Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:22 PM GMT

PDB ID	:	1OP5
Title	:	Crystal Structure of Fab 2G12 bound to Man9GlcNAc2
Authors	:	Calarese, D.A.; Scanlan, C.N.; Zwick, M.B.; Deechongkit, S.; Mimura, Y.; Kunert, R.; Stanfield, R.L.; Kelly, J.W.; Rudd, P.M.; Dwek, R.A.; Katinger, H.; Burton, D.R.; Wilson, I.A.
Deposited on	:	2003-03-04
Resolution	:	3.00 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:

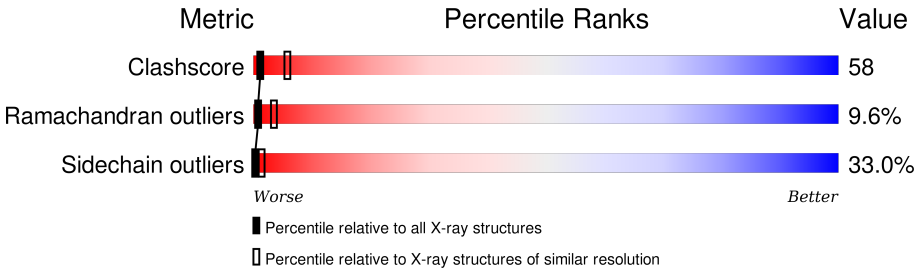
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 3.00 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))
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	K	212	25% 43% 25% 7%
1	L	212	30% 42% 25% ·
2	H	225	22% 43% 29% 7%
2	M	225	20% 46% 29% 5%

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	MAN	K	218	-	-	X	-
4	MAN	H	237	-	-	X	-
4	MAN	L	214	-	-	X	-
4	MAN	M	230	-	-	X	-
6	MAN	H	234	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6848 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 FAB 2G12, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	212	Total	C	N	O	S	0	0	0
			1620	1016	273	326	5			
1	K	212	Total	C	N	O	S	0	0	0
			1620	1016	273	326	5			

- Molecule 2 is a protein called FAB 2G12, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	225	Total	C	N	O	S	0	0	0
			1676	1051	287	331	7			
2	M	225	Total	C	N	O	S	0	0	0
			1676	1051	287	331	7			

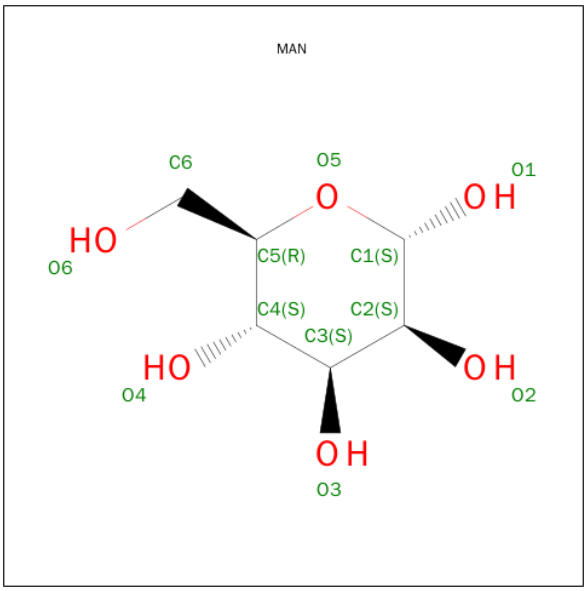
- Molecule 3 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	K	6	Total	C	N	O	0	0
			73	40	2	31		

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	M	2	Total	C	O	0	0
			22	12	10		
4	M	2	Total	C	O	0	0
			22	12	10		
4	H	2	Total	C	O	0	0
			22	12	10		
4	L	2	Total	C	O	0	0
			22	12	10		

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	M	1	Total	C	O		0	0
			11	6	5			

- Molecule 6 is a polymer of unknown type called SUGAR (ALPHA-D-MANNOSE).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	H	7	Total	C	N	O	0	0
			84	46	2	36		

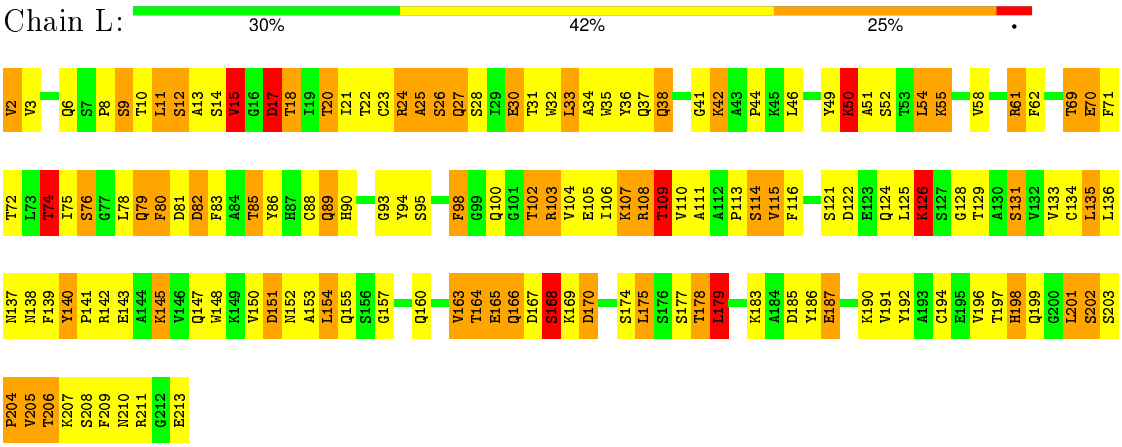
3 Residue-property plots (i)

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.

Note EDS was not executed.

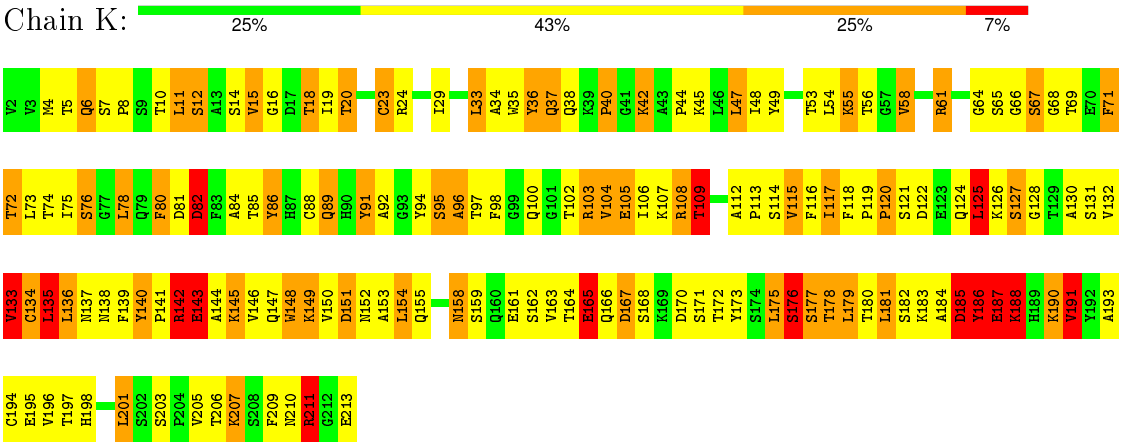
- Molecule 1: FAB 2G12, light chain

Chain L:



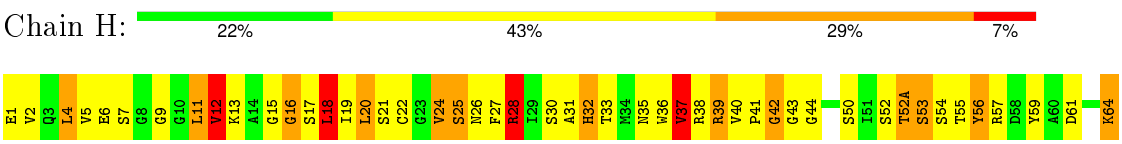
- Molecule 1: FAB 2G12, light chain

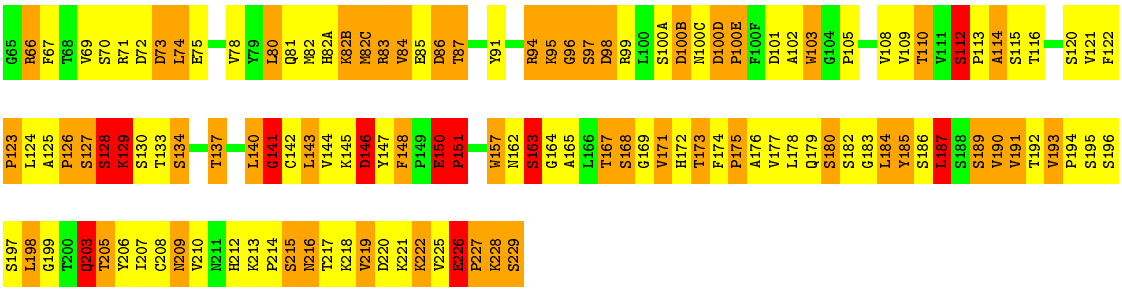
Chain K:



- Molecule 2: FAB 2G12, heavy chain

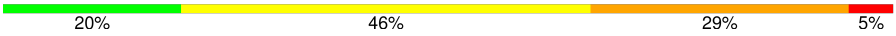
Chain H:

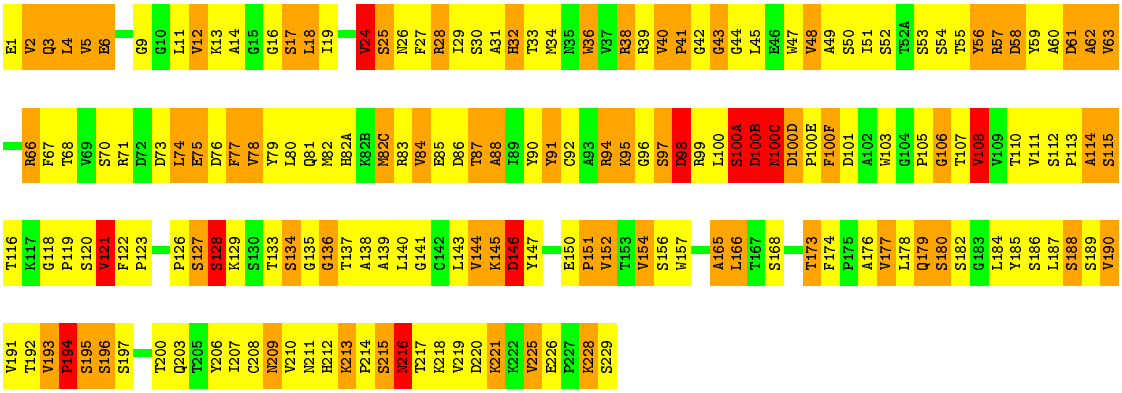




- Molecule 2: FAB 2G12, heavy chain

Chain M:





4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	135.82Å 145.71Å 148.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	105.41 – 3.00	Depositor
% Data completeness (in resolution range)	97.5 (105.41-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.248 , 0.329	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6848	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	K	1.49	15/1656 (0.9%)	1.47	14/2251 (0.6%)
1	L	1.75	22/1656 (1.3%)	1.62	26/2251 (1.2%)
2	H	2.15	34/1715 (2.0%)	1.72	35/2337 (1.5%)
2	M	1.54	17/1714 (1.0%)	1.66	28/2333 (1.2%)
All	All	1.75	88/6741 (1.3%)	1.62	103/9172 (1.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	K	0	1
1	L	0	1
2	H	0	4
2	M	0	9
All	All	0	15

All (88) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	222	LYS	CE-NZ	41.93	2.53	1.49
2	H	112	SER	C-N	19.01	1.70	1.34
2	H	229	SER	CB-OG	16.80	1.64	1.42
2	H	228	LYS	CE-NZ	14.28	1.84	1.49
2	H	128	SER	CB-OG	12.46	1.58	1.42
1	L	2	VAL	CB-CG2	11.89	1.77	1.52
1	L	165	GLU	CD-OE2	10.76	1.37	1.25
2	M	75	GLU	CD-OE1	9.94	1.36	1.25
2	H	123	PRO	C-O	9.51	1.42	1.23
1	L	70	GLU	CD-OE1	8.89	1.35	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	2	VAL	CB-CG1	8.78	1.71	1.52
2	H	64	LYS	CD-CE	8.62	1.72	1.51
2	M	44	GLY	N-CA	8.48	1.58	1.46
2	M	36	TRP	CB-CG	-8.41	1.35	1.50
1	K	71	PHE	CE2-CZ	8.10	1.52	1.37
2	H	229	SER	C-O	7.69	1.38	1.23
1	L	80	PHE	CE1-CZ	7.63	1.51	1.37
1	L	165	GLU	CG-CD	7.61	1.63	1.51
2	H	12	VAL	CB-CG1	-7.51	1.37	1.52
1	K	186	TYR	CD1-CE1	7.46	1.50	1.39
1	L	62	PHE	CB-CG	-7.28	1.39	1.51
1	L	42	LYS	CD-CE	7.17	1.69	1.51
1	K	71	PHE	CG-CD1	7.16	1.49	1.38
1	L	168	SER	CA-CB	7.09	1.63	1.52
1	K	186	TYR	CD2-CE2	6.96	1.49	1.39
1	L	80	PHE	CG-CD2	6.78	1.49	1.38
1	L	30	GLU	CD-OE1	6.76	1.33	1.25
2	H	157	TRP	CB-CG	-6.65	1.38	1.50
1	L	50	LYS	CD-CE	6.63	1.67	1.51
2	M	190	VAL	CB-CG2	-6.55	1.39	1.52
1	L	105	GLU	CD-OE1	-6.44	1.18	1.25
2	H	129	LYS	CD-CE	6.32	1.67	1.51
2	H	228	LYS	CB-CG	6.32	1.69	1.52
2	H	28	ARG	CB-CG	6.29	1.69	1.52
1	K	117	ILE	CA-CB	6.25	1.69	1.54
2	H	37	VAL	CB-CG1	-6.21	1.39	1.52
1	L	18	THR	CA-CB	-6.20	1.37	1.53
1	L	98	PHE	CD2-CE2	6.10	1.51	1.39
1	L	80	PHE	CE2-CZ	6.07	1.48	1.37
1	K	186	TYR	CG-CD2	6.05	1.47	1.39
2	H	226	GLU	CD-OE2	6.03	1.32	1.25
2	M	83	ARG	NE-CZ	5.98	1.40	1.33
2	M	43	GLY	N-CA	5.97	1.55	1.46
1	K	80	PHE	CE2-CZ	5.95	1.48	1.37
2	M	190	VAL	CB-CG1	-5.94	1.40	1.52
2	M	24	VAL	CB-CG2	-5.92	1.40	1.52
2	H	229	SER	CA-CB	5.91	1.61	1.52
1	L	166	GLN	CG-CD	5.90	1.64	1.51
2	M	24	VAL	CA-CB	-5.88	1.42	1.54
2	M	100(B)	ASP	CB-CG	5.75	1.63	1.51
1	K	186	TYR	CE1-CZ	5.71	1.46	1.38
2	H	103	TRP	CE3-CZ3	-5.69	1.28	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	9	SER	C-O	5.61	1.34	1.23
2	H	150	GLU	CD-OE1	5.61	1.31	1.25
2	M	28	ARG	NE-CZ	5.58	1.40	1.33
2	M	1	GLU	CD-OE1	5.57	1.31	1.25
1	K	67	SER	N-CA	5.54	1.57	1.46
2	H	64	LYS	CE-NZ	5.53	1.62	1.49
2	H	24	VAL	CB-CG2	-5.53	1.41	1.52
2	H	28	ARG	NE-CZ	5.53	1.40	1.33
2	H	177	VAL	CA-CB	5.50	1.66	1.54
2	H	148	PHE	CE2-CZ	5.44	1.47	1.37
2	M	108	VAL	CA-CB	-5.44	1.43	1.54
2	M	24	VAL	CB-CG1	-5.43	1.41	1.52
2	H	228	LYS	CD-CE	5.41	1.64	1.51
1	K	58	VAL	CA-CB	-5.40	1.43	1.54
1	L	38	GLN	CB-CG	-5.38	1.38	1.52
2	M	154	VAL	CA-CB	-5.37	1.43	1.54
2	H	84	VAL	CB-CG2	-5.36	1.41	1.52
2	H	185	TYR	CB-CG	-5.36	1.43	1.51
1	K	207	LYS	CB-CG	5.32	1.67	1.52
2	H	177	VAL	CB-CG2	5.24	1.63	1.52
2	H	148	PHE	CD1-CE1	5.24	1.49	1.39
1	L	107	LYS	CD-CE	5.23	1.64	1.51
2	H	44	GLY	C-O	5.23	1.32	1.23
1	L	70	GLU	CD-OE2	5.21	1.31	1.25
1	K	96	ALA	CA-CB	-5.20	1.41	1.52
1	K	143	GLU	CG-CD	5.20	1.59	1.51
1	L	165	GLU	CD-OE1	5.20	1.31	1.25
1	K	165	GLU	CD-OE1	5.20	1.31	1.25
2	H	108	VAL	CB-CG2	-5.19	1.42	1.52
2	H	109	VAL	CB-CG2	-5.18	1.42	1.52
1	K	86	TYR	CB-CG	-5.18	1.43	1.51
2	H	82	MET	CB-CG	-5.14	1.34	1.51
2	H	203	GLN	CG-CD	5.14	1.62	1.51
2	M	100(C)	ASN	C-N	5.13	1.45	1.34
2	M	77	PHE	CE1-CZ	-5.09	1.27	1.37
2	H	37	VAL	CA-CB	-5.05	1.44	1.54

