



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:03 PM GMT

PDB ID : 1IGT  
Title : STRUCTURE OF IMMUNOGLOBULIN  
Authors : Harris, L.J.; Larson, S.B.; Hasel, K.W.; McPherson, A.  
Deposited on : 1996-10-25  
Resolution : 2.80 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](mailto: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.

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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

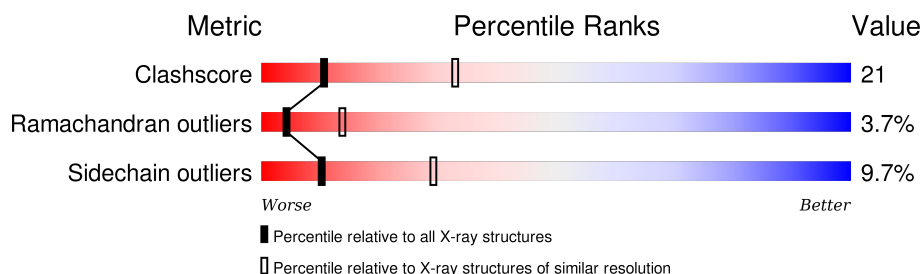
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)

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  $\geq 3$ , 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	214	
1	C	214	
2	B	444	
2	D	444	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	B	477	X	-	-	-
4	FUC	D	476	X	-	-	-
4	NAG	D	477	X	-	-	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12956 atoms, of which 2522 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 IGG2A INTACT ANTIBODY - MAB231.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	214	Total	C	H	N	O	S	0	0	0
			2033	1029	386	276	336	6			
1	C	214	Total	C	H	N	O	S	0	0	0
			2033	1029	386	276	336	6			

- Molecule 2 is a protein called IGG2A INTACT ANTIBODY - MAB231.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	444	Total	C	H	N	O	S	9	0	0
			4232	2191	772	576	671	22			
2	D	444	Total	C	H	N	O	S	9	0	0
			4232	2191	772	576	671	22			

- 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	0	0
			213	62	103	4	44		

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

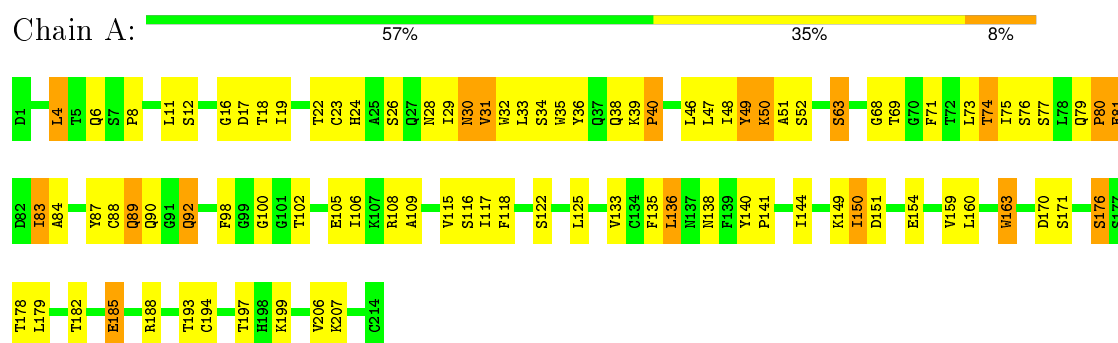
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	D	9	Total	C	H	N	O	0	0
			213	62	103	4	44		

### 3 Residue-property plots

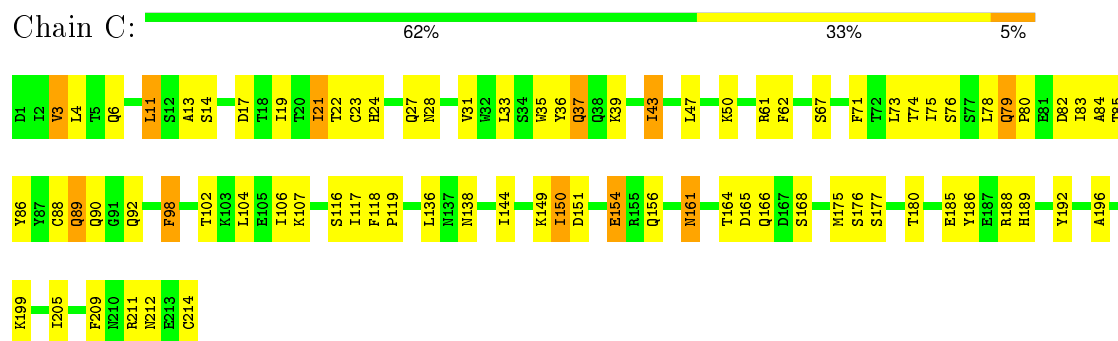
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

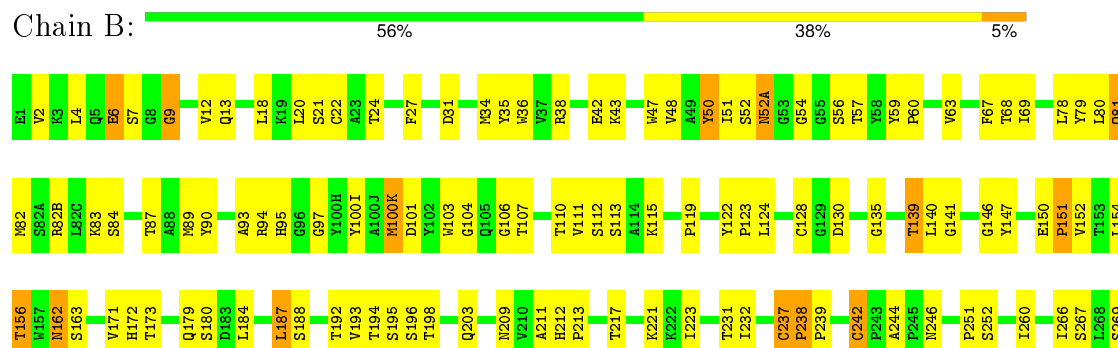
#### • Molecule 1: IGG2A INTACT ANTIBODY - MAB231

