



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:00 PM UTC

PDB ID : 8HQ1 / pdb_00008hq1
Title : Crystal Structure Of Human Lgi1-Adam22 Complex In Space Group C2
Authors : Liu, H.L.; Lin, Z.H.; Xu, F.
Deposited on : 2022-12-13
Resolution : 4.17 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

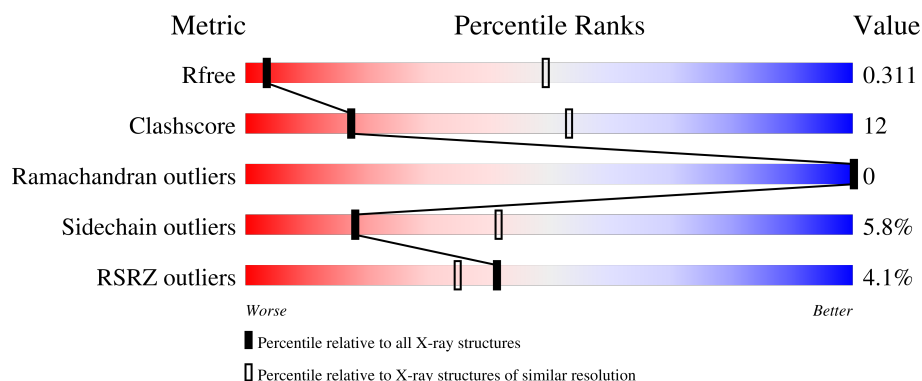
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.17 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}	180053	1026 (4.50-3.86)
Clashscore	190562	1071 (4.50-3.86)
Ramachandran outliers	187476	1014 (4.52-3.84)
Sidechain outliers	187428	1000 (4.52-3.84)
RSRZ outliers	180081	1023 (4.50-3.86)

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

Mol	Chain	Length	Quality of chain
1	A	486	 5% 75% 22% .
1	B	486	 4% 73% 23% .
1	C	486	 4% 72% 24% .
2	D	526	 4% 69% 28% ..
2	E	526	 4% 71% 25% ..

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Mol	Chain	Length	Quality of chain
2	F	526	3% 70% 26% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23997 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 Disintegrin and metalloproteinase domain-containing protein 22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	486	Total	C	N	O	S	0	0	0
			3728	2303	643	731	51			
1	B	486	Total	C	N	O	S	0	0	0
			3728	2303	643	731	51			
1	C	486	Total	C	N	O	S	0	0	0
			3728	2303	643	731	51			

- Molecule 2 is a protein called Leucine-rich glioma-inactivated protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	515	Total	C	N	O	S	0	0	0
			4183	2694	696	778	15			
2	E	515	Total	C	N	O	S	0	0	0
			4183	2694	696	778	15			
2	F	515	Total	C	N	O	S	0	0	0
			4183	2694	696	778	15			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	32	HIS	-	expression tag	UNP O95970
D	33	HIS	-	expression tag	UNP O95970
D	34	HIS	-	expression tag	UNP O95970
D	35	HIS	-	expression tag	UNP O95970
D	36	HIS	-	expression tag	UNP O95970
D	37	HIS	-	expression tag	UNP O95970
D	38	HIS	-	expression tag	UNP O95970
E	32	HIS	-	expression tag	UNP O95970
E	33	HIS	-	expression tag	UNP O95970
E	34	HIS	-	expression tag	UNP O95970
E	35	HIS	-	expression tag	UNP O95970
E	36	HIS	-	expression tag	UNP O95970

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Chain	Residue	Modelled	Actual	Comment	Reference
E	37	HIS	-	expression tag	UNP O95970
E	38	HIS	-	expression tag	UNP O95970
F	32	HIS	-	expression tag	UNP O95970
F	33	HIS	-	expression tag	UNP O95970
F	34	HIS	-	expression tag	UNP O95970
F	35	HIS	-	expression tag	UNP O95970
F	36	HIS	-	expression tag	UNP O95970
F	37	HIS	-	expression tag	UNP O95970
F	38	HIS	-	expression tag	UNP O95970

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		
3	F	1	Total	C	N	O	0	0
			14	8	1	5		
3	F	1	Total	C	N	O	0	0
			14	8	1	5		
3	F	1	Total	C	N	O	0	0
			14	8	1	5		

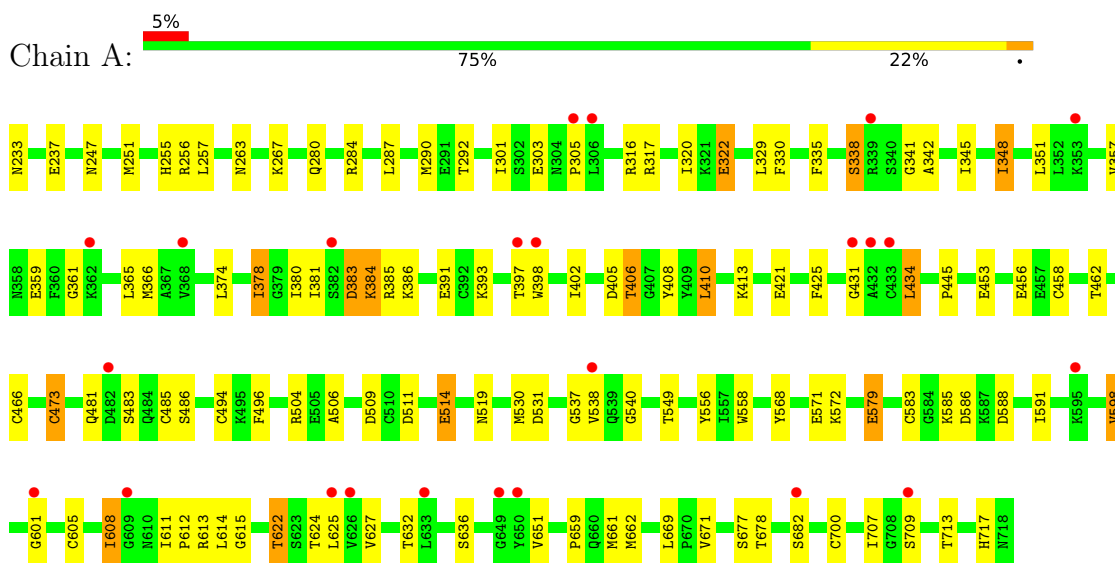
- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Ca	0	0
			3	3		
4	B	3	Total	Ca	0	0
			3	3		
4	C	3	Total	Ca	0	0
			3	3		
4	D	1	Total	Ca	0	0
			1	1		
4	E	1	Total	Ca	0	0
			1	1		
4	F	1	Total	Ca	0	0
			1	1		

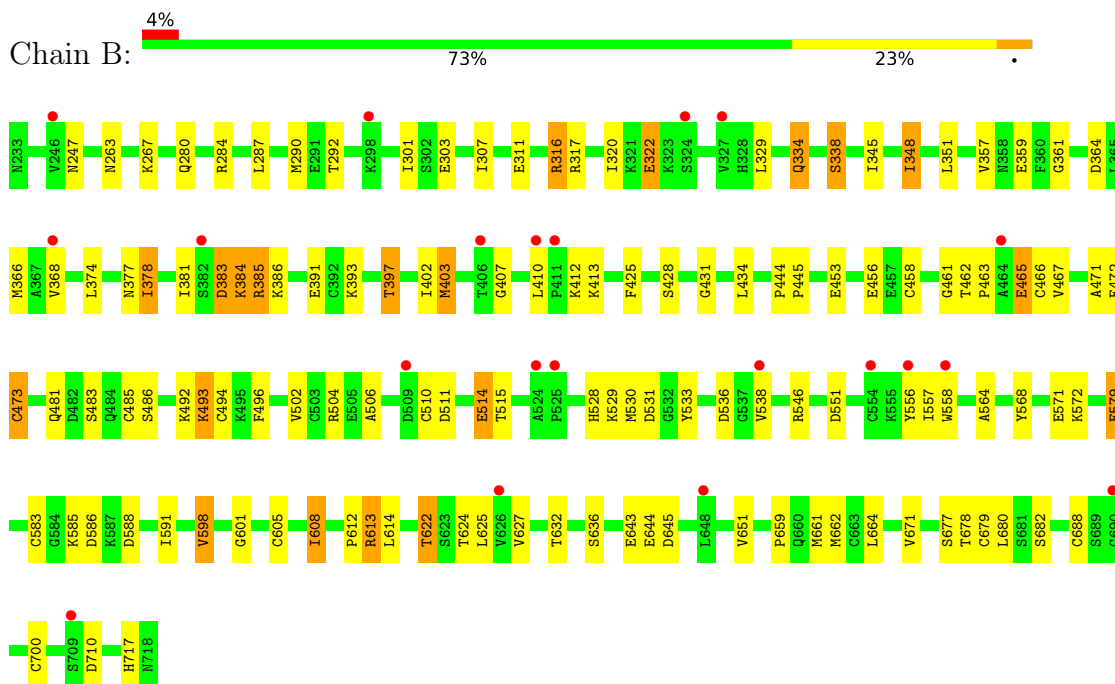
3 Residue-property plots

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

- Molecule 1: Disintegrin and metalloproteinase domain-containing protein 22



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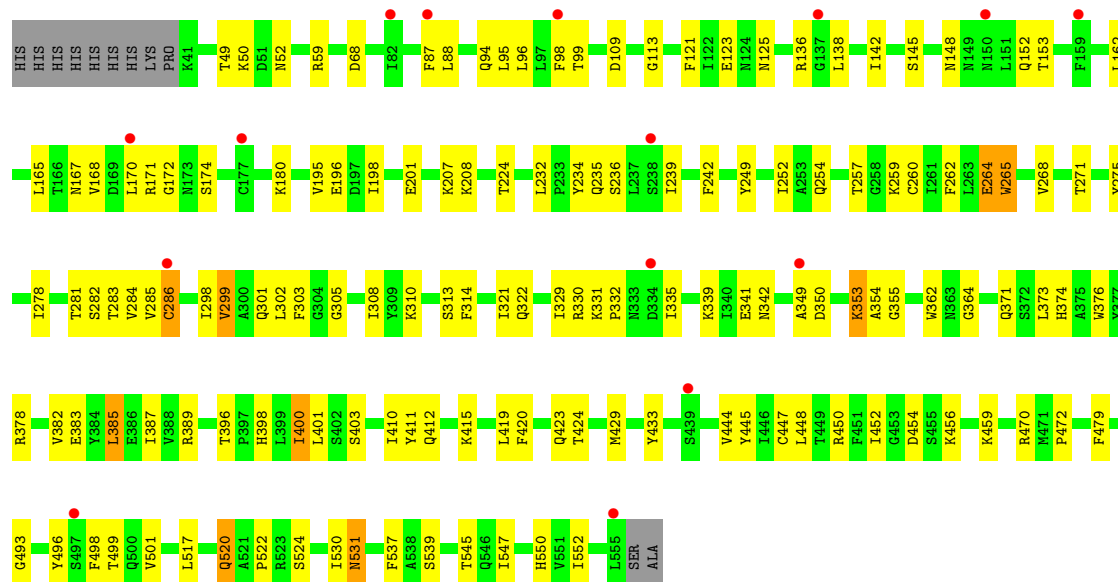


