



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 06:08 PM BST

PDB ID : 3B2V
Title : Crystal structure of the extracellular region of the epidermal growth factor receptor in complex with the Fab fragment of IMC-11F8
Authors : Ferguson, K.M.; Li, S.; Kussie, P.
Deposited on : 2007-10-19
Resolution : 3.30 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

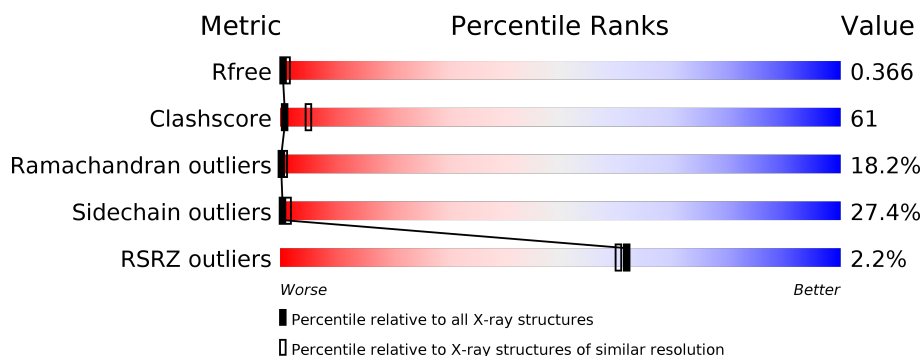
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	L	213	
2	H	223	
3	A	624	
4	B	3	
5	C	2	
5	D	2	

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	NAG	C	1	X	-	-	-
6	NAG	A	5041	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5645 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 IMC-11F8 FAB Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	213	Total	C	N	O	S	0	0	0
			1432	883	240	304	5			

- Molecule 2 is a protein called IMC-11F8 FAB Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	217	Total	C	N	O	S	0	0	0
			1533	962	253	313	5			

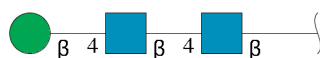
- Molecule 3 is a protein called Epidermal growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	375	Total	C	N	O	S	0	0	0
			2559	1561	451	513	34			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	619	HIS	-	expression tag	UNP P00533
A	620	HIS	-	expression tag	UNP P00533
A	621	HIS	-	expression tag	UNP P00533
A	622	HIS	-	expression tag	UNP P00533
A	623	HIS	-	expression tag	UNP P00533
A	624	HIS	-	expression tag	UNP P00533

- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



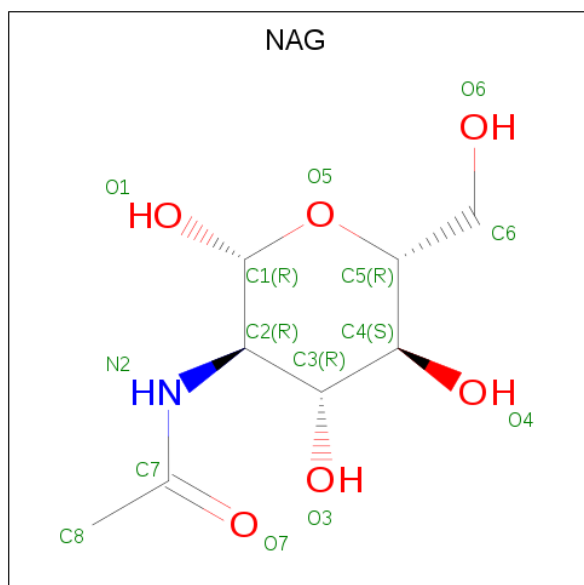
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	B	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

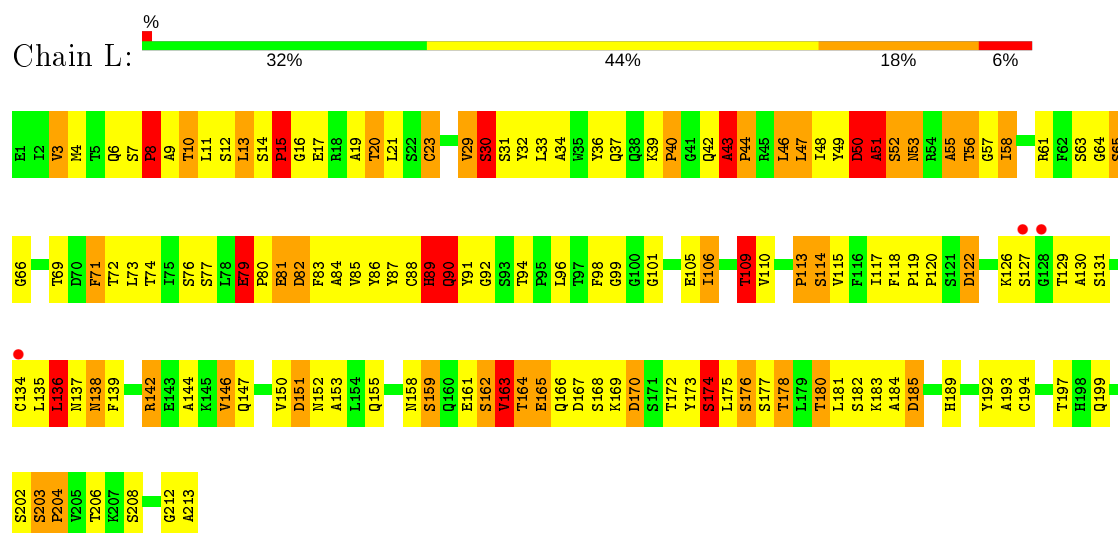


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			12	8	1	3		

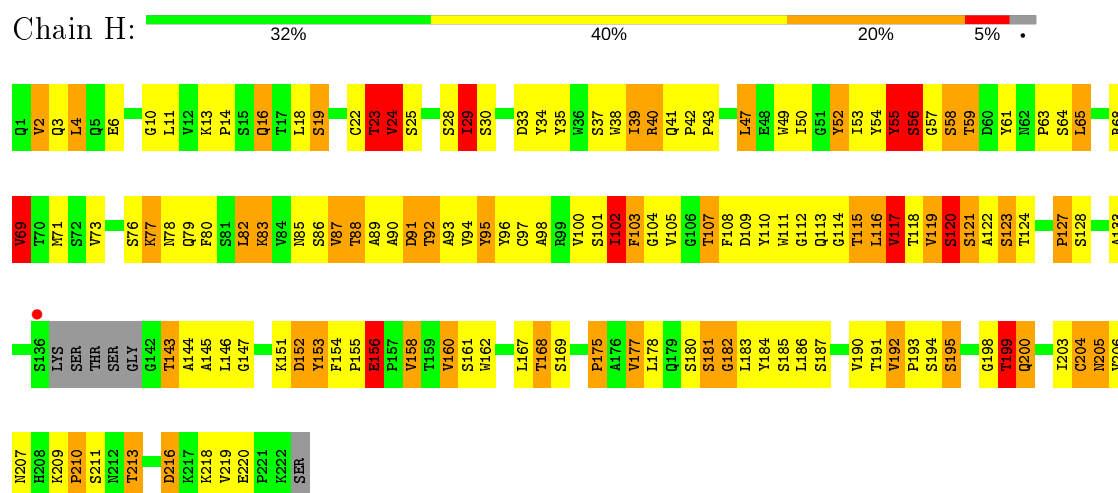
3 Residue-property plots

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: IMC-11F8 FAB Light chain

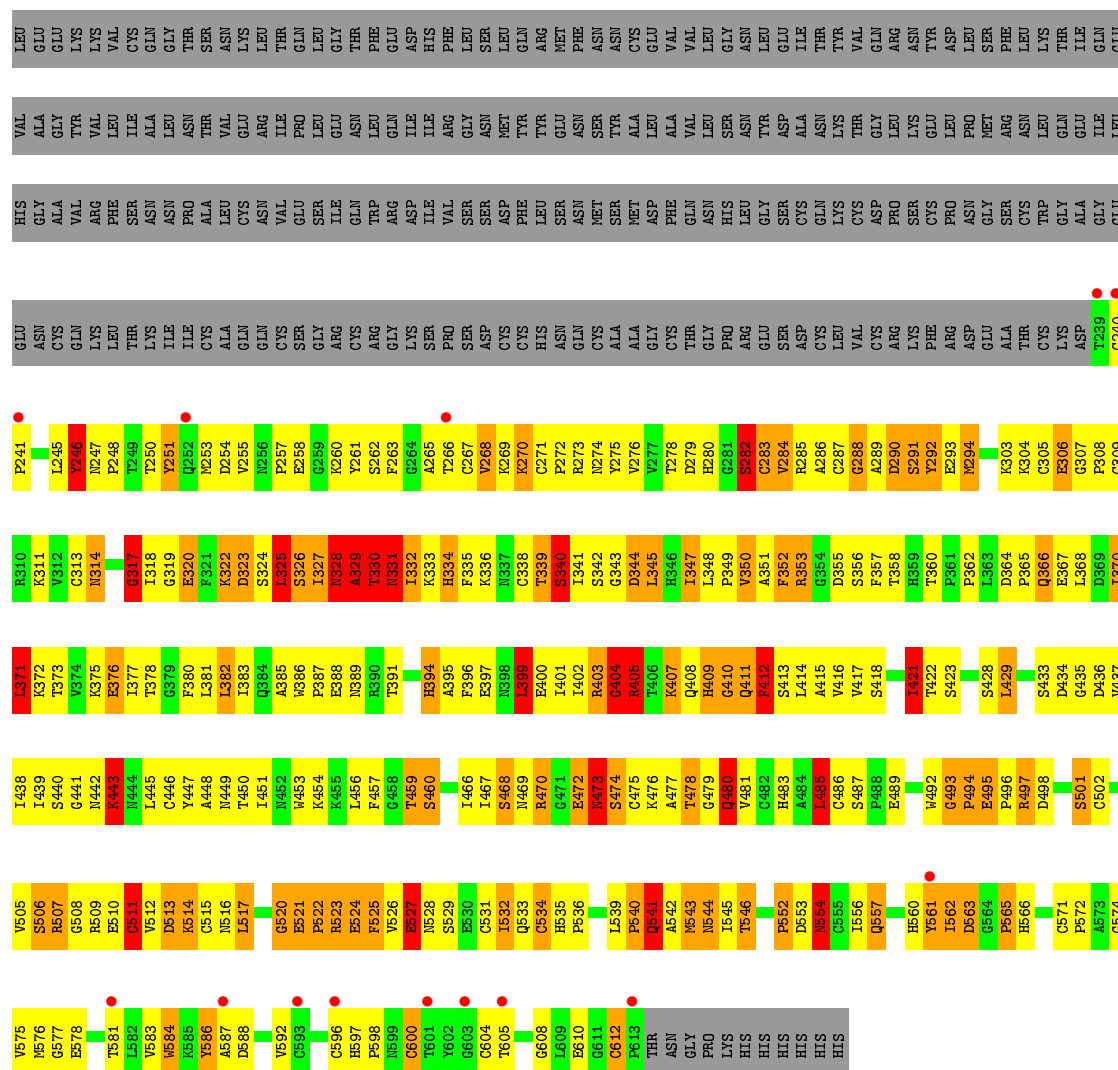


• Molecule 2: IMC-11F8 FAB Heavy chain



• Molecule 3: Epidermal growth factor receptor





- Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B: 100%

MAG1
MAG2
EM3

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C: 50%

MAG1
MAG2

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D: 100%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	68.74Å 266.24Å 156.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.04 – 3.30 41.04 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.1 (41.04-3.30) 99.3 (41.04-3.30)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.01 (at 3.32Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.282 , 0.367 0.285 , 0.366	Depositor DCC
R_{free} test set	1120 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	62.9	Xtriage
Anisotropy	0.319	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.18 , 70.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	5645	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

