Full wwPDB X-ray Structure Validation Report (i)

Mar 8, 2023 – 01:05 AM EST

PDB ID	:	1R1A
Title	:	CRYSTAL STRUCTURE OF HUMAN RHINOVIRUS SEROTYPE 1A (HRV1A)
Authors	:	Kim, S.; Rossmann, M.G.
Deposited on	:	1989-03-15
Resolution	:	3.20 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

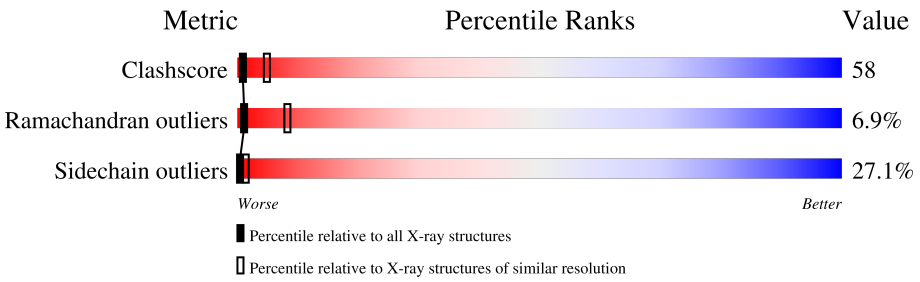
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

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 3.20 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	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	1	287	18% 43% 25% 13% •
2	2	263	19% 36% 31% 10% •
3	3	238	19% 47% 26% 8%
4	4	44	9% 16% 9% 9% 57%
5	A	2	100%

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
5	GLC	A	1	X	-	X	-
5	FRU	A	2	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6246 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 HUMAN RHINOVIRUS 1A COAT PROTEIN (SUBUNIT VP1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	1	283	2262	1431	389	430	12	0	0	0

- Molecule 2 is a protein called HUMAN RHINOVIRUS 1A COAT PROTEIN (SUBUNIT VP2).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	2	253	1979	1249	349	371	10	0	0	0

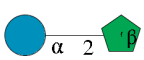
- Molecule 3 is a protein called HUMAN RHINOVIRUS 1A COAT PROTEIN (SUBUNIT VP3).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	3	238	1831	1169	297	348	17	0	0	0

- Molecule 4 is a protein called HUMAN RHINOVIRUS 1A COAT PROTEIN (SUBUNIT VP4).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	4	19	151	96	25	30	0	0	0

- Molecule 5 is an oligosaccharide called beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
5	A	2	23	12	11	0	0	0

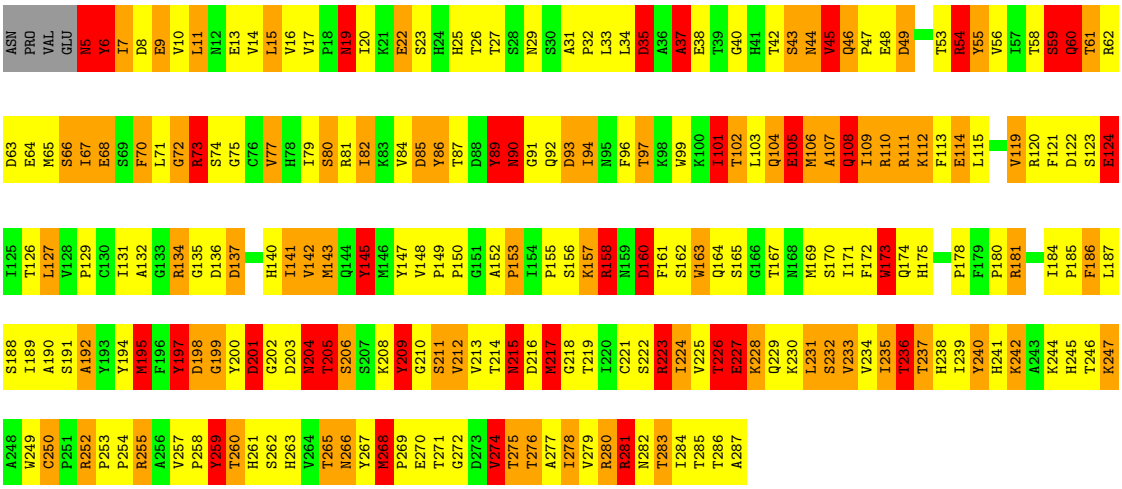
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

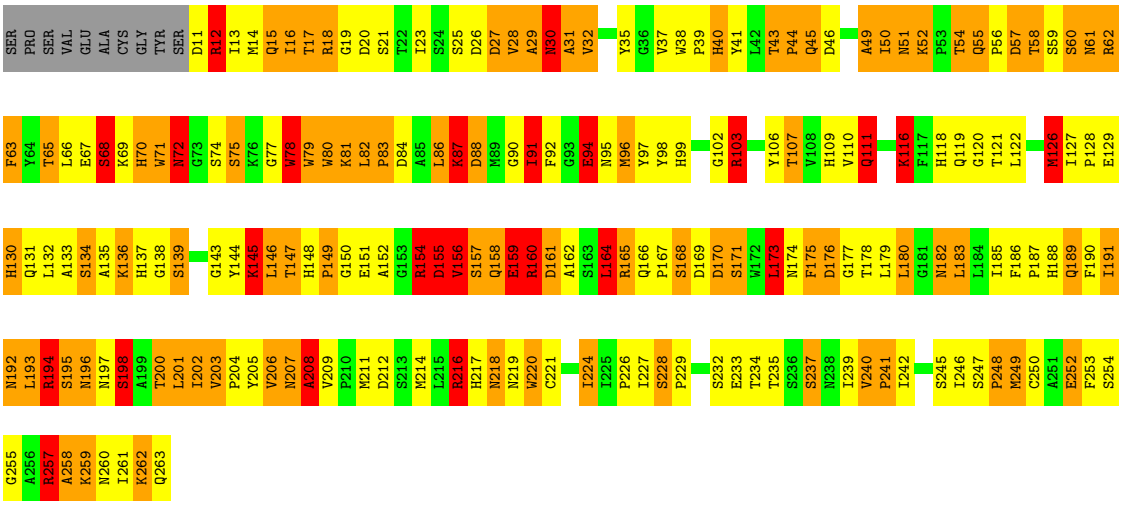
• Molecule 1: HUMAN RHINOVIRUS 1A COAT PROTEIN (SUBUNIT VP1)

Chain 1: 18% 43% 25% 13%



• Molecule 2: HUMAN RHINOVIRUS 1A COAT PROTEIN (SUBUNIT VP2)

Chain 2: 19% 36% 31% 10%



- Molecule 3: HUMAN RHINOVIRUS 1A COAT PROTEIN (SUBUNIT VP3)

Chain 3: 19% 47% 26% 8%

G1 L2 P3 V4 Y5 I6 T7 P8 G9 S10 M14 T15 T16 D17 D18 M19 Q20 S21 P22 C23 A24 L25 P26 W27 Y28 T31 K32 E33 I34 S35 I36 P37 G38 E39 V40 K41 N42 L43 I44 E45 M46 C47 Q48 V49 D50 T51 L52 I53 P54 V55 N56 N57 V58 G59 N60 N61 V62 G63

N64 V65 S66 M67 Y68 L72 G73 N74 Q75 T76 G77 M78 A79 Q80 K81 V82 F83 S84 V87 D88 I89 T90 S91 T92 P93 L94 A95 T96 T97 L98 I99 G100 E101 I102 A103 S104 Y105 Y106 T107 H108 W109 T110 G111 S112 L113 R114 F115 S116 F117 M118 F119 G120 G121 T122 A123 N124 T125 T126

L127 K128 L129 L130 L131 A132 Y133 T134 P135 P136 E140 P141 T142 T143 R144 K145 D146 A147 M148 L149 H152 W155 D156 V157 G158 L159 Q160 S161 T162 I163 S164 L165 V166 V167 P168 W169 A172 S173 H174 F175 R176 L177 T178 N181 K182 Y183 S184 M185 A186 G187 Y188 I189 T190 C191 W192

Y193 Q194 T195 N196 L197 P200 P201 S202 T203 P204 Q205 T206 A207 D208 M209 L210 C211 F212 V213 S214 A215 C216 K217 D218 F219 C220 L221 R222 M223 A224 R225 D226 T227 D228 L229 H230 I231 Q232 S233 G234 P235 I236 E237 Q238

- Molecule 4: HUMAN RHINOVIRUS 1A COAT PROTEIN (SUBUNIT VP4)

Chain 4: 9% 16% 9% 9% 57%

GLY ALA GLY VAL SER ARG GLN ASN VAL GLY THR HIS SER THR GLN ASN SER VAL SER ASN GLY SER SER LEU ASN Y26 F27 N28 I29 N30 Y31 F32 K33 D34 A35 A36 S37 S38 G39 A40 S41 R42 L43 D44

- Molecule 5: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain A: 100%

GLC1 FRU2

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α, β, γ	341.30Å 341.30Å 465.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 3.20	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-3.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.293 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6246	wwPDB-VP
Average B, all atoms (Å^2)	14.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GLC, FRU

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	1	0.98	0/2322	2.61	150/3162 (4.7%)
2	2	0.95	0/2033	2.60	151/2770 (5.5%)
3	3	0.93	0/1878	2.47	112/2570 (4.4%)
4	4	1.25	0/154	3.16	21/206 (10.2%)
All	All	0.96	0/6387	2.58	434/8708 (5.0%)

There are no bond length outliers.