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	98	ASP	CB-CG-OD2	10.81	128.03	118.30
2	M	96	GLY	N-CA-C	10.18	138.55	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	M	100(B)	ASP	CB-CG-OD2	10.05	127.34	118.30
2	M	61	ASP	CB-CG-OD2	9.67	127.01	118.30
1	K	167	ASP	CB-CG-OD2	9.45	126.80	118.30
1	L	61	ARG	NE-CZ-NH2	-9.26	115.67	120.30
2	H	100(D)	ASP	CB-CG-OD2	9.03	126.42	118.30
1	L	17	ASP	CB-CG-OD2	8.92	126.33	118.30
2	H	39	ARG	NE-CZ-NH1	-8.67	115.96	120.30
1	L	2	VAL	CB-CA-C	-8.56	95.14	111.40
2	M	78	VAL	CB-CA-C	-8.30	95.62	111.40
1	L	2	VAL	CG1-CB-CG2	8.21	124.04	110.90
2	H	187	LEU	CA-CB-CG	8.09	133.91	115.30
2	M	76	ASP	CB-CG-OD2	7.98	125.48	118.30
2	M	18	LEU	CB-CG-CD1	-7.94	97.50	111.00
2	H	86	ASP	CB-CG-OD2	7.88	125.39	118.30
2	M	92	CYS	CA-CB-SG	-7.75	100.05	114.00
1	K	61	ARG	NE-CZ-NH1	7.72	124.16	120.30
1	K	82	ASP	CB-CG-OD2	7.68	125.21	118.30
1	K	185	ASP	CB-CG-OD2	7.64	125.18	118.30
1	L	75	ILE	CG1-CB-CG2	-7.59	94.70	111.40
2	M	108	VAL	CB-CA-C	-7.51	97.13	111.40
2	H	39	ARG	NE-CZ-NH2	7.46	124.03	120.30
1	K	125	LEU	CA-CB-CG	7.37	132.25	115.30
2	H	28	ARG	NE-CZ-NH1	7.31	123.96	120.30
1	L	74	THR	OG1-CB-CG2	-7.16	93.53	110.00
1	L	8	PRO	N-CD-CG	-7.05	92.62	103.20
2	H	67	PHE	CB-CA-C	-7.04	96.32	110.40
2	H	64	LYS	CD-CE-NZ	7.03	127.88	111.70
1	K	151	ASP	CB-CG-OD2	7.02	124.62	118.30
1	K	135	LEU	CB-CG-CD1	-6.97	99.16	111.00
1	L	103	ARG	NE-CZ-NH2	-6.90	116.85	120.30
1	L	170	ASP	CB-CG-OD2	6.88	124.49	118.30
2	M	91	TYR	CB-CA-C	-6.87	96.67	110.40
2	M	121	VAL	N-CA-C	6.83	129.45	111.00
2	H	6	GLU	OE1-CD-OE2	6.77	131.42	123.30
2	H	80	LEU	CB-CG-CD1	-6.70	99.62	111.00
1	K	81	ASP	CB-CG-OD2	6.63	124.27	118.30
2	H	228	LYS	CD-CE-NZ	-6.59	96.54	111.70
2	H	95	LYS	C-N-CA	-6.49	108.67	122.30
2	H	105	PRO	N-CD-CG	-6.47	93.49	103.20
2	H	146	ASP	CB-CG-OD2	6.47	124.12	118.30
1	K	148	TRP	N-CA-C	-6.46	93.55	111.00
2	M	121	VAL	CB-CA-C	-6.42	99.21	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	M	56	TYR	CA-CB-CG	6.40	125.55	113.40
2	M	39	ARG	NE-CZ-NH1	-6.35	117.12	120.30
2	M	28	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	L	102	THR	CA-CB-CG2	-6.29	103.60	112.40
2	H	18	LEU	CA-CB-CG	-6.25	100.93	115.30
2	H	101	ASP	CB-CG-OD1	6.22	123.90	118.30
1	K	133	VAL	N-CA-C	6.13	127.55	111.00
1	L	82	ASP	CB-CG-OD1	6.10	123.79	118.30
1	L	167	ASP	CB-CG-OD2	6.08	123.78	118.30
2	H	84	VAL	CB-CA-C	-6.06	99.89	111.40
1	L	17	ASP	CB-CG-OD1	-6.05	112.85	118.30
2	H	4	LEU	CB-CG-CD1	6.04	121.27	111.00
1	L	42	LYS	CB-CA-C	6.01	122.41	110.40
1	L	38	GLN	CB-CA-C	-5.99	98.42	110.40
2	H	28	ARG	NE-CZ-NH2	-5.96	117.32	120.30
2	M	83	ARG	NE-CZ-NH1	5.92	123.26	120.30
2	H	57	ARG	NE-CZ-NH1	5.87	123.23	120.30
2	M	100(D)	ASP	CB-CG-OD2	5.84	123.56	118.30
1	L	202	SER	CB-CA-C	5.82	121.17	110.10
2	M	58	ASP	CB-CG-OD2	5.79	123.51	118.30
1	L	41	GLY	C-N-CA	-5.76	107.29	121.70
1	L	85	THR	CA-CB-CG2	-5.73	104.38	112.40
2	M	75	GLU	CG-CD-OE2	-5.72	106.87	118.30
2	H	5	VAL	CB-CA-C	-5.70	100.56	111.40
1	K	15	VAL	CG1-CB-CG2	-5.67	101.83	110.90
1	K	103	ARG	NE-CZ-NH1	5.59	123.10	120.30
2	H	82(C)	MET	CB-CG-SD	-5.56	95.71	112.40
2	H	84	VAL	CG1-CB-CG2	-5.50	102.10	110.90
2	H	32	HIS	CB-CA-C	-5.47	99.46	110.40
1	L	185	ASP	CB-CG-OD2	5.46	123.22	118.30
1	L	179	LEU	CB-CG-CD2	5.44	120.24	111.00
2	M	177	VAL	CB-CA-C	-5.44	101.07	111.40
2	M	56	TYR	CB-CA-C	-5.42	99.55	110.40
2	H	78	VAL	N-CA-C	-5.32	96.64	111.00
2	M	63	VAL	CB-CA-C	-5.30	101.34	111.40
2	M	194	PRO	N-CD-CG	-5.28	95.27	103.20
2	H	73	ASP	N-CA-CB	5.27	120.09	110.60
2	M	82(C)	MET	CG-SD-CE	-5.25	91.80	100.20
2	M	5	VAL	CB-CA-C	-5.24	101.44	111.40
1	K	73	LEU	CB-CG-CD1	-5.24	102.09	111.00
2	H	141	GLY	N-CA-C	5.20	126.10	113.10
2	H	20	LEU	CB-CG-CD1	-5.19	102.18	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	109	THR	OG1-CB-CG2	-5.18	98.08	110.00
2	M	95	LYS	N-CA-C	5.18	125.00	111.00
2	M	4	LEU	CB-CG-CD2	-5.17	102.20	111.00
1	K	40	PRO	N-CD-CG	-5.17	95.45	103.20
1	L	24	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	L	15	VAL	CB-CA-C	-5.13	101.66	111.40
2	H	18	LEU	CB-CA-C	-5.11	100.50	110.20
2	H	114	ALA	N-CA-C	-5.10	97.22	111.00
2	H	87	THR	CA-CB-CG2	-5.10	105.26	112.40
2	M	61	ASP	CB-CG-OD1	-5.08	113.73	118.30
2	M	95	LYS	CA-C-N	5.07	126.35	116.20
2	H	18	LEU	N-CA-C	-5.06	97.33	111.00
2	H	184	LEU	CA-CB-CG	-5.06	103.66	115.30
1	L	54	LEU	CB-CG-CD1	-5.05	102.42	111.00
2	H	96	GLY	N-CA-C	5.04	125.70	113.10
1	L	140	TYR	N-CA-C	-5.01	97.48	111.00
1	L	191	VAL	CB-CA-C	-5.00	101.89	111.40

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	128	SER	Peptide
2	H	141	GLY	Peptide
2	H	42	GLY	Peptide
2	H	96	GLY	Peptide
1	K	19	ILE	Peptide
1	L	25	ALA	Peptide
2	M	100(A)	SER	Peptide
2	M	123	PRO	Peptide
2	M	145	LYS	Peptide
2	M	151	PRO	Peptide
2	M	215	SER	Peptide
2	M	40	VAL	Peptide
2	M	42	GLY	Peptide
2	M	88	ALA	Peptide
2	M	97	SER	Peptide

5.2 Too-close contacts (i)

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	K	1620	0	1551	199	0
1	L	1620	0	1551	181	0
2	H	1676	0	1628	184	0
2	M	1676	0	1628	198	0
3	K	73	0	63	15	0
4	H	22	0	17	7	0
4	L	22	0	19	6	0
4	M	44	0	38	15	0
5	M	11	0	10	3	0
6	H	84	0	72	15	0
All	All	6848	0	6577	771	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 58.

