Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:31 PM GMT

PDB ID	:	1FZA
Title	:	CRYSTAL STRUCTURE OF FIBRINOGEN FRAGMENT D
Authors	:	Spraggon, G.; Everse, S.J.; Doolittle, R.F.
Deposited on	:	1997-08-05
Resolution	:	2.90 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 (i)) were used in the production of this report:

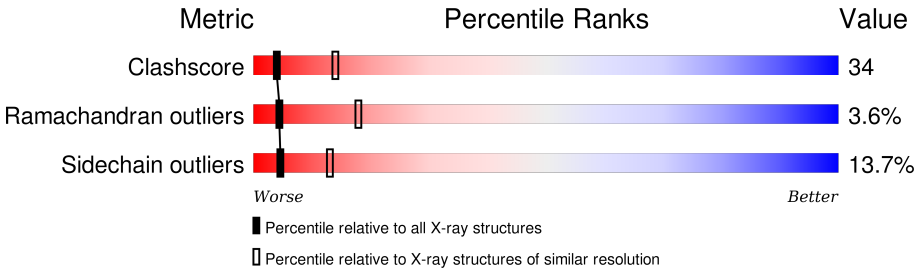
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	87	39% 41% 16% • •
1	D	87	38% 43% 16% • •
2	B	328	40% 45% 10% 5%
2	E	328	41% 45% 10% 5%
3	C	319	43% 46% 7% • •
3	F	319	42% 47% 7% • •

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11418 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 FIBRINOGEN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	85	Total	C	N	O	S	0	0	0
			697	432	132	130	3			
1	D	85	Total	C	N	O	S	0	0	0
			697	432	132	130	3			

- Molecule 2 is a protein called FIBRINOGEN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	313	Total	C	N	O	S	0	0	0
			2517	1571	444	480	22			
2	E	313	Total	C	N	O	S	0	0	0
			2517	1571	444	480	22			

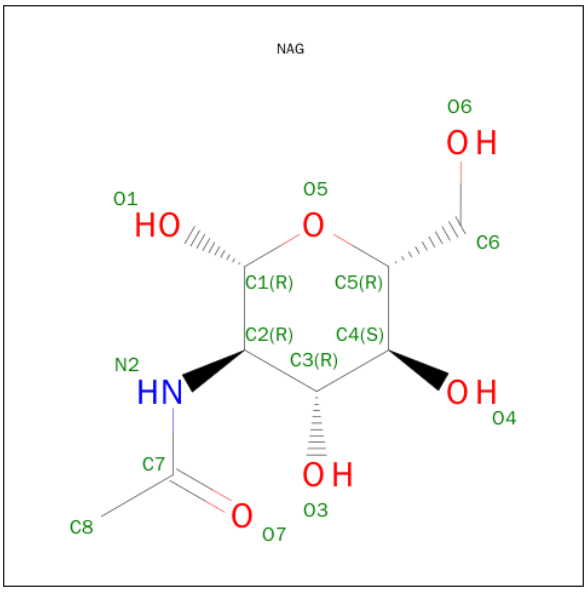
- Molecule 3 is a protein called FIBRINOGEN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	309	Total	C	N	O	S	0	0	0
			2480	1574	415	478	13			
3	F	309	Total	C	N	O	S	0	0	0
			2480	1574	415	478	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	88	LYS	ILE	CONFLICT	UNP P02679
F	88	LYS	ILE	CONFLICT	UNP P02679

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total Ca 1 1	0	0
5	F	1	Total Ca 1 1	0	0

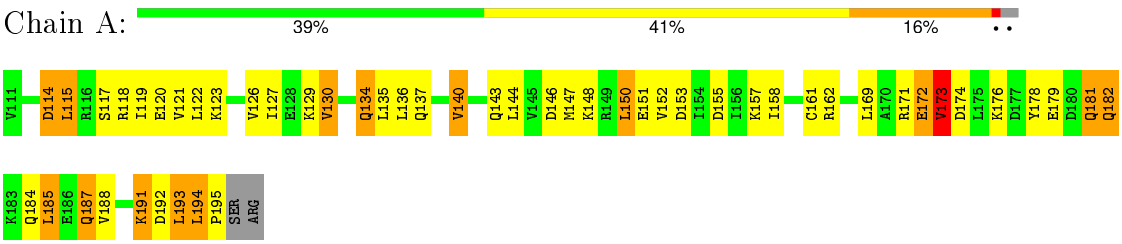
3 Residue-property plots (i)

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.

Note EDS was not executed.

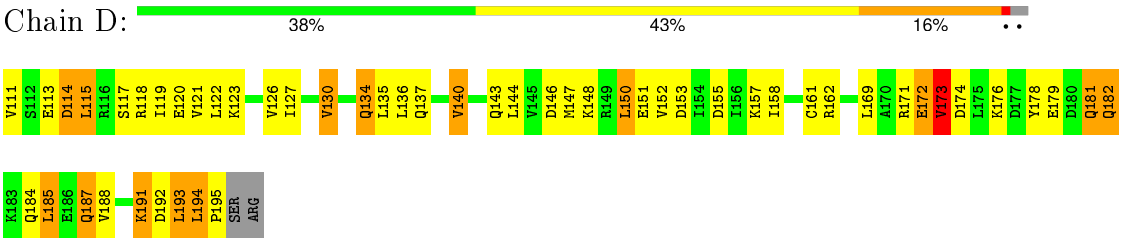
- Molecule 1: FIBRINOGEN

Chain A:



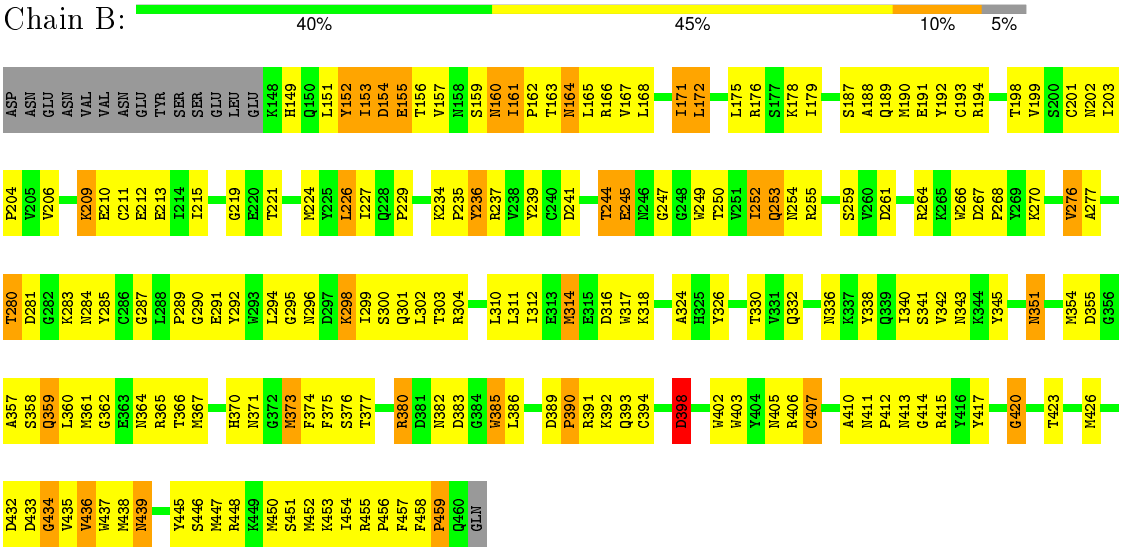
- Molecule 1: FIBRINOGEN

Chain D:



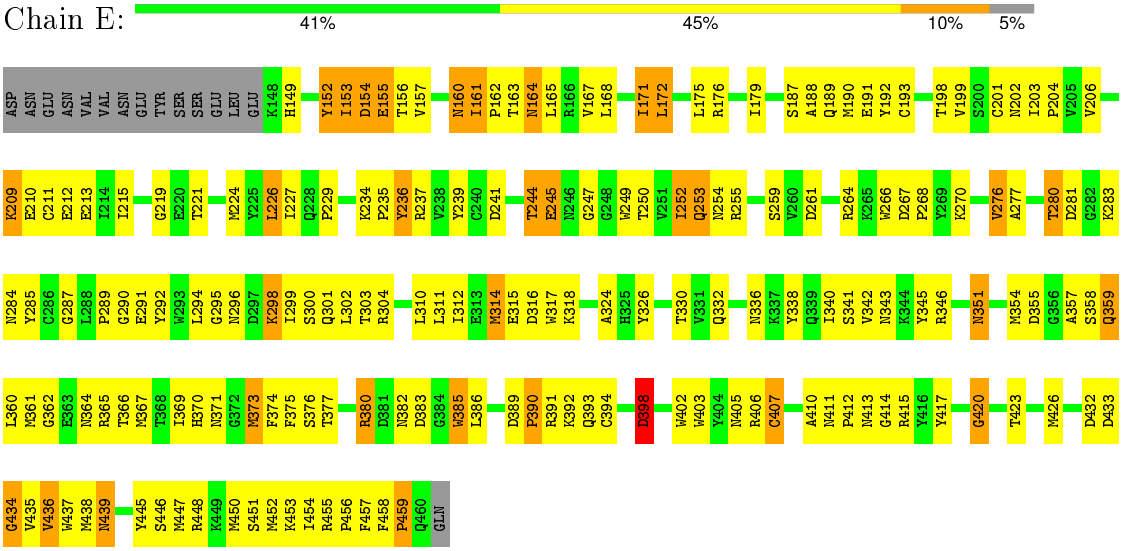
- Molecule 2: FIBRINOGEN

Chain B:



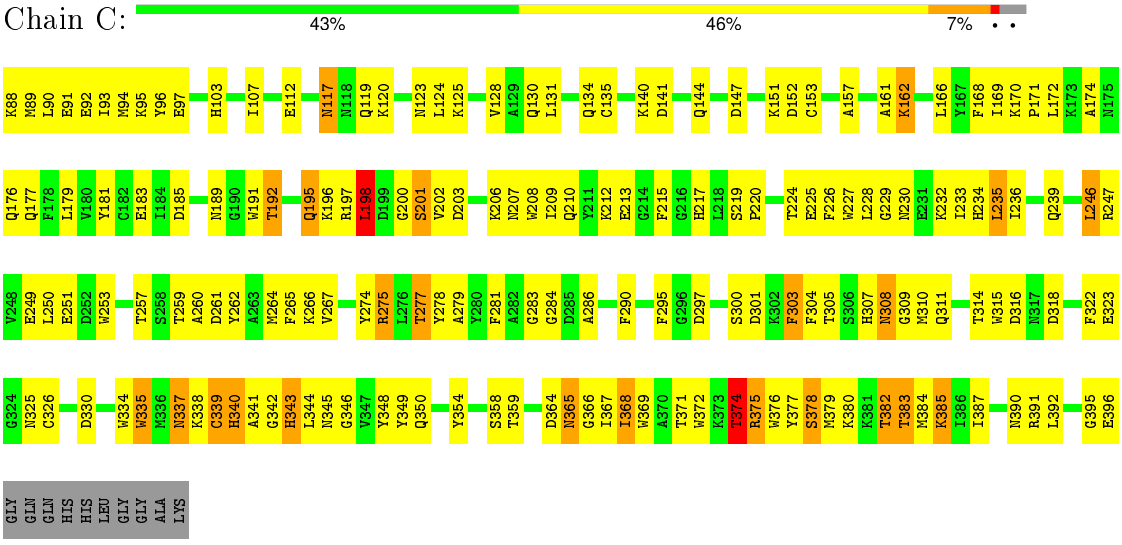
- Molecule 2: FIBRINOGEN

Chain E:



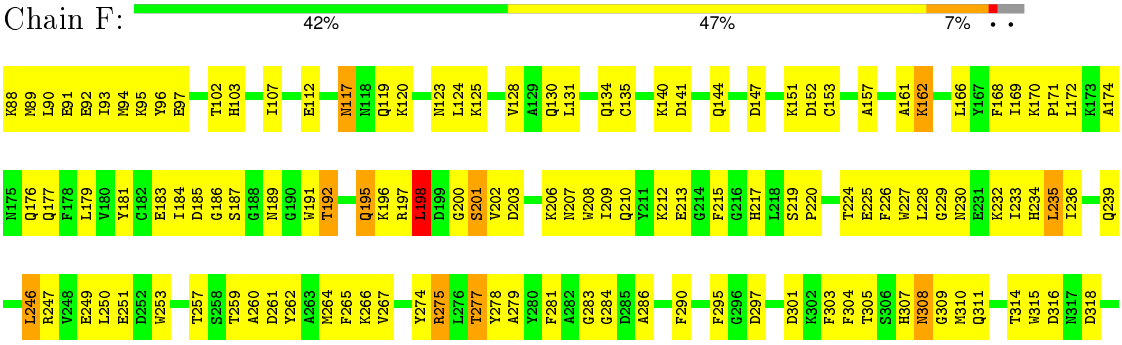
- Molecule 3: FIBRINOGEN

Chain C:



- Molecule 3: FIBRINOGEN

Chain F:




F322
E323
S324
N325
C326
D330
W334
W335
M336
M337
K338
G339
H340
A341
G342
H343
L344
N345
G346
V347
Y348
Y349
Q350
Y354
S358
T359
D364
M365
G366
I367
I368
W369
A370
T371
W372
K373
F374
A375
W376
Y377
S378
M379
K380
K381
T382
T383
M384
K385
I386
I387
N390
R391
G395
E396
GLY
GLN
GLN
HIS
HIS
LEU
GLY
GLY
ALA
LYS

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	107.72Å 48.08Å 167.56Å 90.00° 105.70° 90.00°	Depositor
Resolution (Å)	30.00 – 2.90	Depositor
% Data completeness (in resolution range)	87.1 (30.00-2.90)	Depositor
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.263 , 0.363	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11418	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.56	0/699	0.75	0/933
1	D	0.56	0/699	0.75	0/933
2	B	0.57	0/2581	0.84	1/3487 (0.0%)
2	E	0.57	0/2581	0.84	1/3487 (0.0%)
3	C	0.51	0/2546	0.71	0/3440
3	F	0.51	0/2546	0.71	0/3440
All	All	0.55	0/11652	0.77	2/15720 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
2	E	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	247	GLY	N-CA-C	-5.09	100.39	113.10
2	B	247	GLY	N-CA-C	-5.07	100.43	113.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	236	TYR	Sidechain
2	E	236	TYR	Sidechain

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	697	0	744	51	0
1	D	697	0	744	50	3
2	B	2517	0	2380	176	4
2	E	2517	0	2380	180	0
3	C	2480	0	2333	180	3
3	F	2480	0	2332	180	4
4	B	14	0	13	2	0
4	E	14	0	13	3	0
5	C	1	0	0	0	0
5	F	1	0	0	0	0
All	All	11418	0	10939	764	7

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 34.

