



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 31, 2017 – 03:41 AM EDT

PDB ID : 3SDA  
Title : Crystal structure of autoreactive-Valpha14-Vbeta6 NKT TCR in complex with CD1d-beta-galactosylceramide  
Authors : Clarke, A.J.; Rossjohn, J.  
Deposited on : unknown  
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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

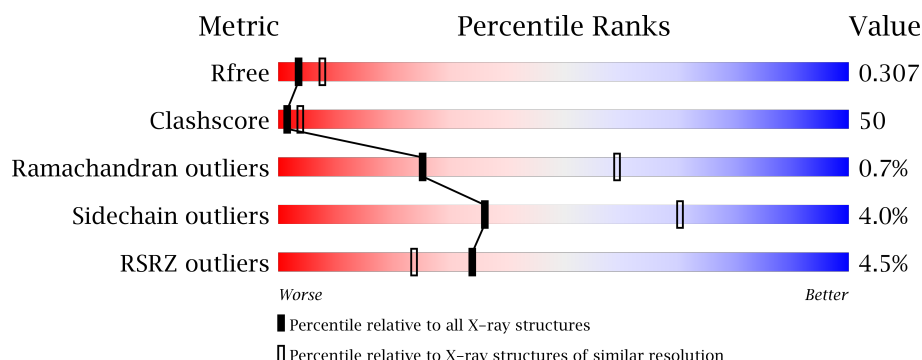
# 1 Overall quality at a glance

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))
$R_{free}$	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (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.

Mol	Chain	Length	Quality of chain
1	A	302	<div> <div>0.1%</div> <div>54%</div> <div>40%</div> <div>0.1%</div> <div>0.1%</div> </div>
2	B	99	<div> <div>3%</div> <div>54%</div> <div>44%</div> <div>0.1%</div> <div>0.1%</div> </div>
3	C	207	<div> <div>8%</div> <div>43%</div> <div>47%</div> <div>5%</div> <div>5%</div> </div>
4	D	245	<div> <div>6%</div> <div>42%</div> <div>51%</div> <div>0.1%</div> <div>0.1%</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	GCY	A	601	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6739 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Antigen-presenting glycoprotein CD1d1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	290	Total	C	N	O	S	10	0	0
			2333	1486	406	427	14			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	201	HIS	ASP	SEE REMARK 999	UNP P11609
A	280	GLY	-	EXPRESSION TAG	UNP P11609
A	281	SER	-	EXPRESSION TAG	UNP P11609
A	282	LEU	-	EXPRESSION TAG	UNP P11609
A	283	HIS	-	EXPRESSION TAG	UNP P11609
A	284	HIS	-	EXPRESSION TAG	UNP P11609
A	285	ILE	-	EXPRESSION TAG	UNP P11609
A	286	LEU	-	EXPRESSION TAG	UNP P11609
A	287	ASP	-	EXPRESSION TAG	UNP P11609
A	288	ALA	-	EXPRESSION TAG	UNP P11609
A	289	GLN	-	EXPRESSION TAG	UNP P11609
A	290	LYS	-	EXPRESSION TAG	UNP P11609
A	291	MET	-	EXPRESSION TAG	UNP P11609
A	292	VAL	-	EXPRESSION TAG	UNP P11609
A	293	TRP	-	EXPRESSION TAG	UNP P11609
A	294	ASN	-	EXPRESSION TAG	UNP P11609
A	295	HIS	-	EXPRESSION TAG	UNP P11609
A	296	ARG	-	EXPRESSION TAG	UNP P11609
A	297	HIS	-	EXPRESSION TAG	UNP P11609
A	298	HIS	-	EXPRESSION TAG	UNP P11609
A	299	HIS	-	EXPRESSION TAG	UNP P11609
A	300	HIS	-	EXPRESSION TAG	UNP P11609
A	301	HIS	-	EXPRESSION TAG	UNP P11609
A	302	HIS	-	EXPRESSION TAG	UNP P11609

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	3	0	0
			814	520	138	149	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	85	ALA	ASP	SEE REMARK 999	UNP P01887

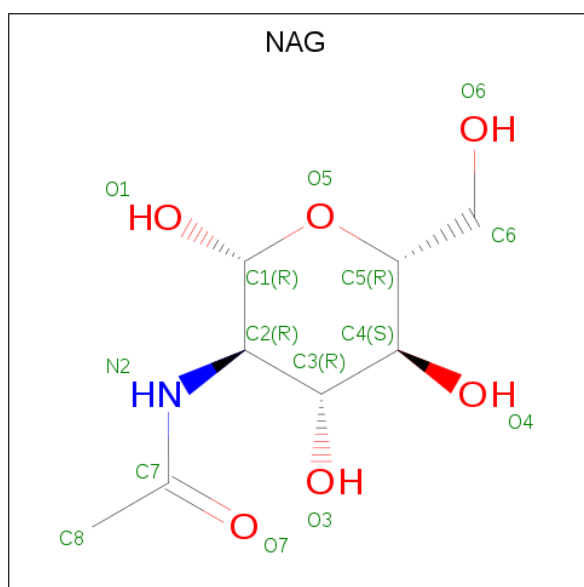
- Molecule 3 is a protein called NKT TCR Valpha14 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	196	Total	C	N	O	S	5	0	0
			1511	937	260	307	7			

- Molecule 4 is a protein called NKT TCR autoreactive-Vbeta6 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	239	Total	C	N	O	S	7	0	0
			1900	1202	326	365	7			

- Molecule 5 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



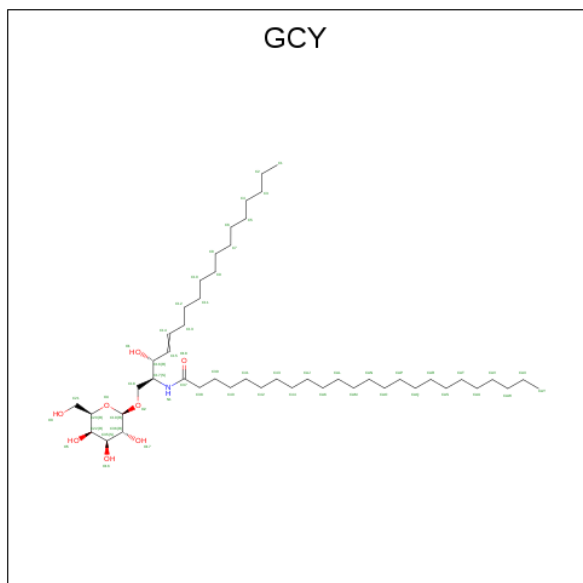
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 6 is N-[(2S,3R)-1-(beta-D-galactopyranosyloxy)-3-hydroxyoctadec-4-en-2-yl]tetracosanamide (three-letter code: GCY) (formula: C<sub>48</sub>H<sub>93</sub>NO<sub>8</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			57	48	1	8		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			6	3	3		

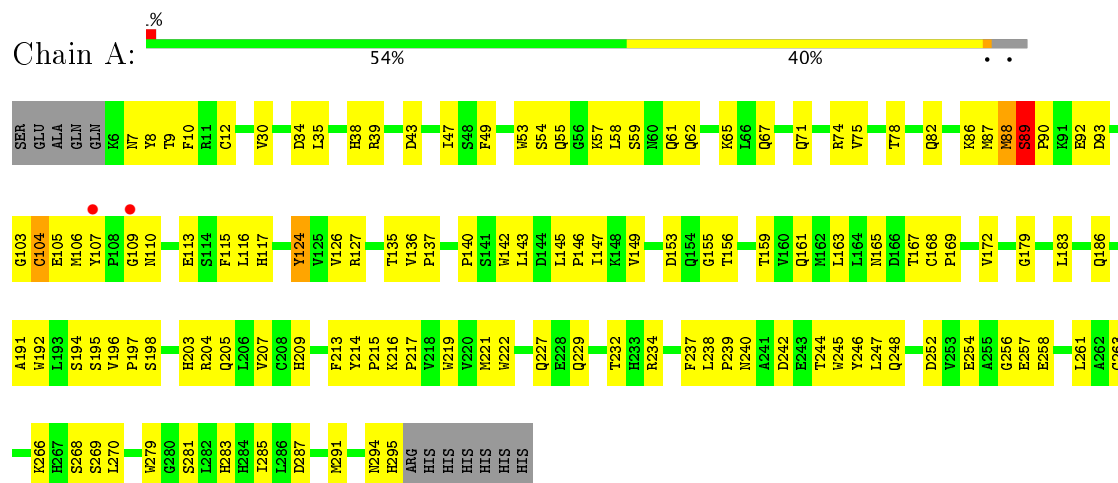
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	19	Total	O	0	0
			19	19		
8	B	12	Total	O	0	0
			12	12		
8	C	16	Total	O	0	0
			16	16		
8	D	15	Total	O	0	0
			15	15		