All (771) 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:L:2:VAL:CG2	1:L:2:VAL:CB	1.77	1.58
2:M:82:MET:CE	2:M:82:MET:SD	2.01	1.48
2:H:112:SER:C	2:H:113:PRO:N	1.70	1.45
1:K:113:PRO:HD3	1:K:198:HIS:CD2	1.50	1.44
2:H:229:SER:OG	2:H:229:SER:CB	1.64	1.42
2:H:228:LYS:NZ	2:H:228:LYS:CE	1.84	1.39
1:L:175:LEU:HD23	1:L:175:LEU:O	1.36	1.21
1:L:20:THR:HB	1:L:74:THR:CG2	1.72	1.19
1:K:166:GLN:HG3	1:K:173:TYR:CE1	1.79	1.17
2:M:2:VAL:HG11	2:M:94:ARG:HH12	1.08	1.17
1:K:91:TYR:HE1	2:M:100(C):ASN:O	1.25	1.14
1:K:113:PRO:CD	1:K:198:HIS:HD2	1.60	1.14
2:H:184:LEU:H	2:H:184:LEU:HD12	1.03	1.10
2:M:112:SER:C	2:M:113:PRO:N	2.05	1.10
2:H:83:ARG:HG3	2:H:83:ARG:HH11	1.11	1.09
1:L:113:PRO:HD3	1:L:198:HIS:HD2	1.11	1.09
2:M:48:VAL:HG12	2:M:49:ALA:H	1.02	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:48:VAL:HG12	2:M:49:ALA:N	1.58	1.07
1:L:133:VAL:HG22	1:L:178:THR:HG23	1.28	1.07
2:H:228:LYS:HD3	2:H:229:SER:OG	1.56	1.06
2:M:2:VAL:HG11	2:M:94:ARG:NH1	1.71	1.05
2:M:94:ARG:HG2	2:M:101:ASP:OD1	1.55	1.05
2:H:184:LEU:H	2:H:184:LEU:CD1	1.63	1.04
1:L:6:GLN:HB2	1:L:100:GLN:NE2	1.71	1.04
1:L:175:LEU:HD23	1:L:175:LEU:C	1.77	1.04
1:L:175:LEU:CD2	1:L:175:LEU:O	2.06	1.03
2:H:18:LEU:HB2	2:H:82(C):MET:CE	1.89	1.03
2:H:125:ALA:O	2:H:127:SER:HB3	1.58	1.03
2:H:184:LEU:N	2:H:184:LEU:HD12	1.65	1.02
1:K:91:TYR:CE1	2:M:100(C):ASN:O	2.13	1.02
2:H:17:SER:OG	2:H:82(A):HIS:HD2	1.42	1.02
2:M:113:PRO:HD2	2:M:114:ALA:H	1.25	1.01
2:H:212:HIS:CD2	2:H:215:SER:HB3	1.96	1.00
2:M:211:ASN:HD21	2:M:218:LYS:HD3	1.23	1.00
1:K:166:GLN:HG3	1:K:173:TYR:HE1	0.87	1.00
6:H:232:BMA:H62	6:H:234:MAN:H3	1.43	1.00
4:L:214:MAN:C1	6:H:234:MAN:O3	2.09	0.99
1:L:151:ASP:O	1:L:152:ASN:HB2	1.57	0.99
1:L:20:THR:HB	1:L:74:THR:HG23	1.45	0.98
2:M:138:ALA:HB2	2:M:193:VAL:HG22	1.46	0.98
1:K:8:PRO:HG3	1:K:11:LEU:HD22	1.44	0.97
2:H:52:SER:O	2:H:71:ARG:NH1	1.98	0.97
2:H:35:ASN:OD1	2:H:50:SER:HB3	1.63	0.96
1:L:6:GLN:CB	1:L:100:GLN:HE22	1.79	0.95
2:H:226:GLU:HB2	2:H:227:PRO:HD2	1.49	0.94
3:K:219:MAN:O2	5:M:234:MAN:H2	1.67	0.94
3:K:217:MAN:O2	4:M:230:MAN:C1	2.14	0.94
2:M:154:VAL:CG1	2:M:156:SER:N	2.30	0.94
1:K:163:VAL:CG2	1:K:175:LEU:HD12	1.97	0.94
1:L:113:PRO:HD3	1:L:198:HIS:CD2	2.01	0.94
2:M:48:VAL:CG1	2:M:49:ALA:N	2.30	0.94
1:K:18:THR:HG23	1:K:76:SER:HA	1.50	0.94
2:H:98:ASP:C	2:H:98:ASP:OD1	2.03	0.94
2:M:88:ALA:HB3	2:M:90:TYR:CE1	2.03	0.93
2:M:194:PRO:O	2:M:196:SER:N	1.99	0.93
2:M:173:THR:HG23	2:M:189:SER:HB2	1.48	0.93
1:K:145:LYS:HD3	1:K:147:GLN:HE21	1.33	0.92
2:M:113:PRO:CD	2:M:114:ALA:H	1.76	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:126:PRO:HG3	2:H:140:LEU:HD12	1.52	0.92
1:L:20:THR:HB	1:L:74:THR:HG22	1.52	0.92
2:H:75:GLU:HG3	2:M:57:ARG:NH1	1.83	0.92
1:K:18:THR:CG2	1:K:76:SER:HA	1.99	0.91
2:H:66:ARG:NH1	2:H:86:ASP:OD2	2.03	0.91
1:L:6:GLN:CA	1:L:100:GLN:HE22	1.84	0.91
2:M:187:LEU:HD12	2:M:188:SER:N	1.86	0.90
1:K:149:LYS:HE3	1:K:195:GLU:OE1	1.72	0.90
1:L:108:ARG:NH1	1:L:109:THR:HG23	1.87	0.90
2:H:100(A):SER:O	2:H:100(C):ASN:N	2.05	0.90
2:M:211:ASN:ND2	2:M:218:LYS:HD3	1.85	0.90
2:M:84:VAL:O	2:M:86:ASP:N	2.05	0.89
1:K:65:SER:HB3	1:K:72:THR:HG23	1.54	0.89
2:M:90:TYR:N	2:M:107:THR:O	2.06	0.89
1:L:110:VAL:HG22	1:L:141:PRO:HD3	1.54	0.88
2:H:83:ARG:NH1	2:H:83:ARG:HG3	1.74	0.88
1:K:163:VAL:HG23	1:K:175:LEU:HD12	1.56	0.88
2:H:212:HIS:CE1	2:H:214:PRO:HG2	2.08	0.88
1:L:2:VAL:CG2	1:L:2:VAL:HB	2.03	0.87
1:L:133:VAL:HG22	1:L:178:THR:CG2	2.04	0.87
2:M:138:ALA:HB3	2:M:193:VAL:H	1.39	0.87
2:M:154:VAL:HG12	2:M:156:SER:N	1.88	0.87
2:M:140:LEU:HD13	2:M:225:VAL:HG11	1.53	0.87
1:K:113:PRO:CD	1:K:198:HIS:CD2	2.45	0.86
1:L:143:GLU:N	1:L:143:GLU:OE2	2.09	0.85
2:M:6:GLU:OE1	2:M:105:PRO:HD2	1.77	0.85
2:H:27:PHE:O	2:H:27:PHE:CD1	2.30	0.85
2:M:52:SER:HB3	2:M:56:TYR:HB2	1.57	0.85
4:L:214:MAN:C1	6:H:234:MAN:HO3	1.86	0.84
1:L:106:ILE:O	1:L:106:ILE:HG22	1.76	0.83
2:H:18:LEU:HB2	2:H:82(C):MET:HE1	1.59	0.83
1:K:89:GLN:HB2	1:K:98:PHE:CD2	2.14	0.83
2:H:66:ARG:HG2	2:H:82(A):HIS:O	1.79	0.82
1:L:18:THR:HG23	1:L:76:SER:HA	1.60	0.82
1:K:166:GLN:CG	1:K:173:TYR:HE1	1.83	0.82
2:H:81:GLN:NE2	2:H:82(A):HIS:HE1	1.77	0.82
2:M:208:CYS:O	2:M:220:ASP:HA	1.80	0.82
1:K:133:VAL:HG22	1:K:178:THR:HG23	1.60	0.81
1:K:147:GLN:HB2	1:K:195:GLU:HB3	1.63	0.81
1:L:85:THR:HG22	1:L:86:TYR:N	1.94	0.81
2:H:226:GLU:CB	2:H:227:PRO:HD2	2.10	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:154:VAL:HG13	2:M:156:SER:H	1.46	0.80
2:H:17:SER:OG	2:H:82(A):HIS:CD2	2.31	0.80
2:H:24:VAL:HG11	2:H:27:PHE:CZ	2.17	0.80
2:H:83:ARG:HH11	2:H:83:ARG:CG	1.91	0.80
1:L:11:LEU:HD12	1:L:11:LEU:C	2.02	0.80
1:L:183:LYS:O	1:L:187:GLU:HB2	1.81	0.80
1:K:175:LEU:HD23	1:K:176:SER:H	1.46	0.79
1:L:20:THR:CB	1:L:74:THR:HG22	2.11	0.79
2:H:172:HIS:HB2	2:H:190:VAL:HG23	1.65	0.79
2:M:128:SER:HB2	2:M:133:THR:HG21	1.64	0.79
2:H:178:LEU:HD11	2:H:183:GLY:O	1.82	0.79
1:K:125:LEU:O	1:K:183:LYS:HD2	1.83	0.79
3:K:217:MAN:O2	4:M:230:MAN:C2	2.31	0.78
2:M:29:ILE:HG23	2:M:34:MET:CE	2.12	0.78
6:H:232:BMA:C6	6:H:234:MAN:H3	2.12	0.78
2:H:175:PRO:HB2	1:K:162:SER:OG	1.84	0.78
1:L:20:THR:CB	1:L:74:THR:CG2	2.57	0.78
2:M:113:PRO:CD	2:M:114:ALA:N	2.47	0.78
2:M:187:LEU:C	2:M:187:LEU:HD12	2.04	0.78
2:H:2:VAL:HG22	2:H:27:PHE:HD2	1.48	0.77
2:M:212:HIS:CE1	2:M:214:PRO:HD2	2.19	0.77
2:H:143:LEU:HD11	2:H:145:LYS:HB2	1.64	0.77
2:H:2:VAL:HG22	2:H:27:PHE:CD2	2.20	0.77
2:M:177:VAL:CG1	2:M:178:LEU:N	2.47	0.77
2:M:60:ALA:O	2:M:63:VAL:HG22	1.84	0.77
2:M:152:VAL:HG12	2:M:152:VAL:O	1.85	0.77
1:L:38:GLN:OE1	2:H:39:ARG:NH1	2.17	0.77
2:M:5:VAL:O	2:M:5:VAL:HG12	1.84	0.77
1:L:6:GLN:HB2	1:L:100:GLN:HE22	1.34	0.77
1:L:124:GLN:HE22	1:L:131:SER:HB2	1.48	0.77
1:L:6:GLN:CB	1:L:100:GLN:NE2	2.43	0.76
2:H:12:VAL:HG13	2:H:18:LEU:HD12	1.68	0.76
3:K:218:MAN:O3	4:M:232:MAN:H5	1.85	0.76
2:M:112:SER:O	2:M:113:PRO:CA	2.34	0.76
1:K:137:ASN:HD21	1:K:138:ASN:HD22	1.34	0.76
1:K:113:PRO:HB3	1:K:139:PHE:HB3	1.68	0.75
2:H:121:VAL:HG21	2:H:219:VAL:HG11	1.66	0.75
2:H:124:LEU:N	2:H:141:GLY:O	2.20	0.75
1:L:135:LEU:HD11	2:M:190:VAL:HG21	1.66	0.75
2:H:186:SER:OG	2:H:187:LEU:N	2.19	0.75
1:K:137:ASN:ND2	1:K:138:ASN:HD22	1.84	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:151:ASP:O	1:L:152:ASN:CB	2.35	0.75
2:M:127:SER:O	2:M:128:SER:OG	2.06	0.74
2:H:173:THR:HG23	2:H:189:SER:OG	1.86	0.74
3:K:217:MAN:O2	4:M:230:MAN:H2	1.88	0.74
2:M:32:HIS:CD2	2:M:94:ARG:HE	2.05	0.73
1:L:10:THR:HG22	1:L:11:LEU:H	1.53	0.73
2:M:138:ALA:CB	2:M:193:VAL:HG22	2.18	0.73
1:K:145:LYS:HD3	1:K:147:GLN:NE2	2.03	0.73
2:M:97:SER:O	2:M:100:LEU:HB2	1.89	0.73
1:L:108:ARG:HD3	1:L:109:THR:O	1.88	0.73
2:M:177:VAL:HG12	2:M:178:LEU:N	2.04	0.73
1:K:6:GLN:O	1:K:100:GLN:NE2	2.13	0.73
2:H:35:ASN:OD1	2:H:50:SER:CB	2.36	0.73
6:H:233:MAN:O2	4:H:237:MAN:C2	2.37	0.72
2:M:145:LYS:O	2:M:146:ASP:HB2	1.88	0.72
2:M:154:VAL:CG1	2:M:156:SER:H	1.99	0.72
2:M:87:THR:HG23	2:M:110:THR:HG22	1.70	0.72
1:L:150:VAL:HB	1:L:155:GLN:NE2	2.03	0.72
1:K:163:VAL:HG23	1:K:175:LEU:CD1	2.19	0.72
1:L:10:THR:HG22	1:L:11:LEU:N	2.03	0.72
2:M:18:LEU:HB2	2:M:82(C):MET:HE1	1.70	0.72
2:M:113:PRO:HD2	2:M:114:ALA:N	2.01	0.72
2:M:173:THR:HG23	2:M:189:SER:CB	2.17	0.72
1:K:33:LEU:CD1	1:K:89:GLN:O	2.37	0.72
1:K:44:PRO:HG2	2:M:103:TRP:CD2	2.26	0.71
1:L:85:THR:CG2	1:L:86:TYR:N	2.53	0.71
2:M:112:SER:O	2:M:113:PRO:HA	1.90	0.71
3:K:218:MAN:O3	4:M:232:MAN:C5	2.39	0.71
2:H:222:LYS:NZ	2:H:222:LYS:CE	2.53	0.71
1:K:4:MET:CE	1:K:23:CYS:SG	2.78	0.71
1:K:112:ALA:HB1	1:K:201:LEU:HD13	1.72	0.71
1:K:186:TYR:O	1:K:188:LYS:N	2.22	0.70
1:L:170:ASP:OD1	1:L:170:ASP:C	2.27	0.70
1:L:163:VAL:HG23	1:L:175:LEU:HB2	1.71	0.70
2:H:215:SER:O	2:H:216:ASN:HB3	1.91	0.70
2:H:81:GLN:HE21	2:H:82(A):HIS:CE1	2.09	0.70
1:K:91:TYR:O	1:K:91:TYR:CD1	2.43	0.70
1:K:132:VAL:HB	1:K:179:LEU:HD23	1.73	0.70
2:H:81:GLN:NE2	2:H:82(A):HIS:CE1	2.59	0.70
4:L:214:MAN:C5	6:H:234:MAN:HO3	2.04	0.70
1:K:15:VAL:HG13	1:K:78:LEU:O	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:33:LEU:HD12	1:K:34:ALA:N	2.06	0.70
2:M:29:ILE:HG23	2:M:34:MET:HE1	1.74	0.70
2:H:226:GLU:HB2	2:H:227:PRO:CD	2.21	0.69
2:H:212:HIS:HD2	2:H:215:SER:HB3	1.52	0.69
1:K:8:PRO:CG	1:K:11:LEU:HD22	2.18	0.69
1:K:124:GLN:O	1:K:127:SER:HB3	1.91	0.69
2:M:111:VAL:O	2:M:112:SER:C	2.28	0.69
1:K:89:GLN:CB	1:K:98:PHE:CD2	2.76	0.69
1:K:167:ASP:HB3	1:K:171:SER:H	1.58	0.69
4:M:230:MAN:O3	4:M:231:MAN:C1	2.36	0.69
1:L:104:VAL:HG12	1:L:104:VAL:O	1.92	0.69
2:M:100(C):ASN:O	2:M:100(C):ASN:CG	2.32	0.68
3:K:219:MAN:O2	5:M:234:MAN:C2	2.42	0.68
1:K:186:TYR:HE2	1:K:211:ARG:HD2	1.59	0.68
1:L:93:GLY:O	1:L:94:TYR:CD2	2.47	0.68
2:M:97:SER:O	2:M:100:LEU:CB	2.42	0.68
2:M:216:ASN:HD22	2:M:216:ASN:N	1.93	0.67
1:L:3:VAL:H	1:L:26:SER:CB	2.07	0.67
1:L:32:TRP:CE3	2:H:100(C):ASN:ND2	2.63	0.67
2:H:143:LEU:HD12	2:H:143:LEU:C	2.15	0.67
1:K:132:VAL:O	1:K:148:TRP:CH2	2.47	0.67
4:L:214:MAN:H5	6:H:234:MAN:O3	1.94	0.67
2:M:144:VAL:HG11	2:M:152:VAL:HG21	1.77	0.67
2:M:94:ARG:CG	2:M:101:ASP:OD1	2.40	0.67
1:K:23:CYS:HB2	1:K:35:TRP:CZ2	2.30	0.67
1:L:154:LEU:HD12	1:L:155:GLN:H	1.59	0.67
2:H:209:ASN:N	2:H:209:ASN:HD22	1.93	0.66
1:K:186:TYR:CE2	1:K:211:ARG:HD2	2.31	0.66
1:K:85:THR:HA	1:K:103:ARG:HA	1.78	0.66
2:H:98:ASP:OD1	2:H:98:ASP:O	2.13	0.66
2:H:229:SER:HG	2:H:229:SER:CB	2.07	0.66
1:K:142:ARG:O	1:K:143:GLU:C	2.34	0.66
2:M:107:THR:OG1	2:M:108:VAL:N	2.28	0.66
3:K:218:MAN:HO3	4:M:232:MAN:C1	2.08	0.65
1:L:113:PRO:CA	1:L:139:PHE:HB3	2.26	0.65
1:K:115:VAL:O	1:K:116:PHE:CG	2.50	0.65
6:H:235:MAN:C1	6:H:236:MAN:O5	2.44	0.65
2:H:75:GLU:HG3	2:M:57:ARG:HH11	1.61	0.65
1:L:163:VAL:HG13	1:L:164:THR:O	1.97	0.65
2:M:121:VAL:HG12	2:M:121:VAL:O	1.95	0.65
2:H:15:GLY:O	2:H:16:GLY:O	2.15	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:170:ASP:OD1	1:K:172:THR:OG1	2.06	0.65
1:K:116:PHE:CD2	1:K:135:LEU:HD13	2.32	0.64
2:M:2:VAL:HG12	2:M:27:PHE:CD2	2.32	0.64
1:K:159:SER:HA	1:K:179:LEU:HA	1.79	0.64
2:H:209:ASN:N	2:H:209:ASN:ND2	2.43	0.64
1:L:192:TYR:O	1:L:208:SER:HB2	1.97	0.64
1:K:38:GLN:HB2	1:K:44:PRO:HA	1.79	0.64
2:M:121:VAL:HG13	2:M:122:PHE:N	2.12	0.64
2:H:228:LYS:NZ	2:H:228:LYS:CD	2.61	0.64
2:M:152:VAL:CG1	2:M:152:VAL:O	2.45	0.64
1:L:133:VAL:HG12	1:L:134:CYS:N	2.13	0.64
1:L:14:SER:O	1:L:17:ASP:HB2	1.98	0.64
2:H:126:PRO:HG2	2:H:226:GLU:O	1.97	0.64
1:K:151:ASP:OD1	1:K:191:VAL:HG23	1.98	0.64
2:M:111:VAL:O	2:M:112:SER:O	2.15	0.64
2:M:38:ARG:HD3	2:M:48:VAL:HG21	1.80	0.64
2:M:121:VAL:O	2:M:221:LYS:NZ	2.24	0.64
1:K:172:THR:C	1:K:173:TYR:HD1	2.00	0.63
1:K:108:ARG:HD3	1:K:109:THR:O	1.97	0.63
2:M:17:SER:OG	2:M:82(A):HIS:HD2	1.80	0.63
1:K:118:PHE:HB2	1:K:133:VAL:O	1.99	0.63
1:K:195:GLU:HA	1:K:206:THR:HG23	1.80	0.63
1:L:50:LYS:O	1:L:52:SER:N	2.29	0.63
2:H:212:HIS:CE1	2:H:214:PRO:CG	2.82	0.62
1:K:36:TYR:CE2	1:K:89:GLN:NE2	2.68	0.62
2:H:179:GLN:O	2:H:180:SER:C	2.36	0.62
1:K:172:THR:O	1:K:173:TYR:HD1	1.82	0.62
1:K:35:TRP:CE3	1:K:88:CYS:HB3	2.34	0.62
2:M:38:ARG:HD3	2:M:48:VAL:CG2	2.28	0.62
1:L:3:VAL:O	1:L:3:VAL:HG12	1.99	0.62
1:L:125:LEU:HD12	1:L:183:LYS:HG2	1.80	0.62
1:L:115:VAL:HG21	1:L:205:VAL:HG11	1.81	0.62
2:M:6:GLU:N	2:M:6:GLU:OE1	2.31	0.62
2:M:12:VAL:O	2:M:111:VAL:HA	1.99	0.62
2:M:100(D):ASP:HB2	4:M:231:MAN:O3	2.00	0.62