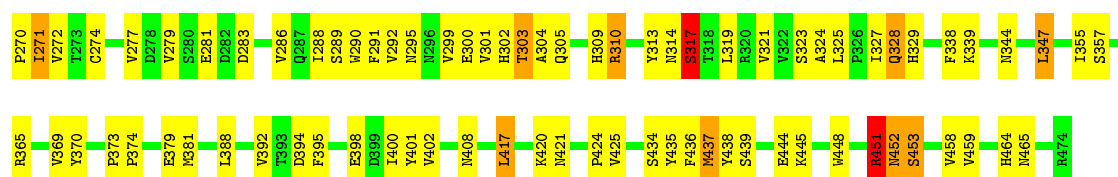


#### • Molecule 1: IGG2A INTACT ANTIBODY - MAB231



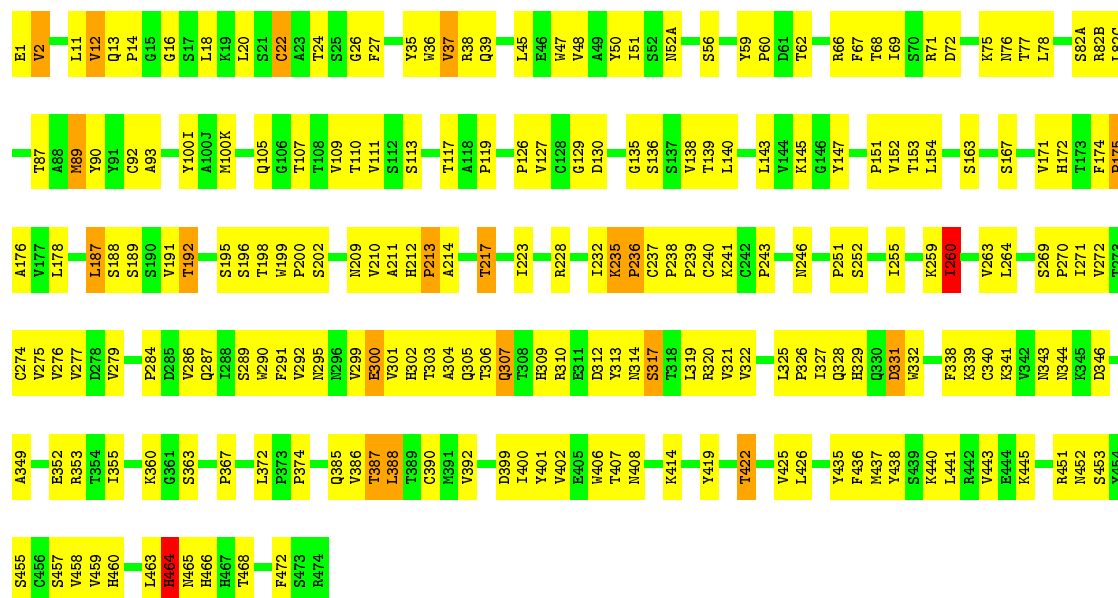
#### • Molecule 2: IGG2A INTACT ANTIBODY - MAB231





• Molecule 2: IGG2A INTACT ANTIBODY - MAB231

Chain D: 51% 44% .



## 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	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.82Å 76.77Å 100.64Å 88.05° 92.35° 97.23°	Depositor
Resolution (Å)	20.00 – 2.80	Depositor
% Data completeness (in resolution range)	86.2 (20.00-2.80)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.209 , 0.297	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12956	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, 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	0/1685	0.72	0/2292
1	C	0.42	0/1685	0.69	0/2292
2	B	0.47	0/3554	0.73	1/4847 (0.0%)
2	D	0.46	0/3554	0.70	0/4847
All	All	0.46	0/10478	0.72	1/14278 (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
2	D	0	1
3	B	1	0
4	D	2	0
All	All	3	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	417	LEU	CA-CB-CG	5.07	126.97	115.30

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	477	NAG	C1
4	D	476	FUC	C1
4	D	477	NAG	C1



All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	35	TYR	Sidechain

## 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	1647	386	1588	71	0
1	C	1647	386	1588	68	0
2	B	3460	772	3377	144	0
2	D	3460	772	3377	155	0
3	B	110	103	94	6	0
4	D	110	103	94	3	0
All	All	10434	2522	10118	436	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 21.