All (434) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	62	ARG	CD-NE-CZ	24.85	158.39	123.60
1	1	134	ARG	NE-CZ-NH1	24.00	132.30	120.30
2	2	216	ARG	NE-CZ-NH2	-22.09	109.25	120.30
1	1	280	ARG	NE-CZ-NH2	-20.39	110.11	120.30
1	1	110	ARG	NE-CZ-NH2	-19.07	110.77	120.30
3	3	146	ASP	CB-CG-OD2	-17.26	102.77	118.30
2	2	257	ARG	NE-CZ-NH2	-16.52	112.04	120.30
3	3	222	ARG	CD-NE-CZ	15.92	145.89	123.60
4	4	42	ARG	NE-CZ-NH1	15.10	127.85	120.30
2	2	155	ASP	CB-CG-OD1	-14.70	105.07	118.30
1	1	110	ARG	CD-NE-CZ	14.29	143.61	123.60
1	1	81	ARG	NE-CZ-NH1	14.06	127.33	120.30
1	1	281	ARG	NE-CZ-NH2	-13.91	113.35	120.30
2	2	154	ARG	NE-CZ-NH1	13.89	127.25	120.30
3	3	226	ASP	CB-CG-OD2	13.80	130.72	118.30
2	2	62	ARG	NE-CZ-NH1	13.79	127.19	120.30
1	1	158	ARG	NE-CZ-NH1	13.66	127.13	120.30
3	3	228	ASP	CB-CG-OD2	-13.33	106.31	118.30
3	3	28	TYR	CB-CG-CD1	13.26	128.95	121.00
1	1	110	ARG	NE-CZ-NH1	13.02	126.81	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	3	183	TYR	CB-CG-CD1	12.41	128.45	121.00
3	3	144	ARG	CD-NE-CZ	12.32	140.85	123.60
1	1	281	ARG	CA-CB-CG	12.20	140.23	113.40
1	1	227	GLU	OE1-CD-OE2	-12.17	108.70	123.30
1	1	6	TYR	CB-CG-CD2	-11.99	113.81	121.00
3	3	114	ARG	NE-CZ-NH1	-11.82	114.39	120.30
1	1	93	ASP	CB-CG-OD2	-11.78	107.70	118.30
3	3	144	ARG	NE-CZ-NH1	11.43	126.02	120.30
1	1	231	LEU	CA-CB-CG	11.30	141.28	115.30
3	3	50	ASP	CB-CG-OD2	-11.21	108.21	118.30
3	3	225	ARG	NE-CZ-NH1	-11.16	114.72	120.30
2	2	67	GLU	OE1-CD-OE2	10.99	136.49	123.30
3	3	50	ASP	CB-CG-OD1	10.99	128.19	118.30
1	1	255	ARG	CD-NE-CZ	10.92	138.89	123.60
1	1	54	ARG	CG-CD-NE	10.81	134.50	111.80
2	2	35	TYR	CB-CG-CD2	10.78	127.47	121.00
4	4	44	ASP	CB-CG-OD1	-10.74	108.63	118.30
2	2	12	ARG	NE-CZ-NH2	-10.30	115.15	120.30
3	3	218	ASP	CB-CG-OD1	-10.29	109.04	118.30
1	1	106	MET	CA-CB-CG	-10.28	95.82	113.30
2	2	162	ALA	CB-CA-C	10.23	125.44	110.10
2	2	12	ARG	CD-NE-CZ	10.20	137.88	123.60
2	2	205	TYR	CB-CG-CD1	10.17	127.10	121.00
2	2	62	ARG	NH1-CZ-NH2	-9.96	108.45	119.40
2	2	11	ASP	CB-CG-OD1	9.86	127.18	118.30
2	2	216	ARG	NE-CZ-NH1	9.85	125.23	120.30
2	2	31	ALA	N-CA-CB	9.82	123.85	110.10
1	1	223	ARG	NE-CZ-NH2	9.73	125.17	120.30
1	1	223	ARG	NE-CZ-NH1	-9.64	115.48	120.30
3	3	67	MET	N-CA-CB	-9.62	93.29	110.60
1	1	8	ASP	CB-CG-OD1	-9.57	109.69	118.30
2	2	154	ARG	C-N-CA	9.56	145.60	121.70
2	2	29	ALA	N-CA-CB	9.55	123.48	110.10
4	4	42	ARG	CD-NE-CZ	9.44	136.81	123.60
2	2	212	ASP	CB-CG-OD1	9.37	126.73	118.30
1	1	105	GLU	CA-CB-CG	9.37	134.00	113.40
2	2	176	ASP	CB-CG-OD1	9.36	126.72	118.30
2	2	165	ARG	NE-CZ-NH1	9.34	124.97	120.30
1	1	59	SER	N-CA-CB	-9.20	96.70	110.50
1	1	281	ARG	NE-CZ-NH1	9.20	124.90	120.30
1	1	9	GLU	OE1-CD-OE2	9.12	134.24	123.30
1	1	134	ARG	NH1-CZ-NH2	-9.04	109.46	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	3	148	MET	CG-SD-CE	9.04	114.66	100.20
3	3	18	ASP	CB-CG-OD2	-8.95	110.25	118.30
2	2	28	VAL	CA-CB-CG1	8.92	124.28	110.90
2	2	165	ARG	NE-CZ-NH2	-8.86	115.87	120.30
1	1	227	GLU	CG-CD-OE1	8.79	135.87	118.30
2	2	154	ARG	NE-CZ-NH2	-8.74	115.93	120.30
1	1	60	GLN	O-C-N	8.73	136.68	122.70
2	2	35	TYR	CB-CG-CD1	-8.70	115.78	121.00
1	1	55	TYR	CB-CG-CD2	-8.69	115.79	121.00
3	3	232	GLN	N-CA-CB	8.68	126.22	110.60
2	2	11	ASP	CB-CG-OD2	-8.65	110.52	118.30
1	1	11	LEU	O-C-N	8.64	136.52	122.70
3	3	222	ARG	NE-CZ-NH1	8.46	124.53	120.30
1	1	108	GLN	C-N-CA	8.46	142.85	121.70
2	2	233	GLU	CG-CD-OE1	8.45	135.19	118.30
1	1	68	GLU	CB-CG-CD	8.36	136.77	114.20
2	2	12	ARG	NE-CZ-NH1	8.32	124.46	120.30
2	2	57	ASP	N-CA-CB	-8.30	95.66	110.60
1	1	187	LEU	CA-C-O	-8.30	102.67	120.10
3	3	28	TYR	CB-CG-CD2	-8.28	116.03	121.00
1	1	181	ARG	NE-CZ-NH2	8.28	124.44	120.30
3	3	226	ASP	OD1-CG-OD2	-8.24	107.65	123.30
2	2	97	TYR	CB-CG-CD2	8.18	125.91	121.00
2	2	126	MET	CA-CB-CG	-8.11	99.52	113.30
1	1	120	ARG	NE-CZ-NH2	8.00	124.30	120.30
2	2	12	ARG	CG-CD-NE	7.99	128.58	111.80
2	2	241	PRO	C-N-CA	7.95	141.57	121.70
1	1	111	ARG	CD-NE-CZ	7.93	134.70	123.60
2	2	26	ASP	CB-CG-OD2	7.89	125.40	118.30
2	2	194	ARG	NE-CZ-NH2	-7.88	116.36	120.30
1	1	181	ARG	CG-CD-NE	7.86	128.30	111.80
2	2	160	ARG	NE-CZ-NH1	-7.83	116.39	120.30
1	1	158	ARG	CD-NE-CZ	7.83	134.56	123.60
1	1	211	SER	O-C-N	7.82	135.22	122.70
2	2	189	GLN	CA-CB-CG	7.82	130.60	113.40
1	1	49	ASP	CB-CG-OD1	-7.81	111.28	118.30
2	2	161	ASP	N-CA-CB	7.78	124.61	110.60
3	3	56	ASN	C-N-CA	7.76	141.11	121.70
2	2	61	ASN	CB-CA-C	7.75	125.89	110.40
1	1	55	TYR	CB-CG-CD1	7.74	125.64	121.00
3	3	235	PRO	C-N-CA	7.72	141.01	121.70
2	2	94	GLU	OE1-CD-OE2	7.70	132.54	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	159	GLU	OE1-CD-OE2	7.68	132.51	123.30
1	1	93	ASP	CB-CG-OD1	7.65	125.19	118.30
1	1	197	TYR	CB-CG-CD1	7.61	125.56	121.00
1	1	73	ARG	NE-CZ-NH1	7.59	124.09	120.30
1	1	280	ARG	NH1-CZ-NH2	7.59	127.75	119.40
2	2	71	TRP	CB-CA-C	7.57	125.55	110.40
3	3	68	TYR	CB-CG-CD1	7.56	125.54	121.00
1	1	134	ARG	CD-NE-CZ	7.55	134.17	123.60
1	1	85	ASP	CB-CG-OD2	-7.54	111.51	118.30
1	1	6	TYR	CB-CG-CD1	7.54	125.52	121.00
2	2	161	ASP	CB-CG-OD2	-7.53	111.52	118.30
3	3	207	ALA	O-C-N	7.51	134.71	122.70
2	2	232	SER	N-CA-CB	7.42	121.62	110.50
1	1	111	ARG	NE-CZ-NH1	-7.42	116.59	120.30
1	1	61	THR	CA-CB-OG1	-7.41	93.44	109.00
2	2	252	GLU	OE1-CD-OE2	7.39	132.16	123.30
3	3	92	THR	CB-CA-C	7.35	131.44	111.60
1	1	89	TYR	CB-CG-CD2	-7.31	116.61	121.00
3	3	161	SER	CB-CA-C	-7.31	96.21	110.10
4	4	34	ASP	CB-CG-OD2	-7.30	111.73	118.30
4	4	37	SER	O-C-N	7.28	134.35	122.70
2	2	147	THR	N-CA-CB	7.21	124.01	110.30
3	3	88	ASP	CB-CG-OD1	7.19	124.77	118.30
1	1	173	TRP	CA-CB-CG	7.17	127.32	113.70
3	3	95	ALA	CA-C-N	7.16	132.95	117.20
2	2	152	ALA	N-CA-CB	-7.16	100.08	110.10
2	2	233	GLU	CG-CD-OE2	-7.16	103.98	118.30
4	4	40	ALA	O-C-N	7.14	134.13	122.70
1	1	228	LYS	CD-CE-NZ	7.13	128.11	111.70
2	2	78	TRP	CA-CB-CG	7.12	127.23	113.70
2	2	62	ARG	NE-CZ-NH2	7.12	123.86	120.30
3	3	232	GLN	O-C-N	7.10	134.05	122.70
2	2	237	SER	CB-CA-C	7.08	123.54	110.10
3	3	120	CYS	CA-CB-SG	-7.04	101.32	114.00
2	2	164	LEU	O-C-N	7.03	133.95	122.70
3	3	218	ASP	N-CA-CB	-7.01	97.98	110.60
2	2	80	TRP	N-CA-CB	7.00	123.19	110.60
1	1	259	TYR	CB-CG-CD2	-6.99	116.81	121.00
1	1	45	VAL	CB-CA-C	6.97	124.65	111.40
2	2	160	ARG	NE-CZ-NH2	6.96	123.78	120.30
2	2	103	ARG	CD-NE-CZ	6.96	133.34	123.60
4	4	42	ARG	NH1-CZ-NH2	-6.96	111.75	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	268	MET	CA-CB-CG	-6.93	101.52	113.30
4	4	31	TYR	CB-CG-CD1	6.91	125.15	121.00
3	3	222	ARG	NH1-CZ-NH2	-6.90	111.81	119.40
2	2	81	LYS	O-C-N	6.85	133.66	122.70
1	1	164	GLN	OE1-CD-NE2	-6.84	106.17	121.90
2	2	160	ARG	N-CA-CB	-6.84	98.30	110.60
1	1	5	ASN	N-CA-CB	6.80	122.84	110.60
2	2	72	ASN	OD1-CG-ND2	6.80	137.54	121.90
3	3	25	LEU	CA-CB-CG	6.78	130.90	115.30
2	2	106	TYR	C-N-CA	6.78	138.65	121.70
1	1	212	VAL	O-C-N	6.74	133.49	122.70
1	1	203	ASP	CB-CG-OD2	-6.74	112.24	118.30
1	1	164	GLN	CG-CD-OE1	6.74	135.07	121.60
2	2	198	SER	CB-CA-C	-6.72	97.33	110.10
1	1	270	GLU	N-CA-CB	6.71	122.68	110.60
3	3	193	TYR	O-C-N	6.68	133.38	122.70
2	2	52	LYS	CA-CB-CG	6.67	128.07	113.40
3	3	26	PRO	O-C-N	6.67	133.37	122.70
3	3	90	THR	N-CA-CB	6.65	122.94	110.30
3	3	73	GLY	CA-C-O	6.64	132.56	120.60
3	3	218	ASP	CA-CB-CG	-6.63	98.81	113.40
4	4	40	ALA	N-CA-CB	6.62	119.37	110.10
3	3	57	ASN	CB-CG-ND2	-6.59	100.88	116.70
2	2	135	ALA	N-CA-CB	-6.59	100.88	110.10
1	1	19	ASN	CB-CG-OD1	-6.58	108.45	121.60
1	1	37	ALA	N-CA-CB	-6.56	100.91	110.10
1	1	70	PHE	O-C-N	6.54	133.17	122.70
2	2	196	ASN	N-CA-CB	-6.53	98.86	110.60
3	3	55	VAL	CB-CA-C	6.51	123.78	111.40
1	1	5	ASN	O-C-N	6.51	133.11	122.70
2	2	50	ILE	CA-CB-CG2	6.48	123.86	110.90
1	1	145	TYR	N-CA-CB	6.47	122.25	110.60
2	2	187	PRO	CB-CA-C	6.46	128.14	112.00
3	3	16	THR	CA-CB-CG2	6.45	121.44	112.40
2	2	183	LEU	O-C-N	6.43	132.99	122.70
3	3	222	ARG	NE-CZ-NH2	6.43	123.52	120.30
1	1	64	GLU	CA-CB-CG	6.42	127.52	113.40
2	2	28	VAL	CG1-CB-CG2	-6.40	100.66	110.90
1	1	199	GLY	O-C-N	6.40	132.93	122.70
2	2	16	ILE	O-C-N	6.39	132.93	122.70
1	1	13	GLU	O-C-N	6.38	132.91	122.70
3	3	172	ALA	CB-CA-C	6.38	119.67	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	105	GLU	CG-CD-OE2	-6.35	105.59	118.30
2	2	68	SER	N-CA-CB	6.35	120.02	110.50
2	2	26	ASP	OD1-CG-OD2	-6.34	111.26	123.30
3	3	235	PRO	CA-C-N	-6.33	103.26	117.20
3	3	160	GLN	N-CA-CB	6.33	121.99	110.60
3	3	235	PRO	CA-C-O	6.30	135.32	120.20
1	1	274	VAL	N-CA-CB	6.29	125.33	111.50
1	1	275	THR	OG1-CB-CG2	6.29	124.45	110.00
2	2	196	ASN	OD1-CG-ND2	6.28	136.34	121.90
3	3	37	PRO	N-CA-CB	6.26	110.81	103.30
1	1	201	ASP	CB-CG-OD2	6.26	123.93	118.30
2	2	248	PRO	N-CA-C	-6.25	95.85	112.10
2	2	161	ASP	O-C-N	6.25	132.69	122.70
1	1	233	VAL	CA-C-N	-6.22	103.51	117.20
4	4	44	ASP	CB-CG-OD2	6.22	123.90	118.30
1	1	77	VAL	O-C-N	6.21	132.64	122.70
2	2	19	GLY	C-N-CA	6.21	137.21	121.70
1	1	233	VAL	CB-CA-C	-6.20	99.61	111.40
2	2	94	GLU	CG-CD-OE2	-6.20	105.89	118.30
3	3	33	GLU	CG-CD-OE2	-6.20	105.90	118.30
4	4	30	ASN	CB-CA-C	6.19	122.79	110.40
1	1	211	SER	CA-C-O	-6.17	107.13	120.10
1	1	86	TYR	CB-CA-C	6.17	122.74	110.40
3	3	94	LEU	CA-C-N	6.17	130.77	117.20
3	3	89	ILE	CB-CA-C	-6.16	99.28	111.60
1	1	223	ARG	CA-CB-CG	6.16	126.95	113.40