1:L:154:LEU:HD12	1:L:155:GLN:N	2.15	0.62
1:K:201:LEU:HB3	1:K:203:SER:O	1.99	0.61
2:H:12:VAL:CG1	2:H:18:LEU:HD12	2.29	0.61
3:K:216:BMA:H62	3:K:218:MAN:C3	2.29	0.61
1:K:38:GLN:HE21	1:K:44:PRO:N	1.98	0.61
2:H:83:ARG:O	2:H:84:VAL:C	2.37	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:6:GLN:HB2	1:L:100:GLN:HE21	1.64	0.61
2:H:19:ILE:HA	2:H:81:GLN:HA	1.81	0.61
2:M:100(F):PHE:CD1	2:M:100(F):PHE:N	2.68	0.61
2:H:219:VAL:HG12	2:H:219:VAL:O	2.01	0.61
1:K:167:ASP:HB3	1:K:171:SER:N	2.15	0.61
2:H:31:ALA:O	4:H:237:MAN:O3	2.19	0.61
1:K:183:LYS:O	1:K:187:GLU:N	2.34	0.61
1:K:15:VAL:HG21	1:K:80:PHE:HD1	1.66	0.61
2:M:100(A):SER:HA	2:M:100(D):ASP:CG	2.21	0.60
2:M:100(F):PHE:HD1	2:M:100(F):PHE:N	1.98	0.60
1:K:29:ILE:HG22	1:K:29:ILE:O	2.01	0.60
2:M:24:VAL:HG11	2:M:27:PHE:CZ	2.37	0.60
2:M:187:LEU:CD1	2:M:188:SER:N	2.63	0.60
1:K:142:ARG:HB2	1:K:173:TYR:HE2	1.65	0.60
1:K:112:ALA:HB1	1:K:201:LEU:CD1	2.32	0.60
1:K:133:VAL:CG2	1:K:178:THR:HG23	2.29	0.60
1:K:36:TYR:HE2	1:K:89:GLN:NE2	1.99	0.60
2:M:17:SER:HA	2:M:82:MET:O	2.01	0.60
2:M:84:VAL:C	2:M:86:ASP:H	2.04	0.60
1:L:38:GLN:NE2	1:L:44:PRO:HD3	2.17	0.59
2:H:4:LEU:HD11	2:H:27:PHE:CZ	2.37	0.59
1:K:33:LEU:HD12	1:K:34:ALA:H	1.66	0.59
2:H:143:LEU:CD1	2:H:145:LYS:HB2	2.32	0.59
1:K:86:TYR:N	1:K:86:TYR:CD1	2.70	0.59
2:H:215:SER:O	2:H:216:ASN:CB	2.49	0.59
2:M:68:THR:HB	2:M:81:GLN:HB2	1.84	0.59
2:H:143:LEU:HD12	2:H:144:VAL:N	2.18	0.59
1:L:143:GLU:CD	1:L:143:GLU:H	1.92	0.59
2:M:126:PRO:O	2:M:127:SER:O	2.20	0.59
2:M:51:ILE:O	2:M:51:ILE:CG2	2.50	0.59
2:M:17:SER:OG	2:M:82(A):HIS:CD2	2.55	0.59
6:H:232:BMA:C6	6:H:234:MAN:C3	2.63	0.59
2:H:147:TYR:N	2:H:184:LEU:HB3	2.18	0.59
3:K:216:BMA:H62	3:K:218:MAN:H3	1.85	0.59
2:M:100(C):ASN:ND2	2:M:100(C):ASN:O	2.35	0.59
1:K:133:VAL:HG12	1:K:134:CYS:O	2.03	0.59
2:H:120:SER:HB3	2:H:122:PHE:CZ	2.39	0.58
2:M:18:LEU:CB	2:M:82(C):MET:HE1	2.33	0.58
1:L:3:VAL:HB	1:L:26:SER:HB2	1.85	0.58
2:H:11:LEU:HD12	2:H:110:THR:HG23	1.84	0.58
1:K:188:LYS:CG	1:K:188:LYS:O	2.50	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:79:GLN:O	1:L:82:ASP:N	2.31	0.58
1:K:48:ILE:HA	1:K:53:THR:O	2.03	0.58
2:M:165:ALA:O	2:M:166:LEU:C	2.42	0.58
3:K:219:MAN:HO2	5:M:234:MAN:H2	1.63	0.58
1:L:106:ILE:CG2	1:L:106:ILE:O	2.48	0.58
1:L:25:ALA:O	1:L:26:SER:C	2.41	0.58
2:M:141:GLY:HA3	2:M:189:SER:O	2.04	0.58
2:H:100(A):SER:OG	2:H:100(D):ASP:OD2	2.16	0.58
4:L:214:MAN:C5	6:H:234:MAN:O3	2.51	0.58
2:H:167:THR:O	2:H:168:SER:C	2.42	0.58
2:H:221:LYS:NZ	2:H:221:LYS:HB3	2.18	0.58
1:L:6:GLN:HG2	1:L:88:CYS:SG	2.43	0.58
1:K:149:LYS:HA	1:K:153:ALA:O	2.04	0.58
1:L:164:THR:HB	1:L:174:SER:O	2.04	0.57
1:L:85:THR:OG1	1:L:103:ARG:HB3	2.04	0.57
2:H:4:LEU:HG	2:H:24:VAL:HG12	1.86	0.57
2:H:137:THR:HA	2:H:194:PRO:HA	1.86	0.57
2:M:25:SER:O	2:M:26:ASN:HB2	2.04	0.57
1:L:164:THR:CG2	1:L:174:SER:H	2.18	0.57
2:M:6:GLU:OE2	2:M:106:GLY:HA2	2.04	0.57
1:K:118:PHE:N	1:K:133:VAL:O	2.36	0.57
1:K:184:ALA:O	1:K:188:LYS:HB3	2.04	0.57
1:L:94:TYR:O	1:L:95:SER:HB3	2.05	0.57
2:M:193:VAL:HG23	2:M:194:PRO:N	2.20	0.57
2:M:121:VAL:HG21	2:M:210:VAL:HG21	1.86	0.57
1:K:142:ARG:HB2	1:K:173:TYR:CE2	2.40	0.57
2:H:147:TYR:H	2:H:184:LEU:HB3	1.69	0.57
1:L:11:LEU:CD1	1:L:11:LEU:C	2.67	0.56
2:M:78:VAL:HG12	2:M:79:TYR:N	2.18	0.56
2:H:228:LYS:CG	2:H:229:SER:H	2.18	0.56
1:L:6:GLN:C	1:L:100:GLN:HE22	2.08	0.56
1:L:25:ALA:CB	1:L:27:GLN:O	2.54	0.56
1:K:20:THR:HB	1:K:74:THR:HG22	1.86	0.56
2:M:38:ARG:HB2	2:M:88:ALA:HB1	1.88	0.56
1:L:71:PHE:O	1:L:72:THR:HG23	2.05	0.56
2:H:213:LYS:N	2:H:214:PRO:CD	2.69	0.56
1:K:148:TRP:CE3	1:K:193:ALA:O	2.58	0.56
1:K:35:TRP:CZ3	1:K:88:CYS:HB3	2.40	0.56
2:M:33:THR:HG23	2:M:52:SER:HA	1.87	0.56
2:H:194:PRO:O	2:H:197:SER:OG	2.14	0.56
1:L:12:SER:HB3	1:L:107:LYS:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:150:VAL:O	1:L:153:ALA:HB3	2.05	0.56
2:M:18:LEU:HD12	2:M:19:ILE:H	1.71	0.56
2:M:112:SER:O	2:M:113:PRO:N	2.40	0.55
1:K:4:MET:HE2	1:K:23:CYS:SG	2.45	0.55
2:M:59:TYR:HB3	2:M:63:VAL:HG23	1.87	0.55
2:H:97:SER:HB3	2:H:100(E):PRO:HD2	1.87	0.55
2:H:122:PHE:O	2:H:143:LEU:HB3	2.06	0.55
1:L:6:GLN:HE22	1:L:102:THR:N	2.04	0.55
1:L:164:THR:HG23	1:L:165:GLU:O	2.07	0.55
1:L:83:PHE:CE2	1:L:106:ILE:HA	2.40	0.55
2:M:128:SER:O	2:M:133:THR:CG2	2.55	0.55
2:M:179:GLN:HG3	2:M:184:LEU:O	2.07	0.55
4:L:214:MAN:H5	6:H:234:MAN:HO3	1.69	0.54
2:H:219:VAL:O	2:H:219:VAL:CG1	2.55	0.54
2:M:67:PHE:HA	2:M:81:GLN:O	2.08	0.54
2:H:87:THR:HG23	2:H:110:THR:HA	1.88	0.54
1:K:23:CYS:HB2	1:K:35:TRP:CH2	2.42	0.54
1:K:23:CYS:SG	1:K:33:LEU:HD21	2.48	0.54
1:K:44:PRO:HG3	2:M:103:TRP:CE3	2.42	0.54
2:H:32:HIS:CE1	2:H:94:ARG:HH11	2.25	0.54
1:K:196:VAL:CG1	1:K:197:THR:N	2.70	0.54
2:H:24:VAL:CG1	2:H:27:PHE:CZ	2.89	0.54
1:K:190:LYS:NZ	1:K:210:ASN:HD22	2.06	0.54
1:L:103:ARG:O	1:L:103:ARG:HG3	2.07	0.54
1:L:44:PRO:HG2	2:H:103:TRP:CE3	2.43	0.54
2:M:18:LEU:HD12	2:M:19:ILE:N	2.23	0.54
1:K:44:PRO:CG	2:M:103:TRP:CE3	2.90	0.54
1:K:164:THR:HG22	1:K:165:GLU:O	2.08	0.54
1:L:11:LEU:HD12	1:L:12:SER:N	2.23	0.54
2:M:212:HIS:CD2	2:M:215:SER:OG	2.60	0.54
1:K:158:ASN:OD1	1:K:158:ASN:N	2.41	0.54
2:M:118:GLY:HA2	2:M:212:HIS:HD2	1.73	0.54
2:M:6:GLU:OE2	2:M:106:GLY:N	2.41	0.54
1:K:33:LEU:HD13	1:K:89:GLN:O	2.07	0.54
1:L:55:LYS:O	1:L:58:VAL:HB	2.08	0.53
2:M:134:SER:O	2:M:136:GLY:N	2.41	0.53
2:M:36:TRP:CD1	2:M:80:LEU:HD13	2.43	0.53
2:H:112:SER:C	2:H:113:PRO:CA	2.70	0.53
1:K:44:PRO:CG	2:M:103:TRP:CD2	2.91	0.53
1:L:136:LEU:HD21	1:L:196:VAL:CG1	2.39	0.53
1:K:139:PHE:HD2	1:K:140:TYR:N	2.06	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:97:SER:HB3	2:H:100(D):ASP:HB3	1.89	0.53
1:K:116:PHE:HD2	1:K:135:LEU:HD13	1.72	0.53
2:M:12:VAL:O	2:M:112:SER:N	2.40	0.53
1:L:141:PRO:HG3	1:L:199:GLN:OE1	2.08	0.53
2:H:27:PHE:O	2:H:28:ARG:C	2.47	0.53
2:H:179:GLN:O	2:H:182:SER:N	2.42	0.53
1:K:112:ALA:CB	1:K:201:LEU:HD13	2.38	0.53
2:H:144:VAL:HB	2:H:187:LEU:HD12	1.91	0.53
2:H:146:ASP:H	2:H:186:SER:HB2	1.73	0.53
1:L:12:SER:CB	1:L:107:LYS:HB2	2.39	0.53
1:L:125:LEU:HD22	1:L:186:TYR:CE2	2.44	0.53
2:H:126:PRO:CG	2:H:140:LEU:HD12	2.33	0.53
2:H:171:VAL:HG23	2:H:191:VAL:CG2	2.39	0.52
1:L:89:GLN:HB2	1:L:98:PHE:CD2	2.45	0.52
1:L:209:PHE:CD1	1:L:209:PHE:C	2.83	0.52
2:H:228:LYS:CD	2:H:229:SER:H	2.22	0.52
1:K:88:CYS:O	1:K:88:CYS:SG	2.68	0.52
1:K:139:PHE:HE2	1:K:142:ARG:HA	1.74	0.52
1:K:103:ARG:CZ	1:K:142:ARG:NH1	2.73	0.52
2:H:175:PRO:HB2	1:K:162:SER:HG	1.74	0.52
1:K:105:GLU:CG	1:K:106:ILE:N	2.73	0.52
1:K:136:LEU:HB2	1:K:175:LEU:HB3	1.90	0.52
2:M:137:THR:HG22	2:M:138:ALA:H	1.73	0.52
6:H:233:MAN:C2	4:H:237:MAN:C1	2.86	0.52
2:M:6:GLU:OE2	2:M:106:GLY:CA	2.58	0.52
2:H:2:VAL:CG2	2:H:27:PHE:CD2	2.92	0.52
1:L:12:SER:HB3	1:L:107:LYS:CA	2.39	0.52
2:H:126:PRO:HG2	2:H:226:GLU:C	2.30	0.52
1:L:37:GLN:HG2	1:L:38:GLN:N	2.25	0.52
2:H:124:LEU:HD13	1:K:118:PHE:CD2	2.44	0.52
2:H:124:LEU:HD22	1:K:118:PHE:HB3	1.92	0.52
2:M:121:VAL:CG2	2:M:210:VAL:HG21	2.40	0.52
1:K:40:PRO:O	1:K:42:LYS:HG2	2.10	0.52
2:H:36:TRP:C	2:H:37:VAL:HG12	2.26	0.52
2:M:66:ARG:HB3	2:M:82(A):HIS:O	2.10	0.51
2:H:222:LYS:HD2	2:H:226:GLU:HG2	1.92	0.51
2:M:4:LEU:HD12	2:M:4:LEU:N	2.25	0.51
1:L:194:CYS:O	1:L:206:THR:HA	2.10	0.51
2:H:228:LYS:HD3	2:H:229:SER:HG	1.67	0.51
4:H:237:MAN:C2	4:H:238:MAN:C5	2.88	0.51
1:L:25:ALA:HB1	1:L:27:GLN:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:172:HIS:HB2	2:H:190:VAL:CG2	2.38	0.51
2:H:102:ALA:C	2:H:103:TRP:CD1	2.84	0.51
2:M:176:ALA:HA	2:M:187:LEU:HB3	1.92	0.51
1:K:128:GLY:O	1:K:183:LYS:HB2	2.09	0.51
1:K:82:ASP:O	1:K:86:TYR:OH	2.23	0.51
2:H:199:GLY:C	2:H:203:GLN:H	2.14	0.51
1:L:125:LEU:CD2	1:L:186:TYR:HE2	2.23	0.51
2:M:147:TYR:N	2:M:147:TYR:CD1	2.78	0.51
2:H:27:PHE:O	2:H:27:PHE:CG	2.64	0.51
1:L:154:LEU:C	1:L:155:GLN:HG2	2.30	0.51
2:M:112:SER:C	2:M:113:PRO:CA	2.74	0.51
1:K:18:THR:HG23	1:K:76:SER:CA	2.33	0.51
2:M:86:ASP:O	2:M:90:TYR:OH	2.18	0.51
2:H:40:VAL:HG23	2:H:41:PRO:O	2.11	0.51
1:K:18:THR:HG22	1:K:75:ILE:O	2.11	0.50
1:K:146:VAL:HG13	1:K:194:CYS:SG	2.50	0.50
1:L:192:TYR:HB2	1:L:209:PHE:CZ	2.47	0.50
2:M:128:SER:O	2:M:133:THR:HG23	2.11	0.50
2:M:51:ILE:O	2:M:51:ILE:HG23	2.11	0.50
1:L:140:TYR:CG	1:L:141:PRO:HA	2.46	0.50
1:L:133:VAL:CG1	1:L:134:CYS:N	2.75	0.50
1:L:125:LEU:O	1:L:183:LYS:HG3	2.11	0.50
1:K:137:ASN:CG	1:K:138:ASN:HD22	2.15	0.50
1:K:139:PHE:CD2	1:K:140:TYR:N	2.80	0.50
1:L:94:TYR:CE1	2:H:56:TYR:CE2	2.99	0.50
1:L:143:GLU:N	1:L:143:GLU:CD	2.63	0.50
1:L:116:PHE:O	1:L:134:CYS:HA	2.11	0.50
2:M:100(B):ASP:OD1	4:M:230:MAN:C1	2.59	0.50
1:K:91:TYR:O	1:K:91:TYR:CG	2.65	0.50
1:L:10:THR:CG2	1:L:11:LEU:N	2.73	0.50
1:K:15:VAL:HG21	1:K:80:PHE:CD1	2.46	0.50
1:L:113:PRO:HA	1:L:139:PHE:HB3	1.93	0.50
2:M:98:ASP:C	2:M:100:LEU:H	2.15	0.50
1:L:12:SER:HB2	1:L:107:LYS:HB2	1.93	0.50
1:L:125:LEU:HD22	1:L:186:TYR:HE2	1.75	0.50
2:H:112:SER:CA	2:H:113:PRO:N	2.69	0.50
2:M:97:SER:O	2:M:100:LEU:HB3	2.11	0.50
1:L:44:PRO:HG2	2:H:103:TRP:CZ3	2.47	0.50
1:K:89:GLN:HB2	1:K:98:PHE:CG	2.47	0.50
3:K:218:MAN:O3	4:M:232:MAN:O5	2.30	0.49
2:M:6:GLU:H	2:M:6:GLU:CD	2.14	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:18:LEU:CB	2:M:82(C):MET:CE	2.90	0.49
1:K:68:GLY:O	1:K:71:PHE:HE1	1.95	0.49
1:L:145:LYS:HB2	1:L:197:THR:HB	1.93	0.49
2:H:226:GLU:CB	2:H:227:PRO:CD	2.84	0.49
1:K:40:PRO:HG3	1:K:165:GLU:CD	2.31	0.49
2:M:211:ASN:HD21	2:M:218:LYS:CD	2.10	0.49
2:H:26:ASN:O	2:H:27:PHE:HB3	2.12	0.49
1:L:125:LEU:CD1	1:L:183:LYS:HG2	2.40	0.49
1:K:187:GLU:HG3	1:K:211:ARG:NH2	2.27	0.49
1:L:121:SER:OG	1:L:124:GLN:N	2.30	0.49
2:H:25:SER:O	2:H:26:ASN:HB2	2.11	0.49
1:K:115:VAL:C	1:K:116:PHE:CD2	2.86	0.49
1:L:121:SER:HG	1:L:124:GLN:H	1.58	0.49
2:M:97:SER:O	2:M:98:ASP:CB	2.61	0.49
1:L:124:GLN:NE2	1:L:131:SER:HB2	2.24	0.49
2:H:212:HIS:NE2	2:H:215:SER:HB3	2.25	0.49
1:K:36:TYR:HA	1:K:45:LYS:O	2.13	0.49
1:L:71:PHE:O	1:L:72:THR:CG2	2.60	0.49
2:H:199:GLY:C	2:H:203:GLN:N	2.66	0.49
1:K:92:ALA:O	2:M:100(C):ASN:OD1	2.30	0.49
2:M:113:PRO:C	2:M:114:ALA:O	2.51	0.49
3:K:217:MAN:HO2	4:M:230:MAN:H2	1.78	0.49
1:L:148:TRP:CD2	1:L:179:LEU:HD22	2.47	0.49
2:M:52:SER:CB	2:M:56:TYR:HB2	2.36	0.49
1:L:70:GLU:C	1:L:71:PHE:CD1	2.86	0.49
1:L:21:ILE:O	1:L:72:THR:HA	2.12	0.49
2:H:178:LEU:HD12	2:H:179:GLN:H	1.78	0.48
1:K:126:LYS:C	1:K:128:GLY:N	2.62	0.48
2:H:59:TYR:CE2	2:H:69:VAL:HG12	2.48	0.48
2:H:113:PRO:O	2:H:114:ALA:C	2.49	0.48
2:H:82(A):HIS:O	2:H:82(B):LYS:C	2.52	0.48
2:H:208:CYS:C	2:H:209:ASN:HD22	2.16	0.48
1:L:50:LYS:HB2	1:L:50:LYS:HE3	1.51	0.48
2:H:178:LEU:HD12	2:H:179:GLN:N	2.27	0.48
1:L:201:LEU:HD13	1:L:201:LEU:HA	1.30	0.48
1:K:142:ARG:O	1:K:144:ALA:N	2.46	0.48
2:M:100(A):SER:HB3	4:M:231:MAN:H3	1.94	0.48
4:M:230:MAN:C2	4:M:231:MAN:C5	2.92	0.48
1:K:142:ARG:HD3	1:K:173:TYR:HE2	1.79	0.48
1:L:83:PHE:HA	1:L:104:VAL:HG12	1.96	0.48
1:K:34:ALA:HA	1:K:49:TYR:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:215:SER:OG	2:M:217:THR:HB	2.13	0.48
1:L:137:ASN:HD21	1:L:138:ASN:HD22	1.61	0.48
2:H:150:GLU:OE1	2:H:176:ALA:HB3	2.14	0.48
2:H:37:VAL:HG23	2:H:38:ARG:N	2.29	0.48
2:M:2:VAL:HG23	2:M:2:VAL:O	2.14	0.48
1:K:185:ASP:N	1:K:185:ASP:OD1	2.47	0.48
1:L:175:LEU:HD22	1:L:175:LEU:O	2.09	0.48
2:M:94:ARG:HG3	2:M:95:LYS:N	2.29	0.48
