



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 06:41 pm GMT

PDB ID : 3RY6
Title : Complex of fcγmariia (CD32) and the FC of human IGG1
Authors : Ramsland, P.A.; Farrugia, W.; Scott, A.M.; Hogarth, P.M.
Deposited on : 2011-05-11
Resolution : 3.80 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

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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
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) : recalc28949

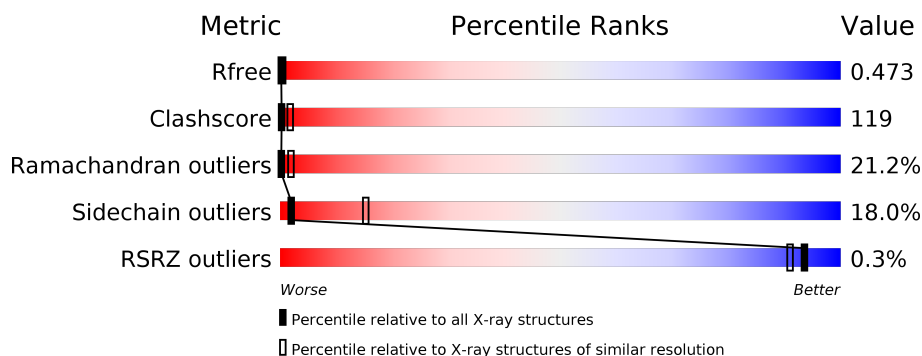
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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	1019 (4.08-3.52)
Clashscore	112137	1030 (4.04-3.56)
Ramachandran outliers	110173	1011 (4.06-3.54)
Sidechain outliers	110143	1005 (4.06-3.54)
RSRZ outliers	101464	1032 (4.08-3.52)

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.

Mol	Chain	Length	Quality of chain
1	A	214	<div> <div>13%</div> <div>58%</div> <div>24%</div> <div>.</div> </div>
1	B	214	<div> <div>14%</div> <div>57%</div> <div>24%</div> <div>6%</div> </div>
2	C	167	<div> <div>%</div> <div>10%</div> <div>59%</div> <div>28%</div> <div>.</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MAN	B	808	-	-	X	-
4	NAG	B	809	-	-	X	-
4	SIA	B	812	-	-	-	X
5	NAG	C	201	-	-	X	-
5	FUL	C	202	-	-	X	-
7	GOL	A	600	-	X	-	-
7	GOL	B	601	-	X	-	-
7	GOL	B	602	-	X	-	-
7	GOL	B	603	-	X	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5145 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 Ig gamma-1 chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1707	1086	289	325	7			
1	B	214	Total	C	N	O	S	0	0	0
			1707	1086	289	325	7			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	272	GLN	GLU	SEE REMARK 999	UNP P01857
A	283	GLN	GLU	SEE REMARK 999	UNP P01857
A	294	GLN	GLU	SEE REMARK 999	UNP P01857
A	312	ASN	ASP	SEE REMARK 999	UNP P01857
A	315	ASP	ASN	SEE REMARK 999	UNP P01857
A	356	GLU	ASP	VARIANT	UNP P01857
A	358	MET	LEU	VARIANT	UNP P01857
B	272	GLN	GLU	SEE REMARK 999	UNP P01857
B	283	GLN	GLU	SEE REMARK 999	UNP P01857
B	294	GLN	GLU	SEE REMARK 999	UNP P01857
B	312	ASN	ASP	SEE REMARK 999	UNP P01857
B	315	ASP	ASN	SEE REMARK 999	UNP P01857
B	356	GLU	ASP	VARIANT	UNP P01857
B	358	MET	LEU	VARIANT	UNP P01857

- Molecule 2 is a protein called Low affinity immunoglobulin gamma Fc region receptor II-a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	167	Total	C	N	O	S	0	0	0
			1331	841	229	256	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	134	ARG	HIS	ENGINEERED MUTATION	UNP P12318

- Molecule 3 is a polymer of unknown type called SUGAR (10-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	10	Total	C	N	O	0	0
			130	73	5	52		

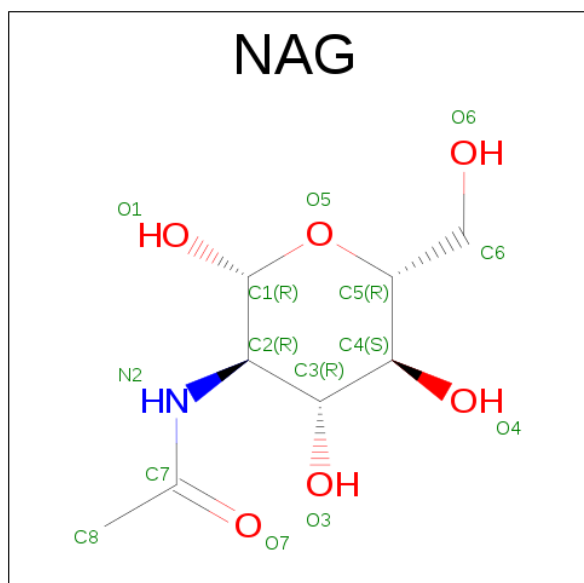
- Molecule 4 is a polymer of unknown type called SUGAR (12-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	12	Total	C	N	O	0	0
			161	90	6	65		

- Molecule 5 is a polymer of unknown type called SUGAR (6-MER).

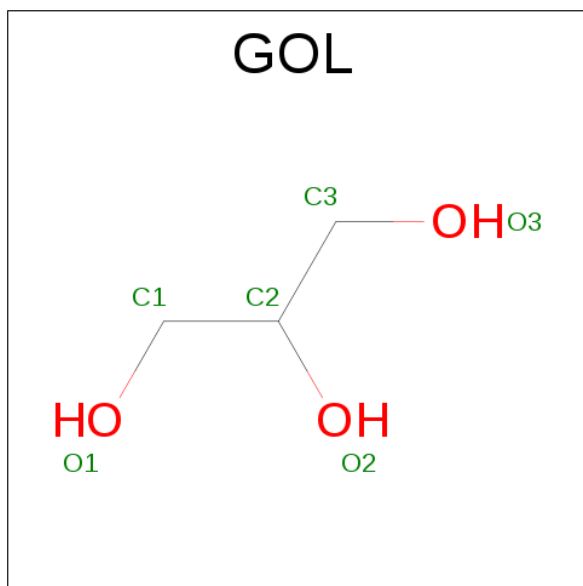
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	6	Total	C	N	O	0	0
			71	40	2	29		

- Molecule 6 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

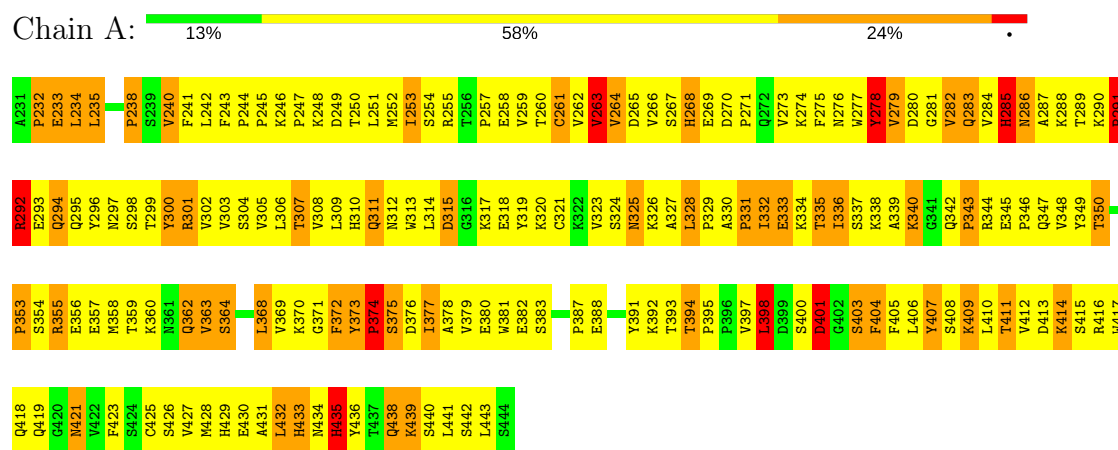


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		

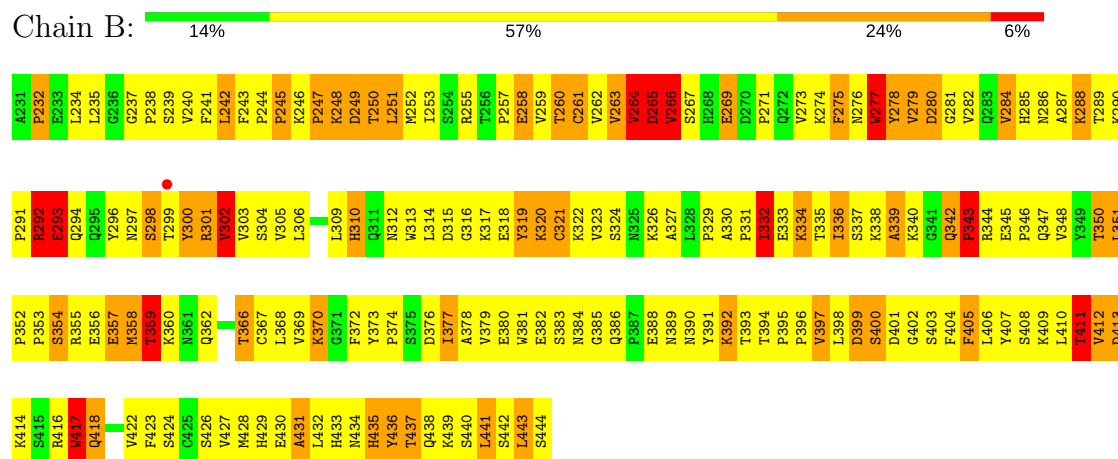
3 Residue-property plots

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.

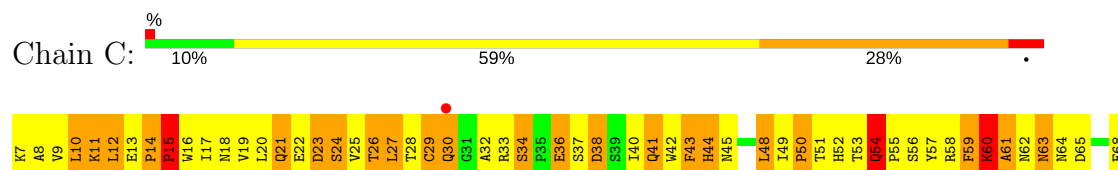
• Molecule 1: Ig gamma-1 chain C region



• Molecule 1: Ig gamma-1 chain C region



• Molecule 2: Low affinity immunoglobulin gamma Fc region receptor II-a



Y69	T70	C71	Q72	T73	G74	Q75	T76	S77	L78	S79	D80	P81	V82	H83	L84	T85	V86	L87	S88	E89	W90	L91	V92	L93	Q94	T95	N96	I97	L98	E99	F100	Q101	E102	G103	E104	T105	I106	M107	L108	R109	G110	H111	S112	W113	K114	D115	K116	P117	L118	V119	K120	V121	T122	F123	F124	Q125	N126	G127	K128
S129	Q130	K131	F132	S133	R134	L135	D136	P137	T138	F139	S140	I141	P142	Q143	A144	N145	H146	S147	H148	S149		Y152	H153	C154	T155	G156	N157	I158	G159	Y160	T161	L162	F163	S164	S165	K166	P167	V168	T169	I170	T171	V172	Q173																

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	153.38Å 255.55Å 58.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.71 – 3.80 29.71 – 3.78	Depositor EDS
% Data completeness (in resolution range)	(Not available) (29.71-3.80) 93.9 (29.71-3.78)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.52 (at 3.75Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.252 , 0.426 0.252 , 0.473	Depositor DCC
R_{free} test set	1147 reflections (11.51%)	DCC
Wilson B-factor (Å ²)	69.5	Xtriage
Anisotropy	0.526	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 283.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.023 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.025 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.79	EDS
Total number of atoms	5145	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.12% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, BMA, NAG, NDG, SIA, GAL, 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	0.50	0/1754	0.76	0/2388
1	B	0.54	0/1754	0.83	1/2388 (0.0%)
2	C	0.49	0/1369	0.80	1/1865 (0.1%)
All	All	0.51	0/4877	0.80	2/6641 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	399	ASP	N-CA-C	-5.86	95.18	111.00
2	C	93	LEU	CA-CB-CG	5.46	127.87	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1707	0	1678	382	0
1	B	1707	0	1679	462	0
2	C	1331	0	1273	351	1
3	A	130	0	110	16	0
4	B	161	0	135	25	0
5	C	71	0	61	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	14	0	13	0	0
7	A	6	0	4	0	0
7	B	18	0	12	3	0
All	All	5145	0	4965	1205	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 119.