### 3 Residue-property plots

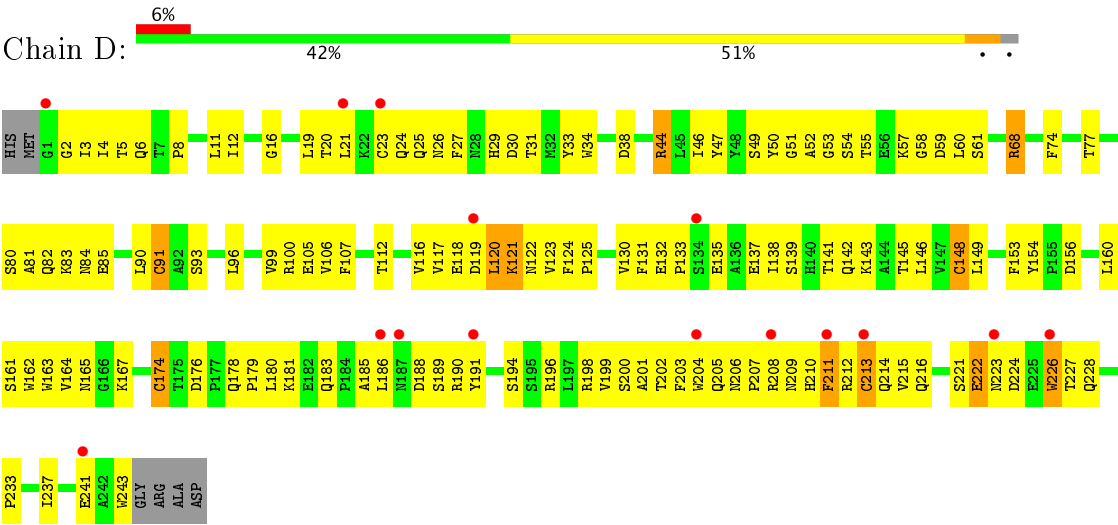
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

#### • Molecule 1: Antigen-presenting glycoprotein CD1d1





● Molecule 4: NKT TCR autoreactive-Vbeta6 chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.75Å 94.75Å 287.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	65.25 – 2.80 65.25 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.0 (65.25-2.80) 97.0 (65.25-2.80)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	0.18	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.67 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.272 , 0.312 0.272 , 0.307	Depositor DCC
$R_{free}$ test set	1634 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	64.9	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 51.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	6739	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	1.51	2/2403 (0.1%)	0.72	0/3266
2	B	1.47	0/840	0.79	2/1140 (0.2%)
3	C	1.28	0/1536	0.78	1/2085 (0.0%)
4	D	1.26	2/1947 (0.1%)	0.75	1/2640 (0.0%)
All	All	1.39	4/6726 (0.1%)	0.75	4/9131 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	12	CYS	CB-SG	-6.61	1.71	1.82
1	A	124	TYR	CD2-CE2	-5.53	1.31	1.39
4	D	106	VAL	CB-CG2	-5.52	1.41	1.52
4	D	105	GLU	CD-OE1	-5.12	1.20	1.25

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	90	CYS	CA-CB-SG	7.63	127.74	114.00
4	D	91	CYS	CA-CB-SG	7.10	126.77	114.00
2	B	80	CYS	CA-CB-SG	7.08	126.75	114.00
2	B	25	CYS	CA-CB-SG	6.40	125.51	114.00

There are no chirality outliers.

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	2333	0	2233	147	1
2	B	814	0	790	73	0
3	C	1511	0	1464	187	0
4	D	1900	0	1829	280	0
5	A	56	0	51	0	0
6	A	57	0	88	9	0
7	B	6	0	8	1	0
8	A	19	0	0	1	0
8	B	12	0	0	0	0
8	C	16	0	0	0	0
8	D	15	0	0	2	0
All	All	6739	0	6463	651	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 50.

