Full wwPDB X-ray Structure Validation Report (i)

Jul 31, 2023 – 01:03 AM EDT

PDB ID	:	1FZE
Title	:	CRYSTAL STRUCTURE OF FRAGMENT DOUBLE-D FROM HUMAN FIBRIN
Authors	:	Everse, S.J.; Spraggon, G.; Veerapandian, L.; Doolittle, R.F.
Deposited on	:	1998-12-23
Resolution	:	3.00 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 (i) 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 (i)) were used in the production of this report:

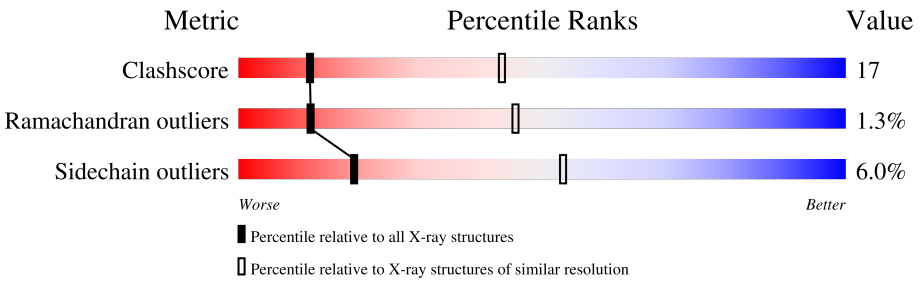
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 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	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	87	47% 41% 5% 7%
1	D	87	55% 33% • 8%
2	B	328	58% 32% • 6%
2	E	328	56% 34% • 6%
3	C	319	63% 29% • 5%
3	F	319	63% 29% • 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	B	470	-	-	X	-
4	NAG	B	471	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 11201 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
			Total	C	N	O	S			
1	A	81	668	414	128	123	3	0	0	0
1	D	80	660	410	127	120	3	0	0	0

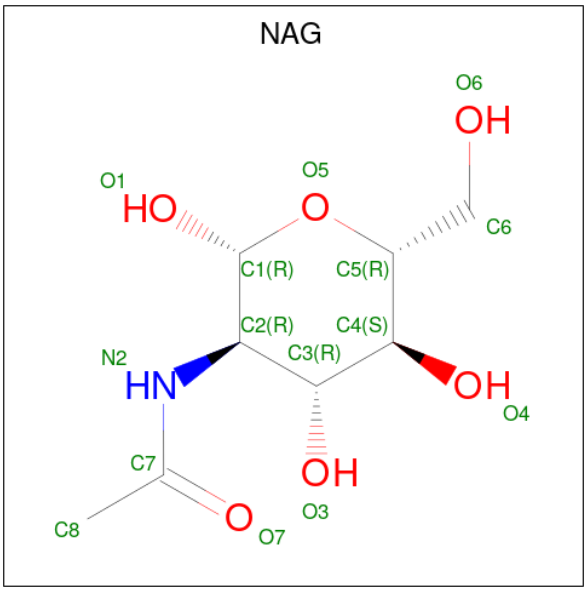
- Molecule 2 is a protein called FIBRINOGEN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	309	2480	1549	435	474	22	0	0	0
2	E	308	2473	1544	434	473	22	0	0	0

- Molecule 3 is a protein called FIBRINOGEN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	303	2433	1545	408	468	12	0	0	0
3	F	302	2425	1539	407	467	12	0	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
5	B	2	2	2	0	0
			Total	Ca		
5	C	1	1	1	0	0
			Total	Ca		
5	E	2	2	2	0	0
			Total	Ca		
5	F	1	1	1	0	0

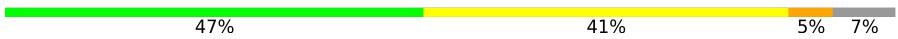
3 Residue-property plots (i)

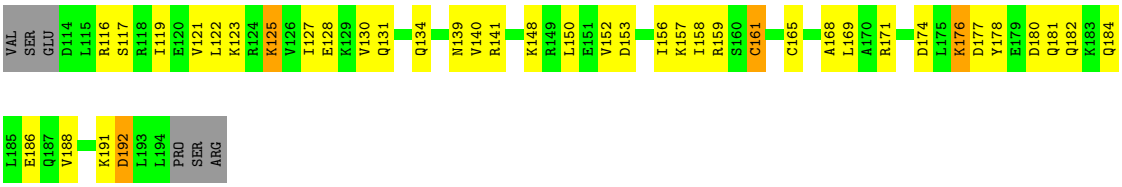
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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