All (436) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:PHE:HB3	2:B:124:LEU:HD12	1.38	1.06
2:D:119:PRO:HB3	2:D:147:TYR:HB3	1.44	0.99
2:D:136:SER:HA	2:D:195:SER:HB3	1.48	0.95
2:D:37:VAL:HG12	2:D:47:TRP:HA	1.55	0.88
2:D:367:PRO:HD3	2:D:460:HIS:HD2	1.42	0.85
1:A:36:TYR:HE2	1:A:89:GLN:HG2	1.43	0.84
2:B:52:SER:HB2	2:B:56:SER:HB2	1.64	0.80
1:A:29:ILE:HA	1:A:92:GLN:HG3	1.65	0.79
2:B:119:PRO:HB3	2:B:147:TYR:HB3	1.66	0.78
2:B:374:PRO:HD3	2:B:388:LEU:HD23	1.66	0.77
2:B:238:PRO:HB2	2:B:239:PRO:HD3	1.65	0.76
1:A:63:SER:HB2	1:A:74:THR:HG23	1.67	0.76
1:A:6:GLN:HE22	1:A:87:TYR:HA	1.51	0.75
1:A:32:TRP:HD1	1:A:92:GLN:HG2	1.51	0.75
2:D:260:ILE:HD13	2:D:260:ILE:H	1.49	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:ILE:HG12	1:C:78:LEU:HD21	1.70	0.74
1:C:37:GLN:HG3	1:C:86:TYR:CE2	2.22	0.74
2:B:87:THR:HG23	2:B:110:THR:HA	1.68	0.74
2:B:6:GLU:HA	2:B:22:CYS:HA	1.69	0.73
2:B:301:VAL:HB	2:B:304:ALA:HB2	1.70	0.73
2:D:290:TRP:NE1	2:D:306:THR:HG21	2.04	0.73
2:B:48:VAL:O	2:B:60:PRO:HD2	1.89	0.73
2:B:9:GLY:HA2	2:B:18:LEU:HD21	1.71	0.72
1:A:188:ARG:HH11	1:A:188:ARG:HB3	1.54	0.72
2:D:276:VAL:HB	2:D:321:VAL:HG12	1.72	0.72
1:C:37:GLN:HG3	1:C:86:TYR:CZ	2.25	0.71
2:B:51:ILE:HG13	2:B:57:THR:HG22	1.73	0.71
2:B:152:VAL:HG12	2:B:212:HIS:HD2	1.55	0.70
1:C:83:ILE:HD12	1:C:168:SER:HA	1.73	0.70
2:B:47:TRP:HZ2	2:B:50:TYR:HB3	1.57	0.70
1:A:118:PHE:CB	2:B:124:LEU:HD12	2.19	0.69
2:B:266:ILE:HG13	2:B:267:SER:H	1.58	0.68
2:B:63:VAL:HB	2:B:67:PHE:CD2	2.29	0.67
1:A:39:LYS:HG2	1:A:83:ILE:O	1.94	0.67
2:D:291:PHE:CD1	2:D:300:GLU:HA	2.28	0.67
1:A:108:ARG:HG2	1:A:109:ALA:N	2.09	0.67
2:B:20:LEU:HD12	2:B:80:LEU:HD23	1.77	0.67
2:B:156:THR:HG23	2:B:209:ASN:HB2	1.77	0.67
1:A:12:SER:HA	1:A:105:GLU:O	1.95	0.66
1:A:115:VAL:HG13	1:A:207:LYS:HG3	1.76	0.66
2:D:390:CYS:HB2	2:D:406:TRP:CZ2	2.30	0.66
2:D:66:ARG:HD2	2:D:82(B):ARG:HB2	1.77	0.66
1:A:8:PRO:HG3	1:A:11:LEU:HG	1.76	0.66
1:C:37:GLN:HB2	1:C:47:LEU:HD11	1.77	0.65
1:C:62:PHE:CD1	1:C:75:ILE:HG13	2.31	0.65
2:B:301:VAL:HB	2:B:304:ALA:CB	2.26	0.65
1:C:4:LEU:HD21	1:C:90:GLN:HG2	1.79	0.65
2:B:83:LYS:O	2:B:111:VAL:HG21	1.97	0.64
1:A:182:THR:OG1	1:A:185:GLU:HB2	1.99	0.63
2:D:163:SER:H	2:D:209:ASN:ND2	1.96	0.63
2:D:272:VAL:HG23	2:D:327:ILE:HG13	1.80	0.63
1:C:106:ILE:H	1:C:166:GLN:HE22	1.46	0.63
2:B:252:SER:HB2	2:B:277:VAL:HG22	1.80	0.63
1:C:136:LEU:HD12	1:C:136:LEU:N	2.14	0.63
1:A:16:GLY:HA2	1:A:77:SER:HA	1.79	0.62
1:A:32:TRP:CD1	1:A:92:GLN:HG2	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:22:CYS:HB3	2:B:78:LEU:HB3	1.80	0.62
2:B:95:HIS:NE2	2:B:97:GLY:O	2.31	0.62
4:D:481:GAL:C6	4:D:481:GAL:H2	2.30	0.62
1:C:22:THR:HG22	1:C:23:CYS:H	1.64	0.62
2:B:4:LEU:HD22	2:B:24:THR:HG22	1.82	0.62
2:B:7:SER:HA	2:B:107:THR:HG21	1.81	0.62
1:C:35:TRP:CZ3	1:C:88:CYS:HB3	2.35	0.61
2:B:140:LEU:HD13	2:B:223:ILE:HG21	1.82	0.61
1:A:11:LEU:CD1	1:A:19:ILE:HD11	2.30	0.61
1:C:84:ALA:HB3	1:C:86:TYR:CE1	2.35	0.61
1:C:36:TYR:HE1	1:C:89:GLN:HB3	1.66	0.61
2:D:465:ASN:O	2:D:466:HIS:HB2	1.99	0.61
1:C:119:PRO:HD2	2:D:228:ARG:HH12	1.65	0.61
2:B:292:VAL:O	2:B:299:VAL:HG12	2.00	0.61
2:D:87:THR:HG23	2:D:110:THR:HA	1.82	0.61
2:B:327:ILE:HG22	2:B:328:GLN:N	2.16	0.61
2:D:292:VAL:O	2:D:299:VAL:HG22	2.01	0.61
1:A:11:LEU:HD12	1:A:19:ILE:HD11	1.82	0.61
2:D:36:TRP:HD1	2:D:69:ILE:HD12	1.66	0.61
2:B:266:ILE:HG13	2:B:267:SER:N	2.16	0.60
3:B:475:NAG:H61	3:B:477:NAG:HN2	1.65	0.60
2:D:139:THR:HB	2:D:192:THR:HG23	1.83	0.60
2:D:275:VAL:HG12	2:D:322:VAL:HG12	1.82	0.60
2:B:84:SER:HA	2:B:111:VAL:HG23	1.83	0.60
2:D:69:ILE:HD11	2:D:78:LEU:HD11	1.84	0.60
1:C:13:ALA:HA	1:C:107:LYS:HE2	1.82	0.60
2:D:290:TRP:HE1	2:D:306:THR:HG21	1.65	0.60
2:B:325:LEU:HD23	2:B:327:ILE:HD11	1.83	0.59
2:D:327:ILE:HD12	2:D:338:PHE:CE1	2.38	0.59
1:C:196:ALA:HB3	1:C:205:ILE:HG23	1.85	0.59
2:D:22:CYS:O	2:D:22:CYS:SG	2.61	0.59
1:C:161:ASN:HA	1:C:177:SER:HA	1.84	0.59
2:D:255:ILE:HG22	2:D:353:ARG:CZ	2.33	0.58
2:D:176:ALA:HB2	2:D:187:LEU:HB2	1.85	0.58
1:C:61:ARG:HH11	1:C:79:GLN:HG3	1.68	0.58
2:B:310:ARG:HG3	2:B:321:VAL:HG22	1.85	0.58
2:B:279:VAL:HG21	2:B:321:VAL:HG23	1.85	0.58
2:D:38:ARG:HA	2:D:89:MET:O	2.04	0.57
2:B:271:ILE:CD1	2:B:324:ALA:HB1	2.33	0.57
1:A:87:TYR:HD2	1:A:100:GLY:O	1.87	0.57
1:C:19:ILE:O	1:C:74:THR:HA	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:438:TYR:OH	2:D:440:LYS:HB2	2.04	0.57
2:B:20:LEU:HB2	2:B:80:LEU:HB3	1.86	0.57
1:C:106:ILE:N	1:C:166:GLN:HE22	2.02	0.57
3:B:481:GAL:C6	3:B:481:GAL:H2	2.35	0.57
1:C:35:TRP:CH2	1:C:88:CYS:HB3	2.39	0.56
1:C:33:LEU:HD13	1:C:71:PHE:CD1	2.40	0.56
1:A:73:LEU:HD12	1:A:74:THR:N	2.19	0.56
2:D:289:SER:HB2	2:D:341:LYS:HB3	1.86	0.56
2:D:211:ALA:HA	2:D:217:THR:O	2.05	0.56
2:B:238:PRO:HB2	2:B:239:PRO:CD	2.35	0.56
2:D:138:VAL:HG22	2:D:140:LEU:HD21	1.87	0.56
1:A:92:GLN:C	1:A:92:GLN:HE21	2.10	0.55