All (651) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:140:LEU:CD1	3:C:178:ALA:O	1.67	1.43
4:D:8:PRO:HD2	4:D:21:LEU:CD2	1.49	1.42
2:B:25:CYS:SG	2:B:80:CYS:CB	2.11	1.39
1:A:89:SER:HB2	1:A:90:PRO:CD	1.45	1.38
3:C:130:ASP:CB	4:D:131:PHE:CD2	2.05	1.37
4:D:30:ASP:HB2	4:D:96:LEU:CD1	1.57	1.34
4:D:23:CYS:SG	4:D:34:TRP:CZ2	2.23	1.31
4:D:226:TRP:CZ2	4:D:228:GLN:HB2	1.65	1.31
4:D:131:PHE:CE1	4:D:149:LEU:HD12	1.70	1.25
3:C:131:SER:HB2	3:C:132:LYS:CA	1.67	1.24
3:C:131:SER:HB2	3:C:132:LYS:C	1.56	1.23
3:C:22:CYS:CB	3:C:90:CYS:SG	2.25	1.23
4:D:176:ASP:OD2	4:D:194:SER:OG	1.56	1.23
2:B:38:GLN:NE2	2:B:45:LYS:CD	2.01	1.22
4:D:4:ILE:CG1	4:D:27:PHE:HE1	1.53	1.22
4:D:131:PHE:CE1	4:D:149:LEU:CD1	2.24	1.20
4:D:4:ILE:HG13	4:D:27:PHE:CE1	1.77	1.20
3:C:22:CYS:SG	3:C:90:CYS:SG	1.36	1.17
2:B:51:MET:SD	2:B:66:ALA:HB2	1.86	1.16
4:D:131:PHE:HE1	4:D:149:LEU:CD1	1.58	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:CYS:SG	1:A:168:CYS:SG	1.36	1.15
2:B:38:GLN:HE21	2:B:45:LYS:CG	1.59	1.14
1:A:89:SER:CB	1:A:90:PRO:CD	2.25	1.13
4:D:176:ASP:CG	4:D:194:SER:OG	1.86	1.12
4:D:4:ILE:HG13	4:D:27:PHE:HE1	0.98	1.10
2:B:63:TYR:OH	7:B:100:GOL:O1	1.68	1.10
4:D:30:ASP:HB2	4:D:96:LEU:HD11	1.10	1.09
3:C:130:ASP:CB	3:C:136:LYS:O	1.99	1.09
3:C:157:ASP:OD1	3:C:158:VAL:HG23	1.51	1.09
4:D:181:LYS:HG2	4:D:191:TYR:CE1	1.87	1.09
4:D:216:GLN:OE1	4:D:237:ILE:HG12	1.52	1.09
2:B:23:LEU:HB2	2:B:70:PHE:CE2	1.86	1.08
1:A:104:CYS:CB	1:A:168:CYS:SG	2.41	1.08
3:C:130:ASP:CB	4:D:131:PHE:CE2	2.36	1.08
2:B:38:GLN:HE21	2:B:45:LYS:CD	1.62	1.08
4:D:8:PRO:HD2	4:D:21:LEU:HD23	1.21	1.08
3:C:22:CYS:SG	3:C:90:CYS:CB	2.40	1.08
3:C:152:GLN:CA	3:C:160:ILE:HD11	1.83	1.07
1:A:135:THR:HG23	1:A:147:ILE:CD1	1.84	1.07
2:B:38:GLN:NE2	2:B:45:LYS:HG2	1.67	1.07
3:C:16:GLU:O	3:C:80:THR:HG23	1.54	1.07
4:D:117:VAL:HG21	4:D:154:TYR:HE2	0.97	1.07
4:D:117:VAL:HG21	4:D:154:TYR:CE2	1.88	1.06
2:B:38:GLN:NE2	2:B:45:LYS:CG	2.17	1.06
4:D:30:ASP:CB	4:D:96:LEU:HD11	1.84	1.06
3:C:136:LYS:O	4:D:131:PHE:HE2	1.38	1.06
3:C:166:LEU:CD1	3:C:166:LEU:H	1.67	1.06
3:C:131:SER:HB2	3:C:132:LYS:HA	1.34	1.04
3:C:152:GLN:HA	3:C:160:ILE:CD1	1.87	1.04
2:B:25:CYS:SG	2:B:80:CYS:SG	1.03	1.03
4:D:206:ASN:HD22	4:D:208:ARG:HB2	1.20	1.03
4:D:117:VAL:CG2	4:D:154:TYR:HE2	1.71	1.02
3:C:136:LYS:O	4:D:131:PHE:CE2	2.14	1.01
4:D:8:PRO:HD2	4:D:21:LEU:HD22	1.33	1.01
4:D:21:LEU:CD1	4:D:112:THR:HG21	1.91	1.00
3:C:127:GLN:HG3	3:C:189:CYS:SG	2.00	1.00
3:C:140:LEU:HD12	3:C:178:ALA:O	0.85	1.00
2:B:51:MET:SD	2:B:66:ALA:CB	2.49	1.00
3:C:135:ASP:HA	3:C:136:LYS:HB2	1.40	1.00
3:C:126:TYR:CE1	4:D:137:GLU:CA	2.45	1.00
4:D:8:PRO:CD	4:D:21:LEU:CD2	2.40	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:PRO:HB2	1:A:142:TRP:CD1	1.97	1.00
3:C:131:SER:HB2	3:C:132:LYS:O	1.62	0.99
2:B:38:GLN:HE21	2:B:45:LYS:HG2	1.19	0.99
4:D:137:GLU:O	4:D:141:THR:OG1	1.79	0.98
3:C:144:PHE:HD1	3:C:148:THR:OG1	1.45	0.98
1:A:89:SER:CB	1:A:90:PRO:HD3	1.86	0.98
1:A:142:TRP:CH2	1:A:143:LEU:HD13	1.98	0.98
2:B:29:GLN:HA	2:B:61:SER:OG	1.63	0.98
2:B:81:ARG:HG3	2:B:92:THR:OG1	1.64	0.98
1:A:205:GLN:HG2	1:A:252:ASP:OD1	1.64	0.98
4:D:185:ALA:H	4:D:186:LEU:HA	1.28	0.98
4:D:49:SER:OG	4:D:68:ARG:HD2	1.64	0.97
2:B:70:PHE:HD1	2:B:78:TYR:CZ	1.82	0.96
4:D:164:VAL:HG22	4:D:165:ASN:H	1.30	0.96
4:D:226:TRP:CE2	4:D:228:GLN:HB2	2.00	0.96
1:A:186:GLN:NE2	1:A:268:SER:OG	1.98	0.96
3:C:130:ASP:CB	4:D:131:PHE:HD2	1.77	0.96
3:C:55:LYS:HG2	3:C:65:THR:HG22	1.48	0.95
4:D:21:LEU:HD11	4:D:112:THR:HG21	1.46	0.95
4:D:30:ASP:HB2	4:D:96:LEU:HD13	1.47	0.95
3:C:60:ARG:NH2	3:C:84:ASP:OD2	1.99	0.94
4:D:160:LEU:HD13	4:D:215:VAL:HG22	1.48	0.94
4:D:164:VAL:HG22	4:D:165:ASN:N	1.79	0.94
3:C:126:TYR:HE1	4:D:137:GLU:CA	1.79	0.94
4:D:181:LYS:HG2	4:D:191:TYR:HE1	1.26	0.94
3:C:131:SER:CB	3:C:132:LYS:C	2.36	0.94
3:C:161:THR:OG1	3:C:179:VAL:N	2.00	0.93
4:D:6:GLN:NE2	4:D:91:CYS:H	1.67	0.93
1:A:145:LEU:HB3	1:A:146:PRO:HD3	1.49	0.93
3:C:131:SER:CB	3:C:132:LYS:HA	1.96	0.93
4:D:226:TRP:CZ2	4:D:228:GLN:CB	2.52	0.93
4:D:131:PHE:HE1	4:D:149:LEU:HD12	1.11	0.93
3:C:134:SER:O	3:C:136:LYS:HB2	1.69	0.91
3:C:166:LEU:HD12	3:C:166:LEU:H	1.33	0.91
4:D:131:PHE:CZ	4:D:149:LEU:HD12	2.04	0.91
4:D:4:ILE:CG1	4:D:27:PHE:CE1	2.45	0.90
2:B:25:CYS:SG	2:B:80:CYS:HB2	2.10	0.90
3:C:126:TYR:HE1	4:D:137:GLU:N	1.70	0.89
2:B:38:GLN:OE1	2:B:81:ARG:NH2	2.05	0.89
3:C:166:LEU:N	3:C:166:LEU:CD1	2.30	0.89
4:D:206:ASN:ND2	4:D:208:ARG:HB2	1.87	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:SER:HB2	1:A:90:PRO:HD3	0.91	0.89
4:D:226:TRP:O	4:D:226:TRP:HD1	1.56	0.89
4:D:117:VAL:CG2	4:D:154:TYR:CE2	2.51	0.88
3:C:166:LEU:HD12	3:C:166:LEU:N	1.89	0.88
3:C:196:SER:O	3:C:197:ILE:HG13	1.74	0.87
3:C:140:LEU:HD13	3:C:179:VAL:HG22	1.56	0.87
4:D:25:GLN:OE1	4:D:29:HIS:HB2	1.74	0.86
1:A:135:THR:CG2	1:A:147:ILE:CD1	2.52	0.86
3:C:140:LEU:HD12	3:C:178:ALA:C	1.95	0.86
3:C:203:PHE:HD1	3:C:204:PHE:N	1.72	0.86
4:D:226:TRP:C	4:D:226:TRP:CD1	2.48	0.86
3:C:140:LEU:HD13	3:C:179:VAL:CG2	2.07	0.85
3:C:128:LEU:HB3	4:D:132:GLU:O	1.76	0.85
2:B:70:PHE:CD1	2:B:78:TYR:CE2	2.64	0.85
3:C:145:ASP:OD1	3:C:146:SER:N	2.10	0.85
1:A:227:GLN:HG3	1:A:227:GLN:O	1.76	0.84
3:C:194:ASN:O	3:C:195:ASN:HB2	1.77	0.84
3:C:203:PHE:O	3:C:204:PHE:CD2	2.30	0.84
3:C:166:LEU:HD13	3:C:166:LEU:H	1.42	0.84
3:C:47:THR:OG1	3:C:56:THR:OG1	1.90	0.84
3:C:126:TYR:CE1	4:D:137:GLU:N	2.46	0.84
2:B:23:LEU:HB2	2:B:70:PHE:HE2	1.41	0.83
1:A:198:SER:HB3	1:A:205:GLN:HG3	1.60	0.83
4:D:131:PHE:CE1	4:D:149:LEU:HD11	2.12	0.83
3:C:202:THR:O	3:C:204:PHE:CE2	2.32	0.82
3:C:140:LEU:CD1	3:C:178:ALA:C	2.47	0.82
