



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:02 PM GMT

PDB ID : 1IGY
Title : STRUCTURE OF IMMUNOGLOBULIN
Authors : Harris, L.J.; McPherson, A.
Deposited on : 1997-10-09
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

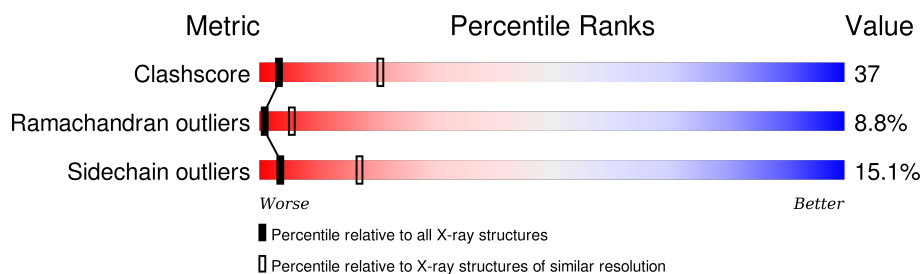
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	213	 38% 49% 12%
1	C	213	 41% 46% 12%
2	B	434	 37% 48% 13% •
2	D	434	 35% 49% 14% •

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
4	FUC	D	476	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12750 atoms, of which 2498 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 IGG1 INTACT ANTIBODY MAB61.1.3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	213	Total	C	H	N	O	S	0	0	0
			2043	1025	393	277	339	9			
1	C	213	Total	C	H	N	O	S	0	0	0
			2043	1025	393	277	339	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	VAL	GLN	CONFLICT	GB 309359
A	?	-	PRO	DELETION	GB 309359
C	7	VAL	GLN	CONFLICT	GB 309359
C	?	-	PRO	DELETION	GB 309359

- Molecule 2 is a protein called IGG1 INTACT ANTIBODY MAB61.1.3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	434	Total	C	H	N	O	S	33	0	0
			4119	2128	753	565	655	18			
2	D	434	Total	C	H	N	O	S	0	0	0
			4119	2128	753	565	655	18			

There are 128 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	3	LYS	GLN	CONFLICT	GB 194362
B	6	GLU	GLN	CONFLICT	GB 194362
B	9	ALA	PRO	CONFLICT	GB 194362
B	12	ALA	GLU	CONFLICT	GB 194362
B	13	ARG	LYS	CONFLICT	GB 194362
B	20	MET	ILE	CONFLICT	GB 194362
B	27	TYR	PHE	CONFLICT	GB 194362
B	28	THR	SER	CONFLICT	GB 194362

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Chain	Residue	Modelled	Actual	Comment	Reference
B	29	PHE	LEU	CONFLICT	GB 194362
B	30	THR	PRO	CONFLICT	GB 194362
B	31	THR	GLY	CONFLICT	GB 194362
B	32	TYR	HIS	CONFLICT	GB 194362
B	33	THR	ASN	CONFLICT	GB 194362
B	35	HIS	ASN	CONFLICT	GB 194362
B	38	LYS	VAL	CONFLICT	GB 194362
B	41	PRO	ASN	CONFLICT	GB 194362
B	43	GLN	LYS	CONFLICT	GB 194362
B	44	GLY	SER	CONFLICT	GB 194362
B	50	TYR	ASN	CONFLICT	GB 194362
B	52	ASN	ASP	CONFLICT	GB 194362
B	53	SER	TYR	CONFLICT	GB 194362
B	54	SER	TYR	CONFLICT	GB 194362
B	55	VAL	GLY	CONFLICT	GB 194362
B	56	TYR	GLY	CONFLICT	GB 194362
B	59	TYR	PHE	CONFLICT	GB 194362
B	61	GLN	PRO	CONFLICT	GB 194362
B	62	ARG	LYS	CONFLICT	GB 194362
B	65	ASP	GLY	CONFLICT	GB 194362
B	71	ARG	VAL	CONFLICT	GB 194362
B	73	ARG	LYS	CONFLICT	GB 194362
B	76	ASN	SER	CONFLICT	GB 194362
B	78	ALA	LEU	CONFLICT	GB 194362
B	79	ASN	TYR	CONFLICT	GB 194362
B	80	ILE	MET	CONFLICT	GB 194362
B	82A	SER	THR	CONFLICT	GB 194362
B	83	THR	GLN	CONFLICT	GB 194362
B	85	ASP	GLU	CONFLICT	GB 194362
B	?	-	ALA	DELETION	GB 194362
B	?	-	ARG	DELETION	GB 194362
B	93	VAL	ARG	CONFLICT	GB 194362
B	95	GLU	ASP	CONFLICT	GB 194362
B	?	-	ASN	DELETION	GB 194362
B	?	-	TYR	DELETION	GB 194362
B	97	GLU	GLY	CONFLICT	GB 194362
B	98	VAL	PHE	CONFLICT	GB 194362
B	101	PRO	THR	CONFLICT	GB 194362
B	108	THR	LEU	CONFLICT	GB 194362
B	113	SER	ALA	CONFLICT	GB 194362
B	199	PRO	THR	CONFLICT	GB 194362
B	200	ARG	TRP	CONFLICT	GB 194362

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Chain	Residue	Modelled	Actual	Comment	Reference
B	263	THR	VAL	CONFLICT	GB 194362
B	265	LEU	THR	CONFLICT	GB 194362
B	268	VAL	LEU	CONFLICT	GB 194362
B	296	ASN	ASP	CONFLICT	GB 194362
B	321	VAL	SER	CONFLICT	GB 194362
B	324	ALA	GLU	CONFLICT	GB 194362
B	363	LYS	ARG	CONFLICT	GB 194362
B	365	ARG	LYS	CONFLICT	GB 194362
B	408	SER	TRP	CONFLICT	GB 194362
B	410	ASP	ASN	CONFLICT	GB 194362
B	415	ALA	PRO	CONFLICT	GB 194362
B	416	PRO	ALA	CONFLICT	GB 194362
B	427	ASP	ASN	CONFLICT	GB 194362
B	430	ASP	ASN	CONFLICT	GB 194362
D	3	LYS	GLN	CONFLICT	GB 194362
D	6	GLU	GLN	CONFLICT	GB 194362
D	9	ALA	PRO	CONFLICT	GB 194362
D	12	ALA	GLU	CONFLICT	GB 194362
D	13	ARG	LYS	CONFLICT	GB 194362
D	20	MET	ILE	CONFLICT	GB 194362
D	27	TYR	PHE	CONFLICT	GB 194362
D	28	THR	SER	CONFLICT	GB 194362
D	29	PHE	LEU	CONFLICT	GB 194362
D	30	THR	PRO	CONFLICT	GB 194362
D	31	THR	GLY	CONFLICT	GB 194362
D	32	TYR	HIS	CONFLICT	GB 194362
D	33	THR	ASN	CONFLICT	GB 194362
D	35	HIS	ASN	CONFLICT	GB 194362
D	38	LYS	VAL	CONFLICT	GB 194362
D	41	PRO	ASN	CONFLICT	GB 194362
D	43	GLN	LYS	CONFLICT	GB 194362
D	44	GLY	SER	CONFLICT	GB 194362
D	50	TYR	ASN	CONFLICT	GB 194362
D	52	ASN	ASP	CONFLICT	GB 194362
D	53	SER	TYR	CONFLICT	GB 194362
D	54	SER	TYR	CONFLICT	GB 194362
D	55	VAL	GLY	CONFLICT	GB 194362
D	56	TYR	GLY	CONFLICT	GB 194362
D	59	TYR	PHE	CONFLICT	GB 194362
D	61	GLN	PRO	CONFLICT	GB 194362
D	62	ARG	LYS	CONFLICT	GB 194362
D	65	ASP	GLY	CONFLICT	GB 194362

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Chain	Residue	Modelled	Actual	Comment	Reference
D	71	ARG	VAL	CONFLICT	GB 194362
D	73	ARG	LYS	CONFLICT	GB 194362
D	76	ASN	SER	CONFLICT	GB 194362
D	78	ALA	LEU	CONFLICT	GB 194362
D	79	ASN	TYR	CONFLICT	GB 194362
D	80	ILE	MET	CONFLICT	GB 194362
D	82A	SER	THR	CONFLICT	GB 194362
D	83	THR	GLN	CONFLICT	GB 194362
D	85	ASP	GLU	CONFLICT	GB 194362
D	?	-	ALA	DELETION	GB 194362
D	?	-	ARG	DELETION	GB 194362
D	93	VAL	ARG	CONFLICT	GB 194362
D	95	GLU	ASP	CONFLICT	GB 194362
D	?	-	ASN	DELETION	GB 194362
D	?	-	TYR	DELETION	GB 194362
D	97	GLU	GLY	CONFLICT	GB 194362
D	98	VAL	PHE	CONFLICT	GB 194362
D	101	PRO	THR	CONFLICT	GB 194362
D	108	THR	LEU	CONFLICT	GB 194362
D	113	SER	ALA	CONFLICT	GB 194362
D	199	PRO	THR	CONFLICT	GB 194362
D	200	ARG	TRP	CONFLICT	GB 194362
D	263	THR	VAL	CONFLICT	GB 194362
D	265	LEU	THR	CONFLICT	GB 194362
D	268	VAL	LEU	CONFLICT	GB 194362
D	296	ASN	ASP	CONFLICT	GB 194362
D	321	VAL	SER	CONFLICT	GB 194362
D	324	ALA	GLU	CONFLICT	GB 194362
D	363	LYS	ARG	CONFLICT	GB 194362
D	365	ARG	LYS	CONFLICT	GB 194362
D	408	SER	TRP	CONFLICT	GB 194362
D	410	ASP	ASN	CONFLICT	GB 194362
D	415	ALA	PRO	CONFLICT	GB 194362
D	416	PRO	ALA	CONFLICT	GB 194362
D	427	ASP	ASN	CONFLICT	GB 194362
D	430	ASP	ASN	CONFLICT	GB 194362

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	9	Total	C	H	N	O	49	0
			213	62	103	4	44		

- Molecule 4 is a polymer of unknown type called SUGAR (9-MER).

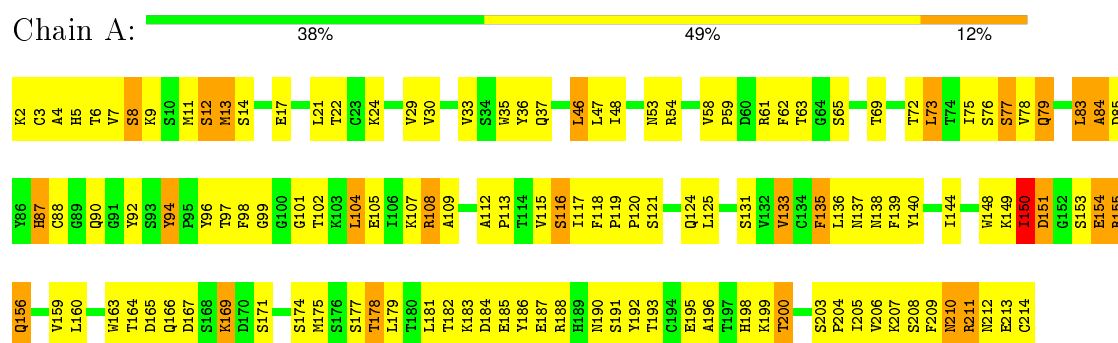
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	9	Total	C	H	N	O	
			213	62	103	4	44	
							28	0