- Chain C: 72% 24% 4%

Item	Value
I707	0.00
T713	0.00
H717	0.00
N718	0.00
E571	0.00
K572	0.00
E579	0.00
G583	0.00
G584	0.00
K585	0.00
D586	0.00
K587	0.00
D588	0.00
I591	0.00
V598	0.00
G601	0.00
G605	0.00
I608	0.00
I611	0.00
P612	0.00
L613	0.00
L614	0.00
T622	0.00
S623	0.00
T624	0.00
L625	0.00
V626	0.00
V627	0.00
T632	0.00
G635	0.00
S636	0.00
E643	0.00
S644	0.00
D645	0.00
V651	0.00
P659	0.00
Q660	0.00
M661	0.00
M662	0.00
L669	0.00
P670	0.00
V671	0.00
S677	0.00
T678	0.00
S682	0.00
G461	0.00
T462	0.00
P463	0.00
A464	0.00
E465	0.00
C466	0.00
C473	0.00
Q481	0.00
T482	0.00
S483	0.00
Q484	0.00
C485	0.00
S486	0.00
C494	0.00
K495	0.00
P496	0.00
Q497	0.00
P498	0.00
V502	0.00
G503	0.00
R504	0.00
E505	0.00
A506	0.00
D509	0.00
C510	0.00
D511	0.00
E514	0.00
T515	0.00
P525	0.00
M530	0.00
D531	0.00
V538	0.00
Q539	0.00
G544	0.00
T549	0.00
R550	0.00
D551	0.00
Q552	0.00
R553	0.00
C554	0.00
K555	0.00
Y556	0.00
I557	0.00
W558	0.00
A564	0.00
V568	0.00
V357	0.00
N358	0.00
F360	0.00
G361	0.00
M366	0.00
A367	0.00
V368	0.00
T369	0.00
L374	0.00
N377	0.00
I378	0.00
G379	0.00
I380	0.00
I381	0.00
S382	0.00
D383	0.00
K384	0.00
R385	0.00
K386	0.00
K393	0.00
T397	0.00
V398	0.00
S399	0.00
G400	0.00
C401	0.00
I402	0.00
M403	0.00
T406	0.00
G407	0.00
Y408	0.00
Y409	0.00
L410	0.00
P411	0.00
K412	0.00
K413	0.00
F414	0.00
E421	0.00
F425	0.00
G431	0.00
L434	0.00
P445	0.00
E453	0.00
E456	0.00
F457	0.00
C458	0.00
N233	0.00
I245	0.00
V246	0.00
N247	0.00
M251	0.00
N263	0.00
K267	0.00
I276	0.00
Q280	0.00
R284	0.00
L287	0.00
M290	0.00
E291	0.00
T292	0.00
W293	0.00
N297	0.00
I301	0.00
S302	0.00
E303	0.00
N304	0.00
P305	0.00
R316	0.00
R317	0.00
I320	0.00
K321	0.00
E322	0.00
K323	0.00
S324	0.00
L329	0.00
F330	0.00
Q334	0.00
F335	0.00
E336	0.00
S337	0.00
S338	0.00
R339	0.00
S340	0.00
G341	0.00
A342	0.00
I345	0.00
I348	0.00
I351	0.00

- [illegible]

- [illegible]



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	373.50Å 232.37Å 80.03Å 90.00° 94.97° 90.00°	Depositor
Resolution (Å)	37.92 – 4.17 37.92 – 4.17	Depositor EDS
% Data completeness (in resolution range)	99.0 (37.92-4.17) 98.9 (37.92-4.17)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 4.13Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155)	Depositor
R, R_{free}	0.266 , 0.314 0.265 , 0.311	Depositor DCC
R_{free} test set	2558 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	172.5	Xtriage
Anisotropy	0.811	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 251.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	23997	wwPDB-VP
Average B, all atoms (Å ²)	264.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.25	0/3792	0.55	1/5105 (0.0%)
1	B	0.24	0/3792	0.55	4/5105 (0.1%)
1	C	0.29	0/3792	0.60	4/5105 (0.1%)
2	D	0.19	0/4290	0.51	3/5821 (0.1%)
2	E	0.15	0/4290	0.41	0/5821
2	F	0.17	0/4290	0.43	0/5821
All	All	0.22	0/24246	0.51	12/32778 (0.0%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	426	ILE	CA-C-N	9.56	129.32	119.76
2	D	426	ILE	C-N-CA	9.56	129.32	119.76
2	D	431	ASP	N-CA-C	8.98	123.86	111.74
1	B	536	ASP	N-CA-C	-6.81	101.99	111.39
1	C	339	ARG	CB-CA-C	5.95	119.55	109.50
1	C	340	SER	N-CA-C	-5.82	106.03	113.01
1	C	400	GLY	O-C-N	5.82	127.91	122.90
1	C	384	LYS	N-CA-C	-5.45	105.73	112.38
1	B	412	LYS	N-CA-C	5.43	120.01	113.17
1	A	384	LYS	N-CA-C	-5.35	105.86	112.38
1	B	384	LYS	N-CA-C	-5.29	106.09	112.54
1	B	383	ASP	N-CA-C	-5.04	100.85	108.67

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3728	0	3580	92	0
1	B	3728	0	3579	99	0
1	C	3728	0	3579	113	0
2	D	4183	0	4101	102	0
2	E	4183	0	4101	101	0
2	F	4183	0	4101	111	0
3	A	42	0	39	2	0
3	B	42	0	39	1	0
3	C	42	0	39	0	0
3	D	42	0	39	0	0
3	E	42	0	39	0	0
3	F	42	0	39	1	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
4	C	3	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
All	All	23997	0	23275	589	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 12.