3:C:166:LEU:HD13	3:C:166:LEU:O	1.79	0.82
4:D:186:LEU:O	4:D:186:LEU:HD12	1.79	0.82
4:D:145:THR:HG22	4:D:198:ARG:HG3	1.61	0.82
4:D:185:ALA:N	4:D:186:LEU:HA	1.87	0.82
4:D:6:GLN:HE22	4:D:90:LEU:HA	1.44	0.82
3:C:126:TYR:CE1	4:D:137:GLU:HA	2.12	0.82
4:D:180:LEU:O	4:D:191:TYR:HA	1.78	0.82
4:D:51:GLY:O	4:D:68:ARG:HD3	1.79	0.82
3:C:144:PHE:CD1	3:C:148:THR:OG1	2.30	0.82
4:D:38:ASP:OD2	4:D:44:ARG:NH2	2.13	0.81
3:C:145:ASP:O	3:C:148:THR:OG1	1.98	0.81
3:C:203:PHE:HD1	3:C:204:PHE:H	1.28	0.81
4:D:216:GLN:OE1	4:D:237:ILE:CG1	2.28	0.81
4:D:226:TRP:NE1	4:D:228:GLN:O	2.12	0.81
3:C:22:CYS:HG	3:C:90:CYS:CB	1.91	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:TRP:HH2	6:A:601:GCY:H2	1.44	0.80
1:A:143:LEU:HD11	6:A:601:GCY:H4	1.60	0.80
4:D:138:ILE:HD12	4:D:138:ILE:H	1.46	0.80
3:C:165:VAL:N	4:D:174:CYS:SG	2.55	0.80
1:A:135:THR:CG2	1:A:147:ILE:HD11	2.11	0.80
2:B:70:PHE:CD1	2:B:78:TYR:CZ	2.69	0.80
3:C:55:LYS:CG	3:C:65:THR:HG22	2.11	0.80
4:D:145:THR:HG22	4:D:198:ARG:CG	2.12	0.80
3:C:161:THR:HG21	3:C:179:VAL:HB	1.64	0.80
4:D:4:ILE:CD1	4:D:27:PHE:HE1	1.94	0.79
2:B:30:PHE:CZ	2:B:54:MET:HE3	2.17	0.79
3:C:86:ALA:O	3:C:88:TYR:CE1	2.35	0.79
4:D:207:PRO:HA	4:D:243:TRP:O	1.82	0.79
4:D:207:PRO:HB3	4:D:243:TRP:O	1.82	0.79
3:C:118:ILE:HD12	3:C:145:ASP:HA	1.65	0.79
3:C:152:GLN:HA	3:C:160:ILE:HD11	0.91	0.79
3:C:194:ASN:O	3:C:195:ASN:CB	2.31	0.79
4:D:117:VAL:HG22	8:D:252:HOH:O	1.81	0.79
4:D:137:GLU:O	4:D:141:THR:N	2.15	0.78
4:D:3:ILE:O	4:D:26:ASN:OD1	2.01	0.78
4:D:226:TRP:O	4:D:226:TRP:CD1	2.36	0.78
4:D:160:LEU:HD13	4:D:215:VAL:CG2	2.14	0.78
1:A:59:SER:CB	1:A:62:GLN:OE1	2.31	0.77
3:C:203:PHE:C	3:C:204:PHE:HD2	1.86	0.77
4:D:47:TYR:CE1	4:D:57:LYS:HG2	2.19	0.77
3:C:198:ILE:HD11	3:C:202:THR:HG21	1.66	0.77
4:D:23:CYS:SG	4:D:34:TRP:CE2	2.77	0.77
1:A:55:GLN:NE2	1:A:58:LEU:O	2.16	0.77
2:B:70:PHE:HD1	2:B:78:TYR:CE2	2.00	0.77
3:C:126:TYR:CE1	4:D:137:GLU:HB2	2.19	0.76
1:A:186:GLN:HE22	1:A:268:SER:HG	1.32	0.76
3:C:177:SER:OG	4:D:196:ARG:HD3	1.83	0.76
2:B:22:ILE:HD13	2:B:69:GLU:HG3	1.67	0.76
3:C:126:TYR:CE1	4:D:137:GLU:CB	2.69	0.76
3:C:22:CYS:HB2	3:C:90:CYS:SG	2.25	0.76
3:C:177:SER:OG	4:D:196:ARG:CD	2.34	0.76
1:A:89:SER:CB	1:A:90:PRO:HD2	2.15	0.76
4:D:23:CYS:SG	4:D:34:TRP:CH2	2.78	0.75
3:C:135:ASP:CA	3:C:136:LYS:HB2	2.17	0.75
4:D:8:PRO:CD	4:D:21:LEU:HD23	2.09	0.74
1:A:57:LYS:O	1:A:57:LYS:HG2	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:203:PHE:C	3:C:204:PHE:CD2	2.61	0.74
6:A:601:GCY:H18	6:A:601:GCY:O17	1.89	0.73
3:C:198:ILE:HD12	3:C:199:PRO:HD2	1.70	0.73
4:D:199:VAL:HG21	4:D:203:PHE:CD1	2.23	0.73
4:D:6:GLN:HE21	4:D:91:CYS:H	1.36	0.73
2:B:30:PHE:CZ	2:B:54:MET:CE	2.71	0.73
4:D:21:LEU:HD13	4:D:112:THR:HG21	1.68	0.73
4:D:8:PRO:CD	4:D:21:LEU:HD22	2.11	0.73
3:C:130:ASP:HA	4:D:131:PHE:HA	1.70	0.72
3:C:22:CYS:SG	3:C:90:CYS:HB3	2.28	0.72
4:D:164:VAL:CG2	4:D:165:ASN:H	2.02	0.72
1:A:135:THR:HG23	1:A:147:ILE:HD13	1.72	0.72
4:D:210:HIS:NE2	4:D:241:GLU:HG3	2.05	0.72
4:D:141:THR:C	4:D:142:GLN:HG2	2.08	0.72
4:D:211:PHE:N	4:D:211:PHE:CD2	2.56	0.72
4:D:135:GLU:HA	4:D:138:ILE:HD13	1.72	0.72
1:A:227:GLN:CG	1:A:227:GLN:O	2.38	0.71
3:C:85:THR:O	3:C:112:LEU:O	2.08	0.71
4:D:3:ILE:HG22	4:D:4:ILE:N	2.05	0.71
4:D:131:PHE:CZ	4:D:149:LEU:CD1	2.70	0.71
1:A:140:PRO:CB	1:A:142:TRP:CD1	2.72	0.70
1:A:242:ASP:OD1	1:A:244:THR:OG1	2.08	0.70
1:A:281:SER:O	1:A:285:ILE:HG13	1.91	0.70
1:A:142:TRP:CH2	6:A:601:GCY:H2	2.27	0.70
2:B:73:THR:OG1	2:B:76:ASP:OD1	2.10	0.69
3:C:131:SER:CB	3:C:132:LYS:O	2.38	0.69
4:D:206:ASN:O	4:D:206:ASN:CG	2.30	0.69
4:D:30:ASP:CB	4:D:96:LEU:CD1	2.51	0.69
4:D:46:ILE:O	4:D:58:GLY:N	2.23	0.69
4:D:135:GLU:CA	4:D:138:ILE:HD13	2.22	0.69
3:C:203:PHE:CD1	3:C:204:PHE:N	2.58	0.69
1:A:110:ASN:O	1:A:110:ASN:OD1	2.10	0.69
3:C:24:TYR:CE1	3:C:71:LYS:HD3	2.27	0.69
4:D:4:ILE:CD1	4:D:27:PHE:CE1	2.74	0.68
4:D:131:PHE:HE1	4:D:149:LEU:CG	2.07	0.68
1:A:135:THR:HG22	1:A:147:ILE:HD11	1.76	0.68
3:C:202:THR:O	3:C:204:PHE:HE2	1.75	0.68
3:C:138:VAL:HG23	3:C:181:TRP:HB3	1.75	0.68
4:D:226:TRP:CD2	4:D:228:GLN:OE1	2.47	0.68
4:D:207:PRO:CA	4:D:243:TRP:O	2.42	0.68
4:D:4:ILE:HA	4:D:24:GLN:O	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:HIS:CD2	1:A:295:HIS:H	2.10	0.67
4:D:202:THR:O	4:D:205:GLN:HB2	1.94	0.67
1:A:74:ARG:NH1	8:A:312:HOH:O	2.25	0.67
3:C:202:THR:O	3:C:204:PHE:CD2	2.47	0.67
4:D:16:GLY:HA2	4:D:80:SER:OG	1.95	0.67
2:B:30:PHE:CE2	2:B:54:MET:HE3	2.28	0.67
4:D:216:GLN:CD	4:D:237:ILE:HG12	2.15	0.67
4:D:122:ASN:O	4:D:124:PHE:CD2	2.47	0.67
2:B:17:ASN:OD1	2:B:73:THR:CA	2.43	0.67
4:D:51:GLY:C	4:D:68:ARG:HD3	2.15	0.67
4:D:160:LEU:CD1	4:D:215:VAL:HG22	2.25	0.66
1:A:30:VAL:HB	1:A:38:HIS:HB2	1.76	0.66
4:D:138:ILE:N	4:D:138:ILE:HD12	2.11	0.66
4:D:11:LEU:HD12	4:D:12:ILE:N	2.11	0.66
1:A:227:GLN:HE21	1:A:229:GLN:HE22	1.43	0.66
4:D:25:GLN:NE2	4:D:29:HIS:O	2.29	0.66
3:C:141:PHE:CZ	3:C:144:PHE:HB3	2.31	0.66
3:C:118:ILE:CD1	3:C:145:ASP:HA	2.25	0.66
3:C:43:LEU:HD12	3:C:43:LEU:N	2.09	0.66
2:B:38:GLN:HE22	2:B:45:LYS:CD	1.89	0.66
1:A:205:GLN:HG2	1:A:252:ASP:CG	2.16	0.65
3:C:127:GLN:CG	3:C:189:CYS:SG	2.82	0.65
3:C:125:VAL:HA	3:C:140:LEU:O	1.97	0.65
4:D:25:GLN:OE1	4:D:93:SER:HB2	1.96	0.65
1:A:191:ALA:HA	1:A:209:HIS:O	1.96	0.65
1:A:78:THR:O	1:A:82:GLN:HG3	1.97	0.65
4:D:145:THR:HG22	4:D:198:ARG:CD	2.27	0.65
4:D:31:THR:HG21	4:D:33:TYR:OH	1.97	0.65
4:D:227:THR:HG23	4:D:228:GLN:N	2.11	0.65
4:D:207:PRO:CB	4:D:243:TRP:O	2.45	0.64
1:A:59:SER:HB2	1:A:62:GLN:OE1	1.95	0.64
2:B:81:ARG:HG3	2:B:92:THR:HG1	1.61	0.64
2:B:30:PHE:HZ	2:B:54:MET:HE3	1.63	0.64
2:B:30:PHE:CE2	2:B:54:MET:CE	2.81	0.64
4:D:4:ILE:HD11	4:D:27:PHE:CE1	2.33	0.64