3 Residue-property plots

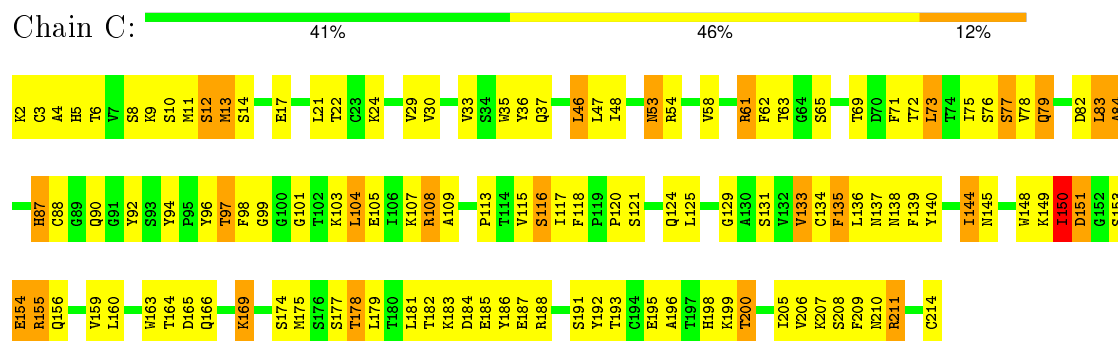
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

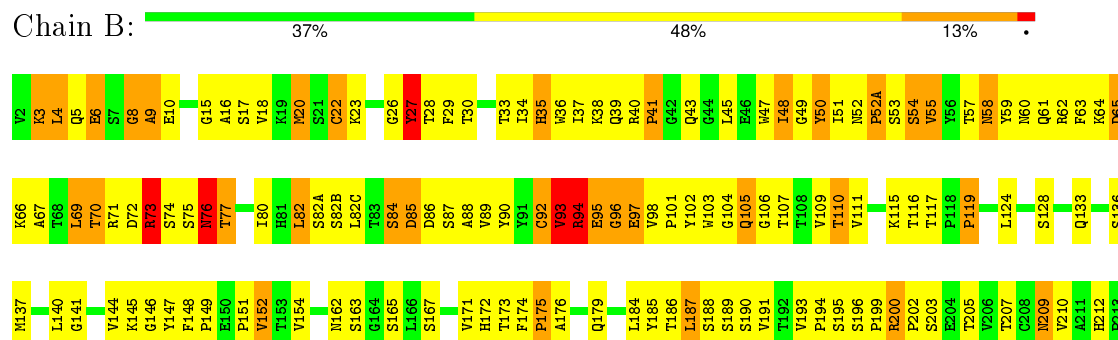
• Molecule 1: IGG1 INTACT ANTIBODY MAB61.1.3

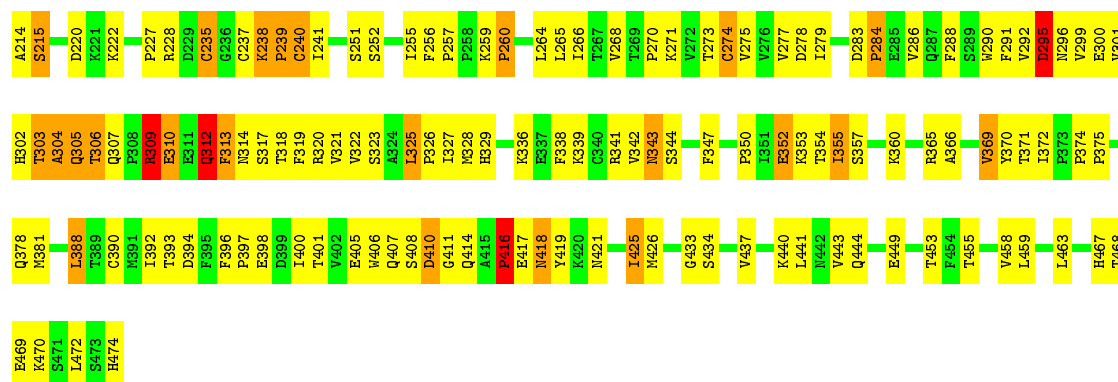


• Molecule 1: IGG1 INTACT ANTIBODY MAB61.1.3

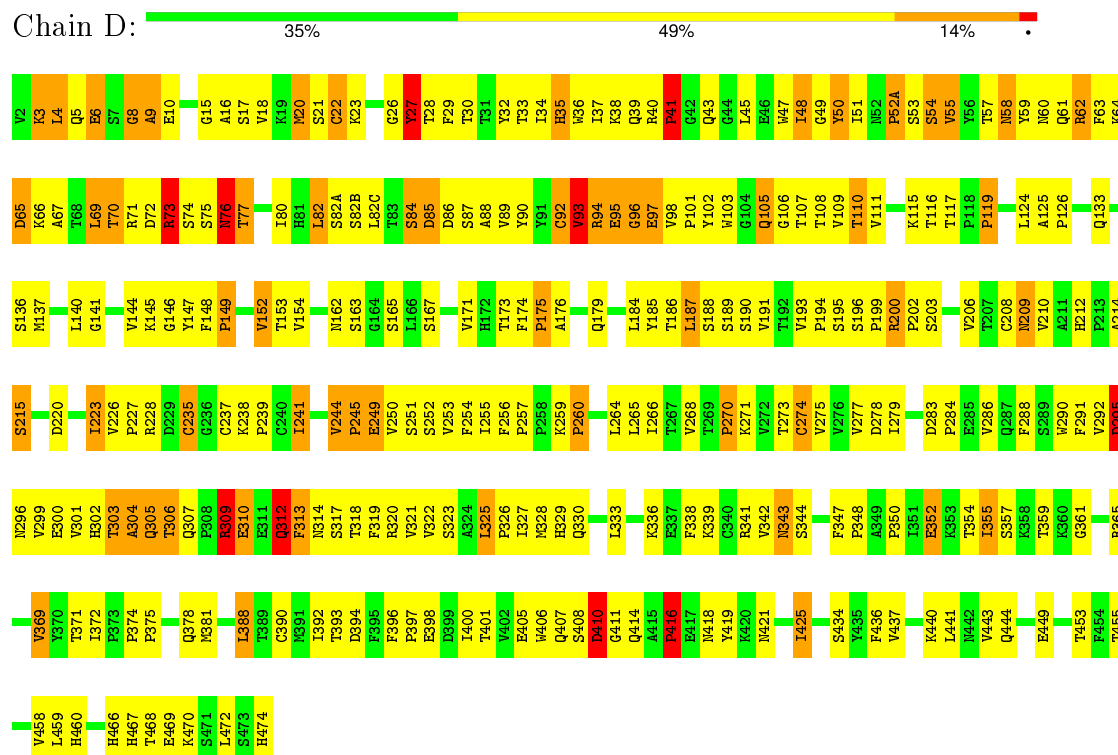


• Molecule 2: IGG1 INTACT ANTIBODY MAB61.1.3





- Molecule 2: IGG1 INTACT ANTIBODY MAB61.1.3



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.65 Å 190.66 Å 73.10 Å 90.00° 109.66° 90.00°	Depositor
Resolution (Å)	20.00 – 3.20	Depositor
% Data completeness (in resolution range)	75.0 (20.00-3.20)	Depositor
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.211 , 0.327	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12750	wwPDB-VP
Average B, all atoms (Å ²)	48.0	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: BMA, NAG, NDG, GAL, FUC, FUL, MAN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.47	0/1687	0.72	0/2288
1	C	0.46	0/1687	0.70	0/2288
2	B	0.47	0/3458	0.76	3/4723 (0.1%)
2	D	0.47	0/3458	0.76	1/4723 (0.0%)
All	All	0.47	0/10290	0.74	4/14022 (0.0%)

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
4	D	1	0

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	96	GLY	N-CA-C	-7.18	95.15	113.10
2	B	96	GLY	N-CA-C	-7.10	95.36	113.10
2	B	240	CYS	CA-CB-SG	-5.53	104.05	114.00
2	B	94	ARG	NE-CZ-NH2	-5.41	117.60	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	D	476	FUC	C1

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1650	393	1570	116	0
1	C	1650	393	1570	114	0
2	B	3366	753	3284	267	2
2	D	3366	753	3284	279	2
3	B	110	103	94	1	0
4	D	110	103	94	2	0
All	All	10252	2498	9896	744	2

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 37.

