Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:56 AM GMT

PDB ID	:	3K72
Title	:	Structure of integrin alphaX beta2
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Deposited on	:	2009-10-11
Resolution	:	3.70 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

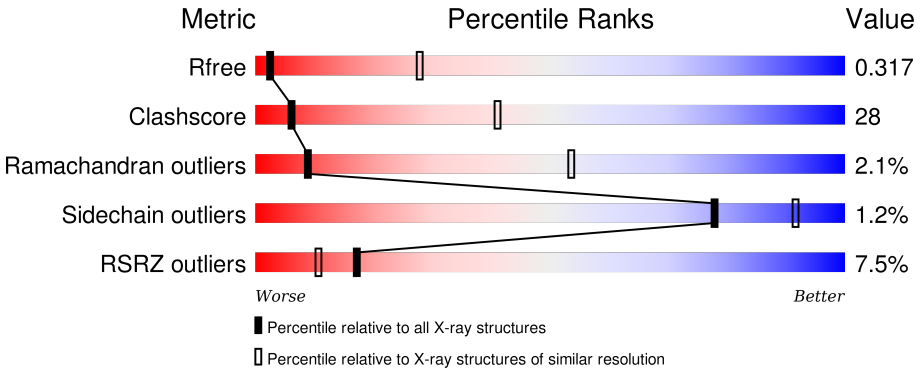
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 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}	91344	1101 (3.90-3.50)
Clashscore	102246	1224 (3.90-3.50)
Ramachandran outliers	100387	1172 (3.90-3.50)
Sidechain outliers	100360	1170 (3.90-3.50)
RSRZ outliers	91569	1108 (3.90-3.50)

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 <=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	1095	3% 43% 35% • 19%
1	C	1095	3% 44% 34% • 19%
2	B	687	10% 62% 34% ••
2	D	687	13% 62% 34% ••

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	NAG	A	3373	X	-	-	-
4	MAN	A	3375	X	-	-	-
4	NAG	C	3373	X	-	-	-
4	MAN	C	3375	X	-	-	-
6	MAN	A	3718	X	-	-	-
6	MAN	A	3882	X	-	-	-
6	NAG	C	3716	-	-	X	-
6	MAN	C	3718	X	-	-	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 24382 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 Integrin alpha-X.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	884	Total	C	N	O	S	0	0	0
			6814	4305	1178	1297	34			
1	C	882	Total	C	N	O	S	0	0	0
			6802	4299	1176	1293	34			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1085	GLY	-	EXPRESSION TAG	UNP P20702
A	1086	CYS	-	EXPRESSION TAG	UNP P20702
A	1087	GLY	-	EXPRESSION TAG	UNP P20702
A	1088	GLY	-	EXPRESSION TAG	UNP P20702
A	1089	LEU	-	EXPRESSION TAG	UNP P20702
A	1090	GLU	-	EXPRESSION TAG	UNP P20702
A	1091	ASN	-	EXPRESSION TAG	UNP P20702
A	1092	LEU	-	EXPRESSION TAG	UNP P20702
A	1093	TYR	-	EXPRESSION TAG	UNP P20702
A	1094	PHE	-	EXPRESSION TAG	UNP P20702
A	1095	GLN	-	EXPRESSION TAG	UNP P20702
C	1085	GLY	-	EXPRESSION TAG	UNP P20702
C	1086	CYS	-	EXPRESSION TAG	UNP P20702
C	1087	GLY	-	EXPRESSION TAG	UNP P20702
C	1088	GLY	-	EXPRESSION TAG	UNP P20702
C	1089	LEU	-	EXPRESSION TAG	UNP P20702
C	1090	GLU	-	EXPRESSION TAG	UNP P20702
C	1091	ASN	-	EXPRESSION TAG	UNP P20702
C	1092	LEU	-	EXPRESSION TAG	UNP P20702
C	1093	TYR	-	EXPRESSION TAG	UNP P20702
C	1094	PHE	-	EXPRESSION TAG	UNP P20702
C	1095	GLN	-	EXPRESSION TAG	UNP P20702

- Molecule 2 is a protein called Integrin beta-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	673	Total	C	N	O	S	0	0	0
			5177	3181	929	1003	64			
2	D	673	Total	C	N	O	S	0	0	0
			5177	3181	929	1003	64			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	678	ASP	-	EXPRESSION TAG	UNP P05107
B	679	GLY	-	EXPRESSION TAG	UNP P05107
B	680	CYS	-	EXPRESSION TAG	UNP P05107
B	681	GLY	-	EXPRESSION TAG	UNP P05107
B	682	GLU	-	EXPRESSION TAG	UNP P05107
B	684	LEU	-	EXPRESSION TAG	UNP P05107
B	685	TYR	-	EXPRESSION TAG	UNP P05107
B	686	PHE	-	EXPRESSION TAG	UNP P05107
B	687	GLN	-	EXPRESSION TAG	UNP P05107
D	678	ASP	-	EXPRESSION TAG	UNP P05107
D	679	GLY	-	EXPRESSION TAG	UNP P05107
D	680	CYS	-	EXPRESSION TAG	UNP P05107
D	681	GLY	-	EXPRESSION TAG	UNP P05107
D	682	GLU	-	EXPRESSION TAG	UNP P05107
D	684	LEU	-	EXPRESSION TAG	UNP P05107
D	685	TYR	-	EXPRESSION TAG	UNP P05107
D	686	PHE	-	EXPRESSION TAG	UNP P05107
D	687	GLN	-	EXPRESSION TAG	UNP P05107

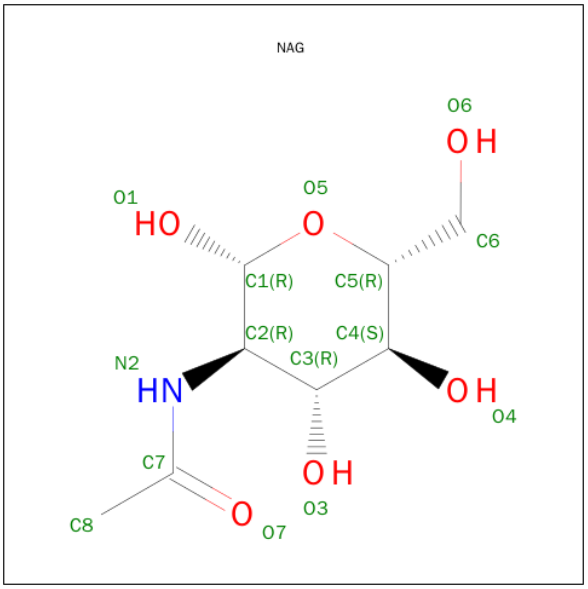
- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	N	O	0	0
			28	16	2	10		
3	C	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	5	Total	C	N	O	0	0
			61	34	2	25		
4	C	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 5 is SUGAR (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 14 8 1 5	0	0
5	B	1	Total C N O 14 8 1 5	0	0
5	B	1	Total C N O 14 8 1 5	0	0
5	C	1	Total C N O 14 8 1 5	0	0
5	C	1	Total C N O 14 8 1 5	0	0
5	D	1	Total C N O 14 8 1 5	0	0
5	D	1	Total C N O 14 8 1 5	0	0

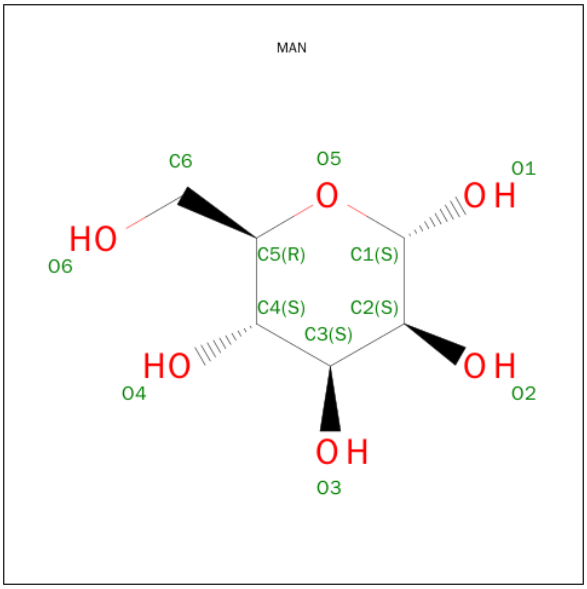
- Molecule 6 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	3	Total C N O 39 22 2 15	0	0
6	A	3	Total C N O 39 22 2 15	0	0
6	C	3	Total C N O 39 22 2 15	0	0

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total Ca 1 1	0	0
7	A	3	Total Ca 3 3	0	0
7	D	1	Total Ca 1 1	0	0
7	C	3	Total Ca 3 3	0	0

- Molecule 8 is SUGAR (ALPHA-D-MANNOSE) (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



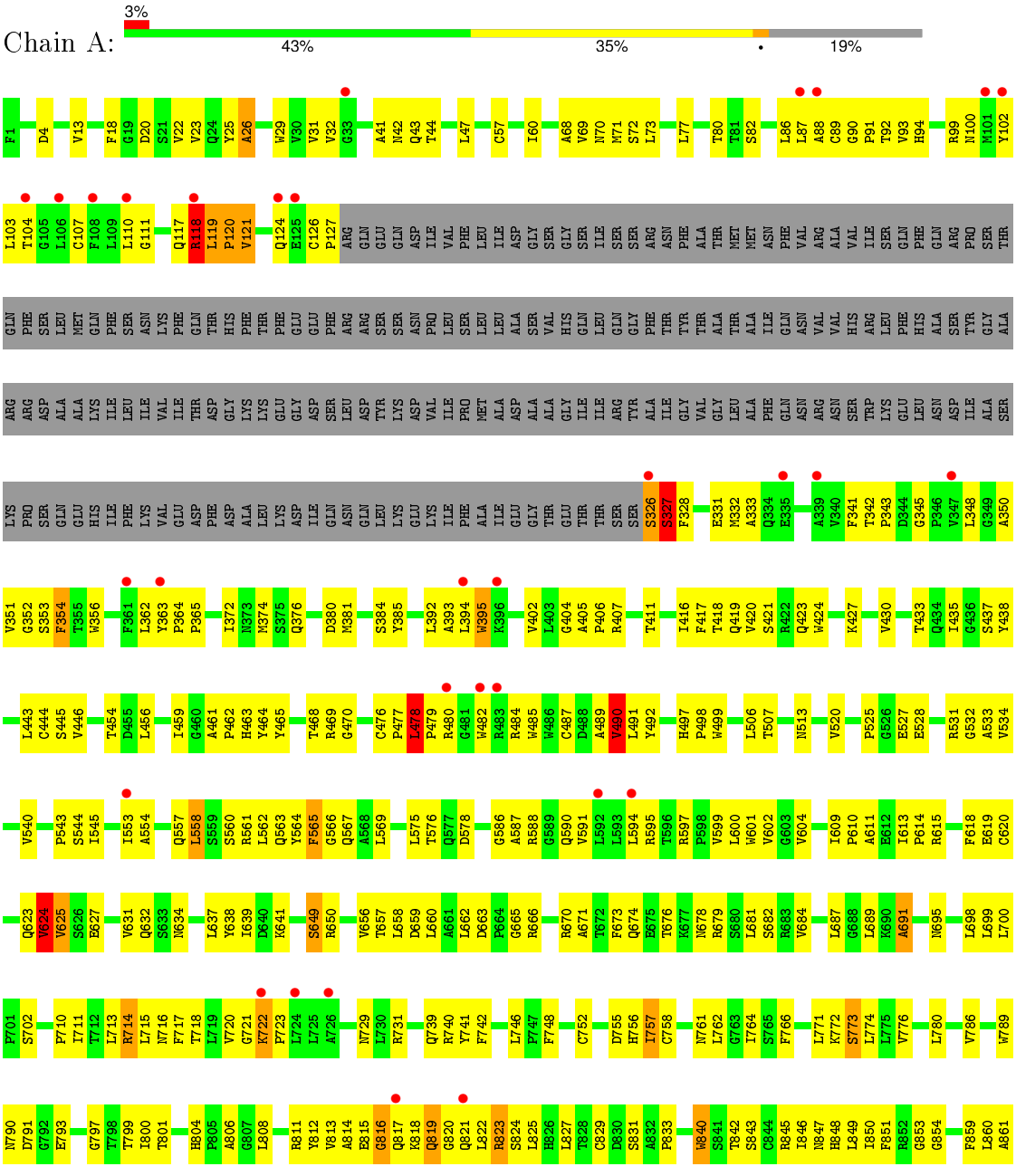
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	1	Total C O 11 6 5	0	0

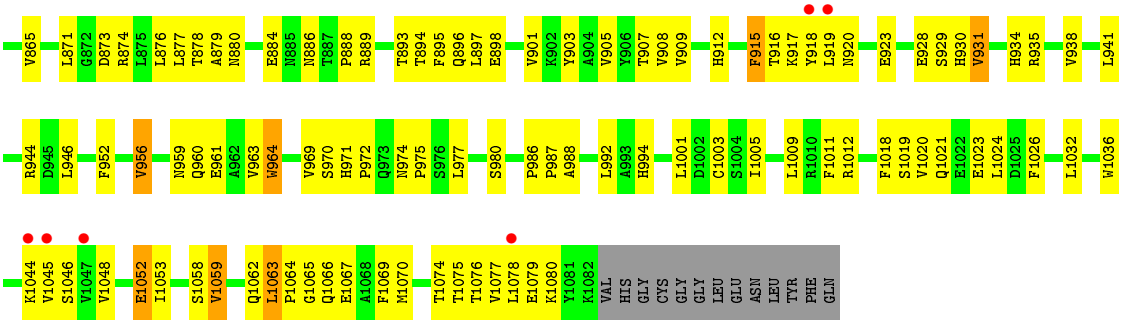
3 Residue-property plots (i)

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

- Molecule 1: Integrin alpha-X

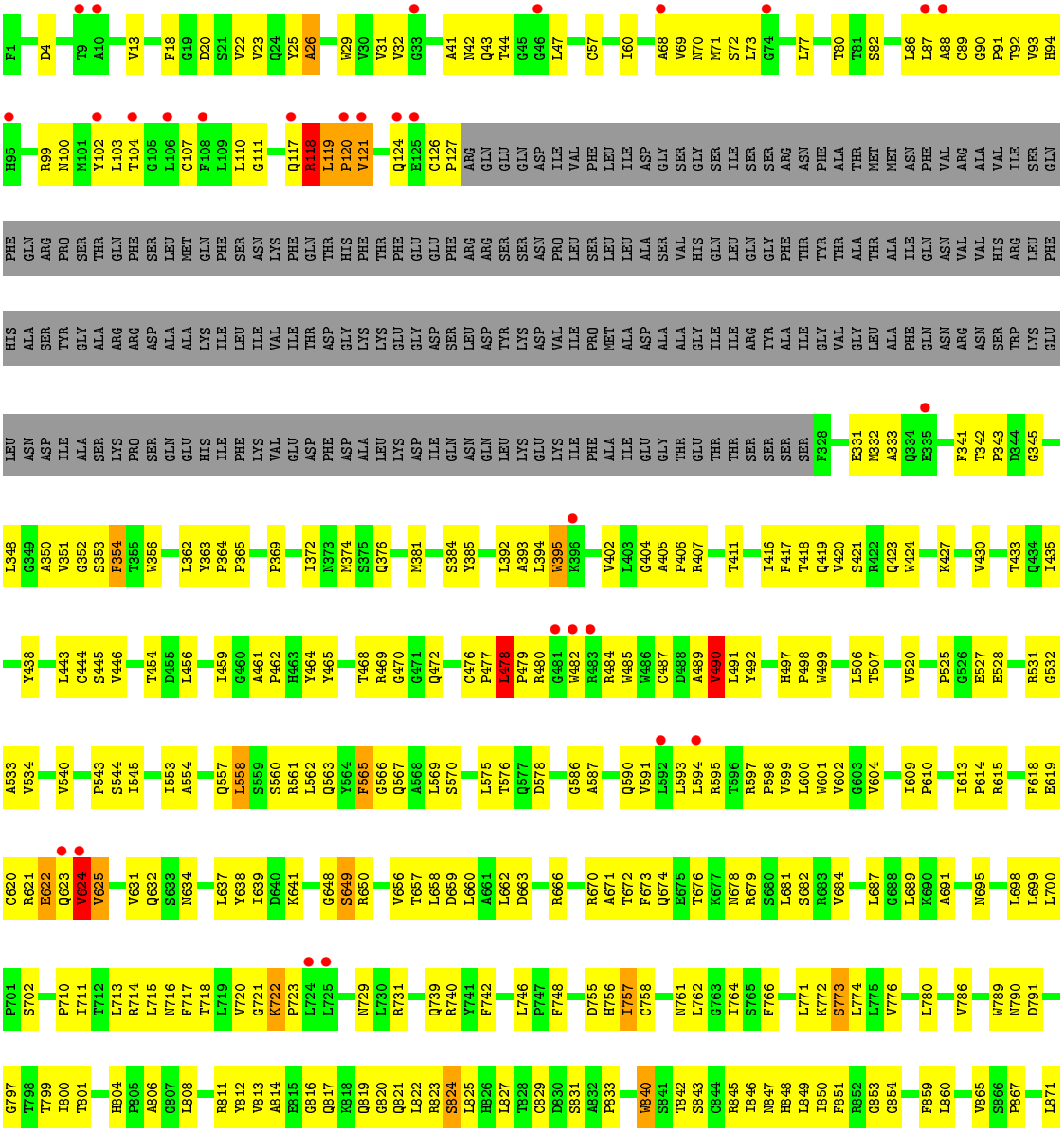
Chain A:

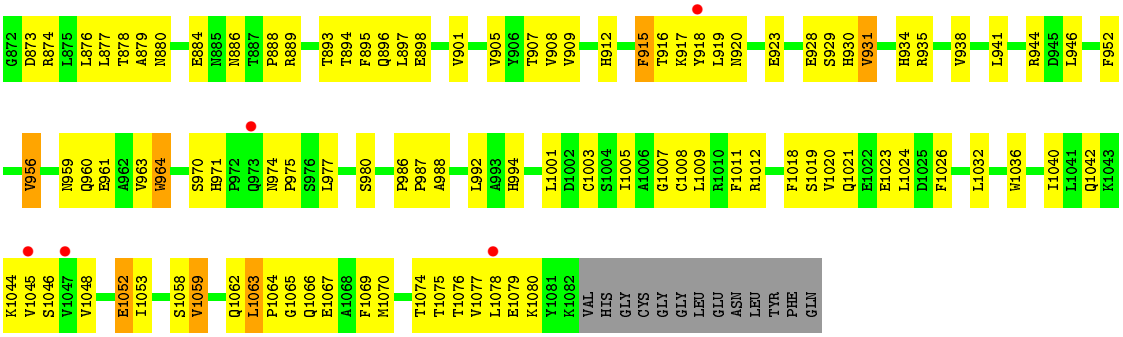




• Molecule 1: Integrin alpha-X

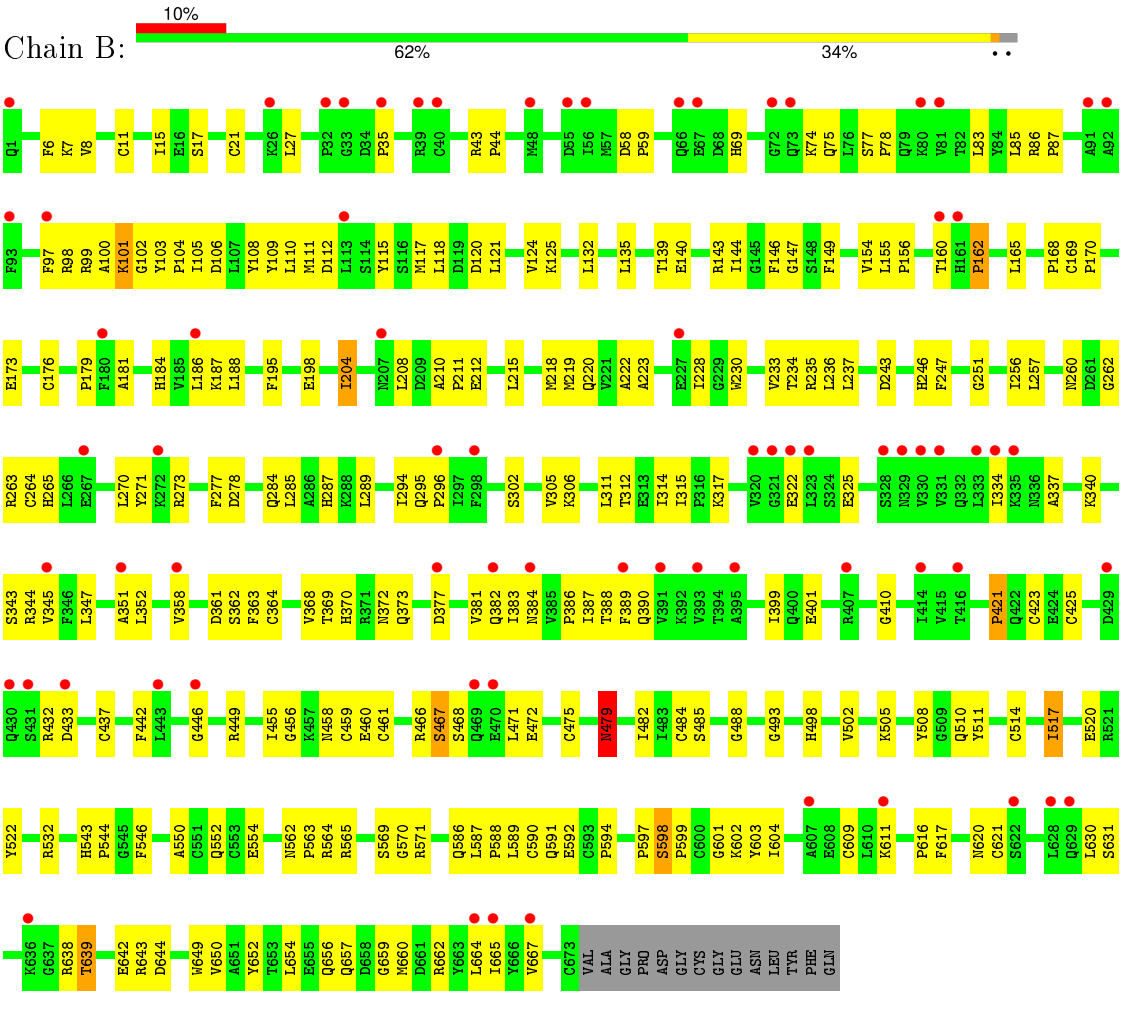
Chain C:





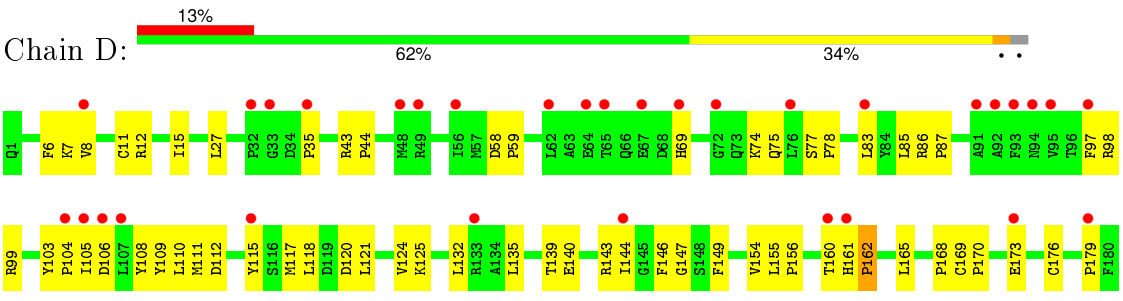
• Molecule 2: Integrin beta-2

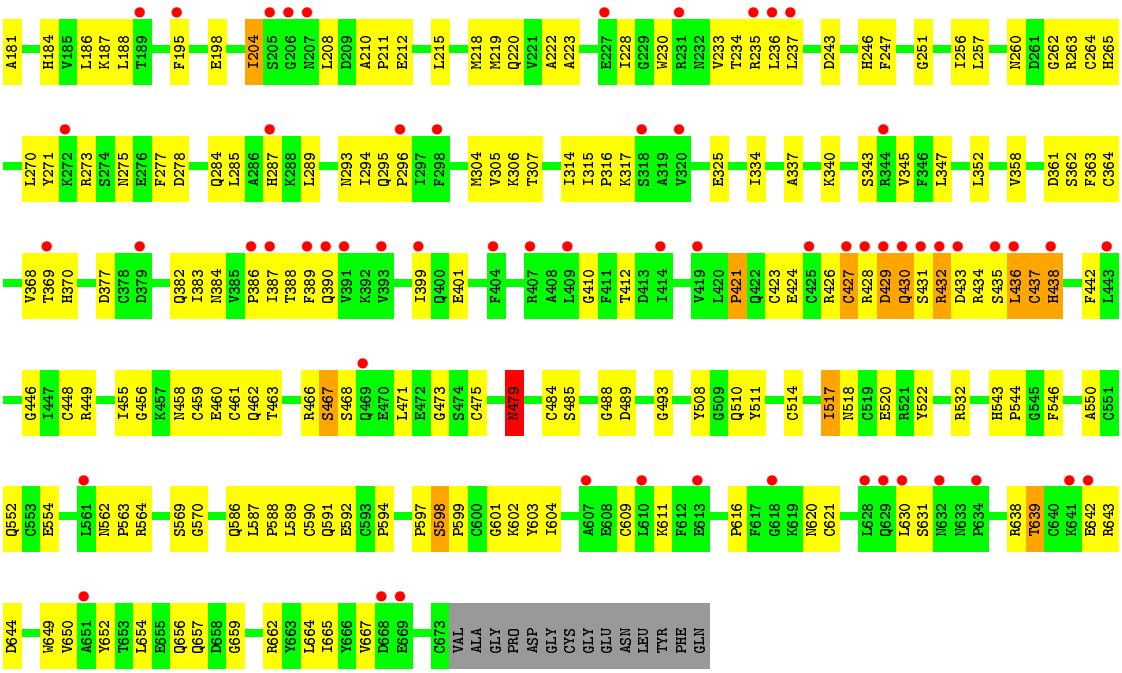
Chain B:



• Molecule 2: Integrin beta-2

Chain D:




A181 H184 V185 L186 K187 L188 T189 F195 E198 I204 S205 G206 N207 L208 D209 A210 P211 E212 L215 M218 M219 Q220 V221 A222 A223 E227 I228 G229 W230 R231 N232 V233 T234 R235 L236 L237 D243 H246 F247 G251 I256 L257 N260 D261 G262 R263 C264 H265
L270 Y271 K272 R273 S274 N275 E276 F277 D278 Q284 L285 A286 H287 K288 L289 N293 I294 Q295 P296 I297 F298 M304 V305 K306 T307 I314 I315 P316 K317 S318 A319 V320 E325 I334 A337 K340 S343 R344 V345 F346 L347 L352 V358 D361 S362 F363 C364
V368 T369 H370 D377 C378 D379 Q382 I383 N384 V385 P386 I387 T388 F389 Q390 V391 K392 V393 I399 Q400 E401 F404 R407 A408 L409 G410 F411 T412 D413 I414 V419 L420 P421 Q422 C423 E424 C425 R426 C427 R428 D429 Q430 S431 R432 D433 R434 S435 L436 C437 H438 F442 L443
G446 I447 C448 R449 I455 G456 K457 N458 C459 E460 C461 Q462 T463 R466 S467 S468 Q469 E470 L471 E472 G473 S474 C475 N479 C484 S485 G488 D489 G493 Y508 G509 Q510 Y511 C514 I517 W518 C519 E520 R521 Y522 R532 H543 P544 G545 F546 A550 C551
Q552 C553 E554 L561 W562 P563 R564 S569 G570 Q586 L587 P588 L589 C590 Q591 E592 C593 P594 P597 S598 P599 Q600 G601 K602 Y603 I604 A607 E608 C609 L610 K611 F612 E613 P616 F617 G618 K619 W620 C621 L628 Q629 L630 S631 W632 W633 P634 R638 T639 C640 K641 E642 R643
D644 W649 V650 A651 Y652 T653 L654 E655 Q656 Q657 D658 G659 R662 Y663 L664 I665 Y666 V667 D668 E669 C673 VAL ALA GLY PRO ASP GLY CYS GLY GLU ASN LEU TYR PHE GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	160.96Å 165.55Å 536.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.48 – 3.70 48.64 – 3.35	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.48-3.70) 99.4 (48.64-3.35)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	1.33 (at 3.33Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.315 , 0.335 0.293 , 0.317	Depositor DCC
R_{free} test set	845 reflections (1.11%)	DCC
Wilson B-factor (Å^2)	92.3	Xtriage
Anisotropy	0.003	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 151.2	EDS
Estimated twinning fraction	0.074 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.22$	Xtriage
Outliers	1 of 102383 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	24382	wwPDB-VP
Average B, all atoms (Å^2)	234.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: CA, NAG, 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	0.43	7/6969 (0.1%)	0.53	3/9480 (0.0%)
1	C	0.38	1/6957 (0.0%)	0.53	2/9464 (0.0%)
2	B	0.29	1/5273 (0.0%)	0.43	0/7119
2	D	0.31	1/5273 (0.0%)	0.43	0/7119
All	All	0.36	10/24472 (0.0%)	0.49	5/33182 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	13
1	C	0	15
2	B	0	2
2	D	0	3
4	A	2	0
4	C	2	0
6	A	2	0
6	C	1	0
All	All	7	33

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	479	ASN	CB-CG	7.36	1.68	1.51
2	B	479	ASN	CB-CG	6.92	1.67	1.51
1	A	326	SER	CB-OG	6.75	1.51	1.42
1	A	327	SER	CA-CB	6.62	1.62	1.52
1	A	326	SER	CA-CB	6.42	1.62	1.52
1	C	478	LEU	CG-CD1	-5.98	1.29	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	478	LEU	CG-CD1	-5.73	1.30	1.51
1	A	326	SER	C-O	5.67	1.34	1.23
1	A	326	SER	CA-C	5.49	1.67	1.52
1	A	327	SER	CB-OG	5.17	1.49	1.42

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	478	LEU	CA-CB-CG	8.42	134.66	115.30
1	A	478	LEU	CA-CB-CG	7.71	133.03	115.30
1	A	478	LEU	CB-CG-CD1	-5.17	102.20	111.00
1	A	118	ARG	NE-CZ-NH1	-5.07	117.76	120.30
1	C	478	LEU	CB-CG-CD1	-5.06	102.39	111.00

All (7) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	3373	NAG	C1
4	A	3375	MAN	C1
6	A	3718	MAN	C1
6	A	3882	MAN	C1
4	C	3373	NAG	C1
4	C	3375	MAN	C1
6	C	3718	MAN	C1

All (33) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1063	LEU	Peptide
1	A	118	ARG	Peptide
1	A	326	SER	Peptide
1	A	327	SER	Peptide
1	A	490	VAL	Peptide
1	A	558	LEU	Peptide
1	A	624	VAL	Peptide
1	A	625	VAL	Peptide
1	A	816	GLY	Peptide
1	A	82	SER	Peptide
1	A	821	GLN	Peptide
1	A	824	SER	Peptide
1	A	889	ARG	Peptide
2	B	100	ALA	Peptide

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Mol	Chain	Res	Type	Group
2	B	425	CYS	Peptide
1	C	1063	LEU	Peptide
1	C	118	ARG	Peptide
1	C	490	VAL	Peptide
1	C	558	LEU	Peptide
1	C	622	GLU	Peptide
1	C	624	VAL	Peptide
1	C	625	VAL	Peptide
1	C	816	GLY	Peptide
1	C	817	GLN	Peptide
1	C	819	GLN	Peptide
1	C	82	SER	Peptide
1	C	820	GLY	Peptide
1	C	821	GLN	Peptide
1	C	824	SER	Peptide
1	C	889	ARG	Peptide
2	D	427	CYS	Peptide
2	D	430	GLN	Peptide
2	D	431	SER	Peptide

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	6814	0	6671	441	0
1	C	6802	0	6661	442	0
2	B	5177	0	4964	236	0
2	D	5177	0	4964	267	0
3	A	28	0	25	0	0
3	C	28	0	25	0	0
4	A	61	0	52	5	0
4	C	61	0	52	7	0
5	A	14	0	12	0	0
5	B	28	0	26	1	0
5	C	28	0	25	0	0
5	D	28	0	26	1	0
6	A	78	0	68	7	0
6	C	39	0	34	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	3	0	0	0	0
7	B	1	0	0	0	0
7	C	3	0	0	0	0
7	D	1	0	0	0	0
8	C	11	0	10	1	0
All	All	24382	0	23615	1353	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 28.