2:D:246:ASN:HA	2:D:349:ALA:CB	2.36	0.55
2:D:20:LEU:HD22	2:D:107:THR:HG21	1.87	0.55
1:A:8:PRO:HG3	1:A:11:LEU:CG	2.37	0.55
2:D:274:CYS:HB2	2:D:290:TRP:CH2	2.42	0.55
2:B:67:PHE:CD1	2:B:82:MET:HA	2.42	0.55
1:C:214:CYS:HB2	2:D:228:ARG:HD3	1.89	0.55
2:B:291:PHE:HB2	2:B:339:LYS:HB3	1.88	0.55
1:A:193:THR:HG23	1:A:206:VAL:HG23	1.90	0.54
2:B:303:THR:HG22	2:B:305:GLN:H	1.72	0.54
2:D:213:PRO:HG2	2:D:214:ALA:H	1.73	0.54
1:C:106:ILE:H	1:C:166:GLN:NE2	2.04	0.54
1:C:21:ILE:HG23	1:C:73:LEU:HB3	1.88	0.54
2:D:374:PRO:HD3	2:D:388:LEU:HD12	1.90	0.54
2:B:152:VAL:HG12	2:B:212:HIS:CD2	2.41	0.54
2:B:272:VAL:HG23	2:B:327:ILE:HG13	1.90	0.54
2:B:452:ASN:ND2	2:B:453:SER:H	2.05	0.54
2:B:123:PRO:HD3	2:B:221:LYS:HG2	1.90	0.54
1:C:80:PRO:O	1:C:83:ILE:HG13	2.08	0.53
2:B:425:VAL:HB	2:B:436:PHE:CE1	2.43	0.53
2:B:408:ASN:HA	2:B:453:SER:O	2.08	0.53
1:C:149:LYS:HA	1:C:154:GLU:O	2.09	0.53
1:C:6:GLN:NE2	1:C:21:ILE:HD11	2.24	0.53
2:B:242:CYS:O	2:B:244:ALA:N	2.42	0.53
1:A:50:LYS:O	1:A:52:SER:N	2.40	0.52
2:B:313:TYR:HE2	3:B:475:NAG:O6	1.92	0.52
2:B:274:CYS:HB2	2:B:290:TRP:CZ2	2.44	0.52
2:D:307:GLN:NE2	2:D:307:GLN:H	2.05	0.52
1:C:35:TRP:O	1:C:47:LEU:HB2	2.09	0.52
2:B:211:ALA:HA	2:B:217:THR:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:52:SER:HB3	2:B:54:GLY:O	2.10	0.52
1:A:73:LEU:HD12	1:A:74:THR:H	1.74	0.52
1:C:119:PRO:HD2	2:D:228:ARG:NH1	2.24	0.52
1:A:115:VAL:HG22	1:A:116:SER:N	2.24	0.52
1:C:175:MET:HG2	1:C:176:SER:N	2.24	0.52
2:B:187:LEU:HD23	2:B:188:SER:N	2.24	0.52
2:B:21:SER:HA	2:B:79:TYR:HD1	1.73	0.52
2:B:12:VAL:O	2:B:111:VAL:HA	2.10	0.52
2:D:400:ILE:HG12	2:D:401:TYR:N	2.25	0.52
2:D:126:PRO:HD3	2:D:140:LEU:HD22	1.92	0.52
2:D:386:VAL:HG23	2:D:443:VAL:HG23	1.92	0.52
2:D:400:ILE:HG12	2:D:401:TYR:H	1.75	0.51
2:D:291:PHE:HD1	2:D:300:GLU:HA	1.74	0.51
2:D:93:ALA:CB	2:D:100(K):MET:HG2	2.40	0.51
2:B:327:ILE:HD12	2:B:338:PHE:CE2	2.45	0.51
1:C:189:HIS:O	1:C:211:ARG:HD3	2.10	0.51
2:B:179:GLN:HG3	2:B:184:LEU:O	2.10	0.51
1:A:87:TYR:CD2	1:A:100:GLY:O	2.63	0.51
2:B:163:SER:H	2:B:209:ASN:ND2	2.08	0.51
1:C:4:LEU:HA	1:C:24:HIS:O	2.11	0.51
2:B:4:LEU:HB2	2:B:104:GLY:HA2	1.92	0.51
2:D:48:VAL:O	2:D:60:PRO:HD3	2.11	0.51
2:D:39:GLN:HG3	2:D:45:LEU:HG	1.91	0.51
3:B:481:GAL:H61	3:B:481:GAL:H2	1.92	0.51
2:B:195:SER:O	2:B:198:THR:N	2.43	0.51
1:A:140:TYR:CD1	1:A:141:PRO:HA	2.45	0.51
1:A:8:PRO:CG	1:A:11:LEU:HG	2.41	0.51
2:D:47:TRP:HZ2	2:D:50:TYR:HB2	1.75	0.50
1:A:33:LEU:HD22	1:A:71:PHE:CB	2.41	0.50
1:A:36:TYR:CE2	1:A:89:GLN:HG2	2.35	0.50
2:D:47:TRP:O	2:D:60:PRO:HG2	2.12	0.50
2:B:47:TRP:O	2:B:60:PRO:HG3	2.11	0.50
2:D:11:LEU:HA	2:D:110:THR:O	2.12	0.50
1:C:31:VAL:HG23	1:C:50:LYS:HG3	1.93	0.50
1:A:133:VAL:HG22	1:A:178:THR:OG1	2.11	0.50
2:D:67:PHE:CD1	2:D:67:PHE:N	2.79	0.50
1:C:88:CYS:O	1:C:88:CYS:SG	2.69	0.50
2:B:171:VAL:HG12	2:B:172:HIS:N	2.27	0.50
2:B:124:LEU:HB2	2:B:141:GLY:O	2.12	0.50
4:D:481:GAL:C6	4:D:481:GAL:C2	2.87	0.50
2:D:309:HIS:HB2	2:D:322:VAL:CG2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:271:ILE:HD12	2:B:324:ALA:HB1	1.93	0.50
1:C:98:PHE:N	1:C:98:PHE:CD1	2.79	0.50
2:B:458:VAL:HG12	2:B:459:VAL:N	2.26	0.49
2:D:24:THR:HG21	2:D:27:PHE:CZ	2.47	0.49
2:D:260:ILE:CG2	2:D:399:ASP:HB3	2.42	0.49
2:B:223:ILE:O	2:B:223:ILE:HG22	2.12	0.49
2:D:463:LEU:CD1	2:D:468:THR:HG22	2.42	0.49
2:D:119:PRO:HB3	2:D:147:TYR:CB	2.29	0.49
2:B:374:PRO:HD3	2:B:388:LEU:CD2	2.40	0.49
2:B:84:SER:HA	2:B:111:VAL:CG2	2.42	0.49
2:D:252:SER:HB2	2:D:277:VAL:CG2	2.42	0.49
2:D:408:ASN:HA	2:D:453:SER:O	2.11	0.49
1:C:150:ILE:HD12	1:C:192:TYR:HE1	1.78	0.49
2:B:2:VAL:HG23	2:B:27:PHE:CE2	2.48	0.49
1:A:24:HIS:HA	1:A:69:THR:O	2.13	0.49
2:B:47:TRP:CZ3	2:B:60:PRO:HD3	2.48	0.49
2:D:246:ASN:HA	2:D:349:ALA:HB3	1.93	0.49
2:D:260:ILE:HG21	2:D:399:ASP:HB3	1.95	0.49
3:B:475:NAG:C6	3:B:477:NAG:HN2	2.26	0.49
1:C:185:GLU:O	1:C:189:HIS:HD2	1.94	0.49
2:D:286:VAL:HG13	2:D:344:ASN:HB2	1.94	0.49
1:A:108:ARG:HG2	1:A:109:ALA:H	1.74	0.49
2:D:327:ILE:HG22	2:D:328:GLN:N	2.27	0.49
3:B:481:GAL:C6	3:B:481:GAL:C2	2.90	0.49
2:B:193:VAL:HG12	2:B:194:THR:N	2.27	0.49
1:C:186:TYR:CE1	1:C:192:TYR:CE2	3.00	0.49
1:C:27:GLN:HG2	1:C:28:ASN:N	2.27	0.49
2:B:290:TRP:CE3	2:B:325:LEU:HD22	2.48	0.49
2:B:59:TYR:HB3	2:B:63:VAL:HG23	1.95	0.49
2:D:152:VAL:HG12	2:D:212:HIS:CD2	2.48	0.49
2:B:59:TYR:OH	2:B:69:ILE:HG22	2.13	0.49
2:D:291:PHE:HA	2:D:301:VAL:HG22	1.95	0.49
2:B:421:ASN:ND2	2:B:439:SER:CB	2.76	0.49
2:D:339:LYS:HG2	2:D:340:CYS:N	2.27	0.48
2:B:400:ILE:HG12	2:B:401:TYR:H	1.78	0.48
2:D:152:VAL:HG12	2:D:212:HIS:HD2	1.78	0.48
1:A:188:ARG:HB3	1:A:188:ARG:NH1	2.26	0.48
1:A:83:ILE:HG13	1:A:106:ILE:HD11	1.95	0.48
1:A:81:GLU:CD	1:A:81:GLU:H	2.15	0.48
2:D:235:LYS:HB2	2:D:236:PRO:HD3	1.94	0.48
1:C:192:TYR:HB2	1:C:209:PHE:CE1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:291:PHE:CE1	2:D:300:GLU:HA	2.49	0.48