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

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	L	1.02	1/1460 (0.1%)	1.19	11/2005 (0.5%)
2	H	1.01	2/1570 (0.1%)	1.16	6/2159 (0.3%)
3	A	1.03	2/2607 (0.1%)	1.17	14/3571 (0.4%)
All	All	1.02	5/5637 (0.1%)	1.17	31/7735 (0.4%)

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	L	0	8
2	H	0	5
3	A	0	11
All	All	0	24

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	534	CYS	CB-SG	-8.21	1.68	1.82
1	L	13	LEU	C-O	5.82	1.34	1.23
2	H	156	GLU	CB-CG	5.45	1.62	1.52
2	H	52	TYR	CE1-CZ	5.18	1.45	1.38
3	A	412	PHE	N-CA	5.11	1.56	1.46

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	382	LEU	CA-CB-CG	-8.96	94.69	115.30
1	L	82	ASP	CB-CG-OD1	-7.54	111.51	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	138	ASN	N-CA-C	-7.42	90.97	111.00
2	H	24	VAL	CB-CA-C	-7.38	97.38	111.40
3	A	371	LEU	CA-CB-CG	-7.04	99.11	115.30
2	H	24	VAL	N-CA-C	-6.92	92.31	111.00
1	L	23	CYS	CB-CA-C	-6.63	97.13	110.40
1	L	88	CYS	CB-CA-C	-6.39	97.62	110.40
3	A	330	THR	C-N-CA	5.95	136.58	121.70
3	A	329	ALA	N-CA-C	-5.94	94.95	111.00
3	A	485	LEU	CA-CB-CG	5.88	128.82	115.30
1	L	50	ASP	CB-CG-OD1	5.86	123.57	118.30
3	A	370	ILE	C-N-CA	5.85	136.33	121.70
2	H	56	SER	N-CA-CB	5.84	119.26	110.50
3	A	493	GLY	N-CA-C	-5.77	98.68	113.10
3	A	405	ARG	N-CA-C	-5.70	95.61	111.00
2	H	29	ILE	CB-CA-C	-5.69	100.22	111.60
1	L	89	HIS	N-CA-C	5.63	126.21	111.00
3	A	478	THR	CB-CA-C	-5.50	96.76	111.60
1	L	47	LEU	CB-CG-CD2	-5.48	101.68	111.00
3	A	436	ASP	CB-CG-OD1	-5.48	113.37	118.30
1	L	23	CYS	CA-CB-SG	5.43	123.78	114.00
1	L	163	VAL	CB-CA-C	-5.43	101.08	111.40
1	L	51	ALA	C-N-CA	5.39	135.18	121.70
1	L	3	VAL	N-CA-C	5.33	125.40	111.00
3	A	331	ASN	N-CA-C	-5.33	96.60	111.00
3	A	473	ASN	N-CA-C	-5.24	96.86	111.00
3	A	399	LEU	CB-CG-CD2	-5.17	102.21	111.00
3	A	502	CYS	N-CA-C	5.11	124.78	111.00
2	H	59	THR	N-CA-C	-5.07	97.31	111.00
2	H	156	GLU	C-N-CD	-5.04	109.52	120.60

There are no chirality outliers.

All (24) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	289	ALA	Peptide
3	A	317	GLY	Peptide
3	A	328	ASN	Peptide
3	A	338	CYS	Peptide
3	A	340	SER	Peptide
3	A	350	VAL	Peptide
3	A	387	PRO	Peptide
3	A	404	GLY	Peptide

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Mol	Chain	Res	Type	Group
3	A	421	ILE	Peptide
3	A	443	LYS	Peptide
3	A	557	GLN	Peptide
2	H	104	GLY	Peptide
2	H	156	GLU	Peptide
2	H	23	THR	Peptide
2	H	69	VAL	Peptide
2	H	82	LEU	Peptide
1	L	101	GLY	Peptide
1	L	23	CYS	Peptide
1	L	42	GLN	Peptide
1	L	43	ALA	Peptide
1	L	55	ALA	Peptide
1	L	56	THR	Peptide
1	L	57	GLY	Peptide
1	L	79	GLU	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	1432	0	1229	149	0
2	H	1533	0	1416	198	0
3	A	2559	0	2201	309	0
4	B	39	0	34	0	0
5	C	28	0	25	1	0
5	D	28	0	25	1	0
6	A	26	0	23	2	0
All	All	5645	0	4953	642	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 61.

