
E	185	GLU	VAL	ENGINEERED MUTATION	UNP Q8WSF8
E	186	ARG	GLN	ENGINEERED MUTATION	UNP Q8WSF8
E	187	PHE	HIS	ENGINEERED MUTATION	UNP Q8WSF8
E	189	GLU	SER	ENGINEERED MUTATION	UNP Q8WSF8
E	192	LYS	PRO	ENGINEERED MUTATION	UNP Q8WSF8

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Chain	Residue	Modelled	Actual	Comment	Reference
E	196	PRO	ILE	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	184	SER	GLN	ENGINEERED MUTATION	UNP Q8WSF8
F	185	GLU	VAL	ENGINEERED MUTATION	UNP Q8WSF8
F	186	ARG	GLN	ENGINEERED MUTATION	UNP Q8WSF8
F	187	PHE	HIS	ENGINEERED MUTATION	UNP Q8WSF8
F	189	GLU	SER	ENGINEERED MUTATION	UNP Q8WSF8
F	192	LYS	PRO	ENGINEERED MUTATION	UNP Q8WSF8
F	196	PRO	ILE	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	184	SER	GLN	ENGINEERED MUTATION	UNP Q8WSF8
G	185	GLU	VAL	ENGINEERED MUTATION	UNP Q8WSF8
G	186	ARG	GLN	ENGINEERED MUTATION	UNP Q8WSF8
G	187	PHE	HIS	ENGINEERED MUTATION	UNP Q8WSF8
G	189	GLU	SER	ENGINEERED MUTATION	UNP Q8WSF8
G	192	LYS	PRO	ENGINEERED MUTATION	UNP Q8WSF8
G	196	PRO	ILE	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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	184	SER	GLN	ENGINEERED MUTATION	UNP Q8WSF8
H	185	GLU	VAL	ENGINEERED MUTATION	UNP Q8WSF8
H	186	ARG	GLN	ENGINEERED MUTATION	UNP Q8WSF8
H	187	PHE	HIS	ENGINEERED MUTATION	UNP Q8WSF8
H	189	GLU	SER	ENGINEERED MUTATION	UNP Q8WSF8
H	192	LYS	PRO	ENGINEERED MUTATION	UNP Q8WSF8
H	196	PRO	ILE	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	184	SER	GLN	ENGINEERED MUTATION	UNP Q8WSF8
I	185	GLU	VAL	ENGINEERED MUTATION	UNP Q8WSF8
I	186	ARG	GLN	ENGINEERED MUTATION	UNP Q8WSF8
I	187	PHE	HIS	ENGINEERED MUTATION	UNP Q8WSF8
I	189	GLU	SER	ENGINEERED MUTATION	UNP Q8WSF8
I	192	LYS	PRO	ENGINEERED MUTATION	UNP Q8WSF8
I	196	PRO	ILE	ENGINEERED MUTATION	UNP Q8WSF8
I	220	SER	-	EXPRESSION TAG	UNP Q8WSF8
I	221	ARG	-	EXPRESSION TAG	UNP Q8WSF8
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	184	SER	GLN	ENGINEERED MUTATION	UNP Q8WSF8
J	185	GLU	VAL	ENGINEERED MUTATION	UNP Q8WSF8
J	186	ARG	GLN	ENGINEERED MUTATION	UNP Q8WSF8
J	187	PHE	HIS	ENGINEERED MUTATION	UNP Q8WSF8
J	189	GLU	SER	ENGINEERED MUTATION	UNP Q8WSF8
J	192	LYS	PRO	ENGINEERED MUTATION	UNP Q8WSF8
J	196	PRO	ILE	ENGINEERED MUTATION	UNP Q8WSF8
J	220	SER	-	EXPRESSION TAG	UNP Q8WSF8
J	221	ARG	-	EXPRESSION TAG	UNP Q8WSF8

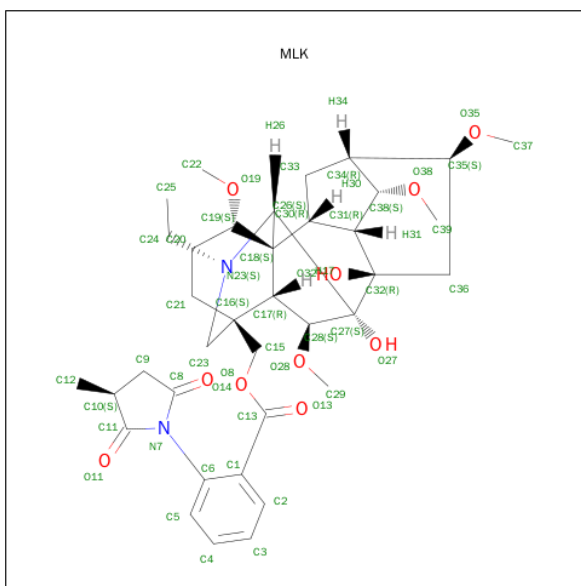
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	I	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	A	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	E	1	Total Mg 1 1	0	0

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

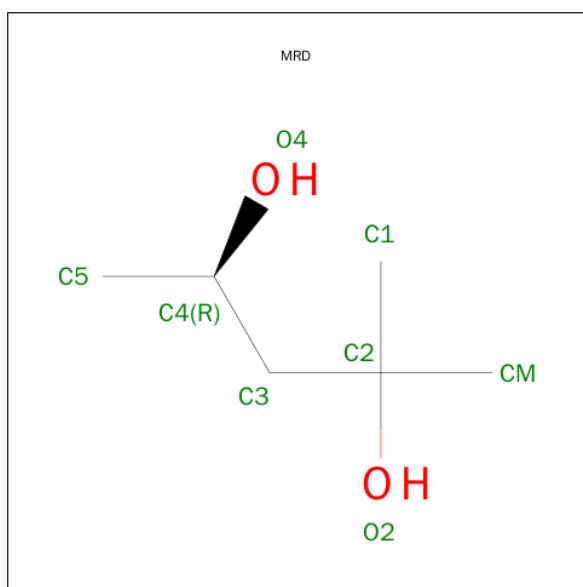
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total C N O 28 16 2 10	0	0
3	D	2	Total C N O 28 16 2 10	0	0
3	E	2	Total C N O 28 16 2 10	0	0
3	G	2	Total C N O 28 16 2 10	0	0

- Molecule 4 is METHYLLYCACONITINE (three-letter code: MLK) (formula: $C_{37}H_{50}N_2O_{10}$).



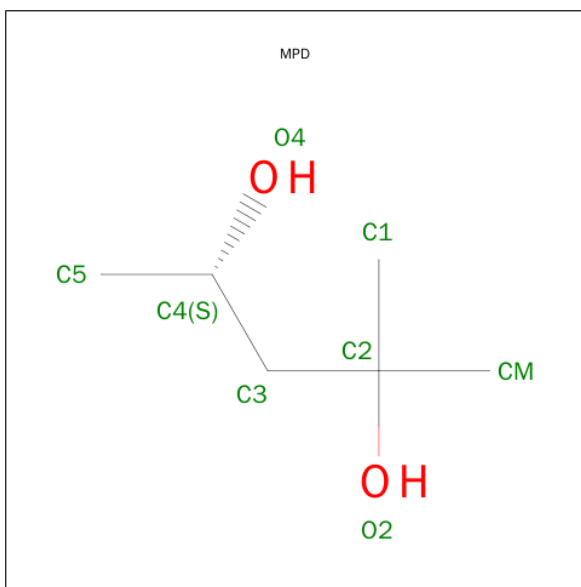
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			49	37	2	10		
4	B	1	Total	C	N	O	0	0
			49	37	2	10		
4	C	1	Total	C	N	O	0	0
			49	37	2	10		
4	D	1	Total	C	N	O	0	0
			49	37	2	10		
4	E	1	Total	C	N	O	0	0
			49	37	2	10		
4	F	1	Total	C	N	O	0	0
			49	37	2	10		
4	G	1	Total	C	N	O	0	0
			49	37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

- Molecule 5 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: $C_6H_{14}O_2$).



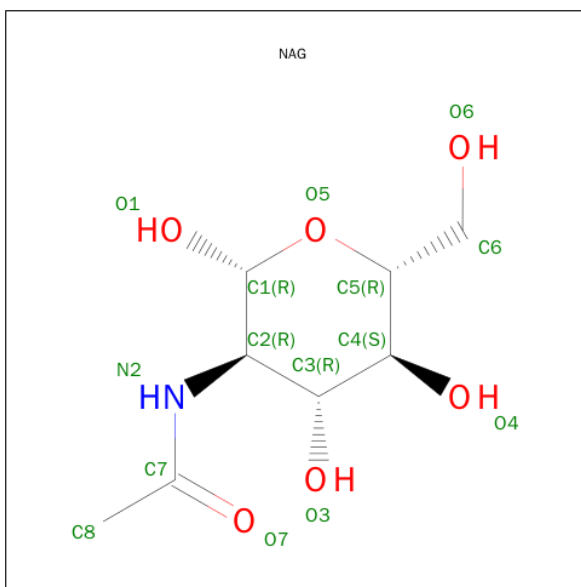
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			8	6	2		
5	B	1	Total	C	O	0	0
			8	6	2		
5	D	1	Total	C	O	0	0
			8	6	2		
5	E	1	Total	C	O	0	0
			8	6	2		
5	F	1	Total	C	O	0	0
			8	6	2		

- Molecule 6 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C₆H₁₄O₂).



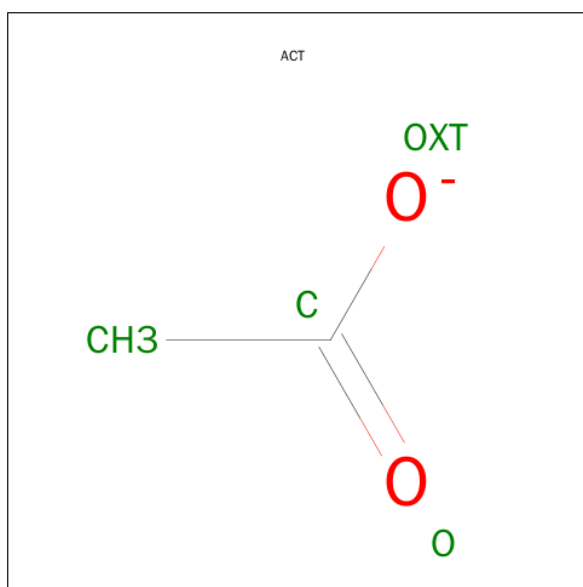
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			8	6	2		
6	A	1	Total	C	O	0	0
			8	6	2		
6	C	1	Total	C	O	0	0
			8	6	2		
6	G	1	Total	C	O	0	0
			8	6	2		
6	G	1	Total	C	O	0	0
			8	6	2		
6	J	1	Total	C	O	0	0
			8	6	2		
6	I	1	Total	C	O	0	0
			8	6	2		

- Molecule 7 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	N	O	0	0
			14	8	1	5		
7	B	1	Total	C	N	O	0	1
			28	16	2	10		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	E	1	Total	C	N	O	0	1
			28	16	2	10		
7	F	1	Total	C	N	O	0	0
			14	8	1	5		
7	I	1	Total	C	N	O	0	0
			14	8	1	5		
7	I	1	Total	C	N	O	0	1
			28	16	2	10		

- Molecule 8 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	G	1	Total	C	O	0	0
			4	2	2		

- Molecule 9 is a polymer of unknown type called SUGAR (3-MER).

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

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	12	Total	O	0	0
			12	12		
10	B	12	Total	O	0	0
			12	12		
10	C	7	Total	O	0	0
			7	7		
10	D	3	Total	O	0	0
			3	3		
10	E	9	Total	O	0	0
			9	9		
10	F	5	Total	O	0	0
			5	5		

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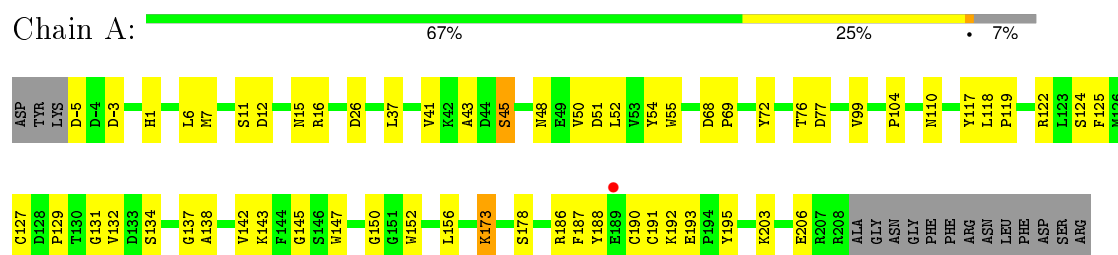
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	G	5	Total 5	O 5	0	0
10	H	5	Total 5	O 5	0	0
10	I	8	Total 8	O 8	0	0
10	J	5	Total 5	O 5	0	0

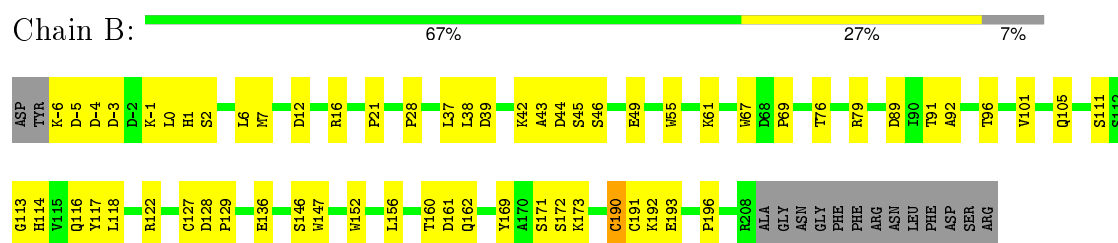
3 Residue-property plots [i](#)

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

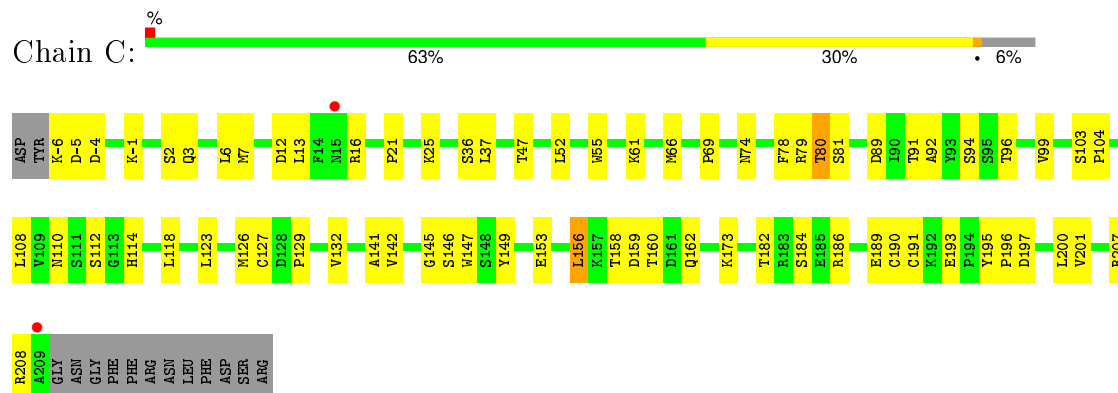
• Molecule 1: Soluble acetylcholine receptor