2:D:463:LEU:HD13	2:D:468:THR:HG22	1.95	0.48
2:B:400:ILE:HG12	2:B:401:TYR:N	2.28	0.48
2:B:281:GLU:HG2	2:B:319:LEU:HD13	1.94	0.48
2:B:36:TRP:NE1	2:B:80:LEU:HB2	2.29	0.48
2:B:47:TRP:HZ2	2:B:50:TYR:CB	2.26	0.48
2:D:332:TRP:HH2	2:D:355:ILE:HG13	1.78	0.48
1:A:150:ILE:HG22	1:A:151:ASP:N	2.28	0.48
1:C:61:ARG:NH1	1:C:79:GLN:HG3	2.28	0.48
2:B:139:THR:HB	2:B:192:THR:HG23	1.96	0.47
1:C:27:GLN:HG2	1:C:28:ASN:H	1.78	0.47
2:D:52(A):ASN:HA	2:D:71:ARG:NH1	2.29	0.47
2:D:303:THR:O	2:D:305:GLN:N	2.47	0.47
2:D:310:ARG:HG3	2:D:321:VAL:HG23	1.96	0.47
2:D:93:ALA:HB3	2:D:100(K):MET:HG2	1.97	0.47
1:C:150:ILE:HD12	1:C:192:TYR:CE1	2.50	0.47
2:D:459:VAL:HA	2:D:466:HIS:O	2.14	0.47
2:D:463:LEU:O	2:D:464:HIS:C	2.52	0.47
1:C:117:ILE:HG13	1:C:118:PHE:N	2.30	0.47
2:D:154:LEU:HD23	2:D:187:LEU:HD21	1.97	0.47
2:D:13:GLN:CD	2:D:13:GLN:H	2.16	0.47
2:D:290:TRP:CD1	2:D:306:THR:HG21	2.50	0.47
2:D:279:VAL:HG23	2:D:319:LEU:HB3	1.97	0.47
2:D:38:ARG:HD3	2:D:90:TYR:CE1	2.50	0.47
2:D:140:LEU:HD13	2:D:223:ILE:HG21	1.97	0.46
2:D:419:TYR:HB3	2:D:441:LEU:HD13	1.98	0.46
1:C:188:ARG:NH1	1:C:189:HIS:NE2	2.63	0.46
2:D:59:TYR:OH	2:D:68:THR:HA	2.15	0.46
1:A:33:LEU:HD22	1:A:71:PHE:CG	2.50	0.46
1:A:79:GLN:HB3	1:A:81:GLU:OE2	2.15	0.46
2:D:270:PRO:O	2:D:271:ILE:HD13	2.16	0.46
2:B:251:PRO:HA	2:B:277:VAL:O	2.16	0.46
2:D:38:ARG:HB3	2:D:90:TYR:CD1	2.51	0.46
1:C:71:PHE:CD1	1:C:71:PHE:N	2.84	0.46
2:D:401:TYR:C	2:D:401:TYR:CD1	2.89	0.46
1:A:31:VAL:O	1:A:31:VAL:HG22	2.15	0.46
2:B:314:ASN:OD1	2:B:317:SER:N	2.49	0.46
2:D:263:VAL:O	2:D:329:HIS:HD2	1.98	0.46
2:B:38:ARG:HB3	2:B:90:TYR:CE2	2.51	0.46
2:B:398:GLU:HG2	2:B:435:TYR:CZ	2.51	0.46
2:D:314:ASN:O	2:D:317:SER:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:161:ASN:HA	1:C:176:SER:O	2.15	0.46
1:A:30:ASN:ND2	1:A:92:GLN:OE1	2.47	0.46
1:A:46:LEU:HD23	1:A:47:LEU:N	2.31	0.46
2:D:191:VAL:HG13	2:D:191:VAL:O	2.16	0.46
1:A:159:VAL:HG12	1:A:160:LEU:H	1.81	0.45
2:B:303:THR:C	2:B:305:GLN:N	2.69	0.45
1:A:149:LYS:HA	1:A:154:GLU:O	2.16	0.45
1:C:17:ASP:O	1:C:78:LEU:HD23	2.16	0.45
1:C:136:LEU:HD23	1:C:144:ILE:HD11	1.97	0.45
2:B:173:THR:HG23	2:B:187:LEU:HD21	1.97	0.45
2:B:392:VAL:HG12	2:B:395:PHE:CE1	2.52	0.45
2:D:171:VAL:HG22	2:D:172:HIS:N	2.31	0.45
2:B:344:ASN:HD21	2:B:347:LEU:HD13	1.80	0.45
2:D:374:PRO:HD3	2:D:388:LEU:CD1	2.47	0.45
2:B:424:PRO:HA	2:B:437:MET:HB3	1.97	0.45
2:D:51:ILE:HG23	2:D:51:ILE:O	2.17	0.45
1:A:115:VAL:HA	1:A:135:PHE:O	2.17	0.45
2:D:407:THR:CG2	2:D:455:SER:HB2	2.47	0.45
1:A:4:LEU:HD21	1:A:90:GLN:HB3	1.98	0.45
1:C:150:ILE:HG22	1:C:151:ASP:N	2.32	0.45
2:D:367:PRO:HD3	2:D:460:HIS:CD2	2.34	0.45
2:D:328:GLN:O	2:D:331:ASP:HB2	2.16	0.45
1:C:78:LEU:HD13	1:C:78:LEU:HA	1.84	0.45
1:C:22:THR:HG22	1:C:23:CYS:N	2.30	0.45
2:D:426:LEU:HD12	2:D:435:TYR:CZ	2.52	0.45
2:B:150:GLU:OE1	2:B:151:PRO:HA	2.17	0.45
1:C:37:GLN:HE22	1:C:39:LYS:HE3	1.81	0.44
1:A:46:LEU:HD12	2:B:101:ASP:HA	1.98	0.44
2:D:239:PRO:O	2:D:241:LYS:N	2.51	0.44
1:C:136:LEU:CD1	1:C:136:LEU:N	2.81	0.44
2:D:392:VAL:HB	2:D:437:MET:HG3	1.99	0.44
2:D:360:LYS:HE3	2:D:360:LYS:HA	1.99	0.44
1:C:78:LEU:O	1:C:79:GLN:HG2	2.17	0.44
2:B:154:LEU:HD23	2:B:156:THR:N	2.32	0.44
2:B:4:LEU:HB2	2:B:104:GLY:CA	2.48	0.44
2:D:299:VAL:HG23	2:D:301:VAL:HG13	1.97	0.44
2:B:42:GLU:O	2:B:43:LYS:HB2	2.17	0.44
2:D:372:LEU:N	2:D:372:LEU:HD12	2.33	0.44
1:A:170:ASP:O	1:A:171:SER:HB2	2.18	0.44
2:B:35:TYR:HE1	2:B:50:TYR:CD1	2.34	0.44
2:B:20:LEU:HD11	2:B:82:MET:SD	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:LEU:HD12	1:A:88:CYS:SG	2.58	0.44
1:A:29:ILE:HD11	1:A:71:PHE:CE1	2.52	0.44
2:B:425:VAL:HG21	2:D:422:THR:HA	1.99	0.44
1:A:34:SER:HA	1:A:48:ILE:O	2.18	0.44
1:A:163:TRP:N	1:A:163:TRP:CE3	2.86	0.44
2:D:387:THR:HG22	2:D:440:LYS:HG3	1.99	0.44
1:C:164:THR:HG22	1:C:165:ASP:O	2.18	0.44
1:C:43:ILE:HD13	1:C:43:ILE:H	1.81	0.44
2:D:322:VAL:HG23	2:D:322:VAL:O	2.18	0.44
2:D:67:PHE:HD1	2:D:67:PHE:N	2.14	0.44
1:A:136:LEU:N	1:A:136:LEU:HD22	2.32	0.44
2:B:421:ASN:HD22	2:B:439:SER:HA	1.83	0.43
2:B:162:ASN:HA	2:B:162:ASN:HD22	1.62	0.43
2:D:82(C):LEU:HB3	2:D:111:VAL:HG21	2.00	0.43
2:D:72:ASP:OD1	2:D:75:LYS:HB2	2.18	0.43
2:B:244:ALA:C	2:B:246:ASN:H	2.21	0.43
2:D:340:CYS:O	2:D:352:GLU:HA	2.19	0.43
2:D:167:SER:O	2:D:171:VAL:HG12	2.18	0.43
2:B:93:ALA:HB1	2:B:100(K):MET:HB3	2.00	0.43
2:B:13:GLN:HA	2:B:112:SER:O	2.18	0.43
2:B:34:MET:HB3	2:B:78:LEU:HD22	1.99	0.43
2:B:47:TRP:CZ2	2:B:50:TYR:HB3	2.46	0.43
2:D:154:LEU:HD13	2:D:210:VAL:CG2	2.47	0.43
2:D:1:GLU:HG2	2:D:2:VAL:H	1.83	0.43
1:A:89:GLN:HG3	1:A:89:GLN:O	2.19	0.43
1:A:16:GLY:CA	1:A:77:SER:HA	2.46	0.43
2:B:365:ARG:HB2	2:B:395:PHE:HA	2.01	0.43
2:B:269:SER:HA	2:B:270:PRO:HD2	1.89	0.43
1:A:28:ASN:OD1	1:A:68:GLY:HA2	2.18	0.43
2:B:310:ARG:CG	2:B:321:VAL:HG22	2.48	0.43