1:A:116:LEU:C	1:A:116:LEU:HD23	2.18	0.64
3:C:125:VAL:O	3:C:125:VAL:HG22	1.96	0.64
2:B:17:ASN:OD1	2:B:73:THR:HA	1.98	0.63
4:D:209:ASN:HB3	4:D:211:PHE:CE2	2.33	0.63
4:D:221:SER:O	4:D:224:ASP:N	2.29	0.63
3:C:136:LYS:C	4:D:131:PHE:HE2	2.02	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:SER:OG	1:A:62:GLN:OE1	2.16	0.63
2:B:96:ASP:C	2:B:96:ASP:OD1	2.34	0.62
3:C:161:THR:CG2	3:C:179:VAL:HB	2.29	0.62
4:D:221:SER:O	4:D:223:ASN:N	2.31	0.62
1:A:294:ASN:O	1:A:295:HIS:C	2.37	0.62
4:D:206:ASN:C	4:D:208:ARG:H	2.01	0.62
4:D:226:TRP:CH2	4:D:228:GLN:HB2	2.27	0.62
3:C:19:VAL:O	3:C:19:VAL:HG12	1.99	0.62
4:D:132:GLU:HB3	4:D:133:PRO:HD2	1.82	0.62
4:D:185:ALA:N	4:D:186:LEU:CA	2.60	0.62
1:A:49:PHE:CD2	1:A:54:SER:HB3	2.35	0.62
3:C:124:ALA:CB	3:C:126:TYR:CE2	2.83	0.62
3:C:196:SER:O	3:C:197:ILE:CG1	2.47	0.62
4:D:164:VAL:O	4:D:165:ASN:C	2.37	0.62
4:D:51:GLY:O	4:D:68:ARG:CD	2.47	0.62
1:A:143:LEU:C	1:A:146:PRO:HD2	2.19	0.61
4:D:145:THR:CG2	4:D:198:ARG:HG3	2.30	0.61
1:A:142:TRP:CZ3	1:A:143:LEU:HD13	2.35	0.61
1:A:143:LEU:O	1:A:146:PRO:HD2	2.01	0.61
1:A:53:TRP:CD2	1:A:179:GLY:HA3	2.35	0.61
3:C:43:LEU:CD1	3:C:43:LEU:N	2.62	0.61
1:A:142:TRP:CH2	1:A:143:LEU:CD1	2.78	0.61
4:D:146:LEU:N	4:D:146:LEU:HD12	2.16	0.61
3:C:166:LEU:HD13	3:C:166:LEU:N	2.07	0.61
4:D:137:GLU:O	4:D:141:THR:CB	2.49	0.60
6:A:601:GCY:O16	3:C:30:ASN:ND2	2.34	0.60
3:C:159:TYR:O	3:C:180:ALA:HA	2.01	0.60
3:C:124:ALA:HB1	3:C:126:TYR:CE2	2.37	0.60
1:A:196:VAL:HG13	1:A:197:PRO:N	2.16	0.60
3:C:166:LEU:HD11	3:C:175:SER:OG	2.02	0.60
4:D:25:GLN:HG3	4:D:25:GLN:O	2.00	0.60
1:A:145:LEU:O	1:A:149:VAL:HG23	2.01	0.60
4:D:213:CYS:O	4:D:213:CYS:SG	2.59	0.60
4:D:221:SER:O	4:D:222:GLU:C	2.39	0.59
1:A:142:TRP:CZ2	1:A:143:LEU:HD13	2.37	0.59
3:C:157:ASP:CG	3:C:158:VAL:HG23	2.23	0.59
3:C:126:TYR:HE1	4:D:137:GLU:HA	1.50	0.59
4:D:206:ASN:O	4:D:208:ARG:N	2.30	0.59
3:C:124:ALA:HB3	3:C:126:TYR:HE2	1.68	0.59
3:C:38:ASP:OD1	3:C:86:ALA:HB2	2.02	0.59
4:D:3:ILE:CG2	4:D:4:ILE:N	2.65	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:85:THR:HG23	3:C:112:LEU:O	2.03	0.59
3:C:131:SER:CA	3:C:132:LYS:C	2.71	0.59
4:D:120:LEU:HD12	4:D:123:VAL:HG23	1.84	0.59
1:A:104:CYS:SG	1:A:168:CYS:CB	2.81	0.58
3:C:140:LEU:HD13	3:C:179:VAL:HG23	1.86	0.58
4:D:189:SER:O	4:D:191:TYR:CE2	2.56	0.58
4:D:30:ASP:O	4:D:68:ARG:NH1	2.36	0.58
4:D:117:VAL:CG1	4:D:119:ASP:O	2.51	0.58
4:D:141:THR:O	4:D:142:GLN:HG2	2.03	0.58
3:C:135:ASP:HA	3:C:136:LYS:CB	2.11	0.58
2:B:10:TYR:CE2	2:B:24:ASN:HB2	2.38	0.58
1:A:59:SER:N	1:A:62:GLN:OE1	2.32	0.57
4:D:138:ILE:H	4:D:138:ILE:CD1	2.13	0.57
1:A:57:LYS:O	1:A:57:LYS:CG	2.53	0.57
2:B:29:GLN:HA	2:B:61:SER:HG	1.69	0.57
2:B:51:MET:SD	2:B:66:ALA:CA	2.93	0.57
4:D:226:TRP:NE1	4:D:228:GLN:N	2.53	0.57
4:D:25:GLN:HE22	4:D:29:HIS:N	2.02	0.57
4:D:20:THR:HG23	4:D:77:THR:HG22	1.84	0.57
4:D:199:VAL:HG22	4:D:203:PHE:HB3	1.85	0.57
1:A:194:SER:OG	1:A:207:VAL:HB	2.05	0.57
1:A:89:SER:HG	1:A:90:PRO:HD2	1.69	0.57
4:D:202:THR:O	4:D:205:GLN:CB	2.53	0.57
4:D:120:LEU:CD1	4:D:123:VAL:HG21	2.35	0.57
4:D:120:LEU:HD12	4:D:123:VAL:CG2	2.34	0.57
4:D:137:GLU:CG	4:D:143:LYS:O	2.52	0.57
1:A:10:PHE:O	1:A:103:GLY:HA3	2.04	0.56
2:B:10:TYR:CE2	2:B:24:ASN:ND2	2.73	0.56
2:B:20:PRO:HA	2:B:71:THR:HG22	1.87	0.56
3:C:32:LEU:HD21	3:C:90:CYS:SG	2.46	0.56
4:D:137:GLU:HG3	4:D:141:THR:HG21	1.87	0.56
1:A:237:PHE:C	1:A:238:LEU:HD23	2.25	0.56
4:D:119:ASP:O	4:D:122:ASN:OD1	2.24	0.56
4:D:132:GLU:HB3	4:D:133:PRO:CD	2.35	0.56
3:C:131:SER:CB	3:C:132:LYS:CA	2.40	0.56
2:B:38:GLN:HE21	2:B:45:LYS:HD3	1.59	0.56
1:A:198:SER:CB	1:A:205:GLN:HG3	2.34	0.56
4:D:148:CYS:HB2	4:D:162:TRP:CZ2	2.39	0.56
4:D:49:SER:OG	4:D:68:ARG:CD	2.48	0.56
4:D:6:GLN:NE2	4:D:91:CYS:N	2.46	0.56
4:D:137:GLU:HG2	4:D:143:LYS:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:136:LYS:O	4:D:131:PHE:CD2	2.60	0.55
4:D:145:THR:CG2	4:D:198:ARG:CD	2.84	0.55
4:D:23:CYS:SG	4:D:34:TRP:HZ2	2.15	0.55
1:A:145:LEU:HB3	1:A:146:PRO:CD	2.28	0.55
1:A:237:PHE:O	1:A:238:LEU:HD23	2.05	0.55
4:D:137:GLU:C	4:D:141:THR:HG1	1.99	0.55
3:C:190:ALA:HA	3:C:204:PHE:HE1	1.71	0.55
4:D:161:SER:OG	4:D:163:TRP:NE1	2.32	0.55
4:D:181:LYS:HE2	4:D:191:TYR:CE1	2.41	0.55
3:C:198:ILE:HD12	3:C:199:PRO:CD	2.36	0.55
4:D:6:GLN:NE2	4:D:90:LEU:HA	2.18	0.55
1:A:104:CYS:HB3	1:A:168:CYS:SG	2.42	0.54
1:A:186:GLN:HB3	1:A:269:SER:HB3	1.89	0.54
3:C:134:SER:O	3:C:136:LYS:HD2	2.07	0.54
4:D:25:GLN:CD	4:D:29:HIS:HB2	2.27	0.54
3:C:167:ASP:OD2	3:C:174:LYS:NZ	2.38	0.54
3:C:198:ILE:HG13	3:C:199:PRO:N	2.23	0.54
4:D:11:LEU:HD12	4:D:12:ILE:H	1.71	0.54
4:D:145:THR:HG22	4:D:198:ARG:HD2	1.90	0.54
4:D:211:PHE:N	4:D:211:PHE:HD2	2.02	0.54
3:C:196:SER:C	3:C:197:ILE:HG13	2.27	0.54
1:A:135:THR:HG23	1:A:147:ILE:HD12	1.84	0.54
2:B:12:ARG:HG3	2:B:12:ARG:HH11	1.72	0.54
1:A:140:PRO:HB2	1:A:142:TRP:NE1	2.22	0.54
4:D:163:TRP:O	4:D:212:ARG:N	2.30	0.54
3:C:126:TYR:CD2	3:C:126:TYR:N	2.75	0.54
1:A:240:ASN:HB2	1:A:244:THR:O	2.08	0.54
3:C:29:ASP:OD1	3:C:29:ASP:N	2.40	0.54
4:D:141:THR:O	4:D:142:GLN:CB	2.55	0.54
1:A:227:GLN:NE2	1:A:229:GLN:HE22	2.04	0.54
3:C:40:GLY:O	3:C:41:LYS:HG2	2.06	0.54
1:A:161:GLN:O	1:A:165:ASN:HB2	2.08	0.54
4:D:122:ASN:O	4:D:124:PHE:CE2	2.61	0.54
3:C:169:ARG:O	3:C:170:SER:CB	2.56	0.53
4:D:99:VAL:HG12	4:D:99:VAL:O	2.08	0.53
3:C:138:VAL:HG22	3:C:180:ALA:O	2.08	0.53
4:D:165:ASN:N	4:D:210:HIS:O	2.41	0.53
1:A:142:TRP:CZ3	1:A:143:LEU:CD1	2.92	0.53
4:D:120:LEU:HD12	4:D:120:LEU:O	2.09	0.53
4:D:185:ALA:HB3	4:D:186:LEU:HA	1.90	0.53
1:A:156:THR:HG23	6:A:601:GCY:H38A	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:ASN:C	1:A:294:ASN:OD1	2.48	0.53