All (1205) 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:C:40:ILE:HG13	2:C:54:GLN:H	1.04	1.19
1:B:377:ILE:HG12	1:B:378:ALA:H	1.10	1.13
1:A:328:LEU:HD23	1:A:329:PRO:HD2	1.22	1.12
1:B:380:GLU:HB2	1:B:426:SER:HB3	1.19	1.12
3:A:809:NAG:H62	3:A:810:GAL:H2	1.27	1.11
1:B:291:PRO:HA	1:B:292:ARG:HH21	1.13	1.10
1:A:301:ARG:HH21	1:A:303:VAL:HG21	1.00	1.10
1:B:292:ARG:HH22	1:B:303:VAL:HG22	0.99	1.09
1:B:432:LEU:HD12	1:B:433:HIS:H	0.96	1.08
2:C:134:ARG:HB3	2:C:134:ARG:HH11	1.10	1.08
1:B:292:ARG:HD2	1:B:293:GLU:H	1.19	1.08
1:A:276:ASN:HA	1:A:285:HIS:HB2	1.31	1.07
2:C:19:VAL:H	2:C:86:VAL:CG2	1.66	1.07
1:A:350:THR:HG21	1:A:441:LEU:HB2	1.35	1.07
4:B:808:MAN:H4	4:B:809:NAG:H82	1.08	1.06
2:C:9:VAL:HG23	2:C:10:LEU:HG	1.32	1.06
1:B:310:HIS:HA	1:B:313:TRP:HB3	1.38	1.06
1:A:266:VAL:HB	1:A:300:TYR:HB2	1.38	1.05
2:C:17:ILE:HB	2:C:84:LEU:HD13	1.32	1.05
4:B:802:FUL:H63	2:C:129:SER:HB3	1.39	1.02
1:A:257:PRO:HB2	1:A:308:VAL:HG13	1.43	1.00
1:B:273:VAL:HB	1:B:324:SER:H	1.22	1.00
1:B:279:VAL:HA	1:B:319:TYR:HA	1.42	0.99
2:C:19:VAL:H	2:C:86:VAL:HG23	1.26	0.99
1:B:252:MET:O	1:B:255:ARG:HG2	1.62	0.99
2:C:98:LEU:HD13	2:C:170:ILE:HA	1.44	0.98
1:B:292:ARG:HH22	1:B:303:VAL:CG2	1.75	0.98
1:B:241:PHE:H	1:B:263:VAL:HG12	1.27	0.98
1:A:274:LYS:HG2	1:A:275:PHE:H	1.28	0.98
2:C:149:SER:HB3	2:C:172:VAL:H	1.29	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:86:VAL:HG22	2:C:87:LEU:H	1.29	0.97
1:B:432:LEU:HD12	1:B:433:HIS:N	1.77	0.97
1:B:432:LEU:CD1	1:B:433:HIS:H	1.77	0.97
1:A:350:THR:HG23	1:A:439:LYS:HB3	1.47	0.97
1:B:292:ARG:NH2	1:B:303:VAL:HG22	1.80	0.97
1:B:362:GLN:HA	1:B:414:LYS:H	1.30	0.97
4:B:808:MAN:H4	4:B:809:NAG:C8	1.95	0.96
1:A:414:LYS:HZ2	1:A:418:GLN:HG3	1.30	0.96
1:B:321:CYS:HB3	1:B:334:LYS:HB2	1.43	0.96
1:A:309:LEU:HB2	1:A:312:ASN:HB3	1.48	0.96
2:C:96:PRO:HG2	2:C:100:PHE:CE2	2.01	0.96
2:C:126:ASN:HB2	2:C:128:LYS:HE3	1.46	0.96
1:B:348:VAL:HG12	1:B:369:VAL:HG13	1.49	0.95
1:A:249:ASP:HA	1:A:255:ARG:HG2	1.46	0.95
2:C:141:ILE:HG22	2:C:144:ALA:HB2	1.49	0.95
1:B:277:TRP:HA	1:B:321:CYS:HA	1.47	0.94
1:B:240:VAL:HA	1:B:263:VAL:HB	1.46	0.94
1:B:346:PRO:HB3	1:B:372:PHE:HB3	1.47	0.94
1:A:301:ARG:NH2	1:A:303:VAL:HG21	1.81	0.94
1:A:301:ARG:HH21	1:A:303:VAL:CG2	1.80	0.94
1:A:253:ILE:HD13	1:A:254:SER:H	1.33	0.94
1:A:344:ARG:HB3	1:A:374:PRO:HD3	1.47	0.94
1:B:291:PRO:HB3	1:B:303:VAL:O	1.69	0.93
1:B:394:THR:HG23	1:B:406:LEU:HB2	1.49	0.93
3:A:809:NAG:C6	3:A:810:GAL:H2	2.00	0.92
2:C:168:VAL:HG22	2:C:169:THR:H	1.32	0.92
2:C:7:LYS:HE2	2:C:76:THR:HG22	1.49	0.92
2:C:86:VAL:HG22	2:C:87:LEU:N	1.85	0.92
2:C:134:ARG:NH1	2:C:134:ARG:HB3	1.85	0.92
1:B:245:PRO:HB2	1:B:257:PRO:HB2	1.52	0.92
1:B:291:PRO:HA	1:B:292:ARG:NH2	1.84	0.91
2:C:40:ILE:HB	2:C:53:THR:HA	1.52	0.91
1:A:428:MET:SD	1:A:436:TYR:HB2	2.10	0.90
1:B:377:ILE:HG12	1:B:378:ALA:N	1.86	0.90
1:A:240:VAL:HG12	1:A:241:PHE:H	1.34	0.90
2:C:17:ILE:HB	2:C:84:LEU:CD1	2.01	0.89
1:A:328:LEU:HD23	1:A:329:PRO:CD	2.01	0.89
1:B:294:GLN:OE1	4:B:812:SIA:H91	1.72	0.89
2:C:43:PHE:CZ	2:C:72:GLN:HB2	2.08	0.89
2:C:40:ILE:HG13	2:C:54:GLN:N	1.87	0.88
2:C:19:VAL:N	2:C:86:VAL:HG23	1.88	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:43:PHE:HA	2:C:48:LEU:HA	1.53	0.88
2:C:96:PRO:HG2	2:C:100:PHE:HE2	1.37	0.88
1:B:429:HIS:O	1:B:435:HIS:HA	1.73	0.87
1:A:364:SER:HA	1:A:411:THR:HG23	1.55	0.87
2:C:118:LEU:HD21	2:C:156:GLY:HA2	1.55	0.87
1:B:380:GLU:CB	1:B:426:SER:HB3	2.04	0.87
1:A:382:GLU:HA	1:A:387:PRO:HA	1.55	0.87
1:B:250:THR:HG22	1:B:313:TRP:HE1	1.39	0.87
1:A:325:ASN:HD21	1:A:327:ALA:HB3	1.37	0.87
1:B:242:LEU:HD12	1:B:261:CYS:HA	1.53	0.87
2:C:103:GLY:HA2	2:C:143:GLN:HA	1.57	0.86
2:C:16:TRP:NE1	2:C:109:ARG:HD3	1.89	0.86
2:C:122:THR:HB	2:C:124:PHE:HE1	1.39	0.86
1:B:289:THR:HA	1:B:305:VAL:O	1.76	0.85
1:A:257:PRO:HD3	1:A:310:HIS:NE2	1.91	0.85
1:B:369:VAL:O	1:B:405:PHE:HA	1.76	0.85
1:B:424:SER:HB2	1:B:440:SER:OG	1.75	0.85
1:A:350:THR:OG1	1:A:439:LYS:HD2	1.74	0.85
1:B:336:ILE:HG13	1:B:337:SER:H	1.41	0.85
1:B:241:PHE:N	1:B:263:VAL:HG12	1.91	0.85
4:B:801:NAG:O5	4:B:802:FUL:H2	1.77	0.85
2:C:41:GLN:HB2	2:C:48:LEU:HD13	1.59	0.85
1:B:391:TYR:HB2	1:B:410:LEU:HA	1.59	0.85
1:A:318:GLU:HG2	1:A:320:LYS:HE3	1.56	0.85
1:A:332:ILE:HG22	1:A:334:LYS:HG2	1.58	0.84
1:B:239:SER:HB3	2:C:120:LYS:NZ	1.91	0.84
1:B:392:LYS:HA	1:B:392:LYS:HE3	1.58	0.84
2:C:101:GLN:O	2:C:104:GLU:HB3	1.77	0.84
2:C:19:VAL:HG22	2:C:86:VAL:HG21	1.57	0.84
1:B:346:PRO:CB	1:B:372:PHE:HB3	2.08	0.84
2:C:40:ILE:HG21	2:C:54:GLN:C	1.98	0.83
1:A:279:VAL:O	1:A:282:VAL:HG23	1.78	0.83
1:B:266:VAL:H	2:C:134:ARG:CZ	1.91	0.83
1:B:266:VAL:HG22	1:B:267:SER:H	1.42	0.83
2:C:93:LEU:HG	2:C:153:HIS:HA	1.59	0.83
1:B:380:GLU:HB2	1:B:426:SER:CB	2.04	0.83
2:C:17:ILE:CB	2:C:84:LEU:HD13	2.08	0.83
1:B:241:PHE:CG	4:B:809:NAG:H83	2.13	0.83
1:A:295:GLN:NE2	1:A:296:TYR:H	1.77	0.83
1:B:245:PRO:HG3	1:B:259:VAL:HG22	1.60	0.83
1:A:240:VAL:HG12	1:A:241:PHE:N	1.93	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:70:THR:HG22	2:C:71:CYS:H	1.43	0.82
1:B:243:PHE:HB2	1:B:262:VAL:HG11	1.59	0.82
1:B:309:LEU:HD13	1:B:310:HIS:N	1.94	0.82
1:B:432:LEU:CD1	1:B:436:TYR:H	1.91	0.82
4:B:808:MAN:C4	4:B:809:NAG:H82	2.03	0.82
1:B:264:VAL:HB	2:C:120:LYS:NZ	1.95	0.82
2:C:27:LEU:HD12	2:C:27:LEU:N	1.94	0.82
1:A:377:ILE:HG12	1:A:378:ALA:H	1.45	0.82
1:B:290:LYS:HB2	1:B:305:VAL:CG1	2.10	0.82
1:B:409:LYS:HG2	1:B:411:THR:OG1	1.80	0.82
1:A:350:THR:HG23	1:A:439:LYS:CB	2.10	0.81
2:C:41:GLN:O	2:C:72:GLN:HB3	1.79	0.81
5:C:201:NAG:H4	5:C:202:FUL:C5	2.10	0.81
2:C:40:ILE:CG1	2:C:54:GLN:H	1.89	0.81
4:B:806:NAG:H61	4:B:807:GAL:O5	1.82	0.80
1:A:425:CYS:SG	1:A:439:LYS:HB2	2.21	0.80
1:B:391:TYR:CB	1:B:410:LEU:HA	2.11	0.80
2:C:12:LEU:HA	2:C:27:LEU:HA	1.62	0.80
1:B:345:GLU:HG2	1:B:432:LEU:H	1.45	0.80
1:B:435:HIS:O	1:B:436:TYR:HB2	1.81	0.80
1:B:273:VAL:HA	1:B:324:SER:O	1.82	0.80
2:C:19:VAL:H	2:C:86:VAL:HG21	1.45	0.79
1:B:321:CYS:SG	1:B:323:VAL:HG23	2.23	0.79
2:C:48:LEU:O	2:C:50:PRO:HD3	1.82	0.79
1:B:246:LYS:HD3	1:B:247:PRO:HD2	1.65	0.78
1:A:232:PRO:O	1:A:233:GLU:HB2	1.81	0.78
2:C:53:THR:O	2:C:54:GLN:HB2	1.82	0.78
1:B:394:THR:CG2	1:B:407:TYR:H	1.96	0.78
1:A:414:LYS:NZ	1:A:418:GLN:HG3	1.98	0.78
1:B:289:THR:HB	1:B:306:LEU:CD1	2.13	0.78
1:B:241:PHE:HB3	1:B:243:PHE:CZ	2.19	0.78
1:B:243:PHE:HD1	1:B:262:VAL:HG22	1.47	0.78
1:B:348:VAL:CG1	1:B:369:VAL:HG13	2.14	0.78
1:A:438:GLN:H	1:A:438:GLN:NE2	1.80	0.77
2:C:57:TYR:CE1	2:C:59:PHE:HB3	2.19	0.77
1:B:278:TYR:HE2	1:B:284:VAL:HA	1.49	0.77
2:C:111:HIS:HD2	2:C:115:ASP:OD1	1.67	0.77
1:A:277:TRP:O	1:A:279:VAL:HG23	1.84	0.77
5:C:201:NAG:H4	5:C:202:FUL:H61	1.64	0.77
1:B:294:GLN:HB3	1:B:301:ARG:HD3	1.66	0.77
2:C:119:VAL:HG23	2:C:120:LYS:HG3	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:432:LEU:HD11	1:B:436:TYR:N	1.98	0.77
1:B:432:LEU:HD11	1:B:435:HIS:N	1.99	0.77
1:A:345:GLU:HG2	1:A:346:PRO:HD2	1.64	0.76
2:C:34:SER:HB3	2:C:37:SER:O	1.83	0.76
1:A:250:THR:HA	1:A:257:PRO:HG3	1.68	0.76
1:B:245:PRO:HD3	1:B:259:VAL:HG13	1.67	0.76
1:B:277:TRP:CD1	1:B:304:SER:HB3	2.20	0.76
1:B:362:GLN:HG2	1:B:413:ASP:HA	1.68	0.76
1:B:432:LEU:CD2	1:B:436:TYR:H	1.99	0.76
2:C:10:LEU:HD13	2:C:11:LYS:HG3	1.67	0.76
1:A:274:LYS:HE2	1:A:276:ASN:OD1	1.84	0.76
5:C:201:NAG:H4	5:C:202:FUL:C6	2.15	0.76
1:A:314:LEU:N	1:A:314:LEU:HD12	2.02	0.76
1:B:266:VAL:H	2:C:134:ARG:NH1	1.83	0.75
1:B:427:VAL:O	1:B:436:TYR:HA	1.86	0.75
1:A:410:LEU:HD12	1:A:411:THR:H	1.51	0.75
1:B:243:PHE:H	1:B:262:VAL:HG13	1.51	0.75
1:A:398:LEU:CD2	1:A:398:LEU:H	1.99	0.75
2:C:92:VAL:HG12	2:C:111:HIS:O	1.86	0.75
1:A:415:SER:O	1:A:419:GLN:HG3	1.86	0.75
1:A:346:PRO:HD3	1:A:431:ALA:HB3	1.68	0.75
1:A:350:THR:HG23	1:A:439:LYS:CG	2.16	0.75
2:C:25:VAL:HG12	2:C:26:THR:H	1.51	0.75
1:A:248:LYS:HB2	1:A:255:ARG:HD3	1.69	0.75
1:A:328:LEU:HD22	1:A:330:ALA:O	1.87	0.75
2:C:40:ILE:HB	2:C:53:THR:CA	2.15	0.75
1:B:277:TRP:HA	1:B:322:LYS:H	1.50	0.75
1:A:350:THR:N	1:A:439:LYS:HG3	2.02	0.74
1:B:239:SER:HB3	2:C:120:LYS:HZ3	1.49	0.74
1:A:309:LEU:H	1:A:309:LEU:HD22	1.52	0.74
1:B:292:ARG:N	1:B:292:ARG:NE	2.35	0.74
2:C:94:GLN:OE1	2:C:111:HIS:HB3	1.87	0.74
2:C:43:PHE:CD1	2:C:70:THR:HB	2.22	0.74
1:A:425:CYS:O	1:A:438:GLN:HA	1.86	0.74
1:A:370:LYS:NZ	1:B:409:LYS:HD3	2.03	0.74
1:B:264:VAL:HA	1:B:299:THR:HG21	1.69	0.74
1:B:273:VAL:HG11	1:B:302:VAL:HG21	1.69	0.73
2:C:16:TRP:CE2	2:C:109:ARG:HD3	2.22	0.73
2:C:152:TYR:N	2:C:168:VAL:HG12	2.03	0.73
1:B:252:MET:HB3	1:B:255:ARG:NE	2.03	0.73
1:B:265:ASP:HA	2:C:134:ARG:HH22	1.54	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:HIS:O	1:B:314:LEU:N	2.21	0.73
1:B:346:PRO:HB3	1:B:372:PHE:CB	2.17	0.73
1:B:430:GLU:HA	1:B:435:HIS:CD2	2.23	0.73
2:C:149:SER:HB3	2:C:172:VAL:N	2.03	0.73
1:A:393:THR:HG23	1:A:407:TYR:O	1.89	0.73
1:A:427:VAL:O	1:A:436:TYR:HA	1.87	0.73
1:B:436:TYR:HD2	1:B:437:THR:H	1.37	0.73
1:B:342:GLN:HB3	1:B:343:PRO:CD	2.18	0.73
5:C:201:NAG:H5	5:C:203:MAN:H2	1.69	0.73
1:B:396:PRO:HG3	1:B:406:LEU:HB3	1.71	0.73
1:B:369:VAL:HB	1:B:406:LEU:HD23	1.70	0.73
1:A:268:HIS:HA	1:A:271:PRO:CG	2.18	0.72
1:A:398:LEU:H	1:A:398:LEU:HD22	1.52	0.72
1:B:243:PHE:HB2	1:B:262:VAL:CG1	2.17	0.72
1:B:342:GLN:HB3	1:B:343:PRO:HD2	1.72	0.72
1:B:396:PRO:HG3	1:B:406:LEU:HD22	1.71	0.72
2:C:10:LEU:HA	2:C:82:VAL:HG22	1.71	0.72
1:A:315:ASP:H	1:A:338:LYS:HZ1	1.36	0.72
1:B:278:TYR:O	1:B:320:LYS:HD2	1.88	0.72
1:B:309:LEU:HD13	1:B:310:HIS:CG	2.24	0.72
1:B:358:MET:O	1:B:359:THR:HG23	1.88	0.72
1:A:373:TYR:HB3	1:A:374:PRO:HD3	1.70	0.72
1:B:306:LEU:HD12	1:B:306:LEU:N	2.04	0.72
2:C:25:VAL:HG12	2:C:26:THR:N	2.05	0.72
1:B:318:GLU:HG2	1:B:319:TYR:H	1.55	0.72
1:B:400:SER:C	1:B:402:GLY:H	1.90	0.72
1:B:241:PHE:O	1:B:262:VAL:O	2.08	0.71
1:A:249:ASP:O	1:A:310:HIS:CE1	2.43	0.71
1:A:295:GLN:OE1	1:A:300:TYR:HD2	1.74	0.71
1:B:278:TYR:HB3	1:B:320:LYS:HD2	1.72	0.71
1:B:248:LYS:HG3	1:B:377:ILE:O	1.91	0.71
1:B:396:PRO:HD3	1:B:406:LEU:HD13	1.71	0.71
2:C:22:GLU:HA	2:C:60:LYS:HD3	1.72	0.71
1:B:432:LEU:HD11	1:B:436:TYR:H	1.52	0.71
5:C:200:NDG:H6C1	5:C:202:FUL:O2	1.91	0.71
3:A:806:NAG:H61	3:A:811:SIA:O9	1.90	0.71
4:B:808:MAN:O3	4:B:809:NAG:H2	1.89	0.71
2:C:43:PHE:N	2:C:43:PHE:CD1	2.56	0.71
1:B:310:HIS:C	1:B:312:ASN:H	1.93	0.71
2:C:9:VAL:HG11	2:C:80:ASP:OD2	1.91	0.71
1:A:400:SER:O	1:A:401:ASP:HB3	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:MET:SD	1:A:436:TYR:HD2	2.14	0.70
1:B:366:THR:HA	1:B:408:SER:O	1.91	0.70
2:C:17:ILE:HB	2:C:84:LEU:HD22	1.73	0.70
1:B:291:PRO:C	1:B:292:ARG:HE	1.95	0.70
1:B:252:MET:HB3	1:B:255:ARG:HE	1.56	0.70
1:B:265:ASP:HA	2:C:134:ARG:NH2	2.06	0.70
1:B:436:TYR:HD2	1:B:437:THR:N	1.90	0.70
1:B:289:THR:OG1	1:B:291:PRO:HD3	1.92	0.70
2:C:86:VAL:CG2	2:C:87:LEU:H	2.03	0.70
2:C:98:LEU:CD1	2:C:170:ILE:HA	2.21	0.69
1:B:245:PRO:CG	1:B:259:VAL:HG22	2.21	0.69
1:A:264:VAL:HG11	3:A:803:NAG:H2	1.73	0.69
1:A:253:ILE:CD1	1:A:254:SER:H	2.03	0.69
1:A:344:ARG:NH1	1:A:345:GLU:O	2.25	0.69
1:A:332:ILE:HG23	1:A:334:LYS:NZ	2.07	0.69
1:B:330:ALA:O	1:B:332:ILE:HD12	1.92	0.69
1:A:290:LYS:HB2	1:A:305:VAL:HG22	1.75	0.69
1:B:266:VAL:HG13	1:B:267:SER:N	2.06	0.69
1:B:322:LYS:HD2	1:B:333:GLU:OE2	1.92	0.69
1:B:292:ARG:CD	1:B:293:GLU:H	2.03	0.69
1:B:373:TYR:CD2	1:B:374:PRO:HA	2.27	0.69
1:A:350:THR:H	1:A:439:LYS:HD2	1.57	0.68
1:A:294:GLN:NE2	1:A:295:GLN:H	1.91	0.68
1:B:320:LYS:HB3	1:B:333:GLU:O	1.93	0.68
1:B:261:CYS:O	1:B:263:VAL:HG13	1.93	0.68
1:B:264:VAL:HB	2:C:120:LYS:HZ2	1.58	0.68
2:C:18:ASN:HA	2:C:86:VAL:HG23	1.76	0.68
1:B:246:LYS:HD3	1:B:247:PRO:CD	2.23	0.68
1:B:438:GLN:HA	1:B:438:GLN:OE1	1.91	0.68
2:C:93:LEU:HD12	2:C:168:VAL:HB	1.76	0.68
2:C:128:LYS:HD2	2:C:128:LYS:C	2.15	0.68
2:C:16:TRP:HE1	2:C:109:ARG:HH11	1.42	0.68
1:B:424:SER:HA	1:B:440:SER:HA	1.76	0.68
2:C:121:VAL:HG12	2:C:122:THR:N	2.09	0.68
1:B:309:LEU:CD1	1:B:310:HIS:H	2.07	0.67
2:C:49:ILE:C	2:C:51:THR:H	1.98	0.67
1:A:439:LYS:NZ	1:A:439:LYS:HA	2.08	0.67
1:B:394:THR:OG1	1:B:395:PRO:HD2	1.95	0.67
2:C:9:VAL:O	2:C:10:LEU:HD12	1.94	0.67
1:A:240:VAL:CG1	1:A:241:PHE:H	2.07	0.67
1:B:436:TYR:CD2	1:B:437:THR:N	2.63	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:125:GLN:HE21	2:C:125:GLN:HA	1.58	0.67
2:C:7:LYS:HE3	2:C:75:GLN:O	1.93	0.67
1:A:242:LEU:HD21	1:A:261:CYS:SG	2.35	0.67
1:B:266:VAL:O	2:C:134:ARG:HD3	1.95	0.67
2:C:84:LEU:HD12	2:C:85:THR:N	2.10	0.67
1:B:277:TRP:CG	1:B:304:SER:HB3	2.30	0.67
2:C:122:THR:OG1	2:C:155:THR:HG23	1.95	0.67
1:B:277:TRP:CA	1:B:322:LYS:H	2.08	0.66
1:B:350:THR:HG22	1:B:439:LYS:O	1.95	0.66
2:C:103:GLY:O	2:C:105:THR:N	2.29	0.66
1:A:263:VAL:CG2	1:A:302:VAL:HB	2.25	0.66
1:A:274:LYS:HG2	1:A:275:PHE:N	2.07	0.66
1:A:345:GLU:HG2	1:A:346:PRO:CD	2.25	0.66
1:A:413:ASP:O	1:A:415:SER:N	2.28	0.66
1:A:253:ILE:HD13	1:A:254:SER:N	2.09	0.66
1:B:278:TYR:OH	1:B:284:VAL:HG13	1.94	0.66
1:B:278:TYR:O	1:B:280:ASP:N	2.28	0.66
2:C:129:SER:O	2:C:130:GLN:HG2	1.96	0.66
1:A:276:ASN:CA	1:A:285:HIS:HB2	2.18	0.65
1:B:239:SER:O	1:B:264:VAL:HG23	1.96	0.65
1:B:432:LEU:HD21	1:B:436:TYR:H	1.61	0.65
1:B:292:ARG:N	1:B:292:ARG:HE	1.92	0.65