2:D:100(I):TYR:CD1	2:D:100(I):TYR:N	2.87	0.43
2:B:95:HIS:NE2	2:B:100(I):TYR:N	2.66	0.43
1:C:6:GLN:HE22	1:C:21:ILE:HD11	1.84	0.43
2:D:419:TYR:HB3	2:D:441:LEU:CD1	2.49	0.43
2:B:436:PHE:O	2:B:437:MET:HB3	2.19	0.43
1:C:188:ARG:HG3	1:C:188:ARG:O	2.19	0.43
2:D:136:SER:CA	2:D:195:SER:HB3	2.34	0.43
1:C:78:LEU:C	1:C:79:GLN:HG2	2.39	0.43
1:C:3:VAL:C	1:C:4:LEU:HD22	2.40	0.43
1:C:36:TYR:OH	1:C:89:GLN:NE2	2.52	0.43
1:A:33:LEU:HD23	1:A:35:TRP:NE1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:251:PRO:HA	2:D:277:VAL:O	2.19	0.42
2:B:194:THR:O	2:B:195:SER:HB3	2.19	0.42
2:D:78:LEU:HD23	2:D:92:CYS:HB2	2.00	0.42
2:D:388:LEU:HD23	2:D:441:LEU:HD23	2.00	0.42
2:D:163:SER:H	2:D:209:ASN:HD21	1.65	0.42
2:B:451:ARG:C	2:B:451:ARG:HD3	2.39	0.42
2:D:12:VAL:HG23	2:D:111:VAL:HG22	2.01	0.42
2:D:199:TRP:HB3	2:D:200:PRO:HD3	2.01	0.42
2:B:103:TRP:N	2:B:103:TRP:CD1	2.88	0.42
1:C:11:LEU:HD22	1:C:11:LEU:HA	1.82	0.42
2:D:138:VAL:O	2:D:138:VAL:HG22	2.18	0.42
1:C:82:ASP:O	1:C:104:LEU:HD23	2.20	0.42
2:D:153:THR:O	2:D:210:VAL:HA	2.19	0.42
2:D:238:PRO:HB3	2:D:239:PRO:HD2	2.01	0.42
1:A:18:THR:HG23	1:A:76:SER:HA	2.02	0.42
2:D:252:SER:O	2:D:276:VAL:HA	2.19	0.42
2:D:401:TYR:HB3	2:D:459:VAL:HG22	2.01	0.42
2:B:68:THR:HB	2:B:81:GLN:CB	2.49	0.42
2:D:260:ILE:H	2:D:260:ILE:CD1	2.17	0.42
2:D:259:LYS:HD2	2:D:259:LYS:N	2.34	0.42
1:A:118:PHE:CD2	2:B:124:LEU:HB3	2.55	0.42
2:B:87:THR:OG1	2:B:111:VAL:HG22	2.20	0.42
2:B:146:GLY:C	2:B:184:LEU:HD12	2.40	0.42
1:A:144:ILE:HG13	1:A:197:THR:O	2.20	0.42
2:D:198:THR:HB	2:D:202:SER:OG	2.20	0.41
1:A:135:PHE:CE1	1:A:176:SER:HB2	2.55	0.41
2:B:252:SER:HB2	2:B:277:VAL:CG2	2.48	0.41
2:D:154:LEU:HD21	2:D:189:SER:HB2	2.03	0.41
2:D:386:VAL:CG2	2:D:443:VAL:HG23	2.50	0.41
2:B:68:THR:HB	2:B:81:GLN:HB2	2.02	0.41
2:B:231:THR:O	2:B:232:ILE:HG23	2.20	0.41
1:C:67:SER:HA	1:C:71:PHE:CE2	2.55	0.41
2:B:421:ASN:ND2	2:B:439:SER:HB2	2.35	0.41
2:D:127:VAL:HG23	2:D:129:GLY:O	2.20	0.41
2:B:272:VAL:HG12	2:B:290:TRP:HH2	1.85	0.41
2:D:139:THR:HA	2:D:192:THR:HA	2.02	0.41
1:A:163:TRP:HE3	1:A:163:TRP:H	1.69	0.41
2:D:154:LEU:CD2	2:D:189:SER:HB2	2.51	0.41
2:B:286:VAL:CG2	2:B:321:VAL:HG21	2.50	0.41
2:B:452:ASN:HD22	2:B:453:SER:H	1.67	0.41
1:A:98:PHE:CD1	1:A:98:PHE:N	2.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:327:ILE:CG2	2:B:328:GLN:N	2.82	0.41
2:D:36:TRP:CD1	2:D:69:ILE:HD12	2.50	0.41
2:D:408:ASN:O	2:D:414:LYS:HG2	2.20	0.41
2:B:400:ILE:CG1	2:B:401:TYR:H	2.33	0.41
2:B:150:GLU:HA	2:B:151:PRO:HA	1.86	0.41
2:D:75:LYS:O	2:D:76:ASN:HB2	2.20	0.41
2:B:374:PRO:HD2	2:B:448:TRP:CZ2	2.54	0.41
2:B:122:TYR:HA	2:B:123:PRO:HD2	1.87	0.41
2:B:94:ARG:NH2	2:B:101:ASP:OD2	2.54	0.41
2:D:287:GLN:HB3	2:D:343:ASN:HB3	2.03	0.41
1:A:117:ILE:HD12	1:A:194:CYS:HB2	2.02	0.41
2:D:310:ARG:HB3	2:D:319:LEU:HD21	2.02	0.41
1:A:38:GLN:C	1:A:84:ALA:HB1	2.41	0.41
4:D:481:GAL:H61	4:D:481:GAL:H2	2.03	0.41
1:A:122:SER:HA	1:A:125:LEU:HD12	2.03	0.41
1:A:49:TYR:N	1:A:49:TYR:CD1	2.89	0.41
2:B:394:ASP:HA	2:B:434:SER:OG	2.21	0.41
2:D:195:SER:O	2:D:198:THR:N	2.54	0.41
1:A:39:LYS:CG	1:A:84:ALA:HB2	2.51	0.41
2:D:264:LEU:O	2:D:466:HIS:HD2	2.03	0.41
2:B:400:ILE:CG1	2:B:401:TYR:N	2.84	0.41
1:A:18:THR:HA	1:A:75:ILE:O	2.21	0.41
2:D:325:LEU:HA	2:D:326:PRO:HD2	1.96	0.41
2:B:288:ILE:HD12	2:B:323:SER:HB2	2.02	0.41
2:B:260:ILE:HA	2:B:260:ILE:HD12	1.81	0.41
2:D:320:ARG:O	2:D:320:ARG:HG3	2.21	0.41
2:B:31:ASP:HA	2:B:52(A):ASN:OD1	2.21	0.41
2:D:269:SER:HA	2:D:270:PRO:HD3	1.81	0.41
2:B:344:ASN:ND2	2:B:347:LEU:HD13	2.36	0.41
2:D:392:VAL:O	2:D:436:PHE:HA	2.20	0.41
2:B:379:GLU:HG2	2:B:379:GLU:O	2.21	0.41
2:D:400:ILE:CG1	2:D:401:TYR:H	2.33	0.40
2:D:400:ILE:CG1	2:D:401:TYR:N	2.84	0.40
2:D:176:ALA:CB	2:D:187:LEU:HB2	2.51	0.40
2:B:451:ARG:HD3	2:B:452:ASN:N	2.36	0.40
2:D:1:GLU:HG2	2:D:2:VAL:N	2.35	0.40
1:C:180:THR:HG21	2:D:145:LYS:HE3	2.02	0.40
2:D:174:PHE:HD2	2:D:188:SER:O	2.03	0.40
2:B:59:TYR:CE1	2:B:69:ILE:HG22	2.56	0.40
2:D:422:THR:OG1	2:D:438:TYR:O	2.39	0.40
1:A:185:GLU:HA	1:A:188:ARG:HG3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:87:THR:HG23	2:D:109:VAL:O	2.21	0.40
2:B:328:GLN:O	2:B:329:HIS:C	2.60	0.40
2:B:35:TYR:CE1	2:B:50:TYR:HB2	2.56	0.40
2:D:66:ARG:HD2	2:D:82(B):ARG:CB	2.50	0.40
2:B:291:PHE:CD1	2:B:300:GLU:HA	2.56	0.40
2:B:90:TYR:O	2:B:106:GLY:HA2	2.22	0.40
2:B:464:HIS:O	2:B:465:ASN:HB2	2.21	0.40
2:B:327:ILE:HG22	2:B:328:GLN:H	1.84	0.40
2:D:237:CYS:HA	2:D:238:PRO:HD3	1.91	0.40
2:D:16:GLY:O	2:D:82(C):LEU:HD12	2.22	0.40
1:C:85:THR:HA	1:C:102:THR:O	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	212/214 (99%)	179 (84%)	24 (11%)	9 (4%)	3	11
1	C	212/214 (99%)	186 (88%)	22 (10%)	4 (2%)	10	32
2	B	442/444 (100%)	365 (83%)	63 (14%)	14 (3%)	5	17
2	D	442/444 (100%)	365 (83%)	56 (13%)	21 (5%)	3	9
All	All	1308/1316 (99%)	1095 (84%)	165 (13%)	48 (4%)	4	14