All (764) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:396:GLU:HA	3:F:187:SER:N	1.59	1.18
1:A:194:LEU:HB3	1:A:195:PRO:HD3	1.33	1.07
3:C:396:GLU:HA	3:F:186:GLY:C	1.74	1.07
1:D:194:LEU:HB3	1:D:195:PRO:HD3	1.33	1.05
3:C:310:MET:SD	3:C:337:ASN:HB2	1.97	1.05
3:F:310:MET:SD	3:F:337:ASN:HB2	1.97	1.05
2:B:198:THR:HG22	3:C:140:LYS:HB3	1.42	1.01
3:F:219:SER:H	3:F:224:THR:HG21	1.26	1.00
2:E:198:THR:HG22	3:F:140:LYS:HB3	1.42	0.99
2:E:351:ASN:HD21	2:E:354:MET:HG2	1.28	0.98
2:B:351:ASN:HD21	2:B:354:MET:HG2	1.28	0.97
2:B:298:LYS:H	2:B:298:LYS:HZ1	1.11	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:219:SER:H	3:C:224:THR:HG21	1.26	0.96
2:E:358:SER:HA	2:E:365:ARG:HH12	1.33	0.94
3:C:396:GLU:HG3	3:F:186:GLY:HA2	1.47	0.93
2:B:167:VAL:HG23	2:B:168:LEU:HD12	1.51	0.92
2:E:303:THR:HB	2:E:330:THR:HA	1.52	0.91
2:B:303:THR:HB	2:B:330:THR:HA	1.52	0.91
3:C:396:GLU:CA	3:F:187:SER:N	2.33	0.91
2:B:358:SER:HA	2:B:365:ARG:HH12	1.33	0.90
2:E:167:VAL:HG23	2:E:168:LEU:HD12	1.51	0.90
3:F:88:LYS:HB3	3:F:92:GLU:HB2	1.53	0.89
3:C:88:LYS:HB3	3:C:92:GLU:HB2	1.53	0.89
1:D:185:LEU:O	1:D:185:LEU:HD12	1.73	0.88
2:E:235:PRO:HG2	3:F:168:PHE:HE2	1.39	0.87
3:F:209:ILE:H	3:F:209:ILE:HD12	1.39	0.87
3:C:209:ILE:H	3:C:209:ILE:HD12	1.39	0.86
2:B:235:PRO:HG2	3:C:168:PHE:HE2	1.39	0.86
1:A:185:LEU:HD12	1:A:185:LEU:O	1.73	0.86
2:E:370:HIS:O	2:E:373:MET:HB2	1.76	0.86
2:E:439:ASN:H	2:E:439:ASN:HD22	1.24	0.86
3:C:340:HIS:CE1	3:C:364:ASP:HB2	2.11	0.85
3:F:340:HIS:CE1	3:F:364:ASP:HB2	2.11	0.85
1:D:158:ILE:HG23	2:E:189:GLN:HE21	1.41	0.84
2:B:439:ASN:HD22	2:B:439:ASN:H	1.24	0.84
2:B:370:HIS:O	2:B:373:MET:HB2	1.76	0.84
2:B:210:GLU:HG2	2:B:212:GLU:H	1.43	0.84
2:E:270:LYS:HA	2:E:296:ASN:HB2	1.61	0.83
1:A:158:ILE:HG23	2:B:189:GLN:HE21	1.41	0.83
2:E:210:GLU:HG2	2:E:212:GLU:H	1.43	0.83
2:E:298:LYS:HZ1	2:E:298:LYS:H	1.27	0.83
2:B:270:LYS:HA	2:B:296:ASN:HB2	1.61	0.82
3:C:396:GLU:HA	3:F:186:GLY:CA	2.09	0.82
3:C:348:TYR:HA	3:C:367:ILE:HD11	1.60	0.81
3:F:348:TYR:HA	3:F:367:ILE:HD11	1.60	0.81
3:C:340:HIS:HE1	3:C:364:ASP:HB2	1.45	0.81
3:F:340:HIS:HE1	3:F:364:ASP:HB2	1.45	0.80
2:E:298:LYS:NZ	2:E:298:LYS:H	1.79	0.80
3:F:318:ASP:HB2	3:F:325:ASN:HD22	1.47	0.80
2:E:276:VAL:HA	2:E:292:TYR:CD2	2.17	0.80
2:B:298:LYS:H	2:B:298:LYS:NZ	1.79	0.79
3:C:318:ASP:HB2	3:C:325:ASN:HD22	1.47	0.79
3:C:260:ALA:HA	3:C:284:GLY:HA3	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:276:VAL:HA	2:B:292:TYR:CD2	2.17	0.78
2:E:351:ASN:ND2	2:E:354:MET:HG2	1.99	0.77
2:B:351:ASN:ND2	2:B:354:MET:HG2	1.99	0.77
3:F:219:SER:H	3:F:224:THR:CG2	1.97	0.77
3:F:374:THR:HG23	3:F:377:TYR:HB2	1.66	0.77
3:F:260:ALA:HA	3:F:284:GLY:HA3	1.65	0.76
3:C:374:THR:HG23	3:C:377:TYR:HB2	1.66	0.76
1:D:191:LYS:HE3	1:D:191:LYS:HA	1.68	0.76
2:B:152:TYR:HD1	2:B:153:ILE:N	1.84	0.76
2:B:235:PRO:HG2	3:C:168:PHE:CE2	2.21	0.76
2:E:295:GLY:O	2:E:299:ILE:HG13	1.86	0.76
2:B:295:GLY:O	2:B:299:ILE:HG13	1.86	0.75
2:E:235:PRO:HG2	3:F:168:PHE:CE2	2.21	0.75
2:E:152:TYR:HD1	2:E:153:ILE:N	1.84	0.75
3:F:278:TYR:H	3:F:308:ASN:HD21	1.35	0.75
1:A:191:LYS:HA	1:A:191:LYS:HE3	1.68	0.75
3:C:322:PHE:HB2	3:C:338:LYS:HA	1.69	0.75
3:C:219:SER:H	3:C:224:THR:CG2	1.97	0.75
3:C:396:GLU:CG	3:F:186:GLY:HA2	2.16	0.74
2:E:373:MET:HG2	2:E:405:ASN:HB2	1.69	0.74
3:C:219:SER:N	3:C:224:THR:HG21	2.03	0.74
3:F:286:ALA:O	3:F:371:THR:HG23	1.89	0.73
3:C:286:ALA:O	3:C:371:THR:HG23	1.88	0.73
3:F:322:PHE:HB2	3:F:338:LYS:HA	1.69	0.73
1:A:140:VAL:HG11	2:B:171:ILE:HD11	1.70	0.73
3:C:195:GLN:HG2	3:C:384:MET:SD	2.29	0.73
2:B:239:TYR:CZ	2:B:289:PRO:HD3	2.24	0.73
3:F:195:GLN:HG2	3:F:384:MET:SD	2.29	0.73
2:E:163:THR:O	2:E:167:VAL:HG22	1.89	0.73
2:B:163:THR:O	2:B:167:VAL:HG22	1.89	0.72
2:B:373:MET:HG2	2:B:405:ASN:HB2	1.70	0.72
2:E:212:GLU:O	2:E:215:ILE:HG22	1.90	0.72
3:C:157:ALA:HA	3:C:161:ALA:HB3	1.72	0.72
2:B:212:GLU:O	2:B:215:ILE:HG22	1.90	0.72
1:D:140:VAL:HG11	2:E:171:ILE:HD11	1.70	0.72
2:E:373:MET:SD	2:E:405:ASN:HB2	2.30	0.72
3:C:278:TYR:H	3:C:308:ASN:HD21	1.35	0.72
2:B:373:MET:SD	2:B:405:ASN:HB2	2.30	0.72
2:E:358:SER:HA	2:E:365:ARG:NH1	2.05	0.71
2:E:239:TYR:CZ	2:E:289:PRO:HD3	2.24	0.71
2:E:294:LEU:HD23	2:E:299:ILE:HG12	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:396:GLU:HG3	3:F:186:GLY:CA	2.20	0.71
2:B:358:SER:HA	2:B:365:ARG:NH1	2.06	0.71
3:F:157:ALA:HA	3:F:161:ALA:HB3	1.72	0.71
2:E:357:ALA:HA	2:E:439:ASN:HD21	1.56	0.71
2:E:351:ASN:O	2:E:355:ASP:HB2	1.91	0.70
2:B:294:LEU:HD23	2:B:299:ILE:HG12	1.72	0.70
3:F:219:SER:N	3:F:224:THR:HG21	2.03	0.70
2:B:439:ASN:HD22	2:B:439:ASN:N	1.90	0.70
2:B:280:THR:OG1	2:B:283:LYS:HB2	1.92	0.70
2:B:351:ASN:O	2:B:355:ASP:HB2	1.91	0.69
1:A:162:ARG:NH1	2:B:259:SER:HB3	2.07	0.69
2:B:357:ALA:HA	2:B:439:ASN:HD21	1.56	0.69
2:E:280:THR:OG1	2:E:283:LYS:HB2	1.92	0.69
2:B:199:VAL:O	3:C:141:ASP:HA	1.93	0.69
2:B:420:GLY:HA3	2:B:445:TYR:CE1	2.27	0.69
3:C:396:GLU:HA	3:F:186:GLY:HA2	1.74	0.69
2:E:199:VAL:O	3:F:141:ASP:HA	1.93	0.69
1:D:162:ARG:NH1	2:E:259:SER:HB3	2.07	0.69
2:E:373:MET:CG	2:E:405:ASN:HB2	2.24	0.68
2:E:420:GLY:HA3	2:E:445:TYR:CE1	2.27	0.68
3:F:307:HIS:HE1	3:F:341:ALA:H	1.42	0.68
3:C:250:LEU:HD22	3:C:379:MET:HG3	1.74	0.68
2:B:316:ASP:HB3	2:B:318:LYS:H	1.58	0.68
3:F:250:LEU:HD22	3:F:379:MET:HG3	1.74	0.68
2:E:316:ASP:HB3	2:E:318:LYS:H	1.58	0.68
2:B:314:MET:HE3	2:B:437:TRP:HB2	1.76	0.68
2:E:314:MET:HE3	2:E:437:TRP:HB2	1.75	0.68
3:C:307:HIS:HE1	3:C:341:ALA:H	1.42	0.67
3:F:308:ASN:HD22	3:F:309:GLY:H	1.43	0.67
2:E:267:ASP:HB3	2:E:268:PRO:CD	2.25	0.67
3:C:307:HIS:CE1	3:C:341:ALA:H	2.13	0.67
2:E:162:PRO:HA	2:E:165:LEU:HD12	1.77	0.67
2:B:357:ALA:HB3	2:B:360:LEU:HD23	1.76	0.67
2:B:267:ASP:HB3	2:B:268:PRO:CD	2.25	0.67
2:B:373:MET:CG	2:B:405:ASN:HB2	2.24	0.67
2:E:439:ASN:N	2:E:439:ASN:HD22	1.90	0.67
2:E:252:ILE:HB	2:E:452:MET:O	1.94	0.67
2:B:252:ILE:HB	2:B:452:MET:O	1.94	0.66
3:F:153:CYS:SG	3:F:192:THR:HB	2.36	0.66
1:A:194:LEU:CB	1:A:195:PRO:HD3	2.18	0.66
2:E:357:ALA:HB3	2:E:360:LEU:HD23	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:153:CYS:SG	3:C:192:THR:HB	2.36	0.66
3:F:307:HIS:CE1	3:F:341:ALA:H	2.13	0.66
2:B:310:LEU:HD21	2:B:312:ILE:HD11	1.76	0.66
2:B:162:PRO:HA	2:B:165:LEU:HD12	1.77	0.66
2:E:310:LEU:HD21	2:E:312:ILE:HD11	1.76	0.66
2:E:252:ILE:HD13	2:E:454:ILE:HB	1.79	0.65
2:B:255:ARG:HA	2:B:291:GLU:HG2	1.78	0.65
2:E:255:ARG:HA	2:E:291:GLU:HG2	1.78	0.65
2:B:252:ILE:HD13	2:B:454:ILE:HB	1.79	0.65
3:C:308:ASN:HD22	3:C:309:GLY:H	1.43	0.65
2:B:345:TYR:CD2	2:B:351:ASN:HB2	2.33	0.64
1:A:162:ARG:HH11	2:B:259:SER:HB3	1.62	0.64
3:C:396:GLU:CB	3:F:186:GLY:HA2	2.28	0.64
2:E:390:PRO:HB3	2:E:393:GLN:OE1	1.97	0.64
2:E:345:TYR:CD2	2:E:351:ASN:HB2	2.33	0.64
1:D:162:ARG:HH11	2:E:259:SER:HB3	1.62	0.64
3:F:92:GLU:O	3:F:95:LYS:HG2	1.98	0.64
2:B:390:PRO:HB3	2:B:393:GLN:OE1	1.97	0.64
3:C:92:GLU:O	3:C:95:LYS:HG2	1.98	0.63
2:E:277:ALA:HA	2:E:289:PRO:HA	1.80	0.63
2:E:202:ASN:ND2	2:E:284:ASN:HB3	2.13	0.63
1:A:193:LEU:HD23	1:A:194:LEU:H	1.63	0.63
1:D:194:LEU:HB3	1:D:195:PRO:CD	2.20	0.63
3:C:153:CYS:SG	3:C:192:THR:HA	2.38	0.63
2:B:202:ASN:ND2	2:B:284:ASN:HB3	2.13	0.63
2:B:277:ALA:HA	2:B:289:PRO:HA	1.80	0.63
3:C:170:LYS:HG2	3:C:174:ALA:HB3	1.81	0.63
1:A:185:LEU:HD12	1:A:185:LEU:C	2.20	0.62
3:F:153:CYS:SG	3:F:192:THR:HA	2.38	0.62
1:D:193:LEU:HD23	1:D:194:LEU:H	1.63	0.62
3:F:209:ILE:H	3:F:209:ILE:CD1	2.12	0.62
2:E:417:TYR:OH	2:E:433:ASP:HB2	1.99	0.62
3:C:209:ILE:H	3:C:209:ILE:CD1	2.12	0.62
3:C:264:MET:HB2	3:C:279:ALA:H	1.65	0.62
3:F:170:LYS:HG2	3:F:174:ALA:HB3	1.81	0.62
3:C:396:GLU:HA	3:F:187:SER:H	1.63	0.62
3:F:367:ILE:HD12	3:F:367:ILE:H	1.65	0.62
3:F:264:MET:HB2	3:F:279:ALA:H	1.65	0.62
3:F:274:TYR:O	3:F:335:TRP:HZ3	1.83	0.62
2:B:417:TYR:OH	2:B:433:ASP:HB2	1.99	0.62
3:C:103:HIS:O	3:C:107:ILE:HD13	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:394:CYS:SG	2:E:407:CYS:N	2.74	0.61
3:F:334:TRP:CZ2	3:F:343:HIS:HA	2.36	0.61
3:C:367:ILE:H	3:C:367:ILE:HD12	1.65	0.61
1:D:151:GLU:HG2	1:D:178:TYR:HE2	1.66	0.61
3:C:125:LYS:O	3:C:128:VAL:HG22	2.01	0.61
3:F:88:LYS:HD3	3:F:92:GLU:HB2	1.83	0.61
2:E:380:ARG:HB2	2:E:380:ARG:HH11	1.65	0.61
2:B:394:CYS:SG	2:B:407:CYS:N	2.73	0.60
3:C:274:TYR:O	3:C:335:TRP:HZ3	1.83	0.60
2:B:380:ARG:HH11	2:B:380:ARG:HB2	1.65	0.60
1:A:151:GLU:HG2	1:A:178:TYR:HE2	1.66	0.60
3:C:88:LYS:HA	3:C:91:GLU:HB2	1.84	0.60