All (1353) 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:B:15:ILE:HG23	2:B:86:ARG:CZ	1.67	1.23
2:D:430:GLN:HB3	2:D:434:ARG:NH2	1.61	1.14
2:D:430:GLN:HG3	2:D:442:PHE:CB	1.78	1.14
2:D:430:GLN:CB	2:D:434:ARG:HH21	1.62	1.10
2:D:430:GLN:HG3	2:D:442:PHE:HB2	1.13	1.09
6:C:3716:NAG:H83	6:C:3716:NAG:H3	1.33	1.08
2:D:430:GLN:HB3	2:D:434:ARG:HH21	0.95	1.07
2:D:15:ILE:HG23	2:D:86:ARG:CZ	1.85	1.07
2:B:15:ILE:HG23	2:B:86:ARG:NH2	1.69	1.06
1:C:94:HIS:NE2	2:D:155:LEU:HD21	1.70	1.06
6:C:3716:NAG:C8	6:C:3716:NAG:H3	1.87	1.04
1:A:94:HIS:NE2	2:B:155:LEU:HD21	1.72	1.03
1:C:822:LEU:HG	1:C:823:ARG:H	1.22	1.02
1:A:119:LEU:N	1:A:120:PRO:HA	1.79	0.97
1:C:119:LEU:N	1:C:120:PRO:HA	1.80	0.96
2:D:430:GLN:CG	2:D:442:PHE:CB	2.43	0.95
1:A:103:LEU:HD11	2:B:155:LEU:HD13	1.46	0.94
1:C:103:LEU:HD11	2:D:155:LEU:HD13	1.47	0.94
1:A:119:LEU:HD21	1:A:124:GLN:HE21	1.32	0.94
1:C:659:ASP:OD2	6:C:3716:NAG:C8	2.18	0.92
1:C:119:LEU:HD21	1:C:124:GLN:HE21	1.33	0.92
2:D:437:CYS:HA	2:D:458:ASN:O	1.71	0.90
1:A:1063:LEU:HD12	1:A:1064:PRO:CA	2.02	0.90
2:D:430:GLN:CB	2:D:434:ARG:NH2	2.28	0.90
2:D:430:GLN:CG	2:D:442:PHE:HB2	2.00	0.90
2:B:155:LEU:HB2	2:B:156:PRO:HA	1.54	0.89
2:D:155:LEU:HB2	2:D:156:PRO:HA	1.55	0.89
1:C:1063:LEU:HD12	1:C:1064:PRO:N	1.87	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1063:LEU:HD12	1:A:1064:PRO:N	1.87	0.89
1:C:659:ASP:OD2	6:C:3716:NAG:C7	2.21	0.88
1:A:484:ARG:NH1	2:B:586:GLN:HG3	1.89	0.88
1:C:1063:LEU:HD12	1:C:1064:PRO:CA	2.02	0.88
1:A:623:GLN:O	1:A:624:VAL:HG22	1.72	0.88
1:C:118:ARG:HG2	1:C:120:PRO:HB3	1.57	0.87
1:C:624:VAL:HG12	1:C:625:VAL:H	1.40	0.87
1:C:812:TYR:CE2	1:C:814:ALA:HB2	2.09	0.87
1:C:624:VAL:HG12	1:C:625:VAL:N	1.90	0.86
2:D:15:ILE:HG23	2:D:86:ARG:NH2	1.89	0.86
1:A:812:TYR:CE2	1:A:814:ALA:HB2	2.12	0.84
6:C:3717:NAG:O3	6:C:3718:MAN:H2	1.78	0.83
1:A:817:GLN:N	1:A:818:LYS:HA	1.92	0.83
1:C:94:HIS:CD2	2:D:155:LEU:HD21	2.14	0.82
2:B:15:ILE:CG2	2:B:86:ARG:CZ	2.54	0.81
2:D:430:GLN:CG	2:D:442:PHE:HB3	2.10	0.81
1:A:118:ARG:HG2	1:A:120:PRO:HB3	1.61	0.81
2:D:430:GLN:HG2	2:D:442:PHE:HB3	1.61	0.81
1:A:756:HIS:O	1:A:757:ILE:HG22	1.80	0.81
1:A:94:HIS:CD2	2:B:155:LEU:HD21	2.17	0.80
2:D:317:LYS:HE3	2:D:410:GLY:CA	2.11	0.80
2:D:317:LYS:HE3	2:D:410:GLY:HA3	1.63	0.79
1:A:731:ARG:O	1:A:731:ARG:HG3	1.83	0.79
1:A:812:TYR:CD2	1:A:814:ALA:HB2	2.17	0.79
1:A:1064:PRO:CG	1:A:1067:GLU:HG3	2.12	0.79
1:A:625:VAL:HG21	1:A:627:GLU:HG3	1.63	0.78
1:C:923:GLU:HB2	1:C:1080:LYS:HB3	1.64	0.78
1:C:1064:PRO:CG	1:C:1067:GLU:HG3	2.13	0.78
2:D:103:TYR:HB3	2:D:104:PRO:HD2	1.66	0.78
1:A:923:GLU:HB2	1:A:1080:LYS:HB3	1.64	0.77
2:B:103:TYR:HB3	2:B:104:PRO:HD2	1.66	0.77
1:A:328:PHE:O	1:A:354:PHE:HA	1.84	0.77
1:C:812:TYR:CD2	1:C:814:ALA:HB2	2.19	0.77
2:B:210:ALA:HB3	2:B:211:PRO:HD3	1.66	0.77
1:A:822:LEU:HG	1:A:823:ARG:H	1.49	0.77
2:D:210:ALA:HB3	2:D:211:PRO:HD3	1.66	0.76
1:C:731:ARG:O	1:C:731:ARG:HG3	1.86	0.76
4:C:3377:MAN:H4	8:C:3378:MAN:C1	2.15	0.76
1:C:822:LEU:CG	1:C:823:ARG:H	1.99	0.75
1:C:721:GLY:C	1:C:723:PRO:HD3	2.07	0.75
1:A:103:LEU:CD1	2:B:155:LEU:HD13	2.16	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:756:HIS:O	1:C:757:ILE:HG22	1.85	0.74
6:C:3716:NAG:C3	6:C:3716:NAG:H83	2.15	0.74
1:C:621:ARG:HH12	1:C:623:GLN:HG2	1.51	0.74
1:A:721:GLY:C	1:A:723:PRO:HD3	2.08	0.74
2:D:471:LEU:O	2:D:493:GLY:HA2	1.88	0.74
1:C:103:LEU:CD1	2:D:155:LEU:HD13	2.17	0.73
2:B:27:LEU:HD21	2:B:446:GLY:HA2	1.70	0.73
1:C:117:GLN:HB2	1:C:121:VAL:HG21	1.71	0.72
2:B:546:PHE:CD2	2:B:554:GLU:O	2.41	0.72
1:A:119:LEU:H	1:A:120:PRO:HA	1.53	0.72
1:A:1064:PRO:HG3	1:A:1067:GLU:CD	2.10	0.72
1:C:1064:PRO:HG3	1:C:1067:GLU:CD	2.09	0.72
1:C:1064:PRO:HG3	1:C:1067:GLU:HG3	1.72	0.72
1:A:484:ARG:NH1	2:B:586:GLN:CG	2.52	0.72
2:B:532:ARG:HD3	2:B:554:GLU:CD	2.09	0.71
1:A:871:LEU:HD11	1:A:901:VAL:HG21	1.72	0.71
2:D:436:LEU:O	2:D:437:CYS:CB	2.39	0.71
1:A:103:LEU:HD13	2:B:156:PRO:HG3	1.73	0.70
1:A:1064:PRO:HG3	1:A:1067:GLU:HG3	1.71	0.70
6:A:3880:NAG:H61	6:A:3881:NAG:O5	1.91	0.70
1:A:117:GLN:HB2	1:A:121:VAL:HG21	1.70	0.70
1:C:871:LEU:HD11	1:C:901:VAL:HG21	1.72	0.70
1:A:1032:LEU:HD21	1:A:1078:LEU:HD21	1.74	0.69
1:C:394:LEU:HD23	1:C:395:TRP:N	2.08	0.69
2:D:427:CYS:HB3	2:D:428:ARG:HB2	1.74	0.69
1:A:103:LEU:CD1	2:B:156:PRO:HG3	2.23	0.69
1:C:119:LEU:H	1:C:120:PRO:HA	1.55	0.69
1:C:721:GLY:C	1:C:723:PRO:CD	2.62	0.68
1:A:394:LEU:HD23	1:A:395:TRP:N	2.08	0.68
1:A:673:PHE:CG	1:A:681:LEU:HD23	2.28	0.68
2:D:104:PRO:HD2	2:D:233:VAL:HG11	1.75	0.68
2:B:104:PRO:HD2	2:B:233:VAL:HG11	1.75	0.68
1:C:673:PHE:CG	1:C:681:LEU:HD23	2.29	0.68
1:A:721:GLY:C	1:A:723:PRO:CD	2.62	0.68
1:C:1032:LEU:HD21	1:C:1078:LEU:HD21	1.75	0.68
1:C:662:LEU:HD11	1:C:673:PHE:CZ	2.28	0.68
1:A:623:GLN:O	1:A:624:VAL:CG2	2.42	0.67
2:D:437:CYS:SG	2:D:458:ASN:HA	2.33	0.67
1:C:604:VAL:HG11	1:C:742:PHE:CD2	2.30	0.67
2:B:597:PRO:O	2:B:598:SER:HB2	1.93	0.67
1:C:103:LEU:HD13	2:D:156:PRO:HG3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1064:PRO:HG3	1:C:1067:GLU:CG	2.25	0.67
1:A:406:PRO:HB3	1:A:438:TYR:CE2	2.30	0.67
1:A:491:LEU:HD11	1:A:545:ILE:HG12	1.76	0.67
1:A:662:LEU:HD11	1:A:673:PHE:CZ	2.30	0.67
1:C:491:LEU:HD11	1:C:545:ILE:HG12	1.76	0.66
1:C:406:PRO:HB3	1:C:438:TYR:CE2	2.31	0.66
2:B:312:THR:CG2	2:B:344:ARG:HH22	2.09	0.66
1:C:825:LEU:HD12	1:C:859:PHE:HB3	1.78	0.66
1:C:364:PRO:HB3	1:C:365:PRO:HD2	1.78	0.66
1:C:599:VAL:O	1:C:599:VAL:HG23	1.96	0.66
1:A:604:VAL:HG11	1:A:742:PHE:CD2	2.30	0.66
2:D:436:LEU:O	2:D:437:CYS:SG	2.53	0.66
1:A:1064:PRO:HG2	1:A:1067:GLU:HG3	1.76	0.66
1:C:119:LEU:HD21	1:C:124:GLN:NE2	2.08	0.65
1:A:1064:PRO:HG3	1:A:1067:GLU:CG	2.24	0.65
1:A:813:VAL:HB	1:A:823:ARG:HH21	1.59	0.65
1:A:822:LEU:CG	1:A:823:ARG:H	2.10	0.65
1:C:364:PRO:CB	1:C:365:PRO:HD2	2.27	0.65
1:C:624:VAL:CG1	1:C:625:VAL:HG13	2.26	0.65
1:C:722:LYS:N	1:C:723:PRO:CD	2.60	0.65
2:D:437:CYS:O	2:D:459:CYS:HB2	1.97	0.65
1:A:484:ARG:HH12	2:B:586:GLN:HG3	1.60	0.65
1:C:833:PRO:HA	1:C:840:TRP:HB2	1.78	0.65
1:C:103:LEU:CD1	2:D:156:PRO:HG3	2.27	0.65
1:A:119:LEU:HD21	1:A:124:GLN:NE2	2.08	0.65
1:C:1064:PRO:HG2	1:C:1067:GLU:HG3	1.77	0.65
1:C:609:ILE:HB	1:C:610:PRO:HD3	1.79	0.64
1:A:833:PRO:HA	1:A:840:TRP:HB2	1.79	0.64
1:C:812:TYR:HE2	1:C:814:ALA:HB2	1.61	0.64
2:B:103:TYR:HB3	2:B:104:PRO:CD	2.27	0.64
1:C:562:LEU:HD11	1:C:590:GLN:HG2	1.79	0.64
2:D:546:PHE:CD2	2:D:554:GLU:O	2.50	0.64
1:A:722:LYS:N	1:A:723:PRO:CD	2.60	0.64
1:A:364:PRO:CB	1:A:365:PRO:HD2	2.27	0.64
2:B:479:ASN:OD1	5:B:3479:NAG:O5	2.12	0.64
1:C:919:LEU:HB2	1:C:1079:GLU:HB3	1.79	0.64
6:A:3881:NAG:H62	6:A:3882:MAN:O5	1.98	0.64
2:D:12:ARG:NH1	2:D:424:GLU:OE2	2.30	0.64
1:C:446:VAL:HG21	1:C:520:VAL:CG1	2.28	0.64
1:A:797:GLY:CA	1:A:884:GLU:HB2	2.28	0.64
2:D:597:PRO:O	2:D:598:SER:CB	2.46	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:103:TYR:HB3	2:D:104:PRO:CD	2.27	0.64
2:B:15:ILE:CG2	2:B:86:ARG:NH2	2.55	0.63
2:D:154:VAL:HA	2:D:160:THR:HG22	1.80	0.63
1:A:364:PRO:HB3	1:A:365:PRO:HD2	1.78	0.63
1:A:446:VAL:HG21	1:A:520:VAL:CG1	2.29	0.63
1:A:625:VAL:CG2	1:A:627:GLU:HG3	2.29	0.63
1:C:18:PHE:CE2	1:C:32:VAL:HG21	2.33	0.63
2:D:532:ARG:HD3	2:D:554:GLU:CD	2.19	0.63
1:A:4:ASP:CG	1:A:597:ARG:NH2	2.51	0.63
1:A:786:VAL:HG11	1:A:859:PHE:CZ	2.33	0.63
2:B:154:VAL:HA	2:B:160:THR:HG22	1.81	0.63
2:D:437:CYS:CA	2:D:458:ASN:O	2.46	0.63
1:C:786:VAL:HG11	1:C:859:PHE:CZ	2.33	0.63
1:A:919:LEU:HB2	1:A:1079:GLU:HB3	1.79	0.63
1:C:44:THR:HG22	1:C:71:MET:HG2	1.81	0.62
1:C:621:ARG:NH1	1:C:623:GLN:HG2	2.14	0.62
1:A:609:ILE:HB	1:A:610:PRO:HD3	1.80	0.62
1:C:47:LEU:HD11	1:C:88:ALA:CB	2.29	0.62
1:A:47:LEU:HD11	1:A:88:ALA:CB	2.28	0.62
2:D:436:LEU:O	2:D:437:CYS:HB2	1.98	0.62
2:B:27:LEU:CD2	2:B:446:GLY:HA2	2.29	0.62
2:B:571:ARG:HH21	2:B:660:MET:CG	2.13	0.62
1:A:18:PHE:CE2	1:A:32:VAL:HG21	2.34	0.62
1:A:562:LEU:HD11	1:A:590:GLN:HG2	1.81	0.62
2:B:597:PRO:O	2:B:598:SER:CB	2.47	0.61
2:D:115:TYR:CD1	2:D:170:PRO:HD2	2.35	0.61
4:A:3374:NAG:O3	4:A:3375:MAN:H2	2.01	0.61
1:C:797:GLY:CA	1:C:884:GLU:HB2	2.30	0.61
1:A:615:ARG:HA	1:A:618:PHE:HB2	1.82	0.61
2:D:587:LEU:HB3	2:D:588:PRO:HA	1.82	0.61
1:A:599:VAL:HG23	1:A:599:VAL:O	1.99	0.61
1:C:43:GLN:HA	1:C:70:ASN:H	1.66	0.61
2:B:571:ARG:HH21	2:B:660:MET:HG3	1.65	0.61
1:A:1063:LEU:HD12	1:A:1064:PRO:HA	1.83	0.61
1:A:789:TRP:CZ2	1:C:772:LYS:HA	2.36	0.61
1:A:362:LEU:HD23	1:A:363:TYR:N	2.16	0.61
2:B:587:LEU:HB3	2:B:588:PRO:HA	1.82	0.61
1:C:118:ARG:HA	1:C:120:PRO:HB3	1.82	0.61
1:C:919:LEU:O	2:D:643:ARG:NH1	2.34	0.61
1:C:578:ASP:OD2	1:C:595:ARG:HD2	2.01	0.61
6:A:3716:NAG:H61	6:A:3717:NAG:O5	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:928:GLU:HG3	1:A:929:SER:N	2.16	0.61
1:A:772:LYS:HA	1:C:789:TRP:CZ2	2.36	0.60
2:B:115:TYR:CD1	2:B:170:PRO:HD2	2.36	0.60
1:C:822:LEU:HG	1:C:823:ARG:N	2.06	0.60
2:B:317:LYS:HE3	2:B:410:GLY:HA3	1.82	0.60
1:C:615:ARG:HA	1:C:618:PHE:HB2	1.83	0.60
1:A:43:GLN:HA	1:A:70:ASN:H	1.65	0.60
1:C:928:GLU:HG3	1:C:929:SER:N	2.17	0.60
1:A:44:THR:HG22	1:A:71:MET:HG2	1.83	0.60
1:C:941:LEU:HD12	1:C:941:LEU:N	2.16	0.60
1:A:941:LEU:HD12	1:A:941:LEU:N	2.16	0.60
1:A:578:ASP:OD2	1:A:595:ARG:HD2	2.02	0.60
2:D:562:ASN:HB2	2:D:563:PRO:HD2	1.84	0.60
2:B:466:ARG:O	2:B:467:SER:OG	2.19	0.60
1:C:119:LEU:O	1:C:119:LEU:HG	2.02	0.59
1:C:833:PRO:HA	1:C:840:TRP:CB	2.32	0.59
1:C:824:SER:H	1:C:825:LEU:HG	1.67	0.59
2:B:562:ASN:HB2	2:B:563:PRO:HD2	1.83	0.59
2:D:220:GLN:HA	2:D:264:CYS:HB3	1.83	0.59
1:A:739:GLN:HB2	1:A:742:PHE:CZ	2.38	0.59
1:C:430:VAL:HG21	1:C:487:CYS:SG	2.43	0.59
2:D:597:PRO:O	2:D:598:SER:HB2	2.03	0.59
1:C:362:LEU:HD23	1:C:363:TYR:N	2.17	0.59
1:A:964:TRP:CB	1:A:1032:LEU:HA	2.32	0.59
1:A:833:PRO:HA	1:A:840:TRP:CB	2.32	0.59
2:D:430:GLN:HB2	2:D:434:ARG:NH2	2.17	0.59
1:A:820:GLY:N	1:A:822:LEU:HB3	2.18	0.59
1:C:739:GLN:HB2	1:C:742:PHE:CZ	2.37	0.59
2:D:289:LEU:HD21	2:D:296:PRO:CD	2.33	0.59
2:B:211:PRO:HB2	2:B:246:HIS:CE1	2.38	0.59
1:A:715:LEU:HD12	1:A:715:LEU:O	2.03	0.59
2:B:289:LEU:HD21	2:B:296:PRO:CD	2.33	0.59
1:A:659:ASP:OD2	6:A:3716:NAG:N2	2.35	0.59
2:B:220:GLN:HA	2:B:264:CYS:HB3	1.83	0.59
1:C:374:MET:HG3	1:C:381:MET:SD	2.43	0.59
1:C:609:ILE:HD12	1:C:632:GLN:OE1	2.03	0.58
2:B:35:PRO:HG2	2:B:510:GLN:CD	2.23	0.58
4:C:3374:NAG:O3	4:C:3375:MAN:H2	2.03	0.58
1:A:468:THR:HG23	1:A:498:PRO:HG3	1.85	0.58
1:A:20:ASP:OD1	1:A:567:GLN:OE1	2.21	0.58
1:C:468:THR:HG23	1:C:498:PRO:HG3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:ARG:HA	1:A:120:PRO:HB3	1.84	0.58
1:A:121:VAL:HG12	1:A:121:VAL:O	2.04	0.58
1:C:479:PRO:HD2	1:C:485:TRP:CD1	2.39	0.58
1:A:374:MET:HG3	1:A:381:MET:SD	2.43	0.58
1:C:964:TRP:CB	1:C:1032:LEU:HA	2.34	0.58
1:C:715:LEU:HD12	1:C:715:LEU:O	2.04	0.58
1:A:479:PRO:HD2	1:A:485:TRP:CD1	2.39	0.58
1:A:119:LEU:HG	1:A:119:LEU:O	2.03	0.57
2:D:211:PRO:HB2	2:D:246:HIS:CE1	2.40	0.57
2:B:461:CYS:SG	2:B:466:ARG:HD3	2.43	0.57
2:B:592:GLU:O	2:B:594:PRO:HD3	2.04	0.57
1:A:602:VAL:HG23	1:A:638:TYR:O	2.04	0.57
1:C:907:THR:CG2	1:C:1053:ILE:HD13	2.34	0.57
1:C:602:VAL:HG23	1:C:638:TYR:O	2.04	0.57
1:C:20:ASP:OD1	1:C:567:GLN:OE1	2.22	0.57
2:D:260:ASN:HA	2:D:277:PHE:CE2	2.39	0.57
2:D:15:ILE:CG2	2:D:86:ARG:CZ	2.74	0.57
1:C:119:LEU:N	1:C:120:PRO:CA	2.61	0.57
1:A:710:PRO:HG3	1:A:884:GLU:OE2	2.05	0.57
1:A:416:ILE:HD11	1:A:485:TRP:CZ2	2.39	0.57
2:B:522:TYR:CD1	2:B:552:GLN:HA	2.38	0.57
1:C:490:VAL:HG12	1:C:491:LEU:N	2.19	0.57
1:A:822:LEU:HG	1:A:823:ARG:N	2.19	0.57
1:C:963:VAL:HA	1:C:1036:TRP:CD1	2.40	0.57
1:A:490:VAL:HG12	1:A:491:LEU:N	2.18	0.57
1:C:986:PRO:CB	1:C:987:PRO:HD2	2.34	0.57
1:A:831:SER:CB	1:A:842:THR:HG22	2.35	0.57
2:D:442:PHE:CZ	2:D:449:ARG:HB2	2.40	0.57
1:C:659:ASP:OD2	6:C:3716:NAG:H81	2.02	0.57
1:A:609:ILE:HD12	1:A:632:GLN:OE1	2.04	0.57
1:C:659:ASP:OD2	6:C:3716:NAG:O7	2.23	0.57
2:B:461:CYS:SG	2:B:466:ARG:CD	2.93	0.57
2:D:35:PRO:HG2	2:D:510:GLN:CD	2.25	0.57
2:D:295:GLN:HG3	2:D:317:LYS:HE2	1.86	0.56
1:C:416:ILE:HD11	1:C:485:TRP:CZ2	2.39	0.56
2:D:165:LEU:HD12	2:D:179:PRO:HG2	1.87	0.56
2:B:442:PHE:CZ	2:B:449:ARG:HB2	2.40	0.56
1:C:624:VAL:HG12	1:C:625:VAL:HG13	1.86	0.56
1:A:919:LEU:CD1	2:B:643:ARG:NH1	2.68	0.56
2:B:570:GLY:HA2	2:B:659:GLY:HA2	1.87	0.56
1:C:121:VAL:HG12	1:C:121:VAL:O	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:772:LYS:O	1:C:772:LYS:HG3	2.05	0.56
1:A:772:LYS:HG3	1:A:772:LYS:O	2.04	0.56
2:B:295:GLN:HG3	2:B:317:LYS:HE2	1.86	0.56
2:B:165:LEU:HD12	2:B:179:PRO:HG2	1.87	0.56
2:D:74:LYS:HD2	2:D:103:TYR:OH	2.06	0.56
2:B:162:PRO:O	2:B:165:LEU:HB3	2.05	0.56
1:A:986:PRO:CB	1:A:987:PRO:HD2	2.36	0.56
2:B:471:LEU:O	2:B:493:GLY:HA2	2.06	0.56
1:C:710:PRO:HG3	1:C:884:GLU:OE2	2.06	0.56
2:D:570:GLY:HA2	2:D:659:GLY:HA2	1.87	0.56
1:A:912:HIS:ND1	1:A:935:ARG:HD2	2.21	0.56
2:D:135:LEU:HD11	2:D:139:THR:HB	1.88	0.56
2:D:317:LYS:CE	2:D:410:GLY:HA3	2.33	0.56
2:B:532:ARG:CD	2:B:554:GLU:HG3	2.36	0.56
1:C:662:LEU:HD11	1:C:673:PHE:CE1	2.41	0.56
1:A:430:VAL:HG21	1:A:487:CYS:SG	2.46	0.56
2:D:162:PRO:O	2:D:165:LEU:HB3	2.05	0.56
1:C:619:GLU:O	1:C:620:CYS:SG	2.64	0.56
2:D:654:LEU:HD13	2:D:665:ILE:HG13	1.88	0.56
1:C:70:ASN:HB3	1:C:94:HIS:ND1	2.21	0.55
2:D:468:SER:HB2	2:D:471:LEU:HG	1.87	0.55
2:B:468:SER:HB2	2:B:471:LEU:HG	1.87	0.55
1:C:780:LEU:O	1:C:865:VAL:HG12	2.06	0.55
1:A:780:LEU:O	1:A:865:VAL:HG12	2.06	0.55
2:D:181:ALA:HB3	2:D:271:TYR:CZ	2.42	0.55
1:C:621:ARG:HG2	1:C:622:GLU:H	1.72	0.55
1:A:469:ARG:NH2	2:B:287:HIS:HB2	2.21	0.55
2:B:289:LEU:HD21	2:B:296:PRO:HD3	1.89	0.55
1:C:89:CYS:O	1:C:91:PRO:HD3	2.07	0.55
1:C:395:TRP:CH2	1:C:480:ARG:HD3	2.41	0.55
1:C:912:HIS:ND1	1:C:935:ARG:HD2	2.21	0.55
1:C:994:HIS:CG	1:C:1005:ILE:HD11	2.41	0.55
1:C:812:TYR:CE2	1:C:814:ALA:CB	2.84	0.55
2:B:87:PRO:CD	2:B:423:CYS:SG	2.94	0.55
1:C:332:MET:SD	2:D:208:LEU:HD13	2.46	0.55
1:C:831:SER:CB	1:C:842:THR:HG22	2.35	0.55
1:A:1052:GLU:OE1	1:C:756:HIS:HA	2.06	0.55
2:D:289:LEU:HD21	2:D:296:PRO:HD3	1.88	0.55
1:A:89:CYS:O	1:A:91:PRO:HD3	2.06	0.55
6:C:3717:NAG:C3	6:C:3718:MAN:H2	2.36	0.55
2:B:181:ALA:HB3	2:B:271:TYR:CZ	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:575:LEU:HD12	1:C:576:THR:N	2.21	0.55
1:C:118:ARG:HA	1:C:120:PRO:CB	2.37	0.55
1:C:722:LYS:N	1:C:723:PRO:HD2	2.22	0.55
1:A:575:LEU:HD12	1:A:576:THR:N	2.22	0.55
1:A:657:THR:HG22	1:A:684:VAL:HG22	1.89	0.55
2:B:58:ASP:N	2:B:59:PRO:HD3	2.21	0.55
1:C:528:GLU:HB2	1:C:531:ARG:HB2	1.89	0.55
2:D:437:CYS:O	2:D:438:HIS:HB2	2.06	0.55
1:A:70:ASN:HB3	1:A:94:HIS:ND1	2.22	0.55
2:B:562:ASN:HB2	2:B:563:PRO:CD	2.37	0.55
1:A:491:LEU:HD12	1:A:491:LEU:C	2.27	0.54
1:C:418:THR:HG21	1:C:482:TRP:CZ2	2.42	0.54
1:A:722:LYS:N	1:A:723:PRO:HD2	2.22	0.54
1:A:465:TYR:HB3	1:A:469:ARG:HA	1.90	0.54
1:A:994:HIS:CG	1:A:1005:ILE:HD11	2.42	0.54
1:A:963:VAL:HA	1:A:1036:TRP:CD1	2.42	0.54
1:C:1063:LEU:HD12	1:C:1064:PRO:HA	1.84	0.54
2:B:295:GLN:CG	2:B:317:LYS:HE2	2.37	0.54
2:B:562:ASN:HB3	2:B:589:LEU:HD13	1.89	0.54
2:B:522:TYR:CE1	2:B:552:GLN:HA	2.42	0.54
1:A:907:THR:CG2	1:A:1053:ILE:HD13	2.37	0.54
1:A:528:GLU:HB2	1:A:531:ARG:HB2	1.89	0.54
1:C:491:LEU:C	1:C:491:LEU:HD12	2.28	0.54
1:C:4:ASP:CG	1:C:597:ARG:NH2	2.61	0.54
1:A:649:SER:O	1:A:650:ARG:HB3	2.07	0.54
1:A:565:PHE:HB2	1:A:587:ALA:HB2	1.90	0.54
2:D:461:CYS:HB3	2:D:466:ARG:HD3	1.88	0.54
2:D:562:ASN:HB2	2:D:563:PRO:CD	2.38	0.54
1:C:31:VAL:HG21	1:C:86:LEU:HD13	1.89	0.54
2:B:135:LEU:HD11	2:B:139:THR:HB	1.90	0.54
1:C:1065:GLY:C	1:C:1066:GLN:HG3	2.28	0.54
2:B:260:ASN:HA	2:B:277:PHE:CE2	2.43	0.54
1:A:418:THR:HG21	1:A:482:TRP:CZ2	2.43	0.54
2:B:587:LEU:N	2:B:587:LEU:HD12	2.23	0.54
2:D:112:ASP:O	2:D:117:MET:HG3	2.08	0.54
2:D:562:ASN:HB3	2:D:589:LEU:HD13	1.88	0.54
2:D:347:LEU:HD22	2:D:389:PHE:CD1	2.43	0.54
1:C:952:PHE:HB2	1:C:1011:PHE:HB2	1.90	0.54
2:B:27:LEU:HD21	2:B:446:GLY:CA	2.37	0.54
2:D:654:LEU:CD1	2:D:665:ILE:HG13	2.38	0.54
1:C:465:TYR:HB3	1:C:469:ARG:HA	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1065:GLY:C	1:A:1066:GLN:HG3	2.27	0.54
2:D:429:ASP:N	2:D:429:ASP:OD1	2.36	0.53
1:A:662:LEU:HD11	1:A:673:PHE:CE1	2.42	0.53
1:C:364:PRO:CB	1:C:365:PRO:CD	2.86	0.53
2:D:115:TYR:HA	2:D:204:ILE:HD13	1.89	0.53
2:B:659:GLY:O	2:B:662:ARG:HG2	2.09	0.53
1:A:80:THR:HB	1:A:341:PHE:CG	2.43	0.53
1:C:657:THR:HG22	1:C:684:VAL:HG22	1.89	0.53
2:D:604:ILE:HD11	2:D:642:GLU:HB2	1.90	0.53
2:D:295:GLN:CG	2:D:317:LYS:HE2	2.38	0.53
2:B:546:PHE:CE2	2:B:554:GLU:HG2	2.43	0.53
2:D:289:LEU:HD23	2:D:315:ILE:HD11	1.90	0.53
2:B:347:LEU:HD22	2:B:389:PHE:CD1	2.43	0.53
2:D:98:ARG:HG2	2:D:98:ARG:O	2.09	0.53
2:B:520:GLU:HB3	2:B:550:ALA:HB2	1.89	0.53
2:D:520:GLU:HB3	2:D:550:ALA:HB2	1.89	0.53
2:D:461:CYS:CB	2:D:466:ARG:HD3	2.38	0.53
1:A:812:TYR:CE2	1:A:814:ALA:CB	2.89	0.53
1:A:364:PRO:CB	1:A:365:PRO:CD	2.86	0.53
1:A:659:ASP:OD2	6:A:3716:NAG:C7	2.56	0.53
2:B:115:TYR:HA	2:B:204:ILE:HD13	1.89	0.53
2:B:343:SER:HA	2:B:381:VAL:O	2.08	0.53
1:A:804:HIS:HB2	1:A:808:LEU:HD11	1.91	0.53
1:C:917:LYS:HE3	1:C:1077:VAL:CG2	2.38	0.53
2:B:654:LEU:HD13	2:B:665:ILE:HG13	1.89	0.53
1:C:804:HIS:HB2	1:C:808:LEU:HD11	1.90	0.53
1:A:657:THR:HG23	1:A:720:VAL:HB	1.90	0.53
1:C:1020:VAL:HG12	1:C:1021:GLN:HG3	1.90	0.53
1:C:565:PHE:HB2	1:C:587:ALA:HB2	1.89	0.53
1:C:333:ALA:HB1	1:C:350:ALA:HB1	1.91	0.53
2:D:74:LYS:HZ2	2:D:103:TYR:HE2	1.57	0.53
2:D:659:GLY:O	2:D:662:ARG:HG2	2.09	0.53
1:A:333:ALA:HB1	1:A:350:ALA:HB1	1.91	0.53
2:D:462:GLN:HG2	2:D:463:THR:N	2.24	0.53
1:C:621:ARG:HG2	1:C:622:GLU:N	2.24	0.53
1:A:595:ARG:HB2	1:A:597:ARG:HH12	1.74	0.53
1:C:80:THR:HB	1:C:341:PHE:CG	2.44	0.53
1:A:917:LYS:HE3	1:A:1077:VAL:CG2	2.38	0.53
2:B:363:PHE:CE2	2:B:369:THR:HG23	2.44	0.53
2:D:87:PRO:CD	2:D:423:CYS:SG	2.97	0.53
1:C:1053:ILE:CG2	1:C:1070:MET:HB2	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:649:SER:O	1:C:650:ARG:HB3	2.09	0.53
2:D:155:LEU:H	2:D:160:THR:CG2	2.22	0.53
1:C:772:LYS:O	1:C:773:SER:HB3	2.09	0.53
1:A:71:MET:HG3	1:A:90:GLY:HA3	1.91	0.53
1:C:657:THR:HG23	1:C:720:VAL:HB	1.91	0.53
1:A:876:LEU:HD12	1:A:876:LEU:C	2.30	0.53
2:B:98:ARG:HG2	2:B:98:ARG:O	2.09	0.53
2:D:466:ARG:O	2:D:467:SER:OG	2.26	0.52
2:D:587:LEU:N	2:D:587:LEU:HD12	2.24	0.52
1:C:595:ARG:HB2	1:C:597:ARG:HH12	1.74	0.52
1:A:755:ASP:O	1:A:756:HIS:HB3	2.09	0.52
2:D:110:LEU:HD11	2:D:237:LEU:HD23	1.91	0.52
2:D:616:PRO:HB2	2:D:620:ASN:HA	1.92	0.52
1:A:118:ARG:HA	1:A:120:PRO:CB	2.39	0.52
1:C:681:LEU:HD12	1:C:681:LEU:C	2.30	0.52
1:C:491:LEU:HD11	1:C:545:ILE:CG1	2.38	0.52
2:B:616:PRO:HB2	2:B:620:ASN:HA	1.90	0.52
2:D:423:CYS:O	2:D:424:GLU:HG2	2.10	0.52
1:A:1020:VAL:HG12	1:A:1021:GLN:HG3	1.92	0.52
2:B:155:LEU:H	2:B:160:THR:CG2	2.23	0.52
1:A:4:ASP:HB2	1:A:597:ARG:CZ	2.40	0.52
2:B:638:ARG:HB2	2:B:654:LEU:O	2.09	0.52
2:B:654:LEU:CD1	2:B:665:ILE:HG13	2.39	0.52
2:D:363:PHE:CE2	2:D:369:THR:HG23	2.44	0.52
2:B:599:PRO:HB2	2:B:603:TYR:HE2	1.74	0.52
2:B:604:ILE:HD11	2:B:642:GLU:HB2	1.91	0.52
1:A:31:VAL:HG21	1:A:86:LEU:HD13	1.91	0.52
2:D:340:LYS:HA	2:D:343:SER:HB2	1.90	0.52
1:C:32:VAL:HG11	1:C:591:VAL:HG11	1.92	0.52
1:C:986:PRO:HB3	1:C:987:PRO:HD2	1.92	0.52
1:C:575:LEU:HD12	1:C:576:THR:CG2	2.39	0.52
2:B:399:ILE:HG13	2:B:421:PRO:HG3	1.92	0.52
1:A:665:GLY:HA3	2:B:498:HIS:HB3	1.92	0.52
1:C:623:GLN:O	1:C:624:VAL:HB	2.10	0.52
1:A:772:LYS:O	1:A:773:SER:HB3	2.09	0.52
1:A:465:TYR:CG	1:A:469:ARG:HG3	2.45	0.52
2:B:289:LEU:HD23	2:B:315:ILE:HD11	1.91	0.52
2:D:461:CYS:SG	2:D:466:ARG:NE	2.83	0.52
1:C:624:VAL:CG1	1:C:625:VAL:N	2.61	0.52
1:A:681:LEU:C	1:A:681:LEU:HD12	2.31	0.52
1:A:491:LEU:HD11	1:A:545:ILE:CG1	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:460:GLU:HG2	2:B:461:CYS:N	2.24	0.52
1:A:952:PHE:HB2	1:A:1011:PHE:HB2	1.90	0.52
2:D:522:TYR:CD1	2:D:552:GLN:HA	2.44	0.52
1:A:831:SER:HA	1:A:842:THR:HG22	1.92	0.52
1:A:332:MET:SD	2:B:208:LEU:HD13	2.50	0.52
1:A:812:TYR:HE2	1:A:814:ALA:HB2	1.68	0.52
1:C:662:LEU:CD1	1:C:673:PHE:CE1	2.93	0.52
1:A:971:HIS:CE1	1:A:974:ASN:HB2	2.45	0.52
2:B:146:PHE:HB2	2:B:195:PHE:CZ	2.45	0.52
1:A:613:ILE:HD12	1:A:748:PHE:CD2	2.45	0.52
2:D:638:ARG:HB2	2:D:654:LEU:O	2.10	0.51
1:A:650:ARG:HD3	1:A:729:ASN:HB3	1.91	0.51