All (744) 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)
2:D:194:PRO:HG2	2:D:199:PRO:HG3	1.27	1.14
1:C:29:VAL:HG13	1:C:92:TYR:HB2	1.23	1.14
2:B:194:PRO:HG2	2:B:199:PRO:HG3	1.27	1.11
1:A:29:VAL:HG13	1:A:92:TYR:HB2	1.27	1.08
2:B:119:PRO:HB3	2:B:147:TYR:HB3	1.38	1.05
2:D:38:LYS:HE2	2:D:90:TYR:HE1	1.25	1.02
2:D:30:THR:HG22	2:D:73:ARG:HB3	1.42	1.00
2:D:119:PRO:HB3	2:D:147:TYR:HB3	1.40	1.00
2:B:38:LYS:HE2	2:B:90:TYR:HE1	1.25	0.98
1:C:214:CYS:HB3	2:D:235:CYS:HA	1.46	0.97
2:B:291:PHE:HB2	2:B:339:LYS:HB2	1.46	0.96
2:D:291:PHE:HB2	2:D:339:LYS:HB2	1.47	0.95
2:B:30:THR:HG22	2:B:73:ARG:HB3	1.48	0.94
2:B:372:ILE:HD11	2:D:375:PRO:HB3	1.49	0.93
2:B:449:GLU:HA	2:B:474:HIS:HD2	1.35	0.92
2:D:449:GLU:HA	2:D:474:HIS:HD2	1.34	0.91
2:B:40:ARG:HH21	2:B:86:ASP:HA	1.40	0.86
2:B:372:ILE:HG21	2:D:372:ILE:HG21	1.54	0.86
2:B:200:ARG:HH21	2:B:227:PRO:HB3	1.41	0.85
2:B:375:PRO:HB3	2:D:372:ILE:HD11	1.57	0.84
2:D:40:ARG:HH21	2:D:86:ASP:HA	1.40	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:94:ARG:O	2:D:101:PRO:HD2	1.77	0.83
2:D:95:GLU:HG3	2:D:96:GLY:H	1.42	0.83
2:B:95:GLU:HG3	2:B:96:GLY:H	1.45	0.82
2:B:94:ARG:O	2:B:101:PRO:HD2	1.80	0.81
2:B:200:ARG:HH11	2:B:200:ARG:HG2	1.46	0.81
2:D:194:PRO:HG2	2:D:199:PRO:CG	2.10	0.80
2:B:38:LYS:HE2	2:B:90:TYR:CE1	2.15	0.80
2:D:38:LYS:HE2	2:D:90:TYR:CE1	2.15	0.80
2:D:20:MET:SD	2:D:82:LEU:HD11	2.22	0.80
2:B:194:PRO:HG2	2:B:199:PRO:CG	2.10	0.79
2:D:200:ARG:HH22	2:D:227:PRO:HD3	1.46	0.79
2:B:140:LEU:HD11	2:B:200:ARG:HD2	1.64	0.79
2:B:200:ARG:NH2	2:B:227:PRO:HB3	1.97	0.79
1:A:78:VAL:HG12	1:A:79:GLN:H	1.49	0.78
2:B:51:ILE:HD13	2:B:71:ARG:HB2	1.65	0.78
2:D:392:ILE:HD11	2:D:437:VAL:HB	1.64	0.77
2:D:140:LEU:HD11	2:D:200:ARG:HD2	1.66	0.77
2:D:60:ASN:HB3	2:D:63:PHE:CZ	2.19	0.77
2:D:40:ARG:HG2	2:D:88:ALA:HB2	1.67	0.77
2:B:60:ASN:HB3	2:B:63:PHE:CZ	2.20	0.77
1:A:190:ASN:OD1	1:A:210:ASN:HB2	1.85	0.76
2:D:51:ILE:HB	2:D:69:LEU:HD21	1.68	0.76
2:D:33:THR:OG1	2:D:95:GLU:HB3	1.86	0.76
1:A:119:PRO:HG2	2:B:228:ARG:HH22	1.50	0.75
2:D:200:ARG:HH11	2:D:200:ARG:HG2	1.51	0.75
2:B:365:ARG:HH21	2:B:394:ASP:HB2	1.51	0.75
2:B:392:ILE:HD11	2:B:437:VAL:HB	1.69	0.75
2:D:29:PHE:HE1	2:D:34:ILE:HD12	1.52	0.74
2:B:27:TYR:HE2	2:B:94:ARG:HE	1.33	0.74
1:A:115:VAL:HG22	1:A:136:LEU:HG	1.70	0.73
1:A:169:LYS:HD3	1:A:169:LYS:H	1.53	0.73
1:C:117:ILE:HG22	1:C:207:LYS:HD2	1.70	0.73
1:C:169:LYS:HD3	1:C:169:LYS:H	1.52	0.73
2:B:33:THR:OG1	2:B:95:GLU:HB3	1.88	0.73
2:D:84:SER:HA	2:D:111:VAL:HB	1.69	0.73
2:B:259:LYS:HD2	2:B:260:PRO:HD2	1.69	0.73
1:C:78:VAL:HG12	1:C:79:GLN:H	1.53	0.73
1:C:135:PHE:HB3	1:C:137:ASN:HD21	1.54	0.72
2:D:82:LEU:HB3	2:D:82(C):LEU:HD21	1.71	0.72
2:B:82:LEU:HB3	2:B:82(C):LEU:HD21	1.71	0.72
2:B:84:SER:HA	2:B:111:VAL:HB	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:PHE:HB3	1:A:137:ASN:HD21	1.53	0.72
2:B:200:ARG:NH1	2:B:200:ARG:HG2	2.03	0.72
1:A:117:ILE:HG22	1:A:207:LYS:HD2	1.72	0.72
1:C:29:VAL:HG13	1:C:92:TYR:CB	2.13	0.72
1:A:65:SER:HB3	1:A:72:THR:OG1	1.89	0.72
2:D:30:THR:HG22	2:D:73:ARG:CB	2.20	0.72
2:B:292:VAL:HG22	2:B:336:LYS:HD3	1.71	0.72
2:D:365:ARG:HH21	2:D:394:ASP:HB2	1.53	0.72
2:B:29:PHE:HE1	2:B:34:ILE:HD12	1.54	0.71
1:A:148:TRP:HZ2	1:A:177:SER:O	1.74	0.71
2:B:40:ARG:HG2	2:B:88:ALA:HB2	1.71	0.71
2:B:51:ILE:HB	2:B:69:LEU:HD21	1.73	0.71
2:B:128:SER:HB2	2:B:235:CYS:SG	2.31	0.71
2:D:259:LYS:HD2	2:D:260:PRO:HD2	1.71	0.71
2:B:6:GLU:HA	2:B:22:CYS:HA	1.73	0.70
2:D:449:GLU:HA	2:D:474:HIS:CD2	2.24	0.70
2:D:251:SER:HA	2:D:278:ASP:HB2	1.73	0.70
2:B:237:CYS:C	2:B:239:PRO:HD3	2.12	0.70
2:D:51:ILE:HD13	2:D:71:ARG:HB2	1.72	0.70
2:D:309:ARG:HB3	2:D:321:VAL:HG13	1.73	0.69
1:C:148:TRP:HZ2	1:C:177:SER:O	1.74	0.69
2:D:48:ILE:HA	2:D:63:PHE:CZ	2.26	0.69
1:C:46:LEU:HD12	2:D:101:PRO:HB3	1.72	0.69
1:A:87:HIS:HB3	1:A:101:GLY:HA2	1.74	0.69
1:A:29:VAL:HG12	1:A:29:VAL:O	1.93	0.69
2:B:449:GLU:HA	2:B:474:HIS:CD2	2.24	0.69
2:B:20:MET:SD	2:B:82:LEU:HD11	2.32	0.69
2:D:200:ARG:HG2	2:D:200:ARG:NH1	2.08	0.69
2:B:3:LYS:HB3	2:B:3:LYS:NZ	2.07	0.69
1:C:29:VAL:CG1	1:C:92:TYR:HB2	2.13	0.68
2:B:251:SER:HA	2:B:278:ASP:HB2	1.73	0.68
2:B:309:ARG:HB3	2:B:321:VAL:HG13	1.75	0.68
2:D:3:LYS:NZ	2:D:3:LYS:HB3	2.08	0.68
2:B:48:ILE:HA	2:B:63:PHE:CZ	2.28	0.68
2:D:226:VAL:HG23	2:D:227:PRO:HD2	1.75	0.68
2:D:92:CYS:O	2:D:92:CYS:SG	2.51	0.68
2:B:29:PHE:CD2	2:B:76:ASN:HA	2.29	0.68
2:B:92:CYS:O	2:B:92:CYS:SG	2.52	0.68
2:D:27:TYR:HE2	2:D:94:ARG:HE	1.40	0.67
2:B:35:HIS:HE1	2:B:95:GLU:HB2	1.59	0.67
1:C:65:SER:HB3	1:C:72:THR:OG1	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:115:VAL:HG22	1:C:136:LEU:HG	1.74	0.67
2:B:105:GLN:HG3	2:B:106:GLY:H	1.60	0.67
2:D:292:VAL:HG22	2:D:336:LYS:HD3	1.77	0.67
1:A:29:VAL:CG1	1:A:92:TYR:HB2	2.18	0.67
2:B:260:PRO:O	2:B:264:LEU:HG	1.93	0.67
1:C:2:LYS:HG2	1:C:2:LYS:O	1.95	0.67
1:A:2:LYS:O	1:A:2:LYS:HG2	1.95	0.67
1:A:149:LYS:HD3	1:A:153:SER:HA	1.77	0.67
1:C:29:VAL:HG12	1:C:29:VAL:O	1.94	0.67
2:B:279:ILE:HG23	2:B:283:ASP:HB2	1.76	0.66
1:C:87:HIS:HB3	1:C:101:GLY:HA2	1.77	0.66
2:D:6:GLU:HA	2:D:22:CYS:HA	1.78	0.66
2:B:38:LYS:HB3	2:B:90:TYR:CD1	2.31	0.66
2:B:30:THR:HG22	2:B:73:ARG:CB	2.24	0.66
1:A:155:ARG:O	1:A:156:GLN:HB2	1.95	0.65
1:C:149:LYS:HB2	1:C:193:THR:HB	1.79	0.65
2:D:313:PHE:HB2	2:D:318:THR:O	1.96	0.65
2:D:154:VAL:HA	2:D:210:VAL:HG12	1.79	0.64
2:D:239:PRO:HB2	2:D:241:ILE:HG12	1.79	0.64
2:D:279:ILE:HG23	2:D:283:ASP:HB2	1.79	0.64
2:B:154:VAL:HA	2:B:210:VAL:HG12	1.78	0.64
2:D:93:VAL:HG12	2:D:94:ARG:H	1.62	0.64
2:D:292:VAL:O	2:D:295:ASP:HB2	1.95	0.64
2:D:29:PHE:CD2	2:D:76:ASN:HA	2.32	0.64
1:C:155:ARG:O	1:C:156:GLN:HB2	1.96	0.64
1:A:35:TRP:HD1	1:A:48:ILE:HD11	1.63	0.64
2:B:26:GLY:O	2:B:27:TYR:HB3	1.98	0.64
2:D:200:ARG:HB3	2:D:202:PRO:HD3	1.78	0.64
2:D:419:TYR:HA	2:D:440:LYS:O	1.97	0.64
2:D:35:HIS:HE1	2:D:95:GLU:HB2	1.63	0.63
2:D:260:PRO:O	2:D:264:LEU:HG	1.99	0.63
1:A:119:PRO:HG2	2:B:228:ARG:NH2	2.13	0.63
2:D:325:LEU:O	2:D:325:LEU:HD23	1.98	0.63
2:B:419:TYR:HA	2:B:440:LYS:O	1.98	0.62
2:D:4:LEU:HD11	2:D:102:TYR:O	1.99	0.62
2:D:136:SER:O	2:D:194:PRO:HA	1.99	0.62
1:C:164:THR:HG22	1:C:174:SER:H	1.64	0.61
1:A:12:SER:HA	1:A:105:GLU:O	2.00	0.61
2:B:64:LYS:O	2:B:66:LYS:HG2	2.00	0.61
2:D:105:GLN:HG3	2:D:106:GLY:H	1.63	0.61
2:B:325:LEU:HD23	2:B:325:LEU:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:TYR:O	1:A:208:SER:HB2	1.99	0.61
2:D:390:CYS:HB2	2:D:406:TRP:CZ2	2.34	0.61
2:B:20:MET:HG3	2:B:36:TRP:CZ3	2.35	0.61
2:B:306:THR:HG21	2:B:325:LEU:HA	1.83	0.61
2:B:313:PHE:HB2	2:B:318:THR:O	2.00	0.61
2:D:51:ILE:CB	2:D:69:LEU:HD21	2.29	0.61
2:D:193:VAL:HB	2:D:194:PRO:HD2	1.83	0.61
2:B:200:ARG:HB3	2:B:202:PRO:HD3	1.83	0.61
1:C:76:SER:O	1:C:77:SER:HB3	2.00	0.61
1:A:182:THR:HB	1:A:185:GLU:CB	2.31	0.61
2:B:292:VAL:O	2:B:295:ASP:HB2	2.01	0.60
1:A:149:LYS:HB2	1:A:193:THR:HB	1.83	0.60
2:D:22:CYS:O	2:D:22:CYS:SG	2.59	0.60
2:B:369:VAL:HG23	2:B:392:ILE:HG22	1.84	0.60
2:D:38:LYS:HB3	2:D:90:TYR:CD1	2.37	0.60
2:D:406:TRP:O	2:D:407:GLN:HG3	2.02	0.60
2:D:72:ASP:O	2:D:74:SER:N	2.34	0.60
2:D:425:ILE:H	2:D:425:ILE:HD13	1.67	0.60
1:C:12:SER:HA	1:C:105:GLU:O	2.02	0.60
2:B:304:ALA:O	2:B:305:GLN:HG2	2.01	0.60
2:D:147:TYR:O	2:D:185:TYR:HB2	2.02	0.59
2:D:341:ARG:HA	2:D:352:GLU:HB3	1.83	0.59
2:D:306:THR:HG21	2:D:325:LEU:HA	1.83	0.59
2:B:238:LYS:HD2	2:B:238:LYS:O	2.02	0.59
1:A:107:LYS:HG2	1:A:140:TYR:OH	2.01	0.59
2:D:392:ILE:HG12	2:D:437:VAL:O	2.02	0.59
1:C:149:LYS:HD3	1:C:153:SER:HA	1.83	0.59
2:B:4:LEU:HD11	2:B:102:TYR:O	2.03	0.59
2:B:193:VAL:HB	2:B:194:PRO:HD2	1.84	0.59
2:B:390:CYS:HB2	2:B:406:TRP:CZ2	2.37	0.59
1:A:164:THR:HG22	1:A:174:SER:H	1.66	0.59
2:D:10:GLU:O	2:D:109:VAL:HA	2.02	0.59
1:C:135:PHE:CD2	2:D:190:SER:HB3	2.37	0.59
2:D:275:VAL:HG23	2:D:321:VAL:O	2.02	0.59
2:B:406:TRP:O	2:B:407:GLN:HG3	2.02	0.59
2:B:10:GLU:O	2:B:109:VAL:HA	2.03	0.58
2:B:93:VAL:HG12	2:B:94:ARG:H	1.68	0.58
1:C:182:THR:HB	1:C:185:GLU:CB	2.33	0.58
2:B:392:ILE:HG12	2:B:437:VAL:O	2.03	0.58
2:D:93:VAL:HG11	2:D:98:VAL:HG12	1.86	0.58