All (589) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:345:ILE:HD12	1:B:381:ILE:CG2	1.66	1.25
1:C:345:ILE:HD12	1:C:381:ILE:CG2	1.72	1.19
1:A:345:ILE:HD12	1:A:381:ILE:CG2	1.72	1.18
1:C:403:MET:HE3	1:C:403:MET:HA	1.20	1.13
2:F:121:PHE:HD2	2:F:145:SER:HB3	1.10	1.09
1:C:345:ILE:HD12	1:C:381:ILE:HG22	1.13	1.06
1:B:345:ILE:HD12	1:B:381:ILE:HG22	1.10	1.06
2:F:121:PHE:CD2	2:F:145:SER:HB3	1.91	1.06
1:A:345:ILE:HD12	1:A:381:ILE:HG22	1.08	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:165:LEU:HD21	2:E:168:VAL:CG2	1.87	1.04
1:B:403:MET:HA	1:B:403:MET:CE	1.89	1.03
1:B:403:MET:HA	1:B:403:MET:HE3	1.04	1.02
1:C:402:ILE:HG21	1:C:414:PHE:CE1	1.93	1.02
1:B:345:ILE:CD1	1:B:381:ILE:HG22	1.90	1.01
1:A:345:ILE:CD1	1:A:381:ILE:HG22	1.91	0.99
1:C:345:ILE:CD1	1:C:381:ILE:HG22	1.95	0.96
1:B:403:MET:HE3	1:B:403:MET:CA	1.98	0.91
1:C:398:TRP:CH2	2:F:284:VAL:HG22	2.05	0.90
1:C:403:MET:HE3	1:C:403:MET:CA	2.01	0.90
2:E:165:LEU:HD21	2:E:168:VAL:HG23	1.55	0.89
2:F:121:PHE:HD2	2:F:145:SER:CB	1.86	0.88
1:C:403:MET:HA	1:C:403:MET:CE	2.03	0.88
1:B:385:ARG:HH11	1:B:385:ARG:HB2	1.36	0.87
2:E:165:LEU:HD21	2:E:168:VAL:HG22	1.57	0.86
2:F:450:ARG:HG2	2:F:452:ILE:O	1.76	0.86
1:B:385:ARG:HH11	1:B:385:ARG:CB	1.87	0.86
2:F:121:PHE:CD2	2:F:145:SER:CB	2.58	0.84
1:A:365:LEU:CD1	1:A:410:LEU:HD11	2.10	0.82
1:C:305:PRO:CD	1:C:337:SER:HB2	2.10	0.81
2:D:429:MET:HE3	2:D:456:LYS:HE3	1.62	0.81
1:A:365:LEU:HD13	1:A:410:LEU:HD11	1.63	0.80
2:D:429:MET:HE3	2:D:456:LYS:CE	2.12	0.79
1:A:586:ASP:HB2	1:A:591:ILE:HD11	1.64	0.79
1:C:410:LEU:HD22	1:C:410:LEU:H	1.48	0.79
1:C:586:ASP:HB2	1:C:591:ILE:HD11	1.64	0.78
1:A:398:TRP:CZ3	2:D:255:PRO:HB2	2.18	0.78
1:A:338:SER:HB2	2:D:354:ALA:HA	1.66	0.78
1:B:586:ASP:HB2	1:B:591:ILE:HD11	1.65	0.77
1:A:365:LEU:HD12	1:A:410:LEU:CD1	2.15	0.76
1:B:345:ILE:HD12	1:B:381:ILE:HG21	1.67	0.76
1:C:483:SER:HA	1:C:494:CYS:O	1.85	0.76
2:F:257:THR:HG23	2:F:259:LYS:H	1.50	0.76
1:A:384:LYS:HG3	1:A:613:ARG:O	1.86	0.76
1:C:340:SER:HB2	1:C:359:GLU:HG2	1.68	0.76
2:E:257:THR:HG23	2:E:259:LYS:H	1.51	0.76
2:D:349:ALA:HB2	2:D:382:VAL:HG23	1.68	0.76
1:B:504:ARG:NH1	1:B:514:GLU:HG3	2.02	0.75
2:F:239:ILE:HD13	2:F:537:PHE:HB3	1.69	0.75
1:B:627:VAL:HG12	1:B:632:THR:HG22	1.67	0.75
2:E:356:PHE:HZ	2:E:376:TRP:CZ2	2.06	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:402:ILE:HG21	1:C:414:PHE:CZ	2.22	0.74
2:F:349:ALA:HB2	2:F:382:VAL:HG23	1.69	0.73
2:E:284:VAL:HG12	2:E:285:VAL:HG23	1.71	0.73
2:F:339:LYS:NZ	2:F:342:ASN:HA	2.04	0.72
2:F:401:LEU:HD12	2:F:401:LEU:O	1.89	0.72
1:C:504:ARG:NH1	1:C:514:GLU:HG3	2.04	0.72
1:C:627:VAL:HG12	1:C:632:THR:HG22	1.69	0.72
2:D:153:THR:HG21	2:D:180:LYS:HE3	1.71	0.72
2:E:144:LEU:HB3	2:E:165:LEU:HD11	1.72	0.72
1:A:365:LEU:HD12	1:A:410:LEU:HD12	1.70	0.71
2:E:165:LEU:CD2	2:E:168:VAL:CG2	2.68	0.71
2:E:339:LYS:NZ	2:E:342:ASN:HA	2.05	0.71
1:B:364:ASP:HB3	1:B:410:LEU:HD22	1.71	0.71
2:F:284:VAL:HG12	2:F:285:VAL:HG23	1.71	0.71
2:E:239:ILE:HD13	2:E:537:PHE:HB3	1.74	0.70
2:E:237:LEU:HD12	2:E:523:ARG:HG3	1.73	0.70
1:A:627:VAL:HG12	1:A:632:THR:HG22	1.74	0.70
2:D:284:VAL:HG12	2:D:285:VAL:HG23	1.74	0.69
1:C:408:TYR:CE2	2:F:433:TYR:HE1	2.10	0.69
2:D:257:THR:HG23	2:D:259:LYS:H	1.57	0.69
1:A:365:LEU:CD1	1:A:410:LEU:CD1	2.70	0.69
1:C:406:THR:HG21	2:F:378:ARG:HH21	1.58	0.68
2:D:353:LYS:HD3	2:D:376:TRP:O	1.93	0.68
1:A:398:TRP:CH2	2:D:255:PRO:HB2	2.29	0.68
2:F:207:LYS:HG2	2:F:208:LYS:HG2	1.76	0.68
2:E:121:PHE:HD1	2:E:145:SER:HB3	1.58	0.68
2:E:349:ALA:HB2	2:E:382:VAL:HG23	1.74	0.68
1:C:305:PRO:CD	1:C:337:SER:CB	2.71	0.67
1:B:462:THR:O	1:B:466:CYS:HB2	1.93	0.67
1:C:305:PRO:HG3	1:C:337:SER:CB	2.24	0.67
2:E:321:ILE:HG22	2:E:322:GLN:HG3	1.76	0.67
2:F:411:TYR:HB3	2:F:420:PHE:HB3	1.77	0.67
1:C:402:ILE:CG2	1:C:414:PHE:CE1	2.75	0.67
1:C:339:ARG:HD2	1:C:339:ARG:N	2.10	0.67
1:C:461:GLY:HA3	1:C:465:GLU:OE2	1.94	0.67
2:D:265:TRP:HA	2:D:271:THR:O	1.93	0.67
1:B:461:GLY:HA3	1:B:465:GLU:OE2	1.94	0.66
1:B:585:LYS:HE3	1:B:588:ASP:HA	1.77	0.66
2:F:339:LYS:HZ2	2:F:342:ASN:HA	1.61	0.66
1:C:305:PRO:HD2	1:C:337:SER:HB2	1.78	0.66
1:C:345:ILE:HD12	1:C:381:ILE:HG21	1.73	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:538:VAL:HG13	1:A:538:VAL:O	1.94	0.65
1:A:585:LYS:HE3	1:A:588:ASP:HA	1.77	0.65
1:A:280:GLN:HE22	1:A:413:LYS:HA	1.60	0.65
2:D:264:GLU:HB3	2:D:275:TYR:CD1	2.30	0.65
2:E:400:ILE:HG12	2:E:410:ILE:HB	1.78	0.65
1:A:247:ASN:HB2	1:A:292:THR:HG23	1.79	0.65
1:A:622:THR:O	1:A:636:SER:HA	1.97	0.65
2:D:454:ASP:HA	2:D:472:PRO:HA	1.79	0.65
2:D:51:ASP:OD2	2:E:542:LYS:HE2	1.96	0.64
2:E:265:TRP:HA	2:E:271:THR:O	1.96	0.64
1:C:380:ILE:HG23	1:C:421:GLU:OE1	1.97	0.64
2:F:424:THR:HG23	3:F:601:NAG:H83	1.79	0.64
1:B:385:ARG:HB2	1:B:385:ARG:NH1	2.10	0.64
1:C:280:GLN:HE22	1:C:413:LYS:HA	1.60	0.64
2:D:432:VAL:HG13	2:D:449:THR:O	1.97	0.64
1:B:557:ILE:O	1:B:613:ARG:HG3	1.98	0.64
2:E:339:LYS:HZ2	2:E:342:ASN:HA	1.61	0.64
1:C:585:LYS:HE3	1:C:588:ASP:HA	1.78	0.63
2:E:264:GLU:HB3	2:E:275:TYR:CD1	2.32	0.63
2:E:429:MET:HE3	2:E:448:LEU:HD22	1.79	0.63
2:E:454:ASP:HA	2:E:472:PRO:HA	1.79	0.63
2:E:49:THR:HB	2:E:52:ASN:HB3	1.80	0.63
1:C:329:LEU:HD23	1:C:357:VAL:HG23	1.81	0.63
2:D:239:ILE:HD13	2:D:537:PHE:HB3	1.81	0.63
1:B:280:GLN:HE22	1:B:413:LYS:HA	1.64	0.63
2:E:207:LYS:HG2	2:E:208:LYS:HG2	1.81	0.63
1:C:462:THR:OG1	1:C:465:GLU:HB3	1.99	0.63
2:F:121:PHE:CE2	2:F:145:SER:HB2	2.33	0.63
2:E:350:ASP:OD2	2:E:355:GLY:HA3	1.99	0.62
2:F:389:ARG:NH1	2:F:412:GLN:HB2	2.14	0.62
1:B:384:LYS:HB2	1:B:612:PRO:O	2.00	0.62
2:D:301:GLN:HB2	2:D:305:GLY:HA3	1.79	0.62
2:F:264:GLU:HB3	2:F:275:TYR:CD1	2.33	0.62
1:A:473:CYS:HB3	1:A:483:SER:HB3	1.82	0.62
1:C:539:GLN:O	1:C:549:THR:HG22	2.00	0.62
2:F:321:ILE:HG22	2:F:322:GLN:HG3	1.82	0.62
2:F:454:ASP:HA	2:F:472:PRO:HA	1.82	0.61
2:D:400:ILE:HG12	2:D:410:ILE:HG22	1.82	0.61
1:A:537:GLY:O	1:A:538:VAL:HG12	2.01	0.61
2:E:121:PHE:CD1	2:E:145:SER:HB3	2.35	0.61
2:D:350:ASP:OD2	2:D:355:GLY:HA3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:49:THR:HB	2:F:52:ASN:HB3	1.84	0.60
2:F:350:ASP:OD2	2:F:355:GLY:HA3	2.01	0.60
2:E:411:TYR:HB3	2:E:420:PHE:HB3	1.82	0.60
1:A:662:MET:HE2	1:A:671:VAL:HG12	1.83	0.60
1:C:305:PRO:HG3	1:C:337:SER:HB3	1.82	0.60
2:E:239:ILE:HG12	2:E:252:ILE:HG12	1.83	0.60
1:C:336:GLU:HG2	2:F:376:TRP:CD1	2.36	0.60
2:F:301:GLN:HB2	2:F:305:GLY:HA3	1.84	0.60
1:B:334:GLN:OE1	2:E:353:LYS:HE2	2.02	0.60
1:B:381:ILE:HD12	1:B:614:LEU:HB3	1.83	0.60
2:F:387:ILE:HG22	2:F:444:VAL:HG21	1.84	0.60
1:A:384:LYS:HB2	1:A:612:PRO:O	2.02	0.60
2:F:385:LEU:HD21	2:F:400:ILE:HD11	1.82	0.60
1:B:538:VAL:HG22	1:B:538:VAL:O	2.02	0.59
2:D:207:LYS:HG2	2:D:208:LYS:HG2	1.85	0.59
1:C:287:LEU:HD21	1:C:290:MET:HE3	1.85	0.59
1:C:538:VAL:O	1:C:538:VAL:HG22	2.01	0.59
1:B:338:SER:HB2	2:E:354:ALA:HA	1.84	0.59
1:C:662:MET:HE2	1:C:671:VAL:HG12	1.85	0.59
1:B:247:ASN:HB2	1:B:292:THR:HG23	1.85	0.58
1:B:504:ARG:HH11	1:B:514:GLU:HG3	1.69	0.58
1:B:384:LYS:HG3	1:B:613:ARG:O	2.04	0.58
1:B:605:CYS:HB2	1:B:608:ILE:HD13	1.85	0.58
1:A:605:CYS:HB2	1:A:608:ILE:HD13	1.85	0.58
1:C:504:ARG:HB3	1:C:514:GLU:HG2	1.85	0.58
1:B:403:MET:CE	1:B:403:MET:CA	2.70	0.58
1:C:398:TRP:HH2	2:F:284:VAL:HG22	1.62	0.58
2:D:473:SER:C	2:D:474:ARG:HD3	2.29	0.58
2:E:144:LEU:HB3	2:E:165:LEU:CD1	2.33	0.58
1:C:305:PRO:CG	1:C:337:SER:CB	2.81	0.57
1:C:605:CYS:HB2	1:C:608:ILE:HD13	1.85	0.57
2:F:456:LYS:HB3	2:F:470:ARG:HG2	1.86	0.57
1:C:334:GLN:HG2	2:F:353:LYS:NZ	2.18	0.57
1:C:340:SER:OG	1:C:369:THR:HG23	2.05	0.57
2:D:262:PHE:HB3	2:D:275:TYR:CE1	2.40	0.57
2:E:295:LEU:HB3	2:E:311:ARG:HB3	1.87	0.57
1:B:493:LYS:HB2	1:B:493:LYS:NZ	2.20	0.57
1:C:383:ASP:HB3	1:C:386:LYS:HB2	1.87	0.57
2:F:239:ILE:HG12	2:F:252:ILE:HG12	1.87	0.57
1:A:398:TRP:CH2	2:D:255:PRO:CB	2.88	0.57
1:C:361:GLY:H	1:C:366:MET:HE2	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:301:GLN:HB2	2:E:305:GLY:HA3	1.87	0.57
1:B:374:LEU:O	1:B:378:ILE:HB	2.05	0.56
2:F:401:LEU:HD12	2:F:401:LEU:C	2.28	0.56
1:B:662:MET:HE2	1:B:671:VAL:HG12	1.87	0.56
1:C:359:GLU:OE2	2:F:353:LYS:HE3	2.06	0.56
1:A:329:LEU:HD23	1:A:357:VAL:HG23	1.87	0.56
1:B:504:ARG:HB3	1:B:514:GLU:HG2	1.86	0.56
1:C:384:LYS:HG3	1:C:613:ARG:O	2.04	0.56
2:F:265:TRP:HA	2:F:271:THR:O	2.06	0.56
2:F:456:LYS:HD3	2:F:470:ARG:HG2	1.88	0.56
1:C:334:GLN:HG2	2:F:353:LYS:HZ1	1.71	0.56
1:A:374:LEU:O	1:A:378:ILE:HB	2.06	0.55
1:C:247:ASN:HB2	1:C:292:THR:HG23	1.87	0.55
2:E:522:PRO:HA	2:E:539:SER:O	2.06	0.55
1:A:625:LEU:HD11	3:A:803:NAG:H82	1.88	0.55
1:A:348:ILE:HD11	1:A:425:PHE:CE2	2.41	0.55
2:D:432:VAL:HG22	2:D:450:ARG:HG3	1.88	0.55
1:B:472:GLU:HB3	1:B:494:CYS:SG	2.46	0.55
2:E:387:ILE:HG22	2:E:444:VAL:HG21	1.89	0.55
1:A:558:TRP:CD1	1:A:608:ILE:HD11	2.42	0.55
2:E:165:LEU:CD2	2:E:168:VAL:HG23	2.33	0.55
2:F:389:ARG:HH12	2:F:412:GLN:HB2	1.70	0.55
1:A:320:ILE:HG23	1:A:322:GLU:HG2	1.88	0.55
1:C:340:SER:HB2	1:C:359:GLU:CG	2.36	0.55
1:C:504:ARG:HH11	1:C:514:GLU:HG3	1.70	0.55