1:A:407:ARG:HG2	2:B:247:PHE:CZ	2.45	0.51
1:C:674:GLN:HB2	1:C:699:LEU:HD11	1.92	0.51
2:D:432:ARG:HD3	2:D:433:ASP:N	2.25	0.51
1:C:532:GLY:HA3	1:C:565:PHE:HD2	1.75	0.51
1:A:848:HIS:HB2	2:B:485:SER:HB3	1.92	0.51
1:A:484:ARG:HH12	2:B:586:GLN:CG	2.19	0.51
1:A:575:LEU:HD12	1:A:576:THR:CG2	2.41	0.51
1:C:650:ARG:HD3	1:C:729:ASN:HB3	1.91	0.51
1:A:461:ALA:N	1:A:462:PRO:HD3	2.26	0.51
1:A:569:LEU:HD12	1:A:569:LEU:O	2.10	0.51
1:A:32:VAL:HG11	1:A:591:VAL:HG11	1.92	0.51
1:A:71:MET:CG	1:A:90:GLY:HA3	2.40	0.51
1:C:531:ARG:HA	1:C:563:GLN:O	2.11	0.51
1:C:470:GLY:HA2	1:C:497:HIS:O	2.09	0.51
1:C:461:ALA:N	1:C:462:PRO:HD3	2.26	0.51
1:A:553:ILE:HG23	1:A:557:GLN:HG3	1.93	0.51
1:C:656:VAL:HG13	1:C:718:THR:O	2.11	0.51
1:A:93:VAL:HB	1:A:104:THR:CG2	2.40	0.51
1:C:118:ARG:HA	1:C:120:PRO:HA	1.93	0.51
1:A:71:MET:SD	1:A:90:GLY:HA3	2.50	0.51
1:C:465:TYR:CG	1:C:469:ARG:HG3	2.46	0.51
2:D:399:ILE:HG13	2:D:421:PRO:HG3	1.93	0.51
1:A:119:LEU:N	1:A:120:PRO:CA	2.60	0.51
2:D:423:CYS:O	2:D:424:GLU:CG	2.58	0.51
1:C:446:VAL:HG12	1:C:456:LEU:CD1	2.41	0.51
1:A:797:GLY:HA3	1:A:884:GLU:HB2	1.93	0.51
1:C:620:CYS:HB3	1:C:702:SER:O	2.11	0.51
1:C:569:LEU:O	1:C:569:LEU:HD12	2.10	0.51
1:C:971:HIS:CE1	1:C:974:ASN:HB2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:83:LEU:HD13	2:D:85:LEU:HB2	1.93	0.51
2:B:364:CYS:HB2	2:B:368:VAL:HB	1.93	0.51
1:A:625:VAL:HG23	1:A:627:GLU:N	2.26	0.51
1:C:831:SER:HA	1:C:842:THR:HG22	1.92	0.51
1:C:420:VAL:HB	1:C:423:GLN:HB2	1.92	0.51
2:D:146:PHE:HB2	2:D:195:PHE:CZ	2.46	0.51
1:C:345:GLY:HA3	1:C:363:TYR:O	2.11	0.51
2:B:105:ILE:HG12	2:B:106:ASP:N	2.26	0.51
2:D:110:LEU:HD13	2:D:218:MET:SD	2.50	0.50
1:C:876:LEU:C	1:C:876:LEU:HD12	2.32	0.50
1:A:674:GLN:HB2	1:A:699:LEU:HD11	1.93	0.50
1:A:470:GLY:HA2	1:A:497:HIS:O	2.10	0.50
2:D:260:ASN:ND2	2:D:277:PHE:HZ	2.09	0.50
1:A:420:VAL:HB	1:A:423:GLN:HB2	1.93	0.50
2:D:184:HIS:CE1	2:D:228:ILE:HG23	2.47	0.50
2:D:364:CYS:HB2	2:D:368:VAL:HB	1.93	0.50
1:C:93:VAL:O	1:C:103:LEU:HA	2.12	0.50
1:A:93:VAL:O	1:A:103:LEU:HA	2.11	0.50
1:C:18:PHE:CZ	1:C:32:VAL:HG21	2.46	0.50
2:D:105:ILE:HG21	2:D:135:LEU:HD13	1.92	0.50
1:A:89:CYS:C	1:A:91:PRO:HD3	2.32	0.50
1:C:848:HIS:O	1:C:849:LEU:HB3	2.12	0.50
2:D:643:ARG:NH2	2:D:649:TRP:CZ2	2.80	0.50
1:A:656:VAL:HG21	1:A:687:LEU:CD1	2.41	0.50
2:B:110:LEU:HD13	2:B:218:MET:SD	2.51	0.50
1:C:920:ASN:OD1	1:C:1080:LYS:HE2	2.11	0.50
1:C:873:ASP:C	1:C:901:VAL:HG12	2.33	0.50
2:B:659:GLY:O	2:B:662:ARG:CG	2.60	0.50
2:D:659:GLY:O	2:D:662:ARG:CG	2.60	0.50
1:A:531:ARG:HA	1:A:563:GLN:O	2.11	0.50
1:A:532:GLY:HA3	1:A:565:PHE:HD2	1.76	0.50
2:B:99:ARG:O	2:B:383:ILE:O	2.30	0.50
1:A:848:HIS:O	1:A:849:LEU:HB3	2.12	0.50
2:B:110:LEU:HD11	2:B:237:LEU:HD23	1.92	0.50
2:B:212:GLU:HG2	2:B:243:ASP:HB2	1.94	0.50
2:D:154:VAL:HG23	2:D:160:THR:HG21	1.92	0.50
1:A:820:GLY:H	1:A:822:LEU:HB3	1.76	0.50
1:A:444:CYS:HB2	1:A:506:LEU:CD1	2.42	0.50
2:B:83:LEU:HD13	2:B:85:LEU:HB2	1.94	0.50
2:B:532:ARG:HD3	2:B:554:GLU:CG	2.42	0.50
1:A:986:PRO:HB3	1:A:987:PRO:HD2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:154:VAL:HG23	2:B:160:THR:HG21	1.92	0.49
1:A:964:TRP:HB3	1:A:1032:LEU:HA	1.93	0.49
1:A:465:TYR:CG	1:A:469:ARG:CG	2.95	0.49
2:D:592:GLU:O	2:D:594:PRO:HD3	2.12	0.49
1:C:419:GLN:HA	1:C:424:TRP:HA	1.94	0.49
1:C:908:VAL:O	1:C:938:VAL:HG23	2.12	0.49
1:C:716:ASN:OD1	1:C:716:ASN:C	2.49	0.49
2:D:532:ARG:CD	2:D:554:GLU:HG3	2.43	0.49
1:A:659:ASP:OD2	6:A:3716:NAG:O7	2.30	0.49
2:B:105:ILE:HG21	2:B:135:LEU:HD13	1.93	0.49
2:D:383:ILE:HG22	2:D:384:ASN:N	2.27	0.49
1:C:71:MET:SD	1:C:90:GLY:HA3	2.52	0.49
1:A:662:LEU:CD1	1:A:673:PHE:CE1	2.95	0.49
1:C:609:ILE:CB	1:C:610:PRO:HD3	2.42	0.49
1:A:18:PHE:CZ	1:A:32:VAL:HG21	2.47	0.49
2:D:105:ILE:HG12	2:D:106:ASP:N	2.27	0.49
2:D:58:ASP:N	2:D:59:PRO:HD3	2.26	0.49
2:D:212:GLU:HG2	2:D:243:ASP:HB2	1.93	0.49
1:A:126:CYS:HB3	1:A:127:PRO:CD	2.42	0.49
1:C:93:VAL:HB	1:C:104:THR:CG2	2.41	0.49
2:B:532:ARG:HD3	2:B:554:GLU:HG3	1.95	0.49
1:A:345:GLY:HA3	1:A:363:TYR:O	2.12	0.49
2:B:437:CYS:HA	2:B:458:ASN:O	2.12	0.49
2:B:546:PHE:HE2	2:B:554:GLU:HG2	1.76	0.49
1:C:964:TRP:HB2	1:C:1032:LEU:HA	1.94	0.49
1:A:47:LEU:HB2	1:A:60:ILE:HG21	1.95	0.49
2:B:260:ASN:ND2	2:B:277:PHE:HZ	2.10	0.49
1:A:666:ARG:HB3	2:B:498:HIS:CD2	2.48	0.49
1:C:553:ILE:HG23	1:C:557:GLN:HG3	1.93	0.49
1:C:126:CYS:HB3	1:C:127:PRO:CD	2.43	0.49
2:D:251:GLY:HA3	2:D:278:ASP:OD1	2.13	0.49
2:B:6:PHE:O	2:B:8:VAL:HG23	2.11	0.49
2:D:11:CYS:O	2:D:15:ILE:HG12	2.13	0.49
1:A:406:PRO:HB3	1:A:438:TYR:CD2	2.47	0.49
1:A:578:ASP:O	1:A:578:ASP:OD1	2.31	0.49
1:C:613:ILE:HD12	1:C:748:PHE:CD2	2.47	0.49
2:D:401:GLU:HA	2:D:421:PRO:HD3	1.94	0.49
2:B:112:ASP:O	2:B:117:MET:HG3	2.12	0.49
1:A:920:ASN:OD1	1:A:1080:LYS:HE2	2.12	0.49
1:A:873:ASP:C	1:A:901:VAL:HG12	2.32	0.49
1:C:681:LEU:HD12	1:C:682:SER:N	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:656:GLN:HG2	2:B:657:GLN:N	2.28	0.49
1:C:89:CYS:C	1:C:91:PRO:HD3	2.33	0.49
1:C:465:TYR:CG	1:C:469:ARG:CG	2.96	0.49
2:D:186:LEU:HD13	2:D:195:PHE:CD1	2.48	0.49
2:D:6:PHE:CG	2:D:7:LYS:N	2.81	0.49
2:D:460:GLU:HG2	2:D:461:CYS:N	2.28	0.49
1:C:71:MET:HG3	1:C:90:GLY:HA3	1.94	0.49
1:A:491:LEU:HD12	1:A:492:TYR:N	2.28	0.49
1:A:362:LEU:HD23	1:A:362:LEU:C	2.33	0.49
2:D:135:LEU:CD1	2:D:139:THR:HB	2.42	0.49
1:A:1053:ILE:CG2	1:A:1070:MET:HB2	2.42	0.49
2:D:345:VAL:HG11	2:D:387:ILE:CD1	2.43	0.49
2:B:251:GLY:HA3	2:B:278:ASP:OD1	2.13	0.49
1:A:850:ILE:HG22	1:A:851:PHE:N	2.27	0.49
2:B:77:SER:HA	2:B:78:PRO:C	2.32	0.49
1:C:624:VAL:HG13	1:C:625:VAL:HG13	1.93	0.49
1:C:406:PRO:HB3	1:C:438:TYR:CD2	2.48	0.49
1:C:446:VAL:CG1	1:C:456:LEU:HD11	2.43	0.49
1:A:986:PRO:HG3	1:A:1003:CYS:O	2.13	0.49
1:A:986:PRO:CB	1:A:987:PRO:CD	2.91	0.49
2:B:6:PHE:CG	2:B:7:LYS:N	2.81	0.49
2:B:455:ILE:HG22	2:B:456:GLY:N	2.28	0.49
2:B:184:HIS:CE1	2:B:228:ILE:HG23	2.48	0.49
1:C:118:ARG:HA	1:C:120:PRO:CA	2.43	0.48
1:A:395:TRP:CH2	1:A:480:ARG:HD3	2.47	0.48
1:A:681:LEU:HD12	1:A:682:SER:N	2.28	0.48
2:D:546:PHE:CE2	2:D:554:GLU:HG2	2.48	0.48
2:B:295:GLN:CD	2:B:317:LYS:HE2	2.34	0.48
2:B:401:GLU:HA	2:B:421:PRO:HD3	1.94	0.48
1:C:908:VAL:HG13	1:C:1069:PHE:HB3	1.95	0.48
2:D:6:PHE:O	2:D:8:VAL:HG23	2.12	0.48
2:D:479:ASN:HB3	5:D:3479:NAG:O7	2.13	0.48
2:B:11:CYS:O	2:B:15:ILE:HG12	2.12	0.48
1:C:1044:LYS:HA	1:C:1079:GLU:HB2	1.95	0.48
2:B:643:ARG:NH2	2:B:649:TRP:CZ2	2.81	0.48
1:C:77:LEU:HD23	1:C:88:ALA:HA	1.95	0.48
1:C:986:PRO:CB	1:C:987:PRO:CD	2.90	0.48
1:A:764:ILE:CD1	1:A:800:ILE:HD11	2.43	0.48
1:A:905:VAL:HG21	1:A:946:LEU:HD22	1.94	0.48
1:C:905:VAL:HG11	1:C:946:LEU:HD21	1.94	0.48
1:C:71:MET:CG	1:C:90:GLY:HA3	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:ARG:HA	1:A:120:PRO:HA	1.95	0.48
1:A:806:ALA:HA	1:A:840:TRP:NE1	2.29	0.48
2:B:135:LEU:CD1	2:B:139:THR:HB	2.43	0.48
1:C:761:ASN:ND2	1:C:791:ASP:HB2	2.28	0.48
2:B:383:ILE:HG22	2:B:384:ASN:N	2.28	0.48
2:D:522:TYR:CE1	2:D:552:GLN:HA	2.48	0.48
1:A:656:VAL:HG13	1:A:718:THR:O	2.12	0.48
1:A:905:VAL:HG11	1:A:946:LEU:HD21	1.94	0.48
2:D:77:SER:HA	2:D:78:PRO:C	2.34	0.48
1:A:928:GLU:HG3	1:A:929:SER:H	1.77	0.48
1:C:20:ASP:OD1	2:D:257:LEU:HD22	2.13	0.48
2:B:121:LEU:O	2:B:125:LYS:HB3	2.13	0.48
2:D:461:CYS:SG	2:D:466:ARG:HD3	2.53	0.48
1:C:918:TYR:C	2:D:643:ARG:NH2	2.67	0.48
1:C:47:LEU:HB2	1:C:60:ILE:HG21	1.95	0.48
2:D:99:ARG:O	2:D:383:ILE:O	2.31	0.48
1:C:905:VAL:HG21	1:C:946:LEU:HD22	1.94	0.48
1:C:850:ILE:HG22	1:C:851:PHE:N	2.28	0.48
1:A:716:ASN:OD1	1:A:716:ASN:C	2.52	0.48
1:C:491:LEU:HD12	1:C:492:TYR:N	2.29	0.48
1:C:928:GLU:HG3	1:C:929:SER:H	1.77	0.48
2:D:285:LEU:O	2:D:289:LEU:HB3	2.14	0.48
1:A:465:TYR:CD1	1:A:469:ARG:HG2	2.48	0.48
2:B:616:PRO:HB3	2:B:621:CYS:SG	2.54	0.48
2:D:432:ARG:HH11	2:D:432:ARG:HG2	1.78	0.48
2:B:432:ARG:O	2:B:433:ASP:HB2	2.14	0.48
1:A:776:VAL:HG21	1:A:903:TYR:CE1	2.49	0.48
1:A:992:LEU:C	1:A:992:LEU:HD23	2.34	0.48
1:A:878:THR:HG22	1:A:896:GLN:HB3	1.94	0.48
2:D:437:CYS:HA	2:D:458:ASN:HB3	1.95	0.48
2:D:437:CYS:O	2:D:458:ASN:O	2.32	0.48
1:C:806:ALA:HA	1:C:840:TRP:NE1	2.28	0.48
1:A:446:VAL:HG12	1:A:456:LEU:CD1	2.43	0.48
2:B:591:GLN:HG2	2:B:592:GLU:N	2.29	0.48
2:D:162:PRO:O	2:D:165:LEU:CB	2.62	0.48
1:C:1058:SER:O	1:C:1059:VAL:HB	2.14	0.48
1:A:639:ILE:HG13	1:A:689:LEU:HA	1.96	0.48
2:D:43:ARG:N	2:D:44:PRO:CD	2.77	0.48
1:A:964:TRP:HB2	1:A:1032:LEU:HA	1.94	0.48
1:C:987:PRO:O	1:C:988:ALA:HB3	2.14	0.48
2:D:591:GLN:HG2	2:D:592:GLU:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:3716:NAG:H61	6:C:3717:NAG:O5	2.13	0.48
1:C:755:ASP:O	1:C:756:HIS:HB3	2.13	0.48
2:B:186:LEU:HD13	2:B:195:PHE:CD1	2.48	0.48
2:B:43:ARG:N	2:B:44:PRO:CD	2.77	0.48
1:A:812:TYR:HD2	1:A:814:ALA:HB2	1.77	0.47
2:D:295:GLN:CD	2:D:317:LYS:HE2	2.34	0.47
1:A:822:LEU:CG	1:A:823:ARG:N	2.77	0.47
1:C:964:TRP:HB3	1:C:1032:LEU:HG	1.96	0.47
2:B:285:LEU:O	2:B:289:LEU:HB3	2.14	0.47
1:A:934:HIS:ND1	1:A:1074:THR:CG2	2.77	0.47
1:A:1020:VAL:O	1:A:1021:GLN:HB2	2.14	0.47
1:C:656:VAL:HG21	1:C:687:LEU:CD1	2.43	0.47
1:A:1058:SER:O	1:A:1059:VAL:HB	2.13	0.47
1:A:430:VAL:O	1:A:430:VAL:HG23	2.14	0.47
1:C:938:VAL:HG12	1:C:1024:LEU:O	2.15	0.47
1:C:905:VAL:CG1	1:C:946:LEU:HD21	2.44	0.47
2:D:656:GLN:HG2	2:D:657:GLN:N	2.28	0.47
1:A:411:THR:HG22	1:A:435:ILE:HA	1.96	0.47
1:C:411:THR:HG22	1:C:435:ILE:HA	1.96	0.47
1:A:631:VAL:HG11	1:A:746:LEU:HD11	1.96	0.47
1:A:118:ARG:CG	1:A:120:PRO:HB3	2.40	0.47
1:A:476:CYS:CB	1:A:487:CYS:HA	2.43	0.47
2:B:347:LEU:HD22	2:B:389:PHE:CG	2.50	0.47
1:A:698:LEU:HD12	1:A:698:LEU:N	2.29	0.47
1:A:1044:LYS:HA	1:A:1079:GLU:HB2	1.95	0.47
1:A:77:LEU:HD23	1:A:88:ALA:HA	1.96	0.47
1:C:1053:ILE:CG2	1:C:1070:MET:CB	2.92	0.47
2:D:347:LEU:HD22	2:D:389:PHE:CG	2.50	0.47
1:A:419:GLN:HA	1:A:424:TRP:HA	1.95	0.47
1:C:764:ILE:CD1	1:C:800:ILE:HD11	2.44	0.47
1:A:445:SER:HB2	1:A:454:THR:HG21	1.97	0.47
1:C:964:TRP:HB3	1:C:1032:LEU:HA	1.95	0.47
1:A:609:ILE:CB	1:A:610:PRO:HD3	2.44	0.47
2:D:223:ALA:HB1	2:D:263:ARG:HA	1.97	0.47
1:A:499:TRP:CZ2	2:B:284:GLN:HG3	2.49	0.47
1:C:600:LEU:HD12	1:C:600:LEU:O	2.15	0.47
1:C:362:LEU:HD23	1:C:362:LEU:C	2.34	0.47
2:B:143:ARG:C	2:B:144:ILE:HD12	2.35	0.47
1:A:110:LEU:N	1:A:110:LEU:HD12	2.29	0.47
1:C:822:LEU:CG	1:C:823:ARG:N	2.72	0.47
1:C:395:TRP:HH2	1:C:480:ARG:CG	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:797:GLY:HA3	1:C:884:GLU:HB2	1.95	0.47
1:C:578:ASP:O	1:C:578:ASP:OD1	2.33	0.47
1:C:748:PHE:CD1	1:C:748:PHE:N	2.82	0.47
4:C:3373:NAG:H3	4:C:3374:NAG:N2	2.30	0.47
1:C:575:LEU:HD12	1:C:576:THR:HG23	1.96	0.47
1:A:848:HIS:HB2	2:B:485:SER:O	2.14	0.47
1:C:444:CYS:HB2	1:C:506:LEU:CD1	2.44	0.47
1:A:880:ASN:OD1	1:A:894:THR:HG22	2.14	0.47
2:B:121:LEU:O	2:B:121:LEU:HD23	2.14	0.47
1:C:886:ASN:O	1:C:888:PRO:HD3	2.15	0.47
1:A:970:SER:O	1:A:1026:PHE:HB2	2.14	0.47
2:D:121:LEU:HD23	2:D:121:LEU:O	2.14	0.47
1:C:476:CYS:CB	1:C:487:CYS:HA	2.44	0.47
1:A:430:VAL:HG13	1:A:485:TRP:CE3	2.49	0.47
2:B:562:ASN:OD1	2:B:564:ARG:HB2	2.15	0.47
2:B:162:PRO:O	2:B:165:LEU:CB	2.62	0.47
1:A:905:VAL:CG1	1:A:946:LEU:HD21	2.45	0.47
2:D:455:ILE:HG22	2:D:456:GLY:N	2.29	0.47
1:C:813:VAL:HG23	1:C:823:ARG:NH1	2.30	0.47
1:C:812:TYR:CE2	1:C:814:ALA:CA	2.98	0.47
1:A:840:TRP:CD1	1:A:840:TRP:N	2.81	0.47
1:C:430:VAL:HG13	1:C:485:TRP:CE3	2.50	0.47
1:C:934:HIS:ND1	1:C:1074:THR:CG2	2.78	0.47
2:D:43:ARG:HB3	2:D:44:PRO:HD3	1.95	0.47
2:D:121:LEU:O	2:D:125:LYS:HB3	2.14	0.47
1:C:601:TRP:CZ2	1:C:641:LYS:HG2	2.50	0.47
1:A:761:ASN:ND2	1:A:791:ASP:HB2	2.30	0.47
1:A:964:TRP:HB3	1:A:1032:LEU:HG	1.96	0.47
1:A:987:PRO:O	1:A:988:ALA:HB3	2.15	0.47
1:C:465:TYR:CD1	1:C:469:ARG:HG2	2.50	0.47
2:B:609:CYS:SG	2:B:616:PRO:HB3	2.55	0.47
2:B:43:ARG:HB3	2:B:44:PRO:HD3	1.96	0.47
2:D:644:ASP:HB3	2:D:650:VAL:HG23	1.97	0.47
1:C:663:ASP:HB3	1:C:666:ARG:HD3	1.97	0.47
1:A:1063:LEU:HD12	1:A:1064:PRO:CB	2.46	0.46
1:C:812:TYR:HE2	1:C:814:ALA:CB	2.23	0.46
1:C:986:PRO:HG3	1:C:1003:CYS:O	2.15	0.46
1:A:831:SER:HB3	1:A:842:THR:HG22	1.97	0.46
2:B:382:GLN:HG3	2:B:383:ILE:H	1.80	0.46
1:A:25:TYR:CE1	1:A:86:LEU:HB2	2.50	0.46
1:A:938:VAL:HG12	1:A:1024:LEU:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:811:ARG:HG3	1:A:811:ARG:O	2.14	0.46
1:A:118:ARG:HA	1:A:120:PRO:CA	2.45	0.46
1:C:376:GLN:HB2	4:C:3373:NAG:O4	2.15	0.46
1:C:565:PHE:HB2	1:C:587:ALA:CB	2.46	0.46
2:D:609:CYS:SG	2:D:616:PRO:HB3	2.55	0.46
1:C:639:ILE:HG13	1:C:689:LEU:HA	1.96	0.46
2:B:345:VAL:HG11	2:B:387:ILE:CD1	2.45	0.46
2:B:15:ILE:HG23	2:B:86:ARG:NH1	2.22	0.46
1:C:721:GLY:O	1:C:723:PRO:HD3	2.15	0.46
1:A:20:ASP:OD1	2:B:257:LEU:HD22	2.16	0.46
2:D:222:ALA:CB	2:D:294:ILE:HD12	2.45	0.46
1:A:601:TRP:CZ2	1:A:641:LYS:HG2	2.50	0.46
1:C:430:VAL:HG22	1:C:485:TRP:HZ3	1.80	0.46
1:A:416:ILE:HG22	1:A:427:LYS:HD3	1.97	0.46
1:A:477:PRO:HG2	1:A:489:ALA:HB2	1.97	0.46
1:C:917:LYS:HE3	1:C:1077:VAL:HG23	1.98	0.46
1:A:1020:VAL:O	1:A:1021:GLN:CB	2.63	0.46
2:B:222:ALA:CB	2:B:294:ILE:HD12	2.46	0.46
2:B:256:ILE:HG13	2:B:256:ILE:O	2.15	0.46
2:D:437:CYS:HA	2:D:458:ASN:C	2.35	0.46
2:D:154:VAL:HA	2:D:160:THR:CG2	2.45	0.46
2:D:468:SER:HB2	2:D:471:LEU:CG	2.45	0.46
1:C:1053:ILE:HG22	1:C:1070:MET:HB2	1.96	0.46
2:D:630:LEU:HD12	2:D:665:ILE:HB	1.98	0.46
1:C:780:LEU:HD23	1:C:780:LEU:C	2.36	0.46
2:B:98:ARG:HB2	2:B:386:PRO:HG3	1.98	0.46
1:A:25:TYR:CG	1:A:26:ALA:N	2.83	0.46
2:D:212:GLU:HG2	2:D:243:ASP:CB	2.45	0.46
2:D:508:TYR:CZ	2:D:514:CYS:HB3	2.51	0.46
1:A:490:VAL:HG12	1:A:491:LEU:CA	2.46	0.46
1:A:456:LEU:HA	1:A:477:PRO:HA	1.97	0.46
1:A:333:ALA:HA	1:A:352:GLY:H	1.80	0.46
1:A:908:VAL:HG13	1:A:1069:PHE:HB3	1.96	0.46
1:A:908:VAL:O	1:A:938:VAL:HG23	2.15	0.46
2:B:155:LEU:HB2	2:B:156:PRO:CA	2.38	0.46
1:C:490:VAL:HG12	1:C:491:LEU:CA	2.46	0.46
1:A:478:LEU:HA	1:A:485:TRP:HE1	1.81	0.46
1:C:961:GLU:HG2	1:C:1036:TRP:HA	1.97	0.46
1:C:25:TYR:CG	1:C:26:ALA:N	2.84	0.46
2:B:186:LEU:HD21	2:B:198:GLU:CB	2.46	0.46
1:A:874:ARG:NH2	1:C:894:THR:O	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:790:ASN:O	1:A:854:GLY:HA2	2.16	0.46
2:D:120:ASP:OD1	2:D:325:GLU:O	2.33	0.46
1:A:827:LEU:HD13	1:A:829:CYS:SG	2.56	0.46
1:C:670:ARG:HG2	1:C:711:ILE:CG2	2.46	0.46
2:B:468:SER:HB2	2:B:471:LEU:CG	2.46	0.46
1:C:831:SER:HB3	1:C:842:THR:HG22	1.98	0.46
2:D:382:GLN:HG3	2:D:383:ILE:H	1.79	0.46
1:C:333:ALA:HA	1:C:352:GLY:H	1.81	0.46
1:A:894:THR:O	1:C:874:ARG:NH2	2.49	0.46
1:C:878:THR:HG22	1:C:896:GLN:HB3	1.97	0.46
1:C:445:SER:HB2	1:C:454:THR:HG21	1.97	0.46
1:C:840:TRP:CD1	1:C:840:TRP:N	2.84	0.46
1:A:446:VAL:CG1	1:A:456:LEU:HD11	2.46	0.46
1:A:780:LEU:HD23	1:A:780:LEU:C	2.36	0.46
2:B:270:LEU:HD23	2:B:271:TYR:O	2.16	0.46
1:C:506:LEU:HA	1:C:569:LEU:HD11	1.97	0.46
1:C:631:VAL:HG11	1:C:746:LEU:HD11	1.98	0.46
1:A:886:ASN:O	1:A:888:PRO:HD3	2.15	0.46
1:C:676:THR:HG23	1:C:678:ASN:H	1.81	0.46
1:A:766:PHE:CE2	1:A:895:PHE:HD2	2.34	0.46
2:D:461:CYS:SG	2:D:466:ARG:CD	3.04	0.46
1:C:1063:LEU:HD12	1:C:1064:PRO:CB	2.46	0.46
4:A:3373:NAG:H3	4:A:3374:NAG:N2	2.31	0.46
1:A:465:TYR:HB3	1:A:469:ARG:HG2	1.97	0.46
1:A:1065:GLY:O	1:A:1066:GLN:HG3	2.16	0.46
1:A:506:LEU:HA	1:A:569:LEU:HD11	1.97	0.46
2:B:212:GLU:HG2	2:B:243:ASP:CB	2.46	0.46
1:A:670:ARG:HG2	1:A:711:ILE:CG2	2.46	0.46
1:C:771:LEU:HD11	1:C:774:LEU:HB2	1.97	0.46
1:C:634:ASN:HB2	1:C:695:ASN:HB3	1.97	0.46
1:A:756:HIS:HA	1:C:1052:GLU:OE1	2.16	0.45
1:C:456:LEU:HA	1:C:477:PRO:HA	1.97	0.45
1:A:73:LEU:HA	1:A:90:GLY:HA2	1.98	0.45
2:D:562:ASN:OD1	2:D:564:ARG:HB2	2.16	0.45
1:C:465:TYR:HB3	1:C:469:ARG:HG2	1.98	0.45
1:A:917:LYS:HE3	1:A:1077:VAL:HG23	1.98	0.45
1:C:698:LEU:N	1:C:698:LEU:HD12	2.31	0.45
2:D:362:SER:HB2	2:D:370:HIS:HB2	1.98	0.45
2:D:345:VAL:HG11	2:D:387:ILE:HD11	1.98	0.45
1:C:766:PHE:C	1:C:766:PHE:CD1	2.89	0.45
1:C:110:LEU:HD12	1:C:110:LEU:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:416:ILE:HG22	1:C:427:LYS:HD3	1.98	0.45
2:D:143:ARG:C	2:D:144:ILE:HD12	2.37	0.45
6:C:3716:NAG:H82	6:C:3716:NAG:H3	1.88	0.45
1:A:395:TRP:HH2	1:A:480:ARG:CG	2.29	0.45
1:A:376:GLN:HB2	4:A:3373:NAG:O4	2.16	0.45
2:D:616:PRO:HB3	2:D:621:CYS:SG	2.56	0.45
1:C:766:PHE:CE2	1:C:895:PHE:HD2	2.34	0.45
1:C:959:ASN:O	1:C:960:GLN:HB3	2.17	0.45
2:B:169:CYS:HB2	2:B:173:GLU:HA	1.98	0.45
1:C:353:SER:C	1:C:354:PHE:CG	2.90	0.45
1:A:676:THR:HG23	1:A:678:ASN:H	1.81	0.45
2:D:643:ARG:NH2	2:D:649:TRP:HZ2	2.14	0.45
1:C:25:TYR:CE1	1:C:86:LEU:HB2	2.51	0.45
1:C:1020:VAL:O	1:C:1021:GLN:CB	2.65	0.45
1:A:25:TYR:HD2	1:A:29:TRP:HB2	1.81	0.45
1:A:342:THR:OG1	1:A:343:PRO:HD2	2.16	0.45
1:C:790:ASN:O	1:C:854:GLY:HA2	2.16	0.45
2:B:362:SER:HB2	2:B:370:HIS:HB2	1.98	0.45
1:A:980:SER:HB3	1:A:1012:ARG:HB3	1.98	0.45
1:C:823:ARG:NH1	1:C:860:LEU:O	2.49	0.45
1:A:961:GLU:HG2	1:A:1036:TRP:HA	1.97	0.45
1:A:663:ASP:HB3	1:A:666:ARG:HD3	1.97	0.45
1:A:799:THR:HA	1:A:845:ARG:HA	1.99	0.45
1:A:897:LEU:HD12	1:A:897:LEU:C	2.37	0.45
1:A:819:GLN:HA	1:A:820:GLY:HA2	1.78	0.45
1:A:721:GLY:O	1:A:723:PRO:HD3	2.16	0.45
2:D:428:ARG:NH1	2:D:428:ARG:HG3	2.32	0.45
1:A:565:PHE:HB2	1:A:587:ALA:CB	2.46	0.45
1:A:764:ILE:HD12	1:A:800:ILE:HD13	1.98	0.45
1:A:800:ILE:HD12	1:A:880:ASN:O	2.17	0.45
2:B:345:VAL:HG11	2:B:387:ILE:HD11	1.99	0.45
1:C:970:SER:O	1:C:1026:PHE:HB2	2.16	0.45
1:C:1048:VAL:HG22	1:C:1075:THR:HB	1.99	0.45
2:B:472:GLU:HA	2:B:475:CYS:CB	2.46	0.45
1:C:71:MET:O	1:C:72:SER:C	2.54	0.45
1:A:25:TYR:O	1:A:26:ALA:C	2.54	0.45
1:A:444:CYS:CB	1:A:506:LEU:CD1	2.94	0.45
2:D:186:LEU:HD21	2:D:198:GLU:CB	2.46	0.45
2:B:223:ALA:HB1	2:B:263:ARG:HA	1.97	0.45
2:B:644:ASP:HB3	2:B:650:VAL:HG23	1.98	0.45
1:A:959:ASN:O	1:A:960:GLN:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1063:LEU:N	1:A:1064:PRO:CD	2.80	0.45
1:C:430:VAL:HG23	1:C:430:VAL:O	2.17	0.45
1:A:797:GLY:N	1:A:884:GLU:HB2	2.32	0.45
1:C:25:TYR:OH	1:C:111:GLY:HA2	2.16	0.45
1:C:31:VAL:HG21	1:C:86:LEU:CD1	2.47	0.45
1:C:800:ILE:HD12	1:C:880:ASN:O	2.16	0.45
1:C:880:ASN:OD1	1:C:894:THR:HG22	2.17	0.45
2:D:109:TYR:CE2	2:D:111:MET:HB2	2.52	0.45
2:D:305:VAL:HG13	2:D:306:LYS:N	2.32	0.45
2:D:256:ILE:O	2:D:256:ILE:HG13	2.17	0.45
1:C:73:LEU:HA	1:C:90:GLY:HA2	1.98	0.45
2:D:169:CYS:HB2	2:D:173:GLU:HA	1.98	0.45
2:D:118:LEU:HD21	2:D:204:ILE:HD13	1.99	0.45
4:C:3375:MAN:O2	4:C:3376:MAN:C1	2.65	0.45
1:C:20:ASP:CG	2:D:257:LEU:HD22	2.38	0.45
1:A:987:PRO:HA	1:C:619:GLU:OE1	2.16	0.45
2:B:599:PRO:O	2:B:603:TYR:CD2	2.70	0.45
2:D:6:PHE:CD2	2:D:7:LYS:N	2.85	0.45
1:C:764:ILE:HD12	1:C:800:ILE:HD13	1.99	0.45
1:C:897:LEU:HD12	1:C:897:LEU:C	2.38	0.45
2:B:630:LEU:HD12	2:B:665:ILE:HB	1.98	0.45
1:A:352:GLY:HA2	1:A:356:TRP:HA	1.99	0.45
1:C:908:VAL:HG12	1:C:909:VAL:N	2.32	0.45
1:A:634:ASN:HB2	1:A:695:ASN:HB3	1.98	0.45
1:C:342:THR:OG1	1:C:343:PRO:HD2	2.17	0.45
2:B:305:VAL:HG13	2:B:306:LYS:N	2.31	0.45
1:C:624:VAL:HG12	1:C:625:VAL:HG22	1.99	0.44
2:B:643:ARG:NH2	2:B:649:TRP:HZ2	2.15	0.44
2:B:118:LEU:HD21	2:B:204:ILE:HD13	1.99	0.44
2:D:285:LEU:C	2:D:287:HIS:N	2.71	0.44
1:A:748:PHE:CD1	1:A:748:PHE:N	2.84	0.44
2:B:83:LEU:O	2:B:83:LEU:HD12	2.16	0.44
2:B:437:CYS:HB3	2:B:459:CYS:SG	2.58	0.44
2:B:6:PHE:CD2	2:B:7:LYS:N	2.85	0.44
1:A:631:VAL:HG11	1:A:746:LEU:CD1	2.47	0.44
1:A:827:LEU:HD12	1:A:827:LEU:O	2.16	0.44
1:C:621:ARG:CG	1:C:622:GLU:H	2.30	0.44
1:A:374:MET:SD	1:A:417:PHE:CZ	3.10	0.44
1:C:1020:VAL:O	1:C:1021:GLN:HB2	2.16	0.44
2:D:222:ALA:HB2	2:D:294:ILE:CD1	2.47	0.44
1:A:762:LEU:HD23	1:A:790:ASN:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:790:ASN:O	1:C:853:GLY:O	2.35	0.44
1:C:980:SER:HB3	1:C:1012:ARG:HB3	2.00	0.44
1:C:418:THR:HB	1:C:427:LYS:CG	2.47	0.44
2:D:149:PHE:HA	2:D:181:ALA:O	2.17	0.44
1:A:1053:ILE:CG2	1:A:1070:MET:CB	2.95	0.44
1:C:25:TYR:HD2	1:C:29:TRP:HB2	1.83	0.44
2:D:75:GLN:O	2:D:97:PHE:CD1	2.71	0.44
1:C:419:GLN:CG	1:C:424:TRP:CD1	3.00	0.44
1:A:764:ILE:CD1	1:A:800:ILE:CD1	2.95	0.44
2:B:334:ILE:HA	2:B:337:ALA:CB	2.48	0.44
1:A:348:LEU:N	1:A:348:LEU:HD12	2.32	0.44
2:B:569:SER:HB2	2:B:590:CYS:O	2.18	0.44
2:B:154:VAL:HA	2:B:160:THR:CG2	2.46	0.44
1:A:1052:GLU:OE2	1:C:757:ILE:HB	2.17	0.44
6:A:3880:NAG:H82	6:A:3880:NAG:O3	2.17	0.44
1:C:477:PRO:HG2	1:C:489:ALA:HB2	1.99	0.44