• Molecule 1: Soluble acetylcholine receptor

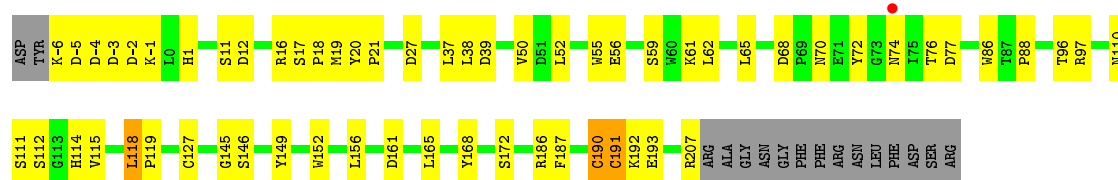


• Molecule 1: Soluble acetylcholine receptor



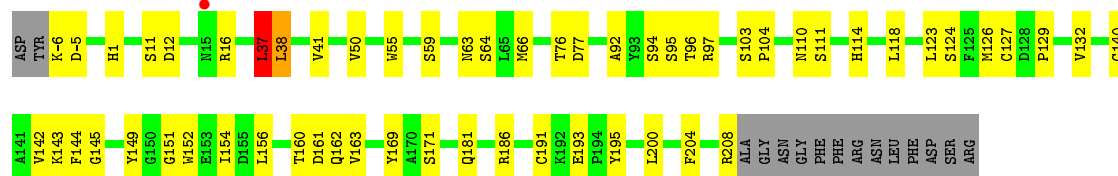
• Molecule 1: Soluble acetylcholine receptor





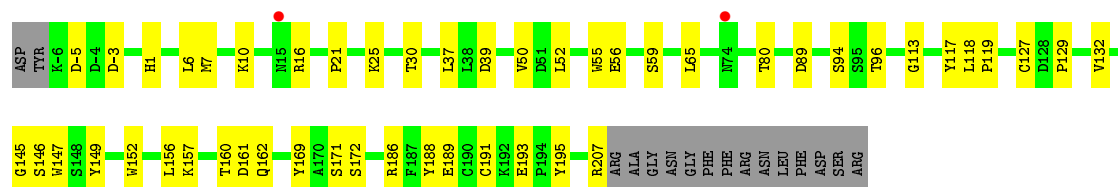
- Molecule 1: Soluble acetylcholine receptor

Chain E: 68% 24% 7%



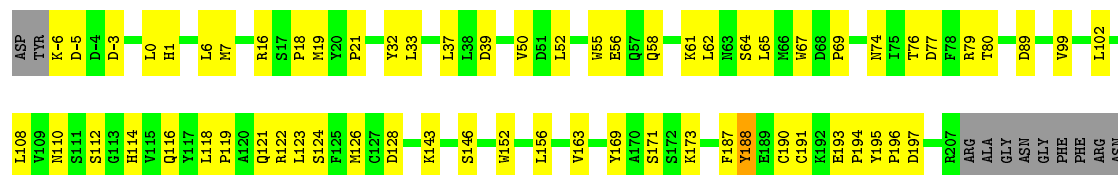
- Molecule 1: Soluble acetylcholine receptor

Chain F: 72% 21% 7%



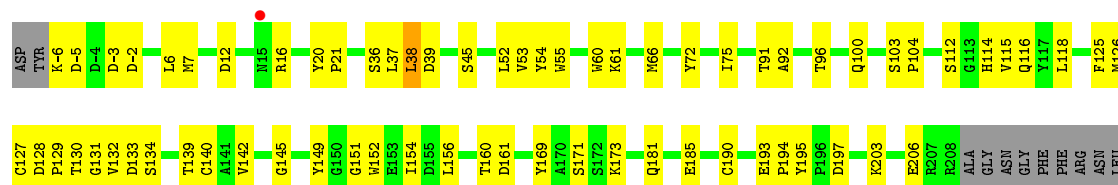
- Molecule 1: Soluble acetylcholine receptor

Chain G: 65% 27% 7%



- Molecule 1: Soluble acetylcholine receptor

Chain H: 64% 29% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.79Å 140.18Å 136.81Å 90.00° 105.20° 90.00°	Depositor
Resolution (Å)	48.05 – 2.90 48.05 – 2.33	Depositor EDS
% Data completeness (in resolution range)	93.5 (48.05-2.90) 64.0 (48.05-2.33)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.66 (at 2.34Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.213 , 0.258 0.213 , 0.259	Depositor DCC
R_{free} test set	1522 reflections (2.41%)	DCC
Wilson B-factor (Å ²)	47.0	Xtriage
Anisotropy	0.694	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 42.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 85106 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	18393	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.86% 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: MG, BMA, NAG, MLK, MPD, ACT, MRD

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	0.45	0/1781	0.69	0/2428
1	B	0.47	0/1796	0.68	0/2446
1	C	0.57	0/1823	0.69	0/2481
1	D	0.47	0/1786	0.62	0/2433
1	E	0.45	0/1800	0.68	1/2449 (0.0%)
1	F	0.43	0/1780	0.67	0/2424
1	G	0.55	0/1760	0.62	0/2398
1	H	0.58	1/1791 (0.1%)	0.69	1/2439 (0.0%)
1	I	0.51	0/1778	0.64	0/2423
1	J	0.53	0/1807	0.67	1/2460 (0.0%)
All	All	0.51	1/17902 (0.0%)	0.66	3/24381 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	127	CYS	CB-SG	-5.22	1.73	1.81

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	38	LEU	CB-CA-C	-5.86	99.06	110.20
1	J	14	PHE	N-CA-C	5.56	126.02	111.00
1	E	37	LEU	CA-CB-CG	-5.49	102.67	115.30

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	1734	0	1647	56	0
1	B	1743	0	1648	68	0
1	C	1764	0	1689	80	0
1	D	1733	0	1645	76	0
1	E	1751	0	1664	77	0
1	F	1733	0	1649	56	0
1	G	1716	0	1621	74	0
1	H	1741	0	1653	67	0
1	I	1728	0	1628	84	0
1	J	1754	0	1672	93	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	E	1	0	0	0	0
2	I	1	0	0	0	0
3	A	28	0	25	3	0
3	D	28	0	25	6	0
3	E	28	0	25	5	0
3	G	28	0	25	4	0
4	A	49	0	50	9	0
4	B	49	0	50	11	0
4	C	49	0	50	18	0
4	D	49	0	50	4	0
4	E	49	0	50	15	0
4	F	49	0	50	20	0
4	G	49	0	50	10	0
4	H	49	0	50	15	0
4	I	49	0	50	15	0
4	J	49	0	50	10	0
5	A	8	0	14	1	0
5	B	8	0	14	2	0
5	D	8	0	14	4	0
5	E	8	0	14	0	0
5	F	8	0	14	3	0
6	A	16	0	28	1	0
6	C	8	0	14	3	0
6	G	16	0	28	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	I	8	0	14	1	0
6	J	8	0	14	0	0
7	B	42	0	39	2	0
7	C	14	0	13	3	0
7	E	28	0	26	2	0
7	F	14	0	13	0	0
7	I	42	0	39	7	0
8	G	4	0	3	0	0
9	H	39	0	34	3	0
9	J	39	0	34	9	0
10	A	12	0	0	0	0
10	B	12	0	0	0	0
10	C	7	0	0	1	0
10	D	3	0	0	0	0
10	E	9	0	0	1	0
10	F	5	0	0	0	0
10	G	5	0	0	0	0
10	H	5	0	0	1	0
10	I	8	0	0	0	0
10	J	5	0	0	0	0
All	All	18393	0	17485	699	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 20.