1:A:295:HIS:N	1:A:295:HIS:CD2	2.76	0.53
1:A:53:TRP:CE3	1:A:179:GLY:HA3	2.43	0.53
3:C:36:LYS:HE2	3:C:86:ALA:HB3	1.91	0.53
3:C:128:LEU:CB	4:D:132:GLU:O	2.52	0.53
4:D:8:PRO:O	4:D:112:THR:OG1	2.20	0.53
1:A:283:HIS:O	1:A:287:ASP:HB2	2.08	0.53
3:C:138:VAL:CG2	3:C:180:ALA:O	2.56	0.53
3:C:52:GLN:HA	3:C:68:LYS:HD2	1.90	0.53
4:D:156:ASP:CG	4:D:156:ASP:O	2.46	0.53
2:B:51:MET:SD	2:B:66:ALA:HA	2.49	0.53
3:C:32:LEU:HD23	3:C:33:ARG:N	2.24	0.53
4:D:83:LYS:O	4:D:84:ASN:HB2	2.08	0.53
3:C:118:ILE:HG22	3:C:120:ASN:H	1.73	0.52
1:A:92:GLU:C	1:A:93:ASP:OD1	2.48	0.52
4:D:125:PRO:HD3	4:D:233:PRO:HB3	1.90	0.52
1:A:196:VAL:HG13	1:A:197:PRO:CD	2.39	0.52
3:C:166:LEU:HB3	4:D:174:CYS:HB2	1.91	0.52
2:B:81:ARG:CG	2:B:92:THR:OG1	2.49	0.52
4:D:216:GLN:OE1	4:D:237:ILE:CD1	2.57	0.52
1:A:104:CYS:SG	1:A:172:VAL:HG21	2.50	0.52
1:A:216:LYS:HD2	1:A:245:TRP:CE2	2.44	0.52
3:C:124:ALA:HB3	3:C:126:TYR:CE2	2.45	0.52
3:C:144:PHE:CZ	3:C:176:ASN:HB3	2.44	0.52
3:C:13:ARG:NH1	3:C:16:GLU:OE2	2.39	0.52
4:D:121:LYS:HG3	4:D:228:GLN:HG2	1.91	0.52
4:D:120:LEU:CD1	4:D:123:VAL:CG2	2.88	0.52
1:A:192:TRP:O	1:A:209:HIS:HD2	1.91	0.51
2:B:13:HIS:HB3	2:B:14:PRO:HD2	1.91	0.51
4:D:31:THR:HG22	4:D:33:TYR:CE1	2.45	0.51
1:A:87:MET:HG3	4:D:50:TYR:CD2	2.45	0.51
3:C:164:CYS:C	4:D:174:CYS:SG	2.88	0.51
1:A:246:TYR:CD2	1:A:246:TYR:C	2.84	0.51
3:C:38:ASP:OD1	3:C:86:ALA:CB	2.58	0.51
3:C:161:THR:HG1	3:C:179:VAL:H	1.46	0.51
3:C:149:ASN:N	3:C:149:ASN:ND2	2.59	0.51
3:C:138:VAL:HG21	3:C:179:VAL:CG1	2.41	0.51
3:C:13:ARG:HB3	3:C:16:GLU:CD	2.31	0.51
1:A:256:GLY:N	1:A:258:GLU:OE1	2.43	0.51
3:C:194:ASN:C	3:C:194:ASN:OD1	2.49	0.50
3:C:151:SER:HB3	3:C:195:ASN:ND2	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:16:GLU:O	3:C:80:THR:CG2	2.42	0.50
4:D:25:GLN:HE22	4:D:29:HIS:CA	2.23	0.50
3:C:128:LEU:N	3:C:128:LEU:HD12	2.26	0.50
3:C:172:ASP:OD2	3:C:172:ASP:O	2.30	0.50
4:D:57:LYS:HB3	4:D:61:SER:CB	2.42	0.50
4:D:212:ARG:HH21	4:D:212:ARG:HG2	1.76	0.50
1:A:196:VAL:HG22	1:A:197:PRO:HD2	1.92	0.50
4:D:156:ASP:O	4:D:156:ASP:OD1	2.30	0.50
1:A:294:ASN:OD1	1:A:294:ASN:O	2.29	0.50
4:D:181:LYS:HE2	4:D:191:TYR:HE1	1.77	0.49
2:B:13:HIS:HB3	2:B:14:PRO:CD	2.41	0.49
3:C:124:ALA:CB	3:C:126:TYR:HE2	2.21	0.49
4:D:185:ALA:H	4:D:186:LEU:CA	2.10	0.49
1:A:155:GLY:O	1:A:159:THR:HG23	2.12	0.49
4:D:181:LYS:HE2	4:D:191:TYR:OH	2.12	0.49
4:D:3:ILE:HG22	4:D:5:THR:HG23	1.95	0.49
1:A:49:PHE:HD2	1:A:54:SER:HB3	1.76	0.49
4:D:49:SER:CB	4:D:68:ARG:HD2	2.43	0.49
1:A:213:PHE:CE2	1:A:245:TRP:HB2	2.47	0.49
3:C:157:ASP:OD1	3:C:158:VAL:N	2.46	0.49
4:D:205:GLN:O	4:D:207:PRO:HD3	2.13	0.49
4:D:221:SER:C	4:D:223:ASN:N	2.62	0.49
4:D:227:THR:CG2	4:D:228:GLN:N	2.75	0.49
4:D:164:VAL:HG12	4:D:167:LYS:O	2.13	0.49
1:A:116:LEU:HD23	1:A:117:HIS:N	2.28	0.49
2:B:23:LEU:HD13	2:B:70:PHE:CZ	2.48	0.49
2:B:27:VAL:HG21	2:B:37:ILE:HD13	1.94	0.49
1:A:198:SER:OG	1:A:203:HIS:CB	2.60	0.49
1:A:58:LEU:HD23	1:A:58:LEU:N	2.28	0.49
4:D:145:THR:CG2	4:D:198:ARG:HD2	2.42	0.48
2:B:30:PHE:HZ	2:B:54:MET:CE	2.20	0.48
3:C:49:LEU:HD23	3:C:56:THR:HG23	1.95	0.48
4:D:4:ILE:CD1	4:D:107:PHE:HB2	2.42	0.48
1:A:219:TRP:CH2	1:A:221:MET:HB2	2.48	0.48
1:A:205:GLN:CG	1:A:252:ASP:OD1	2.50	0.48
2:B:36:GLU:HB2	2:B:83:LYS:HB3	1.94	0.48
1:A:49:PHE:HB3	1:A:54:SER:HB2	1.94	0.48
4:D:137:GLU:O	4:D:141:THR:HG23	2.14	0.48
4:D:57:LYS:HB3	4:D:61:SER:HB3	1.95	0.48
1:A:196:VAL:CG1	1:A:197:PRO:N	2.73	0.48
1:A:196:VAL:HG13	1:A:197:PRO:HD2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:160:ILE:HG13	3:C:160:ILE:O	2.14	0.48
4:D:117:VAL:HG23	4:D:154:TYR:OH	2.14	0.48
4:D:206:ASN:C	4:D:208:ARG:N	2.65	0.48
4:D:58:GLY:C	4:D:60:LEU:H	2.16	0.48
1:A:216:LYS:N	1:A:217:PRO:HD2	2.28	0.48
4:D:2:GLY:HA2	4:D:26:ASN:ND2	2.29	0.48
3:C:171:MET:SD	4:D:143:LYS:NZ	2.86	0.47
3:C:37:GLN:O	3:C:86:ALA:HB1	2.13	0.47
3:C:10:LEU:HD23	3:C:112:LEU:HD13	1.97	0.47
4:D:26:ASN:N	4:D:26:ASN:OD1	2.48	0.47
1:A:254:GLU:O	1:A:257:GLU:HB2	2.14	0.47
4:D:186:LEU:C	4:D:186:LEU:HD12	2.35	0.47
4:D:188:ASP:HB3	8:D:252:HOH:O	2.13	0.47
1:A:294:ASN:CG	1:A:294:ASN:O	2.52	0.47
4:D:141:THR:O	4:D:142:GLN:CG	2.62	0.47
3:C:141:PHE:HZ	3:C:199:PRO:HG2	1.79	0.47
3:C:86:ALA:O	3:C:88:TYR:CD1	2.68	0.47
4:D:117:VAL:CG2	4:D:154:TYR:CZ	2.97	0.47
1:A:219:TRP:CE3	1:A:266:LYS:HG3	2.50	0.47
2:B:17:ASN:OD1	2:B:73:THR:C	2.52	0.47
3:C:143:ASP:OD1	3:C:143:ASP:N	2.47	0.47
3:C:63:SER:HB2	3:C:76:HIS:HB2	1.97	0.47
4:D:204:TRP:O	4:D:204:TRP:CD2	2.68	0.47
1:A:126:VAL:HG12	1:A:127:ARG:N	2.28	0.47
2:B:38:GLN:NE2	2:B:45:LYS:HD3	2.11	0.47
1:A:67:GLN:O	1:A:71:GLN:HG3	2.15	0.46
2:B:20:PRO:CA	2:B:71:THR:HG22	2.45	0.46
2:B:27:VAL:HG21	2:B:37:ILE:CD1	2.46	0.46
4:D:25:GLN:NE2	4:D:29:HIS:HB2	2.31	0.46
2:B:10:TYR:CZ	2:B:24:ASN:HB2	2.50	0.46
4:D:130:VAL:HG13	4:D:130:VAL:O	2.15	0.46
1:A:116:LEU:C	1:A:116:LEU:CD2	2.84	0.46
1:A:140:PRO:HG2	1:A:142:TRP:HE1	1.79	0.46
4:D:25:GLN:OE1	4:D:93:SER:CB	2.63	0.46
6:A:601:GCY:O17	6:A:601:GCY:C18	2.59	0.46
3:C:127:GLN:CG	3:C:139:CYS:SG	3.04	0.46
3:C:149:ASN:H	3:C:149:ASN:ND2	2.13	0.46
4:D:54:SER:O	4:D:55:THR:CG2	2.64	0.46
1:A:291:MET:HG2	2:B:15:PRO:O	2.16	0.46
1:A:9:THR:OG1	1:A:105:GLU:HG3	2.15	0.46
1:A:234:ARG:HG3	1:A:247:LEU:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:TRP:CE3	2:B:14:PRO:HG3	2.51	0.46
1:A:198:SER:OG	1:A:203:HIS:HB3	2.16	0.46
2:B:41:LYS:O	2:B:42:ASN:HB2	2.15	0.46
3:C:134:SER:O	3:C:136:LYS:CB	2.54	0.46
2:B:70:PHE:CD1	2:B:78:TYR:CD2	3.04	0.46
1:A:88:MET:O	1:A:90:PRO:HD2	2.16	0.45
4:D:120:LEU:HD11	4:D:123:VAL:HG21	1.98	0.45
4:D:68:ARG:HG3	4:D:74:PHE:CD1	2.51	0.45
1:A:103:GLY:HA3	1:A:115:PHE:CZ	2.50	0.45