2:D:273:ARG:O	2:D:277:PHE:HB3	2.18	0.44
1:C:1065:GLY:O	1:C:1066:GLN:HG3	2.17	0.44
2:D:361:ASP:HB2	2:D:390:GLN:HB3	1.98	0.44
1:A:22:VAL:HG22	1:A:23:VAL:N	2.32	0.44
2:D:639:THR:HG23	2:D:639:THR:O	2.18	0.44
1:A:1048:VAL:HG22	1:A:1075:THR:HB	1.99	0.44
2:B:543:HIS:HB3	2:B:544:PRO:HD2	1.99	0.44
2:D:543:HIS:HB3	2:D:544:PRO:HD2	1.99	0.44
1:A:513:ASN:HA	1:A:599:VAL:HG21	2.00	0.44
2:D:139:THR:HG22	2:D:140:GLU:N	2.33	0.44
1:A:93:VAL:HB	1:A:104:THR:HG22	2.00	0.44
1:C:873:ASP:O	1:C:901:VAL:HG12	2.17	0.44
2:B:479:ASN:N	2:B:479:ASN:OD1	2.43	0.44
1:A:430:VAL:HG22	1:A:485:TRP:HZ3	1.83	0.44
1:C:25:TYR:O	1:C:26:ALA:C	2.55	0.44
2:B:75:GLN:O	2:B:97:PHE:CD1	2.71	0.44
1:A:25:TYR:OH	1:A:111:GLY:HA2	2.17	0.44
2:B:222:ALA:HB2	2:B:294:ILE:CD1	2.48	0.44
1:C:631:VAL:HG11	1:C:746:LEU:CD1	2.48	0.44
2:D:27:LEU:HG	2:D:446:GLY:HA2	2.00	0.44
1:C:107:CYS:SG	1:C:348:LEU:HD21	2.58	0.44
1:C:348:LEU:HD12	1:C:348:LEU:N	2.32	0.44
1:A:771:LEU:HD11	1:A:774:LEU:HB2	1.99	0.44
1:C:73:LEU:C	1:C:73:LEU:HD12	2.38	0.44
1:A:812:TYR:HE2	1:A:814:ALA:CB	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:873:ASP:O	1:A:901:VAL:HG12	2.17	0.44
2:B:665:ILE:HD12	2:B:665:ILE:N	2.33	0.44
1:A:848:HIS:ND1	1:A:848:HIS:O	2.50	0.44
2:D:479:ASN:OD1	2:D:479:ASN:N	2.41	0.44
2:D:569:SER:HB2	2:D:590:CYS:O	2.17	0.44
2:B:109:TYR:CE2	2:B:111:MET:HB2	2.52	0.44
1:A:1063:LEU:HG	1:A:1064:PRO:HD3	2.00	0.44
2:B:285:LEU:C	2:B:287:HIS:N	2.71	0.44
1:C:25:TYR:CD1	1:C:86:LEU:HB2	2.53	0.44
1:C:352:GLY:HA2	1:C:356:TRP:HA	1.99	0.44
2:D:83:LEU:O	2:D:83:LEU:HD12	2.18	0.44
2:D:144:ILE:HG22	2:D:195:PHE:CZ	2.53	0.44
1:C:876:LEU:HB3	1:C:898:GLU:HG3	2.00	0.44
2:B:169:CYS:CB	2:B:173:GLU:HA	2.48	0.44
1:A:87:LEU:HD21	1:A:348:LEU:HD11	1.98	0.44
1:C:87:LEU:HD21	1:C:348:LEU:HD11	1.99	0.44
2:B:219:MET:HE2	2:B:262:GLY:HA2	2.00	0.44
1:A:1001:LEU:O	1:A:1001:LEU:HD23	2.17	0.44
1:C:560:SER:O	1:C:561:ARG:HG2	2.18	0.44
1:C:813:VAL:CG2	1:C:823:ARG:NH1	2.81	0.44
4:A:3374:NAG:C3	4:A:3375:MAN:H2	2.47	0.44
2:B:149:PHE:HA	2:B:181:ALA:O	2.18	0.44
1:C:650:ARG:HD3	1:C:729:ASN:CB	2.48	0.44
1:A:31:VAL:HG21	1:A:86:LEU:CD1	2.48	0.44
1:C:507:THR:HG22	1:C:569:LEU:CD1	2.48	0.44
1:C:420:VAL:HG12	1:C:421:SER:N	2.32	0.44
1:C:764:ILE:CD1	1:C:800:ILE:CD1	2.96	0.44
1:A:741:TYR:CD2	2:B:502:VAL:HG22	2.52	0.44
2:D:437:CYS:O	2:D:438:HIS:CB	2.66	0.43
2:D:437:CYS:SG	2:D:448:CYS:CB	3.05	0.43
1:A:786:VAL:CG1	1:A:859:PHE:CZ	2.99	0.43
1:A:73:LEU:C	1:A:73:LEU:HD12	2.39	0.43
1:C:1053:ILE:HG22	1:C:1070:MET:CB	2.48	0.43
2:D:270:LEU:HD23	2:D:271:TYR:O	2.17	0.43
2:B:87:PRO:HD3	2:B:423:CYS:SG	2.59	0.43
2:D:237:LEU:HD13	2:D:294:ILE:HG23	2.00	0.43
2:D:432:ARG:HD3	2:D:433:ASP:H	1.83	0.43
1:A:419:GLN:CG	1:A:424:TRP:CD1	3.00	0.43
1:A:671:ALA:HB2	1:A:700:LEU:HD23	2.00	0.43
2:B:352:LEU:CD2	2:B:358:VAL:HG23	2.48	0.43
1:A:484:ARG:NH1	2:B:586:GLN:CB	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:815:GLU:HB3	1:A:819:GLN:NE2	2.33	0.43
2:D:169:CYS:CB	2:D:173:GLU:HA	2.48	0.43
1:A:658:LEU:O	1:A:659:ASP:OD1	2.36	0.43
2:D:132:LEU:HA	2:D:135:LEU:HB3	1.99	0.43
2:D:105:ILE:HG21	2:D:135:LEU:CD1	2.48	0.43
2:B:340:LYS:HA	2:B:343:SER:HB2	1.98	0.43
2:D:304:MET:HE3	2:D:307:THR:HG21	2.00	0.43
1:C:22:VAL:HG22	1:C:23:VAL:N	2.33	0.43
1:A:68:ALA:HA	1:A:93:VAL:HG13	1.99	0.43
1:C:907:THR:HG21	1:C:1053:ILE:HD13	2.00	0.43
2:D:665:ILE:HD12	2:D:665:ILE:N	2.33	0.43
1:A:525:PRO:HA	1:A:532:GLY:HA2	1.99	0.43
2:B:132:LEU:HA	2:B:135:LEU:HB3	1.99	0.43
1:A:107:CYS:SG	1:A:348:LEU:HD21	2.58	0.43
2:B:361:ASP:HB2	2:B:390:GLN:HB3	1.99	0.43
1:A:893:THR:O	1:A:893:THR:HG23	2.18	0.43
1:C:658:LEU:O	1:C:659:ASP:OD1	2.37	0.43
1:C:739:GLN:HB2	1:C:742:PHE:CE1	2.52	0.43
2:D:87:PRO:HD3	2:D:423:CYS:SG	2.59	0.43
2:D:285:LEU:O	2:D:287:HIS:N	2.51	0.43
1:C:20:ASP:OD2	2:D:257:LEU:HD22	2.18	0.43
1:C:1003:CYS:HB3	1:C:1008:CYS:HB2	1.88	0.43
1:A:649:SER:O	1:A:650:ARG:CB	2.67	0.43
2:B:273:ARG:O	2:B:277:PHE:HB3	2.18	0.43
2:D:98:ARG:HB2	2:D:386:PRO:HG3	1.99	0.43
1:A:25:TYR:CD1	1:A:86:LEU:HB2	2.53	0.43
1:A:420:VAL:HG12	1:A:421:SER:N	2.32	0.43
1:C:848:HIS:HB2	2:D:485:SER:HB3	2.01	0.43
1:A:801:THR:HG22	1:A:843:SER:CB	2.49	0.43
1:A:13:VAL:HG21	1:A:57:CYS:HB2	2.01	0.43
1:C:1001:LEU:O	1:C:1001:LEU:HD23	2.18	0.43
2:D:532:ARG:O	2:D:543:HIS:HB2	2.19	0.43
1:C:4:ASP:HB2	1:C:597:ARG:CZ	2.49	0.43
1:A:71:MET:O	1:A:72:SER:C	2.55	0.43
1:A:934:HIS:ND1	1:A:1074:THR:HB	2.33	0.43
1:A:619:GLU:O	1:A:620:CYS:SG	2.76	0.43
1:A:560:SER:O	1:A:561:ARG:HG2	2.18	0.43
2:D:601:GLY:O	2:D:602:LYS:HB2	2.19	0.43
2:D:631:SER:HB3	2:D:664:LEU:HD11	2.01	0.43
1:A:600:LEU:O	1:A:600:LEU:HD12	2.17	0.43
1:C:992:LEU:HD23	1:C:992:LEU:C	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:120:ASP:OD1	2:B:325:GLU:O	2.36	0.43
1:A:93:VAL:HB	1:A:104:THR:HG23	2.01	0.43
1:C:757:ILE:O	1:C:758:CYS:HB2	2.19	0.43
2:D:118:LEU:HD21	2:D:204:ILE:CD1	2.48	0.43
1:A:650:ARG:HD3	1:A:729:ASN:CB	2.48	0.43
2:B:105:ILE:HG21	2:B:135:LEU:CD1	2.48	0.43
1:C:848:HIS:O	1:C:848:HIS:ND1	2.51	0.43
1:A:711:ILE:HD11	1:A:746:LEU:HD13	2.00	0.43
1:A:827:LEU:CD1	1:A:829:CYS:SG	3.07	0.43
1:C:762:LEU:HD23	1:C:790:ASN:HA	1.99	0.43
1:C:41:ALA:O	1:C:42:ASN:C	2.57	0.43
1:A:41:ALA:O	1:A:42:ASN:C	2.56	0.43
2:D:334:ILE:HA	2:D:337:ALA:CB	2.49	0.43
2:D:352:LEU:CD2	2:D:358:VAL:HG23	2.48	0.43
1:A:69:VAL:HG12	1:A:70:ASN:N	2.34	0.43
2:D:643:ARG:CZ	2:D:649:TRP:CZ2	3.02	0.43
1:C:478:LEU:HA	1:C:485:TRP:HE1	1.83	0.43
2:B:652:TYR:HB3	2:B:667:VAL:HA	1.99	0.43
1:A:372:ILE:O	1:A:372:ILE:HG13	2.19	0.43
2:B:639:THR:HG23	2:B:639:THR:O	2.19	0.43
1:C:13:VAL:HG21	1:C:57:CYS:HB2	2.01	0.43
2:D:154:VAL:HG22	2:D:155:LEU:N	2.34	0.43
2:B:154:VAL:HG22	2:B:155:LEU:N	2.34	0.43
1:A:374:MET:SD	1:A:417:PHE:CE2	3.12	0.43
1:C:944:ARG:N	1:C:1020:VAL:HG21	2.34	0.43
1:C:671:ALA:HB2	1:C:700:LEU:HD23	2.01	0.43
2:B:188:LEU:HD12	2:B:230:TRP:HA	2.00	0.43
1:C:69:VAL:HG12	1:C:70:ASN:N	2.34	0.43
1:C:621:ARG:CG	1:C:622:GLU:N	2.82	0.43
1:C:757:ILE:HD12	1:C:757:ILE:HA	1.91	0.43
1:A:739:GLN:HB2	1:A:742:PHE:CE1	2.53	0.43
1:C:609:ILE:CD1	1:C:632:GLN:OE1	2.66	0.43
1:C:402:VAL:HG12	1:C:443:LEU:HD22	2.01	0.43
1:A:566:GLY:O	1:A:567:GLN:C	2.56	0.43
1:A:575:LEU:HD12	1:A:576:THR:HG23	1.99	0.43
2:D:75:GLN:O	2:D:97:PHE:HA	2.19	0.43
2:D:363:PHE:HB2	2:D:388:THR:HB	2.00	0.43
1:A:507:THR:HG22	1:A:569:LEU:CD1	2.48	0.43
1:C:392:LEU:HG	1:C:393:ALA:N	2.34	0.43
2:B:508:TYR:CZ	2:B:514:CYS:HB3	2.54	0.43
1:A:99:ARG:HG3	1:A:100:ASN:OD1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:LEU:HG	1:A:393:ALA:N	2.33	0.43
1:C:827:LEU:HD13	1:C:829:CYS:SG	2.58	0.43
6:C:3716:NAG:O3	6:C:3717:NAG:H2	2.19	0.43
1:A:353:SER:C	1:A:354:PHE:CG	2.91	0.43
1:C:404:GLY:O	1:C:406:PRO:HD3	2.19	0.43
1:C:786:VAL:CG1	1:C:859:PHE:CZ	2.99	0.43
1:A:418:THR:HB	1:A:427:LYS:CG	2.48	0.43
1:A:919:LEU:HG	2:B:643:ARG:CZ	2.49	0.43
2:B:118:LEU:HD21	2:B:204:ILE:CD1	2.49	0.43
1:C:525:PRO:HA	1:C:532:GLY:HA2	2.00	0.43
1:C:1023:GLU:O	1:C:1024:LEU:C	2.57	0.43
2:B:120:ASP:O	2:B:124:VAL:HB	2.18	0.43
2:B:234:THR:HG22	2:B:235:ARG:N	2.34	0.43
2:D:652:TYR:HB3	2:D:667:VAL:HA	2.00	0.43
1:C:594:LEU:HD12	1:C:594:LEU:N	2.34	0.43
2:B:108:TYR:CE2	2:B:147:GLY:HA3	2.54	0.43
1:C:609:ILE:HB	1:C:610:PRO:CD	2.46	0.42
4:A:3375:MAN:O2	4:A:3376:MAN:C1	2.66	0.42
1:C:797:GLY:H	1:C:884:GLU:HB2	1.84	0.42
1:C:797:GLY:N	1:C:884:GLU:HB2	2.33	0.42
1:A:660:LEU:CD2	1:A:715:LEU:HB3	2.49	0.42
1:C:575:LEU:CD1	1:C:576:THR:HG23	2.49	0.42
1:C:534:VAL:HG23	1:C:565:PHE:CZ	2.54	0.42
2:B:144:ILE:HG22	2:B:195:PHE:CZ	2.53	0.42
2:D:432:ARG:HG2	2:D:432:ARG:NH1	2.34	0.42
2:D:120:ASP:O	2:D:124:VAL:HB	2.19	0.42
1:A:766:PHE:CZ	1:A:877:LEU:HD12	2.54	0.42
1:A:620:CYS:HB3	1:A:702:SER:O	2.19	0.42
2:B:601:GLY:O	2:B:602:LYS:HB2	2.19	0.42
2:D:219:MET:HE2	2:D:262:GLY:HA2	2.01	0.42
2:D:108:TYR:CE2	2:D:147:GLY:HA3	2.54	0.42
1:A:1018:PHE:O	1:A:1019:SER:C	2.57	0.42
1:C:1018:PHE:O	1:C:1019:SER:C	2.55	0.42
1:C:659:ASP:OD2	6:C:3716:NAG:H82	2.11	0.42
1:C:812:TYR:HD2	1:C:814:ALA:HB2	1.81	0.42
2:B:139:THR:HG22	2:B:140:GLU:N	2.34	0.42
1:A:905:VAL:O	1:A:1062:GLN:HG3	2.18	0.42
1:A:790:ASN:O	1:A:853:GLY:O	2.37	0.42
2:D:611:LYS:HG2	2:D:667:VAL:HB	2.01	0.42
2:D:473:GLY:C	2:D:475:CYS:H	2.22	0.42
2:B:631:SER:HB3	2:B:664:LEU:HD11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:799:THR:HA	1:C:845:ARG:HA	2.00	0.42
1:A:477:PRO:C	1:A:479:PRO:HD3	2.40	0.42
1:C:660:LEU:CD2	1:C:715:LEU:HB3	2.49	0.42
1:C:1009:LEU:HD22	1:C:1011:PHE:CE1	2.54	0.42
1:A:1009:LEU:HD22	1:A:1011:PHE:CE1	2.54	0.42
1:A:444:CYS:HB2	1:A:506:LEU:HD12	2.02	0.42
1:C:444:CYS:CB	1:C:506:LEU:CD1	2.96	0.42
1:A:908:VAL:HG12	1:A:909:VAL:N	2.33	0.42
1:C:527:GLU:HG3	1:C:533:ALA:CB	2.50	0.42
2:D:438:HIS:ND1	2:D:460:GLU:HA	2.34	0.42
1:C:93:VAL:HB	1:C:104:THR:HG22	2.02	0.42
1:C:68:ALA:HA	1:C:93:VAL:HG13	2.01	0.42
1:C:813:VAL:HG23	1:C:823:ARG:HH12	1.84	0.42
1:C:407:ARG:HG2	2:D:247:PHE:CZ	2.54	0.42
1:C:459:ILE:HD12	1:C:487:CYS:SG	2.60	0.42
2:B:98:ARG:HD2	2:B:384:ASN:OD1	2.19	0.42
2:B:611:LYS:HG2	2:B:667:VAL:HB	2.01	0.42
1:A:594:LEU:HD12	1:A:594:LEU:N	2.35	0.42
2:D:428:ARG:HH11	2:D:428:ARG:HG3	1.84	0.42
1:A:491:LEU:HD21	1:A:545:ILE:HG12	2.02	0.42
1:A:797:GLY:H	1:A:884:GLU:HB2	1.85	0.42
1:A:446:VAL:HG12	1:A:456:LEU:HD11	2.01	0.42
2:B:643:ARG:CZ	2:B:649:TRP:CZ2	3.02	0.42
2:B:176:CYS:HB2	2:B:204:ILE:O	2.19	0.42
2:B:285:LEU:O	2:B:287:HIS:N	2.52	0.42
1:A:351:VAL:HG23	1:A:352:GLY:N	2.35	0.42
1:A:876:LEU:HB3	1:A:898:GLU:HG3	2.01	0.42
1:A:1058:SER:O	1:A:1059:VAL:CB	2.67	0.42
1:A:1023:GLU:O	1:A:1024:LEU:C	2.58	0.42
1:A:564:TYR:CZ	1:A:588:ARG:HD2	2.53	0.42
1:C:372:ILE:O	1:C:372:ILE:HG13	2.19	0.42
1:A:402:VAL:HG12	1:A:443:LEU:HD22	2.02	0.42
1:C:446:VAL:HG12	1:C:456:LEU:HD11	2.00	0.42
1:C:374:MET:SD	1:C:417:PHE:CZ	3.12	0.42
1:A:534:VAL:HG23	1:A:565:PHE:CZ	2.54	0.42
1:C:351:VAL:HG23	1:C:352:GLY:N	2.34	0.42
1:C:102:TYR:CG	1:C:331:GLU:HB3	2.55	0.42
1:C:801:THR:HG22	1:C:843:SER:CB	2.49	0.42
1:C:893:THR:HG23	1:C:893:THR:O	2.20	0.42
2:D:188:LEU:HD12	2:D:230:TRP:HA	2.01	0.42
1:C:93:VAL:HB	1:C:104:THR:HG23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:609:ILE:CD1	1:A:632:GLN:OE1	2.67	0.42
1:C:772:LYS:O	1:C:773:SER:CB	2.68	0.42
1:C:597:ARG:HA	1:C:598:PRO:HD3	1.90	0.42
2:D:315:ILE:HA	2:D:316:PRO:HD3	1.87	0.42
2:D:186:LEU:HD21	2:D:198:GLU:HB2	2.02	0.42
2:B:237:LEU:HD13	2:B:294:ILE:HG23	2.01	0.42
2:D:27:LEU:CD2	2:D:446:GLY:HA2	2.50	0.42
2:B:219:MET:CE	2:B:262:GLY:HA2	2.50	0.42
2:D:234:THR:HG22	2:D:235:ARG:N	2.34	0.42
2:B:74:LYS:HD2	2:B:103:TYR:OH	2.20	0.42
1:C:385:TYR:CE2	1:C:407:ARG:HD3	2.55	0.42
2:D:532:ARG:HD3	2:D:554:GLU:HG3	2.02	0.42
1:C:614:PRO:O	1:C:615:ARG:HB3	2.20	0.42
1:C:905:VAL:O	1:C:1062:GLN:HG3	2.20	0.42
1:A:1023:GLU:HG2	1:A:1023:GLU:O	2.19	0.42
2:D:27:LEU:HD21	2:D:446:GLY:HA2	2.02	0.42
1:A:975:PRO:HG2	1:A:977:LEU:HD11	2.02	0.42
1:C:916:THR:O	1:C:1076:THR:HG23	2.20	0.42
1:C:717:PHE:CE1	1:C:740:ARG:HA	2.55	0.42
1:C:811:ARG:O	1:C:811:ARG:HG3	2.19	0.42
1:A:384:SER:HB2	1:A:405:ALA:HB1	2.02	0.42
2:B:155:LEU:HD12	2:B:155:LEU:C	2.40	0.42
2:B:215:LEU:HD12	2:B:246:HIS:O	2.19	0.42
2:D:215:LEU:HD12	2:D:246:HIS:O	2.20	0.42
1:C:491:LEU:HD21	1:C:545:ILE:HG12	2.01	0.42
1:A:918:TYR:O	1:A:919:LEU:C	2.58	0.42
1:A:614:PRO:O	1:A:615:ARG:HB3	2.19	0.42
1:A:660:LEU:HB3	1:A:713:LEU:HD21	2.01	0.42
4:C:3373:NAG:O3	4:C:3374:NAG:C7	2.68	0.42
2:D:265:HIS:HB2	2:D:273:ARG:HG3	2.01	0.42
1:C:915:PHE:CZ	1:C:917:LYS:HB2	2.55	0.42
2:B:186:LEU:HD21	2:B:198:GLU:HB2	2.02	0.42
2:B:234:THR:CG2	2:B:236:LEU:HD13	2.50	0.42
1:C:827:LEU:HD12	1:C:827:LEU:O	2.19	0.42
1:C:799:THR:HG22	1:C:845:ARG:HB3	2.02	0.42
1:A:102:TYR:CG	1:A:331:GLU:HB3	2.54	0.42
1:A:437:SER:HA	1:A:463:HIS:O	2.20	0.42
1:A:860:LEU:HD23	1:A:861:ALA:N	2.34	0.42
2:B:484:CYS:HB2	2:B:488:GLY:O	2.19	0.42
1:C:1063:LEU:N	1:C:1064:PRO:CD	2.83	0.42
1:A:772:LYS:O	1:A:773:SER:CB	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:3374:NAG:C3	4:C:3375:MAN:H2	2.49	0.42
2:B:363:PHE:HB2	2:B:388:THR:HB	2.01	0.42
1:A:656:VAL:HG21	1:A:687:LEU:HD12	2.01	0.42
1:A:435:ILE:HD13	2:B:311:LEU:HB2	2.02	0.42
1:A:799:THR:HG22	1:A:845:ARG:HB3	2.02	0.42
1:C:484:ARG:NH1	2:D:586:GLN:HG3	2.35	0.42
1:A:930:HIS:O	1:A:931:VAL:C	2.58	0.42
2:D:429:ASP:HB2	2:D:430:GLN:H	1.66	0.41
1:A:327:SER:O	1:A:328:PHE:O	2.38	0.41
1:C:721:GLY:O	1:C:722:LYS:HB2	2.19	0.41
1:A:721:GLY:O	1:A:722:LYS:HB2	2.19	0.41
1:C:613:ILE:HA	1:C:614:PRO:HD3	1.86	0.41
1:A:71:MET:HA	1:A:92:THR:C	2.40	0.41
1:A:433:THR:HG23	1:A:464:TYR:CE1	2.55	0.41
1:A:956:VAL:O	1:A:963:VAL:HG23	2.20	0.41
1:A:944:ARG:N	1:A:1020:VAL:HG21	2.34	0.41
1:A:385:TYR:CE2	1:A:407:ARG:HD3	2.55	0.41
2:B:611:LYS:CB	2:B:667:VAL:HB	2.50	0.41
2:B:17:SER:HB2	2:B:21:CYS:SG	2.60	0.41
1:C:99:ARG:HG3	1:C:100:ASN:OD1	2.20	0.41
1:C:499:TRP:CZ2	2:D:284:GLN:HG3	2.55	0.41
1:C:71:MET:HA	1:C:92:THR:C	2.40	0.41
2:B:587:LEU:N	2:B:587:LEU:CD1	2.83	0.41
2:B:75:GLN:O	2:B:97:PHE:HA	2.19	0.41
2:B:75:GLN:CD	2:B:98:ARG:O	2.58	0.41
1:A:25:TYR:HB3	1:A:29:TRP:O	2.19	0.41
1:A:444:CYS:HB3	1:A:506:LEU:HD13	2.01	0.41
1:C:444:CYS:HB3	1:C:506:LEU:HD13	2.02	0.41
1:A:698:LEU:C	1:A:699:LEU:HD12	2.41	0.41
1:A:800:ILE:HD11	1:A:879:ALA:HB1	2.02	0.41
1:A:766:PHE:CD1	1:A:766:PHE:C	2.93	0.41
2:B:188:LEU:CD1	2:B:230:TRP:HA	2.50	0.41
2:D:187:LYS:HG2	2:D:188:LEU:N	2.36	0.41
2:D:234:THR:CG2	2:D:236:LEU:HD13	2.51	0.41
2:D:484:CYS:HB2	2:D:488:GLY:O	2.20	0.41
1:A:533:ALA:HA	1:A:554:ALA:HA	2.02	0.41
1:C:433:THR:HG23	1:C:464:TYR:CE1	2.55	0.41
1:C:94:HIS:CD2	2:D:155:LEU:CD2	2.97	0.41
1:A:103:LEU:HD12	2:B:156:PRO:HB3	2.01	0.41
1:C:599:VAL:O	1:C:599:VAL:CG2	2.67	0.41
1:C:477:PRO:C	1:C:479:PRO:HD3	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:ASP:O	1:A:381:MET:HB3	2.20	0.41
1:C:566:GLY:O	1:C:567:GLN:C	2.59	0.41
1:A:1065:GLY:O	1:A:1066:GLN:CG	2.68	0.41
2:D:98:ARG:HD2	2:D:384:ASN:OD1	2.21	0.41
1:C:1075:THR:O	1:C:1075:THR:HG23	2.20	0.41
1:A:1075:THR:HG23	1:A:1075:THR:O	2.20	0.41
1:A:969:VAL:O	1:A:969:VAL:HG13	2.20	0.41
2:B:565:ARG:HA	2:B:565:ARG:HD3	1.84	0.41
1:C:384:SER:HB2	1:C:405:ALA:HB1	2.02	0.41
1:C:637:LEU:HD11	1:C:658:LEU:HD21	2.02	0.41
2:D:155:LEU:C	2:D:155:LEU:HD12	2.41	0.41
2:D:155:LEU:HB2	2:D:156:PRO:CA	2.39	0.41
2:B:27:LEU:CG	2:B:446:GLY:HA2	2.51	0.41
2:B:532:ARG:O	2:B:543:HIS:HB2	2.19	0.41
1:A:604:VAL:CG1	1:A:742:PHE:CD2	3.03	0.41
2:D:462:GLN:CG	2:D:463:THR:N	2.84	0.41
2:D:222:ALA:HB2	2:D:294:ILE:HD12	2.02	0.41
1:C:1023:GLU:O	1:C:1023:GLU:HG2	2.20	0.41
1:C:711:ILE:HD11	1:C:746:LEU:HD13	2.02	0.41
1:C:766:PHE:CZ	1:C:877:LEU:HD12	2.55	0.41
1:A:634:ASN:HA	1:A:695:ASN:HA	2.03	0.41
1:C:827:LEU:CD1	1:C:829:CYS:SG	3.08	0.41
2:D:611:LYS:CB	2:D:667:VAL:HB	2.51	0.41
2:D:517:ILE:HD12	2:D:518:ASN:N	2.35	0.41
2:D:438:HIS:CE1	2:D:460:GLU:CB	3.04	0.41
1:C:103:LEU:HD12	2:D:156:PRO:HB3	2.02	0.41
1:C:756:HIS:O	1:C:756:HIS:CG	2.74	0.41
2:D:75:GLN:CD	2:D:98:ARG:O	2.59	0.41
1:C:915:PHE:CD1	1:C:1074:THR:CG2	3.03	0.41
1:A:915:PHE:CZ	1:A:917:LYS:HB2	2.55	0.41
1:A:799:THR:HG22	1:A:845:ARG:CB	2.51	0.41
2:B:472:GLU:HA	2:B:475:CYS:HB3	2.02	0.41
2:B:101:LYS:HG2	2:B:102:GLY:H	1.85	0.41
1:A:916:THR:O	1:A:1076:THR:HG23	2.20	0.41
2:D:599:PRO:HB2	2:D:603:TYR:HE2	1.85	0.41
1:C:920:ASN:O	1:C:1080:LYS:HG2	2.20	0.41
1:C:831:SER:CA	1:C:842:THR:HG22	2.50	0.41
1:C:1065:GLY:O	1:C:1066:GLN:CG	2.69	0.41
2:D:98:ARG:HD3	2:D:386:PRO:HG3	2.02	0.41
1:C:649:SER:O	1:C:650:ARG:CB	2.68	0.41
1:C:1058:SER:O	1:C:1059:VAL:CB	2.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:671:ALA:O	1:C:672:THR:HG23	2.20	0.41
1:C:1040:ILE:CD1	1:C:1042:GLN:HB2	2.51	0.41
2:B:505:LYS:HA	2:B:517:ILE:HG21	2.02	0.41
1:C:543:PRO:O	1:C:544:SER:HB3	2.21	0.41
1:A:1045:VAL:HG22	1:A:1046:SER:N	2.35	0.41
1:A:610:PRO:O	1:A:611:ALA:C	2.58	0.41
2:B:98:ARG:HD3	2:B:386:PRO:HG3	2.02	0.41
2:D:352:LEU:HD22	2:D:358:VAL:HG23	2.03	0.41
2:B:187:LYS:HG2	2:B:188:LEU:N	2.36	0.41
2:D:652:TYR:CD2	2:D:652:TYR:O	2.74	0.41
1:A:624:VAL:HG23	1:A:625:VAL:H	1.86	0.41
2:D:74:LYS:NZ	2:D:103:TYR:HE2	2.18	0.41
1:C:492:TYR:CD2	1:C:492:TYR:O	2.74	0.41
2:D:176:CYS:HB2	2:D:204:ILE:O	2.21	0.41
1:A:464:TYR:O	1:A:465:TYR:HB3	2.21	0.41
1:C:713:LEU:C	1:C:713:LEU:HD23	2.41	0.41
2:D:161:HIS:HA	2:D:162:PRO:HA	1.81	0.41
1:A:915:PHE:CD1	1:A:1074:THR:CG2	3.04	0.41
1:C:533:ALA:HA	1:C:554:ALA:HA	2.03	0.41
1:A:527:GLU:HG3	1:A:533:ALA:CB	2.50	0.41
1:C:464:TYR:HD2	1:C:472:GLN:HB2	1.86	0.41
1:C:1045:VAL:HG22	1:C:1046:SER:N	2.36	0.41
1:A:717:PHE:CE1	1:A:740:ARG:HA	2.55	0.41
1:A:328:PHE:HB2	1:A:354:PHE:O	2.21	0.41
1:A:404:GLY:O	1:A:406:PRO:HD3	2.21	0.41
1:C:918:TYR:C	2:D:643:ARG:HH22	2.24	0.41
1:C:402:VAL:CG1	1:C:443:LEU:HD22	2.50	0.41
1:A:586:GLY:HA2	1:A:591:VAL:HG23	2.03	0.41
1:A:562:LEU:HD23	1:A:562:LEU:HA	1.84	0.41
1:A:599:VAL:CG2	1:A:599:VAL:O	2.68	0.41
1:C:941:LEU:CD1	1:C:941:LEU:N	2.84	0.41
1:A:713:LEU:HD23	1:A:713:LEU:C	2.41	0.41
1:C:374:MET:SD	1:C:417:PHE:CE2	3.14	0.41
1:A:831:SER:CA	1:A:842:THR:HG22	2.50	0.41
2:D:168:PRO:CG	2:D:179:PRO:HG3	2.51	0.41
1:A:534:VAL:HG23	1:A:565:PHE:CE2	2.56	0.41
1:C:648:GLY:O	1:C:649:SER:O	2.39	0.41
1:C:698:LEU:C	1:C:699:LEU:HD12	2.42	0.41
1:A:849:LEU:HA	2:B:482:ILE:HG22	2.03	0.41
1:C:444:CYS:HB2	1:C:506:LEU:HD12	2.03	0.41
1:A:946:LEU:HD12	1:A:946:LEU:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:305:VAL:HG13	2:B:306:LYS:HG3	2.02	0.41
1:C:975:PRO:HG2	1:C:977:LEU:HD11	2.02	0.41
2:D:293:ASN:OD1	2:D:412:THR:HG22	2.21	0.41
1:C:776:VAL:HG12	1:C:867:PRO:O	2.21	0.41
2:B:302:SER:HB3	2:B:322:GLU:CG	2.51	0.41
1:A:823:ARG:NH1	1:A:825:LEU:O	2.54	0.41
1:C:402:VAL:HG22	1:C:416:ILE:HG23	2.03	0.41
1:A:4:ASP:OD2	1:A:597:ARG:NH2	2.54	0.41
2:D:169:CYS:HA	2:D:170:PRO:HD3	1.84	0.41
2:D:260:ASN:OD1	2:D:260:ASN:C	2.60	0.41
2:D:181:ALA:HB3	2:D:271:TYR:CE2	2.56	0.41
2:B:265:HIS:HB2	2:B:273:ARG:HG3	2.02	0.41
2:D:110:LEU:CD1	2:D:218:MET:SD	3.09	0.41
2:B:352:LEU:HD22	2:B:358:VAL:HG23	2.03	0.41
1:C:824:SER:N	1:C:825:LEU:HG	2.34	0.40
1:A:459:ILE:HD12	1:A:487:CYS:SG	2.61	0.40
1:C:363:TYR:CD1	1:C:369:PRO:HB3	2.56	0.40
1:A:907:THR:HG21	1:A:1053:ILE:HD13	2.03	0.40
1:C:507:THR:HG21	1:C:570:SER:HA	2.03	0.40
2:D:368:VAL:HG11	2:D:370:HIS:ND1	2.36	0.40
1:C:593:LEU:C	1:C:594:LEU:HD12	2.41	0.40
2:D:230:TRP:CE3	2:D:235:ARG:HD3	2.57	0.40
1:C:930:HIS:O	1:C:931:VAL:C	2.58	0.40
1:C:121:VAL:O	1:C:121:VAL:CG1	2.69	0.40
1:C:918:TYR:O	1:C:919:LEU:C	2.58	0.40
2:D:587:LEU:N	2:D:587:LEU:CD1	2.84	0.40
1:C:660:LEU:HB3	1:C:713:LEU:HD21	2.02	0.40
2:D:654:LEU:HD13	2:D:665:ILE:CG1	2.51	0.40
1:C:934:HIS:ND1	1:C:1074:THR:HB	2.35	0.40
1:C:648:GLY:O	1:C:649:SER:C	2.60	0.40
2:D:256:ILE:HG21	2:D:275:ASN:O	2.22	0.40
1:A:402:VAL:CG1	1:A:443:LEU:HD22	2.50	0.40
1:A:543:PRO:O	1:A:544:SER:HB3	2.21	0.40
1:A:103:LEU:HD21	2:B:155:LEU:CD2	2.52	0.40
1:A:920:ASN:O	1:A:1080:LYS:HG2	2.21	0.40
1:C:604:VAL:CG1	1:C:742:PHE:CD2	3.02	0.40
1:C:438:TYR:CD1	2:D:247:PHE:HE1	2.39	0.40
1:A:637:LEU:HD11	1:A:658:LEU:HD21	2.03	0.40
1:C:956:VAL:O	1:C:963:VAL:HG23	2.21	0.40
1:C:800:ILE:HD11	1:C:879:ALA:HB1	2.03	0.40
2:B:230:TRP:CE3	2:B:235:ARG:HD3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:799:THR:HG22	1:C:845:ARG:CB	2.51	0.40
2:B:372:ASN:O	2:B:373:GLN:HG3	2.22	0.40
1:A:756:HIS:O	1:A:756:HIS:CG	2.74	0.40
1:A:757:ILE:O	1:A:758:CYS:HB2	2.22	0.40
1:C:586:GLY:HA2	1:C:591:VAL:HG23	2.03	0.40
1:A:638:TYR:HB3	1:A:691:ALA:HA	2.03	0.40
2:B:168:PRO:CG	2:B:179:PRO:HG3	2.52	0.40
1:C:43:GLN:HG2	1:C:44:THR:HG23	2.03	0.40
1:A:804:HIS:CB	1:A:808:LEU:HD11	2.52	0.40
1:A:971:HIS:N	1:A:972:PRO:HD3	2.36	0.40
1:C:897:LEU:HD12	1:C:897:LEU:O	2.22	0.40
1:A:752:CYS:HB2	1:A:793:GLU:OE2	2.21	0.40
1:A:714:ARG:C	1:A:714:ARG:HD2	2.42	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	880/1095 (80%)	667 (76%)	192 (22%)	21 (2%)	7 51
1	C	878/1095 (80%)	664 (76%)	195 (22%)	19 (2%)	8 52
2	B	671/687 (98%)	518 (77%)	141 (21%)	12 (2%)	11 56
2	D	671/687 (98%)	512 (76%)	146 (22%)	13 (2%)	10 55
All	All	3100/3564 (87%)	2361 (76%)	674 (22%)	65 (2%)	9 53