1:B:432:LEU:HD13	1:B:436:TYR:O	1.96	0.65
1:B:275:PHE:CE1	1:B:304:SER:HB2	2.32	0.65
2:C:146:HIS:HA	2:C:172:VAL:CG1	2.26	0.65
5:C:201:NAG:H4	5:C:202:FUL:H5	1.77	0.65
1:A:432:LEU:HD13	1:A:435:HIS:HA	1.79	0.65
1:B:395:PRO:O	1:B:397:VAL:HG22	1.95	0.65
1:B:394:THR:O	1:B:406:LEU:HD12	1.96	0.65
1:A:344:ARG:HB3	1:A:373:TYR:HB3	1.77	0.65
1:A:435:HIS:N	1:A:435:HIS:CD2	2.64	0.65
2:C:7:LYS:HB2	2:C:30:GLN:O	1.95	0.65
5:C:200:NDG:H4	5:C:201:NAG:N2	2.09	0.65
1:B:279:VAL:HB	1:B:282:VAL:HG23	1.79	0.65
1:B:333:GLU:O	1:B:335:THR:HG23	1.95	0.65
1:B:383:SER:HB2	1:B:416:ARG:HH11	1.62	0.65
1:A:412:VAL:HB	1:A:416:ARG:HD3	1.78	0.65
1:B:250:THR:HG22	1:B:313:TRP:NE1	2.09	0.65
1:B:279:VAL:HG13	1:B:319:TYR:HB3	1.79	0.65
1:B:338:LYS:O	1:B:339:ALA:C	2.35	0.64
2:C:106:ILE:O	2:C:140:SER:HA	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:PRO:HG3	1:A:372:PHE:HB2	1.78	0.64
1:A:412:VAL:HG11	1:A:423:PHE:CZ	2.31	0.64
1:B:248:LYS:NZ	1:B:378:ALA:HA	2.13	0.64
1:A:360:LYS:HG2	1:A:362:GLN:H	1.62	0.64
1:B:310:HIS:CA	1:B:313:TRP:HB3	2.22	0.64
1:A:407:TYR:HE2	1:B:366:THR:HG21	1.61	0.64
2:C:97:HIS:O	2:C:98:LEU:HD23	1.97	0.64
1:A:414:LYS:HG2	1:A:418:GLN:HG2	1.78	0.64
1:B:346:PRO:CA	1:B:372:PHE:HB3	2.28	0.64
1:B:265:ASP:OD2	2:C:120:LYS:HD2	1.96	0.64
1:A:346:PRO:HG3	1:A:372:PHE:CB	2.27	0.64
1:A:370:LYS:HZ1	1:B:409:LYS:HD3	1.62	0.64
1:B:388:GLU:HG2	1:B:410:LEU:HD11	1.79	0.64
2:C:60:LYS:O	2:C:61:ALA:HB2	1.96	0.64
2:C:118:LEU:HD21	2:C:156:GLY:CA	2.26	0.64
1:A:398:LEU:HD22	1:A:398:LEU:N	2.13	0.64
1:A:350:THR:H	1:A:439:LYS:CD	2.10	0.64
1:B:243:PHE:CD1	1:B:262:VAL:HG22	2.32	0.64
2:C:74:GLY:O	2:C:75:GLN:HG2	1.98	0.64
2:C:19:VAL:N	2:C:86:VAL:CG2	2.47	0.64
1:A:246:LYS:HG2	1:A:249:ASP:CG	2.17	0.64
1:A:268:HIS:HB3	1:A:300:TYR:CE1	2.33	0.64
1:A:358:MET:CE	1:A:363:VAL:HG11	2.28	0.64
1:B:245:PRO:HD3	1:B:259:VAL:HA	1.78	0.64
1:B:290:LYS:HB2	1:B:305:VAL:HG11	1.80	0.64
1:B:346:PRO:HG3	1:B:429:HIS:CB	2.28	0.64
2:C:41:GLN:HB3	2:C:49:ILE:O	1.98	0.64
1:B:291:PRO:CA	1:B:292:ARG:HH21	2.01	0.63
1:B:309:LEU:HD13	1:B:310:HIS:H	1.61	0.63
2:C:107:MET:C	2:C:108:LEU:HD22	2.19	0.63
1:A:238:PRO:HG3	1:A:265:ASP:O	1.98	0.63
1:B:330:ALA:O	1:B:332:ILE:CD1	2.46	0.63
2:C:9:VAL:HA	2:C:29:CYS:SG	2.38	0.63
1:A:346:PRO:CA	1:A:372:PHE:HB3	2.29	0.63
1:B:320:LYS:HD3	1:B:333:GLU:HB2	1.80	0.63
2:C:34:SER:C	2:C:36:GLU:H	1.99	0.63
1:B:249:ASP:HA	1:B:255:ARG:HD2	1.81	0.63
2:C:113:TRP:O	2:C:116:LYS:HG3	1.99	0.63
2:C:40:ILE:HG21	2:C:54:GLN:O	1.98	0.63
2:C:10:LEU:CA	2:C:82:VAL:HG22	2.29	0.63
1:A:380:GLU:O	1:A:426:SER:N	2.25	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:312:ASN:HB2	1:B:317:LYS:CG	2.28	0.63
1:A:253:ILE:HD13	1:A:253:ILE:N	2.13	0.62
2:C:17:ILE:CB	2:C:84:LEU:HD22	2.29	0.62
1:B:249:ASP:O	1:B:252:MET:HB2	2.00	0.62
1:A:309:LEU:HB2	1:A:312:ASN:CB	2.26	0.62
1:A:313:TRP:C	1:A:314:LEU:HD12	2.19	0.62
2:C:98:LEU:HD21	2:C:169:THR:O	2.00	0.62
1:A:248:LYS:O	1:A:251:LEU:N	2.29	0.62
1:A:373:TYR:O	1:A:375:SER:N	2.32	0.62
2:C:9:VAL:HA	2:C:29:CYS:HA	1.81	0.62
1:A:350:THR:H	1:A:439:LYS:CG	2.12	0.62
2:C:43:PHE:HE1	2:C:71:CYS:C	2.03	0.62
1:A:278:TYR:CG	1:A:281:GLY:HA2	2.34	0.62
1:B:243:PHE:N	1:B:262:VAL:HG13	2.15	0.62
1:B:394:THR:HG21	1:B:407:TYR:H	1.63	0.62
2:C:41:GLN:CB	2:C:48:LEU:HD13	2.29	0.62
1:A:301:ARG:NH1	3:A:803:NAG:H81	2.15	0.62
1:B:242:LEU:HD12	1:B:261:CYS:CA	2.28	0.62
1:B:287:ALA:O	1:B:288:LYS:HB2	1.99	0.62
1:B:367:CYS:O	1:B:407:TYR:HA	2.00	0.62
2:C:17:ILE:HB	2:C:84:LEU:CD2	2.30	0.62
1:B:348:VAL:HG23	1:B:439:LYS:HG3	1.81	0.62
2:C:43:PHE:CE1	2:C:72:GLN:HB2	2.35	0.62
1:B:300:TYR:O	1:B:302:VAL:N	2.33	0.61
1:B:321:CYS:O	1:B:333:GLU:HA	1.99	0.61
2:C:146:HIS:HA	2:C:172:VAL:HG12	1.81	0.61
1:A:277:TRP:O	1:A:278:TYR:C	2.38	0.61
1:A:301:ARG:HE	1:A:303:VAL:HG23	1.65	0.61
2:C:28:THR:HA	2:C:55:PRO:O	1.99	0.61
1:A:274:LYS:HB3	1:A:324:SER:HB3	1.81	0.61
1:A:342:GLN:HB3	1:A:343:PRO:HD2	1.82	0.61
1:A:350:THR:H	1:A:439:LYS:HG3	1.64	0.61
1:B:251:LEU:HD22	1:B:251:LEU:C	2.20	0.61
2:C:49:ILE:O	2:C:49:ILE:HG23	1.99	0.61
2:C:10:LEU:CB	2:C:82:VAL:HG22	2.30	0.61
1:B:291:PRO:CB	1:B:303:VAL:O	2.46	0.61
1:B:352:PRO:HB2	1:B:353:PRO:HD2	1.81	0.61
1:B:377:ILE:CG1	1:B:378:ALA:H	1.93	0.61
1:B:379:VAL:HA	1:B:426:SER:O	2.01	0.61
2:C:134:ARG:O	2:C:135:LEU:HB3	2.01	0.61
1:A:259:VAL:HG23	1:A:259:VAL:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:LYS:HE3	1:B:378:ALA:CB	2.31	0.61
1:B:315:ASP:CG	1:B:316:GLY:H	2.04	0.61
2:C:118:LEU:HD22	2:C:121:VAL:HG22	1.83	0.61
1:A:253:ILE:N	1:A:253:ILE:CD1	2.63	0.61
1:A:382:GLU:O	1:A:388:GLU:HG2	2.01	0.61
1:B:276:ASN:O	1:B:277:TRP:C	2.39	0.61
1:B:433:HIS:CD2	1:B:434:ASN:HD22	2.19	0.61
1:B:348:VAL:O	1:B:439:LYS:HE3	2.00	0.61
1:A:248:LYS:HA	1:A:251:LEU:HB2	1.82	0.61
1:B:247:PRO:HB2	1:B:376:ASP:OD1	2.01	0.61
1:A:407:TYR:CE2	1:B:366:THR:HG21	2.35	0.61
1:B:379:VAL:HG22	1:B:427:VAL:HG22	1.82	0.61
2:C:27:LEU:CD1	2:C:27:LEU:N	2.64	0.61
1:A:344:ARG:HB3	1:A:374:PRO:CD	2.25	0.60
2:C:7:LYS:CE	2:C:76:THR:HG22	2.28	0.60
2:C:17:ILE:O	2:C:84:LEU:HD11	2.01	0.60
1:B:266:VAL:HG12	2:C:134:ARG:CD	2.32	0.60
1:B:432:LEU:HD21	1:B:436:TYR:N	2.16	0.60
1:A:289:THR:HA	1:A:306:LEU:CD1	2.32	0.60
1:A:290:LYS:HB2	1:A:305:VAL:CG2	2.31	0.60
1:A:257:PRO:CB	1:A:308:VAL:HG13	2.23	0.60
1:A:348:VAL:HA	1:A:368:LEU:O	2.02	0.60
1:A:252:MET:HG3	1:A:255:ARG:H	1.67	0.60
1:A:360:LYS:HB2	1:A:360:LYS:NZ	2.15	0.60
1:B:277:TRP:HA	1:B:322:LYS:N	2.16	0.60
1:B:368:LEU:HD21	1:B:370:LYS:HB3	1.82	0.60
1:A:364:SER:CA	1:A:411:THR:HG23	2.30	0.60
1:A:429:HIS:O	1:A:435:HIS:HB3	2.02	0.60
4:B:805:MAN:C1	4:B:806:NAG:H83	2.31	0.60
2:C:17:ILE:HG12	2:C:95:THR:O	2.01	0.60
1:A:292:ARG:HD2	1:A:292:ARG:O	2.02	0.60
1:A:347:GLN:O	1:A:369:VAL:HA	2.01	0.60
1:B:344:ARG:HG3	1:B:344:ARG:NH1	2.17	0.60
1:A:357:GLU:OE1	1:A:364:SER:N	2.34	0.60
2:C:48:LEU:HD12	2:C:48:LEU:C	2.22	0.60
1:A:368:LEU:HD23	1:A:406:LEU:O	2.01	0.60
1:B:320:LYS:HG2	1:B:335:THR:CG2	2.31	0.60
1:B:432:LEU:CD1	1:B:436:TYR:N	2.60	0.60
2:C:84:LEU:HD12	2:C:85:THR:H	1.65	0.59
1:A:325:ASN:ND2	1:A:327:ALA:HB3	2.14	0.59
1:A:428:MET:SD	1:A:436:TYR:CD2	2.94	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:HIS:C	1:B:286:ASN:HD22	2.05	0.59
1:B:261:CYS:HB3	1:B:303:VAL:HA	1.84	0.59
1:B:320:LYS:HD3	1:B:333:GLU:CB	2.33	0.59
1:B:435:HIS:O	1:B:436:TYR:CB	2.49	0.59
1:B:246:LYS:HB3	1:B:249:ASP:OD1	2.02	0.59
1:B:291:PRO:CA	1:B:292:ARG:HE	2.16	0.59
2:C:121:VAL:HG12	2:C:122:THR:H	1.66	0.59
2:C:13:GLU:O	2:C:15:PRO:HD3	2.02	0.59
1:A:406:LEU:HD12	1:A:406:LEU:C	2.22	0.59
1:A:414:LYS:HZ2	1:A:418:GLN:CG	2.10	0.59
2:C:86:VAL:CG2	2:C:87:LEU:N	2.58	0.59
1:A:289:THR:HA	1:A:306:LEU:HD11	1.84	0.59
1:A:357:GLU:OE2	1:A:363:VAL:HG12	2.03	0.59
5:C:201:NAG:C6	5:C:202:FUL:H5	2.32	0.59
1:A:234:LEU:HG	1:A:235:LEU:H	1.68	0.58
1:A:246:LYS:N	1:A:246:LYS:HD3	2.17	0.58
1:B:277:TRP:CE2	1:B:304:SER:O	2.56	0.58
1:B:290:LYS:H	1:B:305:VAL:HG13	1.67	0.58
2:C:100:PHE:CE2	2:C:106:ILE:HG23	2.38	0.58
1:A:432:LEU:HD12	1:A:432:LEU:N	2.18	0.58
1:A:262:VAL:HA	1:A:302:VAL:O	2.03	0.58
1:A:350:THR:CG2	1:A:441:LEU:HD12	2.33	0.58
1:B:273:VAL:CG1	1:B:302:VAL:HG21	2.34	0.58
2:C:26:THR:HA	2:C:57:TYR:O	2.03	0.58
1:A:409:LYS:HB3	1:A:409:LYS:NZ	2.18	0.58
1:B:368:LEU:C	1:B:368:LEU:HD23	2.24	0.58
1:B:275:PHE:CZ	1:B:303:VAL:O	2.57	0.58
1:B:293:GLU:CB	1:B:300:TYR:HA	2.33	0.58
1:B:392:LYS:HA	1:B:392:LYS:CE	2.33	0.58
1:A:377:ILE:HD11	1:A:427:VAL:CG1	2.34	0.58
3:A:811:SIA:N5	3:A:811:SIA:H8	2.19	0.58
1:B:277:TRP:HA	1:B:321:CYS:CA	2.27	0.58
1:B:289:THR:HG23	1:B:291:PRO:CD	2.34	0.58
2:C:172:VAL:O	2:C:173:GLN:HB3	2.04	0.58
2:C:20:LEU:C	2:C:21:GLN:HG3	2.24	0.58
1:B:430:GLU:O	1:B:431:ALA:O	2.22	0.58
1:A:312:ASN:HD21	1:A:317:LYS:HD2	1.69	0.57
1:A:344:ARG:NE	1:A:371:GLY:O	2.36	0.57
1:B:264:VAL:HB	2:C:120:LYS:HZ1	1.66	0.57
1:B:273:VAL:O	1:B:274:LYS:HB2	2.04	0.57
2:C:122:THR:HB	2:C:124:PHE:CE1	2.30	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:168:VAL:HG22	2:C:169:THR:N	2.12	0.57
1:A:264:VAL:O	1:A:265:ASP:HB2	2.03	0.57
1:B:286:ASN:N	1:B:286:ASN:HD22	2.02	0.57
2:C:100:PHE:CG	2:C:106:ILE:HG12	2.39	0.57
2:C:162:LEU:HD22	2:C:162:LEU:N	2.18	0.57
2:C:17:ILE:CG1	2:C:84:LEU:HD13	2.34	0.57
1:A:432:LEU:HD12	1:A:432:LEU:H	1.69	0.57
1:A:434:ASN:O	1:A:436:TYR:N	2.36	0.57
1:A:381:TRP:HB2	1:A:388:GLU:HB2	1.86	0.57
2:C:120:LYS:HE3	2:C:134:ARG:HH22	1.68	0.57
1:A:260:THR:HB	1:A:303:VAL:HG13	1.86	0.57
1:A:344:ARG:HH11	1:A:345:GLU:N	2.03	0.57
1:B:290:LYS:N	1:B:291:PRO:HD3	2.20	0.57
1:B:243:PHE:CZ	4:B:808:MAN:H62	2.39	0.57
1:B:309:LEU:CD1	1:B:310:HIS:N	2.65	0.57
1:B:391:TYR:HB3	1:B:410:LEU:HA	1.86	0.57
1:A:274:LYS:O	1:A:275:PHE:CD2	2.58	0.57
1:A:372:PHE:O	1:A:404:PHE:HB2	2.04	0.57
1:B:239:SER:HB3	2:C:120:LYS:HZ2	1.69	0.57
4:B:810:GAL:O4	4:B:811:SIA:H32	2.04	0.57
2:C:93:LEU:HD23	2:C:154:CYS:SG	2.44	0.57
1:A:245:PRO:HB3	1:A:258:GLU:N	2.20	0.57
1:A:378:ALA:O	1:A:427:VAL:HA	2.05	0.57
2:C:40:ILE:O	2:C:52:HIS:O	2.23	0.57
2:C:42:TRP:CZ2	2:C:55:PRO:O	2.58	0.57
1:A:328:LEU:HD22	1:A:330:ALA:H	1.70	0.57
1:B:318:GLU:HG2	1:B:319:TYR:N	2.20	0.57
2:C:125:GLN:NE2	2:C:126:ASN:H	2.03	0.57
2:C:42:TRP:HZ2	2:C:55:PRO:O	1.87	0.57
1:A:246:LYS:N	1:A:249:ASP:HB2	2.20	0.56
1:A:353:PRO:HB3	1:A:357:GLU:OE2	2.04	0.56
1:A:350:THR:HG23	1:A:439:LYS:HG3	1.87	0.56
1:B:294:GLN:H	1:B:301:ARG:HB3	1.68	0.56
1:B:280:ASP:HB2	1:B:318:GLU:HB3	1.86	0.56
2:C:111:HIS:CD2	2:C:115:ASP:OD1	2.55	0.56
1:A:425:CYS:O	1:A:438:GLN:CA	2.53	0.56
1:B:278:TYR:O	1:B:279:VAL:C	2.43	0.56
1:A:270:ASP:OD2	1:A:326:LYS:HB3	2.04	0.56
1:A:314:LEU:HB3	1:A:338:LYS:HZ3	1.69	0.56
1:B:383:SER:CB	1:B:416:ARG:HH11	2.17	0.56
2:C:125:GLN:HE21	2:C:125:GLN:CA	2.18	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:ILE:HG23	1:A:378:ALA:N	2.18	0.56
1:B:239:SER:CB	2:C:120:LYS:HZ3	2.18	0.56
1:B:400:SER:C	1:B:402:GLY:N	2.59	0.56
2:C:25:VAL:O	2:C:58:ARG:HA	2.05	0.56
2:C:28:THR:O	2:C:29:CYS:SG	2.63	0.56
2:C:40:ILE:CB	2:C:53:THR:HA	2.30	0.56
1:A:247:PRO:HD2	1:A:248:LYS:HZ2	1.70	0.56
1:B:412:VAL:HG23	1:B:413:ASP:N	2.20	0.56
2:C:41:GLN:HB2	2:C:48:LEU:CD1	2.34	0.56
1:A:245:PRO:HD3	1:A:259:VAL:CG1	2.36	0.56
1:A:249:ASP:HB3	1:A:257:PRO:HA	1.86	0.56
1:A:301:ARG:HG3	3:A:803:NAG:H81	1.87	0.56
2:C:10:LEU:HA	2:C:82:VAL:CG2	2.34	0.56
1:A:252:MET:HB3	1:A:255:ARG:HB2	1.88	0.56
1:A:371:GLY:O	1:A:403:SER:HB2	2.05	0.56
2:C:49:ILE:O	2:C:51:THR:N	2.39	0.56
2:C:42:TRP:CE3	2:C:70:THR:O	2.58	0.56
1:A:242:LEU:HD11	1:A:321:CYS:HB3	1.86	0.56
1:B:362:GLN:HA	1:B:414:LYS:N	2.10	0.56
2:C:145:ASN:C	2:C:147:SER:H	2.09	0.56
1:A:234:LEU:O	1:A:235:LEU:HB2	2.05	0.56
1:A:248:LYS:HG3	1:A:255:ARG:NH1	2.21	0.56
1:B:291:PRO:HA	1:B:292:ARG:HE	1.70	0.56
1:B:393:THR:HG22	1:B:394:THR:N	2.21	0.56
2:C:96:PRO:HG2	2:C:100:PHE:CZ	2.39	0.56
1:B:279:VAL:O	1:B:281:GLY:N	2.39	0.56
1:B:260:THR:HA	1:B:277:TRP:HZ2	1.70	0.55
1:B:394:THR:HG22	1:B:407:TYR:H	1.71	0.55
2:C:14:PRO:O	2:C:15:PRO:C	2.43	0.55
2:C:40:ILE:HG23	2:C:73:THR:HB	1.88	0.55
1:A:319:TYR:O	1:A:336:ILE:HG23	2.06	0.55
1:B:353:PRO:HG3	1:B:417:TRP:HE1	1.71	0.55
1:B:348:VAL:CG2	1:B:439:LYS:HG3	2.36	0.55
2:C:157:ASN:HB2	2:C:162:LEU:HD13	1.89	0.55
1:A:335:THR:C	1:A:336:ILE:HG22	2.26	0.55
2:C:116:LYS:HB3	2:C:117:PRO:HD2	1.87	0.55
1:A:295:GLN:OE1	1:A:300:TYR:CD2	2.58	0.55
1:A:392:LYS:O	1:A:408:SER:HA	2.07	0.55
1:B:251:LEU:HD22	1:B:252:MET:N	2.21	0.55
2:C:9:VAL:HG21	2:C:80:ASP:OD2	2.06	0.55
1:A:293:GLU:HG3	1:A:294:GLN:N	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:809:NAG:H5	3:A:810:GAL:O5	2.07	0.55
1:B:249:ASP:HB3	1:B:255:ARG:HG3	1.89	0.55
1:B:383:SER:CB	1:B:416:ARG:NH1	2.70	0.55
1:B:241:PHE:CD1	4:B:809:NAG:H83	2.42	0.55
2:C:158:ILE:O	2:C:160:TYR:N	2.40	0.55
2:C:27:LEU:HD12	2:C:27:LEU:H	1.69	0.55
1:A:267:SER:O	1:A:269:GLU:N	2.39	0.55
1:A:360:LYS:HB2	1:A:360:LYS:HZ3	1.71	0.55
1:B:310:HIS:C	1:B:312:ASN:N	2.60	0.55
2:C:133:SER:OG	2:C:136:ASP:HB3	2.07	0.55
2:C:152:TYR:O	2:C:168:VAL:HG12	2.07	0.55
1:A:347:GLN:HB3	1:A:349:TYR:CE2	2.42	0.55
1:B:289:THR:OG1	1:B:305:VAL:N	2.36	0.55
1:B:332:ILE:O	1:B:334:LYS:HD2	2.06	0.55
1:B:338:LYS:O	1:B:339:ALA:O	2.25	0.55
1:B:359:THR:O	1:B:414:LYS:HD3	2.06	0.55
2:C:90:TRP:HD1	2:C:90:TRP:O	1.90	0.55
1:A:414:LYS:HG2	1:A:418:GLN:CG	2.37	0.55
1:A:432:LEU:CD1	1:A:435:HIS:HA	2.37	0.55
2:C:85:THR:HG22	2:C:86:VAL:H	1.72	0.55
1:A:263:VAL:HG23	1:A:302:VAL:HB	1.87	0.55
1:A:344:ARG:NH1	1:A:345:GLU:N	2.55	0.55
1:B:289:THR:HB	1:B:306:LEU:HD11	1.86	0.55
1:B:291:PRO:HA	1:B:292:ARG:CZ	2.36	0.55
1:B:288:LYS:O	1:B:306:LEU:HA	2.07	0.55
2:C:58:ARG:O	2:C:58:ARG:HG2	2.07	0.54
1:B:248:LYS:HE3	1:B:378:ALA:HB2	1.88	0.54
1:B:296:TYR:CD2	1:B:299:THR:HB	2.42	0.54
2:C:54:GLN:HB3	2:C:57:TYR:H	1.72	0.54
1:A:309:LEU:N	1:A:309:LEU:HD22	2.22	0.54
1:A:373:TYR:HB3	1:A:374:PRO:CD	2.37	0.54
2:C:158:ILE:HD12	2:C:163:PHE:CE1	2.42	0.54
1:A:245:PRO:HB2	1:A:249:ASP:HB3	1.90	0.54
1:B:289:THR:HA	1:B:305:VAL:C	2.27	0.54
1:B:346:PRO:HB3	1:B:372:PHE:CD2	2.43	0.54
1:A:332:ILE:HG23	1:A:334:LYS:HZ3	1.71	0.54
1:B:293:GLU:HB2	1:B:300:TYR:HA	1.90	0.54