1:B:348:ILE:HD11	1:B:425:PHE:CE2	2.41	0.55
2:F:310:LYS:HB3	2:F:321:ILE:HG13	1.87	0.55
2:D:359:ILE:HD11	2:D:373:LEU:HD11	1.89	0.55
2:F:396:THR:HB	2:F:398:HIS:HE1	1.72	0.55
1:B:329:LEU:HD23	1:B:357:VAL:HG23	1.88	0.55
1:C:401:CYS:O	1:C:411:PRO:HB3	2.06	0.54
2:F:121:PHE:CD2	2:F:145:SER:HB2	2.42	0.54
1:B:317:ARG:HG3	1:B:351:LEU:HD21	1.89	0.54
1:C:398:TRP:NE1	1:C:409:TYR:CG	2.75	0.54
2:F:174:SER:HB2	2:F:201:GLU:HG2	1.90	0.54
1:A:386:LYS:HG2	1:A:391:GLU:OE2	2.08	0.54
1:B:383:ASP:HB3	1:B:386:LYS:HB2	1.90	0.54
1:B:473:CYS:HB3	1:B:483:SER:HB3	1.88	0.54
2:E:262:PHE:HB3	2:E:275:TYR:CE1	2.43	0.54
1:A:381:ILE:HD12	1:A:614:LEU:HB3	1.89	0.54
1:C:397:THR:HG22	2:F:282:SER:OG	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:558:TRP:CD1	1:C:608:ILE:HD11	2.42	0.54
2:D:239:ILE:HG12	2:D:252:ILE:HG12	1.89	0.54
1:B:502:VAL:HG22	1:B:515:THR:HG22	1.89	0.54
2:E:174:SER:HB2	2:E:201:GLU:HG2	1.90	0.54
1:A:256:ARG:O	1:A:257:LEU:HB2	2.07	0.54
1:B:558:TRP:CD1	1:B:608:ILE:HD11	2.43	0.54
1:B:402:ILE:HG12	1:B:413:LYS:O	2.08	0.53
1:B:680:LEU:O	1:B:688:CYS:HA	2.08	0.53
2:D:165:LEU:HD11	2:D:167:ASN:O	2.08	0.53
2:E:359:ILE:HD11	2:E:373:LEU:HD11	1.90	0.53
1:A:287:LEU:HD21	1:A:290:MET:HE3	1.90	0.53
2:D:87:PHE:HZ	2:D:98:PHE:HZ	1.57	0.53
1:A:255:HIS:O	1:A:256:ARG:HB2	2.08	0.53
1:A:410:LEU:H	1:A:410:LEU:HD22	1.73	0.53
1:B:368:VAL:HG21	1:B:410:LEU:HD11	1.91	0.53
2:D:353:LYS:HE2	2:D:376:TRP:O	2.09	0.53
2:E:286:CYS:SG	2:E:299:VAL:HB	2.48	0.53
1:A:398:TRP:CZ3	2:D:255:PRO:CB	2.88	0.53
1:C:348:ILE:HD11	1:C:425:PHE:CE2	2.44	0.53
2:F:153:THR:HG21	2:F:180:LYS:HE3	1.90	0.53
1:C:384:LYS:HB2	1:C:612:PRO:O	2.08	0.53
1:A:402:ILE:HG12	1:A:413:LYS:O	2.08	0.53
1:C:410:LEU:H	1:C:410:LEU:CD2	2.20	0.52
2:E:192:ASN:N	2:E:192:ASN:HD22	2.06	0.52
2:E:216:SER:HA	2:E:219:PHE:HD2	1.75	0.52
1:B:287:LEU:HD21	1:B:290:MET:HE3	1.90	0.52
2:D:387:ILE:HG22	2:D:444:VAL:HG21	1.91	0.52
2:F:262:PHE:HB3	2:F:275:TYR:CE1	2.44	0.52
1:B:361:GLY:H	1:B:366:MET:HE2	1.75	0.52
2:D:171:ARG:NH1	2:D:196:GLU:HG3	2.25	0.52
1:B:556:TYR:O	1:B:613:ARG:HD2	2.10	0.52
1:C:385:ARG:HG3	1:C:611:ILE:HG23	1.92	0.52
1:A:385:ARG:HG3	1:A:611:ILE:HG23	1.92	0.52
1:A:462:THR:O	1:A:466:CYS:HB2	2.08	0.51
1:B:402:ILE:HG12	1:B:413:LYS:C	2.35	0.51
2:D:174:SER:HB2	2:D:201:GLU:HG2	1.92	0.51
1:A:361:GLY:H	1:A:366:MET:HE2	1.74	0.51
1:C:374:LEU:O	1:C:378:ILE:HB	2.10	0.51
2:F:450:ARG:CG	2:F:452:ILE:O	2.53	0.51
1:C:340:SER:OG	1:C:369:THR:CG2	2.59	0.51
1:C:305:PRO:HD3	1:C:337:SER:HB2	1.89	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:123:GLU:CD	2:E:474:ARG:HH12	2.19	0.51
2:D:142:ILE:O	2:D:165:LEU:HD12	2.11	0.51
1:C:401:CYS:C	1:C:411:PRO:HB3	2.36	0.51
2:F:171:ARG:NH1	2:F:196:GLU:HG3	2.26	0.51
1:C:484:GLN:HB3	1:C:496:PHE:CE2	2.46	0.51
2:D:236:SER:O	2:D:539:SER:HB2	2.10	0.51
2:F:522:PRO:HA	2:F:539:SER:O	2.11	0.51
1:A:556:TYR:O	1:A:613:ARG:HD3	2.11	0.51
1:B:622:THR:O	1:B:636:SER:HA	2.10	0.51
2:D:522:PRO:HA	2:D:539:SER:O	2.11	0.51
2:D:168:VAL:HB	2:D:195:VAL:HG22	1.93	0.50
2:F:165:LEU:HD11	2:F:167:ASN:O	2.10	0.50
1:A:345:ILE:HD12	1:A:381:ILE:HG21	1.79	0.50
1:A:384:LYS:CG	1:A:613:ARG:O	2.59	0.50
2:E:396:THR:HB	2:E:398:HIS:HE1	1.75	0.50
2:F:298:ILE:HG13	2:F:308:ILE:HG12	1.93	0.50
2:D:152:GLN:HA	2:D:174:SER:O	2.11	0.50
1:B:307:ILE:O	1:B:311:GLU:HG2	2.11	0.50
1:B:368:VAL:CG2	1:B:410:LEU:HD11	2.42	0.50
1:A:504:ARG:HH11	1:A:514:GLU:HG3	1.76	0.50
1:B:462:THR:H	1:B:465:GLU:HG2	1.77	0.50
2:F:142:ILE:O	2:F:165:LEU:HD12	2.12	0.50
1:A:303:GLU:CD	1:A:303:GLU:H	2.20	0.50
1:A:317:ARG:HG3	1:A:351:LEU:HD21	1.94	0.50
1:A:386:LYS:HB3	1:A:391:GLU:HB3	1.94	0.50
1:B:359:GLU:OE2	2:E:353:LYS:HE3	2.12	0.50
2:E:281:THR:O	2:E:301:GLN:HB3	2.12	0.50
1:A:624:THR:HG22	1:A:625:LEU:H	1.77	0.49
1:C:320:ILE:HG23	1:C:322:GLU:HG2	1.93	0.49
1:C:551:ASP:HA	1:C:564:ALA:HB2	1.94	0.49
2:E:216:SER:HA	2:E:219:PHE:CD2	2.47	0.49
2:F:281:THR:O	2:F:301:GLN:HB3	2.12	0.49
2:F:350:ASP:CG	2:F:355:GLY:HA3	2.37	0.49
1:B:453:GLU:HB2	1:B:456:GLU:OE2	2.12	0.49
1:B:458:CYS:HB2	1:B:486:SER:HB2	1.94	0.49
2:D:232:LEU:HB2	2:D:545:THR:HB	1.94	0.49
1:B:473:CYS:HB3	1:B:483:SER:CB	2.43	0.49
1:B:530:MET:HE2	1:B:531:ASP:O	2.12	0.49
1:C:398:TRP:NE1	1:C:409:TYR:CD2	2.76	0.49
1:B:320:ILE:HG23	1:B:322:GLU:HG2	1.93	0.49
2:F:530:ILE:HG22	2:F:531:ASN:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:492:LYS:HG2	1:B:493:LYS:HD3	1.95	0.49
1:B:303:GLU:H	1:B:303:GLU:CD	2.21	0.49
1:B:624:THR:HG22	1:B:625:LEU:H	1.76	0.49
2:F:332:PRO:HA	2:F:349:ALA:O	2.13	0.49
2:D:472:PRO:HB2	2:D:474:ARG:HH12	1.78	0.49
2:F:152:GLN:HA	2:F:174:SER:O	2.13	0.49
1:B:445:PRO:HA	1:B:453:GLU:OE2	2.13	0.49
2:D:281:THR:O	2:D:301:GLN:HB3	2.12	0.49
1:C:398:TRP:CH2	2:F:284:VAL:CG2	2.90	0.49
1:C:624:THR:HG22	1:C:625:LEU:H	1.77	0.49
1:A:348:ILE:HD11	1:A:425:PHE:HE2	1.77	0.48
1:A:384:LYS:HE3	1:A:615:GLY:N	2.28	0.48
2:E:232:LEU:HB2	2:E:545:THR:HB	1.96	0.48
2:F:429:MET:HE3	2:F:448:LEU:HD22	1.93	0.48
1:C:381:ILE:HD12	1:C:614:LEU:HB3	1.95	0.48
1:C:462:THR:O	1:C:466:CYS:HB2	2.13	0.48
1:C:622:THR:O	1:C:636:SER:HA	2.13	0.48
2:F:49:THR:HG22	2:F:50:LYS:N	2.29	0.48
2:F:88:LEU:HD23	2:F:113:GLY:HA3	1.95	0.48
1:C:251:MET:HE3	1:C:330:PHE:HB3	1.94	0.48
1:C:473:CYS:HB3	1:C:483:SER:CB	2.44	0.48
2:D:298:ILE:HG13	2:D:308:ILE:HG12	1.96	0.48
1:A:445:PRO:HA	1:A:453:GLU:OE2	2.14	0.48
2:D:396:THR:HB	2:D:398:HIS:HE1	1.79	0.48
2:D:530:ILE:HB	2:D:533:ARG:HB2	1.96	0.48
2:D:295:LEU:HB3	2:D:311:ARG:HB3	1.96	0.48
2:E:262:PHE:HB3	2:E:275:TYR:CZ	2.49	0.48
2:D:332:PRO:HA	2:D:349:ALA:O	2.14	0.48
2:E:49:THR:HG22	2:E:50:LYS:N	2.28	0.48
1:C:303:GLU:CD	1:C:303:GLU:H	2.22	0.48
1:A:483:SER:HA	1:A:494:CYS:O	2.14	0.47
1:B:348:ILE:HD11	1:B:425:PHE:HE2	1.77	0.47
1:B:348:ILE:HD13	1:B:431:GLY:HA2	1.96	0.47
1:C:408:TYR:HE2	2:F:433:TYR:HE1	1.57	0.47
2:D:49:THR:HG22	2:D:50:LYS:N	2.29	0.47
2:F:419:LEU:HD23	2:F:419:LEU:HA	1.63	0.47
2:E:168:VAL:HB	2:E:195:VAL:HG22	1.96	0.47
2:E:265:TRP:H	2:E:265:TRP:CD1	2.33	0.47
2:E:332:PRO:HA	2:E:349:ALA:O	2.14	0.47
1:C:502:VAL:HG22	1:C:515:THR:HG22	1.95	0.47
1:B:385:ARG:HG3	1:B:386:LYS:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:152:GLN:HA	2:E:174:SER:O	2.14	0.47
2:E:429:MET:SD	2:E:456:LYS:HE3	2.55	0.47
2:F:550:HIS:NE2	2:F:552:ILE:HD11	2.29	0.47
1:A:485:CYS:HB3	1:A:496:PHE:CE1	2.50	0.47
2:D:232:LEU:HD11	2:D:547:ILE:HD11	1.97	0.47
2:F:168:VAL:HB	2:F:195:VAL:HG22	1.97	0.47
2:F:415:LYS:HB2	2:F:415:LYS:NZ	2.29	0.47
1:A:380:ILE:HG23	1:A:421:GLU:OE1	2.14	0.47
1:A:402:ILE:HG12	1:A:413:LYS:C	2.40	0.47
1:B:403:MET:N	1:B:403:MET:SD	2.88	0.47
1:C:348:ILE:HD11	1:C:425:PHE:HE2	1.79	0.47
2:D:472:PRO:HB2	2:D:474:ARG:HH22	1.79	0.47
1:C:530:MET:HE2	1:C:531:ASP:O	2.15	0.47
2:D:121:PHE:CD1	2:D:145:SER:HB3	2.50	0.47
2:E:87:PHE:HZ	2:E:98:PHE:HZ	1.63	0.47
2:E:142:ILE:HA	2:E:165:LEU:HA	1.96	0.47
2:E:144:LEU:CB	2:E:165:LEU:CD1	2.93	0.47
2:F:260:CYS:HB3	2:F:278:ILE:HB	1.96	0.47
2:F:339:LYS:HZ1	2:F:342:ASN:HA	1.78	0.47
1:B:504:ARG:HB3	1:B:514:GLU:CG	2.45	0.46
2:F:501:VAL:HG21	2:F:517:LEU:HD13	1.97	0.46
1:B:445:PRO:HA	1:B:453:GLU:CD	2.40	0.46
2:F:283:THR:HG22	2:F:301:GLN:HG2	1.97	0.46
2:F:232:LEU:HD11	2:F:547:ILE:HD11	1.96	0.46
1:A:320:ILE:CG2	1:A:322:GLU:HG2	2.46	0.46
1:A:530:MET:HB2	1:A:530:MET:HE3	1.84	0.46
1:C:317:ARG:HG3	1:C:351:LEU:HD21	1.97	0.46
2:E:187:TRP:O	2:E:191:THR:HG22	2.16	0.46
2:F:286:CYS:SG	2:F:299:VAL:HB	2.55	0.46
2:F:373:LEU:HD22	2:F:411:TYR:CE2	2.51	0.46
1:C:398:TRP:NE1	1:C:409:TYR:CD1	2.82	0.46
1:A:348:ILE:HD13	1:A:431:GLY:HA2	1.98	0.46
1:A:530:MET:HE2	1:A:531:ASP:O	2.15	0.46
1:A:540:GLY:HA3	1:A:549:THR:HG22	1.98	0.46
1:C:348:ILE:HD13	1:C:431:GLY:HA2	1.98	0.46
2:E:298:ILE:HG13	2:E:308:ILE:HG12	1.98	0.46
2:E:530:ILE:HB	2:E:533:ARG:HB2	1.97	0.46
1:B:385:ARG:HH11	1:B:385:ARG:CG	2.28	0.46
1:B:462:THR:HB	1:B:463:PRO:HD2	1.97	0.46
1:B:659:PRO:O	1:B:661:MET:HG3	2.16	0.46
1:C:305:PRO:HB2	1:C:342:ALA:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:49:THR:HB	2:D:52:ASN:HB2	1.98	0.46
2:D:484:ILE:O	2:D:487:TYR:HB2	2.15	0.46
1:A:453:GLU:HB2	1:A:456:GLU:OE2	2.14	0.46
2:D:180:LYS:O	2:D:183:TRP:CD1	2.69	0.46
1:A:383:ASP:HB3	1:A:386:LYS:HB2	1.98	0.46
2:D:530:ILE:HG22	2:D:531:ASN:H	1.80	0.46
2:F:170:LEU:HB2	2:F:198:ILE:HG21	1.96	0.46
1:C:659:PRO:O	1:C:661:MET:HG3	2.15	0.45
2:F:329:ILE:HA	2:F:350:ASP:OD2	2.15	0.45
1:A:378:ILE:HD11	1:A:434:LEU:HD21	1.97	0.45
1:C:473:CYS:HB3	1:C:483:SER:HB3	1.98	0.45
2:E:478:VAL:HB	2:E:523:ARG:O	2.15	0.45
2:F:234:TYR:HE1	2:F:252:ILE:HG21	1.80	0.45
2:D:109:ASP:OD1	2:D:136:ARG:HD2	2.16	0.45
1:A:538:VAL:O	1:A:538:VAL:CG1	2.63	0.45
1:C:506:ALA:HB1	1:C:511:ASP:HB3	1.98	0.45
2:E:339:LYS:HZ1	2:E:342:ASN:HA	1.79	0.45
1:B:485:CYS:HB3	1:B:496:PHE:CE1	2.51	0.45
2:D:501:VAL:HG21	2:D:517:LEU:HD13	1.97	0.45
1:A:255:HIS:O	1:A:256:ARG:CB	2.64	0.45
1:A:458:CYS:HB2	1:A:486:SER:HB2	1.98	0.45
1:A:506:ALA:HB1	1:A:511:ASP:HB3	1.99	0.45
1:C:263:ASN:O	1:C:267:LYS:HG3	2.16	0.45
1:C:485:CYS:HB3	1:C:496:PHE:CE1	2.51	0.45