All (65) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	757	ILE
2	B	162	PRO

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Mol	Chain	Res	Type
2	B	598	SER
1	C	624	VAL
1	C	757	ILE
2	D	162	PRO
2	D	438	HIS
2	D	598	SER
1	A	490	VAL
1	A	624	VAL
1	A	649	SER
1	A	722	LYS
1	A	931	VAL
1	A	956	VAL
2	B	314	ILE
1	C	490	VAL
1	C	649	SER
1	C	722	LYS
1	C	931	VAL
1	C	956	VAL
2	D	314	ILE
2	D	436	LEU
2	D	437	CYS
1	A	773	SER
1	A	847	ASN
1	C	773	SER
1	C	847	ASN
1	A	26	ALA
1	A	354	PHE
1	A	691	ALA
2	B	69	HIS
2	B	101	LYS
2	B	639	THR
1	C	354	PHE
1	C	558	LEU
1	C	691	ALA
2	D	435	SER
2	D	639	THR
1	A	327	SER
1	A	558	LEU
1	A	819	GLN
1	A	846	ILE
1	C	26	ALA
1	C	846	ILE

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Mol	Chain	Res	Type
2	D	69	HIS
1	A	121	VAL
2	B	351	ALA
2	B	377	ASP
2	B	617	PHE
1	C	121	VAL
2	D	377	ASP
1	A	816	GLY
2	D	517	ILE
1	A	120	PRO
1	A	540	VAL
1	A	1059	VAL
2	B	204	ILE
2	B	517	ILE
1	C	120	PRO
1	C	1007	GLY
2	D	204	ILE
2	B	421	PRO
1	C	540	VAL
1	C	1059	VAL
2	D	421	PRO