All (699) 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:C:110:ASN:HD21	7:C:250:NAG:C1	1.05	1.65
1:J:110:ASN:HD21	9:J:250:NAG:C1	1.07	1.58
1:D:16:ARG:HG3	1:J:16:ARG:CD	1.44	1.46
1:D:16:ARG:CG	1:J:16:ARG:HD3	1.44	1.43
1:E:160:THR:HG22	1:E:162:GLN:H	0.99	1.12
9:J:250:NAG:H61	9:J:251:NAG:HN2	1.12	1.10
1:C:160:THR:HG22	1:C:162:GLN:H	1.08	1.10
1:D:16:ARG:CD	1:J:16:ARG:HD3	1.82	1.10
1:C:7:MET:HE3	1:D:21:PRO:HD3	1.21	1.09
1:E:16:ARG:CD	1:I:16:ARG:HE	1.69	1.05
4:F:301:MLK:H371	1:J:116:GLN:NE2	1.75	1.02
1:J:160:THR:HG22	1:J:162:GLN:H	1.24	1.00
1:H:16:ARG:HG2	1:H:16:ARG:HH11	1.24	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:ARG:HD3	1:G:16:ARG:HD3	1.46	0.98
1:J:110:ASN:HD21	9:J:250:NAG:C2	1.78	0.97
1:C:16:ARG:HB2	1:F:16:ARG:NH2	1.78	0.97
1:A:12:ASP:O	1:A:16:ARG:HB3	1.65	0.96
1:C:16:ARG:HD3	1:F:16:ARG:CD	1.95	0.96
1:B:-6:LYS:HG3	1:B:-5:ASP:H	1.32	0.95
1:I:29:LEU:HD11	1:I:60:TRP:HB2	1.48	0.95
1:F:160:THR:HG22	1:F:162:GLN:H	1.31	0.95
1:D:1:HIS:HE1	1:I:-3:ASP:OD1	1.49	0.93
1:D:-3:ASP:OD2	1:I:1:HIS:HE1	1.39	0.93
1:J:110:ASN:ND2	9:J:250:NAG:C2	2.31	0.92
1:E:160:THR:HG22	1:E:162:GLN:N	1.84	0.92
3:A:250:NAG:H62	3:A:251:NAG:HN2	1.33	0.92
1:E:94:SER:HB3	1:E:142:VAL:HG23	1.51	0.92
1:J:52:LEU:HD23	1:J:54:TYR:CD2	2.05	0.92
1:F:65:LEU:O	1:F:113:GLY:HA2	1.70	0.91
1:C:16:ARG:HD3	1:F:16:ARG:HD2	1.52	0.91
1:J:52:LEU:HD23	1:J:54:TYR:HD2	1.36	0.90
1:H:12:ASP:HA	1:H:16:ARG:HD3	1.55	0.87
1:D:86:TRP:CZ3	1:D:88:PRO:HD3	2.10	0.86
7:I:275[B]:NAG:H3	7:I:275[B]:NAG:H83	1.55	0.86
4:F:301:MLK:H371	1:J:116:GLN:HE22	1.34	0.86
1:H:37:LEU:HD11	1:H:52:LEU:HD22	1.58	0.86
1:A:55:TRP:CZ3	4:B:301:MLK:H292	2.11	0.85
1:D:16:ARG:HG3	1:J:16:ARG:HD3	0.85	0.84
1:E:16:ARG:HD2	1:I:16:ARG:HE	1.41	0.84
1:D:1:HIS:CE1	1:I:-3:ASP:OD1	2.31	0.84
1:J:110:ASN:CG	9:J:250:NAG:C1	2.46	0.84
1:J:160:THR:CG2	1:J:162:GLN:H	1.90	0.83
3:A:250:NAG:H62	3:A:251:NAG:N2	1.91	0.83
1:C:160:THR:HG22	1:C:162:GLN:N	1.92	0.83
1:H:118:LEU:HD23	1:H:118:LEU:O	1.76	0.83
1:E:76:THR:O	1:E:110:ASN:HB2	1.78	0.83
1:C:186[A]:ARG:HD2	4:C:301:MLK:H4	1.62	0.82
1:E:16:ARG:HH22	1:I:12:ASP:CG	1.83	0.82
1:D:-3:ASP:OD2	1:I:1:HIS:CE1	2.29	0.81
1:B:16:ARG:HD3	1:G:16:ARG:CD	2.09	0.81
3:D:251:NAG:O7	3:D:251:NAG:C3	2.29	0.81
1:E:208[A]:ARG:HA	1:E:208[A]:ARG:HE	1.46	0.80
1:E:16:ARG:NH2	1:I:12:ASP:HA	1.96	0.80
1:D:16:ARG:CG	1:J:16:ARG:CD	2.27	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:TRP:O	4:C:301:MLK:H253	1.82	0.80
1:E:16:ARG:CZ	1:I:16:ARG:HG3	2.11	0.79
1:D:16:ARG:HG3	1:J:16:ARG:NE	1.98	0.79
3:A:250:NAG:C6	3:A:251:NAG:HN2	1.95	0.78
1:A:99:VAL:HG23	10:E:326:HOH:O	1.83	0.78
1:G:190:CYS:SG	1:G:191:CYS:N	2.57	0.78
9:J:250:NAG:H61	9:J:251:NAG:N2	1.96	0.78
1:G:116:GLN:HE22	4:H:301:MLK:C37	1.96	0.77
1:H:16:ARG:NH1	1:H:16:ARG:HG2	1.96	0.77
3:D:251:NAG:O7	3:D:251:NAG:H3	1.84	0.77
1:A:55:TRP:HB3	1:A:118[B]:LEU:HD21	1.66	0.77
1:E:16:ARG:HH22	1:I:12:ASP:HA	1.50	0.77
1:E:208[A]:ARG:NE	1:E:208[A]:ARG:HA	2.00	0.77
1:C:16:ARG:HD3	1:F:16:ARG:NE	2.01	0.76
1:J:55:TRP:HB3	1:J:118:LEU:HD11	1.68	0.75
1:G:-6:LYS:HG3	1:G:-5:ASP:H	1.51	0.75
1:E:160:THR:CG2	1:E:162:GLN:H	1.91	0.75
1:G:39:ASP:HB2	1:H:126:MET:HE1	1.69	0.75
1:A:6:LEU:HD23	1:B:21:PRO:HB2	1.68	0.74
1:H:7:MET:HE1	1:I:18:PRO:HG2	1.67	0.74
1:D:152:TRP:HB2	1:D:193:GLU:OE2	1.87	0.74
1:C:186[A]:ARG:HD2	4:C:301:MLK:C4	2.17	0.74
1:C:55:TRP:HB3	1:C:118:LEU:HD11	1.70	0.74
1:H:37:LEU:HD11	1:H:52:LEU:CD2	2.17	0.73
1:I:112:SER:OG	7:I:250:NAG:H82	1.87	0.73
1:B:160:THR:HG22	1:B:162:GLN:H	1.54	0.72
1:B:-6:LYS:CG	1:B:-5:ASP:H	2.02	0.72
1:A:190:CYS:SG	1:A:191:CYS:N	2.63	0.72
1:H:139:THR:OG1	1:H:203:LYS:HD2	1.89	0.72
1:F:152:TRP:CE3	1:F:193:GLU:HG3	2.24	0.72
1:J:160:THR:HG22	1:J:162:GLN:N	2.02	0.72
1:E:143:LYS:HD2	4:E:301:MLK:C5	2.20	0.72
1:I:160:THR:HG22	1:I:162:GLN:H	1.55	0.72
1:C:7:MET:CE	1:D:21:PRO:HD3	2.12	0.71
1:G:16:ARG:CZ	1:G:16:ARG:HB3	2.18	0.71
1:I:56:GLU:O	1:I:119:PRO:HD2	1.90	0.71
1:I:36:SER:HB3	1:I:164:ASP:HB3	1.71	0.71
1:H:16:ARG:HH11	1:H:16:ARG:CG	2.00	0.71
1:J:152:TRP:CE3	1:J:193:GLU:HG3	2.25	0.71
1:G:116:GLN:HE22	4:H:301:MLK:H373	1.54	0.71
1:J:152:TRP:CD2	1:J:193:GLU:HG3	2.26	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:12:ASP:OD1	1:J:16:ARG:NH1	2.24	0.70
1:E:16:ARG:HG2	1:I:16:ARG:NE	2.06	0.70
1:D:-5:ASP:O	1:D:-2:ASP:HB2	1.91	0.70
1:E:12:ASP:HA	1:E:16:ARG:HD3	1.73	0.70
1:I:79:ARG:HD3	1:J:149:TYR:CE1	2.27	0.69
1:I:17:SER:OG	1:I:18:PRO:HD2	1.93	0.69
1:A:173:LYS:NZ	1:B:45:SER:O	2.25	0.69
1:G:188:TYR:HE2	1:G:195:TYR:CD2	2.10	0.69
1:F:152:TRP:CD2	1:F:193:GLU:HG3	2.28	0.69
1:D:76:THR:O	1:D:110:ASN:HB2	1.93	0.69
1:H:-6:LYS:HG3	1:H:-5:ASP:H	1.58	0.69
4:E:301:MLK:H152	4:E:301:MLK:C29	2.23	0.68
1:E:16:ARG:CG	1:I:16:ARG:HE	2.06	0.68
1:B:116:GLN:HG2	1:B:118:LEU:HD11	1.75	0.68
1:C:118:LEU:HD23	4:D:301:MLK:H242	1.75	0.68
4:G:301:MLK:O28	4:G:301:MLK:H31	1.93	0.68
1:B:16:ARG:HB2	1:G:16:ARG:HD2	1.75	0.67
1:C:13:LEU:HD23	6:C:306:MPD:H31	1.76	0.67
1:A:55:TRP:CH2	4:B:301:MLK:H292	2.29	0.67
1:B:169:TYR:CZ	1:B:171:SER:HB2	2.29	0.67
1:C:94:SER:HB2	1:C:126:MET:HE2	1.75	0.67
1:C:7:MET:HE3	1:D:21:PRO:CD	2.14	0.67
1:D:11:SER:HB3	1:D:16:ARG:NH1	2.08	0.67
1:B:91:THR:HG22	1:B:92:ALA:O	1.94	0.67
1:F:117:TYR:CE2	1:F:119:PRO:HG3	2.30	0.67
1:F:189:GLU:O	1:F:189:GLU:HG3	1.95	0.67
5:A:305:MRD:H1C1	5:A:305:MRD:O4	1.93	0.67
1:I:195:TYR:CE1	4:I:301:MLK:H331	2.30	0.66
1:E:-6:LYS:HD2	1:E:-5:ASP:H	1.60	0.66
1:F:195:TYR:CE2	4:F:301:MLK:H331	2.30	0.66
1:H:116:GLN:HE22	4:I:301:MLK:H373	1.59	0.66
4:F:301:MLK:O8	1:J:55:TRP:HH2	1.79	0.66
1:J:183:ARG:HH12	1:J:185:GLU:CG	2.09	0.66
1:H:133:ASP:HA	1:H:206:GLU:HG3	1.77	0.66
1:A:52:LEU:HD23	1:A:54:TYR:CD2	2.31	0.66
1:D:161:ASP:O	1:D:161:ASP:OD1	2.13	0.66
4:C:301:MLK:H3	10:C:333:HOH:O	1.96	0.65
1:E:16:ARG:NH2	1:I:12:ASP:CG	2.49	0.65
1:B:16:ARG:HG2	1:B:16:ARG:O	1.97	0.65
4:I:301:MLK:H242	4:I:301:MLK:O27	1.97	0.65
1:I:57:GLN:NE2	1:I:116:GLN:HE22	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:-6:LYS:HG3	1:C:-5:ASP:H	1.62	0.65
1:G:116:GLN:NE2	4:H:301:MLK:H373	2.12	0.65
1:D:77:ASP:HB3	1:D:110:ASN:CB	2.28	0.64
1:E:160:THR:CG2	1:E:161:ASP:N	2.61	0.64
1:G:39:ASP:HB2	1:H:126:MET:CE	2.27	0.64
1:E:16:ARG:HH22	1:I:12:ASP:CA	2.10	0.63
1:E:208[A]:ARG:CA	1:E:208[A]:ARG:HE	2.10	0.63
1:E:145:GLY:HA2	1:E:156:LEU:HD11	1.80	0.63
1:B:136:GLU:CD	1:B:136:GLU:H	2.02	0.63
1:C:195:TYR:CD1	4:C:301:MLK:H222	2.34	0.63
1:B:105:GLN:HG2	1:B:117:TYR:OH	1.98	0.63
1:E:1:HIS:CE1	1:H:-3:ASP:OD1	2.52	0.63
1:J:56:GLU:O	1:J:119:PRO:HD2	1.99	0.63
1:H:169:TYR:CZ	1:H:171:SER:HB2	2.34	0.62
1:I:152:TRP:HB2	1:I:193:GLU:OE2	1.99	0.62
4:I:301:MLK:H252	4:I:301:MLK:H362	1.80	0.62
1:A:178:SER:OG	1:A:203:LYS:HE3	2.00	0.62
1:I:50:VAL:HG21	1:I:127:CYS:SG	2.39	0.62
1:D:77:ASP:HB3	1:D:110:ASN:HB3	1.80	0.62
1:C:94:SER:CB	1:C:126:MET:HE2	2.28	0.62
1:H:16:ARG:NH1	1:H:16:ARG:CG	2.58	0.62
1:F:172:SER:O	1:F:207:ARG:NH1	2.32	0.62
1:A:125:PHE:CE1	1:A:142:VAL:HG22	2.35	0.62
1:E:16:ARG:NE	1:I:16:ARG:HE	1.98	0.62
1:C:13:LEU:CD2	6:C:306:MPD:H31	2.31	0.61
9:H:252:BMA:H3	10:H:338:HOH:O	1.99	0.61
1:J:76:THR:O	1:J:110:ASN:HB2	2.00	0.61
1:C:16:ARG:CD	1:F:16:ARG:HD2	2.27	0.61
4:A:301:MLK:H242	1:E:118:LEU:HD13	1.82	0.61
1:E:12:ASP:HA	1:E:16:ARG:CD	2.30	0.61
4:B:301:MLK:H31	4:B:301:MLK:O28	1.99	0.61
1:G:62:LEU:HB2	1:G:65:LEU:HD12	1.82	0.61
1:G:118:LEU:HD13	4:H:301:MLK:O27	2.01	0.61
1:J:110:ASN:ND2	9:J:250:NAG:H2	2.16	0.61
5:D:305:MRD:H5C2	5:D:305:MRD:O2	2.01	0.61
1:H:7:MET:HE2	1:I:21:PRO:HD3	1.83	0.61
1:I:125:PHE:CD1	1:I:142:VAL:HG22	2.37	0.60
1:J:177:LEU:HD12	1:J:203:LYS:HG2	1.81	0.60
1:J:132:VAL:HG23	1:J:205:ARG:HA	1.83	0.60
1:E:16:ARG:NH2	1:I:16:ARG:HG3	2.15	0.60
1:D:39:ASP:HB2	1:E:126:MET:HE1	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:301:MLK:O28	4:J:301:MLK:H31	2.01	0.60
4:H:301:MLK:O27	4:H:301:MLK:H242	2.01	0.60
1:H:7:MET:CE	1:I:21:PRO:HD3	2.31	0.60
1:G:188:TYR:CE2	1:G:195:TYR:CD2	2.90	0.60
1:G:56:GLU:O	1:G:119:PRO:HD2	2.01	0.60
1:I:195:TYR:HE1	4:I:301:MLK:H222	1.67	0.59
1:A:125:PHE:CD1	1:A:142:VAL:HG22	2.37	0.59
1:H:72:TYR:O	1:H:75:ILE:HG13	2.03	0.59
1:I:195:TYR:CE1	4:I:301:MLK:H222	2.37	0.59
1:H:6:LEU:HD23	1:I:21:PRO:HB2	1.85	0.59
1:D:39:ASP:HB2	1:E:126:MET:CE	2.32	0.59
1:J:118:LEU:O	1:J:118:LEU:HG	2.03	0.59
4:B:301:MLK:H252	4:B:301:MLK:H362	1.85	0.59
1:I:114:HIS:CG	7:I:250:NAG:H5	2.37	0.59
4:E:301:MLK:H152	4:E:301:MLK:H292	1.82	0.59
1:J:110:ASN:OD1	9:J:250:NAG:C1	2.50	0.58
1:C:37:LEU:HD11	1:C:52:LEU:HD11	1.85	0.58
1:J:-6:LYS:NZ	1:J:-6:LYS:HB2	2.18	0.58
1:C:99:VAL:HG22	1:C:123:LEU:HD13	1.84	0.58
1:D:114:HIS:ND1	3:D:250:NAG:H5	2.18	0.58
1:C:153:GLU:OE1	1:C:193:GLU:OE2	2.22	0.58
4:F:301:MLK:O27	1:J:118:LEU:CD2	2.52	0.58
1:F:7:MET:CE	1:G:18:PRO:HG2	2.33	0.58
1:G:-6:LYS:HG3	1:G:-5:ASP:N	2.19	0.58
1:A:129:PRO:O	1:A:138:ALA:HB2	2.04	0.58
1:C:16:ARG:HB2	1:F:16:ARG:CZ	2.33	0.58
1:G:89:ASP:O	1:G:89:ASP:CG	2.42	0.58
1:F:55:TRP:CZ3	4:G:301:MLK:H292	2.39	0.58
1:G:61:LYS:HE2	1:G:112:SER:O	2.03	0.58
1:C:186[A]:ARG:CD	4:C:301:MLK:H4	2.33	0.57
1:J:184:SER:O	1:J:196:PRO:HA	2.04	0.57
1:B:79:ARG:NH1	1:C:153:GLU:OE2	2.38	0.57
1:G:76:THR:HB	3:G:250:NAG:C8	2.33	0.57
1:B:7:MET:HE2	1:C:21:PRO:HD3	1.86	0.57
1:F:195:TYR:HE2	4:F:301:MLK:H222	1.69	0.57
1:E:16:ARG:CG	1:I:16:ARG:NE	2.67	0.57
4:G:301:MLK:H252	4:G:301:MLK:H362	1.86	0.57
1:F:89:ASP:O	1:F:146:SER:HA	2.04	0.57
4:G:301:MLK:H242	4:G:301:MLK:O27	2.04	0.57
4:I:301:MLK:H31	4:I:301:MLK:O28	2.05	0.57
1:D:37:LEU:HD13	1:D:52:LEU:HD22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:186:ARG:NH2	1:F:188:TYR:CE2	2.72	0.57
1:C:195:TYR:HD1	4:C:301:MLK:H222	1.69	0.57
1:E:152:TRP:CD2	1:E:193:GLU:HG3	2.40	0.57
1:E:11:SER:OG	1:I:16:ARG:NH2	2.38	0.57
1:B:122:ARG:HD2	1:C:96:THR:O	2.05	0.57
1:J:28:PRO:HB3	1:J:152:TRP:O	2.05	0.56
3:E:251:NAG:O7	3:E:251:NAG:H3	2.04	0.56
1:D:37:LEU:HD12	1:D:37:LEU:C	2.26	0.56
1:D:12:ASP:O	1:D:16:ARG:HB2	2.05	0.56
1:C:158:THR:CG2	1:C:160:THR:O	2.54	0.56
5:F:305:MRD:O2	5:F:305:MRD:H5C3	2.06	0.56
4:E:301:MLK:H242	4:E:301:MLK:O27	2.06	0.56
1:H:169:TYR:HB2	1:I:126:MET:CE	2.36	0.56
1:F:195:TYR:CD2	4:F:301:MLK:H19	2.42	0.55
1:G:77:ASP:HB3	1:G:110:ASN:HB3	1.86	0.55
1:G:55:TRP:CH2	4:H:301:MLK:H292	2.40	0.55
1:J:160:THR:CG2	1:J:161:ASP:N	2.70	0.55
1:B:118:LEU:HD22	4:C:301:MLK:H242	1.89	0.55
1:C:-6:LYS:HG3	1:C:-5:ASP:N	2.21	0.55
1:E:38:LEU:HD11	1:E:55:TRP:CE2	2.41	0.55
1:E:16:ARG:HH22	1:I:12:ASP:CB	2.19	0.55
1:A:1:HIS:CE1	1:G:-3:ASP:OD1	2.58	0.55
1:D:-6:LYS:CG	1:D:-5:ASP:H	2.19	0.55
4:H:301:MLK:H362	4:H:301:MLK:H252	1.87	0.55
1:F:149:TYR:HE2	5:F:305:MRD:HMC3	1.72	0.55
1:I:173:LYS:HG2	1:J:48:ASN:ND2	2.21	0.55
1:I:110:ASN:OD1	1:I:114:HIS:HB2	2.07	0.55
1:A:-3:ASP:OD1	1:G:1:HIS:CE1	2.60	0.55
1:C:80:THR:HG23	1:C:81:SER:O	2.07	0.55
4:A:301:MLK:H242	4:A:301:MLK:O27	2.07	0.54
1:D:56:GLU:O	1:D:119:PRO:HD2	2.07	0.54
1:H:145:GLY:HA2	1:H:156:LEU:HD11	1.90	0.54
1:C:61:LYS:HD2	1:C:114:HIS:NE2	2.22	0.54
1:J:61:LYS:HE2	1:J:112:SER:O	2.07	0.54
1:I:129:PRO:O	1:I:132:VAL:CG2	2.55	0.54
1:D:50:VAL:CG2	1:D:127:CYS:SG	2.96	0.54
1:D:39:ASP:OD2	1:E:126:MET:HG2	2.08	0.54
1:C:160:THR:CG2	1:C:162:GLN:HB2	2.38	0.54
1:B:55:TRP:CH2	4:C:301:MLK:H292	2.43	0.54
1:B:12:ASP:OD1	1:G:16:ARG:NH2	2.41	0.54
4:B:301:MLK:O27	4:B:301:MLK:H242	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:THR:CG2	1:B:162:GLN:H	2.21	0.54
1:G:122:ARG:HD2	1:H:96:THR:O	2.08	0.54
1:E:95:SER:HB3	1:E:123:LEU:HD11	1.89	0.54
7:E:275[B]:NAG:C7	7:E:275[B]:NAG:O3	2.56	0.54
1:D:145:GLY:HA2	1:D:156:LEU:HD11	1.89	0.54
1:F:21:PRO:HB2	1:J:6:LEU:HD23	1.90	0.54
1:F:6:LEU:HD23	1:G:21:PRO:HB2	1.89	0.53
1:D:17:SER:HB3	1:D:18:PRO:HD2	1.89	0.53
1:D:152:TRP:CD2	1:D:193:GLU:HG3	2.44	0.53
1:H:61:LYS:HD2	1:H:114:HIS:CE1	2.43	0.53
1:G:169:TYR:CZ	1:G:171:SER:HB2	2.42	0.53
1:A:122:ARG:HD2	1:B:96:THR:O	2.07	0.53
1:G:152:TRP:CZ3	1:G:193:GLU:HB2	2.43	0.53
1:A:77:ASP:HB3	1:A:110:ASN:HB3	1.90	0.53
1:E:160:THR:HG22	1:E:161:ASP:N	2.23	0.53
1:F:65:LEU:O	1:F:113:GLY:CA	2.52	0.53
1:J:183:ARG:HH12	1:J:185:GLU:HG2	1.73	0.53
5:B:305:MRD:H5C1	1:C:149:TYR:OH	2.08	0.53
1:B:39:ASP:HB2	1:C:126:MET:SD	2.49	0.53
1:D:37:LEU:HD12	1:D:38:LEU:N	2.23	0.53
1:B:-6:LYS:CG	1:B:-5:ASP:N	2.72	0.53
1:J:37:LEU:HD21	1:J:52:LEU:HD21	1.90	0.53
1:D:86:TRP:NE1	5:D:305:MRD:H3C2	2.24	0.53
1:C:78:PHE:O	1:C:108:LEU:HD12	2.08	0.53
1:I:173:LYS:HD2	1:J:46:SER:O	2.09	0.53
1:D:55:TRP:CZ3	4:E:301:MLK:H292	2.44	0.53
1:D:-6:LYS:HG2	1:D:-5:ASP:H	1.73	0.53
1:A:37:LEU:HD21	1:A:52:LEU:HD21	1.90	0.53
1:I:57:GLN:HG3	1:I:118:LEU:HD21	1.91	0.53
4:J:301:MLK:H292	4:J:301:MLK:H152	1.90	0.53
1:E:16:ARG:HD2	1:I:16:ARG:NE	2.19	0.53
1:H:118:LEU:CD2	1:H:118:LEU:O	2.52	0.53
4:H:301:MLK:H292	4:H:301:MLK:H152	1.90	0.53
1:F:160:THR:HG22	1:F:161:ASP:N	2.24	0.52
1:H:55:TRP:CH2	4:I:301:MLK:H292	2.45	0.52
1:B:161:ASP:OD1	1:B:162:GLN:NE2	2.42	0.52
3:G:251:NAG:O7	3:G:251:NAG:H3	2.09	0.52
1:A:145:GLY:HA2	1:A:156:LEU:HD11	1.92	0.52
1:G:37:LEU:HG	1:G:52:LEU:HD11	1.89	0.52
1:C:118:LEU:HG	1:C:118:LEU:O	2.09	0.52
1:I:3:GLN:O	1:I:7:MET:HG3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:11:SER:O	1:E:16:ARG:HG3	2.10	0.52
1:E:-6:LYS:HD2	1:E:-5:ASP:N	2.24	0.52
1:E:195:TYR:CE1	4:E:301:MLK:H331	2.44	0.52
4:E:301:MLK:O28	4:E:301:MLK:H31	2.09	0.52
1:J:89:ASP:O	1:J:146:SER:HA	2.10	0.52
1:A:152:TRP:CZ3	1:A:193:GLU:HB2	2.45	0.52
1:J:77:ASP:HB3	1:J:110:ASN:HB3	1.92	0.52
1:I:169:TYR:CZ	1:I:171:SER:HB2	2.44	0.52
1:C:184:SER:HB2	1:C:197:ASP:OD1	2.10	0.52
1:H:185:GLU:OE2	1:H:194:PRO:CB	2.58	0.52
1:D:50:VAL:HG21	1:D:127:CYS:SG	2.51	0.51
1:D:16:ARG:CD	1:J:16:ARG:CD	2.72	0.51
1:H:100:GLN:HB3	1:I:98:PRO:HG3	1.91	0.51
1:F:188:TYR:O	1:F:191:CYS:O	2.28	0.51
1:J:37:LEU:CD2	1:J:52:LEU:HD21	2.40	0.51
1:I:114:HIS:HB2	7:I:250:NAG:C1	2.40	0.51
1:I:171:SER:HB3	1:J:128:ASP:HB2	1.93	0.51
1:C:186[A]:ARG:HD2	4:C:301:MLK:C3	2.39	0.51
1:D:-6:LYS:HD2	1:D:-5:ASP:OD1	2.11	0.51
1:F:169:TYR:CZ	1:F:171:SER:HB2	2.46	0.51
1:B:-6:LYS:HG3	1:B:-5:ASP:N	2.13	0.51
1:G:79:ARG:HD3	1:G:108:LEU:CD1	2.40	0.51
1:F:147:TRP:O	4:F:301:MLK:H253	2.10	0.51
1:C:91:THR:HG22	1:C:92:ALA:O	2.11	0.51
1:C:186[B]:ARG:HH11	4:C:301:MLK:C4	2.24	0.51
5:B:305:MRD:O2	5:B:305:MRD:H5C2	2.11	0.51
1:A:152:TRP:CD2	1:A:193:GLU:HG3	2.46	0.51
1:A:55:TRP:CB	1:A:118[B]:LEU:HD21	2.39	0.51
1:J:183:ARG:NH1	1:J:185:GLU:HG2	2.26	0.51
1:F:10:LYS:HE2	1:F:80:THR:CG2	2.41	0.51
4:F:301:MLK:H35	4:F:301:MLK:H26	1.93	0.51
1:G:7:MET:HE2	1:H:21:PRO:HD3	1.93	0.51
1:J:183:ARG:NH1	1:J:185:GLU:CG	2.74	0.51
1:G:7:MET:CE	1:H:21:PRO:HD3	2.42	0.50
1:I:52:LEU:O	1:I:122:ARG:HA	2.11	0.50
1:C:6:LEU:HD23	1:D:21:PRO:HB2	1.93	0.50
1:A:117:TYR:C	1:A:118[A]:LEU:HD12	2.31	0.50
4:F:301:MLK:H371	1:J:116:GLN:HE21	1.68	0.50
1:J:186[A]:ARG:HD2	4:J:301:MLK:H3	1.92	0.50
1:D:61:LYS:HE2	1:D:112:SER:O	2.11	0.50
1:C:207:ARG:O	1:C:208:ARG:HD2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:301:MLK:H293	4:B:301:MLK:H152	1.92	0.50
1:E:103:SER:HB2	1:E:104:PRO:HD2	1.92	0.50
1:C:145:GLY:HA2	1:C:156:LEU:HD21	1.93	0.50
1:F:25:LYS:HG2	1:F:152:TRP:HB3	1.93	0.50
1:F:149:TYR:CE2	5:F:305:MRD:HMC3	2.46	0.50
1:C:61:LYS:HE3	1:C:112:SER:O	2.12	0.50
1:C:129:PRO:O	1:C:132:VAL:HB	2.11	0.50
4:F:301:MLK:C24	1:J:118:LEU:HD23	2.42	0.50
9:H:250:NAG:O7	9:H:250:NAG:H3	2.11	0.50
1:B:-1:LYS:O	1:B:2:SER:HB3	2.12	0.50
1:F:10:LYS:HE2	1:F:80:THR:HG22	1.94	0.50
1:B:-3:ASP:OD1	1:B:1:HIS:CD2	2.65	0.50
1:D:16:ARG:NE	1:J:16:ARG:HD3	2.23	0.49
1:B:152:TRP:CZ3	1:B:193:GLU:HB2	2.47	0.49
1:E:163:VAL:HG21	1:E:200:LEU:CD1	2.42	0.49
1:D:-6:LYS:HG2	1:D:-5:ASP:N	2.27	0.49