1:B:372:PHE:HB2	1:B:429:HIS:NE2	2.22	0.54
1:B:399:ASP:HB2	1:B:405:PHE:CD2	2.42	0.54
1:B:266:VAL:HG12	2:C:134:ARG:NE	2.23	0.54
2:C:44:HIS:HA	2:C:68:GLU:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:PRO:HD2	1:A:248:LYS:NZ	2.23	0.54
1:A:346:PRO:HA	1:A:372:PHE:HB3	1.90	0.54
2:C:41:GLN:NE2	2:C:50:PRO:O	2.40	0.54
1:A:301:ARG:HD3	1:A:302:VAL:N	2.22	0.54
1:A:371:GLY:N	1:A:404:PHE:O	2.40	0.54
2:C:93:LEU:HD13	2:C:93:LEU:O	2.07	0.54
1:A:279:VAL:C	1:A:281:GLY:N	2.58	0.54
1:A:381:TRP:CB	1:A:388:GLU:HB2	2.38	0.54
1:B:251:LEU:CD2	1:B:252:MET:SD	2.96	0.54
2:C:162:LEU:HD22	2:C:162:LEU:H	1.73	0.54
1:A:292:ARG:NH1	1:A:292:ARG:N	2.56	0.54
1:A:302:VAL:O	1:A:303:VAL:HG23	2.08	0.54
1:B:346:PRO:HB3	1:B:372:PHE:CG	2.43	0.54
1:A:233:GLU:HG3	1:B:235:LEU:HA	1.88	0.54
1:B:290:LYS:N	1:B:305:VAL:HG13	2.22	0.54
1:B:344:ARG:HH11	1:B:344:ARG:HG3	1.71	0.54
1:B:391:TYR:HB2	1:B:410:LEU:CA	2.35	0.54
1:B:243:PHE:HE2	4:B:809:NAG:H82	1.72	0.54
2:C:145:ASN:O	2:C:147:SER:N	2.40	0.54
5:C:201:NAG:O6	5:C:202:FUL:H5	2.07	0.54
1:A:312:ASN:HD21	1:A:317:LYS:CD	2.21	0.53
1:B:290:LYS:H	1:B:305:VAL:CG1	2.21	0.53
2:C:85:THR:O	2:C:86:VAL:HB	2.07	0.53
1:A:278:TYR:CD2	1:A:281:GLY:HA2	2.43	0.53
1:A:428:MET:HA	1:A:435:HIS:O	2.08	0.53
1:B:250:THR:CG2	1:B:313:TRP:HE1	2.17	0.53
2:C:18:ASN:CA	2:C:86:VAL:HG23	2.39	0.53
1:B:266:VAL:C	2:C:134:ARG:HD3	2.28	0.53
2:C:12:LEU:HD23	2:C:12:LEU:O	2.08	0.53
2:C:157:ASN:OD1	2:C:162:LEU:HD13	2.09	0.53
1:A:294:GLN:NE2	1:A:295:GLN:N	2.56	0.53
1:A:332:ILE:CG2	1:A:334:LYS:NZ	2.70	0.53
1:A:315:ASP:N	1:A:338:LYS:HZ1	2.04	0.53
1:B:251:LEU:C	1:B:253:ILE:H	2.12	0.53
1:B:345:GLU:OE1	1:B:347:GLN:HB2	2.08	0.53
1:B:367:CYS:HB2	1:B:381:TRP:CH2	2.44	0.53
1:B:393:THR:HA	1:B:408:SER:HA	1.91	0.53
1:B:346:PRO:HG3	1:B:429:HIS:HB2	1.89	0.53
1:A:262:VAL:HG12	1:A:263:VAL:H	1.73	0.53
1:A:321:CYS:SG	1:A:323:VAL:HG23	2.48	0.53
1:B:267:SER:C	1:B:269:GLU:H	2.11	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:LEU:HD13	1:B:310:HIS:ND1	2.23	0.53
1:B:368:LEU:HD23	1:B:369:VAL:N	2.23	0.53
1:B:399:ASP:HB3	1:B:403:SER:O	2.09	0.53
1:A:329:PRO:HD3	2:C:113:TRP:CH2	2.43	0.53
2:C:40:ILE:HG22	2:C:42:TRP:HE1	1.72	0.53
1:A:245:PRO:HD3	1:A:259:VAL:HG13	1.89	0.53
1:A:257:PRO:HB2	1:A:308:VAL:CG1	2.30	0.53
2:C:70:THR:HG22	2:C:71:CYS:N	2.19	0.53
1:A:284:VAL:O	1:A:285:HIS:CB	2.56	0.53
1:B:247:PRO:HG2	1:B:248:LYS:H	1.74	0.53
1:B:396:PRO:CD	1:B:406:LEU:HD13	2.38	0.53
1:B:243:PHE:HE2	4:B:809:NAG:C8	2.21	0.53
1:B:276:ASN:HB2	1:B:322:LYS:HE2	1.91	0.53
2:C:16:TRP:CZ2	2:C:109:ARG:HB2	2.44	0.53
2:C:40:ILE:CG2	2:C:42:TRP:HE1	2.22	0.53
1:A:377:ILE:HG13	1:A:429:HIS:HB2	1.91	0.53
1:A:417:TRP:HA	1:A:421:ASN:HD21	1.74	0.53
1:B:277:TRP:CE3	1:B:306:LEU:HD13	2.44	0.53
2:C:124:PHE:HB3	2:C:127:GLY:O	2.09	0.53
2:C:149:SER:CA	2:C:172:VAL:HG23	2.39	0.52
1:A:249:ASP:HA	1:A:255:ARG:CG	2.31	0.52
1:A:407:TYR:CD1	1:A:407:TYR:N	2.77	0.52
1:B:232:PRO:O	1:B:235:LEU:HD11	2.09	0.52
2:C:125:GLN:C	2:C:127:GLY:N	2.62	0.52
2:C:48:LEU:O	2:C:50:PRO:CD	2.57	0.52
1:A:439:LYS:HZ3	1:A:439:LYS:HA	1.75	0.52
1:B:434:ASN:C	1:B:435:HIS:ND1	2.62	0.52
2:C:113:TRP:C	2:C:115:ASP:H	2.12	0.52
1:B:235:LEU:HD12	1:B:235:LEU:N	2.24	0.52
2:C:10:LEU:N	2:C:29:CYS:SG	2.82	0.52
1:A:279:VAL:C	1:A:281:GLY:H	2.13	0.52
2:C:8:ALA:H	2:C:30:GLN:HB2	1.75	0.52
1:A:267:SER:C	1:A:269:GLU:H	2.12	0.52
1:A:287:ALA:C	1:A:289:THR:H	2.12	0.52
4:B:801:NAG:H4	4:B:803:NAG:N2	2.25	0.52
2:C:132:PHE:HD2	2:C:132:PHE:O	1.92	0.52
2:C:17:ILE:HD12	2:C:84:LEU:HD13	1.90	0.52
1:A:242:LEU:HB3	1:A:336:ILE:HD13	1.91	0.52
1:A:397:VAL:HB	1:A:405:PHE:CZ	2.44	0.52
1:B:430:GLU:HA	1:B:435:HIS:CG	2.44	0.52
2:C:34:SER:C	2:C:36:GLU:N	2.62	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:MET:HB3	1:A:255:ARG:CB	2.40	0.52
1:B:373:TYR:CZ	1:B:374:PRO:HB3	2.44	0.52
1:B:391:TYR:HB2	1:B:409:LYS:O	2.10	0.52
2:C:98:LEU:HD11	2:C:169:THR:O	2.09	0.52
1:A:428:MET:SD	1:A:436:TYR:CB	2.93	0.52
2:C:114:LYS:O	2:C:115:ASP:HB2	2.10	0.52
2:C:90:TRP:CD1	2:C:90:TRP:O	2.63	0.52
1:A:249:ASP:O	1:A:310:HIS:HE1	1.91	0.52
1:B:320:LYS:C	1:B:334:LYS:O	2.49	0.52
2:C:144:ALA:HB1	2:C:148:HIS:CD2	2.45	0.52
2:C:85:THR:HG22	2:C:86:VAL:N	2.25	0.52
1:A:234:LEU:HG	1:A:235:LEU:N	2.25	0.51
1:B:248:LYS:HZ2	1:B:378:ALA:HA	1.74	0.51
1:B:245:PRO:HD3	1:B:259:VAL:HG22	1.92	0.51
1:B:372:PHE:HB2	1:B:429:HIS:CD2	2.45	0.51
1:B:266:VAL:N	2:C:134:ARG:CZ	2.69	0.51
2:C:25:VAL:O	2:C:26:THR:OG1	2.24	0.51
2:C:48:LEU:HD12	2:C:48:LEU:O	2.11	0.51
1:A:249:ASP:O	1:A:257:PRO:HG3	2.11	0.51
1:A:313:TRP:HB3	1:A:314:LEU:HD12	1.93	0.51
1:A:348:VAL:HG12	1:A:439:LYS:HG2	1.91	0.51
1:B:245:PRO:CD	1:B:259:VAL:HG22	2.41	0.51
1:B:413:ASP:O	1:B:416:ARG:N	2.42	0.51
1:B:431:ALA:O	1:B:432:LEU:HG	2.10	0.51
1:A:379:VAL:HA	1:A:426:SER:O	2.09	0.51
1:B:381:TRP:CG	1:B:410:LEU:HD13	2.46	0.51
2:C:132:PHE:CD2	2:C:132:PHE:C	2.84	0.51
2:C:16:TRP:HE1	2:C:109:ARG:NH1	2.05	0.51
2:C:89:GLU:OE2	2:C:166:LYS:HE3	2.10	0.51
1:B:394:THR:CG2	1:B:407:TYR:N	2.71	0.51
2:C:170:ILE:HG22	2:C:171:THR:N	2.25	0.51
2:C:62:ASN:HB2	2:C:65:ASP:OD1	2.09	0.51
1:A:332:ILE:HG22	1:A:334:LYS:CG	2.36	0.51
1:A:353:PRO:CB	1:A:363:VAL:HG12	2.40	0.51
1:B:393:THR:CG2	1:B:394:THR:N	2.74	0.51
2:C:17:ILE:HB	2:C:84:LEU:CG	2.40	0.51
1:A:268:HIS:HA	1:A:271:PRO:CD	2.41	0.51
1:B:251:LEU:HD22	1:B:252:MET:SD	2.51	0.51
1:A:295:GLN:HE22	1:A:299:THR:N	2.09	0.51
1:A:302:VAL:HG12	1:A:303:VAL:N	2.26	0.51
1:A:314:LEU:N	1:A:314:LEU:CD1	2.72	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:GLU:O	1:A:360:LYS:HB3	2.11	0.51
1:A:251:LEU:HD13	1:A:428:MET:HB3	1.92	0.51
1:B:241:PHE:O	1:B:243:PHE:N	2.43	0.51
2:C:21:GLN:OE1	2:C:88:SER:HB2	2.11	0.51
1:A:318:GLU:CG	1:A:320:LYS:HE3	2.34	0.51
1:B:432:LEU:HD12	1:B:434:ASN:H	1.75	0.51
2:C:149:SER:HB2	2:C:171:THR:HA	1.93	0.51
2:C:99:GLU:OE2	2:C:171:THR:OG1	2.29	0.51
1:A:383:SER:HB2	1:A:388:GLU:CD	2.31	0.51
1:B:275:PHE:HZ	1:B:302:VAL:O	1.94	0.51
2:C:60:LYS:HZ2	2:C:60:LYS:HB2	1.75	0.51
1:A:324:SER:O	1:A:325:ASN:CB	2.58	0.50
1:B:433:HIS:NE2	1:B:434:ASN:ND2	2.58	0.50
2:C:81:PRO:HB2	2:C:83:HIS:CE1	2.46	0.50
2:C:98:LEU:HB3	2:C:99:GLU:OE1	2.11	0.50
1:B:245:PRO:HD3	1:B:259:VAL:CG1	2.38	0.50
2:C:15:PRO:O	2:C:16:TRP:C	2.49	0.50
2:C:173:GLN:HG3	2:C:173:GLN:O	2.12	0.50
2:C:52:HIS:ND1	2:C:57:TYR:CE1	2.78	0.50
2:C:60:LYS:O	2:C:61:ALA:CB	2.59	0.50
1:A:292:ARG:HG2	1:A:293:GLU:O	2.11	0.50
1:B:235:LEU:HD23	1:B:329:PRO:HG3	1.92	0.50
1:B:279:VAL:O	1:B:282:VAL:N	2.45	0.50
1:B:346:PRO:O	1:B:348:VAL:HG13	2.10	0.50
1:B:391:TYR:HA	1:B:409:LYS:O	2.10	0.50
1:B:432:LEU:HD11	1:B:435:HIS:CA	2.41	0.50
1:A:380:GLU:HG2	1:A:381:TRP:N	2.26	0.50
1:A:433:HIS:C	1:A:435:HIS:H	2.14	0.50
1:B:251:LEU:N	1:B:251:LEU:HD13	2.26	0.50
1:B:297:ASN:O	1:B:298:SER:HB2	2.11	0.50
1:B:355:ARG:O	1:B:358:MET:HB2	2.11	0.50
2:C:27:LEU:O	2:C:56:SER:HA	2.11	0.50
1:A:283:GLN:HG2	1:A:285:HIS:H	1.75	0.50
1:A:291:PRO:O	1:A:292:ARG:HB3	2.11	0.50
1:B:305:VAL:HG22	1:B:305:VAL:O	2.11	0.50
1:B:321:CYS:SG	1:B:323:VAL:CG2	2.95	0.50
1:B:336:ILE:HG13	1:B:337:SER:N	2.19	0.50
1:A:309:LEU:HB3	1:A:311:GLN:OE1	2.10	0.50
1:A:415:SER:O	1:A:419:GLN:N	2.35	0.50
1:A:432:LEU:CD1	1:A:432:LEU:H	2.18	0.50
1:B:373:TYR:CG	1:B:374:PRO:HA	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:10:LEU:HB3	2:C:82:VAL:HG22	1.93	0.50
2:C:111:HIS:CG	2:C:112:SER:N	2.79	0.50
2:C:25:VAL:HG23	2:C:60:LYS:O	2.11	0.50
1:A:421:ASN:ND2	1:A:421:ASN:N	2.59	0.50
1:B:291:PRO:HA	1:B:292:ARG:NE	2.26	0.50
2:C:125:GLN:HB3	2:C:130:GLN:CG	2.42	0.50
1:A:309:LEU:CD2	1:A:309:LEU:H	2.24	0.49
1:A:360:LYS:HG2	1:A:362:GLN:N	2.26	0.49
1:A:380:GLU:HG2	1:A:381:TRP:H	1.77	0.49
1:A:383:SER:OG	1:A:416:ARG:NH2	2.45	0.49
1:B:261:CYS:C	1:B:303:VAL:HG12	2.33	0.49
2:C:113:TRP:C	2:C:115:ASP:N	2.65	0.49
1:A:270:ASP:N	1:A:271:PRO:HD3	2.28	0.49
1:A:333:GLU:N	1:A:333:GLU:OE1	2.45	0.49
1:B:238:PRO:HA	1:B:265:ASP:CB	2.41	0.49
1:B:243:PHE:HZ	4:B:808:MAN:H62	1.77	0.49
1:B:260:THR:HG1	1:B:304:SER:H	1.57	0.49
2:C:27:LEU:HB2	2:C:42:TRP:CZ3	2.47	0.49
1:A:406:LEU:C	1:A:407:TYR:CD1	2.85	0.49
1:B:234:LEU:C	1:B:235:LEU:HD12	2.33	0.49
1:B:334:LYS:HD2	1:B:334:LYS:H	1.77	0.49
1:A:262:VAL:HA	1:A:303:VAL:HG22	1.93	0.49
1:A:421:ASN:HD22	1:A:421:ASN:N	2.10	0.49
1:B:275:PHE:CZ	1:B:302:VAL:O	2.66	0.49
1:B:277:TRP:CZ2	1:B:304:SER:O	2.66	0.49
1:B:391:TYR:CD1	1:B:391:TYR:C	2.85	0.49
1:B:443:LEU:HD12	1:B:443:LEU:C	2.32	0.49
2:C:42:TRP:CZ3	2:C:71:CYS:SG	3.05	0.49
1:B:433:HIS:CD2	1:B:434:ASN:ND2	2.79	0.49
1:A:435:HIS:N	1:A:435:HIS:HD2	2.11	0.49
1:B:237:GLY:O	1:B:265:ASP:OD2	2.31	0.49
1:B:444:SER:H	7:B:601:GOL:C2	2.23	0.49
2:C:157:ASN:CB	2:C:162:LEU:HD13	2.42	0.49
2:C:40:ILE:HB	2:C:53:THR:C	2.33	0.49
1:A:285:HIS:CG	1:A:286:ASN:N	2.80	0.49
1:A:295:GLN:CD	1:A:296:TYR:H	2.15	0.49
1:A:312:ASN:OD1	1:A:319:TYR:OH	2.31	0.49
1:A:319:TYR:O	1:A:336:ILE:CG2	2.61	0.49
1:A:360:LYS:O	1:A:414:LYS:HD3	2.13	0.49
2:C:105:THR:OG1	2:C:142:PRO:HA	2.13	0.49
2:C:84:LEU:CD1	2:C:85:THR:N	2.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:312:ASN:HB2	1:B:317:LYS:HD2	1.94	0.49
1:A:342:GLN:HB3	1:A:343:PRO:CD	2.42	0.49
1:A:406:LEU:C	1:A:407:TYR:HD1	2.15	0.49
1:B:382:GLU:O	1:B:423:PHE:HA	2.13	0.49
1:B:297:ASN:O	1:B:298:SER:CB	2.61	0.49
2:C:134:ARG:CB	2:C:134:ARG:HH11	2.02	0.48
1:A:246:LYS:O	1:A:249:ASP:HB2	2.13	0.48
1:A:377:ILE:HG12	1:A:378:ALA:N	2.22	0.48
1:A:407:TYR:HD1	1:A:407:TYR:N	2.12	0.48
1:A:350:THR:CG2	1:A:439:LYS:HB3	2.31	0.48
1:B:241:PHE:H	1:B:263:VAL:CG1	2.13	0.48
1:B:430:GLU:HA	1:B:435:HIS:NE2	2.28	0.48
2:C:100:PHE:CZ	2:C:106:ILE:HG23	2.47	0.48
2:C:38:ASP:OD1	2:C:40:ILE:HD11	2.12	0.48
2:C:96:PRO:HD2	2:C:107:MET:O	2.13	0.48
1:A:403:SER:OG	1:A:404:PHE:N	2.46	0.48
1:B:289:THR:HB	1:B:306:LEU:HD12	1.91	0.48
1:B:417:TRP:CH2	1:B:442:SER:O	2.66	0.48
2:C:162:LEU:CD2	2:C:162:LEU:H	2.26	0.48
1:B:289:THR:HG23	1:B:291:PRO:HD3	1.94	0.48
2:C:169:THR:O	2:C:170:ILE:HG13	2.14	0.48
2:C:97:HIS:O	2:C:98:LEU:CD2	2.61	0.48
2:C:9:VAL:HG21	2:C:80:ASP:HB2	1.94	0.48
1:A:257:PRO:HD3	1:A:310:HIS:HE2	1.73	0.48
1:B:284:VAL:C	1:B:286:ASN:H	2.17	0.48
1:B:321:CYS:O	1:B:334:LYS:N	2.46	0.48
2:C:128:LYS:O	2:C:129:SER:O	2.31	0.48
1:B:309:LEU:HB3	1:B:312:ASN:OD1	2.13	0.48
2:C:113:TRP:HE3	2:C:116:LYS:HE2	1.77	0.48
2:C:84:LEU:CG	2:C:85:THR:N	2.75	0.48
1:A:434:ASN:C	1:A:436:TYR:H	2.15	0.48
1:B:293:GLU:HB3	1:B:300:TYR:HA	1.94	0.48
1:B:279:VAL:CA	1:B:319:TYR:HA	2.29	0.48
1:B:373:TYR:C	1:B:373:TYR:CD1	2.87	0.48
2:C:152:TYR:N	2:C:168:VAL:CG1	2.76	0.48
1:A:433:HIS:O	1:A:435:HIS:N	2.45	0.48
1:B:260:THR:OG1	1:B:303:VAL:HB	2.14	0.48
1:B:243:PHE:HD1	1:B:262:VAL:CG2	2.23	0.48
2:C:170:ILE:CG2	2:C:171:THR:N	2.77	0.48
5:C:201:NAG:C5	5:C:203:MAN:H2	2.42	0.48
2:C:138:THR:HG22	2:C:139:PHE:H	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:PRO:HA	1:A:374:PRO:HG2	1.96	0.47
1:B:246:LYS:HD3	1:B:247:PRO:N	2.29	0.47
1:B:418:GLN:OE1	1:B:443:LEU:HD21	2.13	0.47
2:C:145:ASN:C	2:C:147:SER:N	2.68	0.47
2:C:9:VAL:CA	2:C:29:CYS:HA	2.42	0.47
2:C:100:PHE:O	2:C:104:GLU:HB3	2.14	0.47
1:A:268:HIS:C	1:A:271:PRO:HD3	2.35	0.47
1:B:377:ILE:CG1	1:B:378:ALA:N	2.62	0.47
2:C:62:ASN:HB2	2:C:64:ASN:OD1	2.15	0.47
2:C:123:PHE:N	2:C:123:PHE:CD1	2.81	0.47
2:C:49:ILE:HG13	2:C:51:THR:OG1	2.14	0.47
1:B:399:ASP:O	1:B:401:ASP:N	2.46	0.47
4:B:802:FUL:H61	2:C:128:LYS:HB2	1.96	0.47
1:A:253:ILE:H	1:A:253:ILE:CD1	2.26	0.47
1:A:301:ARG:C	1:A:301:ARG:HD3	2.35	0.47
1:B:312:ASN:HB2	1:B:317:LYS:HG3	1.94	0.47
1:B:381:TRP:CB	1:B:410:LEU:HD13	2.44	0.47
2:C:108:LEU:N	2:C:108:LEU:HD22	2.30	0.47
2:C:122:THR:HB	2:C:155:THR:HG22	1.97	0.47
2:C:32:ALA:H	2:C:75:GLN:CD	2.18	0.47
2:C:34:SER:HB3	2:C:37:SER:C	2.34	0.47
1:A:275:PHE:HE1	1:A:291:PRO:CB	2.27	0.47
1:A:345:GLU:HA	1:A:346:PRO:HD3	1.45	0.47
1:B:251:LEU:C	1:B:253:ILE:N	2.67	0.47
2:C:16:TRP:HH2	2:C:107:MET:HG3	1.79	0.47
2:C:163:PHE:HB3	2:C:164:SER:H	1.50	0.47
2:C:40:ILE:HG22	2:C:42:TRP:NE1	2.30	0.47
1:A:297:ASN:OD1	1:A:299:THR:HG23	2.14	0.47
1:B:248:LYS:CG	1:B:377:ILE:O	2.61	0.47
2:C:52:HIS:ND1	2:C:57:TYR:HE1	2.12	0.47
1:B:310:HIS:O	1:B:312:ASN:N	2.47	0.47
1:B:443:LEU:HA	7:B:601:GOL:H11	1.97	0.47
1:A:414:LYS:HG2	1:A:414:LYS:O	2.15	0.47
1:A:380:GLU:O	1:A:425:CYS:HA	2.14	0.47
1:A:432:LEU:O	1:A:433:HIS:O	2.33	0.47
1:B:266:VAL:HG21	1:B:300:TYR:HB2	1.97	0.47
1:B:303:VAL:HG23	1:B:304:SER:N	2.30	0.47
2:C:49:ILE:C	2:C:51:THR:N	2.65	0.47
1:A:370:LYS:NZ	1:B:411:THR:HG23	2.29	0.47
1:A:264:VAL:HG12	3:A:803:NAG:H82	1.97	0.47
1:B:394:THR:CG2	1:B:406:LEU:HB2	2.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:149:SER:N	2:C:172:VAL:HG23	2.30	0.47
2:C:48:LEU:HD12	2:C:50:PRO:N	2.30	0.47
2:C:26:THR:OG1	2:C:58:ARG:HA	2.15	0.47
1:A:249:ASP:N	1:A:255:ARG:HD3	2.30	0.46
1:B:395:PRO:O	1:B:396:PRO:C	2.54	0.46
2:C:149:SER:HB3	2:C:172:VAL:HG23	1.96	0.46
1:A:253:ILE:CG1	1:A:254:SER:N	2.78	0.46
1:A:245:PRO:HB3	1:A:258:GLU:H	1.80	0.46
1:A:332:ILE:HG22	1:A:332:ILE:O	2.15	0.46
1:B:240:VAL:HB	1:B:263:VAL:HG11	1.97	0.46
1:B:306:LEU:CD1	1:B:306:LEU:N	2.73	0.46
1:B:309:LEU:CD1	1:B:310:HIS:ND1	2.78	0.46