All (642) 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)
3:A:483:HIS:CD2	3:A:496:PRO:HG3	1.52	1.43
1:L:51:ALA:CB	1:L:52:SER:HB2	1.50	1.39
1:L:51:ALA:HB3	1:L:52:SER:CB	1.51	1.38
2:H:24:VAL:HG21	2:H:78:ASN:O	1.24	1.32
2:H:24:VAL:CG2	2:H:78:ASN:O	1.79	1.30
3:A:311:LYS:O	3:A:339:THR:HG22	1.25	1.27
3:A:328:ASN:HB2	3:A:329:ALA:CB	1.65	1.24
3:A:459:THR:CG2	3:A:460:SER:H	1.40	1.22
3:A:328:ASN:CB	3:A:329:ALA:HB3	1.70	1.19
3:A:459:THR:CG2	3:A:460:SER:N	1.98	1.17
1:L:202:SER:CB	1:L:203:SER:HB3	1.76	1.16
3:A:527:GLU:O	3:A:527:GLU:HG3	1.42	1.14
3:A:459:THR:HG23	3:A:460:SER:N	1.40	1.14
3:A:483:HIS:CD2	3:A:496:PRO:CG	2.31	1.13
2:H:6:GLU:HB3	2:H:115:THR:HG22	1.33	1.09
3:A:403:ARG:CG	3:A:403:ARG:HH11	1.66	1.09
2:H:2:VAL:HA	2:H:25:SER:O	1.50	1.08
1:L:212:GLY:HA2	1:L:213:ALA:HB3	1.17	1.08
3:A:311:LYS:O	3:A:339:THR:CG2	2.02	1.08
1:L:47:LEU:HD23	1:L:58:ILE:HG21	1.29	1.08
2:H:116:LEU:HD12	2:H:117:VAL:H	1.05	1.07
2:H:199:THR:HG23	2:H:200:GLN:H	1.13	1.07
3:A:403:ARG:HG3	3:A:403:ARG:HH11	0.87	1.03
3:A:347:ILE:HD12	3:A:347:ILE:N	1.73	1.03
1:L:212:GLY:HA2	1:L:213:ALA:CB	1.87	1.03
2:H:22:CYS:O	2:H:79:GLN:HB3	1.59	1.02
3:A:487:SER:HB3	3:A:501:SER:O	1.60	1.02
1:L:135:LEU:HG	1:L:136:LEU:H	1.25	1.02
1:L:6:GLN:NE2	1:L:86:TYR:O	1.93	1.01
3:A:403:ARG:HG3	3:A:403:ARG:NH1	1.69	1.01
3:A:319:GLY:HA3	3:A:320:GLU:CB	1.91	1.00
3:A:483:HIS:HD2	3:A:496:PRO:CD	1.75	0.99
3:A:330:THR:HG22	3:A:331:ASN:HA	1.43	0.99
3:A:348:LEU:O	3:A:351:ALA:HB2	1.61	0.99
2:H:127:PRO:HB3	2:H:153:TYR:HB3	1.45	0.98
3:A:328:ASN:HB2	3:A:329:ALA:HB3	0.99	0.98
3:A:291:SER:HB3	3:A:305:CYS:SG	2.03	0.98
3:A:343:GLY:H	3:A:378:THR:HB	1.28	0.98
3:A:483:HIS:HD2	3:A:496:PRO:CG	1.70	0.97
2:H:6:GLU:HB3	2:H:115:THR:CG2	1.93	0.97
1:L:98:PHE:HD1	2:H:47:LEU:HB2	1.29	0.97
3:A:347:ILE:HD12	3:A:347:ILE:H	1.28	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:47:LEU:HA	1:L:58:ILE:HD12	1.47	0.96
3:A:339:THR:HG23	3:A:340:SER:H	1.30	0.96
3:A:583:VAL:HA	3:A:584:TRP:CB	1.96	0.95
2:H:203:ILE:HA	2:H:218:LYS:HA	1.49	0.95
2:H:160:VAL:HB	2:H:206:VAL:HG22	1.48	0.94
1:L:98:PHE:CD1	2:H:47:LEU:HB2	2.02	0.94
3:A:339:THR:HG23	3:A:340:SER:N	1.78	0.94
3:A:326:SER:OG	3:A:327:ILE:N	1.94	0.93
3:A:330:THR:HG22	3:A:331:ASN:CA	1.98	0.93
2:H:116:LEU:HD12	2:H:117:VAL:N	1.84	0.92
3:A:376:GLU:HB2	3:A:401:ILE:HG23	1.50	0.92
3:A:505:VAL:HG23	3:A:529:SER:O	1.69	0.92
3:A:479:GLY:HA2	3:A:481:VAL:HG23	1.52	0.91
2:H:181:SER:O	2:H:183:LEU:N	2.04	0.91
1:L:39:LYS:HD2	1:L:84:ALA:HB2	1.51	0.91
3:A:505:VAL:CG2	3:A:529:SER:O	2.19	0.91
2:H:68:ARG:NH2	2:H:91:ASP:OD1	2.04	0.91
2:H:61:TYR:CE2	2:H:71:MET:HG3	2.07	0.89
2:H:6:GLU:CB	2:H:115:THR:HG22	2.02	0.89
2:H:4:LEU:HB3	2:H:97:CYS:SG	2.12	0.88
3:A:328:ASN:OD1	3:A:330:THR:N	2.05	0.88
3:A:342:SER:HA	3:A:378:THR:OG1	1.74	0.87
2:H:205:ASN:HA	2:H:216:ASP:HB3	1.57	0.86
3:A:348:LEU:O	3:A:351:ALA:CB	2.23	0.86
2:H:199:THR:CG2	2:H:200:GLN:H	1.87	0.86
3:A:291:SER:OG	3:A:304:LYS:HA	1.75	0.85
3:A:483:HIS:HD2	3:A:496:PRO:HD3	1.39	0.85
2:H:4:LEU:O	2:H:112:GLY:HA3	1.76	0.84
3:A:314:ASN:N	3:A:314:ASN:HD22	1.74	0.84
3:A:442:ASN:O	3:A:443:LYS:HB3	1.76	0.84
2:H:55:TYR:O	2:H:55:TYR:CD1	2.30	0.84
3:A:366:GLN:O	3:A:368:LEU:N	2.11	0.84
3:A:353:ARG:HH11	3:A:353:ARG:HG2	1.43	0.83
3:A:505:VAL:HG11	3:A:515:CYS:SG	2.16	0.83
3:A:540:PRO:O	3:A:541:GLN:HB2	1.78	0.83
3:A:479:GLY:C	3:A:481:VAL:H	1.80	0.83
2:H:199:THR:HG23	2:H:200:GLN:N	1.94	0.83
2:H:28:SER:O	2:H:30:SER:N	2.11	0.83
1:L:55:ALA:N	1:L:58:ILE:HD11	1.93	0.83
3:A:380:PHE:HB2	3:A:413:SER:O	1.78	0.83
2:H:2:VAL:HG21	2:H:110:TYR:CE2	2.13	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:39:ILE:HG23	2:H:49:TRP:HA	1.58	0.83
3:A:487:SER:CB	3:A:501:SER:O	2.26	0.82
1:L:47:LEU:CA	1:L:58:ILE:HD12	2.09	0.82
3:A:507:ARG:HB3	3:A:512:VAL:HG21	1.61	0.82
1:L:12:SER:HA	1:L:105:GLU:O	1.79	0.82
1:L:117:ILE:HD12	1:L:194:CYS:SG	2.18	0.82
2:H:145:ALA:HB2	2:H:191:THR:HG22	1.62	0.82
2:H:181:SER:C	2:H:183:LEU:H	1.82	0.82
2:H:61:TYR:HE2	2:H:71:MET:HG3	1.39	0.82
1:L:106:ILE:H	1:L:106:ILE:HD13	1.43	0.82
3:A:328:ASN:CB	3:A:329:ALA:CB	2.40	0.82
2:H:93:ALA:O	2:H:116:LEU:CD1	2.28	0.81
3:A:532:ILE:HD13	3:A:532:ILE:N	1.95	0.81
3:A:371:LEU:H	3:A:373:THR:HG22	1.45	0.81
3:A:375:LYS:HA	3:A:399:LEU:HA	1.63	0.81
3:A:314:ASN:N	3:A:314:ASN:ND2	2.27	0.80
2:H:65:LEU:CD2	2:H:69:VAL:HG13	2.12	0.80
1:L:55:ALA:H	1:L:58:ILE:HD11	1.44	0.79
3:A:438:ILE:O	3:A:438:ILE:HG23	1.81	0.79
3:A:352:PHE:O	3:A:362:PRO:HB3	1.81	0.79
1:L:135:LEU:O	1:L:136:LEU:HB2	1.83	0.79
1:L:212:GLY:CA	1:L:213:ALA:HB3	2.08	0.79
3:A:339:THR:CG2	3:A:340:SER:H	1.96	0.79
2:H:18:LEU:O	2:H:83:LYS:HA	1.82	0.78
1:L:203:SER:H	1:L:204:PRO:CD	1.95	0.78
3:A:335:PHE:O	3:A:336:LYS:C	2.22	0.77
3:A:483:HIS:CD2	3:A:496:PRO:HD3	2.18	0.77
3:A:328:ASN:CA	3:A:329:ALA:CB	2.61	0.77
2:H:55:TYR:CG	2:H:55:TYR:O	2.37	0.77
3:A:483:HIS:CD2	3:A:496:PRO:CD	2.64	0.76
3:A:347:ILE:N	3:A:347:ILE:CD1	2.49	0.76
1:L:96:LEU:HD23	1:L:96:LEU:N	1.98	0.76
2:H:122:ALA:HB1	2:H:123:SER:HB3	1.67	0.76
3:A:447:TYR:O	3:A:449:ASN:N	2.19	0.76
1:L:185:ASP:O	1:L:189:HIS:HD2	1.69	0.76
3:A:291:SER:CB	3:A:305:CYS:SG	2.74	0.76
1:L:64:GLY:HA2	1:L:65:SER:HB3	1.68	0.76
3:A:339:THR:CG2	3:A:340:SER:N	2.49	0.75
1:L:131:SER:HB3	1:L:180:THR:HA	1.67	0.75
1:L:36:TYR:OH	2:H:107:THR:CG2	2.35	0.75
1:L:117:ILE:HG21	1:L:208:SER:HA	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:40:ARG:HG2	2:H:50:ILE:HD11	1.69	0.75
1:L:8:PRO:O	1:L:10:THR:N	2.21	0.74
3:A:561:TYR:O	3:A:562:ILE:HB	1.87	0.74
3:A:389:ASN:HD22	6:A:3891:NAG:H83	1.51	0.74
1:L:36:TYR:OH	2:H:107:THR:HG23	1.86	0.74
1:L:170:ASP:OD2	1:L:172:THR:HG22	1.88	0.74
1:L:47:LEU:CD2	1:L:58:ILE:HG21	2.16	0.74
3:A:347:ILE:CD1	3:A:347:ILE:H	2.00	0.74
2:H:35:TYR:HD2	2:H:52:TYR:CD2	2.04	0.74
3:A:522:PRO:HD2	3:A:523:ARG:N	2.03	0.74
2:H:88:THR:HG23	2:H:91:ASP:OD1	1.88	0.74
2:H:68:ARG:HH22	2:H:91:ASP:CG	1.91	0.73
3:A:400:GLU:HA	3:A:428:SER:O	1.88	0.73
3:A:507:ARG:HB3	3:A:512:VAL:CG2	2.18	0.73
3:A:505:VAL:HG22	3:A:506:SER:N	2.04	0.73
3:A:284:VAL:HG23	3:A:285:ARG:N	2.03	0.72
2:H:23:THR:HA	2:H:24:VAL:HG22	1.70	0.72
1:L:8:PRO:HG2	1:L:8:PRO:O	1.89	0.72
3:A:403:ARG:CG	3:A:403:ARG:NH1	2.31	0.72
3:A:376:GLU:HB2	3:A:401:ILE:CG2	2.18	0.71
3:A:514:LYS:HG2	3:A:515:CYS:N	2.05	0.71
3:A:571:CYS:SG	3:A:572:PRO:HD2	2.31	0.71
3:A:516:ASN:HB2	3:A:524:GLU:HG2	1.72	0.71
2:H:116:LEU:CD1	2:H:117:VAL:H	1.96	0.71
2:H:102:ILE:HB	2:H:103:PHE:HD2	1.56	0.71
3:A:328:ASN:HA	3:A:329:ALA:HB2	1.73	0.71
2:H:22:CYS:O	2:H:23:THR:OG1	2.09	0.70
3:A:459:THR:HG22	3:A:460:SER:N	2.03	0.70
3:A:377:ILE:HD12	3:A:399:LEU:CD1	2.21	0.70
2:H:153:TYR:CD2	2:H:153:TYR:C	2.64	0.70
2:H:145:ALA:HB2	2:H:191:THR:CG2	2.21	0.70
3:A:479:GLY:C	3:A:481:VAL:N	2.44	0.70
1:L:64:GLY:HA2	1:L:65:SER:CB	2.22	0.69
3:A:394:HIS:ND1	3:A:395:ALA:N	2.40	0.69
1:L:202:SER:CA	1:L:203:SER:HB3	2.21	0.69
2:H:35:TYR:CD2	2:H:52:TYR:CE2	2.81	0.69
3:A:527:GLU:O	3:A:527:GLU:CG	2.30	0.69
2:H:2:VAL:CA	2:H:25:SER:O	2.35	0.69
1:L:175:LEU:HD23	1:L:176:SER:N	2.08	0.69
1:L:33:LEU:HD13	1:L:71:PHE:CG	2.27	0.68
3:A:403:ARG:HA	3:A:433:SER:HB2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:8:PRO:CG	1:L:8:PRO:O	2.39	0.68
2:H:92:THR:HG23	2:H:118:THR:HA	1.75	0.68
3:A:439:ILE:HG22	3:A:442:ASN:HD22	1.58	0.68
2:H:180:SER:O	2:H:182:GLY:N	2.19	0.68
1:L:47:LEU:O	1:L:58:ILE:HD12	1.94	0.68
3:A:447:TYR:C	3:A:449:ASN:H	1.96	0.67
2:H:2:VAL:HG21	2:H:110:TYR:HE2	1.54	0.67
3:A:467:ILE:O	3:A:468:SER:HB2	1.95	0.67
2:H:133:ALA:HB2	2:H:220:GLU:O	1.95	0.67
2:H:151:LYS:HA	2:H:185:SER:OG	1.94	0.67
3:A:371:LEU:N	3:A:373:THR:HG22	2.10	0.67
1:L:65:SER:OG	1:L:72:THR:O	2.13	0.67
2:H:160:VAL:CG2	2:H:161:SER:N	2.58	0.66
3:A:412:PHE:CE2	3:A:438:ILE:HB	2.29	0.66
3:A:352:PHE:N	3:A:352:PHE:CD1	2.61	0.66
3:A:459:THR:HG23	3:A:460:SER:H	0.58	0.66
3:A:526:VAL:HG12	3:A:527:GLU:N	2.11	0.66
2:H:100:VAL:CG1	2:H:101:SER:N	2.57	0.66
1:L:4:MET:HE2	1:L:90:GLN:HG2	1.76	0.66
2:H:143:THR:HA	2:H:194:SER:H	1.59	0.66
3:A:349:PRO:HB3	3:A:385:ALA:HB2	1.78	0.66
3:A:402:ILE:HD12	3:A:429:LEU:CD1	2.25	0.66
2:H:160:VAL:CG2	2:H:161:SER:H	2.09	0.66
1:L:47:LEU:HA	1:L:58:ILE:CD1	2.24	0.66
1:L:131:SER:CB	1:L:180:THR:HA	2.25	0.66
3:A:472:GLU:HA	3:A:475:CYS:HB2	1.78	0.65
2:H:22:CYS:C	2:H:23:THR:HG1	1.99	0.65
1:L:49:TYR:CD2	1:L:50:ASP:OD1	2.48	0.65
3:A:320:GLU:O	3:A:334:HIS:CD2	2.49	0.65
3:A:522:PRO:HD2	3:A:523:ARG:H	1.59	0.65
2:H:88:THR:O	2:H:119:VAL:HG11	1.96	0.65
1:L:49:TYR:HD2	1:L:50:ASP:OD1	1.79	0.65
1:L:71:PHE:CD2	1:L:71:PHE:N	2.63	0.65
1:L:37:GLN:HE21	1:L:86:TYR:HE2	1.42	0.65
3:A:272:PRO:O	3:A:274:ASN:N	2.29	0.65
3:A:364:ASP:O	3:A:365:PRO:C	2.35	0.65
3:A:352:PHE:HD1	3:A:352:PHE:H	1.45	0.65
1:L:80:PRO:HA	1:L:106:ILE:HG13	1.79	0.65
2:H:116:LEU:O	2:H:117:VAL:HG12	1.96	0.65
2:H:127:PRO:HA	2:H:152:ASP:O	1.97	0.64
3:A:349:PRO:CA	3:A:385:ALA:HB2	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:135:LEU:CG	1:L:136:LEU:H	1.98	0.64
3:A:332:ILE:HG13	3:A:370:ILE:HD12	1.80	0.64
2:H:160:VAL:HG23	2:H:161:SER:H	1.60	0.64
2:H:120:SER:O	2:H:121:SER:O	2.16	0.64
1:L:162:SER:OG	2:H:175:PRO:HG2	1.98	0.64
3:A:278:THR:HG22	3:A:280:HIS:H	1.63	0.64
3:A:522:PRO:CD	3:A:523:ARG:N	2.59	0.64
2:H:107:THR:HG23	2:H:108:PHE:N	2.13	0.64