1:E:16:ARG:NH2	1:I:12:ASP:OD1	2.45	0.49
1:C:118:LEU:CD2	4:D:301:MLK:O27	2.61	0.49
1:C:-6:LYS:CG	1:C:-5:ASP:H	2.19	0.49
1:B:38:LEU:N	1:B:38:LEU:HD12	2.27	0.49
1:D:16:ARG:NE	1:J:16:ARG:HG2	2.27	0.49
1:H:197:ASP:OD2	4:H:301:MLK:H4	2.13	0.49
1:H:132:VAL:HG22	1:H:206:GLU:HG2	1.94	0.49
1:C:89:ASP:O	1:C:146:SER:HA	2.12	0.49
1:I:146:SER:OG	1:I:149:TYR:HB2	2.11	0.49
1:D:16:ARG:HG3	1:J:16:ARG:CZ	2.42	0.49
1:D:16:ARG:NE	1:J:16:ARG:CD	2.75	0.49
3:D:251:NAG:O7	3:D:251:NAG:O3	2.30	0.49
1:H:169:TYR:HB2	1:I:126:MET:HE1	1.94	0.49
1:F:129:PRO:O	1:F:132:VAL:HB	2.12	0.49
1:A:147:TRP:O	4:A:301:MLK:H253	2.12	0.49
1:G:89:ASP:O	1:G:146:SER:HA	2.13	0.49
1:G:79:ARG:HG3	1:H:149:TYR:CE1	2.47	0.49
1:J:50:VAL:HG23	1:J:127:CYS:HB3	1.95	0.49
1:F:195:TYR:CZ	4:F:301:MLK:H331	2.47	0.49
1:E:195:TYR:CZ	4:E:301:MLK:H331	2.48	0.49
4:H:301:MLK:O28	4:H:301:MLK:H31	2.12	0.49
1:G:195:TYR:CZ	4:G:301:MLK:H331	2.48	0.49
1:A:45:SER:HA	1:A:129:PRO:HG2	1.95	0.49
1:H:151:GLY:HA2	1:H:154:ILE:O	2.12	0.49
1:B:12:ASP:OD1	1:G:16:ARG:CZ	2.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:114:HIS:CB	3:E:250:NAG:H62	2.42	0.49
1:A:131:GLY:O	1:A:137:GLY:HA2	2.12	0.49
4:H:301:MLK:H26	4:H:301:MLK:H252	1.49	0.48
1:D:172:SER:O	1:D:207:ARG:HD3	2.13	0.48
4:I:301:MLK:H292	4:I:301:MLK:H152	1.95	0.48
1:C:156:LEU:HB2	1:C:196:PRO:HB2	1.94	0.48
1:B:190:CYS:SG	1:B:191:CYS:N	2.87	0.48
1:E:114:HIS:CG	3:E:250:NAG:C6	2.96	0.48
1:G:32:TYR:O	1:G:58:GLN:HA	2.14	0.48
1:A:48:ASN:ND2	1:E:171:SER:O	2.46	0.48
1:H:116:GLN:NE2	4:I:301:MLK:H373	2.26	0.48
4:D:301:MLK:H362	4:D:301:MLK:H252	1.96	0.48
1:F:56:GLU:O	1:F:119:PRO:HD2	2.13	0.48
1:J:112:SER:HG	1:J:114:HIS:HD1	1.60	0.48
1:F:145:GLY:HA2	1:F:156:LEU:HD11	1.96	0.48
1:D:19:MET:HG3	1:D:20:TYR:N	2.28	0.48
1:E:160:THR:HG23	1:E:161:ASP:H	1.78	0.48
1:I:7:MET:CE	1:J:21:PRO:HD3	2.44	0.48
1:D:190:CYS:SG	1:D:191:CYS:N	2.87	0.48
1:G:-6:LYS:CG	1:G:-5:ASP:H	2.17	0.47
1:B:44:ASP:OD2	1:B:46:SER:OG	2.29	0.47
1:H:20:TYR:CD2	1:H:21:PRO:HD2	2.50	0.47
1:B:169:TYR:OH	1:B:171:SER:HB2	2.14	0.47
1:G:102:LEU:HD12	1:G:121:GLN:C	2.34	0.47
1:E:92:ALA:HB2	1:E:144:PHE:CE1	2.49	0.47
1:H:195:TYR:CD1	4:H:301:MLK:H222	2.50	0.47
1:C:141:ALA:HA	1:C:200:LEU:O	2.14	0.47
4:B:301:MLK:H152	4:B:301:MLK:C29	2.45	0.47
1:B:160:THR:HG22	1:B:161:ASP:N	2.29	0.47
1:G:67:TRP:O	1:G:69:PRO:HD3	2.14	0.47
1:I:103:SER:HB3	1:I:120:ALA:HB3	1.97	0.47
4:C:301:MLK:O27	4:C:301:MLK:H242	2.15	0.47
1:B:-3:ASP:OD1	1:F:1:HIS:CE1	2.67	0.47
1:B:156:LEU:HB2	1:B:196:PRO:HB2	1.97	0.47
1:B:-4:ASP:O	1:B:0:LEU:HD13	2.14	0.47
1:I:29:LEU:HD12	1:I:30:THR:H	1.80	0.47
1:D:118:LEU:HD13	4:E:301:MLK:O27	2.14	0.47
1:H:169:TYR:CG	1:I:126:MET:HE3	2.49	0.47
1:A:143:LYS:HD3	4:A:301:MLK:C5	2.45	0.47
4:J:301:MLK:H362	4:J:301:MLK:H26	1.59	0.47
1:J:-6:LYS:HG3	1:J:-5:ASP:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:114:HIS:CG	9:H:250:NAG:H5	2.49	0.47
1:I:50:VAL:CG2	1:I:127:CYS:SG	3.03	0.47
1:G:197:ASP:OD2	4:G:301:MLK:H3	2.14	0.47
1:F:7:MET:HE1	1:G:18:PRO:HG2	1.96	0.47
1:F:-3:ASP:OD2	1:F:1:HIS:CD2	2.68	0.47
1:I:136:GLU:N	1:I:136:GLU:OE1	2.48	0.47
1:A:156:LEU:HA	1:A:156:LEU:HD23	1.65	0.47
1:A:132:VAL:O	1:A:206:GLU:HG3	2.15	0.47
7:I:275[A]:NAG:O7	7:I:275[A]:NAG:O3	2.30	0.46
1:B:89:ASP:O	1:B:146:SER:HA	2.15	0.46
1:C:103:SER:HB2	1:C:104:PRO:CD	2.45	0.46
1:J:183:ARG:HH12	1:J:185:GLU:CD	2.18	0.46
1:H:185:GLU:HG2	1:H:194:PRO:HB3	1.97	0.46
1:C:103:SER:HB2	1:C:104:PRO:HD2	1.97	0.46
1:G:187:PHE:CZ	1:G:194:PRO:HB3	2.50	0.46
1:G:-3:ASP:O	1:G:1:HIS:HD2	1.97	0.46
1:G:102:LEU:HD11	1:G:122:ARG:HB2	1.97	0.46
1:B:67:TRP:O	1:B:69:PRO:HD3	2.15	0.46
1:B:16:ARG:CB	1:G:16:ARG:HD2	2.44	0.46
4:C:301:MLK:H202	4:C:301:MLK:H223	1.50	0.46
1:G:76:THR:HB	3:G:250:NAG:H82	1.97	0.46
1:D:50:VAL:HG23	1:D:127:CYS:SG	2.56	0.46
4:C:301:MLK:H292	4:C:301:MLK:H152	1.96	0.46
1:G:156:LEU:HB2	1:G:196:PRO:HB2	1.98	0.46
1:G:79:ARG:HD3	1:G:108:LEU:HD12	1.97	0.46
4:F:301:MLK:H28	4:F:301:MLK:H152	1.79	0.46
1:A:118[B]:LEU:HD22	1:B:147:TRP:HZ2	1.80	0.46
1:E:160:THR:CG2	1:E:161:ASP:H	2.29	0.46
1:C:12:ASP:HA	1:C:16:ARG:HB3	1.98	0.46
4:H:301:MLK:H202	4:H:301:MLK:H223	1.49	0.46
1:A:190:CYS:HG	1:A:191:CYS:N	2.10	0.46
1:F:96:THR:O	1:J:122:ARG:HD2	2.16	0.46
1:D:37:LEU:HD13	1:D:52:LEU:CD2	2.46	0.46
1:F:10:LYS:CE	1:F:80:THR:HG22	2.46	0.45
1:C:173:LYS:HA	1:C:173:LYS:HD2	1.78	0.45
4:F:301:MLK:N23	4:F:301:MLK:O19	2.47	0.45
1:J:132:VAL:HG21	1:J:174:TYR:CE1	2.52	0.45
1:G:16:ARG:HB3	1:G:16:ARG:NH1	2.30	0.45
1:E:38:LEU:HD11	1:E:55:TRP:CD2	2.52	0.45
1:G:50:VAL:O	1:G:124:SER:HA	2.16	0.45
1:C:-1:LYS:O	1:C:2:SER:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:114:HIS:CG	3:D:250:NAG:H5	2.51	0.45
1:I:19:MET:HE3	1:I:20:TYR:O	2.16	0.45
1:G:-6:LYS:CG	1:G:-5:ASP:N	2.79	0.45
1:E:149:TYR:HB2	1:E:154:ILE:HD12	1.99	0.45
4:J:301:MLK:H152	4:J:301:MLK:C29	2.47	0.45
4:J:301:MLK:H362	4:J:301:MLK:H252	1.98	0.45
1:B:152:TRP:CE3	1:B:193:GLU:HB2	2.51	0.45
1:I:0:LEU:HA	1:I:0:LEU:HD12	1.88	0.45
1:H:116:GLN:HE22	4:I:301:MLK:C37	2.26	0.45
1:H:39:ASP:OD2	1:I:126:MET:HG2	2.16	0.45
1:A:76:THR:O	1:A:110:ASN:HB2	2.17	0.45
1:C:145:GLY:HA2	1:C:156:LEU:CD2	2.47	0.45
1:H:131:GLY:O	1:H:134:SER:HB3	2.16	0.45
1:E:76:THR:HB	3:E:250:NAG:H83	1.99	0.45
1:B:37:LEU:N	1:B:37:LEU:HD23	2.32	0.45
1:D:12:ASP:OD2	1:D:72:TYR:OH	2.29	0.44
4:F:301:MLK:H293	4:F:301:MLK:H17	1.74	0.44
1:D:86:TRP:HE1	5:D:305:MRD:H3C2	1.80	0.44
4:G:301:MLK:H26	4:G:301:MLK:H362	1.56	0.44
4:A:301:MLK:H202	4:A:301:MLK:H223	1.72	0.44
1:J:190:CYS:SG	1:J:191:CYS:N	2.90	0.44
1:F:160:THR:HG22	1:F:162:GLN:N	2.13	0.44
4:A:301:MLK:H293	4:A:301:MLK:H17	1.49	0.44
1:B:7:MET:CE	1:C:21:PRO:HD3	2.46	0.44
1:H:66:MET:HG2	1:H:112:SER:O	2.16	0.44
6:A:223:MPD:HM1	6:A:223:MPD:O4	2.16	0.44
1:H:12:ASP:CA	1:H:16:ARG:HD3	2.37	0.44
1:F:195:TYR:CE2	4:F:301:MLK:H222	2.50	0.44
1:I:188:TYR:CE2	4:I:301:MLK:H30	2.52	0.44
1:H:20:TYR:HA	1:H:21:PRO:HD3	1.87	0.44
1:F:30:THR:HG21	1:F:157:LYS:HG3	1.99	0.44
1:F:37:LEU:HA	1:F:37:LEU:HD12	1.52	0.44
1:H:173:LYS:HD2	1:H:173:LYS:HA	1.85	0.44
1:C:69:PRO:O	1:C:74:ASN:N	2.49	0.44
1:I:-5:ASP:CG	1:I:-4:ASP:H	2.21	0.44
1:E:114:HIS:CG	3:E:250:NAG:H62	2.53	0.44
1:A:7:MET:HE2	1:B:21:PRO:HD3	1.98	0.44
1:I:7:MET:HE1	1:J:21:PRO:HD3	1.99	0.44
1:E:163:VAL:HG21	1:E:200:LEU:HD11	1.99	0.44
1:F:37:LEU:HD11	1:F:52:LEU:HD11	1.98	0.44
1:H:152:TRP:CG	1:H:193:GLU:HG3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:68:ASP:OD2	1:D:70:ASN:HB2	2.17	0.44
1:C:110:ASN:C	1:C:110:ASN:OD1	2.54	0.44
1:A:12:ASP:OD2	1:A:72:TYR:OH	2.35	0.44
1:B:116:GLN:HG2	1:B:118:LEU:CD1	2.45	0.44
1:A:6:LEU:CD2	1:B:21:PRO:HB2	2.43	0.44
1:D:111:SER:OG	3:D:250:NAG:H82	2.17	0.44
1:G:152:TRP:CE3	1:G:193:GLU:HB2	2.53	0.44
1:C:156:LEU:HD12	1:C:156:LEU:HA	1.78	0.44
1:D:59:SER:HA	1:D:115:VAL:O	2.18	0.44
1:I:131:GLY:O	1:I:134:SER:HB3	2.18	0.44
4:F:301:MLK:H242	1:J:118:LEU:HD23	1.99	0.44
7:I:275[B]:NAG:H3	7:I:275[B]:NAG:C8	2.31	0.44
1:J:186[A]:ARG:HD2	4:J:301:MLK:C3	2.48	0.44
1:J:61:LYS:HB2	1:J:114:HIS:CD2	2.53	0.44
1:E:140:CYS:SG	1:E:204:PHE:HE2	2.41	0.44
1:E:143:LYS:HG3	1:E:143:LYS:HZ3	1.64	0.43
1:A:143:LYS:HD3	4:A:301:MLK:C4	2.47	0.43
1:G:-3:ASP:HA	1:G:0:LEU:HD12	1.99	0.43
1:A:152:TRP:HB2	1:A:193:GLU:OE2	2.18	0.43
1:J:156:LEU:HD23	1:J:197:ASP:HA	2.00	0.43
1:H:37:LEU:HD12	1:H:54:TYR:HB3	1.99	0.43
4:B:301:MLK:H26	4:B:301:MLK:H362	1.73	0.43
1:G:76:THR:HB	3:G:250:NAG:H81	1.98	0.43
7:E:275[B]:NAG:O7	7:E:275[B]:NAG:C3	2.62	0.43
1:I:151:GLY:HA2	1:I:154:ILE:O	2.17	0.43
1:H:160:THR:HG23	1:H:181:GLN:HE21	1.83	0.43
1:A:51:ASP:OD1	1:A:124:SER:HB2	2.18	0.43
1:F:195:TYR:CE2	4:F:301:MLK:H19	2.53	0.43
1:G:143:LYS:HD2	4:G:301:MLK:C5	2.47	0.43
1:D:11:SER:O	1:D:16:ARG:HD3	2.18	0.43
1:I:-3:ASP:OD1	1:I:1:HIS:NE2	2.51	0.43
1:E:1:HIS:HE1	1:H:-3:ASP:OD1	2.01	0.43
1:J:132:VAL:HG21	1:J:174:TYR:HE1	1.82	0.43
1:G:77:ASP:HB3	1:G:110:ASN:CB	2.48	0.43
1:A:11:SER:O	1:A:15:ASN:HB2	2.18	0.43
1:B:61:LYS:HA	1:B:113:GLY:O	2.18	0.43
4:B:301:MLK:H332	4:B:301:MLK:O19	2.19	0.43
1:E:169:TYR:CZ	1:E:171:SER:HB2	2.52	0.43
1:G:69:PRO:O	1:G:74:ASN:N	2.48	0.43
1:H:152:TRP:CD2	1:H:193:GLU:HG3	2.53	0.43
1:E:37:LEU:HA	1:E:37:LEU:HD12	1.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:188:TYR:OH	4:F:301:MLK:H293	2.18	0.43
1:E:160:THR:HG21	1:E:162:GLN:HB2	1.99	0.43
1:D:-6:LYS:CG	1:D:-5:ASP:N	2.82	0.43
1:H:169:TYR:HB2	1:I:126:MET:HE3	1.99	0.43
1:J:195:TYR:CE1	4:J:301:MLK:H331	2.54	0.43
7:B:275[B]:NAG:H61	1:C:25:LYS:NZ	2.34	0.43
1:E:16:ARG:CD	1:I:16:ARG:NE	2.55	0.43
1:F:160:THR:CG2	1:F:161:ASP:N	2.81	0.43
1:B:91:THR:HG22	1:B:92:ALA:N	2.33	0.43
1:E:151:GLY:HA2	1:E:154:ILE:O	2.19	0.43
4:H:301:MLK:C29	4:H:301:MLK:H152	2.49	0.43
1:E:143:LYS:HD2	4:E:301:MLK:C4	2.49	0.43
1:A:186:ARG:HH21	4:A:301:MLK:H4	1.83	0.43
1:J:-5:ASP:O	1:J:-2:ASP:HB2	2.18	0.43
7:C:250:NAG:O3	7:C:250:NAG:C8	2.67	0.43
1:D:11:SER:HB3	1:D:16:ARG:CZ	2.48	0.43
1:E:16:ARG:NE	1:I:16:ARG:NE	2.66	0.43
1:E:77:ASP:HB3	1:E:110:ASN:HB3	2.01	0.43
1:A:7:MET:CE	1:B:21:PRO:HD3	2.49	0.43
1:C:66:MET:O	6:C:306:MPD:H32	2.18	0.43
1:J:173:LYS:HB3	1:J:174:TYR:CD2	2.54	0.43
1:D:62:LEU:HB2	1:D:65:LEU:HD12	2.00	0.43
1:I:55:TRP:CH2	4:J:301:MLK:H292	2.54	0.43
1:A:41:VAL:HG11	1:B:49:GLU:OE2	2.19	0.43
4:E:301:MLK:H26	4:E:301:MLK:H362	1.73	0.42
1:G:128:ASP:OD1	1:G:128:ASP:C	2.57	0.42
1:A:50:VAL:O	1:A:124:SER:HA	2.19	0.42
1:F:50:VAL:HG21	1:F:127:CYS:SG	2.59	0.42
1:C:118:LEU:HD21	4:D:301:MLK:O27	2.18	0.42
1:A:104:PRO:HG2	1:B:89:ASP:HB2	2.00	0.42
4:A:301:MLK:C8	4:A:301:MLK:O13	2.67	0.42
1:B:28:PRO:HB3	1:B:152:TRP:O	2.18	0.42
1:E:129:PRO:O	1:E:132:VAL:HB	2.19	0.42
4:C:301:MLK:H31	4:C:301:MLK:O28	2.19	0.42
4:I:301:MLK:H362	4:I:301:MLK:H26	1.70	0.42
1:B:6:LEU:HD23	1:C:21:PRO:HB2	2.01	0.42
1:A:187:PHE:O	1:A:188:TYR:CD2	2.73	0.42
1:J:94:SER:O	1:J:126:MET:HG3	2.18	0.42
1:A:150:GLY:HA2	1:A:195:TYR:CD1	2.54	0.42
1:G:99:VAL:HG22	1:G:123:LEU:CD1	2.50	0.42
1:I:125:PHE:CD1	1:I:142:VAL:CG2	3.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:-5:ASP:OD1	1:J:-4:ASP:N	2.53	0.42
1:G:61:LYS:HG3	1:G:114:HIS:CE1	2.54	0.42
1:J:70:ASN:HA	1:J:70:ASN:HD22	1.70	0.42
1:D:-4:ASP:HB2	1:D:-1:LYS:HD2	2.01	0.42
1:I:33:LEU:O	1:I:158:THR:HG22	2.19	0.42
4:B:301:MLK:H202	4:B:301:MLK:H223	1.51	0.42
1:B:89:ASP:OD1	1:B:89:ASP:N	2.52	0.42
1:H:103:SER:HB2	1:H:104:PRO:CD	2.50	0.42
1:H:52:LEU:HD23	1:H:52:LEU:HA	1.76	0.42
1:G:89:ASP:O	1:G:89:ASP:OD1	2.36	0.42
1:G:33:LEU:HA	1:G:33:LEU:HD23	1.88	0.42
1:H:128:ASP:OD1	1:H:129:PRO:HD2	2.19	0.42
1:B:12:ASP:OD1	1:G:16:ARG:NE	2.52	0.42
7:I:275[A]:NAG:O3	7:I:275[A]:NAG:C7	2.68	0.42
4:G:301:MLK:H252	4:G:301:MLK:H26	1.75	0.42
1:E:63:ASN:HA	1:E:66:MET:HG3	2.01	0.42
1:J:99:VAL:H	1:J:99:VAL:HG23	1.54	0.42
1:E:161:ASP:HA	1:E:181:GLN:O	2.20	0.42
1:C:158:THR:HG21	1:C:160:THR:O	2.19	0.42
1:J:160:THR:HG23	1:J:161:ASP:N	2.34	0.42
1:D:61:LYS:HE3	1:D:114:HIS:CE1	2.55	0.42
1:F:7:MET:HE3	1:G:19:MET:O	2.20	0.42
1:I:9:LEU:HA	1:I:72:TYR:CE2	2.54	0.42
1:J:60:TRP:CD1	1:J:62:LEU:HD13	2.55	0.42
1:J:76:THR:HB	9:J:250:NAG:H81	2.01	0.42
1:I:29:LEU:HD12	1:I:30:THR:N	2.34	0.42
1:H:197:ASP:OD2	4:H:301:MLK:C4	2.68	0.42
1:G:-6:LYS:HA	1:G:-6:LYS:HD2	1.83	0.42
1:F:39:ASP:HB2	1:G:126:MET:SD	2.60	0.42
1:H:38:LEU:HB2	1:H:53:VAL:O	2.20	0.42
4:C:301:MLK:H293	4:C:301:MLK:H17	1.91	0.41
4:E:301:MLK:H152	4:E:301:MLK:H293	1.98	0.41
4:I:301:MLK:H293	4:I:301:MLK:H17	1.80	0.41
1:I:193:GLU:HA	1:I:194:PRO:HD3	1.81	0.41
1:J:60:TRP:HD1	1:J:62:LEU:HD13	1.85	0.41
1:B:114:HIS:CG	7:B:250:NAG:H5	2.55	0.41
1:A:68:ASP:HA	1:A:69:PRO:HD2	1.95	0.41
1:D:86:TRP:CD1	5:D:305:MRD:H3C2	2.55	0.41
1:J:183:ARG:HG2	1:J:184:SER:N	2.35	0.41
1:J:94:SER:OG	1:J:142:VAL:HG23	2.20	0.41
1:J:33:LEU:O	1:J:158:THR:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:LYS:HB3	1:C:47:THR:HG22	2.02	0.41
1:J:59:SER:HA	1:J:115:VAL:O	2.20	0.41
1:F:118:LEU:HD22	4:G:301:MLK:H242	2.02	0.41
1:C:79:ARG:HD3	1:D:149:TYR:CE1	2.55	0.41
1:I:204:PHE:CD2	1:I:204:PHE:N	2.89	0.41
1:D:165:LEU:HA	1:D:165:LEU:HD23	1.88	0.41
1:D:186:ARG:HG3	1:D:187:PHE:N	2.35	0.41
1:A:52:LEU:O	1:A:122:ARG:HA	2.21	0.41
1:C:3:GLN:NE2	1:D:27:ASP:OD2	2.46	0.41
1:B:101:VAL:HG23	1:B:101:VAL:O	2.19	0.41
4:F:301:MLK:O27	1:J:118:LEU:HD23	2.20	0.41
1:I:16:ARG:HA	1:I:16:ARG:HH11	1.86	0.41
1:D:55:TRP:CH2	4:E:301:MLK:H292	2.55	0.41
4:I:301:MLK:H252	4:I:301:MLK:H26	1.79	0.41
1:C:208:ARG:HD2	1:C:208:ARG:HA	1.61	0.41
1:D:146:SER:OG	1:D:149:TYR:HB2	2.20	0.41
1:G:173:LYS:HE3	1:H:45:SER:O	2.21	0.41
1:J:165:LEU:HD23	1:J:165:LEU:HA	1.82	0.41
1:I:63:ASN:HA	1:I:66:MET:HG3	2.01	0.41
1:C:16:ARG:CD	1:F:16:ARG:CD	2.84	0.41
1:J:193:GLU:HG2	1:J:194:PRO:HD2	2.02	0.41
1:B:39:ASP:OD1	1:B:172:SER:HB2	2.21	0.41
1:C:112:SER:HB2	1:C:114:HIS:ND1	2.36	0.41
1:H:185:GLU:OE2	1:H:194:PRO:HB2	2.20	0.41
1:F:-3:ASP:O	1:F:1:HIS:HD2	2.03	0.41
1:B:43:ALA:HB1	1:B:129:PRO:HB3	2.01	0.41
1:A:104:PRO:HD3	1:B:91:THR:OG1	2.21	0.41
1:G:37:LEU:HD13	1:G:163:VAL:HG11	2.03	0.41
1:C:141:ALA:HB2	1:C:201:VAL:HG22	2.01	0.41
1:B:128:ASP:HA	1:B:129:PRO:HD2	1.94	0.41
6:G:222:MPD:H11	6:G:222:MPD:H4	1.60	0.41
1:B:147:TRP:CE2	4:B:301:MLK:H241	2.56	0.41
1:A:178:SER:HG	1:A:203:LYS:HE3	1.86	0.41
1:A:43:ALA:HA	1:A:50:VAL:HG22	2.03	0.41
1:J:67:TRP:O	1:J:69:PRO:HD3	2.20	0.41
6:I:305:MPD:H4	6:I:305:MPD:H12	1.39	0.41
1:F:171:SER:HB3	1:G:128:ASP:HB2	2.03	0.41
1:D:-4:ASP:O	1:D:-1:LYS:HB2	2.21	0.41
1:H:103:SER:HB2	1:H:104:PRO:HD2	2.03	0.41
1:E:66:MET:HA	1:E:111:SER:O	2.21	0.41
1:J:132:VAL:CG2	1:J:205:ARG:HA	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:TRP:CE3	1:B:111:SER:HA	2.56	0.40
1:B:173:LYS:HB3	1:B:173:LYS:HE3	1.93	0.40
1:H:91:THR:HG22	1:H:92:ALA:O	2.21	0.40
1:C:195:TYR:CD1	4:C:301:MLK:H19	2.56	0.40
1:G:-3:ASP:OD2	1:G:1:HIS:CD2	2.74	0.40
1:J:169:TYR:CZ	1:J:171:SER:HB2	2.56	0.40
1:H:60:TRP:CZ2	1:H:115:VAL:HG11	2.56	0.40
1:J:77:ASP:HB3	1:J:110:ASN:CB	2.51	0.40
1:E:96:THR:C	1:E:97[B]:ARG:HG2	2.41	0.40
1:H:125:PHE:CD1	1:H:142:VAL:HB	2.56	0.40
1:C:110:ASN:CG	7:C:250:NAG:C1	2.70	0.40
1:E:-6:LYS:HD3	1:E:-6:LYS:HA	1.83	0.40
4:J:301:MLK:H26	4:J:301:MLK:H252	1.65	0.40
1:J:-6:LYS:HG3	1:J:-5:ASP:H	1.85	0.40
1:D:37:LEU:O	1:D:168:TYR:HD1	2.05	0.40
1:G:6:LEU:HD23	1:H:21:PRO:HB2	2.03	0.40
1:D:96:THR:O	1:D:97[B]:ARG:HG2	2.22	0.40
1:B:118:LEU:HD22	4:C:301:MLK:O27	2.22	0.40
1:E:186:ARG:HD3	4:E:301:MLK:C4	2.52	0.40
1:E:186:ARG:HD3	4:E:301:MLK:C3	2.52	0.40
1:A:186:ARG:HD3	1:A:186:ARG:HA	1.82	0.40
1:E:50:VAL:O	1:E:124:SER:HA	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	214/230 (93%)	208 (97%)	5 (2%)	1 (0%)	34	71
1	B	216/230 (94%)	215 (100%)	1 (0%)	0	100	100
1	C	219/230 (95%)	216 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	215/230 (94%)	212 (99%)	3 (1%)	0	100	100
1	E	215/230 (94%)	208 (97%)	7 (3%)	0	100	100
1	F	214/230 (93%)	212 (99%)	2 (1%)	0	100	100
1	G	212/230 (92%)	208 (98%)	4 (2%)	0	100	100
1	H	215/230 (94%)	213 (99%)	2 (1%)	0	100	100
1	I	214/230 (93%)	211 (99%)	3 (1%)	0	100	100
1	J	217/230 (94%)	215 (99%)	2 (1%)	0	100	100
All	All	2151/2300 (94%)	2118 (98%)	32 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	119	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	197/208 (95%)	190 (96%)	7 (4%)	42	78
1	B	199/208 (96%)	195 (98%)	4 (2%)	63	88
1	C	201/208 (97%)	192 (96%)	9 (4%)	34	70
1	D	198/208 (95%)	193 (98%)	5 (2%)	55	85
1	E	199/208 (96%)	192 (96%)	7 (4%)	43	78
1	F	197/208 (95%)	194 (98%)	3 (2%)	72	92
1	G	195/208 (94%)	192 (98%)	3 (2%)	72	92
1	H	198/208 (95%)	192 (97%)	6 (3%)	48	83
1	I	197/208 (95%)	188 (95%)	9 (5%)	33	69
1	J	200/208 (96%)	194 (97%)	6 (3%)	48	83
All	All	1981/2080 (95%)	1922 (97%)	59 (3%)	48	83