1:B:312:ASN:HB2	1:B:317:LYS:CD	2.45	0.46
1:B:350:THR:O	1:B:351:LEU:HG	2.15	0.46
2:C:84:LEU:HD11	2:C:85:THR:O	2.15	0.46
2:C:40:ILE:CG1	2:C:54:GLN:N	2.65	0.46
2:C:52:HIS:CG	2:C:57:TYR:CE1	3.03	0.46
1:B:241:PHE:O	1:B:243:PHE:CD1	2.68	0.46
2:C:97:HIS:HB2	2:C:100:PHE:CE1	2.50	0.46
2:C:124:PHE:CE1	2:C:155:THR:HG22	2.50	0.46
2:C:168:VAL:CG2	2:C:169:THR:H	2.13	0.46
1:A:328:LEU:HD13	1:A:330:ALA:O	2.15	0.46
1:B:430:GLU:HA	1:B:435:HIS:CE1	2.50	0.46
2:C:97:HIS:CB	2:C:100:PHE:CE1	2.98	0.46
1:A:332:ILE:CG2	1:A:334:LYS:HZ3	2.28	0.46
1:A:401:ASP:OD1	1:A:403:SER:HB3	2.14	0.46
2:C:121:VAL:CG1	2:C:122:THR:N	2.78	0.46
5:C:200:NDG:C4	5:C:201:NAG:N2	2.78	0.46
2:C:29:CYS:O	2:C:30:GLN:O	2.34	0.46
2:C:40:ILE:CB	2:C:54:GLN:N	2.78	0.46
1:A:301:ARG:NH2	1:A:303:VAL:CG2	2.56	0.46
1:B:290:LYS:N	1:B:291:PRO:CD	2.79	0.46
1:B:340:LYS:O	1:B:373:TYR:OH	2.33	0.46
1:A:413:ASP:C	1:A:415:SER:N	2.69	0.46
1:B:301:ARG:HG2	1:B:303:VAL:HG13	1.98	0.46
1:A:301:ARG:HG3	3:A:803:NAG:C8	2.46	0.46
1:A:429:HIS:HB3	1:A:432:LEU:HD11	1.97	0.46
1:B:279:VAL:HG13	1:B:319:TYR:CB	2.44	0.46
1:B:286:ASN:ND2	1:B:286:ASN:N	2.64	0.46
1:B:348:VAL:HG12	1:B:369:VAL:CG1	2.35	0.46
2:C:130:GLN:NE2	2:C:130:GLN:HA	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:LEU:CG	1:A:235:LEU:H	2.25	0.46
1:A:234:LEU:HD23	1:A:234:LEU:H	1.81	0.46
1:A:344:ARG:HG3	1:A:372:PHE:HA	1.97	0.46
1:A:398:LEU:HA	1:A:404:PHE:CE1	2.50	0.46
4:B:805:MAN:C2	4:B:806:NAG:H83	2.46	0.46
2:C:60:LYS:HA	2:C:60:LYS:NZ	2.31	0.46
2:C:98:LEU:HD22	2:C:98:LEU:HA	1.77	0.46
1:A:262:VAL:C	1:A:263:VAL:CG2	2.84	0.45
1:B:331:PRO:O	1:B:332:ILE:O	2.33	0.45
2:C:98:LEU:CD2	2:C:169:THR:O	2.63	0.45
1:A:262:VAL:O	1:A:263:VAL:HG22	2.16	0.45
1:A:353:PRO:HB3	1:A:363:VAL:HG12	1.97	0.45
1:A:414:LYS:NZ	1:A:418:GLN:CG	2.75	0.45
3:A:805:MAN:O3	3:A:806:NAG:H2	2.16	0.45
1:B:245:PRO:HD3	1:B:259:VAL:CB	2.46	0.45
2:C:22:GLU:HB3	2:C:114:LYS:HZ2	1.80	0.45
1:A:346:PRO:CB	1:A:372:PHE:HB3	2.47	0.45
1:B:348:VAL:HG12	1:B:369:VAL:HA	1.99	0.45
1:B:394:THR:HG22	1:B:407:TYR:N	2.30	0.45
2:C:168:VAL:HG13	2:C:169:THR:N	2.31	0.45
2:C:169:THR:C	2:C:170:ILE:HG13	2.36	0.45
1:A:320:LYS:HG3	1:A:335:THR:HA	1.98	0.45
1:B:397:VAL:O	1:B:404:PHE:HD1	1.99	0.45
1:B:417:TRP:HH2	1:B:442:SER:O	2.00	0.45
2:C:96:PRO:CD	2:C:107:MET:O	2.64	0.45
1:A:242:LEU:HD23	1:A:261:CYS:HA	1.98	0.45
1:A:301:ARG:NE	1:A:303:VAL:HG23	2.29	0.45
1:A:350:THR:CA	1:A:439:LYS:HG3	2.46	0.45
1:B:241:PHE:HB3	1:B:243:PHE:CE2	2.51	0.45
1:B:276:ASN:O	1:B:278:TYR:N	2.49	0.45
1:B:357:GLU:O	1:B:359:THR:N	2.49	0.45
2:C:20:LEU:O	2:C:21:GLN:HG3	2.16	0.45
1:A:262:VAL:HA	1:A:303:VAL:CG2	2.47	0.45
1:A:287:ALA:O	1:A:288:LYS:HB3	2.16	0.45
1:A:414:LYS:O	1:A:418:GLN:HG2	2.17	0.45
1:B:287:ALA:O	1:B:288:LYS:CB	2.64	0.45
1:B:396:PRO:CG	1:B:406:LEU:HD13	2.46	0.45
1:A:242:LEU:CD1	1:A:336:ILE:HG21	2.47	0.45
1:A:345:GLU:HA	1:A:431:ALA:CB	2.47	0.45
3:A:802:FUL:H61	3:A:805:MAN:O6	2.17	0.45
1:B:379:VAL:CG1	1:B:380:GLU:N	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:441:LEU:HD22	1:B:441:LEU:C	2.37	0.45
2:C:27:LEU:CD1	2:C:27:LEU:H	2.29	0.45
2:C:42:TRP:HE3	2:C:70:THR:O	2.00	0.45
1:A:334:LYS:O	1:A:336:ILE:HG22	2.16	0.45
1:B:245:PRO:CD	1:B:259:VAL:HA	2.47	0.45
1:B:315:ASP:CG	1:B:316:GLY:N	2.70	0.45
1:B:320:LYS:HG2	1:B:335:THR:HG22	1.98	0.45
1:B:381:TRP:CE3	1:B:424:SER:O	2.70	0.45
4:B:801:NAG:O5	4:B:802:FUL:C2	2.58	0.45
2:C:85:THR:O	2:C:86:VAL:CB	2.64	0.45
1:A:284:VAL:O	1:A:285:HIS:HB3	2.16	0.45
2:C:129:SER:OG	2:C:130:GLN:N	2.43	0.45
5:C:200:NDG:H4	5:C:201:NAG:C7	2.47	0.45
1:A:262:VAL:HG12	1:A:263:VAL:N	2.32	0.44
1:A:283:GLN:CD	1:A:285:HIS:O	2.56	0.44
1:A:332:ILE:HG23	1:A:334:LYS:HZ1	1.78	0.44
1:A:355:ARG:HG2	1:A:356:GLU:N	2.32	0.44
1:A:410:LEU:HD12	1:A:411:THR:N	2.25	0.44
2:C:157:ASN:CG	2:C:162:LEU:HD13	2.37	0.44
2:C:41:GLN:HB3	2:C:50:PRO:HA	1.99	0.44
2:C:53:THR:O	2:C:54:GLN:CB	2.60	0.44
2:C:91:LEU:HB3	2:C:164:SER:O	2.17	0.44
1:A:412:VAL:HG23	1:A:413:ASP:O	2.17	0.44
1:B:241:PHE:CE2	4:B:809:NAG:N2	2.78	0.44
1:B:435:HIS:ND1	1:B:435:HIS:N	2.65	0.44
1:B:443:LEU:HA	7:B:601:GOL:C1	2.48	0.44
2:C:58:ARG:O	2:C:58:ARG:CG	2.65	0.44
1:A:268:HIS:HA	1:A:271:PRO:HD3	1.98	0.44
1:A:332:ILE:O	1:A:334:LYS:HG2	2.17	0.44
2:C:20:LEU:HD12	2:C:111:HIS:CE1	2.53	0.44
2:C:40:ILE:HD13	2:C:73:THR:HB	1.99	0.44
1:B:432:LEU:CD2	1:B:436:TYR:N	2.73	0.44
2:C:78:LEU:HG	2:C:80:ASP:OD1	2.17	0.44
1:A:438:GLN:N	1:A:438:GLN:NE2	2.58	0.44
1:B:278:TYR:HD2	1:B:278:TYR:HA	1.65	0.44
2:C:101:GLN:NE2	2:C:173:GLN:NE2	2.66	0.44
2:C:98:LEU:C	2:C:99:GLU:CD	2.75	0.44
1:A:357:GLU:C	1:A:359:THR:H	2.21	0.44
1:A:344:ARG:HG2	1:A:373:TYR:HB2	2.00	0.44
1:B:252:MET:CB	1:B:255:ARG:NE	2.76	0.44
1:B:359:THR:HB	1:B:360:LYS:H	1.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:33:ARG:O	2:C:34:SER:O	2.35	0.44
2:C:97:HIS:HB3	2:C:98:LEU:H	1.49	0.44
1:A:346:PRO:HD3	1:A:431:ALA:CB	2.43	0.44
1:B:276:ASN:HB2	1:B:322:LYS:CB	2.47	0.44
1:B:241:PHE:CD2	4:B:809:NAG:H83	2.51	0.44
2:C:100:PHE:CB	2:C:106:ILE:HG12	2.48	0.44
2:C:56:SER:OG	2:C:57:TYR:N	2.51	0.44
1:A:441:LEU:HD23	1:A:442:SER:N	2.33	0.44
1:B:262:VAL:HG23	1:B:301:ARG:CZ	2.48	0.44
1:B:293:GLU:OE2	1:B:300:TYR:CZ	2.71	0.44
2:C:56:SER:O	2:C:57:TYR:HB3	2.18	0.44
1:A:314:LEU:HB3	1:A:338:LYS:NZ	2.32	0.43
1:B:279:VAL:CB	1:B:282:VAL:HG23	2.47	0.43
1:B:432:LEU:HD12	1:B:434:ASN:N	2.33	0.43
2:C:13:GLU:N	2:C:26:THR:O	2.50	0.43
1:A:311:GLN:OE1	1:A:311:GLN:N	2.51	0.43
1:A:347:GLN:OE1	1:A:370:LYS:O	2.35	0.43
1:B:245:PRO:HB3	1:B:258:GLU:C	2.38	0.43
1:B:354:SER:O	1:B:357:GLU:HG3	2.18	0.43
2:C:100:PHE:CD2	2:C:106:ILE:HG12	2.52	0.43
1:A:235:LEU:HD11	2:C:117:PRO:HG3	1.99	0.43
2:C:12:LEU:H	2:C:12:LEU:CD2	2.31	0.43
2:C:42:TRP:CD1	2:C:42:TRP:N	2.86	0.43
2:C:91:LEU:HA	2:C:91:LEU:HD12	1.86	0.43
1:A:295:GLN:HE21	1:A:296:TYR:H	1.62	0.43
1:B:290:LYS:HB2	1:B:305:VAL:HG13	1.94	0.43
1:B:423:PHE:N	1:B:423:PHE:CD2	2.84	0.43
1:A:374:PRO:O	1:A:375:SER:HB3	2.18	0.43
1:A:413:ASP:C	1:A:415:SER:H	2.21	0.43
1:B:241:PHE:CZ	4:B:809:NAG:C7	3.00	0.43
2:C:17:ILE:CD1	2:C:84:LEU:HD13	2.48	0.43
1:A:257:PRO:HD3	1:A:310:HIS:CE1	2.51	0.43
1:B:251:LEU:HD21	1:B:252:MET:SD	2.58	0.43
1:B:300:TYR:O	1:B:301:ARG:C	2.57	0.43
1:B:321:CYS:C	1:B:333:GLU:HA	2.39	0.43
1:B:346:PRO:N	1:B:372:PHE:HB3	2.34	0.43
1:B:340:LYS:C	1:B:373:TYR:OH	2.56	0.43
1:A:247:PRO:CD	1:A:248:LYS:HZ2	2.32	0.43
1:B:273:VAL:O	1:B:324:SER:HB3	2.19	0.43
1:B:247:PRO:CB	1:B:376:ASP:OD1	2.66	0.43
1:B:289:THR:C	1:B:291:PRO:HD3	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:102:GLU:O	2:C:104:GLU:N	2.45	0.43
1:A:248:LYS:HB2	1:A:255:ARG:CD	2.42	0.43
1:A:406:LEU:HD12	1:A:407:TYR:N	2.33	0.43
1:A:439:LYS:HZ2	1:A:439:LYS:HA	1.82	0.43
1:B:237:GLY:HA3	2:C:119:VAL:HG11	2.01	0.43
1:B:249:ASP:CA	1:B:255:ARG:HD2	2.48	0.43
1:B:278:TYR:CE2	1:B:284:VAL:HA	2.41	0.43
1:B:321:CYS:HB3	1:B:334:LYS:CB	2.32	0.43
1:B:388:GLU:O	1:B:389:ASN:OD1	2.37	0.43
2:C:43:PHE:HD1	2:C:43:PHE:H	1.65	0.43
2:C:9:VAL:CG2	2:C:80:ASP:HB2	2.49	0.43
1:B:242:LEU:HG	1:B:260:THR:O	2.19	0.43
1:B:432:LEU:HD11	1:B:435:HIS:H	1.78	0.43
4:B:801:NAG:O7	4:B:803:NAG:C1	2.66	0.43
2:C:124:PHE:CD2	2:C:129:SER:HA	2.54	0.42
2:C:43:PHE:HD1	2:C:43:PHE:N	2.13	0.42
2:C:60:LYS:HA	2:C:60:LYS:HZ1	1.84	0.42
1:A:289:THR:HG22	1:A:291:PRO:HD3	2.01	0.42
1:A:305:VAL:O	1:A:306:LEU:HD12	2.18	0.42
1:A:381:TRP:CD1	1:A:391:TYR:CD2	3.07	0.42
1:A:432:LEU:HD13	1:A:435:HIS:CA	2.48	0.42
1:B:292:ARG:O	1:B:293:GLU:OE1	2.37	0.42
2:C:162:LEU:N	2:C:162:LEU:CD2	2.82	0.42
1:A:268:HIS:HA	1:A:271:PRO:HG3	1.98	0.42
1:A:339:ALA:O	1:A:340:LYS:O	2.37	0.42
1:B:250:THR:C	1:B:252:MET:N	2.73	0.42
1:B:432:LEU:CD1	1:B:434:ASN:H	2.32	0.42
2:C:12:LEU:HD23	2:C:12:LEU:H	1.85	0.42
2:C:155:THR:O	2:C:155:THR:HG23	2.20	0.42
2:C:62:ASN:HB2	2:C:63:ASN:H	1.59	0.42
1:A:246:LYS:O	1:A:247:PRO:C	2.57	0.42
1:A:324:SER:O	1:A:325:ASN:HB2	2.19	0.42
1:A:357:GLU:C	1:A:359:THR:N	2.71	0.42
1:B:318:GLU:C	1:B:319:TYR:CG	2.92	0.42
1:B:351:LEU:HD23	1:B:352:PRO:HD2	2.01	0.42
3:A:808:MAN:O3	3:A:809:NAG:C1	2.68	0.42
2:C:133:SER:OG	2:C:136:ASP:CB	2.68	0.42
2:C:173:GLN:CG	2:C:173:GLN:O	2.66	0.42
1:A:260:THR:HA	1:A:304:SER:O	2.20	0.42
1:A:354:SER:O	1:A:357:GLU:N	2.39	0.42
1:A:443:LEU:HG	1:A:443:LEU:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:PRO:HD3	1:B:259:VAL:CA	2.46	0.42
2:C:132:PHE:CD2	2:C:132:PHE:O	2.71	0.42
1:A:257:PRO:O	1:A:258:GLU:OE2	2.37	0.42
1:A:291:PRO:HA	1:A:303:VAL:O	2.20	0.42
1:A:429:HIS:CG	1:A:430:GLU:H	2.37	0.42
3:A:811:SIA:H92	3:A:811:SIA:H6	1.71	0.42
1:B:284:VAL:C	1:B:286:ASN:N	2.72	0.42
1:B:368:LEU:HB2	1:B:407:TYR:CE1	2.54	0.42
1:B:399:ASP:C	1:B:401:ASP:H	2.23	0.42
1:A:355:ARG:HD3	1:A:356:GLU:HG3	2.02	0.42
1:A:429:HIS:CG	1:A:430:GLU:N	2.87	0.42
1:B:417:TRP:HZ3	1:B:442:SER:HA	1.84	0.42
2:C:23:ASP:O	2:C:24:SER:OG	2.23	0.42
1:A:240:VAL:O	1:A:241:PHE:HB2	2.20	0.42
1:A:345:GLU:HA	1:A:431:ALA:HB1	2.02	0.42
2:C:80:ASP:HA	2:C:81:PRO:HD2	1.75	0.42
1:A:277:TRP:CZ3	1:A:321:CYS:HB2	2.55	0.42
1:B:394:THR:OG1	1:B:395:PRO:CD	2.66	0.42
2:C:113:TRP:O	2:C:115:ASP:N	2.53	0.42
2:C:132:PHE:CD2	2:C:133:SER:O	2.73	0.42
1:A:294:GLN:CD	1:A:295:GLN:H	2.23	0.41
1:B:320:LYS:CA	1:B:334:LYS:O	2.68	0.41
1:B:396:PRO:HG3	1:B:406:LEU:CD2	2.46	0.41
2:C:141:ILE:HG22	2:C:144:ALA:CB	2.34	0.41
2:C:43:PHE:CD2	2:C:48:LEU:HB3	2.54	0.41
1:A:383:SER:HB2	1:A:388:GLU:OE1	2.20	0.41
1:A:277:TRP:NE1	1:A:306:LEU:HD13	2.35	0.41
1:A:306:LEU:O	1:A:307:THR:C	2.59	0.41
1:A:312:ASN:ND2	1:A:317:LYS:HD2	2.35	0.41
1:B:247:PRO:O	1:B:249:ASP:N	2.53	0.41
1:B:278:TYR:O	1:B:320:LYS:CD	2.64	0.41
1:B:292:ARG:H	1:B:292:ARG:NE	2.14	0.41
1:B:260:THR:OG1	1:B:303:VAL:CG2	2.68	0.41
1:B:348:VAL:HB	1:B:368:LEU:O	2.20	0.41
5:C:201:NAG:C4	5:C:202:FUL:H5	2.48	0.41
1:B:246:LYS:CD	1:B:247:PRO:HD2	2.45	0.41
1:B:312:ASN:HB2	1:B:317:LYS:CB	2.50	0.41
2:C:125:GLN:HB3	2:C:130:GLN:HG2	2.02	0.41
1:A:275:PHE:HD2	1:A:275:PHE:HA	1.77	0.41
1:A:310:HIS:C	1:A:312:ASN:N	2.72	0.41
1:A:325:ASN:HD21	1:A:327:ALA:CB	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:439:LYS:C	1:A:439:LYS:HD3	2.40	0.41
1:B:251:LEU:CD1	1:B:251:LEU:N	2.84	0.41
1:B:391:TYR:CA	1:B:409:LYS:O	2.68	0.41
2:C:94:GLN:N	2:C:109:ARG:O	2.53	0.41
2:C:42:TRP:HZ2	2:C:55:PRO:C	2.23	0.41
1:A:289:THR:HA	1:A:306:LEU:HD12	2.03	0.41
1:B:279:VAL:CG1	1:B:282:VAL:HG23	2.51	0.41
1:B:262:VAL:HB	1:B:301:ARG:NH2	2.35	0.41
1:B:333:GLU:O	1:B:334:LYS:C	2.58	0.41
1:B:394:THR:O	1:B:406:LEU:CD1	2.66	0.41
2:C:173:GLN:OE1	2:C:173:GLN:CA	2.68	0.41
2:C:18:ASN:O	2:C:94:GLN:HG2	2.21	0.41
2:C:25:VAL:CG1	2:C:26:THR:H	2.25	0.41
1:A:377:ILE:CD1	1:A:429:HIS:HB2	2.51	0.41
1:A:439:LYS:O	1:A:441:LEU:N	2.53	0.41
1:B:243:PHE:CB	1:B:262:VAL:CG1	2.93	0.41
2:C:124:PHE:HB2	2:C:153:HIS:CE1	2.56	0.41
1:B:366:THR:O	1:B:381:TRP:HH2	2.03	0.41
1:B:383:SER:CA	1:B:388:GLU:OE1	2.68	0.41
2:C:83:HIS:O	2:C:84:LEU:HB3	2.20	0.41
1:A:394:THR:OG1	1:A:395:PRO:O	2.39	0.41
1:B:237:GLY:N	1:B:238:PRO:CD	2.84	0.41
1:B:293:GLU:HB3	1:B:300:TYR:CA	2.49	0.41
2:C:143:GLN:NE2	2:C:143:GLN:H	2.18	0.41
2:C:54:GLN:HA	2:C:55:PRO:HD3	1.79	0.41
2:C:75:GLN:O	2:C:76:THR:HG23	2.19	0.41
1:B:336:ILE:HA	1:B:336:ILE:HD12	1.94	0.41
2:C:84:LEU:HG	2:C:85:THR:N	2.30	0.41
1:A:279:VAL:O	1:A:282:VAL:CG2	2.60	0.41
1:A:377:ILE:HD11	1:A:427:VAL:HG12	2.02	0.41
1:B:253:ILE:O	1:B:255:ARG:N	2.54	0.41
2:C:123:PHE:CZ	2:C:139:PHE:HB2	2.56	0.41
1:A:274:LYS:CE	1:A:276:ASN:OD1	2.65	0.40
1:A:323:VAL:O	1:A:331:PRO:HA	2.21	0.40
1:A:337:SER:O	1:A:338:LYS:C	2.60	0.40
1:B:240:VAL:CA	1:B:263:VAL:HB	2.33	0.40
1:B:369:VAL:O	1:B:405:PHE:CA	2.59	0.40
1:B:381:TRP:C	1:B:382:GLU:HG3	2.39	0.40
1:B:427:VAL:HG12	1:B:428:MET:N	2.36	0.40
1:B:243:PHE:CE2	4:B:809:NAG:C8	3.03	0.40
2:C:119:VAL:C	2:C:120:LYS:HG3	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:121:VAL:HB	2:C:133:SER:HB3	2.03	0.40
2:C:40:ILE:HB	2:C:54:GLN:N	2.36	0.40
1:A:260:THR:HB	1:A:303:VAL:CG1	2.51	0.40
1:A:357:GLU:HG2	1:A:357:GLU:O	2.21	0.40
1:A:358:MET:SD	1:A:363:VAL:HG11	2.62	0.40
1:A:373:TYR:CD2	1:A:374:PRO:N	2.89	0.40
1:B:288:LYS:C	1:B:306:LEU:HA	2.42	0.40
2:C:134:ARG:O	2:C:135:LEU:CB	2.66	0.40
5:C:201:NAG:O6	5:C:202:FUL:H3	2.21	0.40
2:C:12:LEU:CA	2:C:27:LEU:HA	2.44	0.40
2:C:49:ILE:HG12	2:C:52:HIS:HD2	1.86	0.40
1:A:277:TRP:CG	1:A:306:LEU:HD22	2.56	0.40
1:A:358:MET:HE1	1:A:363:VAL:HG11	2.02	0.40
1:A:415:SER:C	1:A:419:GLN:HG3	2.42	0.40
1:B:367:CYS:HB2	1:B:381:TRP:CZ2	2.56	0.40
2:C:42:TRP:O	2:C:48:LEU:HB2	2.21	0.40
1:A:243:PHE:HD1	3:A:811:SIA:H91	1.85	0.40
1:B:253:ILE:C	1:B:255:ARG:N	2.74	0.40
1:B:243:PHE:CB	1:B:262:VAL:HG13	2.52	0.40
2:C:32:ALA:O	2:C:75:GLN:HG2	2.22	0.40
2:C:98:LEU:CD1	2:C:169:THR:O	2.69	0.40
3:A:808:MAN:HO3	3:A:809:NAG:C1	2.34	0.40
1:B:344:ARG:HH11	1:B:344:ARG:CG	2.35	0.40
1:B:350:THR:O	1:B:351:LEU:CB	2.69	0.40
1:B:432:LEU:CD1	1:B:435:HIS:H	2.35	0.40
1:B:347:GLN:NE2	1:B:439:LYS:HE3	2.37	0.40
2:C:134:ARG:O	2:C:135:LEU:HD23	2.22	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)
2:C:77:SER:O	2:C:77:SER:O[4_557]	2.14	0.06