2	2	155	ASP	N-CA-CB	6.14	121.66	110.60
4	4	38	SER	O-C-N	6.14	133.65	123.20
2	2	205	TYR	CB-CG-CD2	-6.14	117.32	121.00
1	1	175	HIS	N-CA-CB	-6.12	99.58	110.60
1	1	16	VAL	CG1-CB-CG2	6.12	120.69	110.90
1	1	209	TYR	CB-CG-CD1	6.10	124.66	121.00
4	4	35	ALA	CB-CA-C	6.10	119.25	110.10
1	1	206	SER	O-C-N	6.09	132.44	122.70
2	2	154	ARG	CG-CD-NE	6.07	124.56	111.80
2	2	17	THR	CB-CA-C	6.07	127.98	111.60
3	3	185	MET	CA-CB-CG	6.04	123.57	113.30
2	2	155	ASP	CB-CG-OD2	6.04	123.73	118.30
2	2	107	THR	CA-CB-OG1	-6.04	96.32	109.00
1	1	247	LYS	CB-CA-C	-6.04	98.33	110.40
1	1	227	GLU	CB-CG-CD	6.03	130.49	114.20
2	2	81	LYS	CA-CB-CG	6.03	126.66	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	3	32	LYS	O-C-N	6.02	132.33	122.70
2	2	57	ASP	CB-CG-OD1	-6.02	112.88	118.30
2	2	194	ARG	NH1-CZ-NH2	6.02	126.02	119.40
2	2	82	LEU	CA-CB-CG	-6.01	101.48	115.30
2	2	57	ASP	CB-CG-OD2	-6.01	112.89	118.30
3	3	183	TYR	CB-CG-CD2	-6.00	117.40	121.00
1	1	35	ASP	CB-CG-OD1	6.00	123.69	118.30
1	1	187	LEU	CA-C-N	5.99	130.37	117.20
2	2	262	LYS	CB-CA-C	5.98	122.36	110.40
3	3	15	THR	N-CA-CB	-5.96	98.98	110.30
2	2	160	ARG	CG-CD-NE	5.95	124.29	111.80
1	1	82	ILE	CB-CA-C	-5.92	99.75	111.60
2	2	130	HIS	CA-CB-CG	-5.92	103.53	113.60
3	3	233	SER	CA-C-N	-5.92	104.35	116.20
4	4	26	TYR	CB-CG-CD2	5.92	124.55	121.00
1	1	231	LEU	CB-CA-C	5.92	121.45	110.20
2	2	130	HIS	O-C-N	5.92	132.17	122.70
1	1	71	LEU	CB-CA-C	5.91	121.43	110.20
2	2	87	LYS	CB-CG-CD	5.90	126.94	111.60
2	2	156	VAL	C-N-CA	5.89	136.43	121.70
2	2	157	SER	N-CA-CB	5.89	119.33	110.50
2	2	208	ALA	N-CA-CB	5.89	118.34	110.10
1	1	68	GLU	OE1-CD-OE2	-5.88	116.25	123.30
2	2	91	ILE	N-CA-CB	5.88	124.31	110.80
2	2	49	ALA	CA-C-O	-5.87	107.77	120.10
1	1	55	TYR	O-C-N	5.87	132.09	122.70
2	2	97	TYR	CB-CG-CD1	-5.86	117.48	121.00
1	1	217	MET	CB-CA-C	-5.86	98.69	110.40
3	3	68	TYR	CB-CG-CD2	-5.86	117.49	121.00
3	3	201	PRO	N-CA-C	5.85	127.31	112.10
2	2	252	GLU	CG-CD-OE2	-5.84	106.61	118.30
3	3	105	TYR	CB-CG-CD1	5.83	124.50	121.00
1	1	85	ASP	CB-CG-OD1	5.83	123.55	118.30
1	1	20	ILE	O-C-N	5.83	132.03	122.70
2	2	234	THR	CA-C-O	5.83	132.33	120.10
1	1	49	ASP	OD1-CG-OD2	5.81	134.33	123.30
1	1	89	TYR	CB-CG-CD1	5.79	124.48	121.00
2	2	147	THR	O-C-N	5.79	131.96	122.70
2	2	257	ARG	NE-CZ-NH1	5.79	123.19	120.30
2	2	249	MET	CA-CB-CG	5.79	123.14	113.30
1	1	54	ARG	NE-CZ-NH1	5.79	123.19	120.30
3	3	185	MET	N-CA-CB	5.79	121.02	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	111	ARG	C-N-CA	5.78	136.15	121.70
1	1	215	ASN	O-C-N	5.78	131.94	122.70
1	1	240	TYR	CB-CG-CD2	-5.76	117.55	121.00
1	1	25	HIS	O-C-N	5.75	131.91	122.70
1	1	111	ARG	NE-CZ-NH2	5.75	123.17	120.30
1	1	216	ASP	CB-CA-C	5.75	121.89	110.40
2	2	57	ASP	OD1-CG-OD2	5.75	134.22	123.30
2	2	218	ASN	CA-CB-CG	5.74	126.03	113.40
1	1	226	THR	N-CA-C	5.73	126.48	111.00
3	3	24	ALA	N-CA-CB	-5.73	102.08	110.10
1	1	202	GLY	C-N-CA	5.71	135.99	121.70
1	1	274	VAL	CA-CB-CG1	5.71	119.47	110.90
1	1	250	CYS	CA-CB-SG	5.71	124.28	114.00
2	2	134	SER	CA-C-N	-5.71	104.64	117.20
1	1	16	VAL	CB-CA-C	5.68	122.19	111.40
3	3	45	GLU	OE1-CD-OE2	-5.67	116.49	123.30
1	1	232	SER	CB-CA-C	-5.67	99.33	110.10
1	1	81	ARG	NH1-CZ-NH2	-5.66	113.17	119.40
3	3	229	LEU	CA-CB-CG	5.66	128.32	115.30
2	2	83	PRO	C-N-CA	5.66	135.84	121.70
3	3	103	ALA	CB-CA-C	5.65	118.58	110.10
3	3	76	THR	O-C-N	5.65	132.81	123.20
3	3	160	GLN	O-C-N	5.65	131.74	122.70
1	1	90	ASN	CB-CA-C	5.65	121.70	110.40
2	2	249	MET	CG-SD-CE	5.64	109.23	100.20
2	2	139	SER	N-CA-CB	-5.64	102.04	110.50
1	1	204	ASN	CA-C-N	-5.63	104.81	117.20
3	3	77	GLY	CA-C-O	5.63	130.74	120.60
3	3	18	ASP	OD1-CG-OD2	5.62	133.98	123.30
1	1	198	ASP	CB-CG-OD1	5.62	123.35	118.30
3	3	227	THR	CA-C-O	5.62	131.89	120.10
1	1	122	ASP	CB-CG-OD2	-5.61	113.25	118.30
3	3	212	PHE	CA-CB-CG	5.61	127.35	113.90
2	2	228	SER	N-CA-CB	5.60	118.91	110.50
2	2	26	ASP	CB-CG-OD1	5.59	123.33	118.30
2	2	212	ASP	CB-CG-OD2	-5.59	113.27	118.30
2	2	49	ALA	CA-C-N	5.59	129.50	117.20
3	3	146	ASP	OD1-CG-OD2	5.58	133.91	123.30
2	2	149	PRO	CA-C-N	5.57	127.34	116.20
1	1	274	VAL	CA-C-N	-5.57	104.95	117.20
2	2	134	SER	N-CA-CB	5.57	118.85	110.50
2	2	220	TRP	CA-C-N	-5.57	104.96	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	153	PRO	N-CD-CG	-5.56	94.86	103.20
2	2	83	PRO	CB-CA-C	5.56	125.89	112.00
3	3	146	ASP	CB-CG-OD1	5.56	123.30	118.30
2	2	116	LYS	CB-CA-C	-5.55	99.30	110.40
2	2	119	GLN	CB-CA-C	5.53	121.47	110.40
1	1	68	GLU	CA-CB-CG	5.53	125.57	113.40
3	3	79	ALA	O-C-N	5.53	131.54	122.70
3	3	64	ASN	OD1-CG-ND2	5.52	134.60	121.90
1	1	81	ARG	CD-NE-CZ	5.52	131.33	123.60
3	3	24	ALA	CA-C-N	5.50	129.31	117.20
2	2	194	ARG	NE-CZ-NH1	-5.50	117.55	120.30
1	1	260	THR	CA-C-O	-5.49	108.56	120.10
2	2	54	THR	N-CA-CB	5.49	120.73	110.30
2	2	169	ASP	CA-C-O	5.49	131.62	120.10
2	2	32	VAL	O-C-N	5.47	131.45	122.70
2	2	90	GLY	CA-C-O	5.46	130.43	120.60
2	2	216	ARG	NH1-CZ-NH2	5.45	125.40	119.40
1	1	62	ARG	NE-CZ-NH1	-5.44	117.58	120.30
4	4	40	ALA	N-CA-C	-5.43	96.34	111.00
3	3	169	TRP	CB-CA-C	5.42	121.24	110.40
1	1	270	GLU	O-C-N	5.42	131.37	122.70
2	2	70	HIS	CB-CA-C	-5.42	99.57	110.40
1	1	101	ILE	N-CA-CB	-5.41	98.35	110.80
3	3	218	ASP	C-N-CA	5.41	135.22	121.70
3	3	228	ASP	CB-CA-C	-5.41	99.58	110.40
2	2	20	ASP	CB-CG-OD2	-5.40	113.44	118.30
3	3	58	VAL	CA-CB-CG1	-5.40	102.81	110.90
3	3	234	GLY	N-CA-C	-5.39	99.62	113.10
4	4	26	TYR	CB-CG-CD1	-5.39	117.76	121.00
1	1	124	GLU	CG-CD-OE1	5.39	129.08	118.30
3	3	237	GLU	OE1-CD-OE2	5.38	129.76	123.30
1	1	147	TYR	O-C-N	5.38	131.31	122.70
3	3	8	PRO	C-N-CA	5.38	133.60	122.30
3	3	235	PRO	CB-CA-C	-5.38	98.56	112.00
3	3	183	TYR	CG-CD2-CE2	5.37	125.60	121.30
3	3	225	ARG	NE-CZ-NH2	5.35	122.98	120.30
3	3	203	THR	O-C-N	5.35	131.27	121.10
3	3	88	ASP	OD1-CG-OD2	-5.35	113.14	123.30
1	1	172	PHE	CA-C-O	-5.34	108.88	120.10
1	1	283	THR	O-C-N	5.34	131.25	122.70
4	4	44	ASP	CA-C-O	5.33	131.30	120.10
2	2	150	GLY	O-C-N	5.33	131.24	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	3	175	PHE	CB-CG-CD2	-5.33	117.07	120.80
3	3	95	ALA	CA-C-O	-5.33	108.91	120.10
3	3	233	SER	CA-C-O	5.33	131.29	120.10
2	2	161	ASP	CB-CA-C	-5.33	99.75	110.40
3	3	206	THR	N-CA-C	-5.32	96.64	111.00
2	2	52	LYS	CG-CD-CE	5.31	127.84	111.90
2	2	96	MET	CA-C-N	-5.31	105.51	117.20
2	2	165	ARG	C-N-CA	5.31	134.98	121.70
2	2	111	GLN	CB-CG-CD	5.31	125.40	111.60
2	2	87	LYS	CB-CA-C	5.30	121.00	110.40
3	3	206	THR	OG1-CB-CG2	5.29	122.16	110.00
1	1	201	ASP	CB-CG-OD1	-5.28	113.55	118.30
2	2	150	GLY	CA-C-O	-5.28	111.09	120.60
4	4	29	ILE	O-C-N	5.28	131.15	122.70
3	3	35	SER	N-CA-CB	-5.28	102.58	110.50
2	2	195	SER	CB-CA-C	5.27	120.11	110.10
3	3	108	HIS	CA-CB-CG	5.27	122.56	113.60
3	3	202	SER	CA-C-N	-5.26	105.63	117.20
3	3	10	SER	CB-CA-C	5.25	120.08	110.10
3	3	156	ASP	CB-CG-OD2	-5.25	113.58	118.30
1	1	192	ALA	N-CA-CB	-5.23	102.78	110.10
2	2	11	ASP	O-C-N	5.23	131.07	122.70
2	2	182	ASN	O-C-N	5.22	131.06	122.70
2	2	203	VAL	N-CA-CB	-5.22	100.01	111.50
1	1	158	ARG	NH1-CZ-NH2	-5.22	113.66	119.40
1	1	224	ILE	CB-CG1-CD1	-5.22	99.28	113.90
2	2	82	LEU	N-CA-C	5.22	125.09	111.00
2	2	12	ARG	CB-CA-C	-5.21	99.97	110.40
3	3	114	ARG	NE-CZ-NH2	5.21	122.91	120.30
3	3	92	THR	N-CA-C	-5.21	96.94	111.00
3	3	64	ASN	N-CA-CB	-5.20	101.24	110.60
1	1	287	ALA	CA-C-O	-5.20	109.19	120.10
1	1	242	LYS	CA-C-N	-5.19	105.77	117.20
2	2	173	LEU	CB-CA-C	5.19	120.06	110.20
3	3	24	ALA	CA-C-O	-5.17	109.24	120.10
4	4	26	TYR	O-C-N	5.17	130.97	122.70
2	2	30	ASN	N-CA-CB	-5.16	101.31	110.60
3	3	146	ASP	N-CA-CB	5.16	119.89	110.60
3	3	165	LEU	O-C-N	5.16	130.96	122.70
3	3	76	THR	CA-C-N	-5.16	105.88	116.20
2	2	19	GLY	CA-C-N	-5.15	105.86	117.20
1	1	22	GLU	CG-CD-OE1	5.14	128.58	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	3	181	ASN	O-C-N	5.14	130.92	122.70
2	2	237	SER	CA-C-O	5.13	130.87	120.10
4	4	42	ARG	C-N-CA	-5.13	108.88	121.70
1	1	66	SER	O-C-N	5.11	130.88	122.70
1	1	120	ARG	NH1-CZ-NH2	-5.11	113.78	119.40
3	3	72	LEU	CB-CG-CD2	-5.11	102.32	111.00
1	1	43	SER	CA-C-N	-5.10	105.98	117.20
4	4	38	SER	CA-C-O	-5.10	109.39	120.10
1	1	46	GLN	O-C-N	5.10	130.78	121.10
1	1	163	TRP	CB-CA-C	5.09	120.57	110.40
2	2	50	ILE	CB-CA-C	5.09	121.77	111.60
1	1	189	ILE	C-N-CA	5.08	134.41	121.70
1	1	205	THR	OG1-CB-CG2	5.08	121.70	110.00
1	1	94	ILE	CA-C-N	-5.08	106.02	117.20
1	1	178	PRO	CA-C-N	-5.08	106.02	117.20
3	3	78	MET	CB-CA-C	5.08	120.56	110.40
2	2	40	HIS	CA-CB-CG	-5.07	104.98	113.60
3	3	223	MET	CG-SD-CE	5.06	108.30	100.20
2	2	168	SER	C-N-CA	5.06	134.35	121.70
3	3	227	THR	CA-CB-CG2	-5.06	105.32	112.40
2	2	28	VAL	CB-CA-C	-5.05	101.80	111.40
1	1	195	MET	CG-SD-CE	5.04	108.27	100.20
3	3	131	LEU	CA-CB-CG	5.04	126.89	115.30
1	1	212	VAL	CA-C-N	-5.03	106.13	117.20
3	3	64	ASN	CA-CB-CG	-5.03	102.33	113.40
1	1	223	ARG	CG-CD-NE	5.03	122.36	111.80
2	2	45	GLN	N-CA-CB	5.03	119.65	110.60
1	1	175	HIS	CB-CA-C	5.03	120.45	110.40
1	1	204	ASN	N-CA-CB	5.02	119.64	110.60
1	1	80	SER	CA-C-O	5.02	130.64	120.10
2	2	218	ASN	CB-CG-OD1	-5.02	111.57	121.60
3	3	57	ASN	N-CA-CB	-5.02	101.57	110.60
2	2	79	TRP	CA-CB-CG	5.01	123.22	113.70
1	1	236	THR	CA-CB-CG2	5.01	119.41	112.40
3	3	210	LEU	C-N-CA	-5.00	109.19	121.70
1	1	235	ILE	CA-C-N	-5.00	106.20	117.20