2:D:264:LEU:HD13	2:D:459:LEU:HB3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:75:SER:O	2:B:77:THR:HG22	2.03	0.58
2:B:341:ARG:HA	2:B:352:GLU:HB3	1.84	0.58
2:D:144:VAL:HG23	2:D:187:LEU:HD13	1.84	0.58
2:D:26:GLY:O	2:D:27:TYR:HB3	2.04	0.58
2:D:425:ILE:N	2:D:425:ILE:HD13	2.18	0.58
1:A:76:SER:O	1:A:77:SER:HB3	2.02	0.58
2:B:338:PHE:O	2:B:354:THR:HA	2.03	0.58
2:D:266:ILE:HA	2:D:329:HIS:CE1	2.38	0.58
2:B:136:SER:O	2:B:194:PRO:HA	2.04	0.58
2:D:17:SER:HB3	2:D:82:LEU:O	2.03	0.58
1:A:183:LYS:O	1:A:186:TYR:HB3	2.04	0.57
2:B:51:ILE:CB	2:B:69:LEU:HD21	2.34	0.57
1:A:206:VAL:HG12	1:A:207:LYS:H	1.69	0.57
1:A:214:CYS:SG	2:B:128:SER:OG	2.50	0.57
2:B:264:LEU:HD13	2:B:459:LEU:HB3	1.87	0.57
2:D:162:ASN:HB3	2:D:165:SER:HG	1.69	0.57
2:B:200:ARG:CG	2:B:200:ARG:HH11	2.16	0.57
2:D:87:SER:OG	2:D:110:THR:HA	2.04	0.57
2:B:425:ILE:HD13	2:B:425:ILE:H	1.69	0.57
2:D:338:PHE:O	2:D:354:THR:HA	2.04	0.56
2:D:270:PRO:HG2	2:D:327:ILE:O	2.05	0.56
1:C:192:TYR:O	1:C:208:SER:HB2	2.06	0.56
1:C:24:LYS:HA	1:C:69:THR:O	2.06	0.56
1:A:148:TRP:CZ2	1:A:177:SER:O	2.58	0.56
1:C:163:TRP:O	2:D:175:PRO:HD2	2.05	0.56
2:D:146:GLY:HA2	2:D:184:LEU:HD22	1.87	0.56
1:A:98:PHE:CD2	2:B:45:LEU:HB3	2.41	0.56
1:A:135:PHE:HD1	1:A:135:PHE:H	1.52	0.56
2:B:425:ILE:HD13	2:B:425:ILE:N	2.20	0.56
2:B:72:ASP:O	2:B:74:SER:N	2.39	0.56
2:B:370:TYR:CZ	2:D:378:GLN:HB2	2.41	0.56
2:D:257:PRO:HG3	2:D:355:ILE:CG1	2.34	0.56
1:A:135:PHE:N	1:A:135:PHE:CD1	2.73	0.56
2:B:147:TYR:O	2:B:185:TYR:HB2	2.06	0.56
2:D:288:PHE:HA	2:D:342:VAL:HG12	1.88	0.56
2:D:388:LEU:HD12	2:D:388:LEU:H	1.71	0.56
2:B:93:VAL:HG11	2:B:98:VAL:HG12	1.88	0.55
2:B:171:VAL:HG13	2:B:190:SER:O	2.05	0.55
2:B:309:ARG:HA	2:B:321:VAL:HA	1.89	0.55
2:B:117:THR:O	2:B:147:TYR:HA	2.06	0.55
1:A:213:GLU:O	1:A:214:CYS:HB3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:ASP:O	1:A:188:ARG:HG3	2.07	0.55
2:D:103:TRP:CD1	2:D:103:TRP:N	2.74	0.55
2:D:33:THR:CG2	2:D:52(A):PRO:HD3	2.37	0.55
2:B:103:TRP:N	2:B:103:TRP:CD1	2.74	0.55
1:C:78:VAL:HG12	1:C:79:GLN:N	2.20	0.55
2:D:401:THR:HG22	2:D:459:LEU:HB2	1.89	0.55
1:A:24:LYS:HA	1:A:69:THR:O	2.06	0.55
2:B:57:THR:HG22	2:B:59:TYR:CE1	2.42	0.55
2:B:291:PHE:HD2	2:B:296:ASN:HA	1.71	0.55
1:A:186:TYR:HA	1:A:192:TYR:OH	2.07	0.55
1:C:183:LYS:O	1:C:186:TYR:HB3	2.06	0.55
2:B:34:ILE:HA	2:B:94:ARG:HA	1.89	0.55
2:B:398:GLU:O	2:B:400:ILE:HG22	2.06	0.55
2:B:48:ILE:HG13	2:B:49:GLY:H	1.72	0.55
1:A:115:VAL:HG12	1:A:116:SER:N	2.22	0.55
1:A:105:GLU:HG3	1:A:166:GLN:NE2	2.21	0.54
2:D:75:SER:O	2:D:77:THR:HG22	2.07	0.54
2:D:20:MET:HG3	2:D:36:TRP:CZ3	2.42	0.54
2:D:200:ARG:NH2	2:D:227:PRO:HD3	2.21	0.54
2:B:275:VAL:HG23	2:B:321:VAL:O	2.08	0.54
1:C:193:THR:HA	1:C:208:SER:HB3	1.89	0.54
2:D:214:ALA:O	2:D:215:SER:HB2	2.08	0.54
2:B:214:ALA:O	2:B:215:SER:HB2	2.07	0.54
2:B:119:PRO:CB	2:B:147:TYR:HB3	2.24	0.54
2:D:51:ILE:CA	2:D:69:LEU:HD21	2.38	0.54
2:D:309:ARG:HA	2:D:321:VAL:HA	1.90	0.54
2:B:141:GLY:HA2	2:B:189:SER:O	2.08	0.54
2:B:29:PHE:CD2	2:B:73:ARG:HA	2.43	0.54
2:B:290:TRP:CG	2:B:325:LEU:HD13	2.43	0.54
1:A:214:CYS:HB3	2:B:235:CYS:HA	1.89	0.54
1:C:105:GLU:HG3	1:C:166:GLN:NE2	2.23	0.54
2:B:257:PRO:HG3	2:B:355:ILE:CG1	2.38	0.54
1:C:115:VAL:HG12	1:C:116:SER:N	2.23	0.53
1:A:206:VAL:HG12	1:A:207:LYS:N	2.23	0.53
1:C:205:ILE:HD12	1:C:205:ILE:N	2.23	0.53
1:C:35:TRP:HD1	1:C:48:ILE:HD11	1.71	0.53
2:B:60:ASN:HB3	2:B:63:PHE:HZ	1.72	0.53
1:A:46:LEU:HD12	2:B:101:PRO:HB3	1.90	0.53
2:D:174:PHE:HD2	2:D:188:SER:HG	1.55	0.53
2:D:271:LYS:HA	2:D:326:PRO:HA	1.90	0.53
1:C:120:PRO:HB2	1:C:125:LEU:HD21	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:407:GLN:HA	2:B:416:PRO:HD3	1.89	0.53
2:D:265:LEU:HD13	2:D:268:VAL:CG2	2.38	0.53
2:D:468:THR:HG22	2:D:469:GLU:N	2.24	0.53
2:D:291:PHE:HD2	2:D:296:ASN:HA	1.73	0.53
2:B:3:LYS:HB3	2:B:3:LYS:HZ2	1.71	0.53
1:C:62:PHE:HE1	1:C:75:ILE:HD13	1.74	0.53
2:D:117:THR:O	2:D:147:TYR:HA	2.08	0.53
2:B:51:ILE:CA	2:B:69:LEU:HD21	2.38	0.53
2:D:394:ASP:HA	2:D:434:SER:HB2	1.90	0.53
1:A:120:PRO:HB2	1:A:125:LEU:HD21	1.91	0.53
2:B:66:LYS:HE3	2:B:82(B):SER:HG	1.74	0.53
1:A:184:ASP:HA	1:A:187:GLU:HB2	1.90	0.53
2:B:468:THR:HG22	2:B:469:GLU:N	2.23	0.53
2:B:146:GLY:HA2	2:B:184:LEU:HD22	1.90	0.53
1:A:182:THR:HB	1:A:185:GLU:HB3	1.91	0.53
2:D:304:ALA:O	2:D:305:GLN:HG2	2.08	0.53
2:B:176:ALA:HA	2:B:187:LEU:HB3	1.90	0.53
1:C:206:VAL:HG12	1:C:207:LYS:N	2.24	0.53
2:D:400:ILE:HD11	2:D:458:VAL:CG2	2.39	0.53
1:C:206:VAL:HG12	1:C:207:LYS:H	1.74	0.53
2:D:171:VAL:HG13	2:D:190:SER:O	2.08	0.53
1:C:184:ASP:HA	1:C:187:GLU:HB2	1.90	0.53
2:B:271:LYS:HA	2:B:326:PRO:HA	1.90	0.53
2:B:371:THR:HB	2:B:472:LEU:HG	1.91	0.53
2:B:87:SER:OG	2:B:110:THR:HA	2.09	0.52
1:A:151:ASP:HA	1:A:191:SER:O	2.09	0.52
2:B:288:PHE:HA	2:B:342:VAL:HG12	1.91	0.52
2:D:34:ILE:HG12	2:D:93:VAL:O	2.09	0.52
2:B:38:LYS:NZ	2:B:40:ARG:NH2	2.57	0.52
2:B:154:VAL:HG22	2:B:210:VAL:HG12	1.91	0.52
1:C:182:THR:HB	1:C:185:GLU:HB3	1.92	0.52
1:A:83:LEU:O	1:A:84:ALA:HB2	2.09	0.52
1:C:135:PHE:HD1	1:C:135:PHE:H	1.56	0.52
1:C:186:TYR:HA	1:C:192:TYR:OH	2.09	0.52
2:D:119:PRO:CB	2:D:147:TYR:HB3	2.26	0.52
1:A:62:PHE:HE1	1:A:75:ILE:HD13	1.74	0.52
2:D:141:GLY:HA2	2:D:189:SER:O	2.10	0.52
1:C:98:PHE:CD2	2:D:45:LEU:HB3	2.45	0.52
2:B:375:PRO:HB3	2:D:372:ILE:CD1	2.35	0.52
1:A:135:PHE:CD2	2:B:190:SER:HB3	2.45	0.52
2:B:266:ILE:HA	2:B:329:HIS:CE1	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:ARG:O	1:C:109:ALA:HB3	2.10	0.52
1:C:113:PRO:HA	1:C:139:PHE:HB3	1.92	0.52
2:B:17:SER:HB3	2:B:82:LEU:O	2.10	0.52
1:A:87:HIS:HB3	1:A:101:GLY:CA	2.40	0.52
1:C:148:TRP:CZ2	1:C:177:SER:O	2.61	0.52
1:C:151:ASP:HA	1:C:191:SER:O	2.10	0.52
1:A:195:GLU:HG2	1:A:196:ALA:N	2.25	0.52
2:D:60:ASN:HB3	2:D:63:PHE:HZ	1.70	0.51
2:B:48:ILE:CG1	2:B:49:GLY:H	2.22	0.51
1:C:135:PHE:N	1:C:135:PHE:CD1	2.77	0.51
1:C:90:GLN:NE2	1:C:96:TYR:HD1	2.08	0.51
2:D:57:THR:HG22	2:D:59:TYR:CE1	2.45	0.51
2:D:38:LYS:HE3	2:D:48:ILE:HG21	1.91	0.51
2:B:33:THR:CG2	2:B:52(A):PRO:HD3	2.40	0.51
2:B:144:VAL:HG23	2:B:187:LEU:HD13	1.92	0.51
1:A:178:THR:HG22	1:A:179:LEU:H	1.74	0.51
2:D:66:LYS:HE3	2:D:82(B):SER:HG	1.75	0.51
2:D:95:GLU:CG	2:D:96:GLY:H	2.18	0.51
1:C:135:PHE:C	1:C:136:LEU:HD12	2.31	0.51
2:D:64:LYS:O	2:D:66:LYS:HG2	2.09	0.51
2:B:162:ASN:HB3	2:B:165:SER:HG	1.74	0.51
1:C:83:LEU:O	1:C:84:ALA:HB2	2.10	0.51
1:C:94:TYR:HD1	1:C:94:TYR:H	1.59	0.51
2:D:20:MET:HE2	2:D:90:TYR:HB2	1.93	0.51
2:D:34:ILE:HA	2:D:94:ARG:HA	1.93	0.51
2:B:38:LYS:HZ2	2:B:40:ARG:HH22	1.57	0.51
2:D:200:ARG:CG	2:D:200:ARG:HH11	2.21	0.51
2:D:470:LYS:NZ	2:D:470:LYS:HB3	2.25	0.51
2:D:38:LYS:NZ	2:D:40:ARG:NH2	2.59	0.51
2:D:365:ARG:NH2	2:D:394:ASP:HB2	2.25	0.51
1:C:124:GLN:NE2	1:C:131:SER:H	2.09	0.51
2:B:394:ASP:HA	2:B:434:SER:HB2	1.92	0.51
1:A:78:VAL:HG12	1:A:79:GLN:N	2.20	0.51
2:B:401:THR:HG22	2:B:459:LEU:HB2	1.93	0.51
1:C:22:THR:HG22	1:C:72:THR:HG22	1.93	0.51
1:A:113:PRO:HA	1:A:139:PHE:HB3	1.92	0.51
2:D:37:ILE:HG12	2:D:47:TRP:HA	1.93	0.50
1:C:169:LYS:HD3	1:C:169:LYS:N	2.23	0.50
2:B:470:LYS:HB3	2:B:470:LYS:NZ	2.25	0.50
2:B:205:THR:HG21	2:B:222:LYS:HE3	1.93	0.50
2:B:37:ILE:HG12	2:B:47:TRP:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:290:TRP:CG	2:D:325:LEU:HD13	2.47	0.50
2:D:290:TRP:O	2:D:300:GLU:HA	2.11	0.50
2:D:407:GLN:HA	2:D:416:PRO:HD3	1.93	0.50
2:D:355:ILE:O	2:D:355:ILE:HG23	2.12	0.50
2:D:29:PHE:CE1	2:D:34:ILE:HD12	2.41	0.50
2:B:38:LYS:HE3	2:B:48:ILE:HG21	1.91	0.50
1:A:169:LYS:N	1:A:169:LYS:HD3	2.24	0.50
1:A:124:GLN:NE2	1:A:131:SER:H	2.08	0.50
1:A:29:VAL:HG13	1:A:92:TYR:CB	2.18	0.50
2:D:299:VAL:O	2:D:300:GLU:HB3	2.12	0.50
1:A:87:HIS:N	1:A:87:HIS:ND1	2.59	0.50
1:A:192:TYR:HB2	1:A:209:PHE:CE1	2.47	0.50
2:B:406:TRP:HA	2:B:455:THR:O	2.11	0.50
2:D:48:ILE:CG1	2:D:49:GLY:H	2.25	0.50
2:D:369:VAL:HG23	2:D:392:ILE:HG22	1.92	0.50
1:C:36:TYR:OH	2:D:98:VAL:HB	2.10	0.50
1:A:94:TYR:HD1	1:A:94:TYR:H	1.60	0.50
2:B:270:PRO:HG2	2:B:327:ILE:O	2.12	0.50
2:B:290:TRP:O	2:B:300:GLU:HA	2.12	0.50
2:D:265:LEU:HD13	2:D:268:VAL:HG23	1.93	0.50
2:D:371:THR:HB	2:D:472:LEU:HG	1.92	0.50
2:D:29:PHE:CD2	2:D:73:ARG:HA	2.47	0.49