1:D:185:LEU:C	1:D:185:LEU:HD12	2.19	0.60
1:D:148:LYS:O	1:D:152:VAL:HG23	2.02	0.60
3:C:90:LEU:HA	3:C:93:ILE:HB	1.83	0.60
1:A:193:LEU:HD23	1:A:194:LEU:N	2.17	0.60
3:F:103:HIS:O	3:F:107:ILE:HD13	2.01	0.60
3:F:88:LYS:HA	3:F:91:GLU:HB2	1.84	0.60
3:C:88:LYS:HD3	3:C:92:GLU:HB2	1.83	0.60
2:E:314:MET:HE3	2:E:437:TRP:CB	2.32	0.60
3:C:334:TRP:CZ2	3:C:343:HIS:HA	2.36	0.60
3:F:90:LEU:HA	3:F:93:ILE:HB	1.83	0.60
3:C:334:TRP:CE2	3:C:343:HIS:HB2	2.38	0.59
3:F:125:LYS:O	3:F:128:VAL:HG22	2.01	0.59
2:E:298:LYS:O	2:E:302:LEU:HG	2.03	0.59
3:F:203:ASP:O	3:F:206:LYS:HE2	2.03	0.59
1:D:194:LEU:CB	1:D:195:PRO:HD3	2.18	0.59
2:E:303:THR:CB	2:E:330:THR:HA	2.30	0.59
1:A:143:GLN:NE2	3:C:117:ASN:HB3	2.18	0.59
1:A:148:LYS:O	1:A:152:VAL:HG23	2.02	0.59
3:F:334:TRP:CE2	3:F:343:HIS:HB2	2.38	0.59
2:E:179:ILE:HG21	3:F:120:LYS:HB3	1.83	0.59
3:C:203:ASP:O	3:C:206:LYS:HE2	2.03	0.59
2:B:303:THR:CB	2:B:330:THR:HA	2.30	0.58
1:D:143:GLN:NE2	3:F:117:ASN:HB3	2.18	0.58
3:F:264:MET:HG3	3:F:279:ALA:HB3	1.85	0.58
2:B:179:ILE:HG21	3:C:120:LYS:HB3	1.83	0.58
1:D:193:LEU:HD23	1:D:194:LEU:N	2.17	0.58
2:E:453:LYS:O	2:E:454:ILE:HD12	2.04	0.58
2:E:188:ALA:O	2:E:191:GLU:HB2	2.04	0.58
3:C:396:GLU:C	3:F:187:SER:H	2.06	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:298:LYS:O	2:B:302:LEU:HG	2.02	0.58
2:E:439:ASN:H	2:E:439:ASN:ND2	2.00	0.58
2:B:314:MET:HE3	2:B:437:TRP:CB	2.33	0.58
3:F:166:LEU:HB3	3:F:179:LEU:HD11	1.86	0.58
3:C:396:GLU:C	3:F:187:SER:N	2.57	0.58
1:A:194:LEU:HB3	1:A:195:PRO:CD	2.20	0.58
2:B:439:ASN:H	2:B:439:ASN:ND2	2.00	0.58
2:B:194:ARG:NH2	2:E:191:GLU:OE2	2.37	0.58
2:B:298:LYS:HZ1	2:B:298:LYS:N	1.93	0.57
2:E:210:GLU:HG2	2:E:211:CYS:N	2.18	0.57
2:B:453:LYS:O	2:B:454:ILE:HD12	2.04	0.57
3:F:227:TRP:HZ2	3:F:230:ASN:ND2	2.02	0.57
2:B:210:GLU:HG2	2:B:211:CYS:N	2.18	0.57
1:D:143:GLN:HE22	3:F:117:ASN:CB	2.18	0.57
1:A:143:GLN:HE22	3:C:117:ASN:CB	2.18	0.57
3:F:172:LEU:O	3:F:172:LEU:HD13	2.05	0.57
3:F:307:HIS:O	3:F:310:MET:HB2	2.05	0.57
2:B:405:ASN:C	2:B:407:CYS:N	2.57	0.57
3:C:367:ILE:HD12	3:C:378:SER:OG	2.05	0.57
3:C:264:MET:HG3	3:C:279:ALA:HB3	1.85	0.57
3:C:172:LEU:O	3:C:172:LEU:HD13	2.05	0.57
3:F:308:ASN:HD22	3:F:309:GLY:N	2.03	0.56
2:E:439:ASN:N	2:E:439:ASN:ND2	2.53	0.56
3:C:227:TRP:HZ2	3:C:230:ASN:ND2	2.03	0.56
2:B:188:ALA:O	2:B:191:GLU:HB2	2.04	0.56
3:C:307:HIS:O	3:C:310:MET:HB2	2.05	0.56
1:A:153:ASP:O	1:A:157:LYS:HG2	2.05	0.56
3:F:367:ILE:HD12	3:F:378:SER:OG	2.05	0.56
2:B:234:LYS:HA	2:B:234:LYS:HE2	1.87	0.56
2:B:420:GLY:HA2	2:B:446:SER:O	2.06	0.56
2:E:340:ILE:HG12	2:E:341:SER:N	2.21	0.56
3:C:308:ASN:HD22	3:C:309:GLY:N	2.03	0.56
3:F:189:ASN:ND2	3:F:391:ARG:HH21	2.04	0.56
2:E:405:ASN:C	2:E:407:CYS:N	2.57	0.56
2:B:340:ILE:HG12	2:B:341:SER:N	2.21	0.56
1:D:153:ASP:O	1:D:157:LYS:HG2	2.05	0.56
2:E:266:TRP:CE3	2:E:380:ARG:HD2	2.41	0.56
3:C:166:LEU:HB3	3:C:179:LEU:HD11	1.86	0.55
2:B:436:VAL:HG12	2:B:437:TRP:H	1.71	0.55
2:E:436:VAL:HG12	2:E:437:TRP:H	1.71	0.55
3:F:236:ILE:O	3:F:239:GLN:HG2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:396:GLU:CA	3:F:186:GLY:HA2	2.36	0.55
3:F:304:PHE:O	3:F:338:LYS:HB3	2.07	0.55
2:B:211:CYS:SG	2:B:250:THR:HA	2.46	0.55
2:E:234:LYS:HA	2:E:234:LYS:HE2	1.87	0.55
1:A:134:GLN:O	1:A:137:GLN:HG2	2.07	0.55
2:E:211:CYS:SG	2:E:250:THR:HA	2.46	0.55
3:C:236:ILE:O	3:C:239:GLN:HG2	2.06	0.55
3:C:189:ASN:ND2	3:C:391:ARG:HH21	2.04	0.55
2:E:420:GLY:HA2	2:E:446:SER:O	2.06	0.55
2:B:266:TRP:CE3	2:B:380:ARG:HD2	2.41	0.55
2:E:367:MET:O	2:E:406:ARG:HB2	2.07	0.55
2:B:357:ALA:HA	2:B:439:ASN:ND2	2.21	0.55
1:A:147:MET:HG3	2:B:175:LEU:HD22	1.89	0.55
3:F:209:ILE:N	3:F:209:ILE:HD12	2.17	0.54
2:B:154:ASP:HB2	2:B:157:VAL:HB	1.89	0.54
3:C:267:VAL:HG13	3:C:274:TYR:O	2.07	0.54
2:E:161:ILE:N	2:E:162:PRO:CD	2.70	0.54
3:C:264:MET:O	3:C:278:TYR:HA	2.07	0.54
3:F:267:VAL:HG13	3:F:274:TYR:O	2.07	0.54
3:C:169:ILE:O	3:C:177:GLN:HB2	2.08	0.54
2:E:154:ASP:HB2	2:E:157:VAL:HB	1.89	0.54
4:B:1:NAG:H5	4:B:1:NAG:N2	2.23	0.54
3:C:304:PHE:O	3:C:338:LYS:HB3	2.07	0.54
1:D:134:GLN:O	1:D:137:GLN:HG2	2.07	0.54
2:B:161:ILE:N	2:B:162:PRO:CD	2.70	0.54
1:D:117:SER:O	1:D:121:VAL:HG22	2.08	0.54
1:D:143:GLN:HE22	3:F:117:ASN:HB3	1.72	0.54
3:F:169:ILE:O	3:F:177:GLN:HB2	2.08	0.54
2:B:439:ASN:ND2	2:B:439:ASN:N	2.53	0.54
3:F:264:MET:O	3:F:278:TYR:HA	2.07	0.54
3:F:246:LEU:HG	3:F:246:LEU:O	2.06	0.54
2:B:367:MET:O	2:B:406:ARG:HB2	2.07	0.54
2:B:210:GLU:OE2	2:B:212:GLU:HB3	2.08	0.54
2:E:312:ILE:HB	2:E:324:ALA:HB3	1.90	0.54
3:C:228:LEU:O	3:C:232:LYS:HD2	2.08	0.54
1:A:143:GLN:HE22	3:C:117:ASN:HB3	1.72	0.54
3:F:228:LEU:O	3:F:232:LYS:HD2	2.08	0.54
1:A:176:LYS:H	1:A:176:LYS:HD3	1.73	0.54
3:F:207:ASN:OD1	3:F:209:ILE:N	2.41	0.53
2:E:360:LEU:HB3	2:E:364:ASN:HB3	1.91	0.53
3:F:191:TRP:CE2	3:F:387:ILE:HD12	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:310:MET:SD	3:C:337:ASN:CB	2.87	0.53
3:C:337:ASN:C	3:C:339:CYS:N	2.61	0.53
1:A:117:SER:O	1:A:121:VAL:HG22	2.08	0.53
2:B:226:LEU:HD23	2:B:236:TYR:O	2.08	0.53
3:C:207:ASN:OD1	3:C:209:ILE:N	2.41	0.53
2:E:255:ARG:HH11	2:E:413:ASN:HA	1.73	0.53
2:B:255:ARG:HH11	2:B:413:ASN:HA	1.73	0.53
3:C:249:GLU:HB2	3:C:383:THR:HG23	1.91	0.53
2:B:360:LEU:HB3	2:B:364:ASN:HB3	1.91	0.53
2:E:298:LYS:HZ2	2:E:298:LYS:HB2	1.72	0.53
2:E:226:LEU:HD23	2:E:236:TYR:O	2.08	0.53
2:E:210:GLU:OE2	2:E:212:GLU:HB3	2.08	0.53
3:C:260:ALA:HB2	3:C:286:ALA:HB3	1.90	0.53
3:C:191:TRP:CE2	3:C:387:ILE:HD12	2.43	0.53
1:D:147:MET:HG3	2:E:175:LEU:HD22	1.90	0.53
4:E:1:NAG:H5	4:E:1:NAG:N2	2.23	0.53
3:F:88:LYS:HB3	3:F:92:GLU:CB	2.34	0.52
2:B:210:GLU:HG2	2:B:212:GLU:N	2.18	0.52
3:F:260:ALA:HB2	3:F:286:ALA:HB3	1.90	0.52
2:B:359:GLN:H	2:B:359:GLN:HE21	1.57	0.52
3:C:212:LYS:HG3	3:C:274:TYR:OH	2.09	0.52
1:A:155:ASP:HB2	1:A:173:VAL:HG11	1.91	0.52
1:D:176:LYS:HD3	1:D:176:LYS:H	1.73	0.52
3:F:249:GLU:HB2	3:F:383:THR:HG23	1.91	0.52
1:A:130:VAL:HG23	2:B:161:ILE:HD11	1.92	0.52
2:B:167:VAL:HG23	2:B:168:LEU:H	1.75	0.52
2:E:357:ALA:HA	2:E:439:ASN:ND2	2.21	0.52
3:C:171:PRO:HD2	3:C:174:ALA:HB2	1.92	0.52
2:E:376:SER:HB3	2:E:382:ASN:H	1.75	0.52
2:E:254:ASN:O	2:E:291:GLU:HA	2.10	0.52
2:B:300:SER:HB2	2:B:304:ARG:HH12	1.74	0.52
2:B:376:SER:HB3	2:B:382:ASN:H	1.74	0.52
2:E:300:SER:HB2	2:E:304:ARG:HH12	1.74	0.52
4:E:1:NAG:HN2	4:E:1:NAG:H5	1.75	0.52
1:D:184:GLN:O	1:D:187:GLN:HB3	2.09	0.52
2:E:376:SER:HB3	2:E:382:ASN:N	2.25	0.52
2:E:359:GLN:HE21	2:E:359:GLN:H	1.57	0.52
2:B:312:ILE:HB	2:B:324:ALA:HB3	1.90	0.52
2:B:376:SER:HB3	2:B:382:ASN:N	2.25	0.52
2:E:210:GLU:HG2	2:E:212:GLU:N	2.18	0.52
2:B:254:ASN:O	2:B:291:GLU:HA	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:171:PRO:HD2	3:F:174:ALA:HB2	1.92	0.52
2:E:167:VAL:HG23	2:E:168:LEU:H	1.75	0.52
3:C:246:LEU:HG	3:C:246:LEU:O	2.06	0.52
1:A:184:GLN:O	1:A:187:GLN:HB3	2.09	0.52
3:C:88:LYS:HB3	3:C:92:GLU:CB	2.34	0.51
2:E:296:ASN:HB3	2:E:338:TYR:CE1	2.45	0.51
1:A:179:GLU:O	1:A:182:GLN:HB2	2.10	0.51
3:F:275:ARG:HA	3:F:311:GLN:HA	1.92	0.51
3:C:344:LEU:HA	3:C:367:ILE:HG23	1.92	0.51
3:C:195:GLN:OE1	3:C:382:THR:HG22	2.10	0.51
3:F:212:LYS:HG3	3:F:274:TYR:OH	2.09	0.51
3:C:275:ARG:HA	3:C:311:GLN:HA	1.92	0.51
1:D:130:VAL:HG23	2:E:161:ILE:HD11	1.92	0.51
2:B:296:ASN:HB3	2:B:338:TYR:CE1	2.45	0.51
3:C:330:ASP:O	3:C:365:ASN:HB2	2.10	0.51
1:D:179:GLU:O	1:D:182:GLN:HB2	2.10	0.51
2:B:436:VAL:HG13	2:B:445:TYR:O	2.11	0.51
1:D:155:ASP:HB2	1:D:173:VAL:HG11	1.91	0.51
2:B:342:VAL:H	2:B:371:ASN:ND2	2.09	0.51
1:A:172:GLU:O	1:A:173:VAL:HG13	2.11	0.51
3:F:330:ASP:O	3:F:365:ASN:HB2	2.09	0.51
3:F:195:GLN:OE1	3:F:382:THR:HG22	2.10	0.51
2:E:351:ASN:C	2:E:351:ASN:HD22	2.14	0.51
2:B:266:TRP:HA	2:B:377:THR:HG21	1.93	0.51
3:C:305:THR:HB	3:C:341:ALA:HB2	1.93	0.51
3:F:369:TRP:CD1	3:F:371:THR:HG22	2.46	0.51
4:B:1:NAG:H5	4:B:1:NAG:HN2	1.75	0.50
2:B:155:GLU:HB2	3:C:96:TYR:CZ	2.46	0.50
3:C:369:TRP:CD1	3:C:371:THR:HG22	2.46	0.50
1:D:172:GLU:O	1:D:173:VAL:HG13	2.11	0.50
3:C:185:ASP:OD1	3:C:189:ASN:HB2	2.12	0.50
3:F:367:ILE:O	3:F:378:SER:HA	2.11	0.50
2:E:436:VAL:HG13	2:E:445:TYR:O	2.11	0.50
3:F:119:GLN:HA	3:F:119:GLN:OE1	2.11	0.50
2:B:152:TYR:C	2:B:152:TYR:CD1	2.85	0.50
3:C:227:TRP:CZ2	3:C:230:ASN:ND2	2.80	0.50
3:F:365:ASN:N	3:F:365:ASN:HD22	2.10	0.50
3:F:227:TRP:CZ2	3:F:230:ASN:ND2	2.80	0.50
2:B:351:ASN:C	2:B:351:ASN:HD22	2.14	0.50
2:B:311:LEU:HD12	2:B:312:ILE:H	1.77	0.50