5.3.2 Protein sidechains (i)

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	753/934 (81%)	742 (98%)	11 (2%)	72	90
1	C	751/934 (80%)	740 (98%)	11 (2%)	72	90
2	B	582/592 (98%)	579 (100%)	3 (0%)	92	97
2	D	582/592 (98%)	575 (99%)	7 (1%)	78	91
All	All	2668/3052 (87%)	2636 (99%)	32 (1%)	78	91

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119	LEU
1	A	395	TRP
1	A	478	LEU
1	A	565	PHE
1	A	679	ARG
1	A	714	ARG
1	A	823	ARG
1	A	840	TRP
1	A	915	PHE
1	A	964	TRP
1	A	1052	GLU
2	B	467	SER
2	B	479	ASN
2	B	511	TYR
1	C	118	ARG
1	C	119	LEU
1	C	395	TRP
1	C	478	LEU
1	C	565	PHE
1	C	679	ARG
1	C	714	ARG
1	C	840	TRP
1	C	915	PHE
1	C	964	TRP
1	C	1052	GLU
2	D	426	ARG
2	D	429	ASP
2	D	432	ARG
2	D	467	SER
2	D	479	ASN
2	D	489	ASP
2	D	511	TYR

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	124	GLN
1	A	334	GLN
1	A	434	GLN
1	A	472	GLN
1	A	692	HIS
1	A	819	GLN
2	B	159	ASN

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Mol	Chain	Res	Type
2	B	295	GLN
1	C	124	GLN
1	C	334	GLN
1	C	434	GLN
1	C	472	GLN
1	C	692	HIS
2	D	159	ASN
2	D	295	GLN
2	D	458	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

23 carbohydrates are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	A	3042	1,3	14,14,15	0.51	0	15,19,21	0.77	0
3	NAG	A	3043	3	14,14,15	0.59	0	15,19,21	1.03	1 (6%)
4	NAG	A	3373	1,4	14,14,15	0.58	0	15,19,21	0.83	0
4	NAG	A	3374	4	14,14,15	0.53	0	15,19,21	2.02	1 (6%)
4	MAN	A	3375	4	11,11,12	0.47	0	14,15,17	1.53	2 (14%)
4	MAN	A	3376	4	11,11,12	0.70	0	14,15,17	0.92	1 (7%)
4	MAN	A	3377	4	11,11,12	0.67	0	14,15,17	0.74	0
6	NAG	A	3716	1,6	14,14,15	0.48	0	15,19,21	1.75	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	NAG	A	3717	6	14,14,15	0.71	0	15,19,21	1.59	2 (13%)
6	MAN	A	3718	6	11,11,12	0.78	0	14,15,17	2.90	2 (14%)
6	NAG	A	3880	1,6	14,14,15	0.50	0	15,19,21	2.78	4 (26%)
6	NAG	A	3881	6	14,14,15	0.83	1 (7%)	15,19,21	1.20	2 (13%)
6	MAN	A	3882	6	11,11,12	0.70	0	14,15,17	2.95	4 (28%)
3	NAG	C	3042	1,3	14,14,15	0.48	0	15,19,21	0.73	0
3	NAG	C	3043	3	14,14,15	0.55	0	15,19,21	1.18	1 (6%)
4	NAG	C	3373	1,4	14,14,15	0.57	0	15,19,21	0.89	1 (6%)
4	NAG	C	3374	4	14,14,15	0.51	0	15,19,21	2.09	1 (6%)
4	MAN	C	3375	4	11,11,12	0.43	0	14,15,17	1.50	2 (14%)
4	MAN	C	3376	4	11,11,12	0.71	0	14,15,17	0.90	1 (7%)
4	MAN	C	3377	4	11,11,12	0.62	0	14,15,17	0.73	0
6	NAG	C	3716	1,6	14,14,15	0.57	0	15,19,21	1.49	1 (6%)
6	NAG	C	3717	6	14,14,15	0.53	0	15,19,21	1.21	2 (13%)
6	MAN	C	3718	6	11,11,12	0.90	0	14,15,17	1.36	2 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	3042	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	3043	3	-	0/6/23/26	0/1/1/1
4	NAG	A	3373	1,4	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	A	3374	4	-	0/6/23/26	0/1/1/1
4	MAN	A	3375	4	1/1/4/5	0/2/19/22	0/1/1/1
4	MAN	A	3376	4	-	0/2/19/22	0/1/1/1
4	MAN	A	3377	4	-	0/2/19/22	0/1/1/1
6	NAG	A	3716	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	3717	6	-	0/6/23/26	0/1/1/1
6	MAN	A	3718	6	1/1/4/5	0/2/19/22	0/1/1/1
6	NAG	A	3880	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	3881	6	-	0/6/23/26	0/1/1/1
6	MAN	A	3882	6	1/1/4/5	0/2/19/22	0/1/1/1
3	NAG	C	3042	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	3043	3	-	0/6/23/26	0/1/1/1
4	NAG	C	3373	1,4	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	C	3374	4	-	0/6/23/26	0/1/1/1
4	MAN	C	3375	4	1/1/4/5	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	C	3376	4	-	0/2/19/22	0/1/1/1
4	MAN	C	3377	4	-	0/2/19/22	0/1/1/1
6	NAG	C	3716	1,6	-	0/6/23/26	0/1/1/1
6	NAG	C	3717	6	-	0/6/23/26	0/1/1/1
6	MAN	C	3718	6	1/1/4/5	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	3881	NAG	C1-C2	2.34	1.55	1.52