1:L:198:HIS:CG	1:L:199:GLN:H	2.32	0.48
4:H:237:MAN:C2	4:H:238:MAN:H5	2.44	0.47
1:L:198:HIS:ND1	1:L:199:GLN:N	2.55	0.47
3:K:218:MAN:C3	4:M:232:MAN:C1	2.91	0.47
1:L:128:GLY:O	1:L:183:LYS:HB2	2.14	0.47
1:K:155:GLN:OE1	1:K:158:ASN:ND2	2.39	0.47
1:K:135:LEU:CD2	1:K:135:LEU:C	2.83	0.47
1:L:125:LEU:HG	1:L:183:LYS:HZ3	1.79	0.47
2:M:59:TYR:HB3	2:M:63:VAL:CG2	2.44	0.47
1:K:139:PHE:O	1:K:140:TYR:HB2	2.14	0.47
2:H:52(A):THR:HA	2:H:71:ARG:NH1	2.30	0.47
1:K:142:ARG:CD	1:K:173:TYR:CE2	2.97	0.47
1:K:132:VAL:O	1:K:148:TRP:CZ2	2.66	0.47
2:M:32:HIS:CD2	2:M:94:ARG:NE	2.80	0.47
1:K:196:VAL:HG12	1:K:197:THR:N	2.29	0.47
2:H:174:PHE:O	2:H:175:PRO:C	2.53	0.47
1:K:66:GLY:HA3	1:K:71:PHE:CD2	2.50	0.47
2:H:228:LYS:HD3	2:H:229:SER:H	1.79	0.47
2:H:212:HIS:CE1	2:H:214:PRO:HD2	2.50	0.47
1:L:186:TYR:HD1	1:L:192:TYR:HH	1.62	0.47
2:H:162:ASN:O	2:H:165:ALA:HB3	2.15	0.47
2:M:143:LEU:C	2:M:143:LEU:HD12	2.35	0.47
1:K:5:THR:O	1:K:24:ARG:HB3	2.15	0.47
2:H:228:LYS:CG	2:H:229:SER:N	2.78	0.47
2:H:212:HIS:ND1	2:H:214:PRO:HD2	2.29	0.47
1:L:11:LEU:HD13	1:L:11:LEU:HA	1.50	0.47
2:M:213:LYS:O	2:M:216:ASN:N	2.38	0.47
1:L:55:LYS:HA	1:L:55:LYS:HE2	1.97	0.47
1:K:159:SER:CA	1:K:179:LEU:HA	2.44	0.46
1:K:115:VAL:C	1:K:116:PHE:CG	2.89	0.46
2:H:186:SER:HG	2:H:187:LEU:H	1.63	0.46
1:L:102:THR:HG22	1:L:103:ARG:N	2.28	0.46
1:K:36:TYR:CD2	1:K:36:TYR:N	2.82	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:118:PHE:CB	1:K:133:VAL:O	2.63	0.46
2:M:128:SER:HB2	2:M:133:THR:CG2	2.41	0.46
1:K:148:TRP:HE3	1:K:193:ALA:O	1.97	0.46
2:H:212:HIS:HE1	2:H:214:PRO:HG2	1.72	0.46
1:K:11:LEU:HB3	1:K:104:VAL:HG22	1.98	0.46
2:M:225:VAL:HG12	2:M:225:VAL:O	2.14	0.46
1:L:125:LEU:CD2	1:L:186:TYR:CE2	2.98	0.46
2:M:60:ALA:O	2:M:63:VAL:N	2.40	0.46
1:L:154:LEU:CD1	1:L:155:GLN:H	2.25	0.46
2:M:18:LEU:HA	2:M:18:LEU:HD12	1.25	0.46
2:M:88:ALA:HB3	2:M:90:TYR:CD1	2.47	0.46
2:M:195:SER:OG	2:M:196:SER:N	2.48	0.46
2:H:94:ARG:HB2	2:H:102:ALA:HB3	1.98	0.46
2:H:74:LEU:HD22	2:H:74:LEU:HA	1.76	0.46
2:M:82:MET:CE	2:M:82:MET:HB2	2.46	0.46
6:H:235:MAN:C1	6:H:236:MAN:C5	2.93	0.46
1:K:128:GLY:C	1:K:183:LYS:HB2	2.36	0.46
1:L:13:ALA:HB3	1:L:78:LEU:CD2	2.46	0.46
2:H:125:ALA:O	2:H:126:PRO:C	2.54	0.46
1:L:137:ASN:ND2	1:L:138:ASN:HD22	2.13	0.46
1:K:135:LEU:C	1:K:135:LEU:HD23	2.36	0.46
2:H:213:LYS:N	2:H:214:PRO:HD3	2.30	0.46
1:K:4:MET:HE1	1:K:23:CYS:SG	2.56	0.46
1:K:115:VAL:O	1:K:116:PHE:CD2	2.69	0.46
1:K:140:TYR:CD1	1:K:140:TYR:C	2.88	0.46
2:M:157:TRP:CZ3	2:M:208:CYS:HB3	2.51	0.46
1:K:95:SER:O	1:K:96:ALA:HB2	2.16	0.46
1:L:111:ALA:O	1:L:140:TYR:O	2.33	0.46
2:H:150:GLU:HA	2:H:151:PRO:HA	1.82	0.46
1:K:7:SER:OG	1:K:7:SER:O	2.31	0.46
2:H:32:HIS:O	2:H:71:ARG:NH2	2.43	0.45
1:L:207:LYS:HA	1:L:207:LYS:HD2	1.77	0.45
1:K:135:LEU:HD23	1:K:136:LEU:N	2.31	0.45
2:H:228:LYS:O	2:H:229:SER:O	2.34	0.45
1:L:85:THR:CG2	1:L:86:TYR:H	2.27	0.45
1:K:145:LYS:HB3	1:K:197:THR:HB	1.98	0.45
1:K:147:GLN:HB2	1:K:195:GLU:CB	2.42	0.45
1:K:133:VAL:HG13	1:K:177:SER:O	2.16	0.45
1:L:54:LEU:HD21	1:L:58:VAL:HG12	1.99	0.45
1:L:114:SER:OG	1:L:137:ASN:HB3	2.17	0.45
2:M:87:THR:HG22	2:M:87:THR:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:89:GLN:HB3	1:K:98:PHE:CD2	2.50	0.45
1:L:125:LEU:O	1:L:126:LYS:C	2.54	0.45
2:M:62:ALA:O	2:M:66:ARG:NH2	2.33	0.45
2:H:209:ASN:HA	2:H:220:ASP:OD2	2.17	0.45
2:M:87:THR:CG2	2:M:110:THR:HG22	2.43	0.45
1:L:9:SER:O	1:L:102:THR:HG23	2.17	0.45
2:H:22:CYS:HB2	2:H:36:TRP:CH2	2.51	0.45
1:K:142:ARG:HD3	1:K:173:TYR:CE2	2.52	0.45
1:L:163:VAL:HG23	1:L:175:LEU:CB	2.42	0.45
2:M:29:ILE:CG2	2:M:34:MET:HE2	2.47	0.45
2:M:2:VAL:CG1	2:M:94:ARG:NH1	2.60	0.45
1:L:25:ALA:HB3	1:L:27:GLN:O	2.16	0.45
2:H:40:VAL:O	2:H:43:GLY:HA2	2.17	0.45
2:H:157:TRP:HA	2:H:207:ILE:O	2.17	0.45
1:K:180:THR:CG2	1:K:181:LEU:N	2.80	0.45
1:K:166:GLN:HE21	1:K:171:SER:HB3	1.81	0.44
1:L:35:TRP:CZ3	1:L:88:CYS:HB3	2.52	0.44
1:K:84:ALA:O	1:K:86:TYR:CE1	2.70	0.44
1:L:10:THR:CG2	1:L:11:LEU:H	2.26	0.44
1:K:187:GLU:HA	1:K:211:ARG:CZ	2.47	0.44
2:M:212:HIS:CE1	2:M:214:PRO:CD	2.96	0.44
1:K:108:ARG:O	1:K:109:THR:C	2.56	0.44
1:L:71:PHE:C	1:L:72:THR:HG23	2.37	0.44
1:L:136:LEU:HD21	1:L:196:VAL:HG13	1.99	0.44
1:K:64:GLY:HA2	1:K:72:THR:O	2.17	0.44
2:M:3:GLN:O	2:M:25:SER:N	2.47	0.44
1:L:33:LEU:HG	1:L:34:ALA:N	2.32	0.44
1:L:36:TYR:HE2	1:L:89:GLN:NE2	2.16	0.44
1:L:164:THR:HG22	1:L:174:SER:H	1.81	0.44
1:L:38:GLN:HG3	1:L:44:PRO:HA	1.99	0.44
1:K:89:GLN:CB	1:K:98:PHE:CE2	3.00	0.44
2:H:167:THR:O	2:H:169:GLY:N	2.51	0.44
1:L:33:LEU:HD22	1:L:71:PHE:CD2	2.52	0.44
2:H:163:SER:O	2:H:165:ALA:N	2.41	0.44
1:K:117:ILE:HG21	1:K:209:PHE:HD2	1.83	0.44
1:K:142:ARG:CD	1:K:173:TYR:HE2	2.31	0.44
2:H:18:LEU:HB2	2:H:82(C):MET:HE3	1.92	0.44
1:K:137:ASN:HD21	1:K:138:ASN:ND2	2.10	0.44
1:L:136:LEU:HD21	1:L:196:VAL:HG11	1.99	0.44
2:M:173:THR:CG2	2:M:189:SER:HB2	2.34	0.44
2:M:121:VAL:CG1	2:M:122:PHE:N	2.67	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:49:TYR:HE1	1:L:55:LYS:HE2	1.83	0.44
2:M:212:HIS:O	2:M:215:SER:OG	2.24	0.44
2:H:193:VAL:HA	2:H:194:PRO:HD3	1.79	0.44
2:M:14:ALA:O	2:M:115:SER:HB3	2.17	0.44
1:L:139:PHE:HE2	1:L:142:ARG:O	2.00	0.44
2:H:171:VAL:CG2	2:H:191:VAL:CG2	2.96	0.44
2:M:228:LYS:O	2:M:229:SER:OG	2.30	0.44
2:M:29:ILE:HG23	2:M:34:MET:HE2	1.95	0.43
2:H:157:TRP:CE3	2:H:207:ILE:O	2.71	0.43
1:L:90:HIS:CD2	1:L:90:HIS:C	2.88	0.43
1:K:136:LEU:O	1:K:139:PHE:HD1	2.01	0.43
6:H:232:BMA:H62	6:H:234:MAN:C3	2.21	0.43
2:M:179:GLN:O	2:M:182:SER:N	2.51	0.43
1:K:172:THR:C	1:K:173:TYR:CD1	2.87	0.43
2:M:98:ASP:C	2:M:100:LEU:N	2.71	0.43
1:K:33:LEU:HD13	1:K:33:LEU:HA	1.88	0.43
1:K:146:VAL:HG11	1:K:177:SER:CB	2.48	0.43
1:L:46:LEU:HD23	1:L:55:LYS:HD3	1.99	0.43
2:M:177:VAL:HG13	2:M:178:LEU:N	2.32	0.43
1:K:47:LEU:HA	1:K:58:VAL:HG21	2.01	0.43
1:K:117:ILE:CG2	1:K:209:PHE:HD2	2.30	0.43
1:L:24:ARG:HA	1:L:69:THR:O	2.18	0.43
2:H:144:VAL:HG22	2:H:210:VAL:HG21	1.99	0.43
1:K:147:GLN:OE1	1:K:154:LEU:HD11	2.18	0.43
2:H:75:GLU:HG3	2:M:57:ARG:CZ	2.44	0.43
4:M:230:MAN:C2	4:M:231:MAN:H5	2.48	0.43
2:H:4:LEU:HD11	2:H:27:PHE:HZ	1.84	0.43
2:H:212:HIS:CG	2:H:214:PRO:HD2	2.54	0.43
1:K:68:GLY:O	1:K:71:PHE:CE1	2.70	0.43
2:M:75:GLU:HB3	2:M:77:PHE:HE1	1.84	0.43
1:K:179:LEU:HD11	1:K:181:LEU:HG	2.01	0.43
1:K:84:ALA:O	1:K:86:TYR:CD1	2.72	0.43
2:H:33:THR:OG1	2:H:52:SER:HA	2.18	0.43
2:M:141:GLY:HA2	2:M:157:TRP:CH2	2.54	0.43
2:H:123:PRO:HD2	1:K:121:SER:HB2	2.01	0.43
1:L:175:LEU:HA	2:M:174:PHE:CE2	2.53	0.43
2:H:147:TYR:CE1	2:H:186:SER:HA	2.53	0.43
1:K:89:GLN:HB3	1:K:98:PHE:CE2	2.54	0.43
2:M:119:PRO:HB3	2:M:144:VAL:HG12	2.01	0.43
1:L:124:GLN:HE22	1:L:131:SER:CB	2.26	0.43
2:M:121:VAL:HG21	2:M:210:VAL:CG2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:119:PRO:HA	1:K:120:PRO:HD2	1.47	0.43
2:M:41:PRO:C	2:M:43:GLY:N	2.72	0.43
2:H:121:VAL:O	2:H:221:LYS:HE2	2.19	0.42
2:M:38:ARG:HD3	2:M:48:VAL:HG23	2.00	0.42
1:K:150:VAL:HG23	1:K:155:GLN:NE2	2.34	0.42
1:L:20:THR:CG2	1:L:74:THR:HG22	2.49	0.42
1:K:37:GLN:CG	1:K:38:GLN:N	2.80	0.42
1:K:175:LEU:O	1:K:176:SER:CB	2.67	0.42
2:H:147:TYR:O	2:H:185:TYR:N	2.51	0.42
2:M:18:LEU:HB3	2:M:82(C):MET:CE	2.49	0.42
2:M:66:ARG:O	2:M:82(A):HIS:HB2	2.19	0.42
1:L:14:SER:H	1:L:17:ASP:CG	2.23	0.42
2:H:36:TRP:CE2	2:H:80:LEU:HB2	2.55	0.42
1:K:92:ALA:HB3	1:K:95:SER:O	2.19	0.42
2:H:212:HIS:HD2	2:H:215:SER:CB	2.28	0.42
1:K:94:TYR:CD1	2:M:56:TYR:CE2	3.08	0.42
2:H:113:PRO:O	2:H:115:SER:N	2.52	0.42
1:L:113:PRO:HB3	1:L:139:PHE:HB3	2.02	0.42
2:M:209:ASN:HB3	2:M:220:ASP:OD2	2.20	0.42
1:K:49:TYR:CD1	1:K:49:TYR:N	2.86	0.42
1:K:105:GLU:HG2	1:K:106:ILE:N	2.33	0.42
2:H:129:LYS:HB3	2:H:130:SER:H	1.68	0.42
1:L:30:GLU:HB3	1:L:31:THR:H	1.58	0.42
1:L:175:LEU:CA	2:M:174:PHE:CE2	3.03	0.42
2:H:81:GLN:HE21	2:H:81:GLN:HB3	1.55	0.42
1:L:106:ILE:HB	1:L:166:GLN:CD	2.39	0.42
2:M:18:LEU:HB3	2:M:82(C):MET:HE2	2.01	0.42
2:M:94:ARG:HG2	2:M:101:ASP:CG	2.36	0.42
2:H:144:VAL:CG2	2:H:210:VAL:HG21	2.50	0.42
1:L:186:TYR:HD1	1:L:192:TYR:OH	2.03	0.42
1:K:55:LYS:HD3	1:K:55:LYS:HA	1.79	0.42
2:H:97:SER:OG	2:H:98:ASP:N	2.53	0.42
1:L:102:THR:CG2	1:L:103:ARG:N	2.81	0.42
2:H:102:ALA:O	2:H:103:TRP:CD1	2.73	0.42
2:M:190:VAL:HG23	2:M:191:VAL:N	2.35	0.42
2:H:229:SER:CA	2:H:229:SER:OG	2.57	0.41
1:L:198:HIS:CG	1:L:199:GLN:N	2.88	0.41
1:L:49:TYR:HE1	1:L:55:LYS:CE	2.33	0.41
2:M:100:LEU:O	2:M:100(A):SER:HB2	2.19	0.41
1:L:179:LEU:HA	1:L:179:LEU:HD13	1.75	0.41
1:L:2:VAL:CG2	1:L:2:VAL:CA	2.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:84:VAL:O	2:M:87:THR:N	2.53	0.41
1:K:188:LYS:HG2	1:K:188:LYS:O	2.18	0.41
1:L:154:LEU:HA	1:L:154:LEU:HD12	1.64	0.41
6:H:234:MAN:H61	6:H:235:MAN:C5	2.51	0.41
1:K:161:GLU:HG2	1:K:177:SER:OG	2.20	0.41
1:K:201:LEU:HA	1:K:201:LEU:HD12	1.70	0.41
1:L:94:TYR:HE1	2:H:56:TYR:CE2	2.38	0.41
4:H:237:MAN:C1	4:H:238:MAN:H5	2.50	0.41
3:K:216:BMA:H61	3:K:218:MAN:H2	1.05	0.41
2:M:100:LEU:O	2:M:100(A):SER:CB	2.68	0.41
1:L:11:LEU:HB3	1:L:104:VAL:HA	2.02	0.41
2:H:74:LEU:N	2:H:74:LEU:HD23	2.35	0.41
2:M:203:GLN:O	2:M:206:TYR:CD2	2.74	0.41
1:L:12:SER:HB2	1:L:107:LYS:CB	2.51	0.41
2:M:103:TRP:N	2:M:103:TRP:CD1	2.88	0.41
2:H:210:VAL:HB	2:H:219:VAL:HG12	2.02	0.41
1:K:38:GLN:NE2	1:K:44:PRO:HB3	2.36	0.41
1:K:16:GLY:N	1:K:78:LEU:O	2.52	0.41
1:L:113:PRO:CB	1:L:139:PHE:HB3	2.51	0.41
1:K:133:VAL:HG22	1:K:178:THR:CG2	2.41	0.41
1:L:135:LEU:HD11	2:M:190:VAL:HG11	2.03	0.41
2:M:216:ASN:ND2	2:M:216:ASN:N	2.64	0.41
2:M:47:TRP:HZ2	2:M:50:SER:HB3	1.86	0.41
4:H:237:MAN:H2	4:H:238:MAN:C5	2.50	0.41
2:H:143:LEU:C	2:H:143:LEU:CD1	2.87	0.41
2:H:205:THR:OG1	2:H:206:TYR:N	2.54	0.41
1:K:11:LEU:HD12	1:K:12:SER:H	1.86	0.41
2:H:33:THR:HG22	2:H:35:ASN:HD21	1.85	0.41
2:M:207:ILE:HG22	2:M:208:CYS:N	2.36	0.41
2:M:143:LEU:HD12	2:M:187:LEU:O	2.21	0.41
2:M:127:SER:C	2:M:128:SER:OG	2.59	0.41
2:M:144:VAL:H	2:M:144:VAL:HG23	1.42	0.41
1:K:130:ALA:HB3	1:K:181:LEU:O	2.21	0.41
2:H:11:LEU:N	2:H:11:LEU:CD1	2.84	0.41
2:H:72:ASP:C	2:H:72:ASP:OD1	2.59	0.41
1:L:164:THR:HG21	1:L:174:SER:H	1.85	0.41
1:L:23:CYS:HB2	1:L:35:TRP:CH2	2.55	0.41
1:K:65:SER:N	1:K:72:THR:O	2.54	0.41
1:K:23:CYS:H	1:K:35:TRP:HH2	1.68	0.41
1:K:37:GLN:H	1:K:47:LEU:HD11	1.86	0.41
1:L:94:TYR:CD1	2:H:56:TYR:CD2	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:15:VAL:HG13	1:L:79:GLN:HA	2.02	0.41
2:H:191:VAL:HG12	2:H:193:VAL:HG22	2.03	0.40
2:H:126:PRO:HB3	2:H:198:LEU:HD13	2.03	0.40
2:H:206:TYR:O	2:H:222:LYS:HA	2.21	0.40
1:K:121:SER:O	1:K:125:LEU:HB2	2.20	0.40
2:M:94:ARG:HB3	2:M:101:ASP:OD1	2.22	0.40
1:K:44:PRO:HG2	2:M:103:TRP:CE2	2.56	0.40
1:K:155:GLN:HB3	1:K:158:ASN:HD21	1.85	0.40
2:M:150:GLU:HG3	2:M:185:TYR:CE2	2.56	0.40
1:L:142:ARG:N	1:L:143:GLU:OE2	2.55	0.40
2:H:125:ALA:HA	2:H:126:PRO:HD2	1.99	0.40
2:M:128:SER:O	2:M:133:THR:HG21	2.20	0.40
1:L:49:TYR:O	1:L:50:LYS:C	2.56	0.40
1:K:195:GLU:CA	1:K:206:THR:HG23	2.49	0.40
1:L:12:SER:CB	1:L:107:LYS:CB	3.00	0.40
1:L:136:LEU:N	1:L:136:LEU:HD12	2.37	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	K	210/212 (99%)	158 (75%)	39 (19%)	13 (6%)	2 10
1	L	210/212 (99%)	177 (84%)	24 (11%)	9 (4%)	3 19
2	H	223/225 (99%)	158 (71%)	42 (19%)	23 (10%)	1 3
2	M	221/225 (98%)	155 (70%)	28 (13%)	38 (17%)	0 1
All	All	864/874 (99%)	648 (75%)	133 (15%)	83 (10%)	1 3