2:E:342:VAL:H	2:E:371:ASN:ND2	2.09	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:368:ILE:HD13	3:F:368:ILE:H	1.77	0.50
2:E:314:MET:CE	2:E:437:TRP:CB	2.90	0.50
3:C:265:PHE:CE1	3:C:267:VAL:HG23	2.47	0.50
3:F:337:ASN:C	3:F:339:CYS:N	2.61	0.49
2:B:361:MET:O	2:B:364:ASN:HB2	2.12	0.49
3:C:367:ILE:O	3:C:378:SER:HA	2.11	0.49
3:C:369:TRP:HD1	3:C:372:TRP:HB2	1.76	0.49
3:F:334:TRP:HE3	3:F:345:ASN:ND2	2.10	0.49
2:B:300:SER:HB2	2:B:304:ARG:NH1	2.27	0.49
2:E:155:GLU:HB2	3:F:96:TYR:CZ	2.46	0.49
2:B:314:MET:CE	2:B:437:TRP:CB	2.90	0.49
3:F:265:PHE:CE1	3:F:267:VAL:HG23	2.47	0.49
2:B:340:ILE:HB	2:B:403:TRP:CE2	2.48	0.49
3:C:368:ILE:HD13	3:C:368:ILE:H	1.77	0.49
2:E:361:MET:O	2:E:364:ASN:HB2	2.12	0.49
3:F:344:LEU:HA	3:F:367:ILE:HG23	1.93	0.49
3:C:119:GLN:HA	3:C:119:GLN:OE1	2.11	0.49
2:E:340:ILE:HB	2:E:403:TRP:CE2	2.48	0.49
2:E:412:PRO:HB3	2:E:450:MET:SD	2.53	0.49
3:F:369:TRP:HD1	3:F:372:TRP:HB2	1.76	0.49
2:E:311:LEU:HD12	2:E:312:ILE:H	1.77	0.49
2:E:266:TRP:HA	2:E:377:THR:HG21	1.93	0.49
2:B:340:ILE:HG12	2:B:341:SER:H	1.78	0.49
3:F:305:THR:HB	3:F:341:ALA:HB2	1.93	0.49
3:F:310:MET:SD	3:F:337:ASN:CB	2.87	0.49
2:E:340:ILE:HG12	2:E:341:SER:H	1.78	0.49
2:E:300:SER:HB2	2:E:304:ARG:NH1	2.27	0.49
3:C:209:ILE:N	3:C:209:ILE:HD12	2.17	0.49
2:B:412:PRO:HB3	2:B:450:MET:SD	2.53	0.49
3:C:253:TRP:HA	3:C:380:LYS:HD2	1.95	0.49
1:D:115:LEU:HA	1:D:118:ARG:HH21	1.78	0.49
3:C:266:LYS:O	3:C:277:THR:HG23	2.13	0.49
3:F:185:ASP:OD1	3:F:189:ASN:HB2	2.12	0.49
2:E:276:VAL:O	2:E:290:GLY:N	2.45	0.49
3:C:365:ASN:N	3:C:365:ASN:HD22	2.10	0.49
1:A:122:LEU:HD12	1:A:123:LYS:NZ	2.28	0.49
2:E:224:MET:SD	2:E:237:ARG:HB3	2.53	0.49
3:C:262:TYR:CE2	3:C:281:PHE:HD1	2.31	0.49
2:B:224:MET:SD	2:B:237:ARG:HB3	2.53	0.48
3:F:266:LYS:O	3:F:277:THR:HG23	2.13	0.48
2:E:283:LYS:H	2:E:283:LYS:HE2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:262:TYR:CE2	3:C:290:PHE:HB2	2.48	0.48
2:E:152:TYR:C	2:E:152:TYR:CD1	2.85	0.48
3:C:274:TYR:O	3:C:335:TRP:CZ3	2.65	0.48
3:C:191:TRP:CE3	3:C:387:ILE:HB	2.49	0.48
2:B:276:VAL:O	2:B:290:GLY:N	2.45	0.48
3:F:191:TRP:CZ3	3:F:387:ILE:HB	2.48	0.48
3:F:201:SER:HG	3:F:225:GLU:HG3	1.78	0.48
1:A:115:LEU:HA	1:A:118:ARG:HH21	1.78	0.48
1:D:122:LEU:HD12	1:D:123:LYS:NZ	2.28	0.48
3:C:201:SER:HG	3:C:225:GLU:HG3	1.78	0.48
3:C:191:TRP:CZ3	3:C:387:ILE:HB	2.48	0.48
3:F:262:TYR:CE2	3:F:290:PHE:HB2	2.48	0.48
3:F:123:ASN:HD22	3:F:123:ASN:N	2.12	0.48
3:C:219:SER:OG	3:C:224:THR:HG22	2.13	0.48
3:C:253:TRP:N	3:C:253:TRP:CD1	2.81	0.48
3:F:334:TRP:CD1	3:F:343:HIS:HB2	2.49	0.48
3:C:334:TRP:HE3	3:C:345:ASN:ND2	2.10	0.48
3:F:191:TRP:CE3	3:F:387:ILE:HB	2.49	0.48
3:F:253:TRP:HA	3:F:380:LYS:HD2	1.95	0.48
3:F:208:TRP:HA	3:F:314:THR:HG21	1.95	0.48
3:C:208:TRP:HA	3:C:314:THR:HG21	1.95	0.48
2:B:283:LYS:HE2	2:B:283:LYS:H	1.78	0.48
3:F:247:ARG:HD3	3:F:261:ASP:OD1	2.14	0.48
3:F:262:TYR:CE2	3:F:281:PHE:HD1	2.31	0.48
2:E:385:TRP:HB3	2:E:392:LYS:HZ2	1.78	0.48
1:A:130:VAL:HG22	1:A:192:ASP:OD2	2.14	0.48
3:C:334:TRP:CD2	3:C:343:HIS:HB2	2.49	0.48
2:E:261:ASP:O	2:E:264:ARG:NE	2.41	0.48
3:F:219:SER:OG	3:F:224:THR:HG22	2.13	0.48
2:E:203:ILE:O	3:F:217:HIS:HA	2.14	0.48
2:B:167:VAL:HG23	2:B:168:LEU:N	2.29	0.47
2:E:380:ARG:CB	2:E:380:ARG:HH11	2.27	0.47
2:E:285:TYR:HD1	2:E:285:TYR:H	1.62	0.47
2:B:294:LEU:CD2	2:B:299:ILE:HG12	2.44	0.47
3:C:247:ARG:HD3	3:C:261:ASP:OD1	2.14	0.47
3:C:334:TRP:CD1	3:C:343:HIS:HB2	2.49	0.47
1:D:114:ASP:HB3	3:F:90:LEU:HD21	1.96	0.47
2:B:385:TRP:HB3	2:B:392:LYS:HZ2	1.78	0.47
3:F:181:TYR:HE1	3:F:220:PRO:O	1.98	0.47
2:B:380:ARG:HH11	2:B:380:ARG:CB	2.27	0.47
2:B:203:ILE:O	3:C:217:HIS:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:267:ASP:HB3	2:B:268:PRO:HD2	1.97	0.47
2:B:455:ARG:HG2	2:B:456:PRO:HD2	1.96	0.47
2:E:455:ARG:HG2	2:E:456:PRO:HD2	1.96	0.47
2:B:411:ASN:O	2:B:435:VAL:HA	2.14	0.47
2:E:187:SER:O	2:E:190:MET:HB2	2.15	0.47
2:E:167:VAL:HG23	2:E:168:LEU:N	2.29	0.47
3:C:227:TRP:HZ2	3:C:230:ASN:HD21	1.63	0.47
3:F:225:GLU:O	3:F:226:PHE:HB3	2.15	0.47
1:D:127:ILE:CD1	1:D:193:LEU:HD13	2.44	0.47
2:E:405:ASN:C	2:E:407:CYS:H	2.18	0.47
1:D:158:ILE:HG23	2:E:189:GLN:NE2	2.21	0.47
2:E:215:ILE:HG13	2:E:219:GLY:O	2.15	0.47
2:E:152:TYR:C	2:E:152:TYR:HD1	2.18	0.47
3:F:334:TRP:CD2	3:F:343:HIS:HB2	2.49	0.47
2:B:300:SER:HB2	2:B:332:GLN:O	2.14	0.47
2:E:300:SER:HB2	2:E:332:GLN:O	2.14	0.47
3:F:253:TRP:CD1	3:F:253:TRP:N	2.81	0.47
2:B:326:TYR:CD1	2:B:326:TYR:N	2.83	0.47
3:C:181:TYR:HE1	3:C:220:PRO:O	1.98	0.47
3:C:251:GLU:HG3	3:C:257:THR:HG22	1.97	0.47
2:B:362:GLY:O	2:B:366:THR:HG23	2.15	0.47
3:C:197:ARG:NH1	3:C:346:GLY:O	2.48	0.47
3:F:197:ARG:NH1	3:F:346:GLY:O	2.48	0.47
2:B:410:ALA:HA	2:B:436:VAL:O	2.14	0.47
3:F:151:LYS:HD3	3:F:170:LYS:O	2.15	0.47
3:C:246:LEU:HD22	3:C:265:PHE:CE2	2.50	0.47
1:A:114:ASP:HB3	3:C:90:LEU:HD21	1.96	0.47
3:C:227:TRP:CD1	3:C:229:GLY:HA2	2.50	0.47
1:D:150:LEU:HD22	1:D:150:LEU:HA	1.75	0.47
1:D:130:VAL:HG22	1:D:192:ASP:OD2	2.14	0.47
3:C:225:GLU:O	3:C:226:PHE:HB3	2.15	0.47
3:C:123:ASN:N	3:C:123:ASN:HD22	2.12	0.47
2:E:311:LEU:HD12	2:E:312:ILE:N	2.30	0.47
3:C:151:LYS:HD3	3:C:170:LYS:O	2.15	0.47
3:F:227:TRP:HZ2	3:F:230:ASN:HD21	1.63	0.47
2:B:163:THR:O	2:B:165:LEU:N	2.38	0.46
3:F:246:LEU:HD22	3:F:265:PHE:CE2	2.50	0.46
2:E:411:ASN:O	2:E:435:VAL:HA	2.14	0.46
2:E:163:THR:O	2:E:165:LEU:N	2.38	0.46
2:E:410:ALA:HA	2:E:436:VAL:O	2.15	0.46
2:B:311:LEU:HD12	2:B:312:ILE:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:274:TYR:O	3:F:335:TRP:CZ3	2.65	0.46
1:A:127:ILE:CD1	1:A:193:LEU:HD13	2.44	0.46
2:E:402:TRP:CZ3	2:E:412:PRO:HD2	2.51	0.46
3:F:227:TRP:CD1	3:F:229:GLY:HA2	2.50	0.46
2:E:163:THR:C	2:E:165:LEU:H	2.19	0.46
2:E:374:PHE:O	2:E:403:TRP:HA	2.16	0.46
3:F:343:HIS:ND1	3:F:343:HIS:O	2.49	0.46
2:B:405:ASN:C	2:B:407:CYS:H	2.18	0.46
2:B:215:ILE:HG13	2:B:219:GLY:O	2.15	0.46
2:B:152:TYR:HD1	2:B:152:TYR:C	2.18	0.46
2:B:152:TYR:CD1	2:B:153:ILE:N	2.75	0.46
3:C:343:HIS:O	3:C:343:HIS:ND1	2.49	0.46
3:F:232:LYS:O	3:F:236:ILE:HD12	2.16	0.46
4:E:1:NAG:C5	4:E:1:NAG:N2	2.78	0.46
2:E:415:ARG:O	2:E:434:GLY:HA2	2.15	0.46
2:B:187:SER:O	2:B:190:MET:HB2	2.15	0.46
2:E:326:TYR:N	2:E:326:TYR:CD1	2.83	0.46
2:E:362:GLY:O	2:E:366:THR:HG23	2.15	0.46
2:B:163:THR:C	2:B:165:LEU:H	2.19	0.46
2:B:415:ARG:O	2:B:434:GLY:HA2	2.15	0.46
3:F:251:GLU:HG3	3:F:257:THR:HG22	1.97	0.46
3:F:88:LYS:CD	3:F:92:GLU:HB2	2.45	0.46
3:C:232:LYS:O	3:C:236:ILE:HD12	2.15	0.46
3:C:335:TRP:N	3:C:335:TRP:CD1	2.84	0.46
2:B:209:LYS:HG3	2:B:229:PRO:HA	1.98	0.45
2:B:167:VAL:HG23	2:B:168:LEU:CD1	2.36	0.45
2:E:209:LYS:HG3	2:E:229:PRO:HA	1.98	0.45
2:E:383:ASP:OD1	2:E:385:TRP:CE2	2.69	0.45
2:B:280:THR:OG1	2:B:281:ASP:N	2.49	0.45
3:F:250:LEU:HD22	3:F:379:MET:CG	2.45	0.45
2:B:383:ASP:OD1	2:B:385:TRP:CE2	2.70	0.45
3:F:335:TRP:CD1	3:F:335:TRP:N	2.84	0.45
2:B:241:ASP:HB3	2:B:249:TRP:HB2	1.98	0.45
2:B:261:ASP:O	2:B:264:ARG:NE	2.41	0.45
1:D:126:VAL:HG12	1:D:193:LEU:HD12	1.98	0.45
2:B:402:TRP:CZ3	2:B:412:PRO:HD2	2.51	0.45
3:F:89:MET:HG3	3:F:90:LEU:H	1.82	0.45
1:A:144:LEU:CD1	2:B:175:LEU:HD21	2.46	0.45
3:C:250:LEU:HD22	3:C:379:MET:CG	2.45	0.45
1:D:152:VAL:O	1:D:155:ASP:HB3	2.17	0.45
2:E:267:ASP:HB3	2:E:268:PRO:HD2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:VAL:O	1:A:155:ASP:HB3	2.17	0.45
2:B:374:PHE:O	2:B:403:TRP:HA	2.16	0.45
1:D:144:LEU:CD1	2:E:175:LEU:HD21	2.46	0.45
3:C:200:GLY:O	3:C:202:VAL:N	2.50	0.45
3:F:172:LEU:H	3:F:239:GLN:HE21	1.65	0.45
1:A:126:VAL:HG12	1:A:193:LEU:HD12	1.98	0.45
2:E:351:ASN:O	2:E:351:ASN:ND2	2.41	0.45
3:C:253:TRP:CH2	3:C:350:GLN:HA	2.51	0.45
1:A:115:LEU:HA	1:A:118:ARG:HE	1.82	0.45
3:F:253:TRP:CH2	3:F:350:GLN:HA	2.51	0.45
3:C:235:LEU:HD13	3:C:235:LEU:HA	1.77	0.45
2:E:244:THR:O	2:E:245:GLU:O	2.35	0.45
1:A:188:VAL:HG21	2:B:167:VAL:HG21	1.99	0.44
2:E:241:ASP:HB3	2:E:249:TRP:HB2	1.98	0.44
2:E:201:CYS:O	2:E:203:ILE:HD13	2.17	0.44
3:F:200:GLY:O	3:F:202:VAL:N	2.50	0.44
2:E:191:GLU:O	2:E:193:CYS:N	2.50	0.44
2:B:191:GLU:O	2:B:193:CYS:N	2.50	0.44
2:E:203:ILE:N	2:E:203:ILE:HD13	2.33	0.44
1:D:181:GLN:N	1:D:181:GLN:HE21	2.16	0.44
2:E:294:LEU:CD2	2:E:299:ILE:HG12	2.44	0.44
3:C:89:MET:HG3	3:C:90:LEU:H	1.82	0.44
2:B:244:THR:O	2:B:245:GLU:O	2.35	0.44
2:E:351:ASN:HD21	2:E:354:MET:H	1.65	0.44
2:E:229:PRO:CG	2:E:302:LEU:HD21	2.48	0.44
3:F:349:TYR:HB2	3:F:378:SER:CB	2.48	0.44
2:E:280:THR:HG23	2:E:287:GLY:H	1.83	0.44