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	212/214 (99%)	120 (57%)	50 (24%)	42 (20%)	0	2
1	B	212/214 (99%)	108 (51%)	55 (26%)	49 (23%)	0	1
2	C	165/167 (99%)	78 (47%)	53 (32%)	34 (21%)	0	2
All	All	589/595 (99%)	306 (52%)	158 (27%)	125 (21%)	0	2

All (125) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	234	LEU
1	A	268	HIS
1	A	282	VAL
1	A	285	HIS
1	A	291	PRO
1	A	298	SER
1	A	300	TYR
1	A	325	ASN
1	A	331	PRO
1	A	336	ILE
1	A	340	LYS
1	A	374	PRO
1	A	377	ILE
1	A	401	ASP
1	A	414	LYS
1	A	433	HIS
1	A	435	HIS
1	B	242	LEU
1	B	245	PRO
1	B	247	PRO
1	B	260	THR
1	B	277	TRP
1	B	284	VAL
1	B	288	LYS
1	B	293	GLU
1	B	298	SER
1	B	301	ARG
1	B	320	LYS
1	B	321	CYS
1	B	332	ILE

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Mol	Chain	Res	Type
1	B	350	THR
1	B	351	LEU
1	B	358	MET
1	B	377	ILE
1	B	384	ASN
1	B	431	ALA
1	B	436	TYR
2	C	10	LEU
2	C	11	LYS
2	C	15	PRO
2	C	24	SER
2	C	29	CYS
2	C	30	GLN
2	C	34	SER
2	C	63	ASN
2	C	75	GLN
2	C	86	VAL
2	C	101	GLN
2	C	102	GLU
2	C	104	GLU
2	C	129	SER
2	C	130	GLN
2	C	135	LEU
1	A	233	GLU
1	A	273	VAL
1	A	292	ARG
1	A	315	ASP
1	A	372	PHE
1	A	373	TYR
1	A	403	SER
1	A	440	SER
1	B	250	THR
1	B	279	VAL
1	B	280	ASP
1	B	292	ARG
1	B	334	LYS
1	B	339	ALA
1	B	342	GLN
1	B	359	THR
1	B	398	LEU
1	B	400	SER
2	C	26	THR