1:A:30:VAL:HG21	6:A:601:GCY:HAP	1.98	0.45
4:D:226:TRP:CE2	4:D:228:GLN:CB	2.85	0.45
4:D:201:ALA:O	4:D:202:THR:C	2.54	0.45
3:C:141:PHE:HZ	3:C:144:PHE:HB3	1.80	0.45
1:A:186:GLN:HB3	1:A:186:GLN:HE21	1.58	0.45
1:A:214:TYR:CG	1:A:215:PRO:HA	2.52	0.45
4:D:164:VAL:CG2	4:D:165:ASN:N	2.51	0.45
1:A:92:GLU:O	1:A:93:ASP:OD1	2.34	0.45
3:C:150:VAL:HG12	3:C:150:VAL:O	2.13	0.45
3:C:165:VAL:C	4:D:174:CYS:SG	2.95	0.45
3:C:141:PHE:CZ	3:C:199:PRO:HG2	2.51	0.45
4:D:243:TRP:CD1	4:D:243:TRP:N	2.84	0.45
1:A:109:GLY:HA2	1:A:110:ASN:HA	1.48	0.45
2:B:23:LEU:O	2:B:67:HIS:HA	2.16	0.45
4:D:137:GLU:CD	4:D:143:LYS:O	2.55	0.45
3:C:177:SER:OG	4:D:196:ARG:NE	2.50	0.45
2:B:32:PRO:CB	2:B:33:PRO:HD2	2.46	0.45
3:C:127:GLN:C	3:C:128:LEU:HD12	2.37	0.45
3:C:165:VAL:O	4:D:174:CYS:SG	2.75	0.45
4:D:3:ILE:H	4:D:26:ASN:HD21	1.65	0.45
1:A:143:LEU:HD11	6:A:601:GCY:C4	2.38	0.44
4:D:153:PHE:CE2	4:D:191:TYR:O	2.70	0.44
4:D:226:TRP:CE3	4:D:228:GLN:OE1	2.69	0.44
2:B:51:MET:CE	2:B:66:ALA:HB2	2.45	0.44
3:C:84:ASP:O	3:C:112:LEU:HD23	2.17	0.44
3:C:38:ASP:HA	3:C:86:ALA:HB1	1.98	0.44
1:A:136:VAL:HB	1:A:137:PRO:HD2	1.99	0.44
4:D:8:PRO:CG	4:D:21:LEU:CD2	2.94	0.44
4:D:137:GLU:C	4:D:141:THR:OG1	2.49	0.44
4:D:3:ILE:N	4:D:26:ASN:OD1	2.50	0.44
4:D:54:SER:O	4:D:55:THR:HG23	2.17	0.44
3:C:198:ILE:CG1	3:C:199:PRO:N	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:LEU:HG	1:A:248:GLN:N	2.32	0.44
2:B:32:PRO:O	2:B:84:HIS:HE1	2.01	0.44
4:D:25:GLN:NE2	4:D:29:HIS:H	2.16	0.44
1:A:192:TRP:O	1:A:209:HIS:CD2	2.70	0.44
3:C:55:LYS:HG3	3:C:65:THR:HG22	1.99	0.44
1:A:10:PHE:HD2	1:A:104:CYS:SG	2.41	0.44
1:A:163:LEU:HA	1:A:167:THR:HB	2.00	0.44
3:C:135:ASP:O	3:C:135:ASP:OD1	2.36	0.44
3:C:201:ASP:OD1	3:C:201:ASP:N	2.50	0.44
1:A:34:ASP:N	1:A:34:ASP:OD1	2.42	0.43
1:A:61:GLN:O	1:A:65:LYS:HG3	2.18	0.43
2:B:10:TYR:OH	2:B:26:TYR:HB2	2.17	0.43
2:B:49:VAL:HG12	2:B:50:GLU:N	2.33	0.43
3:C:131:SER:OG	3:C:132:LYS:HA	2.16	0.43
4:D:25:GLN:HE22	4:D:29:HIS:H	1.65	0.43
3:C:97:SER:C	4:D:99:VAL:CG2	2.87	0.43
3:C:160:ILE:HG22	3:C:180:ALA:HB2	2.01	0.43
4:D:137:GLU:O	4:D:141:THR:CG2	2.66	0.43
4:D:137:GLU:HG3	4:D:141:THR:OG1	2.18	0.43
2:B:12:ARG:NH1	2:B:12:ARG:HG3	2.33	0.43
2:B:14:PRO:HA	2:B:15:PRO:HD3	1.84	0.43
2:B:59:ASP:O	2:B:60:TRP:HB2	2.17	0.43
3:C:98:ALA:HA	4:D:99:VAL:HG22	2.00	0.43
4:D:185:ALA:CB	4:D:186:LEU:HA	2.41	0.43
4:D:204:TRP:O	4:D:204:TRP:CE3	2.72	0.43
1:A:53:TRP:CD2	1:A:179:GLY:CA	3.01	0.43
3:C:161:THR:HG23	3:C:179:VAL:O	2.18	0.43
3:C:20:LEU:HD12	3:C:75:LEU:HD23	2.00	0.43
1:A:10:PHE:CD2	1:A:104:CYS:SG	3.12	0.43
4:D:124:PHE:HE2	4:D:190:ARG:HH21	1.66	0.43
1:A:240:ASN:CG	2:B:12:ARG:HD2	2.39	0.43
4:D:120:LEU:O	4:D:121:LYS:C	2.56	0.43
4:D:137:GLU:CG	4:D:141:THR:OG1	2.67	0.43
4:D:52:ALA:HA	4:D:53:GLY:HA2	1.48	0.43
3:C:6:SER:HB2	3:C:7:PRO:HA	2.01	0.42
1:A:107:TYR:HE1	1:A:113:GLU:HG3	1.84	0.42
4:D:4:ILE:HD12	4:D:107:PHE:HB2	2.01	0.42
1:A:145:LEU:N	1:A:146:PRO:CD	2.82	0.42
4:D:209:ASN:O	4:D:243:TRP:HA	2.19	0.42
4:D:226:TRP:CD1	4:D:228:GLN:N	2.87	0.42
1:A:9:THR:HG23	1:A:105:GLU:HG3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:119:ASP:HB2	4:D:122:ASN:OD1	2.20	0.42
4:D:199:VAL:HG22	4:D:200:SER:N	2.34	0.42
4:D:202:THR:C	4:D:205:GLN:HB2	2.38	0.42
1:A:35:LEU:HD12	1:A:183:LEU:HD23	2.00	0.42
1:A:239:PRO:HD2	2:B:26:TYR:CE2	2.55	0.42
1:A:7:ASN:HB3	1:A:8:TYR:CD2	2.54	0.42
3:C:7:PRO:O	3:C:110:THR:HG23	2.20	0.42
4:D:117:VAL:CG2	4:D:154:TYR:OH	2.68	0.42
1:A:291:MET:HB3	1:A:291:MET:HE3	1.75	0.42
4:D:120:LEU:O	4:D:122:ASN:N	2.53	0.42
1:A:43:ASP:C	1:A:43:ASP:OD2	2.58	0.42
4:D:11:LEU:HD22	4:D:21:LEU:HD21	2.01	0.42
1:A:153:ASP:OD1	1:A:153:ASP:C	2.57	0.42
1:A:195:SER:HB3	1:A:279:TRP:HH2	1.84	0.42
2:B:22:ILE:CD1	2:B:69:GLU:HG3	2.44	0.42
3:C:118:ILE:HD13	3:C:144:PHE:O	2.19	0.42
4:D:176:ASP:OD2	4:D:194:SER:CB	2.60	0.42
3:C:95:ARG:HB2	3:C:100:GLY:HA3	2.02	0.41
3:C:128:LEU:N	3:C:128:LEU:CD1	2.83	0.41
4:D:165:ASN:OD1	4:D:165:ASN:O	2.37	0.41
3:C:126:TYR:CZ	4:D:137:GLU:HB2	2.52	0.41
4:D:82:GLN:O	4:D:85:GLU:HB2	2.20	0.41
1:A:240:ASN:ND2	2:B:12:ARG:HD2	2.35	0.41
3:C:122:ASP:N	3:C:123:PRO:CD	2.84	0.41
3:C:126:TYR:N	3:C:126:TYR:HD2	2.16	0.41
1:A:88:MET:C	1:A:89:SER:OG	2.59	0.41
4:D:178:GLN:HA	4:D:179:PRO:HD3	1.74	0.41
2:B:41:LYS:O	2:B:42:ASN:C	2.57	0.41
3:C:80:THR:OG1	3:C:80:THR:O	2.30	0.41
4:D:199:VAL:HG21	4:D:203:PHE:CG	2.55	0.41
4:D:30:ASP:HB3	4:D:96:LEU:HD11	1.91	0.41
3:C:35:PHE:CD1	3:C:43:LEU:HB3	2.56	0.41
4:D:135:GLU:C	4:D:138:ILE:HD13	2.40	0.41
1:A:47:ILE:H	1:A:67:GLN:HE21	1.68	0.41
4:D:54:SER:C	4:D:55:THR:HG23	2.42	0.41
1:A:261:LEU:HD23	1:A:261:LEU:HA	1.80	0.41
3:C:120:ASN:N	3:C:121:PRO:CD	2.83	0.41
3:C:128:LEU:CG	4:D:132:GLU:O	2.69	0.41
4:D:139:SER:O	4:D:142:GLN:NE2	2.54	0.41
4:D:3:ILE:H	4:D:26:ASN:ND2	2.19	0.41
1:A:222:TRP:H	1:A:232:THR:HG21	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:131:PHE:HE1	4:D:149:LEU:HG	1.82	0.41
4:D:100:ARG:HD2	4:D:100:ARG:HH11	1.75	0.40
4:D:81:ALA:HB1	4:D:116:VAL:HG21	2.03	0.40
1:A:135:THR:CG2	1:A:147:ILE:HD12	2.45	0.40
1:A:39:ARG:HD3	2:B:53:ASP:OD2	2.21	0.40
2:B:10:TYR:N	2:B:10:TYR:CD1	2.89	0.40
4:D:185:ALA:HB3	4:D:186:LEU:CA	2.50	0.40
4:D:25:GLN:HE22	4:D:29:HIS:C	2.24	0.40
1:A:124:TYR:CZ	1:A:136:VAL:HG11	2.57	0.40
1:A:82:GLN:O	1:A:86:LYS:HG3	2.22	0.40
1:A:168:CYS:N	1:A:169:PRO:CD	2.85	0.40
3:C:74:THR:HG22	3:C:75:LEU:N	2.36	0.40
4:D:96:LEU:HD12	4:D:96:LEU:N	2.37	0.40
1:A:10:PHE:O	1:A:103:GLY:CA	2.69	0.40
4:D:132:GLU:CB	4:D:133:PRO:CD	2.96	0.40
4:D:199:VAL:CG2	4:D:203:PHE:HB3	2.49	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:SER:OG	1:A:283:HIS:NE2[6_424]	2.06	0.14