2:B:90:TYR:HE2	2:B:109:VAL:HG21	1.77	0.49
2:D:369:VAL:O	2:D:369:VAL:HG13	2.12	0.49
2:D:257:PRO:HG3	2:D:355:ILE:HG12	1.94	0.49
1:A:163:TRP:CE3	1:A:175:MET:HG3	2.47	0.49
2:B:372:ILE:CD1	2:D:375:PRO:HB3	2.33	0.49
1:A:193:THR:HA	1:A:208:SER:HB3	1.94	0.49
2:B:154:VAL:HG22	2:B:210:VAL:CG1	2.42	0.49
2:B:174:PHE:HD2	2:B:188:SER:HG	1.59	0.49
1:C:178:THR:HG22	1:C:179:LEU:H	1.77	0.49
2:B:145:LYS:HG3	2:B:186:THR:HB	1.93	0.49
2:D:136:SER:HA	2:D:195:SER:OG	2.12	0.49
2:D:90:TYR:HE2	2:D:109:VAL:HG21	1.76	0.49
2:B:238:LYS:HB3	2:B:238:LYS:NZ	2.27	0.49
2:D:176:ALA:HA	2:D:187:LEU:HB3	1.93	0.49
1:A:163:TRP:O	2:B:175:PRO:HD2	2.12	0.49
1:C:107:LYS:HG2	1:C:140:TYR:OH	2.12	0.49
2:B:299:VAL:O	2:B:300:GLU:HB3	2.13	0.49
1:C:87:HIS:HB3	1:C:101:GLY:CA	2.40	0.49
1:C:136:LEU:HD12	1:C:136:LEU:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:LEU:O	1:A:183:LYS:HD2	2.13	0.49
2:B:179:GLN:HA	2:B:179:GLN:OE1	2.13	0.49
1:A:205:ILE:N	1:A:205:ILE:HD12	2.28	0.49
1:A:22:THR:HG22	1:A:72:THR:HG22	1.93	0.49
1:A:33:VAL:HG11	1:A:88:CYS:HB2	1.94	0.49
1:A:150:ILE:HB	1:A:154:GLU:HG2	1.93	0.49
2:B:365:ARG:NH2	2:B:394:ASP:HB2	2.23	0.49
2:B:309:ARG:NH1	2:B:310:GLU:HB2	2.28	0.49
2:B:355:ILE:O	2:B:355:ILE:HG23	2.13	0.49
1:A:108:ARG:O	1:A:109:ALA:HB3	2.12	0.49
1:C:199:LYS:HD3	1:C:200:THR:N	2.28	0.49
1:A:212:ASN:O	1:A:214:CYS:N	2.46	0.49
2:B:162:ASN:HB3	2:B:165:SER:OG	2.13	0.49
1:C:192:TYR:HB2	1:C:209:PHE:CE1	2.48	0.48
2:D:209:ASN:HB3	2:D:220:ASP:OD1	2.12	0.48
2:D:40:ARG:HB3	2:D:41:PRO:HD2	1.95	0.48
2:D:48:ILE:HG13	2:D:49:GLY:H	1.77	0.48
1:C:6:THR:HG21	1:C:87:HIS:HA	1.95	0.48
1:C:62:PHE:HD1	1:C:75:ILE:HG12	1.78	0.48
2:D:179:GLN:HA	2:D:179:GLN:OE1	2.13	0.48
1:C:37:GLN:HB2	1:C:47:LEU:HD22	1.94	0.48
2:D:41:PRO:O	2:D:43:GLN:HG2	2.13	0.48
2:B:238:LYS:N	2:B:239:PRO:HD3	2.28	0.48
1:A:150:ILE:HD12	1:A:156:GLN:NE2	2.28	0.48
1:C:87:HIS:ND1	1:C:87:HIS:N	2.61	0.48
1:C:184:ASP:O	1:C:188:ARG:HG3	2.12	0.48
2:D:303:THR:O	2:D:304:ALA:HB2	2.14	0.48
1:A:199:LYS:HD3	1:A:200:THR:N	2.28	0.48
2:B:48:ILE:HG13	2:B:49:GLY:N	2.28	0.48
2:B:400:ILE:HD11	2:B:458:VAL:CG2	2.43	0.48
2:D:162:ASN:HB3	2:D:165:SER:OG	2.12	0.48
1:C:4:ALA:O	1:C:99:GLY:HA2	2.13	0.48
2:D:444:GLN:NE2	2:D:444:GLN:H	2.11	0.48
2:B:444:GLN:NE2	2:B:444:GLN:H	2.11	0.48
1:A:11:MET:O	1:A:104:LEU:HD23	2.13	0.48
1:C:6:THR:HG23	1:C:88:CYS:SG	2.53	0.48
1:A:62:PHE:HD1	1:A:75:ILE:HG12	1.79	0.48
2:B:209:ASN:HB3	2:B:220:ASP:OD1	2.14	0.48
2:D:145:LYS:HG3	2:D:186:THR:HB	1.94	0.48
2:B:40:ARG:HB3	2:B:41:PRO:HD2	1.96	0.48
1:A:33:VAL:CG1	1:A:88:CYS:HB2	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:406:TRP:HA	2:D:455:THR:O	2.13	0.48
2:D:371:THR:HB	2:D:472:LEU:CG	2.44	0.48
2:D:347:PHE:HA	2:D:348:PRO:HD3	1.70	0.48
2:B:388:LEU:HD12	2:B:388:LEU:H	1.78	0.48
1:C:54:ARG:HD2	1:C:58:VAL:HG12	1.96	0.48
2:D:343:ASN:ND2	2:D:350:PRO:HB3	2.28	0.48
2:B:406:TRP:CD1	2:B:419:TYR:HB2	2.49	0.48
2:D:37:ILE:HG22	2:D:38:LYS:N	2.29	0.48
2:D:39:GLN:O	2:D:88:ALA:HB1	2.13	0.48
2:B:290:TRP:HA	2:B:339:LYS:O	2.14	0.48
2:B:200:ARG:HH22	2:B:227:PRO:HD3	1.78	0.48
2:D:51:ILE:HD12	2:D:69:LEU:O	2.13	0.48
2:B:95:GLU:CG	2:B:96:GLY:H	2.23	0.48
2:B:371:THR:HB	2:B:472:LEU:CG	2.44	0.47
2:B:6:GLU:OE1	2:B:104:GLY:HA3	2.14	0.47
2:B:265:LEU:HD13	2:B:268:VAL:CG2	2.43	0.47
2:D:256:PHE:HA	2:D:257:PRO:HD3	1.77	0.47
2:B:115:LYS:HD2	2:B:116:THR:N	2.29	0.47
2:B:116:THR:HA	2:B:148:PHE:O	2.14	0.47
1:A:90:GLN:NE2	1:A:96:TYR:HD1	2.12	0.47
2:D:48:ILE:HG13	2:D:49:GLY:N	2.30	0.47
2:D:50:TYR:CE1	2:D:51:ILE:O	2.68	0.47
2:D:3:LYS:HB3	2:D:3:LYS:HZ3	1.78	0.47
1:C:33:VAL:HG11	1:C:88:CYS:HB2	1.95	0.47
2:D:27:TYR:N	2:D:27:TYR:CD1	2.82	0.47
2:D:51:ILE:HB	2:D:69:LEU:CD2	2.42	0.47
2:D:406:TRP:CD1	2:D:419:TYR:HB2	2.49	0.47
2:D:105:GLN:HG3	2:D:106:GLY:N	2.29	0.47
2:B:89:VAL:HA	2:B:107:THR:O	2.14	0.47
2:D:38:LYS:HZ3	2:D:40:ARG:NH2	2.12	0.47
2:D:115:LYS:HD2	2:D:116:THR:N	2.30	0.47
2:D:252:SER:O	2:D:277:VAL:HG12	2.15	0.47
1:C:35:TRP:CE2	1:C:73:LEU:HB2	2.50	0.47
4:D:480:NAG:O3	4:D:481:GAL:C1	2.62	0.47
2:D:388:LEU:N	2:D:388:LEU:HD12	2.29	0.47
1:C:195:GLU:HG2	1:C:196:ALA:N	2.29	0.47
1:A:63:THR:O	1:A:73:LEU:HA	2.15	0.47
2:B:37:ILE:HG22	2:B:38:LYS:N	2.29	0.47
1:C:125:LEU:O	1:C:183:LYS:HD2	2.14	0.47
2:D:425:ILE:HG12	2:D:436:PHE:CE1	2.50	0.47
2:D:144:VAL:O	2:D:144:VAL:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:63:THR:O	1:C:73:LEU:HA	2.13	0.47
1:A:6:THR:HG21	1:A:87:HIS:HA	1.96	0.46
1:A:182:THR:HB	1:A:185:GLU:HB2	1.95	0.46
2:B:329:HIS:CD2	2:B:329:HIS:H	2.33	0.46
1:C:133:VAL:HG21	2:D:124:LEU:HD13	1.97	0.46
2:D:89:VAL:HA	2:D:107:THR:O	2.15	0.46
3:B:480:NAG:O3	3:B:481:GAL:C1	2.62	0.46
2:D:53:SER:OG	2:D:55:VAL:HG23	2.15	0.46
2:D:398:GLU:O	2:D:400:ILE:HG22	2.15	0.46
1:C:90:GLN:HE22	1:C:96:TYR:HD1	1.64	0.46
2:D:344:SER:HB3	2:D:347:PHE:CD1	2.50	0.46
2:D:309:ARG:NH1	2:D:310:GLU:HB2	2.30	0.46
2:D:241:ILE:H	2:D:241:ILE:HD13	1.81	0.46
1:A:185:GLU:HA	1:A:188:ARG:CZ	2.45	0.46
2:B:256:PHE:HB2	2:B:273:THR:CG2	2.45	0.46
2:D:322:VAL:HG12	2:D:323:SER:N	2.31	0.46
2:D:33:THR:HG23	2:D:52(A):PRO:HD3	1.96	0.46
2:D:126:PRO:O	2:D:228:ARG:HG2	2.15	0.46
1:C:185:GLU:HA	1:C:188:ARG:CZ	2.46	0.46
2:D:329:HIS:H	2:D:329:HIS:CD2	2.34	0.46
2:B:343:ASN:ND2	2:B:350:PRO:HB3	2.30	0.46
2:D:8:GLY:O	2:D:9:ALA:HB2	2.16	0.46
2:B:369:VAL:HA	2:B:392:ILE:HA	1.98	0.46
1:C:210:ASN:O	1:C:211:ARG:CB	2.63	0.46
2:B:27:TYR:N	2:B:27:TYR:CD1	2.84	0.46
2:B:27:TYR:HE2	2:B:94:ARG:NE	2.09	0.46
2:D:125:ALA:O	2:D:228:ARG:HD3	2.16	0.46
2:B:303:THR:O	2:B:304:ALA:HB2	2.16	0.46
2:B:29:PHE:CE1	2:B:34:ILE:HD12	2.42	0.46
1:C:149:LYS:HA	1:C:154:GLU:O	2.16	0.46
1:C:182:THR:HB	1:C:185:GLU:HB2	1.98	0.46
2:B:265:LEU:HD13	2:B:268:VAL:HG23	1.98	0.46
1:C:33:VAL:CG1	1:C:88:CYS:HB2	2.46	0.46
2:D:154:VAL:HG22	2:D:210:VAL:HG12	1.97	0.46
1:A:136:LEU:HD12	1:A:136:LEU:N	2.31	0.46
2:D:200:ARG:HH21	2:D:227:PRO:HB3	1.81	0.46
2:D:50:TYR:N	2:D:69:LEU:HD13	2.31	0.46
2:D:17:SER:OG	2:D:82(A):SER:HA	2.15	0.46
2:D:40:ARG:CG	2:D:88:ALA:HB2	2.43	0.45
2:B:105:GLN:HG3	2:B:106:GLY:N	2.28	0.45
1:C:191:SER:HA	1:C:209:PHE:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:38:LYS:HB3	2:D:90:TYR:CE1	2.51	0.45
2:B:84:SER:HA	2:B:111:VAL:CB	2.45	0.45
1:A:124:GLN:HE22	1:A:131:SER:H	1.63	0.45
1:C:159:VAL:C	1:C:160:LEU:HD12	2.37	0.45
2:D:58:ASN:OD1	2:D:58:ASN:N	2.49	0.45
1:A:214:CYS:SG	2:B:128:SER:CB	3.04	0.45
1:C:90:GLN:OE1	1:C:97:THR:N	2.50	0.45
1:A:133:VAL:HG21	2:B:124:LEU:HD13	1.98	0.45
2:D:57:THR:HG22	2:D:57:THR:O	2.16	0.45
2:D:244:VAL:HG12	2:D:245:PRO:HD2	1.98	0.45
2:B:8:GLY:O	2:B:9:ALA:HB2	2.16	0.45
2:B:38:LYS:HB3	2:B:90:TYR:CE1	2.51	0.45
1:C:150:ILE:HB	1:C:154:GLU:HG2	1.98	0.45
1:A:54:ARG:HD2	1:A:58:VAL:HG12	1.99	0.45
2:D:27:TYR:N	2:D:27:TYR:HD1	2.14	0.45
2:B:39:GLN:O	2:B:88:ALA:HB1	2.17	0.45
1:A:98:PHE:CD2	2:B:45:LEU:CB	2.99	0.45
2:B:264:LEU:CD1	2:B:459:LEU:HB3	2.46	0.45
2:B:252:SER:O	2:B:277:VAL:HG12	2.15	0.45
1:A:9:LYS:HB2	1:A:9:LYS:HE3	1.74	0.45
1:C:98:PHE:CZ	2:D:37:ILE:HD13	2.52	0.45
1:A:149:LYS:HA	1:A:154:GLU:O	2.16	0.45
2:B:388:LEU:N	2:B:388:LEU:HD12	2.32	0.45
2:B:274:CYS:HB3	2:B:290:TRP:CH2	2.52	0.45
2:B:184:LEU:HA	2:B:184:LEU:HD23	1.78	0.45
2:B:274:CYS:HB3	2:B:290:TRP:CZ2	2.52	0.44
1:A:179:LEU:HD23	1:A:179:LEU:C	2.37	0.44
2:B:136:SER:HA	2:B:195:SER:OG	2.16	0.44
2:B:20:MET:HE2	2:B:90:TYR:HB2	1.99	0.44
1:A:6:THR:HG23	1:A:88:CYS:SG	2.57	0.44
1:C:11:MET:O	1:C:104:LEU:HD23	2.16	0.44
2:D:15:GLY:N	2:D:82(C):LEU:O	2.51	0.44
2:D:93:VAL:HG12	2:D:94:ARG:N	2.31	0.44
2:B:4:LEU:HD22	2:B:92:CYS:SG	2.56	0.44
1:C:62:PHE:CE1	1:C:75:ILE:HD13	2.52	0.44
1:A:62:PHE:CE1	1:A:75:ILE:HD13	2.52	0.44
2:D:59:TYR:CE2	2:D:67:ALA:O	2.70	0.44
2:D:196:SER:N	2:D:199:PRO:HD2	2.33	0.44
2:B:34:ILE:HG12	2:B:94:ARG:CB	2.48	0.44
2:D:33:THR:HG22	2:D:52(A):PRO:HD3	2.00	0.44
2:D:313:PHE:HB3	2:D:314:ASN:H	1.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:313:PHE:CE2	2:D:320:ARG:HD3	2.52	0.44
2:D:40:ARG:NE	2:D:85:ASP:O	2.51	0.44
1:A:98:PHE:CZ	2:B:37:ILE:HD13	2.52	0.44