3:F:318:ASP:CG	3:F:325:ASN:HB3	2.38	0.44
3:C:318:ASP:CG	3:C:325:ASN:HB3	2.38	0.44
3:C:161:ALA:C	3:C:162:LYS:HD3	2.38	0.44
2:E:280:THR:OG1	2:E:281:ASP:N	2.49	0.44
2:B:201:CYS:O	2:B:203:ILE:HD13	2.17	0.44
2:B:168:LEU:O	2:B:172:LEU:HB2	2.18	0.44
2:E:168:LEU:O	2:E:172:LEU:HB2	2.18	0.44
3:C:349:TYR:HB2	3:C:378:SER:HB2	1.99	0.44
3:F:206:LYS:HB3	3:F:210:GLN:HB2	2.00	0.44
2:B:203:ILE:HD13	2:B:203:ILE:N	2.33	0.44
1:A:135:LEU:C	1:A:135:LEU:HD13	2.38	0.44
3:C:131:LEU:O	3:C:134:GLN:N	2.49	0.44
2:E:172:LEU:HA	2:E:172:LEU:HD13	1.83	0.44
3:F:161:ALA:C	3:F:162:LYS:HD3	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:124:LEU:O	3:C:128:VAL:HG13	2.18	0.44
2:E:226:LEU:HD23	2:E:236:TYR:C	2.38	0.44
3:C:349:TYR:HB2	3:C:378:SER:CB	2.47	0.43
3:F:124:LEU:O	3:F:128:VAL:HG13	2.18	0.43
2:B:229:PRO:CG	2:B:302:LEU:HD21	2.48	0.43
2:E:167:VAL:HG23	2:E:168:LEU:CD1	2.36	0.43
2:E:360:LEU:HD22	2:E:360:LEU:N	2.33	0.43
2:B:212:GLU:HG3	2:B:213:GLU:N	2.32	0.43
3:F:247:ARG:HG2	3:F:385:LYS:HE2	2.00	0.43
1:D:115:LEU:HA	1:D:118:ARG:HE	1.82	0.43
1:A:127:ILE:HD13	1:A:193:LEU:HD13	2.00	0.43
1:D:127:ILE:HD13	1:D:193:LEU:HD13	2.00	0.43
2:B:298:LYS:HB2	2:B:298:LYS:HZ2	1.82	0.43
2:B:359:GLN:N	2:B:359:GLN:HE21	2.17	0.43
1:A:181:GLN:HE21	1:A:181:GLN:N	2.16	0.43
3:C:88:LYS:CD	3:C:92:GLU:HB2	2.45	0.43
3:C:172:LEU:H	3:C:239:GLN:HE21	1.65	0.43
1:D:135:LEU:C	1:D:135:LEU:HD13	2.38	0.43
2:B:351:ASN:HD21	2:B:354:MET:H	1.65	0.43
1:A:176:LYS:H	1:A:176:LYS:CD	2.29	0.43
2:B:389:ASP:C	2:B:391:ARG:H	2.22	0.43
2:B:360:LEU:HD22	2:B:360:LEU:N	2.33	0.43
3:C:206:LYS:HB3	3:C:210:GLN:HB2	2.00	0.43
1:D:188:VAL:HG21	2:E:167:VAL:HG21	1.99	0.43
3:C:264:MET:CG	3:C:279:ALA:HB3	2.49	0.43
3:F:235:LEU:HD13	3:F:235:LEU:HA	1.77	0.43
3:C:247:ARG:HG2	3:C:385:LYS:HE2	2.00	0.43
1:D:115:LEU:CA	1:D:118:ARG:HE	2.32	0.43
3:C:301:ASP:O	3:C:305:THR:HG23	2.19	0.43
3:F:307:HIS:HE1	3:F:342:GLY:H	1.67	0.43
2:E:168:LEU:HD12	2:E:168:LEU:N	2.34	0.43
2:E:212:GLU:HG3	2:E:213:GLU:N	2.32	0.43
1:A:157:LYS:HE2	2:B:398:ASP:OD2	2.19	0.43
3:F:349:TYR:HB2	3:F:378:SER:HB2	1.99	0.43
2:B:156:THR:O	2:B:160:ASN:HB3	2.18	0.43
2:E:156:THR:O	2:E:160:ASN:HB3	2.18	0.43
2:B:226:LEU:HD23	2:B:236:TYR:C	2.38	0.43
3:C:198:LEU:HD23	3:C:225:GLU:HG2	2.01	0.42
2:E:157:VAL:HA	2:E:160:ASN:HB3	2.00	0.42
2:E:332:GLN:HG2	2:E:336:ASN:HB2	2.01	0.42
3:F:354:TYR:O	3:F:376:TRP:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:423:THR:OG1	2:E:426:MET:HG3	2.19	0.42
2:B:386:LEU:O	2:B:386:LEU:HD12	2.19	0.42
3:F:369:TRP:NE1	3:F:371:THR:CG2	2.82	0.42
2:E:359:GLN:HE21	2:E:359:GLN:N	2.17	0.42
2:E:389:ASP:C	2:E:391:ARG:H	2.22	0.42
2:E:164:ASN:H	2:E:164:ASN:ND2	2.17	0.42
3:F:301:ASP:O	3:F:305:THR:HG23	2.19	0.42
2:B:351:ASN:ND2	2:B:354:MET:H	2.18	0.42
3:C:369:TRP:NE1	3:C:371:THR:CG2	2.82	0.42
3:C:183:GLU:O	3:C:191:TRP:HB2	2.20	0.42
1:A:119:ILE:O	1:A:123:LYS:N	2.52	0.42
3:C:234:HIS:CG	3:C:235:LEU:N	2.87	0.42
2:B:423:THR:OG1	2:B:426:MET:HG3	2.19	0.42
3:C:303:PHE:HD1	3:C:303:PHE:HA	1.68	0.42
2:B:351:ASN:O	2:B:351:ASN:ND2	2.41	0.42
1:D:191:LYS:HG3	1:D:192:ASP:N	2.35	0.42
2:B:375:PHE:CE1	2:B:402:TRP:HA	2.55	0.42
2:E:212:GLU:HG2	2:E:458:PHE:HE2	1.85	0.42
3:C:206:LYS:HE3	3:C:215:PHE:CD2	2.54	0.42
2:B:157:VAL:HA	2:B:160:ASN:HB3	2.00	0.42
3:F:366:GLY:O	3:F:368:ILE:HG23	2.20	0.42
1:A:150:LEU:HD22	1:A:150:LEU:HA	1.75	0.42
3:C:354:TYR:O	3:C:376:TRP:HB3	2.19	0.42
2:B:212:GLU:HG2	2:B:458:PHE:HE2	1.85	0.42
1:A:136:LEU:O	1:A:140:VAL:HG23	2.19	0.42
2:E:276:VAL:O	2:E:289:PRO:HA	2.20	0.42
3:F:206:LYS:HE3	3:F:215:PHE:CD2	2.54	0.42
1:D:157:LYS:HE2	2:E:398:ASP:OD2	2.19	0.42
2:B:414:GLY:HA3	2:B:434:GLY:O	2.19	0.42
3:F:94:MET:HA	3:F:97:GLU:OE2	2.20	0.42
2:B:168:LEU:HD12	2:B:168:LEU:N	2.34	0.42
2:E:370:HIS:CE1	2:E:402:TRP:HE1	2.38	0.42
2:E:375:PHE:CE1	2:E:402:TRP:HA	2.54	0.42
3:C:348:TYR:HA	3:C:367:ILE:CD1	2.41	0.42
3:C:247:ARG:HD2	3:C:259:THR:HB	2.02	0.42
3:F:183:GLU:O	3:F:191:TRP:HB2	2.20	0.42
2:E:227:ILE:HD11	2:E:236:TYR:CE2	2.55	0.42
3:C:366:GLY:O	3:C:368:ILE:HG23	2.20	0.42
1:D:119:ILE:O	1:D:123:LYS:N	2.52	0.42
2:E:204:PRO:HG3	3:F:217:HIS:CD2	2.55	0.42
2:B:276:VAL:O	2:B:289:PRO:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:332:GLN:HG2	2:B:336:ASN:HB2	2.01	0.42
3:F:131:LEU:O	3:F:134:GLN:N	2.49	0.42
2:B:168:LEU:HD12	2:B:168:LEU:H	1.85	0.42
2:B:276:VAL:HA	2:B:292:TYR:CE2	2.53	0.42
3:C:196:LYS:HA	3:C:382:THR:O	2.19	0.42
1:D:136:LEU:O	1:D:140:VAL:HG23	2.19	0.42
2:B:280:THR:HG23	2:B:287:GLY:H	1.83	0.42
2:E:414:GLY:HA3	2:E:434:GLY:O	2.19	0.42
2:E:168:LEU:HD12	2:E:168:LEU:H	1.85	0.42
2:B:317:TRP:CD1	2:B:420:GLY:N	2.85	0.42
3:F:338:LYS:O	3:F:339:CYS:HB2	2.20	0.41
3:F:247:ARG:HD2	3:F:259:THR:HB	2.02	0.41
3:F:198:LEU:HD23	3:F:225:GLU:HG2	2.00	0.41
2:B:164:ASN:ND2	2:B:164:ASN:H	2.17	0.41
3:C:315:TRP:CE2	3:C:316:ASP:HB3	2.55	0.41
3:F:326:CYS:SG	3:F:339:CYS:N	2.93	0.41
3:C:168:PHE:HE1	3:C:179:LEU:HB2	1.85	0.41
2:E:276:VAL:HA	2:E:292:TYR:CE2	2.53	0.41
3:F:196:LYS:HA	3:F:382:THR:O	2.19	0.41
1:A:191:LYS:HG3	1:A:192:ASP:N	2.35	0.41
2:B:370:HIS:CE1	2:B:402:TRP:HE1	2.38	0.41
3:F:346:GLY:O	3:F:367:ILE:HG13	2.20	0.41
3:C:93:ILE:HD12	3:C:93:ILE:N	2.36	0.41
1:A:115:LEU:CA	1:A:118:ARG:HE	2.32	0.41
2:B:204:PRO:HG3	3:C:217:HIS:CD2	2.55	0.41
3:F:295:PHE:CD2	3:F:375:ARG:HD2	2.55	0.41
3:C:94:MET:HA	3:C:97:GLU:OE2	2.20	0.41
3:C:346:GLY:O	3:C:367:ILE:HG13	2.20	0.41
3:F:334:TRP:CE2	3:F:343:HIS:HA	2.55	0.41
1:A:176:LYS:N	1:A:176:LYS:HD3	2.35	0.41
2:E:386:LEU:O	2:E:386:LEU:HD12	2.19	0.41
2:B:285:TYR:HD1	2:B:285:TYR:H	1.62	0.41
3:C:295:PHE:CD2	3:C:375:ARG:HD2	2.55	0.41
3:C:307:HIS:HE1	3:C:342:GLY:H	1.67	0.41
3:F:151:LYS:HD3	3:F:151:LYS:HA	1.80	0.41
3:C:334:TRP:CE2	3:C:343:HIS:HA	2.55	0.41
1:D:114:ASP:HA	1:D:117:SER:HB3	2.03	0.41
3:F:315:TRP:CE2	3:F:316:ASP:HB3	2.55	0.41
3:F:264:MET:CG	3:F:279:ALA:HB3	2.49	0.41
3:F:93:ILE:N	3:F:93:ILE:HD12	2.36	0.41
3:F:213:GLU:O	3:F:232:LYS:HE3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:227:ILE:HD11	2:B:236:TYR:CE2	2.55	0.41
2:E:376:SER:HB3	2:E:382:ASN:HB2	2.03	0.41
1:A:129:LYS:HA	1:A:129:LYS:HD3	1.90	0.41
3:F:330:ASP:HA	3:F:365:ASN:HB3	2.03	0.41
1:D:119:ILE:O	1:D:123:LYS:HB2	2.21	0.41
2:E:351:ASN:ND2	2:E:354:MET:H	2.18	0.41
1:D:176:LYS:HD3	1:D:176:LYS:N	2.35	0.41
2:B:253:GLN:NE2	2:B:451:SER:HA	2.36	0.41
2:E:253:GLN:NE2	2:E:451:SER:HA	2.36	0.41
3:C:337:ASN:C	3:C:339:CYS:H	2.24	0.41
3:C:338:LYS:O	3:C:339:CYS:HB2	2.20	0.41
3:F:305:THR:CB	3:F:341:ALA:HB2	2.51	0.41
3:F:337:ASN:C	3:F:339:CYS:H	2.24	0.41
3:F:168:PHE:HE1	3:F:179:LEU:HB2	1.85	0.41
3:F:168:PHE:CD1	3:F:179:LEU:HD13	2.56	0.41
3:C:232:LYS:O	3:C:233:ILE:C	2.58	0.41
3:C:213:GLU:O	3:C:232:LYS:HE3	2.21	0.41
3:C:247:ARG:CD	3:C:259:THR:HB	2.51	0.41
3:C:246:LEU:O	3:C:261:ASP:HA	2.21	0.41
3:C:330:ASP:HA	3:C:365:ASN:HB3	2.03	0.41
3:F:234:HIS:CG	3:F:235:LEU:N	2.87	0.41
2:B:178:LYS:HE2	2:B:178:LYS:HB2	1.85	0.41
3:C:305:THR:CB	3:C:341:ALA:HB2	2.51	0.41
3:C:326:CYS:SG	3:C:339:CYS:N	2.93	0.41
2:B:276:VAL:HG13	2:B:292:TYR:CE2	2.56	0.41
3:F:246:LEU:O	3:F:261:ASP:HA	2.21	0.41
3:C:168:PHE:CD1	3:C:179:LEU:HD13	2.56	0.40
2:E:276:VAL:HG13	2:E:292:TYR:CE2	2.56	0.40
2:E:351:ASN:C	2:E:351:ASN:ND2	2.74	0.40
2:B:351:ASN:C	2:B:351:ASN:ND2	2.74	0.40
3:C:195:GLN:HA	3:C:226:PHE:O	2.21	0.40
2:E:317:TRP:CD1	2:E:420:GLY:N	2.85	0.40
3:F:247:ARG:CD	3:F:259:THR:HB	2.51	0.40
1:A:114:ASP:HA	1:A:117:SER:HB3	2.03	0.40
3:F:232:LYS:O	3:F:233:ILE:C	2.58	0.40
2:B:376:SER:HB3	2:B:382:ASN:HB2	2.03	0.40
3:F:307:HIS:NE2	3:F:340:HIS:HA	2.36	0.40
2:E:239:TYR:CE1	2:E:289:PRO:HD3	2.56	0.40
3:C:191:TRP:CE3	3:C:385:LYS:HE3	2.56	0.40
2:E:345:TYR:CG	2:E:346:ARG:N	2.90	0.40
3:F:277:THR:HA	3:F:308:ASN:ND2	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:171:PRO:HD2	3:F:174:ALA:CB	2.51	0.40
3:C:212:LYS:HE3	3:C:213:GLU:OE2	2.22	0.40
3:F:184:ILE:HA	3:F:189:ASN:O	2.21	0.40
3:F:253:TRP:CD1	3:F:380:LYS:HB2	2.57	0.40
2:E:383:ASP:OD1	2:E:385:TRP:CD2	2.74	0.40
3:C:392:LEU:HD22	3:F:186:GLY:O	2.20	0.40
2:E:354:MET:HA	2:E:369:ILE:HG23	2.04	0.40
2:E:402:TRP:CG	2:E:403:TRP:N	2.90	0.40
3:C:277:THR:HA	3:C:308:ASN:ND2	2.37	0.40
2:E:315:GLU:HG2	2:E:316:ASP:O	2.22	0.40
3:C:253:TRP:CD1	3:C:380:LYS:HB2	2.57	0.40
1:A:119:ILE:O	1:A:123:LYS:HB2	2.21	0.40
2:B:383:ASP:OD1	2:B:385:TRP:CD2	2.74	0.40
3:F:370:ALA:HA	3:F:373:LYS:O	2.21	0.40