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Mol	Chain	Res	Type
2	C	36	GLU
2	C	45	ASN
2	C	60	LYS
2	C	61	ALA
2	C	94	GLN
2	C	146	HIS
2	C	159	GLY
2	C	168	VAL
1	A	261	CYS
1	A	307	THR
1	A	353	PRO
1	A	375	SER
1	B	248	LYS
1	B	249	ASP
1	B	265	ASP
1	B	326	LYS
1	B	327	ALA
1	B	343	PRO
1	B	418	GLN
2	C	54	GLN
2	C	97	HIS
1	A	232	PRO
1	A	278	TYR
1	A	283	GLN
1	A	286	ASN
1	B	263	VAL
1	B	411	THR
1	B	417	TRP
2	C	14	PRO
2	C	38	ASP
2	C	50	PRO
2	C	89	GLU
2	C	98	LEU
2	C	116	LYS
2	C	163	PHE
1	A	263	VAL
1	A	332	ILE
1	A	335	THR
1	A	279	VAL
1	A	398	LEU
1	B	264	VAL
1	B	385	GLY

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Mol	Chain	Res	Type
1	A	238	PRO
1	B	232	PRO
1	B	244	PRO
1	B	302	VAL
1	B	336	ILE
1	A	240	VAL
1	B	266	VAL
1	A	264	VAL
1	A	343	PRO
1	B	271	PRO
1	B	412	VAL

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	198/198 (100%)	164 (83%)	34 (17%)	2	17
1	B	198/198 (100%)	161 (81%)	37 (19%)	2	13
2	C	154/154 (100%)	126 (82%)	28 (18%)	2	14
All	All	550/550 (100%)	451 (82%)	99 (18%)	2	15

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	235	LEU
1	A	244	PRO
1	A	253	ILE
1	A	263	VAL
1	A	278	TYR
1	A	280	ASP
1	A	285	HIS
1	A	291	PRO
1	A	292	ARG
1	A	294	GLN
1	A	301	ARG

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Mol	Chain	Res	Type
1	A	311	GLN
1	A	328	LEU
1	A	333	GLU
1	A	350	THR
1	A	355	ARG
1	A	362	GLN
1	A	363	VAL
1	A	364	SER
1	A	368	LEU
1	A	374	PRO
1	A	376	ASP
1	A	394	THR
1	A	398	LEU
1	A	401	ASP
1	A	404	PHE
1	A	407	TYR
1	A	409	LYS
1	A	411	THR
1	A	421	ASN
1	A	432	LEU
1	A	435	HIS
1	A	438	GLN
1	A	439	LYS
1	B	251	LEU
1	B	258	GLU
1	B	261	CYS
1	B	264	VAL
1	B	265	ASP
1	B	266	VAL
1	B	269	GLU
1	B	275	PHE
1	B	277	TRP
1	B	278	TYR
1	B	292	ARG
1	B	293	GLU
1	B	300	TYR
1	B	302	VAL
1	B	310	HIS
1	B	319	TYR
1	B	332	ILE
1	B	343	PRO
1	B	354	SER

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Mol	Chain	Res	Type
1	B	356	GLU
1	B	357	GLU
1	B	359	THR
1	B	366	THR
1	B	370	LYS
1	B	386	GLN
1	B	390	ASN
1	B	392	LYS
1	B	397	VAL
1	B	405	PHE
1	B	411	THR
1	B	413	ASP
1	B	417	TRP
1	B	422	VAL
1	B	435	HIS
1	B	437	THR
1	B	441	LEU
1	B	443	LEU
2	C	12	LEU
2	C	15	PRO
2	C	21	GLN
2	C	23	ASP
2	C	27	LEU
2	C	41	GLN
2	C	43	PHE
2	C	44	HIS
2	C	48	LEU
2	C	54	GLN
2	C	59	PHE
2	C	60	LYS
2	C	73	THR
2	C	84	LEU
2	C	97	HIS
2	C	98	LEU
2	C	101	GLN
2	C	111	HIS
2	C	113	TRP
2	C	122	THR
2	C	123	PHE
2	C	125	GLN
2	C	128	LYS
2	C	131	LYS