2:H:116:LEU:O	2:H:117:VAL:CG1	2.46	0.64
3:A:319:GLY:CA	3:A:320:GLU:CB	2.73	0.63
3:A:328:ASN:OD1	3:A:331:ASN:HB3	1.97	0.63
3:A:311:LYS:C	3:A:339:THR:CG2	2.66	0.63
2:H:95:TYR:N	2:H:95:TYR:CD1	2.65	0.63
3:A:378:THR:O	3:A:405:ARG:HB3	1.99	0.63
3:A:349:PRO:CB	3:A:385:ALA:HB2	2.29	0.63
2:H:181:SER:C	2:H:183:LEU:N	2.46	0.63
3:A:352:PHE:O	3:A:362:PRO:CB	2.46	0.63
3:A:332:ILE:CG1	3:A:370:ILE:HD12	2.29	0.63
3:A:493:GLY:H	3:A:498:ASP:HB3	1.62	0.63
3:A:282:SER:O	3:A:283:CYS:HB2	1.98	0.62
3:A:439:ILE:HG22	3:A:442:ASN:ND2	2.13	0.62
3:A:494:PRO:HD2	3:A:495:GLU:H	1.64	0.62
3:A:368:LEU:HD21	3:A:386:TRP:CH2	2.34	0.62
3:A:341:ILE:O	3:A:341:ILE:HG13	1.99	0.62
3:A:324:SER:O	3:A:325:LEU:O	2.18	0.62
1:L:21:LEU:HB2	1:L:73:LEU:HB3	1.81	0.62
3:A:317:GLY:HA2	3:A:322:LYS:CA	2.29	0.62
3:A:454:LYS:HA	3:A:457:PHE:HD1	1.64	0.62
3:A:522:PRO:CD	3:A:523:ARG:H	2.11	0.62
1:L:182:SER:C	1:L:184:ALA:H	2.02	0.62
1:L:47:LEU:C	1:L:58:ILE:HD12	2.20	0.62
3:A:391:THR:OG1	3:A:422:THR:CG2	2.48	0.62
1:L:203:SER:H	1:L:204:PRO:HD3	1.65	0.62
3:A:506:SER:O	3:A:531:CYS:HB2	2.00	0.62
2:H:22:CYS:C	2:H:23:THR:OG1	2.37	0.62
1:L:66:GLY:HA3	1:L:71:PHE:HA	1.82	0.62
2:H:29:ILE:HD11	2:H:79:GLN:HA	1.82	0.62
2:H:40:ARG:HA	2:H:94:VAL:O	2.00	0.62
3:A:366:GLN:C	3:A:368:LEU:H	2.04	0.61
1:L:47:LEU:HD23	1:L:58:ILE:CG2	2.18	0.61
2:H:158:VAL:HG21	2:H:186:LEU:HD22	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:29:ILE:CG2	2:H:29:ILE:O	2.48	0.61
3:A:332:ILE:HG23	3:A:333:LYS:N	2.14	0.61
3:A:291:SER:HB2	3:A:303:LYS:O	2.00	0.61
3:A:535:HIS:CG	3:A:552:PRO:HA	2.35	0.61
2:H:153:TYR:CD2	2:H:153:TYR:O	2.54	0.61
1:L:212:GLY:CA	1:L:213:ALA:CB	2.71	0.61
2:H:167:LEU:HD21	2:H:190:VAL:HG11	1.82	0.60
1:L:170:ASP:C	1:L:170:ASP:OD2	2.39	0.60
1:L:193:ALA:HA	1:L:208:SER:HG	1.66	0.60
3:A:411:GLN:O	3:A:412:PHE:HB2	2.01	0.60
2:H:180:SER:C	2:H:182:GLY:H	2.05	0.60
1:L:164:THR:HG23	1:L:174:SER:O	2.02	0.59
2:H:35:TYR:HD2	2:H:52:TYR:CE2	2.19	0.59
3:A:586:TYR:CB	3:A:587:ALA:HB2	2.32	0.59
2:H:29:ILE:HD11	2:H:79:GLN:CA	2.32	0.59
3:A:328:ASN:HB2	3:A:329:ALA:HB2	1.74	0.59
3:A:526:VAL:CG1	3:A:527:GLU:N	2.66	0.59
3:A:341:ILE:HD11	3:A:345:LEU:HD13	1.84	0.59
3:A:381:LEU:HD12	3:A:382:LEU:H	1.67	0.59
2:H:153:TYR:CE2	2:H:184:TYR:CB	2.86	0.59
1:L:113:PRO:HB3	1:L:136:LEU:HD21	1.85	0.59
1:L:49:TYR:CD1	2:H:105:VAL:HG13	2.38	0.58
2:H:57:GLY:O	2:H:58:SER:C	2.41	0.58
2:H:155:PRO:HD2	2:H:210:PRO:CB	2.33	0.58
3:A:352:PHE:N	3:A:352:PHE:HD1	2.01	0.58
2:H:162:TRP:HB3	2:H:167:LEU:HD23	1.85	0.58
2:H:93:ALA:O	2:H:116:LEU:HD12	2.03	0.58
3:A:292:TYR:CD2	3:A:292:TYR:N	2.67	0.58
3:A:438:ILE:O	3:A:438:ILE:CG2	2.52	0.58
2:H:65:LEU:HD22	2:H:69:VAL:HG13	1.83	0.58
1:L:182:SER:O	1:L:184:ALA:N	2.33	0.58
1:L:193:ALA:HA	1:L:208:SER:OG	2.03	0.58
3:A:473:ASN:O	3:A:474:SER:C	2.41	0.57
2:H:53:ILE:O	2:H:53:ILE:HG23	2.04	0.57
3:A:527:GLU:O	3:A:528:ASN:HB2	2.04	0.57
2:H:33:ASP:O	2:H:34:TYR:CD2	2.57	0.57
1:L:159:SER:HA	1:L:178:THR:O	2.03	0.57
3:A:311:LYS:C	3:A:339:THR:HG22	2.17	0.57
2:H:103:PHE:N	2:H:103:PHE:CD2	2.72	0.57
3:A:314:ASN:H	3:A:314:ASN:ND2	2.00	0.57
3:A:402:ILE:HD12	3:A:429:LEU:HD13	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:365:PRO:O	3:A:366:GLN:C	2.42	0.57
2:H:167:LEU:O	2:H:167:LEU:HG	2.04	0.57
2:H:153:TYR:HD2	2:H:153:TYR:C	2.08	0.57
2:H:38:TRP:NE1	2:H:80:PHE:HE2	2.02	0.57
3:A:240:CYS:HB2	3:A:241:PRO:CD	2.35	0.56
3:A:505:VAL:HG22	3:A:506:SER:H	1.70	0.56
2:H:43:PRO:HD3	2:H:93:ALA:HA	1.86	0.56
2:H:29:ILE:O	2:H:29:ILE:HG22	2.04	0.56
1:L:33:LEU:HD23	1:L:34:ALA:N	2.21	0.56
3:A:495:GLU:O	3:A:498:ASP:HB2	2.06	0.56
1:L:169:LYS:O	1:L:170:ASP:HB3	2.05	0.56
1:L:48:ILE:CG2	1:L:52:SER:H	2.17	0.56
2:H:177:VAL:HG22	2:H:185:SER:O	2.06	0.56
2:H:199:THR:CG2	2:H:200:GLN:N	2.60	0.56
3:A:349:PRO:C	3:A:351:ALA:N	2.59	0.56
1:L:47:LEU:O	1:L:48:ILE:HG13	2.06	0.56
1:L:55:ALA:O	1:L:58:ILE:HG12	2.04	0.56
3:A:292:TYR:N	3:A:292:TYR:HD2	2.03	0.56
2:H:39:ILE:HG23	2:H:49:TRP:CA	2.34	0.55
3:A:324:SER:O	3:A:325:LEU:C	2.45	0.55
2:H:96:TYR:CE2	2:H:114:GLY:HA3	2.42	0.55
1:L:94:THR:O	1:L:94:THR:HG23	2.05	0.55
3:A:391:THR:OG1	3:A:422:THR:HG21	2.07	0.55
2:H:52:TYR:C	2:H:52:TYR:CD2	2.78	0.55
2:H:24:VAL:HG23	2:H:78:ASN:O	1.98	0.55
2:H:100:VAL:HG13	2:H:101:SER:N	2.21	0.55
2:H:177:VAL:HG22	2:H:185:SER:C	2.27	0.55
3:A:317:GLY:HA2	3:A:322:LYS:C	2.27	0.55
2:H:64:SER:OG	2:H:65:LEU:N	2.39	0.55
2:H:35:TYR:CE2	2:H:52:TYR:CE2	2.95	0.55
2:H:40:ARG:CG	2:H:50:ILE:HD11	2.37	0.55
2:H:6:GLU:OE1	2:H:114:GLY:N	2.40	0.54
3:A:400:GLU:O	3:A:429:LEU:HA	2.07	0.54
3:A:439:ILE:CG2	3:A:442:ASN:ND2	2.70	0.54
3:A:305:CYS:HB3	3:A:309:CYS:HA	1.90	0.54
3:A:351:ALA:HB3	3:A:352:PHE:HD1	1.73	0.54
3:A:375:LYS:HD2	3:A:400:GLU:OE2	2.07	0.54
1:L:47:LEU:O	1:L:58:ILE:CD1	2.55	0.54
1:L:33:LEU:CD1	1:L:71:PHE:CD2	2.91	0.54
3:A:404:GLY:HA2	3:A:434:ASP:HB3	1.90	0.54
3:A:381:LEU:HD21	3:A:396:PHE:CE1	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:402:ILE:HD13	3:A:414:LEU:HB2	1.90	0.53
2:H:4:LEU:HD23	2:H:98:ALA:HA	1.90	0.53
3:A:335:PHE:HB2	3:A:370:ILE:HG21	1.89	0.53
1:L:80:PRO:C	1:L:82:ASP:H	2.11	0.53
1:L:92:GLY:O	3:A:468:SER:N	2.42	0.53
3:A:368:LEU:HD21	3:A:386:TRP:CZ3	2.44	0.53
3:A:596:CYS:SG	3:A:597:HIS:N	2.78	0.53
2:H:177:VAL:HG13	2:H:185:SER:O	2.08	0.53
2:H:2:VAL:O	2:H:3:GLN:HB3	2.07	0.53
3:A:293:GLU:CG	3:A:294:MET:H	2.20	0.53
3:A:583:VAL:CA	3:A:584:TRP:CB	2.80	0.53
1:L:50:ASP:O	1:L:52:SER:N	2.41	0.53
3:A:447:TYR:CE2	3:A:480:GLN:O	2.61	0.53
3:A:391:THR:OG1	3:A:422:THR:HG22	2.08	0.53
2:H:144:ALA:N	2:H:192:VAL:O	2.41	0.53
2:H:19:SER:HB3	2:H:83:LYS:HE2	1.90	0.53
3:A:326:SER:HB2	3:A:348:LEU:H	1.73	0.53
2:H:23:THR:OG1	2:H:79:GLN:HG2	2.09	0.53
1:L:164:THR:CG2	1:L:174:SER:HB3	2.39	0.53
3:A:330:THR:HG22	3:A:331:ASN:CB	2.39	0.52
2:H:65:LEU:HD21	2:H:69:VAL:HG13	1.91	0.52
3:A:332:ILE:CG2	3:A:333:LYS:N	2.72	0.52
3:A:479:GLY:CA	3:A:481:VAL:HG23	2.33	0.52
3:A:487:SER:HB3	3:A:501:SER:C	2.28	0.52
2:H:103:PHE:H	2:H:103:PHE:HD2	1.57	0.52
2:H:101:SER:O	2:H:103:PHE:N	2.41	0.52
2:H:57:GLY:O	2:H:58:SER:O	2.26	0.52
1:L:106:ILE:H	1:L:106:ILE:CD1	2.18	0.52
3:A:383:ILE:HD11	3:A:396:PHE:CE1	2.45	0.52
2:H:35:TYR:CD2	2:H:52:TYR:CD2	2.92	0.52
1:L:49:TYR:O	1:L:50:ASP:O	2.28	0.52
2:H:65:LEU:O	2:H:68:ARG:HD3	2.10	0.52
2:H:95:TYR:N	2:H:95:TYR:HD1	2.05	0.52
3:A:341:ILE:CG1	3:A:341:ILE:O	2.53	0.52
2:H:160:VAL:HG22	2:H:161:SER:N	2.25	0.52
2:H:4:LEU:HB3	2:H:22:CYS:SG	2.50	0.52
3:A:268:VAL:HG12	3:A:269:LYS:H	1.75	0.52
3:A:247:ASN:OD1	3:A:248:PRO:HD2	2.10	0.52
2:H:73:VAL:HG12	2:H:73:VAL:O	2.10	0.52
1:L:135:LEU:HG	1:L:136:LEU:N	2.08	0.52
3:A:520:GLY:O	3:A:521:GLU:CB	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:525:PHE:C	3:A:525:PHE:CD1	2.83	0.52
3:A:505:VAL:HG22	3:A:529:SER:O	2.07	0.51
1:L:135:LEU:O	1:L:136:LEU:CB	2.57	0.51
1:L:44:PRO:HG2	2:H:111:TRP:CH2	2.45	0.51
1:L:94:THR:HG22	3:A:469:ASN:O	2.10	0.51
1:L:161:GLU:HA	1:L:176:SER:O	2.11	0.51
1:L:46:LEU:HD13	2:H:107:THR:HG22	1.93	0.51
2:H:10:GLY:O	2:H:117:VAL:HA	2.10	0.51
2:H:204:CYS:O	2:H:206:VAL:N	2.42	0.51
3:A:445:LEU:HB3	3:A:469:ASN:HD22	1.76	0.51
3:A:596:CYS:SG	3:A:600:CYS:HB2	2.51	0.51
2:H:107:THR:CG2	2:H:108:PHE:N	2.73	0.51
1:L:185:ASP:OD2	1:L:185:ASP:N	2.43	0.51
3:A:328:ASN:CB	3:A:329:ALA:HB2	2.34	0.51
2:H:109:ASP:O	2:H:110:TYR:HD1	1.93	0.51
3:A:275:TYR:CB	3:A:284:VAL:O	2.59	0.51
3:A:349:PRO:O	3:A:351:ALA:N	2.43	0.51
3:A:563:ASP:HB3	3:A:566:HIS:O	2.11	0.51
2:H:151:LYS:HG2	2:H:185:SER:OG	2.10	0.51
2:H:28:SER:OG	2:H:28:SER:O	2.28	0.51
1:L:203:SER:H	1:L:204:PRO:HD2	1.74	0.51
3:A:446:CYS:SG	3:A:470:ARG:HD2	2.51	0.50
2:H:23:THR:HG1	2:H:79:GLN:HB3	1.77	0.50
1:L:142:ARG:HH22	1:L:163:VAL:HG21	1.75	0.50
2:H:156:GLU:OE1	2:H:178:LEU:HD12	2.11	0.50
1:L:14:SER:O	1:L:15:PRO:O	2.29	0.50
1:L:29:VAL:O	1:L:31:SER:N	2.45	0.50
3:A:268:VAL:HG12	3:A:269:LYS:N	2.27	0.50
3:A:370:ILE:N	3:A:371:LEU:HB2	2.26	0.50
3:A:383:ILE:HD11	3:A:396:PHE:HE1	1.77	0.50
3:A:417:VAL:HG13	3:A:440:SER:OG	2.11	0.50
3:A:322:LYS:O	3:A:323:ASP:C	2.49	0.50
3:A:413:SER:HB3	3:A:435:GLY:HA3	1.92	0.50
3:A:246:TYR:HD2	3:A:246:TYR:C	2.15	0.50
3:A:284:VAL:HG23	3:A:285:ARG:H	1.77	0.50
3:A:328:ASN:CA	3:A:329:ALA:HB2	2.28	0.49
3:A:382:LEU:HD12	3:A:415:ALA:HB3	1.94	0.49
2:H:122:ALA:CB	2:H:123:SER:HB3	2.39	0.49
2:H:55:TYR:C	2:H:55:TYR:CD1	2.85	0.49
1:L:135:LEU:CG	1:L:136:LEU:N	2.70	0.49
3:A:389:ASN:HD22	6:A:3891:NAG:C8	2.22	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:14:PRO:C	2:H:16:GLN:H	2.15	0.49
2:H:6:GLU:HB3	2:H:115:THR:HG21	1.85	0.49
3:A:541:GLN:OE1	3:A:542:ALA:N	2.45	0.49
2:H:160:VAL:HB	2:H:206:VAL:CG2	2.31	0.49
1:L:138:ASN:C	1:L:172:THR:OG1	2.51	0.49
3:A:332:ILE:HG13	3:A:332:ILE:O	2.12	0.49
3:A:411:GLN:O	3:A:412:PHE:CB	2.61	0.49
2:H:103:PHE:N	2:H:103:PHE:HD2	2.08	0.49
3:A:291:SER:CB	3:A:303:LYS:O	2.61	0.49
3:A:401:ILE:HD11	3:A:403:ARG:HG2	1.94	0.49
3:A:408:GLN:O	3:A:412:PHE:HB2	2.12	0.49
3:A:507:ARG:NE	3:A:524:GLU:OE2	2.45	0.49
2:H:155:PRO:HD2	2:H:210:PRO:HG2	1.94	0.49
3:A:575:VAL:HB	3:A:583:VAL:O	2.13	0.49
2:H:18:LEU:O	2:H:83:LYS:CA	2.57	0.49
1:L:165:GLU:HA	1:L:165:GLU:OE1	2.13	0.49
3:A:260:LYS:CB	3:A:268:VAL:O	2.61	0.49
3:A:353:ARG:NH1	3:A:353:ARG:HG2	2.21	0.49
3:A:473:ASN:O	3:A:476:LYS:N	2.45	0.49