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	51	ALA
1	A	150	ILE
2	B	130	ASP
2	B	317	SER

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Mol	Chain	Res	Type
1	C	138	ASN
1	C	150	ILE
2	D	130	ASP
2	D	284	PRO
2	D	304	ALA
2	D	317	SER
2	D	464	HIS
1	A	138	ASN
2	B	196	SER
2	B	238	PRO
2	B	303	THR
2	D	236	PRO
2	D	240	CYS
2	D	302	HIS
1	A	30	ASN
1	A	199	LYS
2	B	445	LYS
1	C	199	LYS
2	D	196	SER
2	D	235	LYS
2	D	445	LYS
1	A	40	PRO
1	A	80	PRO
2	B	9	GLY
2	B	451	ARG
1	C	76	SER
2	D	26	GLY
2	D	313	TYR
2	B	180	SER
2	B	242	CYS
2	D	243	PRO
2	B	237	CYS
2	D	175	PRO
2	D	232	ILE
2	D	451	ARG
1	A	31	VAL
2	D	260	ILE
1	A	83	ILE
2	D	151	PRO
2	D	213	PRO
2	B	135	GLY
2	B	213	PRO

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Mol	Chain	Res	Type
2	D	135	GLY
2	B	151	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	190/190 (100%)	170 (90%)	20 (10%)	8	24
1	C	190/190 (100%)	175 (92%)	15 (8%)	15	40
2	B	399/399 (100%)	359 (90%)	40 (10%)	9	27
2	D	399/399 (100%)	360 (90%)	39 (10%)	10	28
All	All	1178/1178 (100%)	1064 (90%)	114 (10%)	10	29