## 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	288/302 (95%)	284 (99%)	3 (1%)	1 (0%)	44	77
2	B	97/99 (98%)	95 (98%)	2 (2%)	0	100	100
3	C	192/207 (93%)	181 (94%)	9 (5%)	2 (1%)	18	50
4	D	237/245 (97%)	229 (97%)	5 (2%)	3 (1%)	14	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	814/853 (95%)	789 (97%)	19 (2%)	6 (1%)	25 59

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	89	SER
3	C	195	ASN
3	C	202	THR
4	D	121	LYS
4	D	222	GLU
4	D	59	ASP

### 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	253/264 (96%)	245 (97%)	8 (3%)	44 78
2	B	92/93 (99%)	92 (100%)	0	100 100
3	C	174/186 (94%)	165 (95%)	9 (5%)	27 60
4	D	207/211 (98%)	195 (94%)	12 (6%)	23 55
All	All	726/754 (96%)	697 (96%)	29 (4%)	36 70

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	VAL
1	A	88	MET
1	A	89	SER
1	A	104	CYS
1	A	106	MET
1	A	204	ARG
1	A	263	CYS
1	A	270	LEU
3	C	125	VAL

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Mol	Chain	Res	Type
3	C	126	TYR
3	C	129	ARG
3	C	149	ASN
3	C	166	LEU
3	C	189	CYS
3	C	198	ILE
3	C	201	ASP
3	C	203	PHE
4	D	19	LEU
4	D	44	ARG
4	D	68	ARG
4	D	118	GLU
4	D	120	LEU
4	D	148	CYS
4	D	174	CYS
4	D	183	GLN
4	D	211	PHE
4	D	213	CYS
4	D	214	GLN
4	D	226	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	GLN
1	A	110	ASN
1	A	117	HIS
1	A	186	GLN
1	A	229	GLN
1	A	273	GLN
1	A	283	HIS
1	A	295	HIS
2	B	29	GLN
2	B	31	HIS
2	B	38	GLN
2	B	84	HIS
3	C	30	ASN
3	C	149	ASN
4	D	6	GLN
4	D	165	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
5	NAG	A	303	1	14,14,15	0.48	0	15,19,21	0.92	0
5	NAG	A	304	1	14,14,15	0.54	0	15,19,21	1.50	2 (13%)
5	NAG	A	305	1,5	14,14,15	0.63	0	15,19,21	1.34	2 (13%)
5	NAG	A	306	5	14,14,15	0.65	0	15,19,21	0.91	0
6	GCY	A	601	-	56,57,57	2.04	9 (16%)	61,65,65	1.46	10 (16%)
7	GOL	B	100	-	5,5,5	0.52	0	5,5,5	0.59	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
5	NAG	A	303	1	-	0/6/23/26	0/1/1/1
5	NAG	A	304	1	-	0/6/23/26	0/1/1/1
5	NAG	A	305	1,5	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	306	5	-	0/6/23/26	0/1/1/1
6	GCY	A	601	-	-	0/53/73/73	0/1/1/1
7	GOL	B	100	-	-	0/4/4/4	0/0/0/0

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	601	GCY	O1-C16	-9.32	1.25	1.43
6	A	601	GCY	CAX-CAW	-6.68	1.04	1.51
6	A	601	GCY	C16-C15	-5.40	1.40	1.50
6	A	601	GCY	CAQ-CAP	-2.74	1.35	1.51
6	A	601	GCY	CAN-CAM	-2.47	1.37	1.51
6	A	601	GCY	CAY-CAX	-2.33	1.30	1.49
6	A	601	GCY	O4-C20	2.44	1.50	1.44
6	A	601	GCY	C22-C20	2.70	1.58	1.53
6	A	601	GCY	O2-C19	2.95	1.45	1.40

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	304	NAG	O5-C1-C2	-4.00	105.90	111.47
6	A	601	GCY	C13-C14-C15	-3.85	110.35	125.66
5	A	305	NAG	O4-C4-C3	-3.14	103.53	110.36
6	A	601	GCY	C18-O2-C19	-3.06	107.49	113.76
5	A	304	NAG	C4-C3-C2	-2.44	107.44	111.02
6	A	601	GCY	C19-O4-C20	-2.23	109.52	113.72
6	A	601	GCY	C16-C15-C14	-2.05	122.46	125.22
6	A	601	GCY	O1-C16-C17	2.27	114.01	107.90
5	A	305	NAG	C1-O5-C5	2.30	115.33	112.17
6	A	601	GCY	C18-C17-N1	2.59	113.34	109.76
6	A	601	GCY	O4-C19-O2	3.05	117.25	110.02
6	A	601	GCY	CAV-CAU-CAT	3.14	130.64	114.45
6	A	601	GCY	CAY-CAX-CAW	4.19	146.13	113.42
6	A	601	GCY	CAO-CAN-CAM	4.56	137.97	114.45

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 10 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	601	GCY	9	0
7	B	100	GOL	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	290/302 (96%)	0.05	2 (0%) 87 83	39, 50, 63, 67	9 (3%)
2	B	99/99 (100%)	0.05	3 (3%) 51 39	42, 51, 60, 64	3 (3%)
3	C	196/207 (94%)	0.36	17 (8%) 11 6	38, 59, 114, 117	6 (3%)
4	D	239/245 (97%)	0.40	15 (6%) 21 13	38, 65, 85, 88	5 (2%)
All	All	824/853 (96%)	0.23	37 (4%) 34 24	38, 54, 99, 117	23 (2%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	196	SER	9.6
1	A	109	GLY	7.2
3	C	202	THR	5.6
3	C	195	ASN	4.7
4	D	186	LEU	4.3
3	C	197	ILE	4.0
3	C	150	VAL	3.4
3	C	199	PRO	3.4
3	C	132	LYS	3.3
4	D	208	ARG	3.3
3	C	193	PHE	3.2
3	C	140	LEU	3.0
4	D	213	CYS	2.8
4	D	226	TRP	2.7
1	A	107	TYR	2.6
4	D	1	GLY	2.5
3	C	180	ALA	2.5
3	C	203	PHE	2.5
3	C	191	ASN	2.5
4	D	241	GLU	2.4
4	D	187	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
3	C	201	ASP	2.3
4	D	23	CYS	2.3
2	B	1	ILE	2.3
4	D	191	TYR	2.3
4	D	211	PHE	2.2
4	D	119	ASP	2.2
2	B	11	SER	2.2
3	C	175	SER	2.2
4	D	204	TRP	2.1
3	C	133	SER	2.1
4	D	134	SER	2.1
3	C	148	THR	2.1
2	B	51	MET	2.1
4	D	223	ASN	2.1
4	D	21	LEU	2.1
3	C	119	GLN	2.1

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
6	GCY	A	601	57/57	0.84	0.37	3.40	30,58,68,69	0
5	NAG	A	304	14/15	0.73	0.30	1.35	64,66,67,68	0
7	GOL	B	100	6/6	0.82	0.20	0.93	68,69,69,69	0
5	NAG	A	303	14/15	0.72	0.26	-	75,76,76,77	0
5	NAG	A	306	14/15	0.79	0.33	-	44,47,48,48	0
5	NAG	A	305	14/15	0.94	0.15	-	46,48,49,51	0

## 6.5 Other polymers

There are no such residues in this entry.