2:D:298:ILE:HG22	2:D:335:ILE:HD13	1.99	0.45
2:D:82:ILE:HG22	2:D:110:ALA:HB1	1.99	0.45
2:D:84:GLU:H	2:D:84:GLU:CD	2.25	0.45
2:D:235:GLN:O	2:D:254:GLN:HG3	2.16	0.45
2:D:265:TRP:CD1	2:D:265:TRP:H	2.35	0.45
2:D:472:PRO:HB2	2:D:474:ARG:NH1	2.31	0.45
2:E:235:GLN:O	2:E:254:GLN:HG3	2.17	0.45
2:F:148:ASN:HA	2:F:172:GLY:O	2.17	0.45
2:F:232:LEU:HB2	2:F:545:THR:HB	1.98	0.45
2:F:99:THR:HA	2:F:123:GLU:O	2.17	0.45
2:F:429:MET:SD	2:F:456:LYS:HE3	2.57	0.45
1:C:403:MET:CA	1:C:403:MET:CE	2.76	0.45
2:E:330:ARG:HD2	2:E:354:ALA:HB3	1.99	0.45
1:B:551:ASP:HA	1:B:564:ALA:HB2	1.99	0.45
1:C:497:GLN:HG3	1:C:498:PRO:HD2	1.99	0.45
2:F:265:TRP:CD1	2:F:265:TRP:H	2.35	0.45
2:F:341:GLU:OE2	2:F:415:LYS:HD3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:ILE:HD13	1:A:378:ILE:HA	1.80	0.44
1:A:485:CYS:HB3	1:A:496:PHE:HE1	1.81	0.44
1:B:320:ILE:CG2	1:B:322:GLU:HG2	2.46	0.44
1:B:529:LYS:HB3	1:B:533:TYR:CD2	2.52	0.44
1:C:305:PRO:HD3	1:C:337:SER:CB	2.44	0.44
2:E:410:ILE:HG23	2:E:424:THR:O	2.17	0.44
2:D:148:ASN:HA	2:D:172:GLY:O	2.17	0.44
2:E:493:GLY:HA2	2:E:499:THR:HG23	2.00	0.44
1:C:320:ILE:CG2	1:C:322:GLU:HG2	2.47	0.44
2:F:235:GLN:O	2:F:254:GLN:HG3	2.18	0.44
2:F:371:GLN:HB2	2:F:419:LEU:CD2	2.47	0.44
1:A:233:ASN:O	1:A:237:GLU:HG3	2.17	0.44
2:E:396:THR:HB	2:E:398:HIS:CE1	2.52	0.44
1:A:579:GLU:CD	1:A:579:GLU:H	2.25	0.44
1:A:707:ILE:HG13	1:A:713:THR:HB	1.98	0.44
2:D:49:THR:N	2:D:52:ASN:O	2.51	0.44
2:D:96:LEU:HB3	2:D:120:LEU:HD13	1.99	0.44
2:E:109:ASP:OD1	2:E:136:ARG:HD2	2.18	0.44
2:E:165:LEU:CD2	2:E:168:VAL:HG22	2.37	0.44
2:F:236:SER:O	2:F:539:SER:HB2	2.18	0.44
2:F:401:LEU:HD21	2:F:411:TYR:HE2	1.83	0.44
1:A:659:PRO:O	1:A:661:MET:HG3	2.18	0.44
1:A:700:CYS:HB2	1:A:709:SER:O	2.17	0.44
2:E:357:THR:OG1	2:E:379:ASP:OD2	2.25	0.44
1:B:530:MET:HB2	1:B:530:MET:HE3	1.82	0.44
1:C:339:ARG:N	1:C:339:ARG:CD	2.80	0.44
2:F:109:ASP:OD1	2:F:136:ARG:HD2	2.18	0.44
1:A:263:ASN:O	1:A:267:LYS:HG3	2.18	0.44
1:C:601:GLY:O	1:C:651:VAL:HG23	2.18	0.44
2:D:49:THR:HG22	2:D:50:LYS:H	1.83	0.44
2:D:341:GLU:OE1	2:D:415:LYS:HG3	2.18	0.44
2:F:371:GLN:HB2	2:F:419:LEU:HD21	1.99	0.44
1:C:348:ILE:HG13	1:C:377:ASN:O	2.18	0.43
1:C:643:GLU:HG3	1:C:645:ASP:H	1.83	0.43
2:D:84:GLU:HA	2:D:110:ALA:HA	2.00	0.43
2:D:472:PRO:HB2	2:D:474:ARG:NH2	2.33	0.43
2:E:49:THR:N	2:E:52:ASN:O	2.51	0.43
2:E:224:THR:HG22	2:E:552:ILE:HD12	1.99	0.43
2:E:298:ILE:HG22	2:E:335:ILE:HD13	1.99	0.43
1:A:445:PRO:HA	1:A:453:GLU:CD	2.43	0.43
1:B:386:LYS:HG2	1:B:391:GLU:OE2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:458:CYS:HB2	1:C:486:SER:HB2	1.98	0.43
1:C:579:GLU:H	1:C:579:GLU:CD	2.25	0.43
1:B:643:GLU:HG3	1:B:645:ASP:H	1.81	0.43
1:B:680:LEU:HB3	1:B:710:ASP:HB3	2.00	0.43
1:C:316:ARG:HG3	1:C:317:ARG:N	2.33	0.43
2:D:87:PHE:CZ	2:D:98:PHE:HZ	2.37	0.43
2:D:400:ILE:HA	2:D:409:VAL:O	2.17	0.43
2:E:399:LEU:O	2:E:410:ILE:HA	2.18	0.43
1:A:473:CYS:HB3	1:A:483:SER:CB	2.48	0.43
2:D:296:TYR:CD1	2:D:310:LYS:HB2	2.53	0.43
1:B:316:ARG:HG3	1:B:317:ARG:N	2.32	0.43
1:C:530:MET:HE1	1:C:677:SER:O	2.19	0.43
2:D:330:ARG:HD2	2:D:354:ALA:HB3	2.01	0.43
2:D:94:GLN:HA	2:D:117:LEU:HA	2.00	0.43
2:E:144:LEU:CB	2:E:165:LEU:HD11	2.45	0.43
2:E:148:ASN:HA	2:E:172:GLY:O	2.19	0.43
2:E:501:VAL:HG21	2:E:517:LEU:HD13	2.00	0.43
1:A:335:PHE:CD2	1:A:359:GLU:HB3	2.53	0.43
1:A:530:MET:HE1	1:A:677:SER:O	2.18	0.43
1:B:506:ALA:HB1	1:B:511:ASP:HB3	1.99	0.43
1:B:530:MET:HE1	1:B:677:SER:O	2.18	0.43
2:D:314:PHE:HD1	2:D:314:PHE:HA	1.70	0.43
2:D:447:CYS:HB3	2:D:479:PHE:CD2	2.54	0.43
2:E:550:HIS:NE2	2:E:552:ILE:HD11	2.34	0.43
2:E:530:ILE:HG22	2:E:531:ASN:H	1.83	0.43
2:F:87:PHE:CZ	2:F:96:LEU:HD21	2.54	0.43
1:B:510:CYS:O	1:B:528:HIS:HB2	2.18	0.43
2:D:170:LEU:HB2	2:D:198:ILE:HG21	1.99	0.43
1:C:530:MET:HE3	1:C:530:MET:HB2	1.80	0.43
1:C:707:ILE:HG13	1:C:713:THR:HB	2.01	0.43
2:D:474:ARG:HD3	2:D:474:ARG:N	2.34	0.43
2:E:268:VAL:HG12	2:E:269:GLU:HG3	2.01	0.43
1:A:305:PRO:HB2	1:A:342:ALA:HB2	2.00	0.42
2:D:104:ASP:O	2:D:128:LYS:HB2	2.19	0.42
2:D:385:LEU:HD21	2:D:400:ILE:HD12	1.99	0.42
2:F:87:PHE:HZ	2:F:98:PHE:HZ	1.66	0.42
2:F:396:THR:HB	2:F:398:HIS:CE1	2.51	0.42
2:E:49:THR:HG23	2:F:520:GLN:OE1	2.19	0.42
2:E:505:ASP:HB3	2:E:508:LYS:HB2	2.01	0.42
1:C:445:PRO:HA	1:C:453:GLU:OE2	2.18	0.42
2:D:321:ILE:HG22	2:D:322:GLN:HG3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:493:GLY:HA2	2:D:499:THR:HG23	2.01	0.42
2:D:242:PHE:CZ	2:D:249:TYR:HB2	2.55	0.42
2:F:262:PHE:HB3	2:F:275:TYR:CZ	2.53	0.42
1:B:407:GLY:HA2	2:E:331:LYS:HG3	2.01	0.42
2:D:49:THR:HG23	2:E:520:GLN:OE1	2.19	0.42
2:E:94:GLN:HA	2:E:117:LEU:HA	2.00	0.42
1:B:679:CYS:HB3	1:B:700:CYS:SG	2.59	0.42
2:F:298:ILE:HG22	2:F:335:ILE:HD13	2.02	0.42
2:D:396:THR:HB	2:D:398:HIS:CE1	2.55	0.42
2:E:177:CYS:HA	2:E:181:LEU:HD12	2.02	0.42
1:C:293:TRP:CE3	1:C:297:ASN:HA	2.55	0.42
1:C:338:SER:HB2	1:C:339:ARG:HD2	2.00	0.42
2:D:451:PHE:CE1	2:D:475:GLY:HA2	2.55	0.42
1:A:408:TYR:CE2	2:D:433:TYR:HE1	2.37	0.42
2:D:230:GLN:HB3	2:D:547:ILE:HD12	2.01	0.42
2:F:94:GLN:HB2	2:F:95:LEU:HD12	2.02	0.42
1:A:601:GLY:O	1:A:651:VAL:HG23	2.20	0.42
1:B:625:LEU:HD13	3:B:803:NAG:O7	2.20	0.42
2:E:451:PHE:CE1	2:E:475:GLY:HA2	2.55	0.42
2:F:331:LYS:HA	2:F:331:LYS:HD3	1.83	0.42
2:F:371:GLN:OE1	2:F:420:PHE:HD1	2.03	0.42
2:D:88:LEU:HD23	2:D:113:GLY:HA3	2.02	0.41
2:D:429:MET:CE	2:D:456:LYS:HD2	2.50	0.41
2:E:234:TYR:HE1	2:E:252:ILE:HG21	1.84	0.41
2:E:296:TYR:CE1	2:E:310:LYS:HD2	2.55	0.41
1:A:406:THR:O	2:D:352:SER:HA	2.20	0.41
1:C:453:GLU:HB2	1:C:456:GLU:OE2	2.19	0.41
2:E:356:PHE:HZ	2:E:376:TRP:CH2	2.37	0.41
2:F:49:THR:N	2:F:52:ASN:O	2.53	0.41
2:F:330:ARG:HD2	2:F:354:ALA:HB3	2.01	0.41
1:B:263:ASN:O	1:B:267:LYS:HG3	2.20	0.41
2:D:238:SER:C	2:D:239:ILE:HG13	2.46	0.41
1:B:378:ILE:HA	1:B:378:ILE:HD13	1.82	0.41
1:B:568:TYR:OH	1:B:572:LYS:HE3	2.20	0.41
2:D:333:ASN:HB3	2:D:380:THR:O	2.20	0.41
1:B:428:SER:OG	1:B:546:ARG:HG2	2.21	0.41
1:B:485:CYS:HB3	1:B:496:PHE:HE1	1.86	0.41
1:B:571:GLU:HA	1:B:598:VAL:HG21	2.02	0.41
1:C:246:VAL:O	1:C:329:LEU:HD12	2.20	0.41
2:F:383:GLU:N	2:F:400:ILE:O	2.53	0.41
1:A:519:ASN:HD22	3:A:801:NAG:C7	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:568:TYR:OH	1:A:572:LYS:HE3	2.20	0.41
1:B:348:ILE:HG13	1:B:377:ASN:O	2.21	0.41
1:B:466:CYS:SG	1:B:471:ALA:HA	2.61	0.41
1:C:305:PRO:HG3	1:C:337:SER:OG	2.20	0.41
1:C:398:TRP:CZ2	1:C:409:TYR:CE1	3.09	0.41
1:B:444:PRO:HA	1:B:445:PRO:HD3	1.96	0.41
1:C:571:GLU:HA	1:C:598:VAL:HG21	2.01	0.41
2:D:58:ALA:O	2:D:78:GLY:N	2.50	0.41
2:E:52:ASN:ND2	2:F:496:TYR:HA	2.36	0.41
2:E:385:LEU:HD21	2:E:400:ILE:HD12	2.01	0.41
2:F:362:TRP:CH2	2:F:364:GLY:HA2	2.55	0.41
2:F:410:ILE:O	2:F:423:GLN:HA	2.21	0.41
2:F:123:GLU:O	2:F:125:ASN:ND2	2.54	0.41
2:E:96:LEU:HB3	2:E:120:LEU:HD13	2.03	0.41
2:E:238:SER:C	2:E:239:ILE:HG13	2.46	0.41
1:A:251:MET:HE3	1:A:330:PHE:HB3	2.03	0.41
1:A:405:ASP:OD2	2:D:330:ARG:NH1	2.53	0.41
1:B:579:GLU:CD	1:B:579:GLU:H	2.30	0.41
2:F:456:LYS:HB3	2:F:470:ARG:HA	2.03	0.41
1:A:571:GLU:HA	1:A:598:VAL:HG21	2.03	0.40
1:C:245:ILE:HB	1:C:290:MET:HE2	2.03	0.40
1:C:568:TYR:OH	1:C:572:LYS:HE3	2.21	0.40
2:E:84:GLU:H	2:E:84:GLU:CD	2.29	0.40
1:B:601:GLY:O	1:B:651:VAL:HG23	2.21	0.40
1:C:462:THR:HB	1:C:463:PRO:HD2	2.03	0.40
2:D:262:PHE:HB3	2:D:275:TYR:CZ	2.56	0.40
2:D:310:LYS:HB3	2:D:321:ILE:HG13	2.03	0.40
2:D:432:VAL:HG12	2:D:433:TYR:N	2.36	0.40
2:D:531:ASN:C	2:D:533:ARG:H	2.28	0.40
2:E:54:LEU:HD21	2:F:498:PHE:CE1	2.56	0.40
2:E:94:GLN:HB2	2:E:95:LEU:HD12	2.03	0.40
2:E:242:PHE:CZ	2:E:249:TYR:HB2	2.56	0.40
2:F:445:TYR:CE2	2:F:459:LYS:HB2	2.56	0.40
2:F:447:CYS:HB3	2:F:479:PHE:CD2	2.56	0.40
1:A:341:GLY:CA	1:A:357:VAL:O	2.70	0.40
1:A:504:ARG:HB3	1:A:514:GLU:CG	2.51	0.40
1:B:644:GLU:CD	1:B:644:GLU:H	2.29	0.40
2:F:242:PHE:CZ	2:F:249:TYR:HB2	2.57	0.40
2:F:249:TYR:CE2	2:F:264:GLU:HB2	2.56	0.40
2:F:493:GLY:HA2	2:F:499:THR:HG23	2.03	0.40
1:B:397:THR:H	1:B:397:THR:HG22	1.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:402:ILE:HD13	1:C:402:ILE:HA	1.92	0.40
2:D:265:TRP:HE3	2:D:530:ILE:HG23	1.85	0.40
2:E:84:GLU:HA	2:E:110:ALA:HA	2.03	0.40
2:E:217:LYS:H	2:E:217:LYS:HG3	1.47	0.40
2:D:353:LYS:CD	2:D:376:TRP:O	2.66	0.40
2:E:408:PRO:HG3	2:E:432:VAL:HB	2.03	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	484/486 (100%)	463 (96%)	21 (4%)	0	100	100
1	B	484/486 (100%)	466 (96%)	18 (4%)	0	100	100
1	C	484/486 (100%)	465 (96%)	19 (4%)	0	100	100
2	D	513/526 (98%)	498 (97%)	15 (3%)	0	100	100
2	E	513/526 (98%)	497 (97%)	16 (3%)	0	100	100
2	F	513/526 (98%)	498 (97%)	15 (3%)	0	100	100
All	All	2991/3036 (98%)	2887 (96%)	104 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	420/420 (100%)	394 (94%)	26 (6%)	16	39
1	B	420/420 (100%)	391 (93%)	29 (7%)	14	37
1	C	420/420 (100%)	397 (94%)	23 (6%)	19	43
2	D	473/483 (98%)	444 (94%)	29 (6%)	17	40
2	E	473/483 (98%)	447 (94%)	26 (6%)	19	43
2	F	473/483 (98%)	451 (95%)	22 (5%)	23	46
All	All	2679/2709 (99%)	2524 (94%)	155 (6%)	18	42