3:A:473:ASN:O	3:A:477:ALA:N	2.42	0.49
2:H:87:VAL:HB	2:H:119:VAL:HG21	1.93	0.49
2:H:147:GLY:HA2	2:H:162:TRP:CH2	2.47	0.49
3:A:391:THR:CA	3:A:421:ILE:HG22	2.43	0.48
3:A:532:ILE:CD1	3:A:532:ILE:N	2.57	0.48
2:H:13:LYS:O	2:H:16:GLN:HB2	2.12	0.48
1:L:48:ILE:HG21	1:L:52:SER:H	1.78	0.48
3:A:341:ILE:CD1	3:A:345:LEU:HD13	2.42	0.48
1:L:44:PRO:HD2	2:H:111:TRP:CD2	2.48	0.48
3:A:278:THR:CG2	3:A:280:HIS:H	2.27	0.48
3:A:328:ASN:O	3:A:331:ASN:HB3	2.12	0.48
3:A:246:TYR:CD2	3:A:246:TYR:C	2.85	0.48
2:H:38:TRP:NE1	2:H:80:PHE:CE2	2.81	0.48
3:A:313:CYS:C	3:A:314:ASN:HD22	2.17	0.48
3:A:311:LYS:C	3:A:339:THR:HG21	2.33	0.48
3:A:344:ASP:HA	3:A:380:PHE:H	1.78	0.48
3:A:485:LEU:HD12	3:A:511:CYS:HB3	1.95	0.48
1:L:4:MET:CE	1:L:90:GLN:HB3	2.43	0.48
3:A:250:THR:O	3:A:251:TYR:HB2	2.13	0.48
3:A:525:PHE:CG	3:A:525:PHE:O	2.64	0.48
2:H:111:TRP:CD1	2:H:111:TRP:N	2.79	0.48
2:H:180:SER:C	2:H:182:GLY:N	2.65	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:65:LEU:HD22	2:H:69:VAL:CG1	2.43	0.48
3:A:291:SER:HA	3:A:305:CYS:SG	2.53	0.48
3:A:355:ASP:O	3:A:360:THR:N	2.47	0.48
3:A:467:ILE:O	3:A:467:ILE:HG22	2.13	0.48
1:L:137:ASN:HB3	1:L:138:ASN:HB2	1.95	0.48
3:A:284:VAL:CG2	3:A:285:ARG:N	2.71	0.47
3:A:382:LEU:HA	3:A:382:LEU:HD12	1.48	0.47
2:H:122:ALA:HB1	2:H:123:SER:CB	2.41	0.47
1:L:185:ASP:O	1:L:189:HIS:CD2	2.59	0.47
1:L:33:LEU:HD13	1:L:71:PHE:CD1	2.49	0.47
1:L:167:ASP:OD1	1:L:168:SER:N	2.48	0.47
1:L:13:LEU:HD12	1:L:19:ALA:HB2	1.96	0.47
2:H:2:VAL:CG2	2:H:110:TYR:CE2	2.94	0.47
2:H:53:ILE:HD13	2:H:73:VAL:HG23	1.96	0.47
3:A:263:PHE:C	3:A:265:ALA:H	2.18	0.47
2:H:198:GLY:O	2:H:199:THR:HB	2.14	0.47
1:L:202:SER:CA	1:L:203:SER:CB	2.90	0.47
3:A:356:SER:C	3:A:358:THR:N	2.68	0.47
2:H:147:GLY:C	2:H:162:TRP:HH2	2.17	0.47
3:A:327:ILE:O	3:A:331:ASN:OD1	2.32	0.47
3:A:442:ASN:O	3:A:443:LYS:CB	2.56	0.47
1:L:44:PRO:HD2	2:H:111:TRP:CE3	2.50	0.47
2:H:85:ASN:O	2:H:86:SER:HB2	2.15	0.47
3:A:378:THR:HA	3:A:403:ARG:HB2	1.97	0.47
3:A:505:VAL:CG2	3:A:506:SER:N	2.77	0.47
1:L:192:TYR:O	1:L:208:SER:OG	2.32	0.47
3:A:451:ILE:HG22	3:A:453:TRP:CD1	2.50	0.47
1:L:164:THR:HG23	1:L:174:SER:HB3	1.97	0.47
2:H:161:SER:O	2:H:205:ASN:N	2.48	0.46
2:H:155:PRO:HD2	2:H:210:PRO:HB2	1.96	0.46
1:L:33:LEU:O	1:L:50:ASP:N	2.48	0.46
3:A:343:GLY:H	3:A:378:THR:CB	2.13	0.46
3:A:349:PRO:N	3:A:385:ALA:HB2	2.29	0.46
1:L:150:VAL:C	1:L:152:ASN:H	2.17	0.46
1:L:194:CYS:H	1:L:208:SER:HB2	1.80	0.46
3:A:485:LEU:HD21	3:A:513:ASP:HA	1.96	0.46
3:A:423:SER:HB2	3:A:492:TRP:O	2.16	0.46
1:L:151:ASP:H	1:L:192:TYR:HA	1.80	0.46
3:A:417:VAL:HG13	3:A:440:SER:HG	1.80	0.46
1:L:58:ILE:HG12	1:L:58:ILE:H	1.41	0.46
3:A:266:THR:O	3:A:268:VAL:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:290:ASP:HA	3:A:291:SER:HA	1.61	0.46
1:L:146:VAL:HG12	1:L:147:GLN:H	1.80	0.46
1:L:15:PRO:O	1:L:17:GLU:N	2.49	0.46
3:A:332:ILE:O	3:A:370:ILE:HD12	2.15	0.46
2:H:100:VAL:HG13	2:H:101:SER:H	1.79	0.46
2:H:35:TYR:CE1	2:H:102:ILE:HD13	2.51	0.46
1:L:90:GLN:OE1	1:L:91:TYR:N	2.49	0.46
2:H:41:GLN:HA	2:H:42:PRO:HD2	1.69	0.46
2:H:73:VAL:HG22	2:H:80:PHE:HB2	1.98	0.46
3:A:540:PRO:HA	3:A:546:THR:OG1	2.15	0.46
2:H:11:LEU:HD12	2:H:118:THR:O	2.16	0.45
3:A:261:TYR:O	3:A:262:SER:HB2	2.16	0.45
3:A:514:LYS:HG2	3:A:515:CYS:H	1.79	0.45
3:A:271:CYS:SG	3:A:283:CYS:C	2.95	0.45
3:A:318:ILE:HA	3:A:322:LYS:HA	1.98	0.45
3:A:541:GLN:HG3	3:A:543:MET:HB2	1.99	0.45
1:L:29:VAL:O	1:L:30:SER:C	2.54	0.45
3:A:291:SER:HG	3:A:304:LYS:HA	1.77	0.45
3:A:365:PRO:O	3:A:366:GLN:O	2.34	0.45
1:L:113:PRO:O	1:L:115:VAL:HG23	2.17	0.45
3:A:317:GLY:HA2	3:A:318:ILE:HA	1.77	0.45
3:A:332:ILE:O	3:A:370:ILE:CD1	2.65	0.45
3:A:370:ILE:CA	3:A:371:LEU:HB2	2.46	0.45
3:A:494:PRO:CD	3:A:495:GLU:H	2.29	0.45
2:H:207:ASN:OD1	2:H:213:THR:O	2.35	0.45
2:H:6:GLU:OE2	2:H:97:CYS:N	2.39	0.45
2:H:73:VAL:HG22	2:H:80:PHE:CB	2.47	0.45
1:L:83:PHE:CE2	1:L:165:GLU:HB3	2.51	0.45
1:L:175:LEU:HD23	1:L:176:SER:H	1.81	0.45
3:A:288:GLY:O	3:A:290:ASP:C	2.55	0.45
3:A:577:GLY:O	3:A:578:GLU:HB2	2.17	0.45
1:L:118:PHE:HA	1:L:119:PRO:HD3	1.68	0.45
3:A:524:GLU:HA	3:A:533:GLN:HA	1.98	0.45
2:H:28:SER:O	2:H:29:ILE:C	2.54	0.45
1:L:20:THR:C	1:L:21:LEU:HD12	2.38	0.45
3:A:541:GLN:HG3	3:A:544:ASN:H	1.82	0.45
2:H:119:VAL:O	2:H:120:SER:HB3	2.16	0.45
3:A:370:ILE:N	3:A:371:LEU:CB	2.81	0.44
2:H:144:ALA:O	2:H:191:THR:HA	2.17	0.44
1:L:46:LEU:HG	1:L:47:LEU:N	2.32	0.44
1:L:4:MET:CE	1:L:90:GLN:HG2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:418:SER:HA	3:A:441:GLY:O	2.16	0.44
3:A:485:LEU:HD11	3:A:512:VAL:C	2.37	0.44
3:A:494:PRO:O	3:A:495:GLU:C	2.53	0.44
3:A:531:CYS:N	3:A:532:ILE:HD13	2.33	0.44
1:L:122:ASP:O	1:L:126:LYS:CB	2.65	0.44
3:A:473:ASN:C	3:A:475:CYS:N	2.70	0.44
3:A:576:MET:HA	3:A:577:GLY:HA2	1.83	0.44
2:H:154:PHE:CD2	2:H:155:PRO:HA	2.53	0.44
1:L:36:TYR:OH	2:H:108:PHE:HB2	2.16	0.44
3:A:447:TYR:C	3:A:449:ASN:N	2.65	0.44
5:D:1:NAG:H61	5:D:2:NAG:C1	2.47	0.44
1:L:50:ASP:O	1:L:52:SER:CB	2.66	0.44
3:A:394:HIS:O	3:A:395:ALA:C	2.55	0.44
3:A:494:PRO:HD2	3:A:495:GLU:N	2.30	0.44
3:A:577:GLY:HA2	3:A:581:THR:O	2.17	0.44
2:H:153:TYR:HE2	2:H:156:GLU:HG3	1.82	0.44
2:H:206:VAL:CG1	2:H:207:ASN:N	2.80	0.44
2:H:209:LYS:N	2:H:210:PRO:CD	2.81	0.44
1:L:173:TYR:O	1:L:174:SER:HB2	2.17	0.44
1:L:48:ILE:HA	1:L:53:ASN:O	2.17	0.44
3:A:554:ASN:CG	3:A:554:ASN:O	2.55	0.44
3:A:349:PRO:HA	3:A:351:ALA:HB3	1.99	0.44
3:A:240:CYS:HB2	3:A:241:PRO:HD2	2.00	0.43
1:L:130:ALA:O	1:L:180:THR:O	2.36	0.43
3:A:328:ASN:CG	3:A:329:ALA:HB3	2.33	0.43
3:A:291:SER:CA	3:A:305:CYS:SG	3.06	0.43
2:H:24:VAL:HG22	2:H:78:ASN:O	1.99	0.43
1:L:50:ASP:O	1:L:51:ALA:C	2.56	0.43
1:L:182:SER:C	1:L:184:ALA:N	2.71	0.43
2:H:154:PHE:CD2	2:H:155:PRO:CA	3.02	0.43
3:A:539:LEU:HA	3:A:540:PRO:HD2	1.82	0.43
1:L:6:GLN:OE1	1:L:87:TYR:HA	2.19	0.43
3:A:356:SER:O	3:A:358:THR:N	2.52	0.43
3:A:368:LEU:O	3:A:368:LEU:HG	2.19	0.43
3:A:378:THR:HG22	3:A:405:ARG:HD2	2.01	0.43
2:H:109:ASP:O	2:H:110:TYR:CD1	2.71	0.43
1:L:4:MET:HE3	1:L:90:GLN:HB3	1.99	0.43
3:A:407:LYS:HG3	3:A:410:GLY:C	2.39	0.43
2:H:54:TYR:C	2:H:56:SER:H	2.22	0.43
2:H:87:VAL:O	2:H:87:VAL:HG23	2.19	0.43
1:L:49:TYR:HD2	1:L:50:ASP:CG	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:394:HIS:CG	3:A:395:ALA:N	2.87	0.43
3:A:417:VAL:HA	3:A:440:SER:OG	2.19	0.43
3:A:517:LEU:HB3	3:A:525:PHE:HA	2.01	0.43
2:H:92:THR:CG2	2:H:118:THR:HG23	2.48	0.43
2:H:24:VAL:HG11	2:H:29:ILE:HG13	2.00	0.43
3:A:340:SER:HB2	3:A:376:GLU:N	2.34	0.42
3:A:293:GLU:HG2	3:A:294:MET:H	1.84	0.42
3:A:385:ALA:O	3:A:386:TRP:HB2	2.19	0.42
1:L:79:GLU:CB	1:L:81:GLU:HG3	2.49	0.42
3:A:262:SER:HA	3:A:283:CYS:HB3	2.01	0.42
3:A:383:ILE:CD1	3:A:396:PHE:HE1	2.32	0.42
2:H:162:TRP:CB	2:H:167:LEU:HD23	2.49	0.42
2:H:33:ASP:C	2:H:34:TYR:CD2	2.93	0.42
1:L:109:THR:O	1:L:110:VAL:HG23	2.20	0.42
1:L:36:TYR:O	1:L:86:TYR:HA	2.19	0.42
3:A:535:HIS:ND1	3:A:536:PRO:HD2	2.34	0.42
1:L:11:LEU:HD21	1:L:13:LEU:HD11	2.02	0.42
1:L:64:GLY:HA2	1:L:65:SER:HG	1.84	0.42
3:A:416:VAL:HG12	3:A:416:VAL:O	2.20	0.42
1:L:89:HIS:HA	1:L:98:PHE:HD2	1.84	0.42
1:L:61:ARG:O	1:L:76:SER:HB3	2.19	0.42
3:A:442:ASN:HB2	3:A:469:ASN:HD21	1.85	0.42
3:A:480:GLN:HA	3:A:480:GLN:HE21	1.84	0.42
2:H:155:PRO:HD2	2:H:210:PRO:CG	2.50	0.42
3:A:520:GLY:O	3:A:521:GLU:HB2	2.20	0.42
3:A:366:GLN:C	3:A:368:LEU:N	2.68	0.42
2:H:102:ILE:HB	2:H:103:PHE:H	1.66	0.42
3:A:250:THR:OG1	3:A:254:ASP:OD1	2.37	0.41
1:L:33:LEU:HD12	1:L:71:PHE:CE2	2.55	0.41
3:A:293:GLU:CG	3:A:294:MET:N	2.83	0.41
2:H:4:LEU:O	2:H:97:CYS:SG	2.78	0.41
1:L:43:ALA:HB3	2:H:96:TYR:CZ	2.55	0.41
2:H:143:THR:HA	2:H:194:SER:N	2.31	0.41
2:H:88:THR:OG1	2:H:90:ALA:N	2.36	0.41
2:H:88:THR:HG1	2:H:90:ALA:H	1.59	0.41
1:L:120:PRO:HB3	1:L:130:ALA:HB1	2.01	0.41
3:A:408:GLN:C	3:A:409:HIS:O	2.58	0.41
3:A:545:ILE:O	3:A:546:THR:CB	2.68	0.41
2:H:193:PRO:O	2:H:195:SER:O	2.39	0.41
1:L:139:PHE:CD1	1:L:139:PHE:N	2.88	0.41
3:A:449:ASN:O	3:A:449:ASN:CG	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:561:TYR:O	3:A:562:ILE:CB	2.63	0.41
2:H:33:ASP:C	2:H:34:TYR:CG	2.93	0.41
2:H:63:PRO:O	2:H:64:SER:C	2.59	0.41
3:A:270:LYS:HB3	3:A:270:LYS:HE2	1.76	0.41
3:A:442:ASN:HB2	3:A:469:ASN:ND2	2.35	0.41
3:A:494:PRO:CD	3:A:495:GLU:N	2.83	0.41
5:C:2:NAG:H82	5:C:2:NAG:H2	2.02	0.41
2:H:28:SER:C	2:H:30:SER:N	2.74	0.41
2:H:77:LYS:O	2:H:79:GLN:HG3	2.20	0.41
1:L:173:TYR:N	1:L:173:TYR:CD1	2.89	0.41
3:A:333:LYS:O	3:A:335:PHE:N	2.54	0.41
1:L:161:GLU:HA	1:L:177:SER:HA	2.03	0.41
1:L:39:LYS:HA	1:L:40:PRO:HD2	1.93	0.41
1:L:46:LEU:HD13	2:H:107:THR:CG2	2.50	0.41
1:L:87:TYR:CD1	2:H:47:LEU:HD11	2.56	0.41
3:A:305:CYS:O	3:A:306:GLU:C	2.60	0.40
3:A:353:ARG:HH11	3:A:353:ARG:CG	2.22	0.40
3:A:523:ARG:CB	3:A:534:CYS:HB2	2.51	0.40
3:A:332:ILE:HG12	3:A:370:ILE:HD12	2.03	0.40
2:H:116:LEU:HD13	2:H:116:LEU:HA	1.88	0.40
3:A:250:THR:O	3:A:251:TYR:CB	2.69	0.40
3:A:282:SER:HB2	3:A:283:CYS:H	1.55	0.40
3:A:376:GLU:CB	3:A:401:ILE:HG23	2.36	0.40
2:H:29:ILE:CD1	2:H:79:GLN:CA	2.98	0.40
1:L:47:LEU:HD23	1:L:47:LEU:HA	1.82	0.40
1:L:4:MET:HB2	1:L:99:GLY:HA2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	211/213 (99%)	143 (68%)	33 (16%)	35 (17%)	0	1
2	H	213/223 (96%)	162 (76%)	23 (11%)	28 (13%)	0	1
3	A	373/624 (60%)	207 (56%)	84 (22%)	82 (22%)	0	0
All	All	797/1060 (75%)	512 (64%)	140 (18%)	145 (18%)	0	1