All (83) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	26	SER
1	L	51	ALA
1	L	168	SER
2	H	16	GLY
2	H	53	SER
2	H	100(B)	ASP
2	H	129	LYS
2	H	180	SER
2	H	227	PRO
1	K	152	ASN
1	K	176	SER
1	K	187	GLU
2	M	16	GLY
2	M	30	SER
2	M	48	VAL
2	M	74	LEU
2	M	85	GLU
2	M	98	ASP
2	M	100(A)	SER
2	M	114	ALA
2	M	115	SER
2	M	121	VAL
2	M	127	SER
2	M	139	ALA
2	M	146	ASP
2	M	165	ALA
2	M	166	LEU
2	M	180	SER
2	M	195	SER
1	L	154	LEU
2	H	9	GLY
2	H	134	SER
2	H	163	SER
2	H	164	GLY
1	K	82	ASP
1	K	109	THR
1	K	143	GLU
1	K	188	LYS
1	K	191	VAL
1	K	211	ARG
2	M	2	VAL
2	M	9	GLY
2	M	61	ASP

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Mol	Chain	Res	Type
2	M	100(B)	ASP
2	M	106	GLY
2	M	135	GLY
2	M	136	GLY
2	M	186	SER
2	M	216	ASN
1	L	126	LYS
2	H	42	GLY
2	H	85	GLU
2	H	116	THR
1	K	67	SER
2	M	31	ALA
2	M	73	ASP
1	L	17	ASP
1	L	157	GLY
2	H	146	ASP
2	H	175	PRO
1	K	120	PRO
2	M	40	VAL
2	M	99	ARG
2	M	128	SER
2	M	151	PRO
2	M	193	VAL
1	L	204	PRO
2	H	82(B)	LYS
2	H	100(E)	PRO
2	H	128	SER
2	H	148	PHE
2	H	203	GLN
2	H	216	ASN
1	K	142	ARG
2	M	62	ALA
1	L	81	ASP
1	K	140	TYR
2	M	100(E)	PRO
2	M	41	PRO
2	M	194	PRO
2	H	126	PRO
2	M	84	VAL
2	H	151	PRO