All (155) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	284	ARG
1	A	301	ILE
1	A	316	ARG
1	A	322	GLU
1	A	338	SER
1	A	348	ILE
1	A	378	ILE
1	A	383	ASP
1	A	393	LYS
1	A	397	THR
1	A	406	THR
1	A	410	LEU
1	A	434	LEU
1	A	473	CYS
1	A	481	GLN
1	A	509	ASP
1	A	514	GLU
1	A	579	GLU
1	A	583	CYS
1	A	598	VAL
1	A	608	ILE
1	A	622	THR
1	A	669	LEU
1	A	678	THR
1	A	682	SER
1	A	717	HIS
1	B	284	ARG
1	B	301	ILE
1	B	316	ARG
1	B	322	GLU

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Mol	Chain	Res	Type
1	B	334	GLN
1	B	338	SER
1	B	348	ILE
1	B	378	ILE
1	B	385	ARG
1	B	393	LYS
1	B	397	THR
1	B	403	MET
1	B	434	LEU
1	B	465	GLU
1	B	467	VAL
1	B	473	CYS
1	B	481	GLN
1	B	493	LYS
1	B	514	GLU
1	B	579	GLU
1	B	583	CYS
1	B	598	VAL
1	B	608	ILE
1	B	613	ARG
1	B	622	THR
1	B	664	LEU
1	B	678	THR
1	B	682	SER
1	B	717	HIS
1	C	284	ARG
1	C	301	ILE
1	C	316	ARG
1	C	322	GLU
1	C	348	ILE
1	C	378	ILE
1	C	393	LYS
1	C	401	CYS
1	C	402	ILE
1	C	410	LEU
1	C	434	LEU
1	C	465	GLU
1	C	481	GLN
1	C	514	GLU
1	C	579	GLU
1	C	583	CYS
1	C	598	VAL