There are no chirality outliers.

There are no planarity outliers.

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	1	2262	0	2193	335	1
2	2	1979	0	1920	215	1
3	3	1831	0	1809	226	0
4	4	151	0	136	18	0
5	A	23	0	19	31	0
All	All	6246	0	6077	708	1

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 (708) 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)
1:1:102:THR:CA	5:A:2:FRU:H61	1.09	1.55
1:1:102:THR:HA	5:A:2:FRU:C6	0.95	1.41
2:2:18:ARG:NH1	2:2:249:MET:HE2	1.54	1.21
1:1:23:SER:OG	1:1:53:THR:HG22	1.36	1.19
3:3:42:ASN:HD22	3:3:44:ILE:HG22	1.06	1.13
1:1:254:PRO:HG3	3:3:101:GLU:HG2	1.27	1.12
2:2:18:ARG:HH12	2:2:249:MET:HE2	0.99	1.08
1:1:254:PRO:CG	3:3:101:GLU:HG2	1.81	1.08
3:3:160:GLN:O	3:3:161:SER:HB3	1.48	1.07
1:1:46:GLN:HB3	1:1:47:PRO:CD	1.85	1.06
1:1:102:THR:C	5:A:2:FRU:H61	1.78	1.03
3:3:42:ASN:ND2	3:3:44:ILE:HG22	1.74	1.02
1:1:6:TYR:HB3	1:1:7:ILE:HD13	1.42	1.02
2:2:185:ILE:HD13	3:3:98:LEU:HD22	1.41	1.02
1:1:45:VAL:H	3:3:114:ARG:NH1	1.59	1.01
3:3:117:PHE:HD2	3:3:211:CYS:HB3	1.25	1.01
1:1:142:VAL:CG1	1:1:225:VAL:HB	1.90	1.01
1:1:46:GLN:CB	1:1:47:PRO:HD2	1.89	1.00
2:2:83:PRO:HG2	2:2:218:ASN:HA	1.44	1.00
1:1:7:ILE:HA	1:1:11:LEU:HD23	1.41	1.00
3:3:122:THR:HG22	3:3:123:ALA:H	1.21	1.00
1:1:46:GLN:HB3	1:1:47:PRO:HD2	1.01	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:102:THR:HA	5:A:2:FRU:O6	1.60	0.99
3:3:75:GLN:HA	3:3:75:GLN:NE2	1.75	0.99
3:3:75:GLN:HA	3:3:75:GLN:HE21	1.26	0.99
1:1:278:ILE:HD12	3:3:67:MET:CE	1.93	0.98
3:3:117:PHE:CD2	3:3:211:CYS:HB3	2.00	0.97
3:3:51:THR:HG21	3:3:98:LEU:HB2	1.47	0.96
1:1:113:PHE:O	1:1:115:LEU:N	1.99	0.95
1:1:35:ASP:O	3:3:162:THR:HB	1.69	0.93
1:1:215:ASN:CG	5:A:2:FRU:O3	2.07	0.92
2:2:185:ILE:HD13	3:3:98:LEU:CD2	2.00	0.92
3:3:24:ALA:O	3:3:25:LEU:HB2	1.72	0.90
1:1:96:PHE:CE1	1:1:157:LYS:HA	2.06	0.90
1:1:265:THR:OG1	2:2:133:ALA:HB2	1.69	0.90
1:1:67:ILE:HD11	3:3:40:VAL:HB	1.54	0.88
1:1:173:TRP:CD1	1:1:180:PRO:HD3	2.09	0.88
1:1:141:ILE:HG12	1:1:141:ILE:O	1.69	0.88
2:2:12:ARG:HH11	2:2:12:ARG:HB3	1.36	0.88
3:3:54:PRO:O	3:3:93:PRO:HB2	1.74	0.88
1:1:97:THR:HG23	1:1:222:SER:HB3	1.55	0.87
1:1:75:GLY:O	1:1:77:VAL:HG13	1.74	0.87
1:1:197:TYR:CE1	1:1:214:THR:HG23	2.08	0.87
1:1:254:PRO:HG3	3:3:101:GLU:CG	2.05	0.86
3:3:231:ILE:HD13	3:3:231:ILE:H	1.39	0.86
1:1:190:ALA:O	3:3:31:THR:HG21	1.75	0.86
3:3:58:VAL:O	3:3:61:ASN:HB2	1.76	0.86
1:1:142:VAL:HG12	1:1:225:VAL:HB	1.57	0.86
1:1:171:ILE:HD11	1:1:180:PRO:HB2	1.58	0.86
1:1:17:VAL:HG13	1:1:60:GLN:O	1.76	0.86
2:2:161:ASP:HB2	2:2:164:LEU:HD22	1.55	0.86
3:3:42:ASN:HD22	3:3:44:ILE:CG2	1.87	0.86
3:3:82:VAL:HG12	3:3:83:PHE:HD1	1.38	0.84
3:3:82:VAL:HG12	3:3:83:PHE:N	1.90	0.84
1:1:129:PRO:HG2	1:1:173:TRP:CE2	2.13	0.84
1:1:140:HIS:O	1:1:226:THR:HG21	1.75	0.84
1:1:142:VAL:HG11	1:1:225:VAL:HB	1.60	0.83
2:2:159:GLU:C	2:2:160:ARG:HG2	1.97	0.83
3:3:51:THR:HG21	3:3:98:LEU:CB	2.07	0.83
2:2:161:ASP:HB2	2:2:164:LEU:CD2	2.08	0.82
3:3:102:ILE:HG22	3:3:103:ALA:N	1.92	0.82
2:2:168:SER:OG	2:2:170:ASP:HB2	1.79	0.82
1:1:119:VAL:CG1	1:1:121:PHE:HE2	1.93	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:7:THR:O	3:3:10:SER:HB2	1.80	0.81
1:1:215:ASN:H	1:1:215:ASN:ND2	1.77	0.81
1:1:197:TYR:H	2:2:131:GLN:HE21	1.28	0.80
1:1:23:SER:CB	1:1:53:THR:HG22	2.11	0.80
1:1:204:ASN:C	1:1:206:SER:H	1.82	0.79
1:1:173:TRP:HD1	1:1:180:PRO:HD3	1.45	0.79
2:2:18:ARG:HH12	2:2:249:MET:CE	1.90	0.79
3:3:194:GLN:HA	3:3:194:GLN:HE21	1.48	0.79
2:2:60:SER:OG	2:2:61:ASN:N	2.14	0.78
1:1:45:VAL:H	3:3:114:ARG:HH11	1.31	0.78
2:2:146:LEU:CD1	2:2:166:GLN:HA	2.13	0.78
2:2:12:ARG:HG3	2:2:13:ILE:N	1.99	0.78
1:1:7:ILE:O	1:1:11:LEU:HB2	1.84	0.77
2:2:173:LEU:O	2:2:174:ASN:HB2	1.83	0.77
2:2:146:LEU:HD12	2:2:167:PRO:HD3	1.65	0.77
3:3:231:ILE:H	3:3:231:ILE:CD1	1.97	0.77
1:1:127:LEU:HB2	1:1:180:PRO:HG2	1.67	0.77
1:1:103:LEU:N	5:A:2:FRU:H61	1.99	0.76
1:1:278:ILE:CD1	3:3:67:MET:CE	2.64	0.76
2:2:78:TRP:HZ3	2:2:226:PRO:HD3	1.50	0.76
1:1:255:ARG:HD3	1:1:259:TYR:CE2	2.20	0.76
2:2:126:MET:HG3	2:2:201:LEU:HD12	1.66	0.76
2:2:68:SER:C	2:2:69:LYS:HG2	2.07	0.75
3:3:160:GLN:O	3:3:161:SER:CB	2.32	0.75
3:3:20:GLN:HE22	4:4:30:ASN:HA	1.50	0.74
2:2:65:THR:OG1	2:2:245:SER:OG	2.05	0.74
4:4:26:TYR:CD2	4:4:29:ILE:HD11	2.22	0.74
3:3:75:GLN:OE1	3:3:80:GLN:HG2	1.87	0.74
2:2:257:ARG:HH11	2:2:257:ARG:HG2	1.52	0.74
3:3:81:LYS:HG3	3:3:82:VAL:N	2.01	0.74
1:1:33:LEU:O	3:3:163:ILE:HD12	1.88	0.73
1:1:223:ARG:HH11	1:1:223:ARG:CG	2.00	0.73
1:1:119:VAL:HG13	1:1:121:PHE:CE2	2.24	0.73
2:2:41:TYR:CD2	2:2:55:GLN:OE1	2.41	0.73
2:2:12:ARG:CG	2:2:13:ILE:N	2.51	0.73
1:1:223:ARG:HH11	1:1:223:ARG:HG2	1.53	0.73
3:3:122:THR:HG22	3:3:123:ALA:N	1.99	0.73
1:1:197:TYR:CD1	1:1:214:THR:HG23	2.24	0.73
1:1:210:GLY:O	1:1:213:VAL:HG23	1.89	0.72
1:1:92:GLN:O	1:1:93:ASP:HB2	1.89	0.72
3:3:53:ILE:O	3:3:55:VAL:HG12	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:173:SER:O	3:3:175:PHE:N	2.22	0.72
2:2:183:LEU:HD12	2:2:186:PHE:HD1	1.52	0.72
3:3:125:THR:HG22	3:3:126:THR:N	2.03	0.72
2:2:148:HIS:N	2:2:149:PRO:CD	2.52	0.72
1:1:101:ILE:O	5:A:2:FRU:O6	2.08	0.72
2:2:146:LEU:HD12	2:2:167:PRO:CD	2.19	0.72
2:2:37:VAL:HG21	3:3:37:PRO:HB3	1.72	0.71
1:1:61:THR:HG22	1:1:63:ASP:OD1	1.90	0.71
1:1:242:LYS:NZ	3:3:17:ASP:O	2.22	0.71
2:2:148:HIS:N	2:2:149:PRO:HD3	2.06	0.71
1:1:46:GLN:OE1	3:3:217:LYS:HG3	1.89	0.71
1:1:123:SER:HB3	1:1:241:HIS:NE2	2.05	0.71
1:1:278:ILE:HD12	3:3:67:MET:HE3	1.71	0.71
2:2:207:ASN:HD22	2:2:209:VAL:H	1.37	0.71
1:1:124:GLU:OE2	1:1:181:ARG:HD3	1.91	0.70
1:1:14:VAL:HG11	4:4:43:LEU:HB3	1.74	0.70
3:3:82:VAL:HG12	3:3:83:PHE:CD1	2.25	0.70
1:1:104:GLN:HB3	1:1:110:ARG:HG3	1.72	0.70
1:1:169:MET:CE	1:1:171:ILE:HB	2.21	0.70
3:3:82:VAL:CG1	3:3:83:PHE:HD1	2.04	0.70
1:1:22:GLU:HA	1:1:54:ARG:O	1.91	0.70
1:1:102:THR:OG1	5:A:2:FRU:H5	1.91	0.70
1:1:113:PHE:C	1:1:115:LEU:H	1.93	0.70
2:2:78:TRP:N	2:2:78:TRP:CE3	2.60	0.69
2:2:12:ARG:HD3	2:2:27:ASP:HA	1.74	0.69
1:1:92:GLN:C	1:1:94:ILE:HD12	2.13	0.69
1:1:269:PRO:HG2	1:1:272:GLY:O	1.93	0.69
2:2:41:TYR:HD2	2:2:55:GLN:OE1	1.76	0.69
1:1:281:ARG:HB3	3:3:57:ASN:O	1.93	0.69
1:1:67:ILE:CD1	3:3:40:VAL:HB	2.22	0.69
2:2:78:TRP:HE3	2:2:78:TRP:H	1.39	0.69
1:1:127:LEU:O	1:1:180:PRO:HD2	1.92	0.69
3:3:127:LEU:HA	3:3:196:ASN:O	1.93	0.69
1:1:142:VAL:HG13	1:1:143:MET:N	2.07	0.69
3:3:127:LEU:HG	3:3:128:LYS:N	2.08	0.69
3:3:132:ALA:O	3:3:189:ILE:HA	1.93	0.69
1:1:7:ILE:CA	1:1:11:LEU:HD23	2.21	0.68
1:1:44:ASN:C	1:1:44:ASN:HD22	1.96	0.68
2:2:103:ARG:HB3	2:2:211:MET:HG2	1.76	0.68
2:2:206:VAL:HG12	3:3:37:PRO:HG2	1.75	0.68
1:1:38:GLU:O	2:2:189:GLN:HB2	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:155:PRO:HB3	1:1:163:TRP:HE1	1.57	0.68
1:1:215:ASN:ND2	1:1:215:ASN:N	2.42	0.68
1:1:91:GLY:C	1:1:94:ILE:HD13	2.14	0.68
2:2:56:PRO:HB2	2:2:60:SER:HB3	1.76	0.68
2:2:78:TRP:N	2:2:78:TRP:HE3	1.92	0.68
3:3:42:ASN:HB3	3:3:44:ILE:HG22	1.73	0.68
1:1:278:ILE:HD12	3:3:67:MET:HE1	1.77	0.67
2:2:171:SER:HA	2:2:175:PHE:CE2	2.28	0.67
2:2:78:TRP:CZ3	2:2:226:PRO:HD3	2.30	0.67
1:1:23:SER:OG	1:1:53:THR:CG2	2.31	0.67
2:2:51:ASN:HD22	2:2:51:ASN:H	1.41	0.67
1:1:92:GLN:C	1:1:94:ILE:CD1	2.63	0.66
3:3:42:ASN:ND2	3:3:44:ILE:CG2	2.53	0.66
1:1:135:GLY:HA3	1:1:231:LEU:HB3	1.76	0.66
3:3:89:ILE:HD11	3:3:109:TRP:CG	2.31	0.65
1:1:160:ASP:H	1:1:163:TRP:HD1	1.44	0.65
2:2:126:MET:HE3	2:2:126:MET:HA	1.79	0.65
3:3:201:PRO:O	3:3:202:SER:HB2	1.96	0.65
3:3:87:VAL:HG22	3:3:189:ILE:HG22	1.79	0.65
1:1:186:PHE:HE2	3:3:31:THR:HG22	1.62	0.65
2:2:12:ARG:HB3	2:2:12:ARG:NH1	2.10	0.65
2:2:146:LEU:HD12	2:2:166:GLN:HA	1.77	0.64
3:3:66:SER:C	3:3:68:TYR:H	2.00	0.64
2:2:155:ASP:O	2:2:156:VAL:HB	1.98	0.64
1:1:19:ASN:HB3	1:1:56:VAL:O	1.97	0.64