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-5	ASP
1	A	26	ASP
1	A	45	SER
1	A	127	CYS
1	A	134	SER
1	A	173	LYS
1	A	192	LYS
1	B	76	THR
1	B	127	CYS
1	B	190	CYS
1	B	192	LYS
1	C	36	SER
1	C	80	THR
1	C	127	CYS
1	C	142	VAL
1	C	156	LEU
1	C	182	THR
1	C	189	GLU
1	C	190	CYS
1	C	191	CYS
1	D	74	ASN
1	D	118	LEU
1	D	190	CYS
1	D	191	CYS
1	D	192	LYS
1	E	37	LEU
1	E	38	LEU
1	E	41	VAL
1	E	59	SER
1	E	64	SER
1	E	127	CYS
1	E	191	CYS
1	F	-5	ASP
1	F	59	SER
1	F	94	SER
1	G	64	SER
1	G	80	THR
1	G	188	TYR
1	H	-2	ASP
1	H	36	SER
1	H	130	THR
1	H	140	CYS

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Mol	Chain	Res	Type
1	H	161	ASP
1	H	190	CYS
1	I	45	SER
1	I	64	SER
1	I	116	GLN
1	I	118	LEU
1	I	158	THR
1	I	178	SER
1	I	189	GLU
1	I	190	CYS
1	I	191	CYS
1	J	24	THR
1	J	46	SER
1	J	52	LEU
1	J	64	SER
1	J	160	THR
1	J	191	CYS