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Mol	Chain	Res	Type
1	C	608	ILE
1	C	622	THR
1	C	669	LEU
1	C	678	THR
1	C	682	SER
1	C	717	HIS
2	D	59	ARG
2	D	68	ASP
2	D	138	LEU
2	D	162	LEU
2	D	179	CYS
2	D	221	CYS
2	D	223	ILE
2	D	265	TRP
2	D	286	CYS
2	D	299	VAL
2	D	302	LEU
2	D	313	SER
2	D	314	PHE
2	D	333	ASN
2	D	342	ASN
2	D	353	LYS
2	D	374	HIS
2	D	385	LEU
2	D	403	SER
2	D	419	LEU
2	D	429	MET
2	D	463	SER
2	D	470	ARG
2	D	520	GLN
2	D	524	SER
2	D	531	ASN
2	D	544	ASN
2	D	552	ILE
2	D	553	VAL
2	E	59	ARG
2	E	68	ASP
2	E	162	LEU
2	E	192	ASN
2	E	194	THR
2	E	217	LYS
2	E	264	GLU

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Mol	Chain	Res	Type
2	E	265	TRP
2	E	286	CYS
2	E	299	VAL
2	E	302	LEU
2	E	310	LYS
2	E	313	SER
2	E	314	PHE
2	E	374	HIS
2	E	385	LEU
2	E	403	SER
2	E	410	ILE
2	E	463	SER
2	E	474	ARG
2	E	507	GLU
2	E	520	GLN
2	E	524	SER
2	E	531	ASN
2	E	539	SER
2	E	544	ASN
2	F	59	ARG
2	F	68	ASP
2	F	138	LEU
2	F	162	LEU
2	F	224	THR
2	F	264	GLU
2	F	265	TRP
2	F	268	VAL
2	F	286	CYS
2	F	299	VAL
2	F	302	LEU
2	F	303	PHE
2	F	313	SER
2	F	314	PHE
2	F	353	LYS
2	F	374	HIS
2	F	385	LEU
2	F	400	ILE
2	F	403	SER
2	F	520	GLN
2	F	524	SER
2	F	531	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	427	ASN
1	A	666	HIS
1	B	427	ASN
1	C	247	ASN
1	C	263	ASN
1	C	418	ASN
2	D	374	HIS
2	D	480	GLN
2	D	486	ASN
2	E	52	ASN
2	E	57	ASN
2	E	167	ASN
2	E	480	GLN
2	E	486	ASN
2	F	167	ASN
2	F	423	GLN
2	F	428	ASN
2	F	480	GLN
2	F	485	ASN
2	F	534	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 30 ligands modelled in this entry, 12 are monoatomic - leaving 18 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
3	NAG	B	802	1	14,14,15	0.33	0	17,19,21	0.81	1 (5%)
3	NAG	C	802	1	14,14,15	0.59	0	17,19,21	0.75	1 (5%)
3	NAG	D	601	2	14,14,15	0.72	1 (7%)	17,19,21	0.78	0
3	NAG	E	602	2	14,14,15	0.36	0	17,19,21	0.64	1 (5%)
3	NAG	E	603	2	14,14,15	0.26	0	17,19,21	0.58	0
3	NAG	E	601	2	14,14,15	0.37	0	17,19,21	0.44	0
3	NAG	A	802	1	14,14,15	0.25	0	17,19,21	0.39	0
3	NAG	A	803	1	14,14,15	0.19	0	17,19,21	0.43	0
3	NAG	C	801	1	14,14,15	0.64	0	17,19,21	0.45	0
3	NAG	C	803	1	14,14,15	0.31	0	17,19,21	0.49	0
3	NAG	D	603	2	14,14,15	0.42	0	17,19,21	0.81	1 (5%)
3	NAG	F	602	2	14,14,15	0.26	0	17,19,21	0.41	0
3	NAG	F	603	2	14,14,15	0.55	0	17,19,21	0.73	1 (5%)
3	NAG	F	601	2	14,14,15	0.34	0	17,19,21	0.76	0
3	NAG	D	602	2	14,14,15	0.25	0	17,19,21	0.42	0
3	NAG	A	801	1	14,14,15	0.22	0	17,19,21	0.54	0
3	NAG	B	801	1	14,14,15	0.24	0	17,19,21	0.63	0
3	NAG	B	803	1	14,14,15	0.54	0	17,19,21	1.05	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	802	1	-	2/6/23/26	0/1/1/1
3	NAG	C	802	1	-	0/6/23/26	0/1/1/1
3	NAG	D	601	2	-	0/6/23/26	0/1/1/1
3	NAG	E	602	2	-	2/6/23/26	0/1/1/1
3	NAG	E	603	2	-	0/6/23/26	0/1/1/1
3	NAG	E	601	2	-	1/6/23/26	0/1/1/1
3	NAG	A	802	1	-	2/6/23/26	0/1/1/1
3	NAG	A	803	1	-	0/6/23/26	0/1/1/1
3	NAG	C	801	1	-	1/6/23/26	0/1/1/1
3	NAG	C	803	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	D	603	2	-	2/6/23/26	0/1/1/1
3	NAG	F	602	2	-	0/6/23/26	0/1/1/1
3	NAG	F	603	2	-	2/6/23/26	0/1/1/1
3	NAG	F	601	2	-	1/6/23/26	0/1/1/1
3	NAG	D	602	2	-	0/6/23/26	0/1/1/1
3	NAG	A	801	1	-	0/6/23/26	0/1/1/1
3	NAG	B	801	1	-	0/6/23/26	0/1/1/1
3	NAG	B	803	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	601	NAG	O5-C1	-2.30	1.39	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	803	NAG	C1-O5-C5	3.99	117.53	112.19
3	D	603	NAG	C1-O5-C5	2.92	116.11	112.19
3	F	603	NAG	C1-O5-C5	2.32	115.30	112.19
3	E	602	NAG	C1-O5-C5	2.21	115.15	112.19
3	B	802	NAG	C1-O5-C5	2.14	115.05	112.19
3	C	802	NAG	C3-C4-C5	2.01	113.87	110.23