2:B:256:PHE:HA	2:B:257:PRO:HD3	1.78	0.44
2:D:200:ARG:HH22	2:D:227:PRO:CD	2.23	0.44
1:C:179:LEU:HD23	1:C:179:LEU:C	2.37	0.44
2:B:344:SER:HB3	2:B:347:PHE:CD1	2.53	0.44
2:B:58:ASN:OD1	2:B:58:ASN:N	2.50	0.44
2:B:171:VAL:HG22	2:B:191:VAL:HG23	2.00	0.44
2:D:115:LYS:HZ1	2:D:117:THR:HG22	1.83	0.44
1:A:163:TRP:HA	1:A:175:MET:HB2	1.99	0.44
2:D:89:VAL:HA	2:D:108:THR:HA	2.00	0.44
1:A:7:VAL:HG12	1:A:8:SER:OG	2.18	0.44
1:C:94:TYR:HD2	2:D:47:TRP:CH2	2.35	0.44
1:A:135:PHE:C	1:A:136:LEU:HD12	2.39	0.44
2:B:17:SER:OG	2:B:82(A):SER:HA	2.17	0.43
2:D:163:SER:H	2:D:209:ASN:ND2	2.16	0.43
2:D:152:VAL:HG12	2:D:212:HIS:HA	1.99	0.43
2:B:191:VAL:HG13	2:B:191:VAL:O	2.19	0.43
2:D:84:SER:HA	2:D:111:VAL:CB	2.43	0.43
2:D:6:GLU:OE1	2:D:6:GLU:N	2.51	0.43
2:D:468:THR:HG22	2:D:469:GLU:H	1.83	0.43
1:A:58:VAL:HA	1:A:59:PRO:HD3	1.76	0.43
2:B:15:GLY:N	2:B:82(C):LEU:O	2.51	0.43
2:B:50:TYR:CZ	2:B:51:ILE:O	2.71	0.43
2:D:408:SER:O	2:D:411:GLY:N	2.51	0.43
1:A:22:THR:HG22	1:A:72:THR:HA	2.00	0.43
2:D:401:THR:CG2	2:D:459:LEU:HB2	2.48	0.43
2:D:63:PHE:N	2:D:63:PHE:CD1	2.86	0.43
2:B:20:MET:HG3	2:B:36:TRP:CH2	2.54	0.43
1:C:14:SER:OG	1:C:107:LYS:HB2	2.17	0.43
2:D:208:CYS:HB2	2:D:223:ILE:HD11	2.00	0.43
1:A:37:GLN:HB2	1:A:47:LEU:HD22	2.01	0.43
2:D:93:VAL:CG1	2:D:94:ARG:H	2.24	0.43
2:D:125:ALA:HB1	2:D:227:PRO:HA	1.99	0.43
2:D:70:THR:OG1	2:D:71:ARG:N	2.50	0.43
2:D:4:LEU:HD22	2:D:92:CYS:SG	2.59	0.43
2:D:184:LEU:HA	2:D:184:LEU:HD23	1.76	0.43
2:D:410:ASP:HB2	2:D:411:GLY:H	1.73	0.43
2:B:196:SER:N	2:B:199:PRO:HD2	2.33	0.43
2:B:38:LYS:HZ2	2:B:40:ARG:NH2	2.15	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:27:TYR:HD1	2:B:27:TYR:N	2.15	0.43
2:B:70:THR:OG1	2:B:71:ARG:N	2.52	0.43
2:B:137:MET:HA	2:B:193:VAL:O	2.18	0.43
2:B:313:PHE:HB3	2:B:314:ASN:H	1.55	0.43
2:B:59:TYR:CE2	2:B:67:ALA:O	2.72	0.43
1:C:10:SER:HA	1:C:103:LYS:H	1.83	0.43
2:B:140:LEU:HB2	2:B:191:VAL:CG1	2.49	0.43
2:B:51:ILE:HD13	2:B:71:ARG:CB	2.44	0.43
2:D:392:ILE:HD12	2:D:400:ILE:HD13	2.01	0.43
2:B:309:ARG:CZ	2:B:310:GLU:HB2	2.49	0.43
2:D:374:PRO:HD3	2:D:388:LEU:HG	2.00	0.43
2:B:144:VAL:HG23	2:B:144:VAL:O	2.19	0.43
1:A:85:ASP:HA	1:A:102:THR:O	2.19	0.43
2:B:322:VAL:HG12	2:B:323:SER:N	2.34	0.43
1:A:159:VAL:C	1:A:160:LEU:HD12	2.39	0.43
2:D:90:TYR:HE2	2:D:109:VAL:CG2	2.31	0.43
2:B:33:THR:HG22	2:B:52(A):PRO:HD3	2.00	0.43
2:B:50:TYR:CE1	2:B:51:ILE:O	2.71	0.43
1:A:213:GLU:OE1	1:A:213:GLU:HA	2.18	0.43
2:B:207:THR:HG22	2:B:222:LYS:HG3	2.01	0.43
1:C:61:ARG:HH12	1:C:82:ASP:CG	2.21	0.43
2:B:33:THR:HG23	2:B:52(A):PRO:HD3	2.00	0.42
2:B:255:ILE:HG13	2:B:273:THR:O	2.17	0.42
1:C:124:GLN:HE22	1:C:131:SER:H	1.65	0.42
2:B:426:MET:CE	2:B:433:GLY:HA2	2.49	0.42
2:B:147:TYR:CE1	2:B:185:TYR:HB3	2.54	0.42
2:D:116:THR:HA	2:D:148:PHE:O	2.19	0.42
2:B:95:GLU:HG3	2:B:96:GLY:N	2.24	0.42
2:D:226:VAL:HG22	2:D:227:PRO:O	2.20	0.42
2:D:277:VAL:HG13	2:D:278:ASP:H	1.84	0.42
1:A:35:TRP:CE2	1:A:73:LEU:HB2	2.53	0.42
2:B:257:PRO:HG3	2:B:355:ILE:HG12	2.00	0.42
2:B:26:GLY:O	2:B:27:TYR:CB	2.64	0.42
2:B:200:ARG:NH2	2:B:227:PRO:CB	2.77	0.42
2:B:52:ASN:O	2:B:52(A):PRO:O	2.37	0.42
1:A:121:SER:O	1:A:125:LEU:HG	2.18	0.42
2:D:174:PHE:CD2	2:D:188:SER:O	2.73	0.42
1:A:14:SER:OG	1:A:107:LYS:HB2	2.18	0.42
2:D:206:VAL:O	2:D:223:ILE:HG12	2.19	0.42
2:B:152:VAL:HG12	2:B:212:HIS:HA	2.01	0.42
2:B:93:VAL:CG1	2:B:94:ARG:H	2.29	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:VAL:HA	1:A:135:PHE:O	2.19	0.42
2:D:50:TYR:CZ	2:D:51:ILE:O	2.72	0.42
1:C:121:SER:O	1:C:125:LEU:HG	2.19	0.42
1:A:174:SER:O	2:B:174:PHE:HE1	2.01	0.42
2:B:301:VAL:HG22	2:B:302:HIS:H	1.84	0.42
2:B:40:ARG:NE	2:B:85:ASP:O	2.53	0.42
2:D:32:TYR:O	2:D:71:ARG:NH2	2.50	0.42
2:B:259:LYS:CD	2:B:260:PRO:HD2	2.45	0.42
1:C:22:THR:HG22	1:C:72:THR:HA	2.00	0.42
2:D:256:PHE:HB2	2:D:273:THR:CG2	2.49	0.42
2:B:408:SER:O	2:B:411:GLY:N	2.53	0.42
2:B:291:PHE:CD2	2:B:296:ASN:HA	2.53	0.42
2:D:365:ARG:O	2:D:460:HIS:NE2	2.52	0.42
2:D:274:CYS:HB3	2:D:290:TRP:CZ2	2.55	0.42
1:C:150:ILE:HD12	1:C:156:GLN:NE2	2.34	0.42
2:B:396:PHE:HA	2:B:397:PRO:HA	1.81	0.42
2:B:50:TYR:N	2:B:69:LEU:HD13	2.34	0.42
2:D:310:GLU:H	2:D:321:VAL:HG22	1.84	0.42
2:D:53:SER:O	2:D:54:SER:CB	2.68	0.42
2:B:343:ASN:OD1	2:B:350:PRO:HB3	2.20	0.42
2:D:301:VAL:HG22	2:D:302:HIS:H	1.85	0.42
2:D:147:TYR:CE1	2:D:185:TYR:HB3	2.55	0.42
2:D:274:CYS:HB3	2:D:290:TRP:CH2	2.55	0.42
2:B:53:SER:O	2:B:54:SER:CB	2.67	0.42
1:A:65:SER:O	1:A:72:THR:N	2.53	0.42
1:A:13:MET:HG3	1:A:17:GLU:OE1	2.20	0.42
2:D:140:LEU:HB2	2:D:191:VAL:CG1	2.50	0.41
2:D:191:VAL:HG13	2:D:191:VAL:O	2.20	0.41
2:B:406:TRP:CE3	2:B:441:LEU:HD22	2.54	0.41
1:C:164:THR:CG2	1:C:174:SER:H	2.29	0.41
1:C:174:SER:O	2:D:174:PHE:HE1	2.03	0.41
1:C:118:PHE:CE2	2:D:124:LEU:O	2.73	0.41
1:C:144:ILE:HD12	1:C:145:ASN:H	1.85	0.41
2:D:396:PHE:HA	2:D:397:PRO:HA	1.82	0.41
2:B:283:ASP:HA	2:B:284:PRO:HD2	1.95	0.41
2:D:154:VAL:HG22	2:D:210:VAL:CG1	2.49	0.41
2:B:374:PRO:HD3	2:B:388:LEU:HG	2.01	0.41
1:C:163:TRP:HA	1:C:175:MET:HB2	2.00	0.41
2:B:468:THR:HG22	2:B:469:GLU:H	1.84	0.41
1:A:118:PHE:CE2	2:B:124:LEU:O	2.73	0.41
2:B:312:GLN:HG2	2:B:319:PHE:CE1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:369:VAL:CG2	2:B:392:ILE:HG22	2.50	0.41
2:D:255:ILE:HG13	2:D:273:THR:O	2.19	0.41
2:D:245:PRO:HB2	2:D:249:GLU:H	1.72	0.41
2:B:171:VAL:HG12	2:B:172:HIS:N	2.35	0.41
2:D:153:THR:O	2:D:210:VAL:HA	2.21	0.41
1:A:90:GLN:HE22	1:A:96:TYR:HD1	1.68	0.41
2:B:360:LYS:O	2:B:396:PHE:HE1	2.04	0.41
2:D:38:LYS:HZ2	2:D:40:ARG:HH22	1.68	0.41
2:B:163:SER:H	2:B:209:ASN:ND2	2.19	0.41
2:D:312:GLN:HG2	2:D:319:PHE:CE1	2.55	0.41
1:C:13:MET:HG3	1:C:17:GLU:OE1	2.21	0.41
1:C:9:LYS:HB2	1:C:9:LYS:HE3	1.80	0.41
2:B:353:LYS:HB3	2:B:353:LYS:HE2	1.89	0.41
2:B:417:GLU:O	2:B:418:ASN:HB2	2.20	0.41
2:D:148:PHE:HA	2:D:149:PRO:HA	1.83	0.41
1:C:214:CYS:CB	2:D:235:CYS:HA	2.33	0.41
2:D:290:TRP:HA	2:D:339:LYS:O	2.20	0.41
1:C:136:LEU:N	1:C:136:LEU:CD1	2.83	0.41
1:C:90:GLN:HE22	1:C:96:TYR:HA	1.86	0.41
2:D:137:MET:HA	2:D:193:VAL:O	2.20	0.41
2:B:53:SER:OG	2:B:55:VAL:HG23	2.20	0.41
2:B:369:VAL:O	2:B:369:VAL:HG13	2.21	0.41
2:B:338:PHE:HB2	2:B:355:ILE:HG22	2.03	0.41
2:D:333:LEU:HD13	2:D:466:HIS:HE1	1.86	0.41
2:D:9:ALA:HB2	2:D:20:MET:HB3	2.03	0.41
2:B:63:PHE:N	2:B:63:PHE:CD1	2.89	0.41
1:A:36:TYR:OH	2:B:98:VAL:HB	2.21	0.41
2:D:375:PRO:HG2	2:D:378:GLN:HB3	2.03	0.41
2:D:392:ILE:CD1	2:D:437:VAL:HB	2.42	0.41
2:D:277:VAL:HG21	4:D:477:NDG:C1	2.51	0.41
2:D:327:ILE:HG13	2:D:328:MET:N	2.35	0.41
2:B:76:ASN:ND2	2:B:76:ASN:N	2.69	0.41
2:D:309:ARG:CZ	2:D:310:GLU:HB2	2.51	0.41
2:D:266:ILE:HA	2:D:329:HIS:HE1	1.84	0.41
1:A:112:ALA:N	1:A:200:THR:HG21	2.35	0.41
2:D:343:ASN:CG	2:D:350:PRO:HB3	2.41	0.41
1:A:4:ALA:O	1:A:99:GLY:HA2	2.21	0.41
2:B:51:ILE:HG23	2:B:71:ARG:HH11	1.86	0.40
2:B:392:ILE:HD12	2:B:400:ILE:HD13	2.03	0.40
1:A:191:SER:HA	1:A:209:PHE:O	2.20	0.40
1:C:33:VAL:HG21	1:C:71:PHE:CD2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:406:TRP:CE3	2:D:441:LEU:HD22	2.56	0.40
1:A:167:ASP:O	1:A:171:SER:HA	2.21	0.40
2:B:366:ALA:HB1	2:B:463:LEU:HD23	2.04	0.40
1:A:203:SER:HB2	1:A:204:PRO:HD2	2.03	0.40
2:D:359:THR:O	2:D:359:THR:HG22	2.21	0.40
1:C:129:GLY:H	1:C:183:LYS:HB2	1.86	0.40
1:C:163:TRP:HB3	1:C:164:THR:H	1.72	0.40
2:B:313:PHE:CE2	2:B:320:ARG:HD3	2.56	0.40
1:C:105:GLU:HG3	1:C:166:GLN:HE22	1.85	0.40
2:D:144:VAL:CG2	2:D:187:LEU:HD13	2.51	0.40
1:C:198:HIS:CG	1:C:199:LYS:H	2.39	0.40
2:D:253:VAL:HG22	2:D:254:PHE:N	2.36	0.40
2:B:41:PRO:O	2:B:43:GLN:HG2	2.21	0.40
2:B:375:PRO:HG2	2:B:378:GLN:HB3	2.03	0.40
1:C:65:SER:O	1:C:72:THR:N	2.54	0.40
2:B:343:ASN:CG	2:B:350:PRO:HB3	2.42	0.40
2:B:372:ILE:HG21	2:D:372:ILE:CG2	2.38	0.40
2:B:52(A):PRO:HB2	2:B:53:SER:H	1.75	0.40
2:D:309:ARG:CB	2:D:321:VAL:HG13	2.48	0.40
2:D:163:SER:H	2:D:209:ASN:HD21	1.70	0.40
1:A:198:HIS:CG	1:A:199:LYS:H	2.40	0.40
2:D:238:LYS:HD3	2:D:238:LYS:HA	1.89	0.40
2:D:94:ARG:HG2	2:D:94:ARG:HH11	1.86	0.40
1:C:134:CYS:O	1:C:136:LEU:CD1	2.70	0.40
2:D:259:LYS:CD	2:D:260:PRO:HD2	2.46	0.40
2:D:103:TRP:HD1	2:D:103:TRP:H	1.69	0.40