All (145) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	9	ALA
1	L	15	PRO
1	L	16	GLY
1	L	32	TYR
1	L	52	SER
1	L	65	SER
1	L	90	GLN
1	L	109	THR
1	L	136	LEU
1	L	142	ARG
1	L	170	ASP
1	L	203	SER
1	L	204	PRO
2	H	29	ILE
2	H	56	SER
2	H	76	SER
2	H	113	GLN
2	H	121	SER
2	H	181	SER
2	H	182	GLY
2	H	199	THR
3	A	253	MET
3	A	257	PRO
3	A	258	GLU
3	A	267	CYS
3	A	273	ARG
3	A	279	ASP
3	A	283	CYS
3	A	290	ASP
3	A	308	PRO
3	A	320	GLU
3	A	322	LYS
3	A	325	LEU
3	A	328	ASN

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Mol	Chain	Res	Type
3	A	330	THR
3	A	331	ASN
3	A	350	VAL
3	A	357	PHE
3	A	366	GLN
3	A	367	GLU
3	A	412	PHE
3	A	448	ALA
3	A	494	PRO
3	A	508	GLY
3	A	509	ARG
3	A	513	ASP
3	A	521	GLU
3	A	523	ARG
3	A	540	PRO
3	A	541	GLN
3	A	562	ILE
3	A	584	TRP
3	A	598	PRO
3	A	600	CYS
3	A	610	GLU
1	L	3	VAL
1	L	30	SER
1	L	50	ASP
1	L	51	ALA
1	L	113	PRO
1	L	114	SER
1	L	158	ASN
1	L	174	SER
1	L	181	LEU
1	L	183	LYS
2	H	58	SER
2	H	87	VAL
2	H	102	ILE
2	H	117	VAL
2	H	127	PRO
2	H	200	GLN
2	H	205	ASN
3	A	246	TYR
3	A	286	ALA
3	A	288	GLY
3	A	329	ALA