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

Mol	Chain	Res	Type
1	C	70	ASN
1	C	100	GLN
1	C	110	ASN
1	D	162	GLN
1	E	3	GLN
1	E	57	GLN
1	G	116	GLN
1	H	116	GLN
1	I	116	GLN
1	J	70	ASN
1	J	110	ASN
1	J	116	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 ⓘ

14 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$
3	NAG	A	250	1,3	14,14,15	1.29	1 (7%)	15,19,21	0.75	0
3	NAG	A	251	3	14,14,15	1.29	1 (7%)	15,19,21	0.75	0
3	NAG	D	250	1,3	14,14,15	0.54	0	15,19,21	1.69	1 (6%)
3	NAG	D	251	3	14,14,15	0.96	0	15,19,21	1.59	4 (26%)
3	NAG	E	250	1,3	14,14,15	0.58	0	15,19,21	1.43	1 (6%)
3	NAG	E	251	3	14,14,15	0.64	0	15,19,21	1.31	1 (6%)
3	NAG	G	250	1,3	14,14,15	0.74	0	15,19,21	0.88	1 (6%)
3	NAG	G	251	3	14,14,15	0.54	0	15,19,21	1.01	1 (6%)
9	NAG	H	250	1,9	14,14,15	0.64	0	15,19,21	1.57	4 (26%)
9	NAG	H	251	9	14,14,15	0.59	0	15,19,21	1.03	0
9	BMA	H	252	9	11,11,12	0.44	0	14,15,17	1.08	0
9	NAG	J	250	1,9	14,14,15	0.86	1 (7%)	15,19,21	1.05	1 (6%)
9	NAG	J	251	9	14,14,15	0.45	0	15,19,21	0.93	1 (6%)
9	BMA	J	252	9	11,11,12	0.51	0	14,15,17	0.84	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	250	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	251	3	-	0/6/23/26	0/1/1/1
3	NAG	D	250	1,3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	D	251	3	-	0/6/23/26	0/1/1/1
3	NAG	E	250	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	251	3	-	0/6/23/26	0/1/1/1
3	NAG	G	250	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	251	3	-	0/6/23/26	0/1/1/1
9	NAG	H	250	1,9	-	0/6/23/26	0/1/1/1
9	NAG	H	251	9	-	0/6/23/26	0/1/1/1
9	BMA	H	252	9	-	0/2/19/22	0/1/1/1
9	NAG	J	250	1,9	-	0/6/23/26	0/1/1/1
9	NAG	J	251	9	-	0/6/23/26	0/1/1/1
9	BMA	J	252	9	-	0/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	J	250	NAG	O5-C1	-2.19	1.40	1.43
3	A	251	NAG	O7-C7	4.43	1.33	1.23
3	A	250	NAG	O7-C7	4.45	1.33	1.23

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	H	250	NAG	C1-O5-C5	-3.11	108.30	112.25
3	D	251	NAG	C4-C3-C2	-2.39	107.51	111.23
3	D	251	NAG	C6-C5-C4	-2.38	107.14	113.02
3	D	251	NAG	C3-C4-C5	-2.25	106.28	110.20
9	J	250	NAG	C2-N2-C7	-2.21	120.20	123.04
3	D	251	NAG	C3-C2-N2	-2.21	105.27	110.56
9	H	250	NAG	O7-C7-C8	-2.05	118.31	122.06
9	H	250	NAG	C3-C4-C5	2.05	113.77	110.20
9	J	251	NAG	O5-C5-C6	2.07	111.82	107.35
3	G	251	NAG	C2-N2-C7	2.07	125.70	123.04
3	G	250	NAG	C1-O5-C5	2.63	115.59	112.25
9	H	250	NAG	C2-N2-C7	2.95	126.83	123.04
3	E	251	NAG	C2-N2-C7	3.31	127.29	123.04
3	E	250	NAG	C1-O5-C5	4.50	117.96	112.25
3	D	250	NAG	C1-O5-C5	5.14	118.77	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	250	NAG	3	0
3	A	251	NAG	3	0
3	D	250	NAG	3	0
3	D	251	NAG	3	0
3	E	250	NAG	4	0
3	E	251	NAG	1	0
3	G	250	NAG	3	0
3	G	251	NAG	1	0
9	H	250	NAG	2	0
9	H	252	BMA	1	0
9	J	250	NAG	9	0
9	J	251	NAG	2	0