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	K	176/183 (96%)	108 (61%)	68 (39%)	0 1
1	L	176/183 (96%)	125 (71%)	51 (29%)	0 2
2	H	185/190 (97%)	119 (64%)	66 (36%)	0 1
2	M	185/190 (97%)	132 (71%)	53 (29%)	0 2
All	All	722/746 (97%)	484 (67%)	238 (33%)	0 1

All (238) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	11	LEU
1	L	12	SER
1	L	15	VAL
1	L	20	THR
1	L	22	THR
1	L	27	GLN
1	L	28	SER
1	L	33	LEU
1	L	42	LYS
1	L	50	LYS
1	L	55	LYS
1	L	61	ARG
1	L	69	THR
1	L	74	THR
1	L	76	SER
1	L	79	GLN
1	L	80	PHE
1	L	89	GLN
1	L	108	ARG
1	L	109	THR
1	L	114	SER
1	L	115	VAL
1	L	122	ASP
1	L	126	LYS

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Mol	Chain	Res	Type
1	L	129	THR
1	L	131	SER
1	L	135	LEU
1	L	145	LYS
1	L	147	GLN
1	L	151	ASP
1	L	160	GLN
1	L	163	VAL
1	L	164	THR
1	L	168	SER
1	L	169	LYS
1	L	175	LEU
1	L	177	SER
1	L	178	THR
1	L	179	LEU
1	L	187	GLU
1	L	190	LYS
1	L	198	HIS
1	L	201	LEU
1	L	202	SER
1	L	203	SER
1	L	204	PRO
1	L	205	VAL
1	L	206	THR
1	L	210	ASN
1	L	211	ARG
1	L	213	GLU
2	H	1	GLU
2	H	7	SER
2	H	11	LEU
2	H	12	VAL
2	H	13	LYS
2	H	18	LEU
2	H	20	LEU
2	H	21	SER
2	H	25	SER
2	H	28	ARG
2	H	30	SER
2	H	37	VAL
2	H	52(A)	THR
2	H	53	SER
2	H	54	SER

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Mol	Chain	Res	Type
2	H	55	THR
2	H	56	TYR
2	H	61	ASP
2	H	64	LYS
2	H	66	ARG
2	H	70	SER
2	H	73	ASP
2	H	74	LEU
2	H	83	ARG
2	H	91	TYR
2	H	94	ARG
2	H	95	LYS
2	H	97	SER
2	H	99	ARG
2	H	100(B)	ASP
2	H	110	THR
2	H	112	SER
2	H	127	SER
2	H	128	SER
2	H	129	LYS
2	H	133	THR
2	H	134	SER
2	H	137	THR
2	H	140	LEU
2	H	142	CYS
2	H	143	LEU
2	H	150	GLU
2	H	151	PRO
2	H	163	SER
2	H	167	THR
2	H	168	SER
2	H	171	VAL
2	H	173	THR
2	H	187	LEU
2	H	189	SER
2	H	190	VAL
2	H	191	VAL
2	H	192	THR
2	H	193	VAL
2	H	195	SER
2	H	196	SER
2	H	198	LEU

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Mol	Chain	Res	Type
2	H	203	GLN
2	H	205	THR
2	H	209	ASN
2	H	215	SER
2	H	217	THR
2	H	218	LYS
2	H	219	VAL
2	H	225	VAL
2	H	226	GLU
1	K	6	GLN
1	K	10	THR
1	K	11	LEU
1	K	12	SER
1	K	14	SER
1	K	18	THR
1	K	20	THR
1	K	23	CYS
1	K	33	LEU
1	K	36	TYR
1	K	37	GLN
1	K	42	LYS
1	K	47	LEU
1	K	54	LEU
1	K	55	LYS
1	K	56	THR
1	K	61	ARG
1	K	69	THR
1	K	72	THR
1	K	76	SER
1	K	78	LEU
1	K	89	GLN
1	K	91	TYR
1	K	95	SER
1	K	97	THR
1	K	102	THR
1	K	104	VAL
1	K	105	GLU
1	K	107	LYS
1	K	108	ARG
1	K	109	THR
1	K	114	SER
1	K	115	VAL

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Mol	Chain	Res	Type
1	K	122	ASP
1	K	125	LEU
1	K	127	SER
1	K	131	SER
1	K	133	VAL
1	K	134	CYS
1	K	135	LEU
1	K	136	LEU
1	K	141	PRO
1	K	142	ARG
1	K	143	GLU
1	K	145	LYS
1	K	149	LYS
1	K	154	LEU
1	K	158	ASN
1	K	165	GLU
1	K	168	SER
1	K	175	LEU
1	K	176	SER
1	K	177	SER
1	K	178	THR
1	K	179	LEU
1	K	181	LEU
1	K	182	SER
1	K	185	ASP
1	K	186	TYR
1	K	187	GLU
1	K	188	LYS
1	K	190	LYS
1	K	191	VAL
1	K	201	LEU
1	K	205	VAL
1	K	207	LYS
1	K	211	ARG
1	K	213	GLU
2	M	3	GLN
2	M	6	GLU
2	M	11	LEU
2	M	12	VAL
2	M	13	LYS
2	M	17	SER
2	M	24	VAL

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Mol	Chain	Res	Type
2	M	25	SER
2	M	28	ARG
2	M	32	HIS
2	M	38	ARG
2	M	45	LEU
2	M	53	SER
2	M	54	SER
2	M	55	THR
2	M	57	ARG
2	M	58	ASP
2	M	66	ARG
2	M	70	SER
2	M	71	ARG
2	M	74	LEU
2	M	87	THR
2	M	91	TYR
2	M	94	ARG
2	M	98	ASP
2	M	100(C)	ASN
2	M	100(F)	PHE
2	M	108	VAL
2	M	116	THR
2	M	120	SER
2	M	128	SER
2	M	129	LYS
2	M	134	SER
2	M	144	VAL
2	M	146	ASP
2	M	152	VAL
2	M	168	SER
2	M	173	THR
2	M	179	GLN
2	M	180	SER
2	M	188	SER
2	M	192	THR
2	M	196	SER
2	M	197	SER
2	M	200	THR
2	M	209	ASN
2	M	213	LYS
2	M	216	ASN
2	M	219	VAL

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Mol	Chain	Res	Type
2	M	221	LYS
2	M	225	VAL
2	M	226	GLU
2	M	228	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	27	GLN
1	L	87	HIS
1	L	89	GLN
1	L	100	GLN
1	L	124	GLN
1	L	137	ASN
2	H	32	HIS
2	H	81	GLN
2	H	82(A)	HIS
2	H	212	HIS
1	K	38	GLN
1	K	90	HIS
1	K	137	ASN
1	K	138	ASN
1	K	147	GLN
1	K	210	ASN
2	M	3	GLN
2	M	81	GLN
2	M	82(A)	HIS
2	M	100(C)	ASN
2	M	212	HIS
2	M	216	ASN

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 (i)

21 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	$\#\|Z\| > 2$
6	NAG	H	230	6	15,15,15	1.20	1 (6%)	17,21,21	2.41	7 (41%)
6	NAG	H	231	6	14,14,15	0.86	0	15,19,21	1.59	4 (26%)
6	BMA	H	232	6	11,11,12	1.14	0	14,15,17	2.98	7 (50%)
6	MAN	H	233	4,6	11,11,12	1.46	3 (27%)	14,15,17	2.00	5 (35%)
6	MAN	H	234	6	11,11,12	0.91	0	14,15,17	2.45	5 (35%)
6	MAN	H	235	6	11,11,12	1.81	3 (27%)	14,15,17	3.71	10 (71%)
6	MAN	H	236	6	11,11,12	2.12	4 (36%)	14,15,17	2.90	4 (28%)
4	MAN	H	237	4,6	11,11,12	1.23	2 (18%)	14,15,17	4.21	10 (71%)
4	MAN	H	238	2,4	11,11,12	1.37	2 (18%)	14,15,17	3.41	6 (42%)
3	NAG	K	214	3	15,15,15	1.62	4 (26%)	17,21,21	2.13	6 (35%)
3	NAG	K	215	3	14,14,15	0.96	1 (7%)	15,19,21	2.83	8 (53%)
3	BMA	K	216	3	11,11,12	1.34	2 (18%)	14,15,17	2.82	9 (64%)
3	MAN	K	217	3	11,11,12	1.09	1 (9%)	14,15,17	2.72	6 (42%)
3	MAN	K	218	3,4	11,11,12	1.20	1 (9%)	14,15,17	3.42	7 (50%)
3	MAN	K	219	3	11,11,12	1.70	3 (27%)	14,15,17	2.26	6 (42%)
4	MAN	L	214	4	11,11,12	1.18	2 (18%)	14,15,17	2.91	8 (57%)
4	MAN	L	215	4	11,11,12	1.48	1 (9%)	14,15,17	2.27	4 (28%)
4	MAN	M	230	2,4	11,11,12	1.60	2 (18%)	14,15,17	3.48	8 (57%)
4	MAN	M	231	4	11,11,12	1.15	1 (9%)	14,15,17	3.34	7 (50%)
4	MAN	M	232	3,4	11,11,12	1.00	0	14,15,17	1.88	5 (35%)
4	MAN	M	233	4	11,11,12	1.37	1 (9%)	14,15,17	2.93	6 (42%)

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	NAG	H	230	6	-	0/6/26/26	0/1/1/1
6	NAG	H	231	6	-	0/6/23/26	0/1/1/1
6	BMA	H	232	6	-	0/2/19/22	0/1/1/1
6	MAN	H	233	4,6	-	0/2/19/22	0/1/1/1
6	MAN	H	234	6	-	0/2/19/22	0/1/1/1
6	MAN	H	235	6	-	0/2/19/22	0/1/1/1
6	MAN	H	236	6	-	0/2/19/22	0/1/1/1
4	MAN	H	237	4,6	-	0/2/19/22	0/1/1/1
4	MAN	H	238	2,4	-	0/2/19/22	0/1/1/1
3	NAG	K	214	3	-	0/6/26/26	0/1/1/1
3	NAG	K	215	3	-	0/6/23/26	0/1/1/1
3	BMA	K	216	3	-	0/2/19/22	0/1/1/1
3	MAN	K	217	3	-	0/2/19/22	0/1/1/1
3	MAN	K	218	3,4	-	0/2/19/22	0/1/1/1
3	MAN	K	219	3	-	0/2/19/22	0/1/1/1
4	MAN	L	214	4	-	0/2/19/22	0/1/1/1
4	MAN	L	215	4	-	0/2/19/22	0/1/1/1
4	MAN	M	230	2,4	-	0/2/19/22	0/1/1/1
4	MAN	M	231	4	-	0/2/19/22	0/1/1/1
4	MAN	M	232	3,4	-	0/2/19/22	0/1/1/1
4	MAN	M	233	4	-	0/2/19/22	0/1/1/1