3:3:89:ILE:HD11	3:3:109:TRP:CD2	2.33	0.64
3:3:99:ILE:HG22	3:3:100:GLY:N	2.11	0.64
1:1:278:ILE:CD1	3:3:67:MET:HE1	2.27	0.64
2:2:72:ASN:HB3	2:2:75:SER:N	2.13	0.63
2:2:207:ASN:ND2	2:2:209:VAL:HG22	2.13	0.63
1:1:217:MET:SD	5:A:1:GLC:O3	2.55	0.63
2:2:30:ASN:HD22	2:2:31:ALA:N	1.97	0.63
1:1:244:LYS:HE3	4:4:38:SER:O	1.98	0.63
1:1:260:THR:C	1:1:261:HIS:CD2	2.71	0.63
2:2:174:ASN:C	2:2:175:PHE:HD2	2.02	0.63
1:1:204:ASN:C	1:1:206:SER:N	2.52	0.63
1:1:148:VAL:HG12	1:1:152:ALA:HB3	1.82	0.62
1:1:260:THR:C	1:1:261:HIS:HD2	2.02	0.62
1:1:6:TYR:CB	1:1:7:ILE:HD13	2.25	0.62
1:1:7:ILE:HD13	1:1:7:ILE:N	2.14	0.62
1:1:155:PRO:HB3	1:1:163:TRP:NE1	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:276:THR:OG1	1:1:277:ALA:N	2.31	0.62
2:2:145:LYS:NZ	2:2:263:GLN:HG2	2.15	0.62
1:1:215:ASN:CB	5:A:2:FRU:O3	2.47	0.62
1:1:283:THR:HG22	1:1:285:THR:N	2.15	0.62
1:1:281:ARG:NH2	3:3:84:SER:O	2.33	0.62
3:3:102:ILE:O	3:3:105:TYR:HB2	2.00	0.62
3:3:89:ILE:HA	3:3:94:LEU:HD13	1.80	0.62
1:1:141:ILE:HA	1:1:226:THR:HG21	1.80	0.62
5:A:1:GLC:H5	5:A:2:FRU:H62	1.80	0.62
1:1:37:ALA:HB2	3:3:162:THR:HG21	1.83	0.61
1:1:150:PRO:HG3	1:1:218:GLY:N	2.15	0.61
2:2:84:ASP:HB2	2:2:218:ASN:HD21	1.66	0.61
1:1:223:ARG:HG2	1:1:223:ARG:NH1	2.16	0.61
1:1:14:VAL:HG12	1:1:15:LEU:HD22	1.81	0.61
1:1:91:GLY:O	1:1:157:LYS:CB	2.49	0.61
2:2:91:ILE:O	2:2:92:PHE:C	2.38	0.61
2:2:183:LEU:HD12	2:2:186:PHE:CD1	2.34	0.61
1:1:103:LEU:HG	5:A:1:GLC:H61	1.83	0.61
3:3:91:SER:O	3:3:92:THR:C	2.39	0.61
1:1:94:ILE:HD12	1:1:94:ILE:N	2.16	0.61
1:1:105:GLU:O	1:1:106:MET:HG3	2.01	0.61
1:1:108:GLN:HB3	1:1:109:ILE:HG22	1.83	0.61
3:3:72:LEU:HD11	3:3:209:MET:HB3	1.82	0.60
1:1:140:HIS:O	1:1:226:THR:CG2	2.48	0.60
4:4:43:LEU:O	4:4:44:ASP:C	2.38	0.60
1:1:200:TYR:CD1	1:1:209:TYR:HB2	2.37	0.60
1:1:249:TRP:HA	3:3:39:GLU:HA	1.84	0.60
3:3:90:THR:OG1	3:3:178:THR:O	2.15	0.60
3:3:122:THR:CG2	3:3:123:ALA:H	1.99	0.60
3:3:145:LYS:HA	3:3:148:MET:HE2	1.83	0.60
1:1:79:ILE:HD13	1:1:238:HIS:CE1	2.35	0.60
1:1:102:THR:HA	5:A:2:FRU:C5	2.15	0.60
2:2:84:ASP:OD2	2:2:87:LYS:HE2	2.02	0.60
3:3:95:ALA:O	3:3:97:THR:N	2.34	0.60
1:1:91:GLY:O	1:1:157:LYS:HB3	2.02	0.60
1:1:136:ASP:O	1:1:137:ASP:HB2	2.02	0.59
2:2:207:ASN:HD21	2:2:209:VAL:HG22	1.67	0.59
1:1:22:GLU:CA	1:1:54:ARG:O	2.50	0.59
1:1:204:ASN:HD22	1:1:205:THR:N	2.00	0.59
1:1:45:VAL:H	3:3:114:ARG:HH12	1.45	0.59
3:3:44:ILE:O	3:3:47:CYS:HB2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:127:LEU:CB	1:1:180:PRO:HG2	2.33	0.59
1:1:7:ILE:HD13	1:1:7:ILE:H	1.67	0.59
1:1:102:THR:CB	5:A:2:FRU:C6	2.78	0.59
2:2:144:TYR:O	2:2:146:LEU:N	2.36	0.59
2:2:77:GLY:HA2	2:2:78:TRP:CE3	2.37	0.59
3:3:46:MET:O	3:3:98:LEU:HD23	2.03	0.59
1:1:102:THR:CA	5:A:2:FRU:HO6	2.14	0.58
2:2:257:ARG:HG2	2:2:257:ARG:NH1	2.14	0.58
1:1:66:SER:O	1:1:68:GLU:N	2.37	0.58
3:3:136:PRO:HG3	3:3:176:ARG:HH22	1.68	0.58
1:1:11:LEU:N	1:1:11:LEU:HD22	2.19	0.58
1:1:142:VAL:CG1	1:1:225:VAL:CB	2.76	0.58
1:1:278:ILE:HA	3:3:92:THR:HG21	1.86	0.58
2:2:57:ASP:O	2:2:58:THR:HG22	2.04	0.58
1:1:197:TYR:HD2	1:1:198:ASP:H	1.52	0.58
1:1:44:ASN:C	1:1:44:ASN:ND2	2.58	0.58
1:1:142:VAL:H	1:1:226:THR:HG23	1.67	0.58
1:1:199:GLY:HA2	2:2:216:ARG:O	2.04	0.58
3:3:136:PRO:HG3	3:3:176:ARG:NH2	2.19	0.58
1:1:85:ASP:OD2	1:1:86:TYR:N	2.36	0.58
2:2:154:ARG:HD3	2:2:155:ASP:N	2.19	0.58
3:3:54:PRO:HA	3:3:67:MET:O	2.04	0.58
1:1:99:TRP:CZ3	1:1:101:ILE:HA	2.39	0.57
1:1:110:ARG:O	1:1:114:GLU:HG3	2.04	0.57
1:1:163:TRP:CD2	1:1:223:ARG:HD3	2.39	0.57
2:2:235:THR:C	2:2:237:SER:H	2.06	0.57
3:3:192:TRP:CD1	3:3:192:TRP:N	2.73	0.57
1:1:113:PHE:C	1:1:115:LEU:N	2.52	0.57
1:1:153:PRO:O	1:1:153:PRO:HG2	2.04	0.57
2:2:49:ALA:O	2:2:50:ILE:HG13	2.04	0.57
2:2:158:GLN:HG3	2:2:159:GLU:H	1.68	0.57
3:3:194:GLN:HA	3:3:194:GLN:NE2	2.19	0.57
1:1:7:ILE:H	1:1:7:ILE:CD1	2.17	0.57
3:3:173:SER:O	3:3:174:HIS:C	2.43	0.57
1:1:145:TYR:CD2	1:1:145:TYR:N	2.73	0.57
1:1:104:GLN:OE1	1:1:263:HIS:ND1	2.32	0.56
3:3:87:VAL:O	3:3:89:ILE:N	2.38	0.56
3:3:144:ARG:O	3:3:145:LYS:C	2.44	0.56
1:1:54:ARG:CG	1:1:55:TYR:H	2.16	0.56
1:1:129:PRO:HG2	1:1:173:TRP:CZ2	2.41	0.56
1:1:253:PRO:HD3	2:2:185:ILE:CG2	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:102:THR:CB	5:A:2:FRU:H5	2.35	0.56
1:1:111:ARG:NH1	3:3:230:HIS:HB2	2.20	0.56
3:3:228:ASP:HB3	3:3:229:LEU:HD12	1.88	0.56
1:1:103:LEU:N	5:A:2:FRU:C6	2.67	0.56
2:2:120:GLY:HA3	2:2:193:LEU:HD12	1.86	0.56
1:1:90:ASN:HD22	1:1:158:ARG:HD3	1.70	0.56
1:1:124:GLU:O	1:1:124:GLU:HG3	2.06	0.56
1:1:253:PRO:HD3	2:2:185:ILE:HG21	1.86	0.56
1:1:261:HIS:H	3:3:237:GLU:H	1.52	0.56
2:2:72:ASN:HB3	2:2:74:SER:H	1.70	0.56
1:1:92:GLN:HA	1:1:157:LYS:HG2	1.86	0.56
1:1:255:ARG:NH2	1:1:259:TYR:HA	2.21	0.56
2:2:202:ILE:HD13	2:2:249:MET:CE	2.36	0.56
3:3:42:ASN:CB	3:3:44:ILE:HG22	2.36	0.56
2:2:122:LEU:HD22	2:2:224:ILE:HG13	1.87	0.56
2:2:173:LEU:O	2:2:174:ASN:CB	2.54	0.56
3:3:165:LEU:HD12	3:3:166:VAL:N	2.21	0.56
1:1:67:ILE:HD11	3:3:40:VAL:CB	2.33	0.55
3:3:42:ASN:HB3	3:3:44:ILE:CG2	2.36	0.55
1:1:92:GLN:N	1:1:94:ILE:CD1	2.68	0.55
1:1:119:VAL:HG11	1:1:121:PHE:HE2	1.69	0.55
3:3:81:LYS:HB2	3:3:192:TRP:CE3	2.41	0.55
2:2:83:PRO:HG2	2:2:218:ASN:CA	2.28	0.55
3:3:14:MET:HG2	3:3:16:THR:HG22	1.88	0.55
3:3:83:PHE:CE1	3:3:191:CYS:CB	2.89	0.55
3:3:104:SER:O	3:3:227:THR:HA	2.06	0.55
3:3:107:THR:O	3:3:177:LEU:HD23	2.06	0.55
2:2:84:ASP:O	2:2:87:LYS:HD2	2.07	0.55
1:1:89:TYR:O	1:1:90:ASN:HB2	2.06	0.55
1:1:257:VAL:HG11	1:1:274:VAL:HG21	1.89	0.55
1:1:80:SER:HB3	1:1:237:THR:HG23	1.89	0.55
2:2:127:ILE:HD11	2:2:183:LEU:HD11	1.89	0.55
1:1:19:ASN:HA	1:1:58:THR:HG23	1.88	0.55
1:1:84:VAL:HG21	1:1:233:VAL:HG23	1.88	0.55
1:1:91:GLY:C	1:1:94:ILE:CD1	2.75	0.55
1:1:266:ASN:OD1	2:2:134:SER:N	2.34	0.55
3:3:155:TRP:CD2	3:3:163:ILE:CG2	2.90	0.55
2:2:116:LYS:HB2	3:3:124:ASN:ND2	2.21	0.54
2:2:227:ILE:HG21	3:3:210:LEU:HD11	1.89	0.54
3:3:80:GLN:HA	3:3:80:GLN:NE2	2.23	0.54
3:3:125:THR:CG2	3:3:126:THR:N	2.70	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:61:THR:CG2	1:1:63:ASP:OD1	2.54	0.54
1:1:124:GLU:HG2	1:1:242:LYS:HB3	1.88	0.54
1:1:201:ASP:OD1	1:1:208:LYS:HB2	2.07	0.54
2:2:102:GLY:HA3	2:2:214:MET:HG3	1.88	0.54
3:3:121:GLY:HA2	3:3:207:ALA:HB1	1.88	0.54
1:1:61:THR:HG22	1:1:63:ASP:CG	2.28	0.54
1:1:72:GLY:C	1:1:73:ARG:HG2	2.27	0.54
1:1:84:VAL:HG12	1:1:85:ASP:N	2.22	0.54
3:3:81:LYS:HB2	3:3:192:TRP:CZ3	2.43	0.54
3:3:103:ALA:O	3:3:178:THR:HG21	2.08	0.54
2:2:174:ASN:O	2:2:175:PHE:HB2	2.07	0.54
1:1:169:MET:HE2	1:1:171:ILE:HB	1.89	0.54
2:2:23:ILE:HG21	2:2:109:HIS:CD2	2.42	0.54
1:1:195:MET:CE	5:A:2:FRU:H11	2.37	0.54
2:2:40:HIS:HA	2:2:250:CYS:SG	2.47	0.54
2:2:174:ASN:HB3	2:2:176:ASP:OD1	2.08	0.54
1:1:103:LEU:CG	5:A:1:GLC:H61	2.38	0.54
1:1:269:PRO:CG	1:1:272:GLY:O	2.56	0.54
1:1:283:THR:CG2	1:1:285:THR:HB	2.38	0.54
1:1:215:ASN:H	1:1:215:ASN:HD22	1.51	0.54
1:1:17:VAL:CG1	1:1:60:GLN:O	2.53	0.54
1:1:96:PHE:HE1	1:1:157:LYS:HA	1.70	0.53
1:1:106:MET:O	1:1:107:ALA:O	2.27	0.53
3:3:237:GLU:CG	3:3:238:GLN:H	2.20	0.53
1:1:66:SER:C	1:1:68:GLU:N	2.60	0.53
1:1:103:LEU:H	5:A:2:FRU:C5	2.21	0.53
2:2:235:THR:OG1	2:2:237:SER:HB3	2.08	0.53
3:3:94:LEU:O	3:3:95:ALA:C	2.45	0.53
1:1:33:LEU:HB3	3:3:163:ILE:HD11	1.90	0.53
2:2:103:ARG:CB	2:2:211:MET:HG2	2.38	0.53
3:3:89:ILE:HA	3:3:94:LEU:CD1	2.38	0.53
1:1:200:TYR:HA	1:1:208:LYS:O	2.08	0.53
2:2:174:ASN:C	2:2:175:PHE:CD2	2.82	0.53
2:2:57:ASP:O	2:2:58:THR:CB	2.55	0.53
2:2:122:LEU:O	2:2:190:PHE:HA	2.08	0.53
1:1:89:TYR:HE1	1:1:227:GLU:C	2.12	0.53
2:2:41:TYR:CE2	2:2:55:GLN:OE1	2.62	0.53
1:1:197:TYR:H	2:2:131:GLN:NE2	2.04	0.53
1:1:284:ILE:HG13	1:1:285:THR:N	2.24	0.53
2:2:61:ASN:HB2	2:2:248:PRO:O	2.09	0.53