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Mol	Chain	Res	Type
3	A	334	HIS
3	A	371	LEU
3	A	409	HIS
3	A	410	GLY
3	A	511	CYS
3	A	520	GLY
3	A	543	MET
3	A	563	ASP
3	A	574	GLY
1	L	40	PRO
1	L	155	GLN
1	L	159	SER
2	H	23	THR
2	H	77	LYS
2	H	89	ALA
2	H	120	SER
2	H	168	THR
3	A	251	TYR
3	A	282	SER
3	A	294	MET
3	A	306	GLU
3	A	317	GLY
3	A	323	ASP
3	A	421	ILE
3	A	472	GLU
3	A	474	SER
3	A	480	GLN
3	A	497	ARG
3	A	517	LEU
3	A	522	PRO
3	A	546	THR
3	A	554	ASN
3	A	560	HIS
3	A	561	TYR
3	A	586	TYR
3	A	605	THR
3	A	608	GLY
1	L	8	PRO
1	L	89	HIS
1	L	144	ALA
1	L	151	ASP
2	H	16	GLN

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Mol	Chain	Res	Type
2	H	24	VAL
2	H	123	SER
2	H	210	PRO
2	H	211	SER
2	H	219	VAL
3	A	245	LEU
3	A	339	THR
3	A	404	GLY
3	A	443	LYS
3	A	527	GLU
3	A	553	ASP
1	L	127	SER
1	L	153	ALA
2	H	55	TYR
3	A	268	VAL
3	A	284	VAL
3	A	565	PRO
2	H	175	PRO
3	A	307	GLY
1	L	29	VAL
1	L	43	ALA
3	A	255	VAL
1	L	44	PRO
3	A	592	VAL
3	A	276	VAL
3	A	612	CYS
3	A	552	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	135/181 (75%)	94 (70%)	41 (30%)	0	1
2	H	165/192 (86%)	121 (73%)	44 (27%)	0	1
3	A	254/545 (47%)	187 (74%)	67 (26%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	554/918 (60%)	402 (73%)	152 (27%)	0 1

All (152) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	7	SER
1	L	8	PRO
1	L	10	THR
1	L	15	PRO
1	L	20	THR
1	L	30	SER
1	L	46	LEU
1	L	50	ASP
1	L	53	ASN
1	L	56	THR
1	L	58	ILE
1	L	63	SER
1	L	69	THR
1	L	71	PHE
1	L	74	THR
1	L	77	SER
1	L	79	GLU
1	L	81	GLU
1	L	85	VAL
1	L	90	GLN
1	L	106	ILE
1	L	109	THR
1	L	114	SER
1	L	122	ASP
1	L	129	THR
1	L	134	CYS
1	L	136	LEU
1	L	146	VAL
1	L	162	SER
1	L	163	VAL
1	L	164	THR
1	L	165	GLU
1	L	166	GLN
1	L	174	SER
1	L	176	SER
1	L	178	THR
1	L	180	THR

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Mol	Chain	Res	Type
1	L	185	ASP
1	L	197	THR
1	L	199	GLN
1	L	206	THR
2	H	2	VAL
2	H	4	LEU
2	H	19	SER
2	H	24	VAL
2	H	37	SER
2	H	39	ILE
2	H	40	ARG
2	H	47	LEU
2	H	55	TYR
2	H	59	THR
2	H	65	LEU
2	H	69	VAL
2	H	82	LEU
2	H	83	LYS
2	H	88	THR
2	H	91	ASP
2	H	92	THR
2	H	95	TYR
2	H	102	ILE
2	H	103	PHE
2	H	107	THR
2	H	115	THR
2	H	116	LEU
2	H	117	VAL
2	H	119	VAL
2	H	120	SER
2	H	124	THR
2	H	128	SER
2	H	143	THR
2	H	146	LEU
2	H	152	ASP
2	H	153	TYR
2	H	158	VAL
2	H	160	VAL
2	H	168	THR
2	H	169	SER
2	H	177	VAL
2	H	187	SER

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Mol	Chain	Res	Type
2	H	192	VAL
2	H	195	SER
2	H	199	THR
2	H	204	CYS
2	H	213	THR
2	H	216	ASP
3	A	246	TYR
3	A	270	LYS
3	A	282	SER
3	A	287	CYS
3	A	291	SER
3	A	292	TYR
3	A	314	ASN
3	A	325	LEU
3	A	326	SER
3	A	327	ILE
3	A	330	THR
3	A	331	ASN
3	A	332	ILE
3	A	340	SER
3	A	344	ASP
3	A	345	LEU
3	A	347	ILE
3	A	352	PHE
3	A	353	ARG
3	A	371	LEU
3	A	372	LYS
3	A	376	GLU
3	A	388	GLU
3	A	394	HIS
3	A	397	GLU
3	A	399	LEU
3	A	403	ARG
3	A	405	ARG
3	A	407	LYS
3	A	411	GLN
3	A	429	LEU
3	A	437	VAL
3	A	443	LYS
3	A	450	THR
3	A	456	LEU
3	A	459	THR

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Mol	Chain	Res	Type
3	A	460	SER
3	A	466	ILE
3	A	468	SER
3	A	470	ARG
3	A	473	ASN
3	A	478	THR
3	A	480	GLN
3	A	485	LEU
3	A	486	CYS
3	A	489	GLU
3	A	495	GLU
3	A	497	ARG
3	A	501	SER
3	A	506	SER
3	A	507	ARG
3	A	510	GLU
3	A	511	CYS
3	A	514	LYS
3	A	524	GLU
3	A	525	PHE
3	A	527	GLU
3	A	532	ILE
3	A	541	GLN
3	A	544	ASN
3	A	554	ASN
3	A	556	ILE
3	A	557	GLN
3	A	565	PRO
3	A	588	ASP
3	A	604	CYS
3	A	612	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	42	GLN
1	L	189	HIS
2	H	207	ASN
3	A	314	ASN
3	A	334	HIS
3	A	469	ASN
3	A	480	GLN

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Mol	Chain	Res	Type
3	A	483	HIS
3	A	516	ASN
3	A	544	ASN
3	A	557	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

7 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	$\# Z > 2$
4	NAG	B	1	3,4	14,14,15	1.27	2 (14%)	17,19,21	3.07	7 (41%)
4	NAG	B	2	4	14,14,15	0.89	0	17,19,21	2.67	4 (23%)
4	BMA	B	3	4	11,11,12	1.29	2 (18%)	15,15,17	2.12	5 (33%)
5	NAG	C	1	3,5	14,14,15	0.88	0	17,19,21	2.06	5 (29%)
5	NAG	C	2	5	14,14,15	0.99	1 (7%)	17,19,21	2.85	5 (29%)
5	NAG	D	1	3,5	14,14,15	0.73	0	17,19,21	2.77	9 (52%)
5	NAG	D	2	5	14,14,15	1.02	1 (7%)	17,19,21	2.53	7 (41%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	B	2	4	-	4/6/23/26	0/1/1/1
4	BMA	B	3	4	-	1/2/19/22	0/1/1/1
5	NAG	C	1	3,5	1/1/5/7	2/6/23/26	0/1/1/1
5	NAG	C	2	5	-	4/6/23/26	0/1/1/1
5	NAG	D	1	3,5	-	2/6/23/26	0/1/1/1
5	NAG	D	2	5	-	3/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1	NAG	O5-C1	-2.89	1.39	1.43
4	B	1	NAG	C2-N2	-2.79	1.41	1.46
4	B	3	BMA	C2-C3	2.74	1.56	1.52
4	B	3	BMA	C1-C2	2.08	1.56	1.52
5	D	2	NAG	O5-C1	2.03	1.47	1.43
5	C	2	NAG	C4-C3	2.00	1.57	1.52

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1	NAG	O5-C1-C2	-7.42	99.57	111.29
5	C	2	NAG	C1-C2-N2	6.74	122.00	110.49
5	C	2	NAG	C1-O5-C5	-6.63	103.21	112.19
4	B	2	NAG	C1-O5-C5	-6.38	103.55	112.19
4	B	2	NAG	O5-C5-C6	6.07	116.73	107.20
4	B	1	NAG	C2-N2-C7	-5.78	114.67	122.90
5	C	1	NAG	O4-C4-C3	-5.75	97.06	110.35
5	D	2	NAG	C3-C4-C5	-5.17	101.01	110.24
5	D	1	NAG	C6-C5-C4	-5.12	101.02	113.00
5	D	2	NAG	O5-C5-C6	4.98	115.01	107.20
5	C	2	NAG	C3-C4-C5	4.64	118.51	110.24
4	B	2	NAG	C2-N2-C7	-4.59	116.37	122.90
5	D	2	NAG	O4-C4-C5	4.31	120.00	109.30
4	B	1	NAG	O5-C5-C6	-4.31	100.45	107.20
5	D	1	NAG	C1-O5-C5	4.16	117.83	112.19
4	B	3	BMA	C1-C2-C3	3.96	114.53	109.67
4	B	3	BMA	C1-O5-C5	-3.84	106.99	112.19
5	D	1	NAG	O5-C1-C2	-3.82	105.25	111.29
4	B	2	NAG	C3-C4-C5	-3.74	103.56	110.24
4	B	3	BMA	C2-C3-C4	3.71	117.32	110.89
5	D	2	NAG	C1-O5-C5	3.69	117.19	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	1	NAG	C4-C3-C2	3.68	116.41	111.02
5	D	1	NAG	O4-C4-C3	3.63	118.73	110.35
5	D	1	NAG	O5-C5-C6	-3.50	101.71	107.20
4	B	1	NAG	O6-C6-C5	-3.49	99.33	111.29
5	D	1	NAG	O3-C3-C2	-3.31	102.61	109.47
4	B	1	NAG	O3-C3-C2	-3.24	102.77	109.47
4	B	1	NAG	C4-C3-C2	3.22	115.73	111.02
5	C	1	NAG	C3-C4-C5	-3.05	104.81	110.24
4	B	3	BMA	O2-C2-C1	3.04	115.36	109.15
5	C	2	NAG	O5-C1-C2	-2.87	106.76	111.29
5	C	1	NAG	C4-C3-C2	2.87	115.22	111.02
5	D	1	NAG	C8-C7-N2	2.70	120.66	116.10
5	D	2	NAG	C2-N2-C7	-2.56	119.25	122.90
5	C	1	NAG	O5-C1-C2	2.43	115.13	111.29
5	D	2	NAG	O3-C3-C2	2.37	114.36	109.47
4	B	1	NAG	C1-O5-C5	2.11	115.06	112.19
5	D	1	NAG	O6-C6-C5	-2.10	104.10	111.29
5	D	2	NAG	C8-C7-N2	2.08	119.62	116.10
5	C	2	NAG	C4-C3-C2	2.07	114.05	111.02
5	C	1	NAG	O3-C3-C4	2.06	115.11	110.35
4	B	3	BMA	C6-C5-C4	2.01	117.71	113.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	C	1	NAG	C1