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	603	NAG	O5-C5-C6-O6
3	D	603	NAG	C4-C5-C6-O6
3	B	803	NAG	O5-C5-C6-O6
3	A	802	NAG	O5-C5-C6-O6
3	B	802	NAG	C4-C5-C6-O6
3	E	602	NAG	O5-C5-C6-O6
3	A	802	NAG	C4-C5-C6-O6
3	B	802	NAG	O5-C5-C6-O6
3	B	803	NAG	C4-C5-C6-O6
3	E	602	NAG	C4-C5-C6-O6
3	C	801	NAG	O5-C5-C6-O6
3	E	601	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	F	603	NAG	C3-C2-N2-C7
3	F	603	NAG	C1-C2-N2-C7
3	F	601	NAG	O5-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	803	NAG	1	0
3	F	601	NAG	1	0
3	A	801	NAG	1	0
3	B	803	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	486/486 (100%)	0.40	24 (4%)	35	31	179, 277, 352, 400	0
1	B	486/486 (100%)	0.39	21 (4%)	40	34	174, 277, 342, 379	0
1	C	486/486 (100%)	0.37	21 (4%)	40	34	195, 292, 364, 387	0
2	D	515/526 (97%)	0.48	22 (4%)	40	34	164, 236, 294, 337	0
2	E	515/526 (97%)	0.28	19 (3%)	45	36	188, 253, 311, 357	0
2	F	515/526 (97%)	0.37	15 (2%)	53	41	183, 253, 304, 325	0
All	All	3003/3036 (98%)	0.38	122 (4%)	41	35	164, 260, 342, 400	0

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	410	LEU	5.2
1	A	601	GLY	5.1
1	B	709	SER	5.0
2	D	365	ASN	4.3
2	F	170	LEU	4.0
1	A	398	TRP	3.9
2	D	537	PHE	3.8
1	A	709	SER	3.7
1	A	649	GLY	3.7
2	D	219	PHE	3.6
1	A	432	ALA	3.6
2	E	154	LEU	3.6
2	D	186	GLU	3.5
1	A	339	ARG	3.5
1	C	556	TYR	3.5
1	A	397	THR	3.4
2	D	240	ASP	3.3
2	E	170	LEU	3.3
1	B	406	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	414	PHE	3.2
1	A	650	TYR	3.1
2	D	337	THR	3.1
2	E	153	THR	3.0
1	C	276	ILE	3.0
2	E	234	TYR	3.0
2	D	541	PHE	2.8
1	B	525	PRO	2.8
1	C	381	ILE	2.8
1	A	368	VAL	2.8
1	B	298	LYS	2.8
2	D	151	LEU	2.8
2	F	177	CYS	2.7
2	E	516	GLU	2.7
2	E	146	LEU	2.7
2	D	288	PRO	2.6
1	C	402	ILE	2.6
1	B	411	PRO	2.6
1	B	558	TRP	2.6
1	C	338	SER	2.6
2	F	497	SER	2.6
2	D	127	ILE	2.6
1	B	368	VAL	2.6
1	B	246	VAL	2.5
2	F	286	CYS	2.5
1	A	306	LEU	2.5
1	B	382	SER	2.5
1	A	609	GLY	2.5
1	C	544	GLY	2.5
1	A	362	LYS	2.5
1	B	556	TYR	2.5
1	A	626	VAL	2.5
1	A	625	LEU	2.5
2	D	333	ASN	2.5
2	E	252	ILE	2.5
1	A	633	LEU	2.4
1	B	324	SER	2.4
2	F	238	SER	2.4
2	F	439	SER	2.4
1	A	305	PRO	2.4
1	C	340	SER	2.4
2	D	404	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	368	VAL	2.4
1	B	648	LEU	2.4
2	D	47	THR	2.4
1	C	635	CYS	2.4
1	A	482	ASP	2.4
1	B	538	VAL	2.3
2	F	159	PHE	2.3
1	C	339	ARG	2.3
2	E	151	LEU	2.3
2	D	238	SER	2.3
2	F	150	ASN	2.2
1	B	554	CYS	2.2
1	A	682	SER	2.2
2	D	378	ARG	2.2
1	C	554	CYS	2.2
2	F	137	GLY	2.2
1	C	552	ARG	2.2
1	C	410	LEU	2.2
1	B	690	GLY	2.2
1	C	525	PRO	2.2
1	A	382	SER	2.2
1	B	327	VAL	2.2
1	B	464	ALA	2.2
1	C	464	ALA	2.2
2	D	243	SER	2.2
2	F	87	PHE	2.2
1	A	431	GLY	2.2
2	E	175	PHE	2.2
2	E	261	ILE	2.2
1	A	538	VAL	2.2
1	C	678	THR	2.2
2	E	181	LEU	2.2
1	C	412	LYS	2.1
2	E	333	ASN	2.1
1	B	626	VAL	2.1
1	A	433	CYS	2.1
2	E	219	PHE	2.1
2	F	98	PHE	2.1
2	D	387	ILE	2.1
2	E	130	ILE	2.1
2	F	555	LEU	2.1
2	E	393	THR	2.1

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Mol	Chain	Res	Type	RSRZ
2	E	529	SER	2.1
2	D	303	PHE	2.1
2	F	82	ILE	2.1
1	B	509	ASP	2.1
2	F	334	ASP	2.1
1	B	524	ALA	2.1
2	F	349	ALA	2.1
1	A	353	LYS	2.1
1	A	595	LYS	2.1
2	D	252	ILE	2.1
2	D	386	GLU	2.1
1	C	509	ASP	2.0
1	C	324	SER	2.0
2	D	498	PHE	2.0
2	E	498	PHE	2.0
2	E	437	HIS	2.0
2	D	343	ASN	2.0
1	C	337	SER	2.0
2	E	243	SER	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](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	A	801	14/15	0.42	0.14	264,318,345,361	0
3	NAG	E	602	14/15	0.46	0.13	249,303,313,321	0
3	NAG	E	603	14/15	0.52	0.18	252,287,308,319	0
3	NAG	E	601	14/15	0.53	0.13	239,321,334,342	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	C	803	14/15	0.55	0.13	296,334,345,350	0
3	NAG	B	803	14/15	0.55	0.13	277,311,331,333	0
4	CA	F	604	1/1	0.56	0.17	238,238,238,238	0
3	NAG	D	601	14/15	0.62	0.12	222,312,338,347	0
3	NAG	F	601	14/15	0.63	0.13	305,337,350,355	0
3	NAG	B	801	14/15	0.63	0.11	298,343,353,354	0
3	NAG	A	802	14/15	0.69	0.17	311,345,363,364	0
3	NAG	A	803	14/15	0.70	0.20	332,363,392,393	0
3	NAG	D	603	14/15	0.71	0.12	231,273,279,304	0
3	NAG	F	602	14/15	0.73	0.11	258,308,321,323	0
3	NAG	C	801	14/15	0.74	0.12	330,364,383,389	0
3	NAG	F	603	14/15	0.75	0.14	255,290,335,336	0
3	NAG	D	602	14/15	0.75	0.12	259,284,312,313	0
4	CA	A	804	1/1	0.84	0.16	236,236,236,236	0
3	NAG	B	802	14/15	0.86	0.14	265,305,329,336	0
4	CA	E	604	1/1	0.87	0.12	223,223,223,223	0
3	NAG	C	802	14/15	0.87	0.13	277,309,338,344	0
4	CA	D	604	1/1	0.89	0.10	222,222,222,222	0
4	CA	B	805	1/1	0.96	0.06	213,213,213,213	0
4	CA	C	804	1/1	0.97	0.04	327,327,327,327	0
4	CA	C	805	1/1	0.97	0.09	239,239,239,239	0
4	CA	C	806	1/1	0.97	0.05	342,342,342,342	0
4	CA	A	805	1/1	0.98	0.04	341,341,341,341	0
4	CA	B	806	1/1	0.98	0.06	285,285,285,285	0
4	CA	A	806	1/1	0.98	0.12	239,239,239,239	0
4	CA	B	804	1/1	0.98	0.09	272,272,272,272	0

6.5 Other polymers [i](#)

There are no such residues in this entry.