5.6 Ligand geometry [i](#)

Of 38 ligands modelled in this entry, 5 are monoatomic - leaving 33 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	MPD	A	223	-	6,7,7	0.35	0	7,10,10	1.03	1 (14%)
4	MLK	A	301	-	55,56,56	1.06	4 (7%)	74,92,92	1.87	15 (20%)
5	MRD	A	305	-	6,7,7	0.32	0	7,10,10	0.63	0
6	MPD	A	306	-	6,7,7	0.42	0	7,10,10	0.31	0
7	NAG	B	250	1	14,14,15	0.64	0	15,19,21	1.07	0
7	NAG	B	275[A]	1	14,14,15	0.59	0	15,19,21	0.97	0
7	NAG	B	275[B]	1	14,14,15	0.52	0	15,19,21	1.72	1 (6%)
4	MLK	B	301	-	55,56,56	1.06	4 (7%)	74,92,92	1.76	16 (21%)
5	MRD	B	305	-	6,7,7	0.53	0	7,10,10	0.43	0
7	NAG	C	250	1	14,14,15	1.15	1 (7%)	15,19,21	1.91	2 (13%)
4	MLK	C	301	-	55,56,56	1.13	3 (5%)	74,92,92	1.77	18 (24%)
6	MPD	C	306	-	6,7,7	0.47	0	7,10,10	0.24	0
4	MLK	D	301	-	55,56,56	1.12	5 (9%)	74,92,92	1.66	13 (17%)
5	MRD	D	305	-	6,7,7	0.38	0	7,10,10	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	E	275[A]	1	14,14,15	1.28	1 (7%)	15,19,21	1.08	1 (6%)
7	NAG	E	275[B]	1	14,14,15	0.48	0	15,19,21	1.47	1 (6%)
4	MLK	E	301	-	55,56,56	0.99	4 (7%)	74,92,92	2.14	21 (28%)
5	MRD	E	305	-	6,7,7	0.40	0	7,10,10	0.54	0
7	NAG	F	250	1	14,14,15	0.50	0	15,19,21	1.01	1 (6%)
4	MLK	F	301	-	55,56,56	1.12	3 (5%)	74,92,92	1.72	15 (20%)
5	MRD	F	305	-	6,7,7	0.30	0	7,10,10	0.56	0
6	MPD	G	222	-	6,7,7	0.25	0	7,10,10	0.47	0
4	MLK	G	301	-	55,56,56	1.03	3 (5%)	74,92,92	1.73	18 (24%)
6	MPD	G	305	-	6,7,7	0.51	0	7,10,10	0.39	0
8	ACT	G	308	-	1,3,3	3.69	1 (100%)	0,3,3	0.00	-
4	MLK	H	301	-	55,56,56	1.02	3 (5%)	74,92,92	2.02	20 (27%)
7	NAG	I	250	1	14,14,15	0.60	0	15,19,21	1.27	2 (13%)
7	NAG	I	275[A]	1	14,14,15	1.28	1 (7%)	15,19,21	1.03	1 (6%)
7	NAG	I	275[B]	1	14,14,15	0.69	0	15,19,21	1.61	2 (13%)
4	MLK	I	301	-	55,56,56	1.12	4 (7%)	74,92,92	1.57	16 (21%)
6	MPD	I	305	-	6,7,7	0.44	0	7,10,10	0.99	0
4	MLK	J	301	-	55,56,56	1.07	4 (7%)	74,92,92	1.77	13 (17%)
6	MPD	J	305	-	6,7,7	0.41	0	7,10,10	0.74	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MPD	A	223	-	-	0/5/5/5	0/0/0/0
4	MLK	A	301	-	-	0/24/141/141	0/2/8/8
5	MRD	A	305	-	-	0/5/5/5	0/0/0/0
6	MPD	A	306	-	-	0/5/5/5	0/0/0/0
7	NAG	B	250	1	-	0/6/23/26	0/1/1/1
7	NAG	B	275[A]	1	-	0/6/23/26	0/1/1/1
7	NAG	B	275[B]	1	-	0/6/23/26	0/1/1/1
4	MLK	B	301	-	-	0/24/141/141	0/2/8/8
5	MRD	B	305	-	-	0/5/5/5	0/0/0/0
7	NAG	C	250	1	-	0/6/23/26	0/1/1/1
4	MLK	C	301	-	-	0/24/141/141	0/2/8/8
6	MPD	C	306	-	-	0/5/5/5	0/0/0/0
4	MLK	D	301	-	-	0/24/141/141	0/2/8/8
5	MRD	D	305	-	-	0/5/5/5	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	E	275[A]	1	-	0/6/23/26	0/1/1/1
7	NAG	E	275[B]	1	-	0/6/23/26	0/1/1/1
4	MLK	E	301	-	-	0/24/141/141	0/2/8/8
5	MRD	E	305	-	-	0/5/5/5	0/0/0/0
7	NAG	F	250	1	-	0/6/23/26	0/1/1/1
4	MLK	F	301	-	-	0/24/141/141	0/2/8/8
5	MRD	F	305	-	-	0/5/5/5	0/0/0/0
6	MPD	G	222	-	-	0/5/5/5	0/0/0/0
4	MLK	G	301	-	-	0/24/141/141	0/2/8/8
6	MPD	G	305	-	-	0/5/5/5	0/0/0/0
8	ACT	G	308	-	-	0/0/0/0	0/0/0/0
4	MLK	H	301	-	-	0/24/141/141	0/2/8/8
7	NAG	I	250	1	-	0/6/23/26	0/1/1/1
7	NAG	I	275[A]	1	-	0/6/23/26	0/1/1/1
7	NAG	I	275[B]	1	1/1/5/7	0/6/23/26	0/1/1/1
4	MLK	I	301	-	-	0/24/141/141	0/2/8/8
6	MPD	I	305	-	-	0/5/5/5	0/0/0/0
4	MLK	J	301	-	-	0/24/141/141	0/2/8/8
6	MPD	J	305	-	-	0/5/5/5	0/0/0/0

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	301	MLK	C8-N7	-4.64	1.34	1.40
4	C	301	MLK	C8-N7	-4.40	1.34	1.40
4	D	301	MLK	C8-N7	-4.28	1.34	1.40
4	F	301	MLK	C8-N7	-4.17	1.34	1.40
4	B	301	MLK	C8-N7	-4.04	1.35	1.40
4	J	301	MLK	C8-N7	-4.02	1.35	1.40
4	G	301	MLK	C8-N7	-3.72	1.35	1.40
4	A	301	MLK	C8-N7	-3.67	1.35	1.40
4	E	301	MLK	C8-N7	-3.61	1.35	1.40
4	D	301	MLK	C11-N7	-3.46	1.34	1.39
4	H	301	MLK	C8-N7	-3.45	1.35	1.40
4	F	301	MLK	C11-N7	-3.45	1.34	1.39
4	C	301	MLK	C11-N7	-3.37	1.35	1.39
4	A	301	MLK	C11-N7	-3.30	1.35	1.39
4	J	301	MLK	C11-N7	-3.01	1.35	1.39
4	I	301	MLK	C11-N7	-2.98	1.35	1.39
4	F	301	MLK	C18-C19	-2.79	1.50	1.55
4	H	301	MLK	C11-N7	-2.69	1.36	1.39
4	A	301	MLK	C18-C19	-2.65	1.51	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	301	MLK	C11-N7	-2.49	1.36	1.39
4	D	301	MLK	C6-N7	-2.45	1.41	1.44
4	B	301	MLK	C11-N7	-2.34	1.36	1.39
4	J	301	MLK	C6-N7	-2.34	1.41	1.44
4	G	301	MLK	C18-C19	-2.31	1.51	1.55
4	A	301	MLK	C18-C30	-2.25	1.52	1.56
4	C	301	MLK	C6-N7	-2.18	1.41	1.44
4	D	301	MLK	C18-C19	-2.17	1.51	1.55
4	B	301	MLK	C18-C30	-2.16	1.52	1.56
4	I	301	MLK	C18-C30	-2.14	1.52	1.56
4	D	301	MLK	C18-C30	-2.13	1.52	1.56
4	E	301	MLK	C11-N7	-2.10	1.36	1.39
4	H	301	MLK	C26-N23	-2.08	1.43	1.47
4	E	301	MLK	C18-C19	-2.07	1.52	1.55
4	I	301	MLK	C6-N7	-2.06	1.41	1.44
4	B	301	MLK	C18-C19	-2.05	1.52	1.55
4	J	301	MLK	C18-C30	-2.05	1.52	1.56
4	E	301	MLK	C1-C6	2.40	1.45	1.41
8	G	308	ACT	CH3-C	3.69	1.53	1.48
7	C	250	NAG	C1-C2	3.84	1.57	1.52
7	E	275[A]	NAG	O7-C7	4.43	1.33	1.23
7	I	275[A]	NAG	O7-C7	4.44	1.33	1.23