2:2:158:GLN:CG	2:2:159:GLU:H	2.21	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:66:SER:O	3:3:68:TYR:N	2.42	0.53
1:1:92:GLN:O	1:1:94:ILE:HD11	2.09	0.52
1:1:7:ILE:HA	1:1:11:LEU:CD2	2.28	0.52
1:1:19:ASN:N	1:1:19:ASN:ND2	2.57	0.52
1:1:257:VAL:HG21	2:2:173:LEU:HD11	1.91	0.52
1:1:263:HIS:CE1	5:A:2:FRU:O4	2.61	0.52
3:3:75:GLN:HG2	3:3:80:GLN:HB3	1.91	0.52
4:4:26:TYR:CD2	4:4:29:ILE:CD1	2.91	0.52
1:1:261:HIS:CD2	1:1:261:HIS:N	2.74	0.52
2:2:18:ARG:HG3	2:2:247:SER:OG	2.09	0.52
1:1:200:TYR:CE1	1:1:209:TYR:HB2	2.44	0.52
3:3:169:TRP:CZ3	3:3:176:ARG:HD2	2.44	0.52
1:1:84:VAL:HG12	1:1:85:ASP:H	1.75	0.52
1:1:171:ILE:CD1	1:1:180:PRO:HB2	2.37	0.52
1:1:254:PRO:HG2	3:3:101:GLU:HG2	1.83	0.52
1:1:102:THR:HA	5:A:2:FRU:HO6	1.69	0.52
3:3:83:PHE:CE1	3:3:191:CYS:HB3	2.45	0.52
3:3:136:PRO:HB3	3:3:185:MET:O	2.10	0.52
1:1:119:VAL:CG1	1:1:121:PHE:CE2	2.79	0.51
2:2:14:MET:HG2	2:2:15:GLN:N	2.25	0.51
3:3:7:THR:O	3:3:10:SER:CB	2.53	0.51
1:1:281:ARG:HH11	3:3:57:ASN:HB3	1.74	0.51
1:1:6:TYR:O	1:1:10:VAL:N	2.44	0.51
1:1:46:GLN:O	1:1:49:ASP:HB2	2.10	0.51
2:2:110:VAL:O	2:2:198:SER:HA	2.11	0.51
2:2:190:PHE:O	2:2:196:ASN:ND2	2.43	0.51
2:2:202:ILE:HD13	2:2:249:MET:HE3	1.93	0.51
1:1:197:TYR:CD1	1:1:214:THR:CG2	2.94	0.51
2:2:86:LEU:C	2:2:88:ASP:H	2.14	0.51
2:2:173:LEU:O	2:2:177:GLY:N	2.44	0.51
3:3:99:ILE:CG2	3:3:100:GLY:N	2.73	0.51
3:3:173:SER:C	3:3:175:PHE:N	2.63	0.51
2:2:145:LYS:HZ1	2:2:263:GLN:HG2	1.74	0.51
3:3:181:ASN:OD1	3:3:183:TYR:HB3	2.11	0.51
2:2:12:ARG:O	2:2:28:VAL:HG22	2.10	0.51
3:3:110:THR:O	3:3:219:PHE:HA	2.10	0.51
4:4:42:ARG:HH12	4:4:44:ASP:HB3	1.76	0.51
1:1:7:ILE:O	1:1:11:LEU:HD23	2.11	0.51
1:1:103:LEU:H	5:A:2:FRU:C6	2.24	0.51
1:1:123:SER:HB3	1:1:241:HIS:CD2	2.45	0.51
1:1:143:MET:HG2	1:1:145:TYR:CE2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:271:THR:HG22	1:1:272:GLY:N	2.25	0.50
1:1:42:THR:HG22	1:1:43:SER:O	2.12	0.50
1:1:44:ASN:ND2	1:1:44:ASN:O	2.34	0.50
2:2:154:ARG:HH11	2:2:154:ARG:CG	2.24	0.50
3:3:56:ASN:C	3:3:58:VAL:H	2.12	0.50
3:3:201:PRO:O	3:3:202:SER:CB	2.53	0.50
1:1:92:GLN:C	1:1:94:ILE:HD11	2.31	0.50
4:4:26:TYR:O	4:4:27:PHE:HB2	2.12	0.50
2:2:175:PHE:CD2	2:2:175:PHE:N	2.79	0.50
3:3:72:LEU:HD12	3:3:72:LEU:N	2.26	0.50
3:3:102:ILE:O	3:3:105:TYR:N	2.44	0.50
3:3:141:PRO:HG3	3:3:147:ALA:HB2	1.93	0.50
1:1:184:ILE:HG22	1:1:185:PRO:O	2.12	0.50
1:1:102:THR:CA	5:A:2:FRU:C5	2.85	0.50
1:1:244:LYS:CE	4:4:38:SER:O	2.60	0.50
2:2:137:HIS:CD2	2:2:138:GLY:N	2.79	0.50
2:2:159:GLU:OE1	2:2:159:GLU:HA	2.11	0.50
3:3:25:LEU:N	3:3:26:PRO:HD3	2.27	0.49
3:3:62:VAL:HA	3:3:67:MET:HG3	1.94	0.49
3:3:140:GLU:HB3	3:3:188:TYR:CD1	2.48	0.49
1:1:281:ARG:HH11	3:3:57:ASN:CB	2.26	0.49
1:1:127:LEU:HD12	1:1:239:ILE:HG12	1.95	0.49
1:1:141:ILE:CD1	1:1:235:ILE:HG12	2.43	0.49
3:3:51:THR:HG21	3:3:98:LEU:HB3	1.92	0.49
3:3:200:PRO:O	3:3:203:THR:OG1	2.22	0.49
1:1:186:PHE:CE2	3:3:31:THR:HG22	2.45	0.49
1:1:244:LYS:HZ1	4:4:38:SER:H	1.61	0.49
2:2:70:HIS:ND1	2:2:71:TRP:N	2.60	0.49
3:3:117:PHE:CE1	3:3:131:LEU:HG	2.47	0.49
3:3:14:MET:C	3:3:16:THR:H	2.16	0.49
3:3:118:MET:O	3:3:209:MET:HA	2.12	0.49
3:3:155:TRP:CD2	3:3:163:ILE:HG22	2.48	0.49
2:2:146:LEU:HD11	2:2:166:GLN:HA	1.94	0.49
2:2:174:ASN:ND2	2:2:178:THR:O	2.41	0.49
1:1:7:ILE:O	1:1:11:LEU:N	2.43	0.49
2:2:57:ASP:O	2:2:59:SER:N	2.42	0.49
2:2:146:LEU:HD12	2:2:167:PRO:HD2	1.95	0.49
1:1:173:TRP:HE3	1:1:173:TRP:O	1.95	0.49
3:3:127:LEU:CG	3:3:128:LYS:N	2.75	0.49
3:3:135:PRO:CB	3:3:136:PRO:HD2	2.42	0.49
1:1:103:LEU:HG	5:A:1:GLC:C6	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:261:HIS:H	3:3:237:GLU:N	2.11	0.48
2:2:192:ASN:O	2:2:194:ARG:N	2.46	0.48
1:1:34:LEU:HD23	3:3:162:THR:O	2.12	0.48
1:1:65:MET:O	3:3:42:ASN:CG	2.51	0.48
1:1:191:SER:CB	3:3:34:ILE:HG12	2.43	0.48
1:1:230:LYS:HD3	1:1:231:LEU:HD22	1.95	0.48
1:1:197:TYR:HD2	1:1:198:ASP:N	2.11	0.48
3:3:65:VAL:O	3:3:67:MET:N	2.46	0.48
3:3:231:ILE:CD1	3:3:231:ILE:N	2.70	0.48
2:2:32:VAL:HB	2:2:201:LEU:HD22	1.94	0.48
2:2:81:LYS:HE2	2:2:132:LEU:HD11	1.94	0.48
2:2:174:ASN:C	2:2:176:ASP:H	2.16	0.48
1:1:48:GLU:HA	1:1:53:THR:HG21	1.96	0.48
2:2:15:GLN:HG3	2:2:16:ILE:N	2.29	0.48
2:2:82:LEU:CB	2:2:83:PRO:HD3	2.43	0.48
1:1:45:VAL:N	3:3:114:ARG:NH1	2.43	0.48
1:1:93:ASP:N	1:1:94:ILE:HD12	2.28	0.48
1:1:142:VAL:HG11	1:1:225:VAL:CB	2.39	0.48
1:1:197:TYR:N	2:2:131:GLN:HE21	2.05	0.48
3:3:112:SER:H	3:3:218:ASP:HB3	1.79	0.48
1:1:112:LYS:O	1:1:115:LEU:HB2	2.13	0.48
2:2:30:ASN:HD22	2:2:31:ALA:H	1.62	0.48
1:1:197:TYR:CD2	1:1:198:ASP:N	2.81	0.48
3:3:82:VAL:HG12	3:3:83:PHE:H	1.77	0.48
1:1:204:ASN:HD22	1:1:205:THR:H	1.61	0.47
1:1:257:VAL:HG21	2:2:173:LEU:CD1	2.44	0.47
3:3:155:TRP:CG	3:3:163:ILE:HG21	2.49	0.47
1:1:204:ASN:O	1:1:206:SER:N	2.45	0.47
2:2:128:PRO:HD2	2:2:186:PHE:CD2	2.49	0.47
1:1:15:LEU:CD2	4:4:43:LEU:HD23	2.45	0.47
1:1:86:TYR:CZ	1:1:229:GLN:HB2	2.49	0.47
1:1:119:VAL:HG13	1:1:121:PHE:CD2	2.49	0.47
2:2:12:ARG:CG	2:2:13:ILE:H	2.26	0.47
2:2:107:THR:OG1	2:2:249:MET:CE	2.61	0.47
3:3:61:ASN:ND2	3:3:66:SER:HB2	2.29	0.47
1:1:84:VAL:CG2	1:1:233:VAL:HG23	2.44	0.47
2:2:154:ARG:NH2	2:2:167:PRO:HG2	2.28	0.47
2:2:224:ILE:HD11	2:2:242:ILE:HD13	1.96	0.47
3:3:55:VAL:C	3:3:57:ASN:N	2.67	0.47
3:3:131:LEU:CD1	3:3:191:CYS:SG	3.02	0.47
3:3:124:ASN:HD22	3:3:124:ASN:H	1.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:136:PRO:HD3	3:3:186:ALA:O	2.15	0.47
3:3:155:TRP:CD1	3:3:155:TRP:C	2.87	0.47
2:2:66:LEU:HD23	2:2:80:TRP:CD1	2.50	0.47
2:2:136:LYS:HA	2:2:136:LYS:HD3	1.59	0.47
3:3:219:PHE:CE2	3:3:221:LEU:HD13	2.50	0.47
4:4:27:PHE:O	4:4:28:ASN:HB2	2.14	0.47
1:1:42:THR:HG21	3:3:48:GLN:O	2.15	0.47
2:2:130:HIS:CB	2:2:221:CYS:SG	3.03	0.47
1:1:215:ASN:HB2	5:A:2:FRU:O3	2.15	0.47
1:1:281:ARG:N	3:3:57:ASN:O	2.45	0.47
2:2:82:LEU:HD21	2:2:246:ILE:HD13	1.96	0.47
1:1:38:GLU:C	1:1:40:GLY:H	2.15	0.46
1:1:89:TYR:HD2	1:1:89:TYR:HA	1.49	0.46
2:2:102:GLY:HA3	2:2:214:MET:CG	2.45	0.46
2:2:200:THR:C	2:2:201:LEU:HD23	2.36	0.46
1:1:89:TYR:O	1:1:90:ASN:CB	2.62	0.46
1:1:124:GLU:CD	1:1:181:ARG:HH11	2.18	0.46
2:2:69:LYS:O	2:2:241:PRO:HA	2.15	0.46
2:2:78:TRP:CZ2	2:2:242:ILE:HD12	2.50	0.46
2:2:253:PHE:O	2:2:254:SER:HB3	2.15	0.46
1:1:129:PRO:HA	1:1:237:THR:HA	1.98	0.46
1:1:169:MET:HG2	1:1:170:SER:N	2.30	0.46
3:3:131:LEU:O	3:3:152:HIS:HB2	2.15	0.46
1:1:129:PRO:HG2	1:1:173:TRP:NE1	2.31	0.46
2:2:57:ASP:O	2:2:58:THR:HB	2.15	0.46
2:2:116:LYS:HB2	3:3:124:ASN:HD21	1.79	0.46
2:2:206:VAL:O	2:2:207:ASN:HB2	2.14	0.46
1:1:197:TYR:CE1	1:1:214:THR:CG2	2.91	0.46
2:2:72:ASN:HB3	2:2:75:SER:H	1.78	0.46
1:1:188:SER:OG	1:1:190:ALA:HB3	2.16	0.46
2:2:121:THR:HG22	2:2:227:ILE:HB	1.98	0.46
1:1:184:ILE:HD13	1:1:184:ILE:HG21	1.63	0.46
1:1:197:TYR:HE2	2:2:217:HIS:CG	2.34	0.46
3:3:46:MET:HE3	3:3:102:ILE:HD11	1.97	0.46
1:1:280:ARG:HG3	3:3:62:VAL:HG21	1.98	0.46
2:2:111:GLN:H	2:2:111:GLN:HG2	1.29	0.46
2:2:185:ILE:HD13	3:3:98:LEU:HD21	1.91	0.46
1:1:142:VAL:H	1:1:226:THR:CG2	2.29	0.45
1:1:195:MET:HE1	5:A:2:FRU:H11	1.96	0.45
2:2:46:ASP:HB3	3:3:34:ILE:HB	1.97	0.45
2:2:127:ILE:HG22	2:2:128:PRO:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:164:LEU:O	2:2:166:GLN:HB2	2.16	0.45
1:1:19:ASN:CB	1:1:56:VAL:O	2.63	0.45
3:3:99:ILE:O	3:3:102:ILE:HB	2.16	0.45
3:3:237:GLU:HG3	3:3:238:GLN:H	1.81	0.45
1:1:255:ARG:HH21	1:1:259:TYR:HA	1.80	0.45
2:2:121:THR:OG1	3:3:120:CYS:HB3	2.17	0.45
2:2:174:ASN:ND2	2:2:180:LEU:HA	2.32	0.45
1:1:124:GLU:OE1	1:1:181:ARG:NH1	2.49	0.45
1:1:80:SER:O	1:1:236:THR:HA	2.16	0.45
1:1:283:THR:CG2	1:1:285:THR:H	2.29	0.45
2:2:240:VAL:HA	2:2:241:PRO:HD2	1.88	0.45
3:3:87:VAL:HG22	3:3:189:ILE:CG2	2.45	0.45
3:3:88:ASP:O	3:3:90:THR:N	2.43	0.45
1:1:77:VAL:HG22	1:1:239:ILE:HG22	1.97	0.45