All (7) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:303:PHE:CD2	3:F:277:THR:CG2[2_746]	1.40	0.80
3:C:303:PHE:CE2	3:F:277:THR:CG2[2_746]	1.65	0.55
2:B:159:SER:CB	1:D:114:ASP:OD1[2_545]	1.85	0.35
2:B:162:PRO:CG	1:D:113:GLU:OE1[2_545]	1.93	0.27
3:C:300:SER:CB	3:F:275:ARG:NH1[2_746]	2.06	0.14
2:B:151:LEU:CD2	3:F:102:THR:OG1[2_545]	2.11	0.09
2:B:166:ARG:NE	1:D:111:VAL:CG2[2_545]	2.15	0.05

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	83/87 (95%)	64 (77%)	15 (18%)	4 (5%)	3 10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	83/87 (95%)	64 (77%)	15 (18%)	4 (5%)	3 10
2	B	311/328 (95%)	252 (81%)	47 (15%)	12 (4%)	4 15
2	E	311/328 (95%)	252 (81%)	47 (15%)	12 (4%)	4 15
3	C	307/319 (96%)	243 (79%)	55 (18%)	9 (3%)	6 23
3	F	307/319 (96%)	243 (79%)	55 (18%)	9 (3%)	6 23
All	All	1402/1468 (96%)	1118 (80%)	234 (17%)	50 (4%)	4 18