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	3882	MAN	C1-C2-C3	-7.90	100.19	109.54
6	A	3882	MAN	C1-O5-C5	-5.98	104.65	112.25
4	A	3375	MAN	C2-C3-C4	-2.83	106.24	111.04
4	C	3375	MAN	C2-C3-C4	-2.81	106.27	111.04
6	A	3881	NAG	O4-C4-C5	-2.56	102.44	109.24
6	C	3718	MAN	O5-C1-C2	-2.35	107.04	110.86
4	A	3376	MAN	C1-O5-C5	-2.19	109.46	112.25
4	C	3376	MAN	C1-O5-C5	-2.17	109.50	112.25
6	A	3880	NAG	O4-C4-C3	-2.12	105.56	110.34
6	C	3717	NAG	O3-C3-C4	-2.04	105.73	110.34
4	C	3373	NAG	C1-O5-C5	2.19	115.03	112.25
6	A	3880	NAG	C3-C4-C5	2.43	114.43	110.20
6	A	3880	NAG	O3-C3-C2	2.48	114.03	109.11
6	A	3881	NAG	C1-O5-C5	2.54	115.47	112.25
6	A	3882	MAN	C3-C4-C5	2.54	114.62	110.20
3	A	3043	NAG	C1-O5-C5	2.68	115.65	112.25
6	A	3716	NAG	O3-C3-C2	3.04	115.13	109.11
6	A	3882	MAN	O5-C5-C6	3.05	113.94	107.35
6	C	3717	NAG	C1-O5-C5	3.05	116.12	112.25
6	C	3718	MAN	C1-C2-C3	3.14	113.26	109.54
4	C	3375	MAN	O3-C3-C2	3.25	115.88	110.00
6	C	3716	NAG	O3-C3-C2	3.40	115.85	109.11
3	C	3043	NAG	C1-O5-C5	3.42	116.59	112.25
4	A	3375	MAN	O3-C3-C2	3.44	116.20	110.00
6	A	3717	NAG	C1-O5-C5	3.56	116.77	112.25
6	A	3717	NAG	O4-C4-C3	3.79	118.87	110.34
6	A	3718	MAN	C1-C2-C3	4.72	115.12	109.54
6	A	3716	NAG	C1-O5-C5	4.87	118.43	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	3374	NAG	C1-O5-C5	6.89	120.99	112.25
4	C	3374	NAG	C1-O5-C5	7.18	121.36	112.25
6	A	3718	MAN	C1-O5-C5	9.28	124.02	112.25
6	A	3880	NAG	C1-O5-C5	9.61	124.44	112.25

All (7) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	3375	MAN	C1
4	C	3373	NAG	C1
6	C	3718	MAN	C1
6	A	3882	MAN	C1
4	C	3375	MAN	C1
4	A	3373	NAG	C1
6	A	3718	MAN	C1

There are no torsion outliers.

There are no ring outliers.

17 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	3373	NAG	2	0
4	A	3374	NAG	3	0
4	A	3375	MAN	3	0
4	A	3376	MAN	1	0
6	A	3716	NAG	4	0
6	A	3717	NAG	1	0
6	A	3880	NAG	2	0
6	A	3881	NAG	2	0
6	A	3882	MAN	1	0
4	C	3373	NAG	3	0
4	C	3374	NAG	4	0
4	C	3375	MAN	3	0
4	C	3376	MAN	1	0
4	C	3377	MAN	1	0
6	C	3716	NAG	11	0
6	C	3717	NAG	4	0
6	C	3718	MAN	2	0

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

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	3678	1	14,14,15	0.49	0	15,19,21	0.67	0
5	NAG	B	3094	2	14,14,15	0.59	0	15,19,21	0.94	1 (6%)
5	NAG	B	3479	2	14,14,15	4.26	14 (100%)	15,19,21	2.82	8 (53%)
8	MAN	C	3378	-	11,11,12	0.95	1 (9%)	14,15,17	2.50	4 (28%)
5	NAG	C	3678	1	14,14,15	0.50	0	15,19,21	0.61	0
5	NAG	C	3880	1	14,14,15	0.31	0	15,19,21	1.74	1 (6%)
5	NAG	D	3094	2	14,14,15	0.50	0	15,19,21	0.57	0
5	NAG	D	3479	2	14,14,15	4.69	13 (92%)	15,19,21	2.89	7 (46%)

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	3678	1	-	0/6/23/26	0/1/1/1
5	NAG	B	3094	2	-	0/6/23/26	0/1/1/1
5	NAG	B	3479	2	-	0/6/23/26	0/1/1/1
8	MAN	C	3378	-	-	0/2/19/22	0/1/1/1
5	NAG	C	3678	1	-	0/6/23/26	0/1/1/1
5	NAG	C	3880	1	-	0/6/23/26	0/1/1/1
5	NAG	D	3094	2	-	0/6/23/26	0/1/1/1
5	NAG	D	3479	2	-	0/6/23/26	0/1/1/1

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	3378	MAN	O5-C1	-2.50	1.39	1.43
5	B	3479	NAG	C7-N2	2.25	1.43	1.34
5	B	3479	NAG	O6-C6	2.33	1.52	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	3479	NAG	O3-C3	2.39	1.48	1.43
5	B	3479	NAG	O4-C4	2.92	1.50	1.43
5	B	3479	NAG	O5-C1	2.98	1.48	1.43
5	B	3479	NAG	C6-C5	3.14	1.63	1.51
5	D	3479	NAG	C3-C2	3.19	1.59	1.52
5	D	3479	NAG	C6-C5	3.21	1.63	1.51
5	D	3479	NAG	C7-N2	3.45	1.47	1.34
5	B	3479	NAG	C1-C2	3.85	1.57	1.52
5	D	3479	NAG	C2-N2	3.93	1.53	1.46
5	B	3479	NAG	O3-C3	3.95	1.52	1.43
5	D	3479	NAG	O4-C4	4.00	1.52	1.43
5	B	3479	NAG	O5-C5	4.07	1.52	1.43
5	D	3479	NAG	C4-C3	4.24	1.63	1.52
5	B	3479	NAG	C2-N2	4.35	1.54	1.46
5	B	3479	NAG	C8-C7	4.41	1.59	1.50
5	B	3479	NAG	C3-C2	4.53	1.62	1.52
5	D	3479	NAG	C8-C7	4.87	1.60	1.50
5	B	3479	NAG	C4-C3	5.44	1.66	1.52
5	D	3479	NAG	C1-C2	5.80	1.60	1.52
5	D	3479	NAG	O5-C1	6.09	1.53	1.43
5	D	3479	NAG	O7-C7	6.20	1.37	1.23
5	D	3479	NAG	O5-C5	6.22	1.57	1.43
5	B	3479	NAG	O7-C7	6.24	1.37	1.23
5	B	3479	NAG	C4-C5	6.46	1.66	1.53
5	D	3479	NAG	C4-C5	6.75	1.67	1.53

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	C	3378	MAN	C1-C2-C3	-6.71	101.60	109.54
8	C	3378	MAN	C1-O5-C5	-4.89	106.04	112.25
5	D	3479	NAG	C2-N2-C7	-4.12	117.74	123.04
5	B	3479	NAG	C8-C7-N2	-3.68	109.06	116.11
5	B	3479	NAG	C2-N2-C7	-3.39	118.68	123.04
5	D	3479	NAG	O7-C7-C8	-2.26	117.92	122.06
5	B	3479	NAG	O3-C3-C2	2.24	113.56	109.11
8	C	3378	MAN	O5-C1-C2	2.27	114.54	110.86
5	D	3479	NAG	C3-C4-C5	2.39	114.36	110.20
5	B	3094	NAG	C1-O5-C5	2.58	115.52	112.25
5	B	3479	NAG	O4-C4-C3	2.93	116.94	110.34
5	D	3479	NAG	O5-C5-C6	3.03	113.91	107.35
5	D	3479	NAG	C4-C3-C2	3.09	116.04	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	C	3378	MAN	C3-C4-C5	3.24	115.84	110.20
5	D	3479	NAG	O4-C4-C3	3.24	117.64	110.34
5	B	3479	NAG	O5-C5-C6	3.29	114.48	107.35
5	B	3479	NAG	C1-O5-C5	4.24	117.62	112.25
5	B	3479	NAG	C3-C4-C5	4.30	117.69	110.20
5	B	3479	NAG	O3-C3-C4	4.75	121.04	110.34
5	C	3880	NAG	C1-O5-C5	5.76	119.55	112.25
5	D	3479	NAG	C1-O5-C5	7.60	121.90	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	3479	NAG	1	0
8	C	3378	MAN	1	0
5	D	3479	NAG	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^{th} 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	884/1095 (80%)	0.17	37 (4%)	40	27	106, 204, 303, 383	0
1	C	882/1095 (80%)	0.12	34 (3%)	43	29	112, 207, 304, 401	0
2	B	673/687 (97%)	0.43	72 (10%)	8	6	133, 256, 325, 426	2 (0%)
2	D	673/687 (97%)	0.56	91 (13%)	4	4	144, 258, 332, 424	2 (0%)
All	All	3112/3564 (87%)	0.30	234 (7%)	17	11	106, 233, 318, 426	4 (0%)

All (234) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	433	ASP	11.0
2	D	92	ALA	10.4
2	B	161	HIS	9.3
2	D	432	ARG	9.2
2	B	470	GLU	8.2
2	B	323	LEU	7.9
1	A	482	TRP	7.8
2	B	72	GLY	7.1
2	B	469	GLN	7.0
2	B	92	ALA	7.0
1	C	482	TRP	6.9
2	B	73	GLN	6.6
1	A	396	LYS	6.6
2	B	67	GLU	6.6
2	D	429	ASP	6.5
1	C	108	PHE	6.3
2	D	91	ALA	6.3
2	D	32	PRO	5.9
2	D	430	GLN	5.9
2	D	391	VAL	5.8
1	A	1045	VAL	5.7

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Mol	Chain	Res	Type	RSRZ
2	D	161	HIS	5.5
2	D	95	VAL	5.4
1	C	33	GLY	5.3
2	D	236	LEU	5.2
2	B	160	THR	5.2
1	C	1078	LEU	5.2
2	D	35	PRO	5.1
1	A	483	ARG	5.1
1	A	102	TYR	4.9
2	B	414	ILE	4.9
2	B	32	PRO	4.7
2	D	669	GLU	4.7
2	D	435	SER	4.6
1	A	726	ALA	4.6
1	A	124	GLN	4.5
1	A	326	SER	4.5
1	C	102	TYR	4.4
2	D	393	VAL	4.4
2	D	107	LEU	4.3
2	D	49	ARG	4.3
1	C	624	VAL	4.3
2	B	629	GLN	4.2
2	B	429	ASP	4.2
2	D	189	THR	4.2
1	A	918	TYR	4.1
1	A	87	LEU	4.0
1	A	108	PHE	4.0
2	D	629	GLN	4.0
2	B	446	GLY	3.9
2	D	431	SER	3.9
1	C	623	GLN	3.9
2	B	66	GLN	3.9
1	A	1044	LYS	3.8
1	C	74	GLY	3.8
2	D	33	GLY	3.8
1	A	125	GLU	3.7
2	B	391	VAL	3.7
2	D	106	ASP	3.7
2	D	389	PHE	3.7
1	A	335	GLU	3.7
1	A	1078	LEU	3.6
2	B	35	PRO	3.6

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Mol	Chain	Res	Type	RSRZ
2	D	160	THR	3.6
2	B	1	GLN	3.6
2	D	618	GLY	3.6
2	D	179	PRO	3.5
2	D	668	ASP	3.5
2	D	607	ALA	3.5
1	C	396	LYS	3.5
2	B	622	SER	3.5
2	B	331	VAL	3.5
2	D	634	PRO	3.5
2	B	330	VAL	3.4
2	B	40	CYS	3.4
2	D	72	GLY	3.4
2	D	642	GLU	3.4
2	D	320	VAL	3.4
2	B	358	VAL	3.4
2	B	39	ARG	3.3
1	C	124	GLN	3.3
2	B	667	VAL	3.3
1	C	973	GLN	3.3
2	B	81	VAL	3.3
1	C	117	GLN	3.3
2	D	206	GLY	3.2
2	D	425	CYS	3.2
2	B	430	GLN	3.2
2	B	91	ALA	3.2
2	D	144	ILE	3.2
1	A	592	LEU	3.2
2	D	632	ASN	3.2
2	D	399	ILE	3.2
2	D	69	HIS	3.2
2	D	65	THR	3.1
2	D	379	ASP	3.1
1	C	483	ARG	3.1
2	B	335	LYS	3.1
1	A	594	LEU	3.1
1	C	106	LEU	3.0
2	D	235	ARG	3.0
2	D	93	PHE	3.0
2	D	318	SER	3.0
2	D	641	LYS	3.0
1	C	918	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
2	D	67	GLU	3.0
2	B	345	VAL	3.0
2	D	613	GLU	3.0
2	B	296	PRO	2.9
1	C	594	LEU	2.9
2	D	469	GLN	2.9
2	D	272	LYS	2.9
2	D	651	ALA	2.9
2	B	180	PHE	2.9
2	D	48	MET	2.9
2	B	433	ASP	2.8
2	D	407	ARG	2.8
2	D	97	PHE	2.8
1	A	817	GLN	2.8
2	B	407	ARG	2.8
1	A	106	LEU	2.8
2	B	377	ASP	2.8
2	B	322	GLU	2.7
1	C	88	ALA	2.7
1	C	335	GLU	2.7
2	D	630	LEU	2.7
2	B	351	ALA	2.7
2	B	393	VAL	2.7
2	D	195	PHE	2.7
1	A	394	LEU	2.7
1	C	95	HIS	2.7
2	D	237	LEU	2.7
2	D	427	CYS	2.7
2	B	389	PHE	2.7
2	B	636	LYS	2.7
2	B	665	ILE	2.7
1	A	118	ARG	2.6
2	D	56	ILE	2.6
1	C	87	LEU	2.6
1	A	88	ALA	2.6
1	C	125	GLU	2.6
2	D	369	THR	2.6
2	B	55	ASP	2.6
2	D	231	ARG	2.6
1	A	33	GLY	2.6
2	B	395	ALA	2.6
2	B	26	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	104	PRO	2.5
2	B	664	LEU	2.5
2	B	416	THR	2.5
2	D	404	PHE	2.5
1	A	101	MET	2.5
2	B	431	SER	2.5
2	B	93	PHE	2.5
1	A	361	PHE	2.5
1	C	1045	VAL	2.4
2	B	33	GLY	2.4
2	B	443	LEU	2.4
2	B	48	MET	2.4
2	B	628	LEU	2.4
1	C	592	LEU	2.4
1	C	46	GLY	2.3
1	C	68	ALA	2.3
2	D	287	HIS	2.3
2	D	207	ASN	2.3
1	A	339	ALA	2.3
2	B	113	LEU	2.3
1	A	347	VAL	2.3
1	A	480	ARG	2.3
2	B	384	ASN	2.3
2	D	133	ARG	2.3
2	B	382	GLN	2.3
2	D	298	PHE	2.3
1	C	10	ALA	2.3
2	D	428	ARG	2.3
2	B	97	PHE	2.3
2	D	8	VAL	2.3
2	D	387	ILE	2.3
1	C	725	LEU	2.3
2	B	333	LEU	2.3
1	C	104	THR	2.3
2	D	561	LEU	2.2
2	B	607	ALA	2.2
2	B	298	PHE	2.2
2	D	115	TYR	2.2
2	D	414	ILE	2.2
1	C	724	LEU	2.2
2	B	328	SER	2.2
2	D	205	SER	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	173	GLU	2.2
2	D	610	LEU	2.2
1	C	121	VAL	2.2
2	B	611	LYS	2.2
1	A	553	ILE	2.2
2	D	628	LEU	2.2
1	A	363	TYR	2.2
2	D	386	PRO	2.2
2	D	438	HIS	2.2
2	D	443	LEU	2.2
2	D	76	LEU	2.2
2	B	267	GLU	2.1
1	A	104	THR	2.1
2	B	207	ASN	2.1
2	B	334	ILE	2.1
2	D	344	ARG	2.1
1	C	120	PRO	2.1
1	C	9	THR	2.1
1	A	821	GLN	2.1
2	D	436	LEU	2.1
2	B	329	ASN	2.1
1	A	110	LEU	2.1
2	D	390	GLN	2.1
2	D	94	ASN	2.1
1	A	1047	VAL	2.1
2	B	272	LYS	2.1
1	A	919	LEU	2.1
2	D	105	ILE	2.1
2	B	80	LYS	2.1
1	A	724	LEU	2.1
2	D	83	LEU	2.1
1	C	1047	VAL	2.1
2	D	296	PRO	2.1
2	D	227	GLU	2.1
1	A	722	LYS	2.0
1	C	481	GLY	2.0
2	B	321	GLY	2.0
2	D	64	GLU	2.0
2	B	320	VAL	2.0
2	B	186	LEU	2.0
2	B	56	ILE	2.0
2	B	227	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
2	D	419	VAL	2.0
2	D	62	LEU	2.0
2	D	409	LEU	2.0

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, 95^{th} 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
6	NAG	C	3716	14/15	0.94	0.18	-0.09	90,220,322,330	0
6	NAG	A	3716	14/15	0.93	0.19	-0.56	84,247,290,297	0
6	NAG	A	3880	14/15	0.91	0.20	-0.63	197,234,285,285	0
4	NAG	C	3374	14/15	0.71	0.27	-	205,297,391,446	0
4	MAN	C	3376	11/12	0.53	0.27	-	217,294,356,376	0
4	MAN	A	3376	11/12	0.24	0.46	-	278,313,361,364	0
4	MAN	A	3375	11/12	0.36	0.33	-	221,338,359,359	0
4	NAG	C	3373	14/15	0.82	0.27	-	230,326,381,388	0
3	NAG	C	3043	14/15	0.58	0.43	-	228,295,376,376	0
4	MAN	A	3377	11/12	0.68	0.28	-	241,288,357,366	0
6	MAN	C	3718	11/12	0.76	0.13	-	313,359,401,410	0
6	MAN	A	3882	11/12	0.41	0.57	-	310,353,388,410	0
4	NAG	A	3374	14/15	0.72	0.30	-	273,293,381,415	0
4	MAN	C	3375	11/12	0.58	0.29	-	271,326,353,354	0
3	NAG	A	3043	14/15	0.58	0.27	-	222,255,345,354	0
6	NAG	A	3717	14/15	0.83	0.20	-	225,292,336,341	0
6	NAG	A	3881	14/15	0.77	0.36	-	252,291,337,341	0
3	NAG	A	3042	14/15	0.75	0.30	-	209,289,325,337	0
4	NAG	A	3373	14/15	0.82	0.25	-	181,314,385,389	0
3	NAG	C	3042	14/15	0.81	0.22	-	219,245,283,285	0
4	MAN	C	3377	11/12	0.40	0.32	-	233,301,351,351	0
6	NAG	C	3717	14/15	0.86	0.21	-	237,294,351,395	0
6	MAN	A	3718	11/12	0.47	0.21	-	295,349,390,420	0

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^{th} 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
5	NAG	C	3880	14/15	0.86	0.27	0.76	136,198,243,253	0
7	CA	B	2002	1/1	0.59	0.26	-0.05	608,608,608,608	0
7	CA	C	2005	1/1	0.65	0.17	-0.27	215,215,215,215	0
5	NAG	B	3094	14/15	0.79	0.33	-0.65	232,281,317,341	0
7	CA	C	2006	1/1	0.87	0.17	-0.86	147,147,147,147	0
7	CA	A	2006	1/1	0.93	0.16	-0.96	143,143,143,143	0
7	CA	A	2005	1/1	0.78	0.12	-0.99	193,193,193,193	0
7	CA	D	2002	1/1	0.76	0.10	-1.12	594,594,594,594	0
7	CA	A	2007	1/1	0.67	0.16	-1.32	240,240,240,240	0
7	CA	C	2007	1/1	0.62	0.14	-1.79	237,237,237,237	0
5	NAG	B	3479	14/15	0.82	0.22	-	213,256,300,333	0
8	MAN	C	3378	11/12	0.40	0.54	-	241,288,352,362	0
5	NAG	C	3678	14/15	0.90	0.23	-	177,279,379,392	0
5	NAG	D	3094	14/15	0.78	0.39	-	254,283,315,325	0
5	NAG	A	3678	14/15	0.86	0.26	-	167,304,342,378	0
5	NAG	D	3479	14/15	0.82	0.26	-	191,259,284,291	0

6.5 Other polymers (i)

There are no such residues in this entry.