2:2:182:ASN:O	2:2:185:ILE:HG22	2.16	0.45
2:2:228:SER:HA	2:2:229:PRO:HD2	1.69	0.45
2:2:257:ARG:O	2:2:258:ALA:O	2.35	0.45
1:1:90:ASN:ND2	1:1:158:ARG:HD3	2.31	0.45
1:1:102:THR:CA	5:A:2:FRU:O6	2.35	0.45
3:3:93:PRO:O	3:3:94:LEU:O	2.35	0.45
1:1:97:THR:O	1:1:221:CYS:HA	2.16	0.45
3:3:42:ASN:O	3:3:43:LEU:C	2.54	0.45
3:3:161:SER:OG	3:3:162:THR:N	2.47	0.45
1:1:75:GLY:N	1:1:240:TYR:HD2	2.15	0.45
3:3:101:GLU:HA	3:3:229:LEU:HD22	1.99	0.45
1:1:66:SER:C	1:1:68:GLU:H	2.21	0.45
2:2:61:ASN:HD22	2:2:250:CYS:H	1.65	0.45
4:4:30:ASN:N	4:4:30:ASN:ND2	2.65	0.45
1:1:194:TYR:OH	2:2:207:ASN:ND2	2.50	0.44
1:1:245:HIS:CE1	4:4:38:SER:OG	2.70	0.44
2:2:91:ILE:HG22	2:2:92:PHE:N	2.32	0.44
2:2:103:ARG:HD3	2:2:252:GLU:OE2	2.17	0.44
3:3:25:LEU:N	3:3:26:PRO:CD	2.79	0.44
3:3:173:SER:C	3:3:175:PHE:H	2.20	0.44
1:1:54:ARG:HD2	1:1:56:VAL:HG22	2.00	0.44
1:1:185:PRO:HD3	3:3:23:CYS:SG	2.58	0.44
2:2:18:ARG:HD3	2:2:18:ARG:HA	1.57	0.44
2:2:61:ASN:N	2:2:61:ASN:OD1	2.49	0.44
3:3:66:SER:C	3:3:68:TYR:N	2.69	0.44
3:3:87:VAL:CG2	3:3:189:ILE:HG22	2.46	0.44
1:1:5:ASN:O	1:1:9:GLU:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:7:ILE:O	1:1:11:LEU:CB	2.60	0.44
1:1:90:ASN:HD22	1:1:90:ASN:N	2.16	0.44
2:2:80:TRP:NE1	2:2:151:GLU:O	2.50	0.44
3:3:155:TRP:CD2	3:3:163:ILE:HG21	2.53	0.44
2:2:43:THR:HA	2:2:44:PRO:HD2	1.80	0.44
2:2:83:PRO:CG	2:2:218:ASN:HA	2.31	0.44
2:2:126:MET:HE2	2:2:126:MET:HB3	1.80	0.44
2:2:235:THR:HG23	2:2:235:THR:O	2.17	0.44
3:3:84:SER:OG	3:3:140:GLU:OE1	2.30	0.44
1:1:262:SER:O	1:1:263:HIS:HB2	2.18	0.44
2:2:179:LEU:O	2:2:180:LEU:C	2.56	0.44
3:3:130:LEU:C	3:3:130:LEU:HD23	2.38	0.44
1:1:40:GLY:HA3	2:2:188:HIS:O	2.18	0.44
2:2:79:TRP:CZ3	2:2:81:LYS:HD3	2.52	0.44
3:3:126:THR:O	3:3:197:LEU:HA	2.18	0.44
1:1:96:PHE:CZ	1:1:155:PRO:O	2.71	0.43
2:2:82:LEU:HD23	2:2:82:LEU:HA	1.55	0.43
1:1:149:PRO:HA	1:1:150:PRO:HD3	1.86	0.43
1:1:268:MET:O	2:2:137:HIS:HB2	2.19	0.43
3:3:88:ASP:OD2	3:3:186:ALA:N	2.39	0.43
3:3:159:LEU:HA	3:3:159:LEU:HD23	1.72	0.43
1:1:54:ARG:HG3	1:1:55:TYR:H	1.83	0.43
1:1:74:SER:HB2	3:3:15:THR:HA	2.00	0.43
1:1:215:ASN:CG	5:A:2:FRU:HO3	2.10	0.43
2:2:29:ALA:O	2:2:30:ASN:C	2.56	0.43
1:1:104:GLN:HB3	1:1:104:GLN:HE21	1.64	0.43
1:1:104:GLN:O	3:3:236:ILE:HD11	2.18	0.43
2:2:137:HIS:CD2	2:2:137:HIS:C	2.91	0.43
2:2:171:SER:O	2:2:174:ASN:N	2.38	0.43
3:3:103:ALA:C	3:3:105:TYR:H	2.21	0.43
2:2:191:ILE:HA	2:2:196:ASN:ND2	2.33	0.43
1:1:156:SER:C	1:1:157:LYS:HG3	2.38	0.43
2:2:207:ASN:O	2:2:209:VAL:N	2.51	0.43
3:3:1:GLY:O	3:3:3:PRO:HD3	2.18	0.43
1:1:46:GLN:CB	1:1:47:PRO:CD	2.57	0.43
1:1:192:ALA:HB3	2:2:208:ALA:HB2	2.01	0.43
2:2:37:VAL:HG12	2:2:204:PRO:HB3	2.01	0.43
2:2:43:THR:C	2:2:45:GLN:H	2.22	0.43
2:2:94:GLU:C	2:2:96:MET:H	2.22	0.43
2:2:147:THR:C	2:2:149:PRO:CD	2.87	0.43
1:1:244:LYS:NZ	4:4:38:SER:O	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:54:PRO:HA	3:3:68:TYR:CD2	2.54	0.43
4:4:26:TYR:HD2	4:4:29:ILE:HD11	1.78	0.43
1:1:169:MET:HE1	1:1:171:ILE:CG2	2.49	0.43
1:1:271:THR:O	1:1:272:GLY:C	2.57	0.43
3:3:43:LEU:O	3:3:44:ILE:C	2.56	0.43
2:2:99:HIS:HA	2:2:255:GLY:O	2.19	0.43
2:2:192:ASN:C	2:2:194:ARG:H	2.21	0.43
1:1:58:THR:O	1:1:59:SER:HB3	2.19	0.42
2:2:154:ARG:HH11	2:2:154:ARG:HG2	1.83	0.42
3:3:50:ASP:CA	3:3:214:SER:HB3	2.49	0.42
1:1:260:THR:HB	1:1:261:HIS:CD2	2.53	0.42
2:2:128:PRO:HD3	2:2:220:TRP:CZ3	2.53	0.42
2:2:174:ASN:O	2:2:175:PHE:CB	2.66	0.42
1:1:74:SER:HA	1:1:241:HIS:O	2.20	0.42
1:1:244:LYS:NZ	4:4:38:SER:H	2.16	0.42
1:1:260:THR:HB	1:1:261:HIS:HD2	1.84	0.42
2:2:84:ASP:HB2	2:2:218:ASN:ND2	2.33	0.42
2:2:98:TYR:CE2	2:2:259:LYS:HD2	2.54	0.42
1:1:283:THR:HG22	1:1:285:THR:H	1.83	0.42
2:2:38:TRP:HA	2:2:39:PRO:HD2	1.70	0.42
2:2:65:THR:HA	2:2:245:SER:HA	2.02	0.42
2:2:95:ASN:HB3	2:2:253:PHE:CE2	2.54	0.42
2:2:127:ILE:N	2:2:221:CYS:O	2.53	0.42
2:2:145:LYS:HZ2	2:2:263:GLN:HG2	1.85	0.42
3:3:57:ASN:HD22	3:3:57:ASN:HA	1.21	0.42
3:3:97:THR:O	3:3:98:LEU:C	2.56	0.42
3:3:122:THR:HB	3:3:125:THR:OG1	2.19	0.42
1:1:90:ASN:C	1:1:91:GLY:O	2.57	0.42
1:1:267:TYR:O	1:1:268:MET:C	2.57	0.42
2:2:200:THR:O	2:2:201:LEU:HD23	2.19	0.42
3:3:216:CYS:C	3:3:218:ASP:H	2.23	0.42
3:3:219:PHE:O	3:3:220:CYS:HB2	2.20	0.42
1:1:38:GLU:O	2:2:189:GLN:CB	2.66	0.42
1:1:145:TYR:O	1:1:170:SER:HA	2.19	0.42
2:2:57:ASP:O	2:2:58:THR:CG2	2.67	0.42
1:1:31:ALA:HA	1:1:32:PRO:HD2	1.81	0.42
2:2:58:THR:CG2	2:2:59:SER:N	2.83	0.42
2:2:185:ILE:CD1	3:3:98:LEU:CD2	2.85	0.42
3:3:149:LEU:HD23	3:3:149:LEU:HA	1.73	0.42
3:3:217:LYS:HG3	3:3:217:LYS:H	1.64	0.42
1:1:257:VAL:HA	1:1:258:PRO:HD2	1.69	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:50:ASP:N	3:3:214:SER:HB3	2.34	0.42
3:3:94:LEU:HA	3:3:94:LEU:HD23	1.83	0.42
1:1:92:GLN:N	1:1:94:ILE:HD11	2.35	0.42
2:2:118:HIS:O	3:3:122:THR:HG23	2.19	0.42
2:2:203:VAL:HA	2:2:204:PRO:HD2	1.75	0.42
3:3:83:PHE:CD1	3:3:191:CYS:HB3	2.55	0.42
1:1:103:LEU:CD2	5:A:1:GLC:H61	2.50	0.41
1:1:110:ARG:NE	1:1:114:GLU:OE1	2.53	0.41
1:1:145:TYR:N	1:1:145:TYR:HD2	2.16	0.41
2:2:107:THR:OG1	2:2:249:MET:HE3	2.20	0.41
1:1:132:ALA:HB3	1:1:234:VAL:HG13	2.02	0.41
1:1:190:ALA:C	3:3:31:THR:HG21	2.38	0.41
2:2:175:PHE:HD2	2:2:175:PHE:N	2.18	0.41
2:2:21:SER:OG	2:2:63:PHE:HB2	2.20	0.41
2:2:158:GLN:CG	2:2:159:GLU:N	2.83	0.41
2:2:203:VAL:HG22	2:2:220:TRP:CZ2	2.56	0.41
3:3:2:LEU:HA	3:3:2:LEU:HD23	1.80	0.41
1:1:136:ASP:O	1:1:137:ASP:CB	2.67	0.41
2:2:63:PHE:CD2	2:2:247:SER:HB2	2.55	0.41
3:3:82:VAL:CG1	3:3:83:PHE:CD1	2.94	0.41
1:1:82:ILE:HD13	1:1:82:ILE:HG21	1.81	0.41
2:2:86:LEU:C	2:2:88:ASP:N	2.74	0.41
3:3:144:ARG:O	3:3:145:LYS:O	2.39	0.41
1:1:115:LEU:HA	1:1:115:LEU:HD12	1.76	0.41
3:3:7:THR:HA	3:3:8:PRO:HD3	1.78	0.41
3:3:191:CYS:C	3:3:192:TRP:CD1	2.94	0.41
1:1:131:ILE:HD13	1:1:141:ILE:HG23	2.02	0.41
1:1:145:TYR:HB2	1:1:171:ILE:HG23	2.01	0.41
2:2:37:VAL:CG2	3:3:37:PRO:HB3	2.47	0.41
2:2:143:GLY:N	2:2:165:ARG:O	2.48	0.41
3:3:43:LEU:HA	3:3:43:LEU:HD23	1.78	0.41
3:3:83:PHE:CE1	3:3:191:CYS:HB2	2.56	0.41
3:3:91:SER:C	3:3:92:THR:O	2.58	0.41
1:1:77:VAL:HG22	1:1:239:ILE:O	2.21	0.41
1:1:282:ASN:HD22	1:1:282:ASN:HA	1.55	0.41
3:3:14:MET:C	3:3:16:THR:N	2.74	0.41
3:3:83:PHE:N	3:3:83:PHE:CD1	2.88	0.41
1:1:11:LEU:HD13	1:1:11:LEU:HA	1.77	0.41
1:1:33:LEU:HB3	3:3:163:ILE:CD1	2.51	0.41
1:1:70:PHE:O	1:1:112:LYS:HE2	2.20	0.41
1:1:86:TYR:OH	1:1:229:GLN:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:143:MET:HG3	1:1:223:ARG:O	2.20	0.41
1:1:155:PRO:HG2	1:1:163:TRP:CZ2	2.56	0.41
1:1:255:ARG:NH1	1:1:265:THR:O	2.36	0.41
2:2:126:MET:O	2:2:186:PHE:HB3	2.21	0.41
3:3:75:GLN:HE21	3:3:76:THR:H	1.69	0.41
1:1:97:THR:CG2	1:1:222:SER:HB3	2.39	0.41
3:3:141:PRO:CG	3:3:147:ALA:HB2	2.51	0.41
1:1:23:SER:OG	1:1:53:THR:N	2.49	0.40
1:1:84:VAL:CG1	1:1:85:ASP:H	2.34	0.40
1:1:101:ILE:C	5:A:2:FRU:O6	2.58	0.40
1:1:145:TYR:HE1	1:1:237:THR:HG1	1.69	0.40
1:1:165:SER:C	1:1:167:THR:N	2.74	0.40
2:2:51:ASN:H	2:2:51:ASN:ND2	2.15	0.40
2:2:155:ASP:O	2:2:156:VAL:CB	2.68	0.40
1:1:9:GLU:OE1	4:4:42:ARG:HG3	2.21	0.40
1:1:22:GLU:CB	1:1:54:ARG:O	2.69	0.40
1:1:197:TYR:CE2	2:2:217:HIS:CE1	3.09	0.40
2:2:61:ASN:HD22	2:2:250:CYS:N	2.19	0.40
2:2:109:HIS:CE1	2:2:198:SER:HB3	2.56	0.40
1:1:235:ILE:HG22	1:1:236:THR:N	2.36	0.40
1:1:252:ARG:HB3	1:1:253:PRO:HD2	2.03	0.40
2:2:54:THR:HG22	2:2:253:PHE:HB2	2.02	0.40
1:1:15:LEU:O	1:1:61:THR:HA	2.21	0.40
3:3:15:THR:H	3:3:15:THR:HG22	1.45	0.40
1:1:225:VAL:H	1:1:225:VAL:HG23	1.61	0.40
2:2:147:THR:C	2:2:149:PRO:HD3	2.41	0.40
2:2:192:ASN:HD21	3:3:120:CYS:HA	1.86	0.40
3:3:53:ILE:HD11	3:3:213:VAL:HB	2.04	0.40
3:3:114:ARG:NH2	3:3:215:ALA:O	2.55	0.40
3:3:115:PHE:CE2	3:3:167:VAL:HG21	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:27:THR:OG1	2:2:18:ARG:NH2[2_655]	2.09	0.11