All (2) 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)
2:B:196:SER:H	2:D:23:LYS:HZ3[1_554]	1.25	0.35
2:B:23:LYS:HZ3	2:D:196:SER:H[1_554]	1.33	0.27

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	211/213 (99%)	168 (80%)	32 (15%)	11 (5%)	2	19
1	C	211/213 (99%)	169 (80%)	32 (15%)	10 (5%)	3	22
2	B	432/434 (100%)	301 (70%)	89 (21%)	42 (10%)	1	4
2	D	432/434 (100%)	302 (70%)	80 (18%)	50 (12%)	0	3
All	All	1286/1294 (99%)	940 (73%)	233 (18%)	113 (9%)	1	5

All (113) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	30	VAL
1	A	138	ASN
2	B	9	ALA
2	B	27	TYR
2	B	54	SER
2	B	55	VAL
2	B	61	GLN
2	B	73	ARG
2	B	97	GLU
2	B	215	SER
2	B	304	ALA
2	B	309	ARG
2	B	369	VAL
1	C	30	VAL
1	C	138	ASN
2	D	9	ALA
2	D	54	SER
2	D	55	VAL
2	D	73	ARG
2	D	97	GLU
2	D	215	SER
2	D	250	VAL
2	D	295	ASP
2	D	304	ALA
2	D	309	ARG
2	D	369	VAL
1	A	151	ASP
1	A	211	ARG