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Mol	Chain	Res	Type
2	C	134	ARG
2	C	135	LEU
2	C	136	ASP
2	C	138	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	294	GLN
1	A	295	GLN
1	A	325	ASN
1	A	362	GLN
1	A	419	GLN
1	A	421	ASN
1	A	434	ASN
1	A	435	HIS
1	A	438	GLN
1	B	286	ASN
1	B	311	GLN
1	B	347	GLN
1	B	362	GLN
1	B	384	ASN
1	B	386	GLN
1	B	389	ASN
1	B	390	ASN
1	B	419	GLN
1	B	434	ASN
2	C	44	HIS
2	C	111	HIS
2	C	125	GLN
2	C	143	GLN
2	C	148	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 ⓘ

28 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	NDG	A	801	3	14,14,15	0.77	0	15,19,21	1.26	2 (13%)
3	FUL	A	802	3	9,10,11	0.90	1 (11%)	13,14,16	0.65	0
3	NAG	A	803	3	14,14,15	0.53	0	15,19,21	1.29	3 (20%)
3	BMA	A	804	3	11,11,12	0.60	0	13,15,17	1.02	1 (7%)
3	MAN	A	805	3	11,11,12	0.77	0	13,15,17	0.74	0
3	NAG	A	806	3	14,14,15	0.72	0	15,19,21	1.05	1 (6%)
3	MAN	A	808	3	11,11,12	1.21	1 (9%)	13,15,17	0.88	0
3	NAG	A	809	3	14,14,15	0.88	1 (7%)	15,19,21	0.95	0
3	GAL	A	810	3	11,11,12	0.78	0	13,15,17	1.27	2 (15%)
3	SIA	A	811	3	17,20,21	0.96	1 (5%)	19,28,31	1.23	2 (10%)
4	NAG	B	801	1,4	14,14,15	0.83	1 (7%)	15,19,21	0.91	0
4	FUL	B	802	4	9,10,11	0.62	0	13,14,16	0.73	0
4	NAG	B	803	4	14,14,15	0.74	1 (7%)	15,19,21	0.70	0
4	BMA	B	804	4	11,11,12	1.37	1 (9%)	13,15,17	1.37	2 (15%)
4	MAN	B	805	4	11,11,12	0.81	0	13,15,17	1.00	1 (7%)
4	NAG	B	806	4	14,14,15	0.74	1 (7%)	15,19,21	1.37	2 (13%)
4	GAL	B	807	4	11,11,12	0.99	0	13,15,17	0.60	0
4	MAN	B	808	4	11,11,12	0.96	1 (9%)	13,15,17	1.21	2 (15%)
4	NAG	B	809	4	14,14,15	0.72	0	15,19,21	2.07	5 (33%)
4	GAL	B	810	4	11,11,12	0.50	0	13,15,17	0.44	0
4	SIA	B	811	4	17,20,21	1.00	1 (5%)	19,28,31	0.81	0
4	SIA	B	812	4	17,20,21	1.39	3 (17%)	19,28,31	1.07	2 (10%)
5	NDG	C	200	5	14,14,15	0.92	1 (7%)	15,19,21	1.03	2 (13%)
5	NAG	C	201	5	14,14,15	0.98	1 (7%)	15,19,21	0.75	0
5	FUL	C	202	5	9,10,11	0.90	0	13,14,16	0.80	1 (7%)
5	MAN	C	203	5	11,11,12	0.96	1 (9%)	13,15,17	1.95	3 (23%)
5	MAN	C	204	5	11,11,12	0.67	0	13,15,17	1.53	3 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	BMA	C	205	5	11,11,12	0.56	0	13,15,17	1.12	1 (7%)

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	NDG	A	801	3	-	0/6/23/26	0/1/1/1
3	FUL	A	802	3	-	0/0/17/20	0/1/1/1
3	NAG	A	803	3	-	0/6/23/26	0/1/1/1
3	BMA	A	804	3	-	0/2/19/22	0/1/1/1
3	MAN	A	805	3	-	0/2/19/22	0/1/1/1
3	NAG	A	806	3	-	0/6/23/26	0/1/1/1
3	MAN	A	808	3	-	0/2/19/22	0/1/1/1
3	NAG	A	809	3	-	0/6/23/26	0/1/1/1
3	GAL	A	810	3	-	0/2/19/22	0/1/1/1
3	SIA	A	811	3	-	0/14/34/38	0/1/1/1
4	NAG	B	801	1,4	-	0/6/23/26	0/1/1/1
4	FUL	B	802	4	-	0/0/17/20	0/1/1/1
4	NAG	B	803	4	-	1/6/23/26	0/1/1/1
4	BMA	B	804	4	-	0/2/19/22	0/1/1/1
4	MAN	B	805	4	-	0/2/19/22	0/1/1/1
4	NAG	B	806	4	-	0/6/23/26	0/1/1/1
4	GAL	B	807	4	-	0/2/19/22	0/1/1/1
4	MAN	B	808	4	-	0/2/19/22	0/1/1/1
4	NAG	B	809	4	-	0/6/23/26	0/1/1/1
4	GAL	B	810	4	-	0/2/19/22	0/1/1/1
4	SIA	B	811	4	-	0/14/34/38	0/1/1/1
4	SIA	B	812	4	-	0/14/34/38	0/1/1/1
5	NDG	C	200	5	-	0/6/23/26	0/1/1/1
5	NAG	C	201	5	-	0/6/23/26	0/1/1/1
5	FUL	C	202	5	-	0/0/17/20	0/1/1/1
5	MAN	C	203	5	-	0/2/19/22	0/1/1/1
5	MAN	C	204	5	-	0/2/19/22	0/1/1/1
5	BMA	C	205	5	-	0/2/19/22	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	811	SIA	C6-C5	2.01	1.56	1.53
4	B	806	NAG	C4-C3	2.02	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	812	SIA	C3-C2	2.04	1.55	1.52
5	C	203	MAN	C2-C3	2.14	1.55	1.52
3	A	802	FUL	C2-C3	2.21	1.55	1.52
4	B	803	NAG	C1-C2	2.26	1.55	1.52
3	A	809	NAG	C1-C2	2.31	1.55	1.52
4	B	801	NAG	C1-C2	2.35	1.55	1.52
4	B	812	SIA	O6-C6	2.38	1.47	1.43
5	C	200	NDG	C1-C2	2.39	1.55	1.52
4	B	808	MAN	C2-C3	2.47	1.55	1.52
5	C	201	NAG	C1-C2	2.61	1.56	1.52
3	A	811	SIA	C3-C2	2.90	1.57	1.52
3	A	808	MAN	C2-C3	3.19	1.56	1.52
4	B	812	SIA	C7-C6	3.75	1.57	1.52
4	B	804	BMA	C2-C3	3.75	1.57	1.52

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	809	NAG	C4-C3-C2	-4.95	103.76	111.02
4	B	809	NAG	C2-N2-C7	-3.73	117.50	122.94
3	A	801	NDG	C4-C3-C2	-3.10	106.47	111.02
3	A	801	NDG	C2-N2-C7	-2.90	118.71	122.94
3	A	803	NAG	O5-C1-C2	-2.70	107.71	111.47
4	B	812	SIA	C3-C4-C5	-2.58	108.34	111.46
3	A	811	SIA	C3-C4-C5	-2.47	108.48	111.46
3	A	803	NAG	C2-N2-C7	-2.40	119.44	122.94
4	B	809	NAG	C6-C5-C4	-2.33	107.54	113.00
4	B	809	NAG	O5-C1-C2	-2.26	108.32	111.47
4	B	806	NAG	C2-N2-C7	-2.21	119.72	122.94
5	C	200	NDG	C2-N2-C7	-2.13	119.84	122.94
5	C	200	NDG	C6-C5-C4	2.00	117.69	113.00
3	A	810	GAL	C6-C5-C4	2.06	117.83	113.00
5	C	204	MAN	O5-C1-C2	2.08	114.04	110.79
4	B	812	SIA	C4-C3-C2	2.09	113.67	109.75
4	B	804	BMA	C2-C3-C4	2.10	114.53	110.88
3	A	804	BMA	C3-C4-C5	2.12	113.96	110.22
5	C	202	FUL	C1-C2-C3	2.15	112.37	109.65
5	C	203	MAN	C2-C3-C4	2.17	114.66	110.88
3	A	803	NAG	C3-C4-C5	2.36	114.38	110.22
4	B	808	MAN	C1-C2-C3	2.38	112.67	109.65
4	B	809	NAG	C1-O5-C5	2.54	115.66	112.17
5	C	205	BMA	C1-O5-C5	2.75	115.95	112.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	806	NAG	C4-C3-C2	2.91	115.28	111.02
5	C	203	MAN	C3-C4-C5	2.92	115.36	110.22
4	B	805	MAN	C1-O5-C5	3.10	116.44	112.17
4	B	808	MAN	C1-O5-C5	3.11	116.45	112.17
4	B	806	NAG	C4-C3-C2	3.16	115.66	111.02
5	C	204	MAN	C1-O5-C5	3.20	116.58	112.17
3	A	811	SIA	C4-C3-C2	3.44	116.20	109.75
3	A	810	GAL	C1-C2-C3	3.49	114.07	109.65
5	C	204	MAN	C1-C2-C3	3.62	114.24	109.65
4	B	804	BMA	C1-C2-C3	3.68	114.32	109.65
5	C	203	MAN	C1-C2-C3	5.02	116.02	109.65

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	803	NAG	O7-C7-N2-C2

There are no ring outliers.

23 monomers are involved in 55 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	802	FUL	1	0
3	A	803	NAG	5	0
3	A	805	MAN	2	0
3	A	806	NAG	2	0
3	A	808	MAN	2	0
3	A	809	NAG	5	0
3	A	810	GAL	3	0
3	A	811	SIA	4	0
4	B	801	NAG	4	0
4	B	802	FUL	4	0
4	B	803	NAG	2	0
4	B	805	MAN	2	0
4	B	806	NAG	3	0
4	B	807	GAL	1	0
4	B	808	MAN	6	0
4	B	809	NAG	12	0
4	B	810	GAL	1	0
4	B	811	SIA	1	0
4	B	812	SIA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	200	NDG	4	0
5	C	201	NAG	13	0
5	C	202	FUL	9	0
5	C	203	MAN	2	0

5.6 Ligand geometry [i](#)

5 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
7	GOL	A	600	-	5,5,5	4.75	5 (100%)	5,5,5	4.14	3 (60%)
7	GOL	B	601	-	5,5,5	4.78	5 (100%)	5,5,5	4.14	3 (60%)
7	GOL	B	602	-	5,5,5	4.86	5 (100%)	5,5,5	4.09	3 (60%)
7	GOL	B	603	-	5,5,5	4.85	5 (100%)	5,5,5	4.12	3 (60%)
6	NAG	C	206	2	14,14,15	0.52	0	15,19,21	0.68	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
7	GOL	A	600	-	-	0/4/4/4	0/0/0/0
7	GOL	B	601	-	-	0/4/4/4	0/0/0/0
7	GOL	B	602	-	-	0/4/4/4	0/0/0/0
7	GOL	B	603	-	-	0/4/4/4	0/0/0/0
6	NAG	C	206	2	-	1/6/23/26	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	602	GOL	C3-C2	-8.27	1.21	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	603	GOL	C3-C2	-8.21	1.21	1.52
7	B	601	GOL	C3-C2	-7.94	1.22	1.52
7	A	600	GOL	C3-C2	-7.86	1.23	1.52
7	B	601	GOL	C1-C2	-3.13	1.40	1.52
7	B	603	GOL	C1-C2	-2.99	1.41	1.52
7	A	600	GOL	C1-C2	-2.98	1.41	1.52
7	B	602	GOL	C1-C2	-2.92	1.41	1.52
7	B	602	GOL	O2-C2	-2.82	1.35	1.43
7	B	603	GOL	O2-C2	-2.67	1.35	1.43
7	B	601	GOL	O2-C2	-2.62	1.35	1.43
7	A	600	GOL	O2-C2	-2.56	1.35	1.43
7	B	603	GOL	O3-C3	3.36	1.56	1.42
7	B	602	GOL	O3-C3	3.41	1.56	1.42
7	A	600	GOL	O3-C3	3.70	1.58	1.42
7	B	601	GOL	O3-C3	3.78	1.58	1.42
7	B	601	GOL	O1-C1	4.50	1.61	1.42
7	A	600	GOL	O1-C1	4.67	1.62	1.42
7	B	602	GOL	O1-C1	4.67	1.62	1.42
7	B	603	GOL	O1-C1	4.76	1.62	1.42

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	602	GOL	O1-C1-C2	2.41	122.22	110.07
7	B	601	GOL	O1-C1-C2	2.41	122.23	110.07
7	A	600	GOL	O1-C1-C2	2.46	122.44	110.07
7	B	603	GOL	O1-C1-C2	2.48	122.56	110.07
7	B	602	GOL	O2-C2-C3	5.85	136.44	108.84
7	A	600	GOL	O2-C2-C3	5.96	136.99	108.84
7	B	601	GOL	O2-C2-C3	5.97	137.02	108.84
7	B	603	GOL	O2-C2-C3	5.98	137.07	108.84
7	B	603	GOL	O3-C3-C2	6.41	142.34	110.07
7	B	602	GOL	O3-C3-C2	6.47	142.68	110.07
7	A	600	GOL	O3-C3-C2	6.50	142.82	110.07
7	B	601	GOL	O3-C3-C2	6.51	142.86	110.07

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	206	NAG	O7-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	601	GOL	3	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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	214/214 (100%)	-0.47	0 100 100	1, 28, 70, 118	0
1	B	214/214 (100%)	-0.27	1 (0%) 90 86	1, 33, 72, 108	0
2	C	167/167 (100%)	-0.29	1 (0%) 89 85	1, 35, 76, 113	0
All	All	595/595 (100%)	-0.35	2 (0%) 93 91	1, 31, 74, 118	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	299	THR	3.0
2	C	30	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](#)

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	SIA	B	812	20/21	0.77	0.45	5.57	51,51,138,142	0
5	MAN	C	204	11/12	0.82	0.27	0.52	42,52,64,68	0
4	GAL	B	807	11/12	0.87	0.32	-0.12	31,71,72,72	0
5	NDG	C	200	14/15	0.86	0.22	-0.30	26,27,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	NAG	B	803	14/15	0.81	0.24	-	36,43,59,75	0
4	MAN	B	808	11/12	0.81	0.25	-	37,87,96,106	0
4	NAG	B	806	14/15	0.88	0.18	-	34,47,69,71	0
5	FUL	C	202	10/11	0.83	0.29	-	69,69,69,69	0
5	MAN	C	203	11/12	0.88	0.17	-	68,78,90,94	0
4	NAG	B	801	14/15	0.85	0.22	-	22,71,80,86	0
3	GAL	A	810	11/12	0.79	0.37	-	81,81,82,82	0
3	MAN	A	808	11/12	0.82	0.22	-	15,55,56,56	0
4	SIA	B	811	20/21	0.83	0.26	-	40,40,64,64	0
3	MAN	A	805	11/12	0.93	0.25	-	41,41,67,68	0
3	NAG	A	806	14/15	0.90	0.21	-	17,17,17,62	0
4	NAG	B	809	14/15	0.89	0.15	-	1,1,1,1	0
3	NAG	A	809	14/15	0.84	0.22	-	86,86,87,87	0
3	NAG	A	803	14/15	0.81	0.31	-	25,29,53,63	0
3	NDG	A	801	14/15	0.84	0.32	-	36,36,112,112	0
4	FUL	B	802	10/11	0.89	0.21	-	11,21,32,43	0
3	FUL	A	802	10/11	0.81	0.46	-	65,65,71,81	0
4	GAL	B	810	11/12	0.85	0.28	-	46,131,132,132	0
4	MAN	B	805	11/12	0.83	0.28	-	65,65,65,65	0
5	BMA	C	205	11/12	0.89	0.22	-	71,82,94,98	0
3	BMA	A	804	11/12	0.90	0.40	-	68,78,90,94	0
3	SIA	A	811	20/21	0.74	0.34	-	59,92,97,98	0
4	BMA	B	804	11/12	0.81	0.25	-	54,54,96,141	0
5	NAG	C	201	14/15	0.90	0.26	-	24,81,82,82	0

6.4 Ligands ⓘ

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	NAG	C	206	14/15	0.86	0.29	-	57,61,63,65	0
7	GOL	B	603	6/6	0.66	0.36	-	23,26,27,31	0
7	GOL	B	601	6/6	0.89	0.27	-	23,26,27,31	0
7	GOL	A	600	6/6	0.87	0.25	-	23,26,27,31	0
7	GOL	B	602	6/6	0.86	0.23	-	23,26,27,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.