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	1	NAG	C8-C7-N2-C2
5	D	1	NAG	O7-C7-N2-C2
4	B	1	NAG	O7-C7-N2-C2
5	C	2	NAG	C8-C7-N2-C2
5	C	2	NAG	O7-C7-N2-C2
4	B	2	NAG	C8-C7-N2-C2
4	B	2	NAG	O7-C7-N2-C2
5	D	2	NAG	C8-C7-N2-C2
5	D	2	NAG	O7-C7-N2-C2
4	B	1	NAG	C8-C7-N2-C2
5	C	2	NAG	O5-C5-C6-O6
4	B	2	NAG	O5-C5-C6-O6

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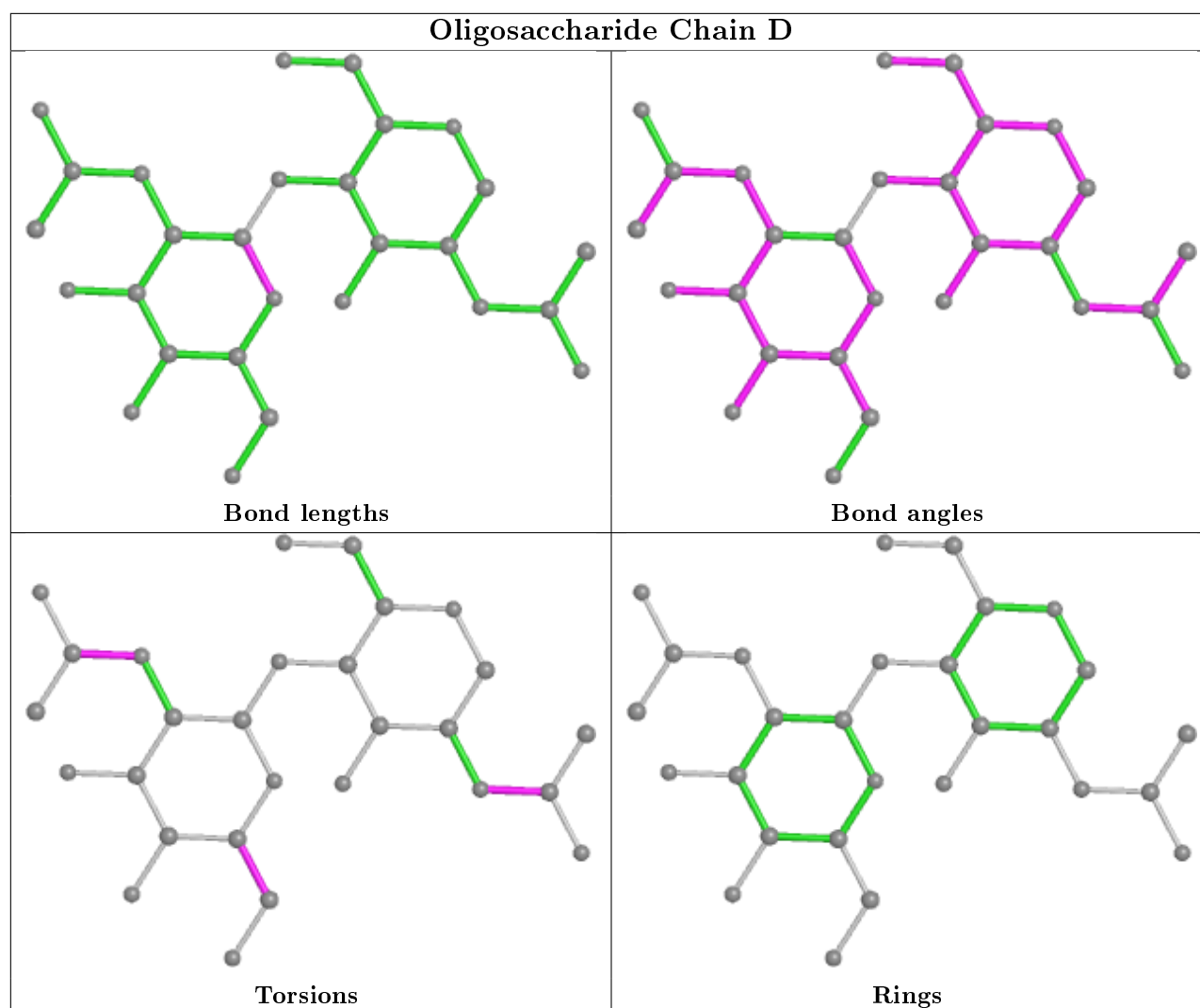
Mol	Chain	Res	Type	Atoms
5	C	1	NAG	C4-C5-C6-O6
5	C	2	NAG	C4-C5-C6-O6
4	B	2	NAG	C4-C5-C6-O6
5	C	1	NAG	O5-C5-C6-O6
5	D	2	NAG	O5-C5-C6-O6
4	B	3	BMA	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	1	NAG	1	0
5	C	2	NAG	1	0
5	D	2	NAG	1	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](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	NAG	A	3891	3	14,14,15	0.79	0	17,19,21	3.06	6 (35%)
6	NAG	A	5041	3	12,12,15	1.06	0	15,16,21	2.61	5 (33%)

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	A	3891	3	-	5/6/23/26	0/1/1/1
6	NAG	A	5041	3	1/1/4/7	0/3/20/26	0/1/1/1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	3891	NAG	O5-C1-C2	-8.62	97.67	111.29
6	A	5041	NAG	C7-N2-C2	7.57	125.71	114.57
6	A	3891	NAG	C1-C2-N2	4.83	118.73	110.49
6	A	3891	NAG	C2-N2-C7	4.67	129.56	122.90
6	A	3891	NAG	C4-C3-C2	-3.60	105.75	111.02
6	A	5041	NAG	O5-C5-C6	3.09	113.97	107.33
6	A	5041	NAG	O4-C4-C5	2.99	116.29	109.67
6	A	5041	NAG	C4-C3-C2	2.74	115.04	111.02
6	A	3891	NAG	O5-C5-C4	2.61	117.17	110.83
6	A	3891	NAG	C3-C4-C5	2.48	114.66	110.24
6	A	5041	NAG	O5-C5-C4	-2.32	105.36	109.52

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	5041	NAG	C1

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	3891	NAG	C8-C7-N2-C2
6	A	3891	NAG	O7-C7-N2-C2
6	A	3891	NAG	O5-C5-C6-O6
6	A	3891	NAG	C1-C2-N2-C7
6	A	3891	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	3891	NAG	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	L	213/213 (100%)	-0.29	3 (1%) 75 75	22, 66, 125, 127	0
2	H	217/223 (97%)	-0.39	1 (0%) 91 91	21, 48, 103, 117	0
3	A	375/624 (60%)	-0.24	14 (3%) 41 38	15, 53, 158, 174	0
All	All	805/1060 (75%)	-0.29	18 (2%) 62 60	15, 53, 146, 174	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	603	GLY	4.7
3	A	596	CYS	4.7
2	H	136	SER	4.5
3	A	587	ALA	4.4
3	A	239	THR	3.0
3	A	593	CYS	3.0
3	A	561	TYR	3.0
3	A	601	THR	2.9
3	A	240	CYS	2.8
1	L	127	SER	2.7
3	A	266	THR	2.4
3	A	581	THR	2.4
3	A	613	PRO	2.3
1	L	128	GLY	2.3
3	A	605	THR	2.2
1	L	134	CYS	2.0
3	A	241	PRO	2.0
3	A	252	GLN	2.0

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

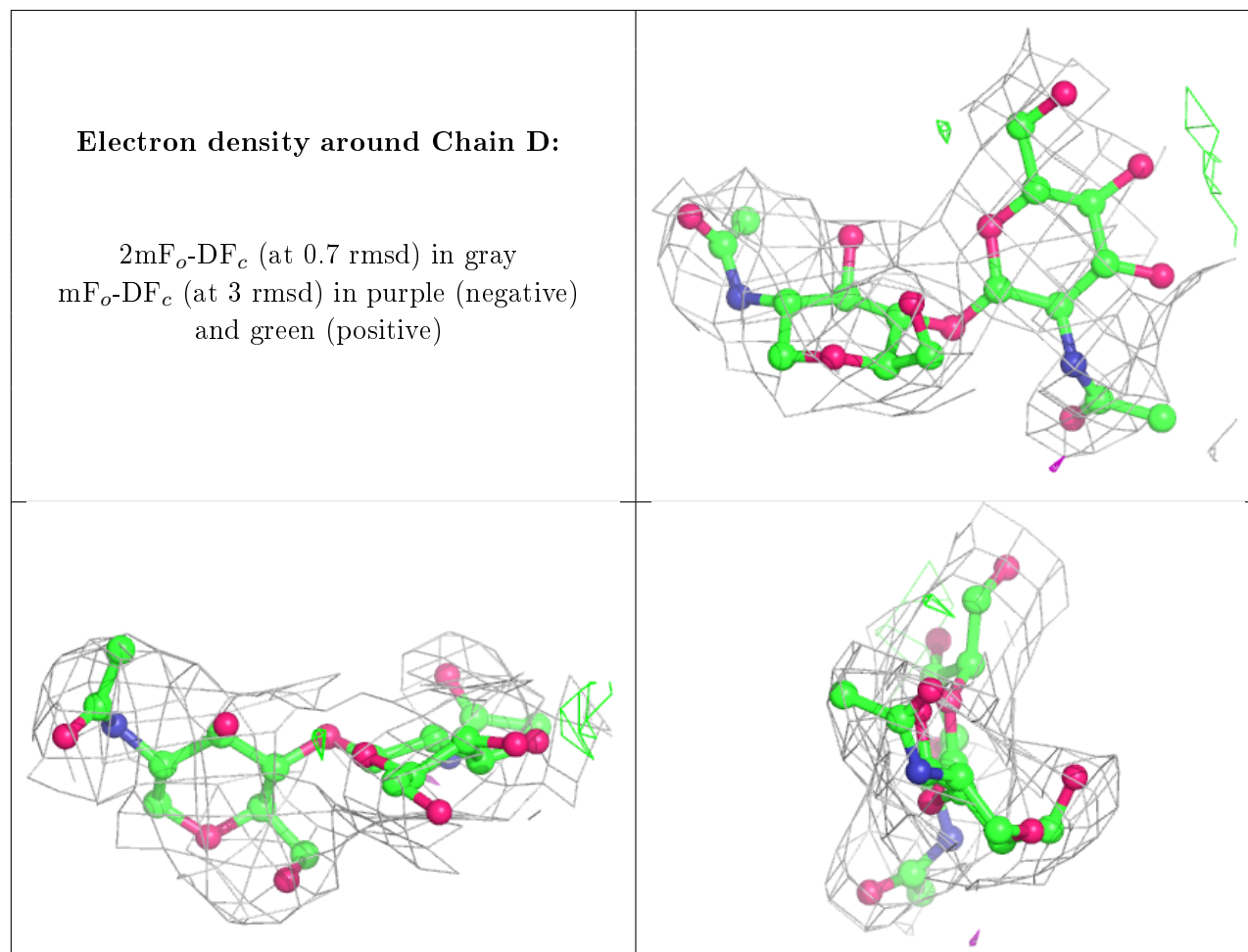
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	C	2	14/15	0.81	0.38	91,93,94,96	0
4	BMA	B	3	11/12	0.85	0.15	70,75,76,77	0
4	NAG	B	2	14/15	0.87	0.18	45,49,57,65	0
5	NAG	D	2	14/15	0.88	0.16	58,61,62,62	0
5	NAG	C	1	14/15	0.91	0.14	78,84,87,88	0
5	NAG	D	1	14/15	0.94	0.14	46,50,51,53	0
4	NAG	B	1	14/15	0.96	0.21	31,35,40,43	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	NAG	A	3891	14/15	0.90	0.14	62,68,71,73	0
6	NAG	A	5041	12/15	0.93	0.14	39,42,45,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.