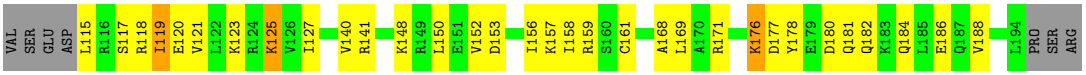
Chain A:





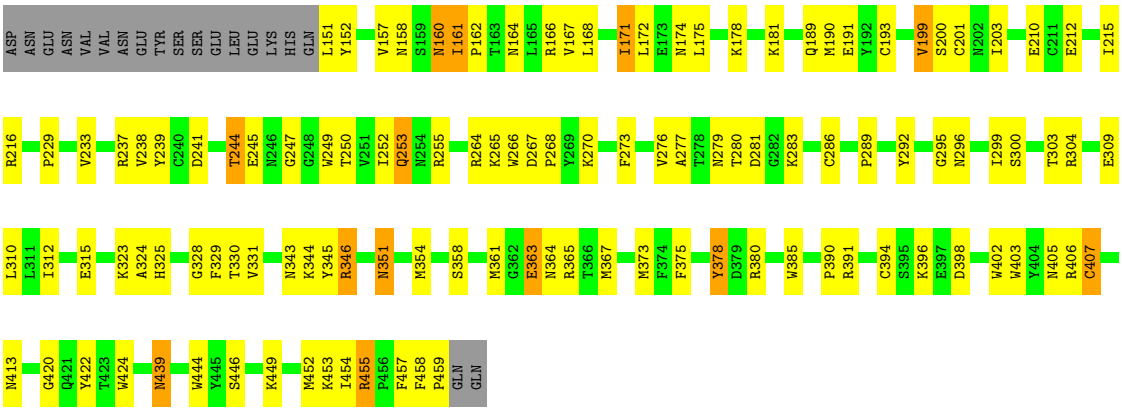
• Molecule 1: FIBRINOGEN

Chain D:



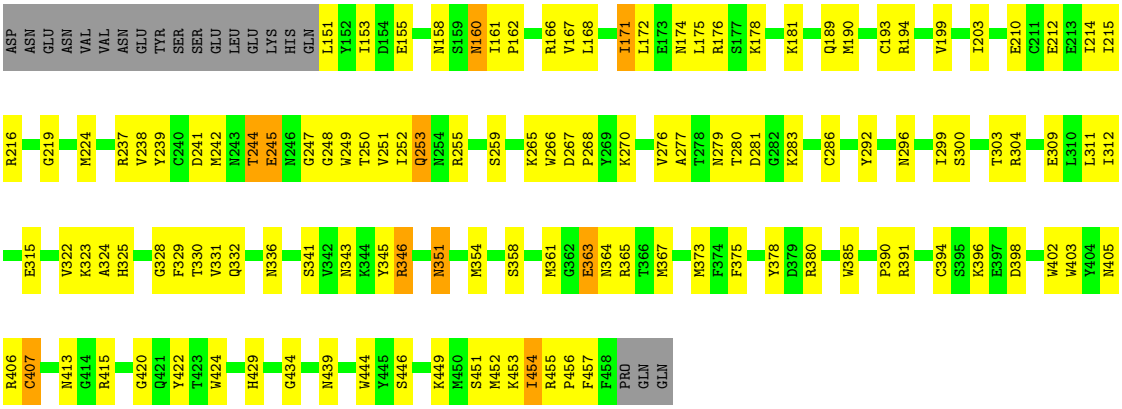
• Molecule 2: FIBRINOGEN

Chain B:



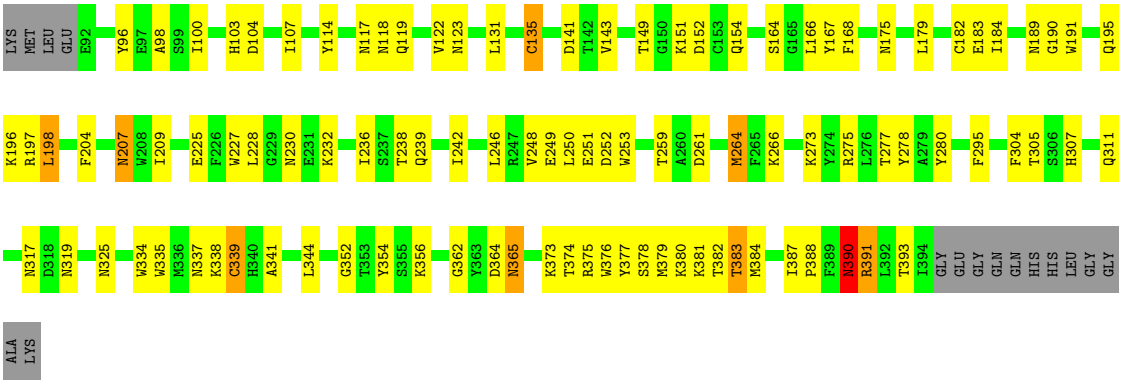
• Molecule 2: FIBRINOGEN

Chain E:



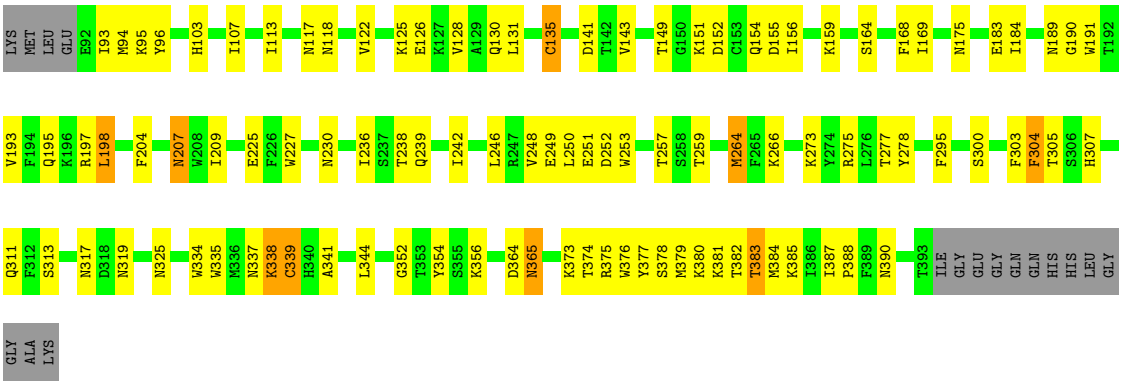
- Molecule 3: FIBRINOGEN

Chain C: 63% 29% • 5%



- Molecule 3: FIBRINOGEN

Chain F: 63% 29% • 5%



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	108.00Å 48.60Å 166.40Å 90.00° 104.40° 90.00°	Depositor
Resolution (Å)	30.00 – 3.00	Depositor
% Data completeness (in resolution range)	96.7 (30.00-3.00)	Depositor
R_{merge}	0.14	Depositor
R_{sym}	0.10	Depositor
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.251 , 0.318	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11201	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.33	0/669	0.56	0/891
1	D	0.35	0/661	0.58	0/880
2	B	0.37	0/2543	0.64	0/3437
2	E	0.37	0/2535	0.64	0/3425
3	C	0.37	0/2499	0.60	0/3379
3	F	0.37	0/2491	0.60	1/3368 (0.0%)
All	All	0.37	0/11398	0.61	1/15380 (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 (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	338	LYS	N-CA-C	-5.13	97.15	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	378	TYR	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	E	378	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	668	0	717	34	4
1	D	660	0	713	27	4
2	B	2480	0	2344	99	19
2	E	2473	0	2337	96	10
3	C	2433	0	2285	78	6
3	F	2425	0	2274	68	15
4	B	28	0	26	10	0
4	E	28	0	26	1	0
5	B	2	0	0	0	0
5	C	1	0	0	0	0
5	E	2	0	0	0	0
5	F	1	0	0	0	0
All	All	11201	0	10722	381	29

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 17.