All (50) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	173	VAL
2	B	245	GLU
2	B	280	THR
2	B	398	ASP
2	B	420	GLY
3	C	201	SER
3	C	339	CYS
1	D	173	VAL
2	E	245	GLU
2	E	280	THR
2	E	398	ASP
2	E	420	GLY
3	F	201	SER
3	F	339	CYS
2	B	153	ILE
2	B	192	TYR
2	B	276	VAL
2	B	407	CYS
2	B	434	GLY
3	C	198	LEU
3	C	283	GLY
3	C	374	THR
2	E	153	ILE
2	E	192	TYR
2	E	276	VAL
2	E	407	CYS
2	E	434	GLY
3	F	198	LEU
3	F	283	GLY
3	F	374	THR

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Mol	Chain	Res	Type
1	A	115	LEU
1	A	194	LEU
2	B	390	PRO
2	B	459	PRO
3	C	275	ARG
3	C	358	SER
1	D	115	LEU
1	D	194	LEU
2	E	390	PRO
2	E	459	PRO
3	F	275	ARG
3	F	358	SER
1	A	114	ASP
1	D	114	ASP
2	B	244	THR
3	C	176	GLN
2	E	244	THR
3	F	176	GLN
3	C	395	GLY
3	F	395	GLY

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	80/82 (98%)	62 (78%)	18 (22%)	1 3
1	D	80/82 (98%)	62 (78%)	18 (22%)	1 3
2	B	271/286 (95%)	237 (88%)	34 (12%)	6 17
2	E	271/286 (95%)	237 (88%)	34 (12%)	6 17
3	C	261/267 (98%)	229 (88%)	32 (12%)	6 17
3	F	261/267 (98%)	229 (88%)	32 (12%)	6 17
All	All	1224/1270 (96%)	1056 (86%)	168 (14%)	4 13

All (168) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	120	GLU
1	A	130	VAL
1	A	134	GLN
1	A	140	VAL
1	A	146	ASP
1	A	150	LEU
1	A	161	CYS
1	A	169	LEU
1	A	171	ARG
1	A	172	GLU
1	A	173	VAL
1	A	174	ASP
1	A	181	GLN
1	A	182	GLN
1	A	185	LEU
1	A	187	GLN
1	A	191	LYS
1	A	193	LEU
2	B	149	HIS
2	B	152	TYR
2	B	154	ASP
2	B	155	GLU
2	B	160	ASN
2	B	161	ILE
2	B	164	ASN
2	B	171	ILE
2	B	172	LEU
2	B	176	ARG
2	B	206	VAL
2	B	209	LYS
2	B	221	THR
2	B	226	LEU
2	B	252	ILE
2	B	253	GLN
2	B	298	LYS
2	B	301	GLN
2	B	314	MET
2	B	343	ASN
2	B	351	ASN
2	B	359	GLN
2	B	373	MET
2	B	380	ARG
2	B	385	TRP

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Mol	Chain	Res	Type
2	B	398	ASP
2	B	432	ASP
2	B	436	VAL
2	B	438	MET
2	B	439	ASN
2	B	447	MET
2	B	448	ARG
2	B	457	PHE
2	B	459	PRO
3	C	112	GLU
3	C	117	ASN
3	C	130	GLN
3	C	135	CYS
3	C	144	GLN
3	C	147	ASP
3	C	152	ASP
3	C	162	LYS
3	C	192	THR
3	C	195	GLN
3	C	198	LEU
3	C	235	LEU
3	C	246	LEU
3	C	277	THR
3	C	297	ASP
3	C	303	PHE
3	C	308	ASN
3	C	323	GLU
3	C	335	TRP
3	C	337	ASN
3	C	340	HIS
3	C	343	HIS
3	C	359	THR
3	C	365	ASN
3	C	368	ILE
3	C	374	THR
3	C	375	ARG
3	C	378	SER
3	C	382	THR
3	C	383	THR
3	C	385	LYS
3	C	390	ASN
1	D	120	GLU

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Mol	Chain	Res	Type
1	D	130	VAL
1	D	134	GLN
1	D	140	VAL
1	D	146	ASP
1	D	150	LEU
1	D	161	CYS
1	D	169	LEU
1	D	171	ARG
1	D	172	GLU
1	D	173	VAL
1	D	174	ASP
1	D	181	GLN
1	D	182	GLN
1	D	185	LEU
1	D	187	GLN
1	D	191	LYS
1	D	193	LEU
2	E	149	HIS
2	E	152	TYR
2	E	154	ASP
2	E	155	GLU
2	E	160	ASN
2	E	161	ILE
2	E	164	ASN
2	E	171	ILE
2	E	172	LEU
2	E	176	ARG
2	E	206	VAL
2	E	209	LYS
2	E	221	THR
2	E	226	LEU
2	E	252	ILE
2	E	253	GLN
2	E	298	LYS
2	E	301	GLN
2	E	314	MET
2	E	343	ASN
2	E	351	ASN
2	E	359	GLN
2	E	373	MET
2	E	380	ARG
2	E	385	TRP

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Mol	Chain	Res	Type
2	E	398	ASP
2	E	432	ASP
2	E	436	VAL
2	E	438	MET
2	E	439	ASN
2	E	447	MET
2	E	448	ARG
2	E	457	PHE
2	E	459	PRO
3	F	112	GLU
3	F	117	ASN
3	F	130	GLN
3	F	135	CYS
3	F	144	GLN
3	F	147	ASP
3	F	152	ASP
3	F	162	LYS
3	F	192	THR
3	F	195	GLN
3	F	198	LEU
3	F	235	LEU
3	F	246	LEU
3	F	277	THR
3	F	297	ASP
3	F	303	PHE
3	F	308	ASN
3	F	323	GLU
3	F	335	TRP
3	F	337	ASN
3	F	340	HIS
3	F	343	HIS
3	F	359	THR
3	F	365	ASN
3	F	368	ILE
3	F	374	THR
3	F	375	ARG
3	F	378	SER
3	F	382	THR
3	F	383	THR
3	F	385	LYS
3	F	390	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	GLN
1	A	143	GLN
1	A	181	GLN
2	B	160	ASN
2	B	174	ASN
2	B	180	GLN
2	B	189	GLN
2	B	228	GLN
2	B	253	GLN
2	B	256	GLN
2	B	271	GLN
2	B	339	GLN
2	B	343	ASN
2	B	351	ASN
2	B	359	GLN
2	B	371	ASN
2	B	439	ASN
3	C	117	ASN
3	C	123	ASN
3	C	136	GLN
3	C	176	GLN
3	C	189	ASN
3	C	230	ASN
3	C	234	HIS
3	C	239	GLN
3	C	307	HIS
3	C	308	ASN
3	C	317	ASN
3	C	319	ASN
3	C	325	ASN
3	C	329	GLN
3	C	337	ASN
3	C	361	ASN
3	C	365	ASN
1	D	137	GLN
1	D	143	GLN
1	D	181	GLN
2	E	160	ASN
2	E	174	ASN
2	E	180	GLN
2	E	189	GLN
2	E	228	GLN

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Mol	Chain	Res	Type
2	E	253	GLN
2	E	256	GLN
2	E	271	GLN
2	E	339	GLN
2	E	343	ASN
2	E	351	ASN
2	E	359	GLN
2	E	371	ASN
2	E	439	ASN
3	F	117	ASN
3	F	123	ASN
3	F	136	GLN
3	F	176	GLN
3	F	189	ASN
3	F	230	ASN
3	F	234	HIS
3	F	239	GLN
3	F	307	HIS
3	F	308	ASN
3	F	317	ASN
3	F	319	ASN
3	F	325	ASN
3	F	329	GLN
3	F	361	ASN
3	F	365	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
4	NAG	B	1	-	14,14,15	0.55	0	15,19,21	0.82	1 (6%)
4	NAG	E	1	-	14,14,15	0.54	0	15,19,21	0.81	1 (6%)

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
4	NAG	B	1	-	-	0/6/23/26	0/1/1/1
4	NAG	E	1	-	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1	NAG	C2-N2-C7	-2.31	120.08	123.04
4	E	1	NAG	C2-N2-C7	-2.29	120.09	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1	NAG	2	0
4	E	1	NAG	3	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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