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	215	MAN	O5-C1	-4.27	1.36	1.43
4	M	230	MAN	C2-C3	-3.06	1.48	1.52
4	H	238	MAN	O4-C4	-2.93	1.35	1.43
4	M	230	MAN	O5-C1	-2.89	1.38	1.43
6	H	233	MAN	C4-C5	-2.76	1.47	1.53
3	K	216	BMA	C2-C3	-2.58	1.49	1.52
4	M	231	MAN	O5-C5	-2.51	1.37	1.43
3	K	218	MAN	O2-C2	-2.41	1.37	1.43
3	K	216	BMA	O5-C5	-2.21	1.38	1.43
4	L	214	MAN	O5-C1	-2.19	1.40	1.43
6	H	233	MAN	O5-C5	-2.13	1.38	1.43
4	H	237	MAN	O5-C5	-2.03	1.39	1.43
4	L	214	MAN	C4-C5	-2.02	1.48	1.53
3	K	214	NAG	C4-C5	2.08	1.57	1.53
6	H	233	MAN	C2-C3	2.12	1.55	1.52
3	K	214	NAG	C3-C2	2.18	1.57	1.53
3	K	219	MAN	C4-C5	2.25	1.57	1.53
6	H	235	MAN	C2-C3	2.28	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	217	MAN	C1-C2	2.34	1.57	1.52
4	H	237	MAN	C1-C2	2.40	1.57	1.52
3	K	215	NAG	C1-C2	2.61	1.56	1.52
4	H	238	MAN	C2-C3	2.64	1.56	1.52
3	K	219	MAN	C2-C3	2.67	1.56	1.52
6	H	236	MAN	C2-C3	2.68	1.56	1.52
3	K	214	NAG	C2-N2	2.70	1.50	1.45
6	H	235	MAN	C1-C2	3.09	1.59	1.52
6	H	236	MAN	C1-C2	3.17	1.59	1.52
3	K	219	MAN	C4-C3	3.22	1.60	1.52
6	H	230	NAG	C1-C2	3.23	1.56	1.53
6	H	236	MAN	O5-C1	3.32	1.49	1.43
6	H	236	MAN	C4-C5	3.60	1.60	1.53
4	M	233	MAN	C2-C3	3.60	1.57	1.52
6	H	235	MAN	C4-C5	3.70	1.60	1.53
3	K	214	NAG	C1-C2	4.06	1.57	1.53

All (138) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	238	MAN	C1-C2-C3	-9.32	98.51	109.54
4	M	230	MAN	O2-C2-C3	-7.97	94.08	110.12
4	M	231	MAN	C1-C2-C3	-7.79	100.33	109.54
4	H	237	MAN	O3-C3-C4	-6.72	95.20	110.34
3	K	215	NAG	C1-O5-C5	-6.14	104.45	112.25
3	K	217	MAN	C1-O5-C5	-5.93	104.72	112.25
4	L	215	MAN	C3-C4-C5	-5.82	100.06	110.20
4	M	230	MAN	C1-O5-C5	-5.81	104.87	112.25
4	L	214	MAN	C6-C5-C4	-5.81	98.69	113.02
4	H	237	MAN	O4-C4-C3	-5.75	97.40	110.34
6	H	234	MAN	C1-O5-C5	-5.67	105.05	112.25
4	M	231	MAN	O5-C5-C6	-5.66	95.09	107.35
3	K	216	BMA	C2-C3-C4	-5.25	102.13	111.04
6	H	235	MAN	O4-C4-C3	-4.98	99.12	110.34
3	K	216	BMA	O3-C3-C2	-4.74	101.43	110.00
4	M	230	MAN	O3-C3-C4	-4.60	99.97	110.34
6	H	230	NAG	C3-C2-N2	-4.53	101.29	110.66
3	K	215	NAG	C4-C3-C2	-4.43	104.34	111.23
6	H	232	BMA	C6-C5-C4	-4.29	102.44	113.02
4	H	237	MAN	O5-C5-C6	-4.02	98.64	107.35
6	H	235	MAN	O5-C5-C6	-4.00	98.69	107.35
3	K	218	MAN	O3-C3-C2	-3.99	102.80	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	M	233	MAN	C3-C4-C5	-3.97	103.28	110.20
4	M	232	MAN	O2-C2-C3	-3.96	102.14	110.12
4	H	237	MAN	C2-C3-C4	-3.94	104.35	111.04
4	H	237	MAN	C6-C5-C4	-3.87	103.46	113.02
4	L	214	MAN	C2-C3-C4	-3.87	104.47	111.04
4	M	230	MAN	O3-C3-C2	-3.87	103.01	110.00
3	K	216	BMA	O5-C5-C6	-3.62	99.51	107.35
3	K	217	MAN	O6-C6-C5	-3.59	99.46	111.33
4	H	237	MAN	O2-C2-C3	-3.35	103.38	110.12
3	K	219	MAN	O2-C2-C3	-3.32	103.45	110.12
4	M	233	MAN	O2-C2-C1	-3.28	102.63	109.21
6	H	232	BMA	O3-C3-C4	-3.24	103.05	110.34
3	K	216	BMA	O2-C2-C3	-3.23	103.62	110.12
4	M	232	MAN	O3-C3-C2	-3.23	104.17	110.00
4	M	233	MAN	O5-C1-C2	-3.17	105.72	110.86
4	L	215	MAN	O6-C6-C5	-3.12	101.02	111.33
6	H	232	BMA	O5-C5-C6	-3.00	100.86	107.35
4	L	214	MAN	O2-C2-C1	-2.96	103.27	109.21
6	H	234	MAN	O2-C2-C1	-2.94	103.31	109.21
3	K	216	BMA	O3-C3-C4	-2.90	103.82	110.34
4	M	230	MAN	C3-C4-C5	-2.87	105.19	110.20
6	H	233	MAN	O5-C1-C2	-2.76	106.37	110.86
6	H	231	NAG	C3-C2-N2	-2.70	104.09	110.56
6	H	232	BMA	O2-C2-C1	-2.70	103.79	109.21
3	K	216	BMA	C6-C5-C4	-2.60	106.60	113.02
3	K	214	NAG	C8-C7-N2	-2.59	111.15	116.11
3	K	215	NAG	C3-C4-C5	-2.58	105.70	110.20
4	M	231	MAN	O6-C6-C5	-2.55	102.89	111.33
6	H	231	NAG	O4-C4-C5	-2.55	102.49	109.24
6	H	233	MAN	O4-C4-C5	-2.54	102.52	109.24
4	H	237	MAN	O6-C6-C5	-2.50	103.06	111.33
3	K	216	BMA	O5-C1-C2	-2.48	106.83	110.86
6	H	233	MAN	C6-C5-C4	-2.48	106.89	113.02
3	K	217	MAN	O4-C4-C3	-2.46	104.79	110.34
4	L	214	MAN	O5-C1-C2	-2.26	107.19	110.86
3	K	216	BMA	O2-C2-C1	-2.23	104.74	109.21
6	H	234	MAN	O6-C6-C5	-2.19	104.09	111.33
3	K	216	BMA	O6-C6-C5	-2.14	104.25	111.33
4	L	214	MAN	O4-C4-C5	-2.01	103.91	109.24
4	M	230	MAN	O5-C5-C6	2.00	111.68	107.35
3	K	219	MAN	C1-O5-C5	2.00	114.79	112.25
3	K	214	NAG	O5-C5-C4	2.04	113.51	109.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	M	231	MAN	O3-C3-C4	2.09	115.04	110.34
3	K	218	MAN	C6-C5-C4	2.16	118.35	113.02
4	M	232	MAN	C3-C4-C5	2.19	114.01	110.20
4	L	214	MAN	O5-C5-C6	2.21	112.14	107.35
6	H	230	NAG	C1-O5-C5	2.29	117.71	113.47
6	H	230	NAG	O3-C3-C4	2.30	115.51	110.34
6	H	234	MAN	O5-C5-C6	2.30	112.33	107.35
4	M	231	MAN	O5-C1-C2	2.31	114.60	110.86
3	K	215	NAG	C3-C2-N2	2.32	116.11	110.56
3	K	217	MAN	O5-C5-C6	2.36	112.46	107.35
3	K	215	NAG	O3-C3-C4	2.36	115.66	110.34
4	M	232	MAN	C1-O5-C5	2.38	115.27	112.25
3	K	214	NAG	C1-O5-C5	2.43	117.96	113.47
6	H	231	NAG	C1-O5-C5	2.43	115.34	112.25
6	H	232	BMA	O2-C2-C3	2.56	115.27	110.12
4	H	238	MAN	C3-C4-C5	2.59	114.72	110.20
6	H	230	NAG	C2-N2-C7	2.64	129.88	123.10
6	H	235	MAN	C2-C3-C4	2.65	115.55	111.04
4	M	232	MAN	O5-C1-C2	2.71	115.25	110.86
4	H	238	MAN	O2-C2-C1	2.74	114.71	109.21
3	K	219	MAN	O6-C6-C5	2.84	120.71	111.33
4	L	215	MAN	O4-C4-C5	2.89	116.91	109.24
3	K	214	NAG	O7-C7-N2	2.93	127.83	121.86
3	K	215	NAG	O5-C5-C6	2.95	113.73	107.35
4	M	230	MAN	O4-C4-C5	2.99	117.16	109.24
3	K	218	MAN	O3-C3-C4	3.12	117.36	110.34
4	L	215	MAN	O3-C3-C2	3.14	115.67	110.00
6	H	231	NAG	O3-C3-C4	3.28	117.73	110.34
6	H	233	MAN	C2-C3-C4	3.29	116.62	111.04
3	K	219	MAN	O4-C4-C5	3.31	118.01	109.24
3	K	217	MAN	O5-C1-C2	3.36	116.31	110.86
6	H	235	MAN	C3-C4-C5	3.37	116.08	110.20
4	M	230	MAN	C1-C2-C3	3.38	113.54	109.54
3	K	218	MAN	O4-C4-C5	3.38	118.20	109.24
4	H	238	MAN	O5-C1-C2	3.43	116.43	110.86
3	K	219	MAN	C1-C2-C3	3.49	113.67	109.54
6	H	235	MAN	O2-C2-C1	3.52	116.27	109.21
3	K	215	NAG	O3-C3-C2	3.59	116.23	109.11
6	H	232	BMA	C3-C4-C5	3.61	116.48	110.20
6	H	235	MAN	O5-C1-C2	3.62	116.72	110.86
6	H	235	MAN	C1-O5-C5	3.71	116.96	112.25
4	M	231	MAN	C2-C3-C4	3.75	117.40	111.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	K	219	MAN	O4-C4-C3	3.77	118.83	110.34
6	H	235	MAN	O4-C4-C5	3.81	119.33	109.24
3	K	214	NAG	C2-N2-C7	3.87	133.04	123.10
6	H	234	MAN	C3-C4-C5	3.88	116.95	110.20
6	H	236	MAN	O4-C4-C5	3.93	119.64	109.24
6	H	230	NAG	O5-C5-C4	3.96	117.11	109.68
6	H	236	MAN	C6-C5-C4	3.96	122.78	113.02
4	H	237	MAN	C1-C2-C3	4.02	114.30	109.54
6	H	230	NAG	C4-C3-C2	4.12	116.14	110.43
4	M	233	MAN	O4-C4-C3	4.12	119.62	110.34
6	H	233	MAN	C1-O5-C5	4.13	117.49	112.25
3	K	218	MAN	C1-C2-C3	4.19	114.50	109.54
4	H	238	MAN	C1-O5-C5	4.20	117.58	112.25
3	K	215	NAG	C6-C5-C4	4.22	123.43	113.02
4	L	214	MAN	C1-C2-C3	4.26	114.58	109.54
6	H	230	NAG	C3-C4-C5	4.44	117.94	110.20
4	M	233	MAN	O2-C2-C3	4.49	119.14	110.12
3	K	214	NAG	C4-C3-C2	4.74	117.01	110.43
4	H	238	MAN	O2-C2-C3	4.81	119.79	110.12
4	M	231	MAN	O2-C2-C1	4.83	118.89	109.21
4	L	214	MAN	C1-O5-C5	4.99	118.58	112.25
3	K	217	MAN	O2-C2-C1	5.42	120.08	109.21
4	M	233	MAN	O5-C5-C6	5.82	119.94	107.35
6	H	236	MAN	C1-C2-C3	5.83	116.44	109.54
6	H	235	MAN	C6-C5-C4	6.06	127.97	113.02
4	H	237	MAN	O5-C1-C2	6.25	121.00	110.86
6	H	235	MAN	C1-C2-C3	6.38	117.09	109.54
6	H	236	MAN	C1-O5-C5	6.45	120.43	112.25
4	H	237	MAN	O4-C4-C5	6.53	126.54	109.24
3	K	218	MAN	C1-O5-C5	6.71	120.77	112.25
6	H	232	BMA	C1-O5-C5	7.12	121.28	112.25
3	K	218	MAN	O5-C1-C2	7.16	122.47	110.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	H	232	BMA	4	0
6	H	233	MAN	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	H	234	MAN	11	0
6	H	235	MAN	3	0
6	H	236	MAN	2	0
4	H	237	MAN	7	0
4	H	238	MAN	4	0
3	K	216	BMA	3	0
3	K	217	MAN	4	0
3	K	218	MAN	8	0
3	K	219	MAN	3	0
4	L	214	MAN	6	0
4	M	230	MAN	8	0
4	M	231	MAN	5	0
4	M	232	MAN	5	0

5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	MAN	M	234	-	11,11,12	0.90	0	14,15,17	3.39	6 (42%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MAN	M	234	-	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	M	234	MAN	C3-C4-C5	-5.81	100.07	110.20
5	M	234	MAN	O2-C2-C1	-2.35	104.49	109.21
5	M	234	MAN	O2-C2-C3	2.89	115.92	110.12
5	M	234	MAN	O5-C5-C6	3.79	115.55	107.35
5	M	234	MAN	O4-C4-C3	6.15	124.18	110.34
5	M	234	MAN	C1-O5-C5	7.37	121.60	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	M	234	MAN	3	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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.