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Mol	Chain	Res	Type
2	B	8	GLY
2	B	16	ALA
2	B	50	TYR
2	B	52(A)	PRO
2	B	62	ARG
2	B	65	ASP
2	B	76	ASN
2	B	203	SER
2	B	295	ASP
2	B	306	THR
2	B	310	GLU
2	B	312	GLN
2	B	317	SER
2	B	355	ILE
2	B	453	THR
1	C	151	ASP
1	C	211	ARG
2	D	8	GLY
2	D	16	ALA
2	D	27	TYR
2	D	50	TYR
2	D	52(A)	PRO
2	D	61	GLN
2	D	62	ARG
2	D	76	ASN
2	D	203	SER
2	D	237	CYS
2	D	306	THR
2	D	310	GLU
2	D	312	GLN
2	D	317	SER
2	D	355	ILE
2	D	361	GLY
2	D	453	THR
1	A	53	ASN
1	A	150	ILE
2	B	48	ILE
2	B	95	GLU
2	B	167	SER
2	B	284	PRO
1	C	53	ASN
1	C	150	ILE

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Mol	Chain	Res	Type
2	D	48	ILE
2	D	65	ASP
2	D	84	SER
2	D	95	GLU
2	D	167	SER
2	D	249	GLU
2	D	284	PRO
2	D	357	SER
2	B	286	VAL
2	B	303	THR
2	B	357	SER
2	B	410	ASP
2	B	416	PRO
1	C	8	SER
1	C	200	THR
2	D	245	PRO
2	D	286	VAL
2	D	303	THR
2	D	330	GLN
2	D	416	PRO
1	A	8	SER
1	A	77	SER
1	A	84	ALA
1	A	156	GLN
1	A	200	THR
2	B	84	SER
2	B	239	PRO
2	B	313	PHE
1	C	77	SER
1	C	84	ALA
2	D	313	PHE
2	D	410	ASP
2	D	119	PRO
2	B	41	PRO
2	B	93	VAL
2	B	119	PRO
2	D	41	PRO
2	D	93	VAL
2	D	223	ILE
2	D	241	ILE
2	D	270	PRO
2	B	149	PRO

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Mol	Chain	Res	Type
2	D	149	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	188/188 (100%)	160 (85%)	28 (15%)	4	17
1	C	188/188 (100%)	162 (86%)	26 (14%)	4	21
2	B	390/390 (100%)	329 (84%)	61 (16%)	3	15
2	D	390/390 (100%)	330 (85%)	60 (15%)	3	16
All	All	1156/1156 (100%)	981 (85%)	175 (15%)	3	17

All (175) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	CYS
1	A	5	HIS
1	A	12	SER
1	A	13	MET
1	A	21	LEU
1	A	46	LEU
1	A	61	ARG
1	A	73	LEU
1	A	79	GLN
1	A	83	LEU
1	A	87	HIS
1	A	94	TYR
1	A	97	THR
1	A	104	LEU
1	A	108	ARG
1	A	116	SER
1	A	133	VAL
1	A	135	PHE
1	A	144	ILE
1	A	150	ILE

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Mol	Chain	Res	Type
1	A	154	GLU
1	A	155	ARG
1	A	165	ASP
1	A	169	LYS
1	A	178	THR
1	A	181	LEU
1	A	210	ASN
1	A	211	ARG
2	B	3	LYS
2	B	4	LEU
2	B	5	GLN
2	B	6	GLU
2	B	18	VAL
2	B	20	MET
2	B	22	CYS
2	B	27	TYR
2	B	28	THR
2	B	35	HIS
2	B	58	ASN
2	B	65	ASP
2	B	69	LEU
2	B	70	THR
2	B	73	ARG
2	B	76	ASN
2	B	77	THR
2	B	80	ILE
2	B	82	LEU
2	B	85	ASP
2	B	92	CYS
2	B	93	VAL
2	B	94	ARG
2	B	97	GLU
2	B	105	GLN
2	B	110	THR
2	B	133	GLN
2	B	151	PRO
2	B	152	VAL
2	B	173	THR
2	B	175	PRO
2	B	187	LEU
2	B	200	ARG
2	B	209	ASN

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Mol	Chain	Res	Type
2	B	235	CYS
2	B	238	LYS
2	B	240	CYS
2	B	241	ILE
2	B	260	PRO
2	B	274	CYS
2	B	295	ASP
2	B	305	GLN
2	B	307	GLN
2	B	309	ARG
2	B	312	GLN
2	B	325	LEU
2	B	328	MET
2	B	343	ASN
2	B	352	GLU
2	B	381	MET
2	B	388	LEU
2	B	393	THR
2	B	405	GLU
2	B	410	ASP
2	B	414	GLN
2	B	416	PRO
2	B	418	ASN
2	B	421	ASN
2	B	425	ILE
2	B	443	VAL
2	B	467	HIS
1	C	3	CYS
1	C	5	HIS
1	C	12	SER
1	C	13	MET
1	C	21	LEU
1	C	46	LEU
1	C	53	ASN
1	C	61	ARG
1	C	73	LEU
1	C	79	GLN
1	C	83	LEU
1	C	87	HIS
1	C	97	THR
1	C	104	LEU
1	C	108	ARG

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Mol	Chain	Res	Type
1	C	116	SER
1	C	133	VAL
1	C	135	PHE
1	C	144	ILE
1	C	150	ILE
1	C	154	GLU
1	C	155	ARG
1	C	165	ASP
1	C	169	LYS
1	C	178	THR
1	C	181	LEU
2	D	3	LYS
2	D	4	LEU
2	D	5	GLN
2	D	6	GLU
2	D	18	VAL
2	D	20	MET
2	D	21	SER
2	D	22	CYS
2	D	27	TYR
2	D	28	THR
2	D	35	HIS
2	D	41	PRO
2	D	58	ASN
2	D	62	ARG
2	D	65	ASP
2	D	69	LEU
2	D	70	THR
2	D	73	ARG
2	D	76	ASN
2	D	77	THR
2	D	80	ILE
2	D	82	LEU
2	D	85	ASP
2	D	92	CYS
2	D	93	VAL
2	D	94	ARG
2	D	97	GLU
2	D	105	GLN
2	D	110	THR
2	D	133	GLN
2	D	152	VAL

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Mol	Chain	Res	Type
2	D	173	THR
2	D	175	PRO
2	D	187	LEU
2	D	200	ARG
2	D	209	ASN
2	D	235	CYS
2	D	244	VAL
2	D	260	PRO
2	D	274	CYS
2	D	295	ASP
2	D	305	GLN
2	D	307	GLN
2	D	309	ARG
2	D	312	GLN
2	D	325	LEU
2	D	343	ASN
2	D	352	GLU
2	D	381	MET
2	D	388	LEU
2	D	393	THR
2	D	405	GLU
2	D	410	ASP
2	D	414	GLN
2	D	416	PRO
2	D	418	ASN
2	D	421	ASN
2	D	425	ILE
2	D	443	VAL
2	D	467	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	GLN
1	A	137	ASN
2	B	5	GLN
2	B	35	HIS
2	B	43	GLN
2	B	135	ASN
2	B	312	GLN
2	B	329	HIS
2	B	334	ASN

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Mol	Chain	Res	Type
2	B	414	GLN
2	B	423	GLN
2	B	444	GLN
2	B	465	ASN
2	B	474	HIS
1	C	124	GLN
1	C	137	ASN
2	D	5	GLN
2	D	35	HIS
2	D	43	GLN
2	D	135	ASN
2	D	312	GLN
2	D	329	HIS
2	D	334	ASN
2	D	414	GLN
2	D	444	GLN
2	D	465	ASN
2	D	466	HIS
2	D	474	HIS

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 ⓘ

18 carbohydrates are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	B	475	3,2	14,14,15	1.12	1 (7%)	15,19,21	1.19	2 (13%)
3	FUL	B	476	3	10,10,11	0.39	0	14,14,16	0.58	0
3	NDG	B	477	3	14,14,15	0.70	0	15,19,21	0.90	1 (6%)
3	BMA	B	478	3	11,11,12	0.73	0	14,15,17	0.59	0
3	MAN	B	479	3	11,11,12	0.55	0	14,15,17	0.65	0
3	NAG	B	480	3	14,14,15	0.55	0	15,19,21	0.76	0
3	GAL	B	481	3	11,11,12	0.71	0	14,15,17	0.58	0
3	MAN	B	482	3	11,11,12	0.68	0	14,15,17	0.59	0
3	NAG	B	483	3	14,14,15	0.39	0	15,19,21	0.60	0
4	NAG	D	475	2,4	14,14,15	0.81	0	15,19,21	1.25	1 (6%)
4	FUC	D	476	4	10,10,11	0.43	0	14,14,16	0.66	0
4	NDG	D	477	4	14,14,15	0.64	0	15,19,21	0.95	2 (13%)
4	BMA	D	478	4	11,11,12	0.83	0	14,15,17	0.50	0
4	MAN	D	479	4	11,11,12	0.41	0	14,15,17	0.63	0
4	NAG	D	480	4	14,14,15	0.54	0	15,19,21	0.76	0
4	GAL	D	481	4	11,11,12	0.63	0	14,15,17	0.52	0
4	MAN	D	482	4	11,11,12	0.69	0	14,15,17	0.58	0
4	NAG	D	483	4	14,14,15	0.42	0	15,19,21	0.60	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	475	3,2	-	0/6/23/26	0/1/1/1
3	FUL	B	476	3	-	0/0/17/20	0/1/1/1
3	NDG	B	477	3	-	0/6/23/26	0/1/1/1
3	BMA	B	478	3	-	0/2/19/22	0/1/1/1
3	MAN	B	479	3	-	0/2/19/22	0/1/1/1
3	NAG	B	480	3	-	0/6/23/26	0/1/1/1
3	GAL	B	481	3	-	0/2/19/22	0/1/1/1
3	MAN	B	482	3	-	0/2/19/22	0/1/1/1
3	NAG	B	483	3	-	0/6/23/26	0/1/1/1
4	NAG	D	475	2,4	-	0/6/23/26	0/1/1/1
4	FUC	D	476	4	1/1/5/5	0/0/17/20	0/1/1/1
4	NDG	D	477	4	-	0/6/23/26	0/1/1/1
4	BMA	D	478	4	-	0/2/19/22	0/1/1/1
4	MAN	D	479	4	-	0/2/19/22	0/1/1/1
4	NAG	D	480	4	-	0/6/23/26	0/1/1/1
4	GAL	D	481	4	-	0/2/19/22	0/1/1/1
4	MAN	D	482	4	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	D	483	4	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	475	NAG	C1-C2	2.44	1.55	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	477	NDG	C2-N2-C7	-2.03	120.43	123.04
3	B	475	NAG	C2-N2-C7	-2.01	120.46	123.04
4	D	477	NDG	C1-O-C5	2.46	115.37	112.25
3	B	477	NDG	C1-O-C5	2.48	115.40	112.25
3	B	475	NAG	C1-O5-C5	3.37	116.52	112.25
4	D	475	NAG	C1-O5-C5	3.66	116.89	112.25

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	D	476	FUC	C1

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	480	NAG	1	0
3	B	481	GAL	1	0
4	D	477	NDG	1	0
4	D	480	NAG	1	0
4	D	481	GAL	1	0

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

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

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

6.3 Carbohydrates ⓘ

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

6.4 Ligands ⓘ

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

6.5 Other polymers ⓘ

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