All (177) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	301	MLK	C9-C10-C11	-7.89	98.16	103.89
4	E	301	MLK	C9-C10-C11	-6.85	98.92	103.89
4	F	301	MLK	C33-C34-C35	-5.44	102.39	112.03
4	F	301	MLK	C16-C17-C28	-5.22	101.81	112.70
4	H	301	MLK	C16-C17-C28	-5.16	101.94	112.70
4	D	301	MLK	C16-C17-C28	-4.93	102.43	112.70
4	C	301	MLK	C16-C17-C28	-4.66	102.99	112.70
4	B	301	MLK	C16-C17-C28	-4.66	102.99	112.70
4	A	301	MLK	C16-C17-C28	-4.52	103.28	112.70
4	C	301	MLK	C33-C34-C35	-4.50	104.05	112.03
7	I	275[B]	NAG	C1-O5-C5	-4.48	106.56	112.25
4	I	301	MLK	C16-C17-C28	-4.43	103.46	112.70
4	E	301	MLK	C16-C17-C28	-4.42	103.48	112.70
4	D	301	MLK	C9-C10-C11	-4.19	100.84	103.89
4	F	301	MLK	C37-O35-C35	-4.09	102.97	114.09
4	J	301	MLK	C16-C17-C28	-3.95	104.47	112.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	301	MLK	C16-C17-C28	-3.94	104.49	112.70
4	H	301	MLK	C33-C34-C35	-3.85	105.20	112.03
4	A	301	MLK	C29-O28-C28	-3.77	107.17	114.39
4	B	301	MLK	C29-O28-C28	-3.73	107.26	114.39
4	I	301	MLK	C38-C34-C35	-3.69	106.86	111.86
4	D	301	MLK	C33-C34-C35	-3.69	105.49	112.03
4	E	301	MLK	C38-C34-C35	-3.65	106.91	111.86
4	J	301	MLK	C38-C34-C35	-3.65	106.92	111.86
4	B	301	MLK	C11-N7-C8	-3.60	109.43	112.46
4	H	301	MLK	C29-O28-C28	-3.55	107.60	114.39
4	J	301	MLK	C37-O35-C35	-3.54	104.47	114.09
4	G	301	MLK	C33-C34-C35	-3.50	105.82	112.03
4	J	301	MLK	C33-C34-C35	-3.46	105.89	112.03
4	J	301	MLK	C29-O28-C28	-3.43	107.83	114.39
4	J	301	MLK	C9-C10-C11	-3.35	101.46	103.89
4	I	301	MLK	C33-C34-C35	-3.34	106.11	112.03
4	E	301	MLK	C33-C34-C35	-3.33	106.13	112.03
4	A	301	MLK	C33-C34-C35	-3.27	106.23	112.03
4	I	301	MLK	C21-C16-C23	-3.22	108.20	111.47
4	G	301	MLK	C37-O35-C35	-3.19	105.43	114.09
4	G	301	MLK	C38-C34-C35	-3.18	107.56	111.86
4	D	301	MLK	C37-O35-C35	-3.17	105.48	114.09
4	A	301	MLK	C39-O38-C38	-3.05	105.97	114.59
4	B	301	MLK	C18-C30-C31	-3.05	113.58	117.24
4	G	301	MLK	C39-O38-C38	-3.03	106.03	114.59
4	J	301	MLK	C39-O38-C38	-3.02	106.07	114.59
4	E	301	MLK	C29-O28-C28	-3.00	108.64	114.39
4	G	301	MLK	C29-O28-C28	-3.00	108.65	114.39
4	H	301	MLK	C15-C16-C17	-2.99	107.22	112.25
4	E	301	MLK	C39-O38-C38	-2.88	106.46	114.59
4	A	301	MLK	C38-C34-C35	-2.83	108.03	111.86
4	H	301	MLK	C22-O19-C19	-2.82	105.44	113.63
4	E	301	MLK	C10-C11-N7	-2.82	106.50	108.06
4	D	301	MLK	C29-O28-C28	-2.82	109.00	114.39
4	C	301	MLK	C29-O28-C28	-2.80	109.03	114.39
4	I	301	MLK	C9-C10-C11	-2.80	101.86	103.89
4	E	301	MLK	O14-C13-O13	-2.80	118.52	123.66
4	C	301	MLK	C9-C10-C11	-2.79	101.86	103.89
4	F	301	MLK	C29-O28-C28	-2.78	109.08	114.39
4	J	301	MLK	C18-C30-C31	-2.77	113.92	117.24
4	C	301	MLK	C18-C17-C16	-2.76	106.61	108.70
4	C	301	MLK	C39-O38-C38	-2.75	106.82	114.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	301	MLK	C39-O38-C38	-2.75	106.82	114.59
4	B	301	MLK	C18-C17-C16	-2.71	106.65	108.70
7	I	250	NAG	C2-N2-C7	-2.70	119.56	123.04
4	H	301	MLK	C37-O35-C35	-2.70	106.75	114.09
4	A	301	MLK	C37-O35-C35	-2.69	106.80	114.09
4	A	301	MLK	O14-C13-O13	-2.68	118.74	123.66
4	I	301	MLK	C29-O28-C28	-2.67	109.29	114.39
4	A	301	MLK	C21-C16-C23	-2.63	108.79	111.47
4	E	301	MLK	C18-C30-C31	-2.60	114.12	117.24
4	A	301	MLK	C22-O19-C19	-2.60	106.08	113.63
4	E	301	MLK	C37-O35-C35	-2.59	107.05	114.09
4	B	301	MLK	C39-O38-C38	-2.58	107.30	114.59
4	D	301	MLK	C39-O38-C38	-2.55	107.38	114.59
4	B	301	MLK	C33-C34-C35	-2.54	107.53	112.03
4	I	301	MLK	C18-C17-C16	-2.51	106.80	108.70
4	G	301	MLK	C18-C30-C31	-2.51	114.23	117.24
4	H	301	MLK	C21-C16-C23	-2.50	108.93	111.47
6	A	223	MPD	C2-C3-C4	-2.49	104.90	116.66
4	I	301	MLK	C37-O35-C35	-2.46	107.41	114.09
4	G	301	MLK	O8-C8-C9	-2.45	124.12	127.41
4	C	301	MLK	C22-O19-C19	-2.45	106.53	113.63
4	F	301	MLK	O14-C13-O13	-2.43	119.19	123.66
4	H	301	MLK	C18-C30-C31	-2.41	114.36	117.24
4	F	301	MLK	C18-C17-C16	-2.40	106.89	108.70
4	D	301	MLK	C38-C34-C35	-2.38	108.64	111.86
4	B	301	MLK	C37-O35-C35	-2.38	107.64	114.09
4	B	301	MLK	C38-C34-C35	-2.37	108.66	111.86
4	C	301	MLK	O14-C13-O13	-2.35	119.34	123.66
4	E	301	MLK	C19-C18-C26	-2.35	112.21	116.62
4	E	301	MLK	C11-N7-C8	-2.34	110.49	112.46
4	C	301	MLK	C37-O35-C35	-2.33	107.75	114.09
4	H	301	MLK	O8-C8-C9	-2.28	124.35	127.41
4	H	301	MLK	C2-C1-C13	-2.21	114.14	118.68
7	C	250	NAG	O7-C7-C8	-2.20	118.03	122.06
7	E	275[A]	NAG	C4-C3-C2	-2.19	107.82	111.23
4	F	301	MLK	C39-O38-C38	-2.18	108.43	114.59
7	I	275[A]	NAG	C4-C3-C2	-2.17	107.85	111.23
4	A	301	MLK	C15-C16-C17	-2.17	108.61	112.25
4	D	301	MLK	C18-C30-C31	-2.15	114.66	117.24
4	J	301	MLK	O14-C13-O13	-2.14	119.72	123.66
7	I	275[B]	NAG	C3-C4-C5	-2.12	106.49	110.20
4	E	301	MLK	C22-O19-C19	-2.11	107.50	113.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	301	MLK	C22-O19-C19	-2.09	107.58	113.63
4	G	301	MLK	O11-C11-C10	-2.07	122.95	126.70
4	E	301	MLK	C2-C1-C13	-2.07	114.42	118.68
4	I	301	MLK	C39-O38-C38	-2.04	108.84	114.59
4	C	301	MLK	C38-C34-C35	-2.03	109.11	111.86
4	F	301	MLK	C18-C30-C31	-2.03	114.80	117.24
4	I	301	MLK	C18-C30-C31	-2.01	114.83	117.24
4	C	301	MLK	O8-C8-N7	2.00	125.86	123.94
4	B	301	MLK	C18-C17-C28	2.01	105.73	102.98
4	C	301	MLK	O14-C15-C16	2.01	110.75	108.31
4	A	301	MLK	C15-O14-C13	2.03	121.03	116.64
4	C	301	MLK	C18-C17-C28	2.09	105.84	102.98
4	I	301	MLK	C10-C11-N7	2.09	109.21	108.06
4	B	301	MLK	C23-C16-C17	2.10	110.15	108.22
4	F	301	MLK	C18-C17-C28	2.11	105.88	102.98
4	I	301	MLK	C1-C6-N7	2.16	122.92	121.07
4	E	301	MLK	C21-C20-C19	2.16	115.14	110.65
4	G	301	MLK	C23-C16-C17	2.20	110.25	108.22
4	H	301	MLK	C18-C17-C28	2.22	106.03	102.98
4	D	301	MLK	C23-N23-C24	2.23	114.14	111.19
4	D	301	MLK	O14-C15-C16	2.24	111.04	108.31
4	F	301	MLK	C23-C16-C17	2.29	110.33	108.22
4	I	301	MLK	O11-C11-N7	2.33	126.72	124.33
4	C	301	MLK	C23-C16-C17	2.35	110.38	108.22
4	H	301	MLK	C23-N23-C24	2.35	114.31	111.19
4	H	301	MLK	O19-C19-C18	2.36	113.48	108.46
4	E	301	MLK	C21-C16-C23	2.40	113.91	111.47
4	J	301	MLK	C23-N23-C24	2.41	114.38	111.19
4	G	301	MLK	C6-N7-C11	2.48	126.67	123.19
4	D	301	MLK	O8-C8-N7	2.48	126.32	123.94
4	G	301	MLK	C9-C8-N7	2.52	110.11	108.07
4	F	301	MLK	O35-C35-C34	2.55	115.64	108.80
4	F	301	MLK	O8-C8-N7	2.62	126.45	123.94
4	G	301	MLK	C15-O14-C13	2.63	122.33	116.64
4	I	301	MLK	C15-O14-C13	2.67	122.42	116.64
4	C	301	MLK	O11-C11-N7	2.72	127.12	124.33
4	H	301	MLK	O14-C13-C1	2.73	117.13	112.16
4	A	301	MLK	O8-C8-N7	2.76	126.59	123.94
4	G	301	MLK	O14-C13-C1	2.79	117.24	112.16
7	F	250	NAG	C1-O5-C5	2.80	115.80	112.25
4	F	301	MLK	C10-C11-N7	2.80	109.60	108.06
4	I	301	MLK	C23-C16-C17	2.80	110.80	108.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	301	MLK	C6-N7-C11	2.81	127.14	123.19
4	H	301	MLK	C15-O14-C13	2.83	122.76	116.64
4	G	301	MLK	C10-C11-N7	2.91	109.66	108.06
4	H	301	MLK	C21-C16-C17	2.91	113.78	110.05
4	C	301	MLK	O19-C19-C18	2.94	114.72	108.46
4	G	301	MLK	O11-C11-N7	2.95	127.36	124.33
4	E	301	MLK	O14-C15-C16	2.97	111.92	108.31
4	I	301	MLK	O14-C13-C1	3.15	117.89	112.16
4	B	301	MLK	C6-N7-C11	3.29	127.81	123.19
4	B	301	MLK	C1-C6-N7	3.34	123.94	121.07
7	I	250	NAG	C1-O5-C5	3.36	116.52	112.25
4	C	301	MLK	O14-C13-C1	3.40	118.36	112.16
4	B	301	MLK	O8-C8-N7	3.44	127.25	123.94
4	H	301	MLK	O11-C11-N7	3.52	127.95	124.33
4	J	301	MLK	O11-C11-N7	3.53	127.95	124.33
4	F	301	MLK	O14-C13-C1	3.76	119.01	112.16
4	D	301	MLK	O14-C13-C1	3.85	119.17	112.16
4	B	301	MLK	O11-C11-N7	3.93	128.37	124.33
4	B	301	MLK	O14-C13-C1	4.00	119.44	112.16
4	A	301	MLK	C23-C16-C17	4.07	111.97	108.22
4	J	301	MLK	O14-C13-C1	4.12	119.66	112.16
4	D	301	MLK	C1-C6-N7	4.25	124.73	121.07
4	H	301	MLK	O8-C8-N7	4.37	128.14	123.94
4	A	301	MLK	O14-C13-C1	4.41	120.18	112.16
7	E	275[B]	NAG	C1-O5-C5	4.58	118.06	112.25
4	G	301	MLK	C1-C6-N7	4.58	125.01	121.07
4	E	301	MLK	O14-C13-C1	4.65	120.62	112.16
4	E	301	MLK	O11-C11-N7	4.72	129.17	124.33
4	F	301	MLK	C1-C6-N7	4.84	125.23	121.07
4	J	301	MLK	C1-C6-N7	4.90	125.28	121.07
7	C	250	NAG	C1-O5-C5	5.83	119.64	112.25
7	B	275[B]	NAG	C1-O5-C5	6.01	119.88	112.25
4	C	301	MLK	C1-C6-N7	6.29	126.48	121.07
4	E	301	MLK	C1-C6-N7	7.14	127.21	121.07
4	H	301	MLK	C1-C6-N7	7.37	127.41	121.07

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	I	275[B]	NAG	C1

There are no torsion outliers.

There are no ring outliers.

25 monomers are involved in 157 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	223	MPD	1	0
4	A	301	MLK	9	0
5	A	305	MRD	1	0
7	B	250	NAG	1	0
7	B	275[B]	NAG	1	0
4	B	301	MLK	11	0
5	B	305	MRD	2	0
7	C	250	NAG	3	0
4	C	301	MLK	18	0
6	C	306	MPD	3	0
4	D	301	MLK	4	0
5	D	305	MRD	4	0
7	E	275[B]	NAG	2	0
4	E	301	MLK	15	0
4	F	301	MLK	20	0
5	F	305	MRD	3	0
6	G	222	MPD	1	0
4	G	301	MLK	10	0
4	H	301	MLK	15	0
7	I	250	NAG	3	0
7	I	275[A]	NAG	2	0
7	I	275[B]	NAG	2	0
4	I	301	MLK	15	0
6	I	305	MPD	1	0
4	J	301	MLK	10	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.50	1 (0%) 91 90	47, 67, 93, 117	5 (2%)
1	B	215/230 (93%)	-0.49	0 100 100	44, 61, 92, 122	2 (0%)
1	C	216/230 (93%)	-0.45	2 (0%) 85 84	40, 63, 96, 112	2 (0%)
1	D	214/230 (93%)	-0.53	1 (0%) 91 90	48, 67, 103, 114	1 (0%)
1	E	215/230 (93%)	-0.40	1 (0%) 91 90	44, 64, 96, 116	3 (1%)
1	F	214/230 (93%)	-0.39	2 (0%) 85 84	45, 65, 99, 118	0
1	G	214/230 (93%)	-0.53	0 100 100	47, 60, 93, 106	1 (0%)
1	H	215/230 (93%)	-0.48	1 (0%) 91 90	42, 61, 95, 109	0
1	I	214/230 (93%)	-0.43	0 100 100	48, 67, 105, 116	0
1	J	215/230 (93%)	-0.46	0 100 100	48, 63, 101, 119	2 (0%)
All	All	2146/2300 (93%)	-0.46	8 (0%) 93 92	40, 64, 97, 122	16 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	15	ASN	4.5
1	E	15	ASN	4.3
1	C	209	ALA	3.2
1	F	15	ASN	2.9
1	D	74	ASN	2.5
1	C	15	ASN	2.4
1	F	74	ASN	2.2
1	A	189	GLU	2.1

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 ⓘ

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
9	NAG	J	250	14/15	0.85	0.23	3.65	91,105,119,132	0
3	NAG	D	250	14/15	0.88	0.22	3.15	87,103,113,123	0
3	NAG	A	250	14/15	0.91	0.16	1.13	93,107,120,132	0
3	NAG	G	250	14/15	0.86	0.14	0.37	81,99,110,112	0
3	NAG	E	250	14/15	0.88	0.12	0.13	95,111,123,124	0
3	NAG	E	251	14/15	0.89	0.13	-	123,134,142,144	0
3	NAG	A	251	14/15	0.56	0.23	-	122,138,143,143	0
9	NAG	H	250	14/15	0.86	0.19	-	86,105,111,128	0
9	BMA	J	252	11/12	0.53	0.24	-	139,148,152,158	0
3	NAG	D	251	14/15	0.78	0.18	-	118,130,135,136	0
9	NAG	H	251	14/15	0.54	0.25	-	106,136,147,152	0
3	NAG	G	251	14/15	0.86	0.12	-	103,126,135,140	0
9	NAG	J	251	14/15	0.56	0.22	-	123,136,148,149	0
9	BMA	H	252	11/12	0.74	0.17	-	126,140,146,148	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(Å ²)	Q<0.9
5	MRD	B	305	8/8	0.90	0.27	7.62	66,75,86,95	0
7	NAG	E	275[A]	14/15	0.59	0.39	7.46	105,111,115,117	14
6	MPD	A	223	8/8	0.93	0.25	5.35	62,83,87,91	0
5	MRD	D	305	8/8	0.86	0.25	5.26	72,74,86,90	0
7	NAG	I	275[A]	14/15	0.66	0.26	5.12	96,99,103,105	14
6	MPD	G	222	8/8	0.87	0.25	4.52	68,76,91,92	0
7	NAG	E	275[B]	14/15	0.59	0.39	4.23	91,112,121,123	14
6	MPD	J	305	8/8	0.88	0.27	3.98	64,82,89,97	0
5	MRD	E	305	8/8	0.84	0.26	3.91	69,85,99,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
7	NAG	B	275[A]	14/15	0.67	0.35	3.70	78,98,105,106	14
7	NAG	I	275[B]	14/15	0.66	0.26	3.25	81,95,102,103	14
7	NAG	C	250	14/15	0.87	0.19	3.18	91,102,110,116	0
6	MPD	G	305	8/8	0.88	0.23	2.12	65,75,93,94	0
6	MPD	A	306	8/8	0.90	0.18	1.67	84,97,105,105	0
6	MPD	I	305	8/8	0.88	0.21	1.43	79,80,90,92	0
5	MRD	F	305	8/8	0.93	0.22	1.39	75,77,85,90	0
5	MRD	A	305	8/8	0.89	0.18	1.20	70,76,83,86	0
7	NAG	B	250	14/15	0.91	0.19	1.15	87,95,105,106	0
4	MLK	G	301	49/49	0.94	0.20	1.10	72,89,103,108	0
8	ACT	G	308	4/4	0.85	0.19	0.48	74,85,89,90	0
4	MLK	J	301	49/49	0.94	0.20	0.44	72,92,103,113	0
4	MLK	I	301	49/49	0.92	0.17	0.31	76,95,105,108	0
4	MLK	H	301	49/49	0.93	0.16	0.26	67,83,97,101	0
4	MLK	D	301	49/49	0.92	0.16	0.22	75,93,105,110	0
4	MLK	C	301	49/49	0.91	0.18	-0.04	64,90,98,102	0
4	MLK	B	301	49/49	0.93	0.17	-0.07	69,87,104,111	0
4	MLK	E	301	49/49	0.94	0.16	-0.09	69,87,102,108	0
4	MLK	F	301	49/49	0.92	0.14	-0.34	72,92,105,115	0
6	MPD	C	306	8/8	0.86	0.15	-0.37	82,87,97,100	0
7	NAG	F	250	14/15	0.89	0.14	-0.46	91,99,108,108	0
4	MLK	A	301	49/49	0.91	0.14	-0.56	78,90,100,103	0
7	NAG	I	250	14/15	0.83	0.14	-	82,98,103,104	0
2	MG	I	222	1/1	0.98	0.21	-	34,34,34,34	0
2	MG	A	222	1/1	0.97	0.26	-	37,37,37,37	0
2	MG	C	222	1/1	0.97	0.29	-	57,57,57,57	0
7	NAG	B	275[B]	14/15	0.67	0.35	-	93,98,103,103	14
2	MG	E	222	1/1	0.96	0.29	-	57,57,57,57	0
2	MG	B	222	1/1	0.97	0.22	-	47,47,47,47	0

6.5 Other polymers ⓘ

There are no such residues in this entry.