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	17	ASP
1	A	22	THR
1	A	23	CYS
1	A	26	SER
1	A	40	PRO
1	A	49	TYR
1	A	50	LYS
1	A	63	SER
1	A	74	THR
1	A	80	PRO
1	A	81	GLU
1	A	89	GLN
1	A	92	GLN
1	A	102	THR
1	A	136	LEU
1	A	163	TRP
1	A	176	SER
1	A	179	LEU

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Mol	Chain	Res	Type
1	A	185	GLU
2	B	6	GLU
2	B	50	TYR
2	B	52(A)	ASN
2	B	81	GLN
2	B	82(B)	ARG
2	B	89	MET
2	B	100(K)	MET
2	B	113	SER
2	B	115	LYS
2	B	128	CYS
2	B	139	THR
2	B	156	THR
2	B	162	ASN
2	B	187	LEU
2	B	203	GLN
2	B	237	CYS
2	B	271	ILE
2	B	283	ASP
2	B	289	SER
2	B	295	ASN
2	B	302	HIS
2	B	309	HIS
2	B	310	ARG
2	B	317	SER
2	B	328	GLN
2	B	347	LEU
2	B	355	ILE
2	B	357	SER
2	B	369	VAL
2	B	370	TYR
2	B	373	PRO
2	B	381	MET
2	B	402	VAL
2	B	417	LEU
2	B	420	LYS
2	B	437	MET
2	B	444	GLU
2	B	451	ARG
2	B	452	ASN
2	B	453	SER
1	C	3	VAL

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Mol	Chain	Res	Type
1	C	11	LEU
1	C	14	SER
1	C	21	ILE
1	C	37	GLN
1	C	43	ILE
1	C	79	GLN
1	C	89	GLN
1	C	92	GLN
1	C	98	PHE
1	C	116	SER
1	C	154	GLU
1	C	156	GLN
1	C	161	ASN
1	C	212	ASN
2	D	2	VAL
2	D	12	VAL
2	D	14	PRO
2	D	18	LEU
2	D	22	CYS
2	D	37	VAL
2	D	56	SER
2	D	62	THR
2	D	77	THR
2	D	82(A)	SER
2	D	89	MET
2	D	105	GLN
2	D	113	SER
2	D	117	THR
2	D	143	LEU
2	D	175	PRO
2	D	178	LEU
2	D	187	LEU
2	D	192	THR
2	D	217	THR
2	D	260	ILE
2	D	295	ASN
2	D	300	GLU
2	D	307	GLN
2	D	312	ASP
2	D	331	ASP
2	D	346	ASP
2	D	363	SER

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Mol	Chain	Res	Type
2	D	385	GLN
2	D	387	THR
2	D	388	LEU
2	D	402	VAL
2	D	422	THR
2	D	425	VAL
2	D	452	ASN
2	D	457	SER
2	D	458	VAL
2	D	464	HIS
2	D	472	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	30	ASN
1	A	37	GLN
1	A	92	GLN
1	A	124	GLN
1	A	210	ASN
2	B	162	ASN
2	B	179	GLN
2	B	203	GLN
2	B	209	ASN
2	B	295	ASN
2	B	421	ASN
1	C	37	GLN
1	C	89	GLN
1	C	189	HIS
2	D	209	ASN
2	D	307	GLN
2	D	368	GLN
2	D	385	GLN
2	D	460	HIS
2	D	466	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	0.90	1 (7%)	15,19,21	1.61	3 (20%)
3	FUL	B	476	3	10,10,11	0.54	0	14,14,16	0.54	0
3	NAG	B	477	3	14,14,15	0.67	0	15,19,21	1.28	2 (13%)
3	BMA	B	478	3	11,11,12	0.47	0	14,15,17	0.92	1 (7%)
3	MAN	B	479	3	11,11,12	0.58	0	14,15,17	0.57	0
3	NAG	B	480	3	14,14,15	0.49	0	15,19,21	0.50	0
3	GAL	B	481	3	11,11,12	0.56	0	14,15,17	0.63	0
3	MAN	B	482	3	11,11,12	0.35	0	14,15,17	0.58	0
3	NAG	B	483	3	14,14,15	0.45	0	15,19,21	0.58	0
4	NAG	D	475	2,4	14,14,15	0.82	0	15,19,21	0.68	0
4	FUC	D	476	4	10,10,11	0.42	0	14,14,16	0.65	0
4	NAG	D	477	4	14,14,15	0.84	0	15,19,21	0.79	1 (6%)
4	BMA	D	478	4	11,11,12	0.51	0	14,15,17	0.63	0
4	MAN	D	479	4	11,11,12	0.67	0	14,15,17	0.74	1 (7%)
4	NAG	D	480	4	14,14,15	0.61	0	15,19,21	0.72	1 (6%)
4	GAL	D	481	4	11,11,12	0.52	0	14,15,17	0.82	1 (7%)
4	MAN	D	482	4	11,11,12	0.45	0	14,15,17	0.55	0
4	NAG	D	483	4	14,14,15	0.47	0	15,19,21	0.63	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	NAG	B	477	3	1/1/7/7	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	NAG	D	477	4	1/1/7/7	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
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	2.42	1.55	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	475	NAG	C4-C3-C2	-4.05	104.93	111.23
3	B	477	NAG	C3-C4-C5	-3.14	104.73	110.20
3	B	475	NAG	C2-N2-C7	-2.90	119.32	123.04
3	B	475	NAG	C3-C4-C5	-2.44	105.94	110.20
4	D	480	NAG	C2-N2-C7	-2.24	120.16	123.04
3	B	478	BMA	C1-C2-C3	2.14	112.07	109.54
4	D	479	MAN	C1-C2-C3	2.22	112.17	109.54
4	D	481	GAL	C1-O5-C5	2.22	115.07	112.25
4	D	477	NAG	C1-O5-C5	2.32	115.20	112.25
3	B	477	NAG	C1-O5-C5	2.40	115.29	112.25

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	D	477	NAG	C1
3	B	477	NAG	C1

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Mol	Chain	Res	Type	Atom
4	D	476	FUC	C1

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	475	NAG	3	0
3	B	477	NAG	2	0
3	B	481	GAL	3	0
4	D	481	GAL	3	0

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

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

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

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

### 6.3 Carbohydrates [i](#)

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

### 6.4 Ligands [i](#)

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

### 6.5 Other polymers [i](#)

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