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	1	281/287 (98%)	217 (77%)	46 (16%)	18 (6%)	1 10
2	2	251/263 (95%)	201 (80%)	35 (14%)	15 (6%)	1 12
3	3	236/238 (99%)	178 (75%)	38 (16%)	20 (8%)	1 4
4	4	17/44 (39%)	9 (53%)	7 (41%)	1 (6%)	1 12
All	All	785/832 (94%)	605 (77%)	126 (16%)	54 (7%)	1 8

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	59	SER
1	1	72	GLY
1	1	107	ALA
1	1	108	GLN
1	1	114	GLU
1	1	158	ARG
1	1	226	THR
2	2	145	LYS
2	2	157	SER
2	2	258	ALA
3	3	57	ASN
3	3	88	ASP
3	3	89	ILE
3	3	94	LEU
3	3	96	THR
1	1	29	ASN
1	1	37	ALA
1	1	67	ILE
1	1	90	ASN
1	1	227	GLU
2	2	91	ILE
2	2	129	GLU

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Mol	Chain	Res	Type
2	2	155	ASP
2	2	193	LEU
2	2	208	ALA
2	2	257	ARG
3	3	59	GLY
3	3	66	SER
3	3	67	MET
3	3	95	ALA
3	3	159	LEU
3	3	161	SER
3	3	174	HIS
3	3	184	SER
1	1	6	TYR
1	1	137	ASP
2	2	30	ASN
2	2	156	VAL
3	3	74	ASN
3	3	201	PRO
3	3	219	PHE
3	3	229	LEU
4	4	27	PHE
1	1	160	ASP
1	1	266	ASN
2	2	260	ASN
1	1	205	THR
1	1	268	MET
2	2	87	LYS
2	2	259	LYS
3	3	220	CYS
3	3	121	GLY
2	2	44	PRO
3	3	82	VAL

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	1	254/258 (98%)	184 (72%)	70 (28%)	0 1
2	2	219/227 (96%)	158 (72%)	61 (28%)	0 1
3	3	209/209 (100%)	157 (75%)	52 (25%)	0 2
4	4	15/35 (43%)	9 (60%)	6 (40%)	0 0
All	All	697/729 (96%)	508 (73%)	189 (27%)	0 1

All (189) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	5	ASN
1	1	6	TYR
1	1	7	ILE
1	1	15	LEU
1	1	19	ASN
1	1	26	THR
1	1	35	ASP
1	1	44	ASN
1	1	45	VAL
1	1	54	ARG
1	1	60	GLN
1	1	73	ARG
1	1	87	THR
1	1	89	TYR
1	1	90	ASN
1	1	97	THR
1	1	101	ILE
1	1	102	THR
1	1	104	GLN
1	1	105	GLU
1	1	108	GLN
1	1	109	ILE
1	1	112	LYS
1	1	119	VAL
1	1	124	GLU
1	1	126	THR
1	1	127	LEU
1	1	134	ARG
1	1	141	ILE
1	1	142	VAL
1	1	143	MET
1	1	145	TYR
1	1	157	LYS

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Mol	Chain	Res	Type
1	1	158	ARG
1	1	160	ASP
1	1	161	PHE
1	1	162	SER
1	1	173	TRP
1	1	174	GLN
1	1	186	PHE
1	1	195	MET
1	1	197	TYR
1	1	201	ASP
1	1	204	ASN
1	1	209	TYR
1	1	211	SER
1	1	212	VAL
1	1	215	ASN
1	1	217	MET
1	1	219	THR
1	1	223	ARG
1	1	224	ILE
1	1	227	GLU
1	1	228	LYS
1	1	232	SER
1	1	236	THR
1	1	237	THR
1	1	246	THR
1	1	247	LYS
1	1	250	CYS
1	1	252	ARG
1	1	259	TYR
1	1	265	THR
1	1	274	VAL
1	1	275	THR
1	1	276	THR
1	1	278	ILE
1	1	279	VAL
1	1	281	ARG
1	1	286	THR
2	2	12	ARG
2	2	15	GLN
2	2	17	THR
2	2	18	ARG
2	2	25	SER

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Mol	Chain	Res	Type
2	2	27	ASP
2	2	30	ASN
2	2	43	THR
2	2	51	ASN
2	2	52	LYS
2	2	55	GLN
2	2	58	THR
2	2	60	SER
2	2	62	ARG
2	2	63	PHE
2	2	65	THR
2	2	68	SER
2	2	72	ASN
2	2	75	SER
2	2	78	TRP
2	2	86	LEU
2	2	87	LYS
2	2	88	ASP
2	2	94	GLU
2	2	103	ARG
2	2	111	GLN
2	2	116	LYS
2	2	126	MET
2	2	136	LYS
2	2	139	SER
2	2	145	LYS
2	2	146	LEU
2	2	154	ARG
2	2	158	GLN
2	2	159	GLU
2	2	160	ARG
2	2	164	LEU
2	2	170	ASP
2	2	171	SER
2	2	173	LEU
2	2	175	PHE
2	2	180	LEU
2	2	191	ILE
2	2	192	ASN
2	2	194	ARG
2	2	195	SER
2	2	197	ASN

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Mol	Chain	Res	Type
2	2	198	SER
2	2	200	THR
2	2	201	LEU
2	2	202	ILE
2	2	206	VAL
2	2	207	ASN
2	2	216	ARG
2	2	219	ASN
2	2	224	ILE
2	2	239	ILE
2	2	240	VAL
2	2	257	ARG
2	2	261	ILE
2	2	262	LYS
3	3	2	LEU
3	3	4	VAL
3	3	5	TYR
3	3	7	THR
3	3	19	MET
3	3	21	SER
3	3	23	CYS
3	3	32	LYS
3	3	39	GLU
3	3	50	ASP
3	3	55	VAL
3	3	56	ASN
3	3	60	ASN
3	3	61	ASN
3	3	65	VAL
3	3	66	SER
3	3	75	GLN
3	3	84	SER
3	3	90	THR
3	3	92	THR
3	3	99	ILE
3	3	116	SER
3	3	119	PHE
3	3	126	THR
3	3	127	LEU
3	3	134	THR
3	3	140	GLU
3	3	142	THR

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Mol	Chain	Res	Type
3	3	143	THR
3	3	148	MET
3	3	157	VAL
3	3	159	LEU
3	3	161	SER
3	3	177	LEU
3	3	182	LYS
3	3	189	ILE
3	3	192	TRP
3	3	194	GLN
3	3	196	ASN
3	3	201	PRO
3	3	205	GLN
3	3	208	ASP
3	3	209	MET
3	3	210	LEU
3	3	211	CYS
3	3	212	PHE
3	3	213	VAL
3	3	216	CYS
3	3	217	LYS
3	3	228	ASP
3	3	231	ILE
3	3	236	ILE
4	4	26	TYR
4	4	29	ILE
4	4	33	LYS
4	4	42	ARG
4	4	43	LEU
4	4	44	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	44	ASN
1	1	90	ASN
1	1	95	ASN
1	1	140	HIS
1	1	159	ASN
1	1	168	ASN
1	1	204	ASN
1	1	215	ASN

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Mol	Chain	Res	Type
1	1	261	HIS
1	1	282	ASN
2	2	15	GLN
2	2	30	ASN
2	2	51	ASN
2	2	72	ASN
2	2	109	HIS
2	2	111	GLN
2	2	131	GLN
2	2	192	ASN
2	2	197	ASN
2	2	207	ASN
2	2	218	ASN
2	2	219	ASN
3	3	20	GLN
3	3	42	ASN
3	3	56	ASN
3	3	57	ASN
3	3	61	ASN
3	3	75	GLN
3	3	80	GLN
3	3	124	ASN
3	3	194	GLN
3	3	196	ASN
4	4	30	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

2 monosaccharides 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	$\#\|Z\| > 2$
5	GLC	A	1	5	11,11,12	2.22	2 (18%)	15,15,17	5.30	8 (53%)
5	FRU	A	2	1,5	11,12,12	1.20	1 (9%)	10,18,18	2.23	2 (20%)

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	GLC	A	1	5	1/1/4/5	2/2/19/22	0/1/1/1
5	FRU	A	2	1,5	-	5/5/24/24	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1	GLC	O5-C1	-6.29	1.33	1.43
5	A	1	GLC	C2-C3	-2.75	1.48	1.52
5	A	2	FRU	C1-C2	2.23	1.55	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1	GLC	O3-C3-C2	15.15	139.00	109.99
5	A	1	GLC	C1-O5-C5	6.99	121.67	112.19
5	A	1	GLC	O5-C5-C6	6.67	117.67	107.20
5	A	1	GLC	O2-C2-C3	6.49	123.13	110.14
5	A	2	FRU	O2-C2-O5	5.67	120.45	109.50
5	A	1	GLC	C3-C4-C5	-4.65	101.95	110.24
5	A	1	GLC	O2-C2-C1	-3.21	102.58	109.15
5	A	1	GLC	C1-C2-C3	3.02	113.38	109.67
5	A	2	FRU	C6-C5-C4	-2.84	108.25	115.09
5	A	1	GLC	O4-C4-C5	-2.25	103.70	109.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	1	GLC	C1

All (7) torsion outliers are listed below:

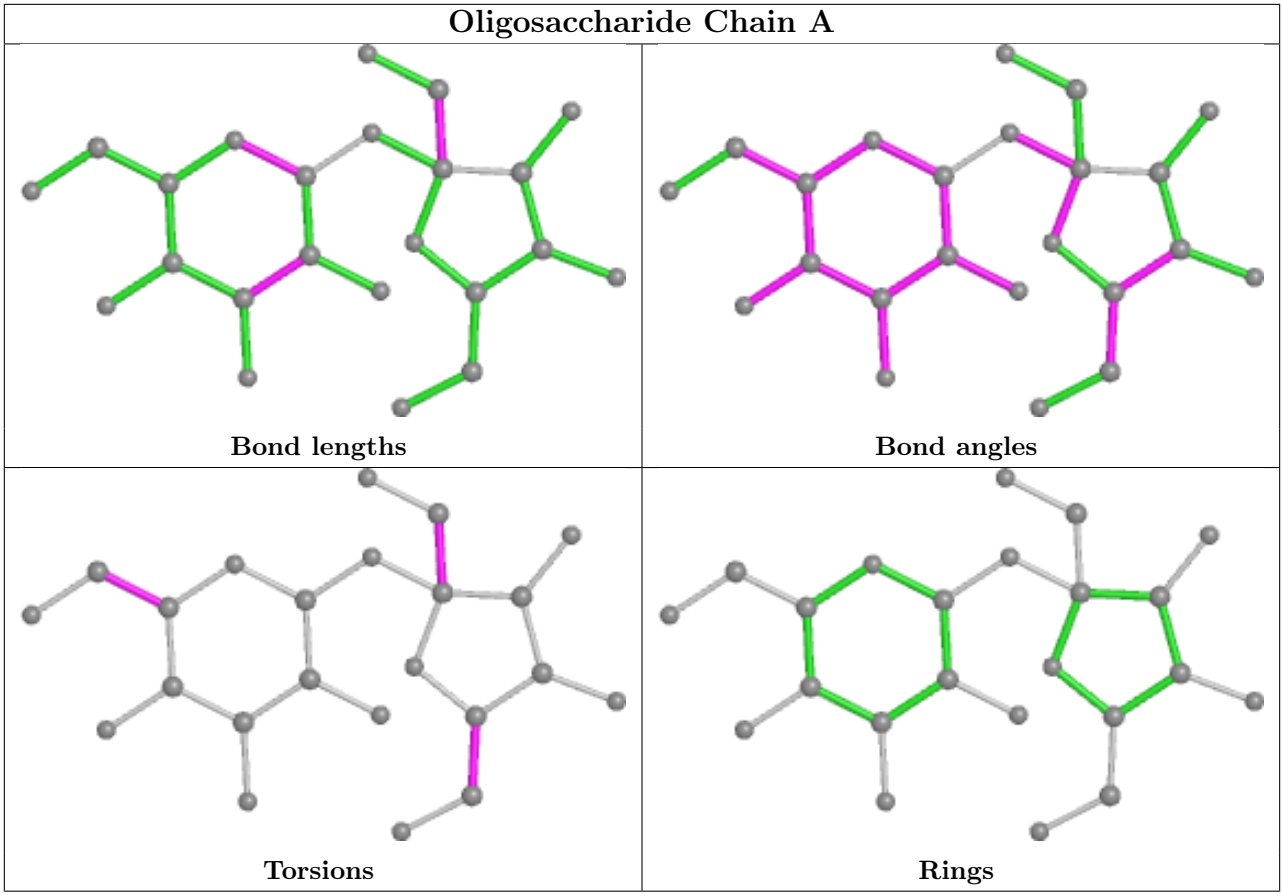
Mol	Chain	Res	Type	Atoms
5	A	2	FRU	O1-C1-C2-C3
5	A	2	FRU	O1-C1-C2-O2
5	A	2	FRU	O5-C5-C6-O6
5	A	1	GLC	O5-C5-C6-O6
5	A	1	GLC	C4-C5-C6-O6
5	A	2	FRU	O1-C1-C2-O5
5	A	2	FRU	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1	GLC	6	0
5	A	2	FRU	26	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry (i)

There are no ligands in this entry.

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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.