All (381) 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:D:115:LEU:HA	1:D:118:ARG:HD3	1.38	1.00
1:A:140:VAL:HG11	2:B:171:ILE:HD11	1.52	0.91
1:A:161:CYS:HA	3:C:135:CYS:HB3	1.56	0.86
4:B:470:NAG:H3	4:B:471:NAG:C4	2.03	0.86
4:B:470:NAG:H3	4:B:471:NAG:H4	1.58	0.86
2:E:373:MET:SD	2:E:405:ASN:HB2	2.16	0.84
3:F:183:GLU:HB3	3:F:191:TRP:HB2	1.59	0.84
2:B:373:MET:SD	2:B:405:ASN:HB2	2.21	0.81
3:C:183:GLU:HB3	3:C:191:TRP:HB2	1.62	0.81
2:B:373:MET:HG3	2:B:405:ASN:HB2	1.63	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:253:TRP:HA	3:C:380:LYS:HD2	1.64	0.78
2:E:373:MET:HG3	2:E:405:ASN:HB2	1.65	0.78
3:C:373:LYS:HG2	3:C:377:TYR:CD2	2.19	0.78
3:F:373:LYS:HG2	3:F:377:TYR:CD2	2.21	0.76
3:F:253:TRP:HA	3:F:380:LYS:HD2	1.66	0.76
1:A:139:ASN:HB3	3:C:114:TYR:CE2	2.22	0.74
3:F:249:GLU:HB2	3:F:383:THR:HG23	1.69	0.74
3:C:249:GLU:HB2	3:C:383:THR:HG23	1.69	0.74
3:F:305:THR:HB	3:F:341:ALA:HB2	1.70	0.73
4:B:470:NAG:H5	4:B:471:NAG:H62	1.69	0.73
2:B:373:MET:CG	2:B:405:ASN:HB2	2.20	0.72
2:E:373:MET:CG	2:E:405:ASN:HB2	2.20	0.72
2:E:358:SER:HA	2:E:365:ARG:NH1	2.06	0.71
1:A:188:VAL:HG21	2:B:167:VAL:HG11	1.74	0.70
2:B:358:SER:HA	2:B:365:ARG:NH1	2.06	0.70
3:C:305:THR:HB	3:C:341:ALA:HB2	1.72	0.70
2:E:212:GLU:HG3	2:E:216:ARG:HH11	1.56	0.70
1:A:177:ASP:O	1:A:181:GLN:HG2	1.91	0.70
1:D:140:VAL:HG11	2:E:171:ILE:HD11	1.74	0.70
1:D:188:VAL:HG21	2:E:167:VAL:HG11	1.75	0.68
1:D:168:ALA:HA	2:E:189:GLN:HE22	1.59	0.67
2:B:351:ASN:ND2	2:B:354:MET:H	1.92	0.67
1:D:177:ASP:O	1:D:181:GLN:HG2	1.94	0.67
4:B:470:NAG:C1	4:B:471:NAG:H4	2.25	0.67
3:F:184:ILE:HA	3:F:189:ASN:O	1.94	0.67
2:B:439:ASN:H	2:B:439:ASN:HD22	1.42	0.66
2:B:212:GLU:HG3	2:B:216:ARG:HH11	1.61	0.65
2:B:160:ASN:H	2:B:162:PRO:HD2	1.61	0.65
3:C:227:TRP:HZ2	3:C:230:ASN:HD21	1.43	0.65
2:E:351:ASN:ND2	2:E:354:MET:H	1.93	0.65
2:B:201:CYS:O	3:C:143:VAL:HG21	1.96	0.65
3:C:197:ARG:HA	3:C:225:GLU:HG3	1.77	0.65
2:E:351:ASN:C	2:E:351:ASN:HD22	2.01	0.64
2:E:276:VAL:HA	2:E:292:TYR:CD1	2.32	0.64
4:B:470:NAG:C3	4:B:471:NAG:H4	2.27	0.64
1:D:125:LYS:HA	1:D:125:LYS:HE3	1.80	0.64
1:A:125:LYS:HE3	1:A:125:LYS:HA	1.80	0.64
2:B:323:LYS:HE2	2:B:325:HIS:HB2	1.78	0.63
2:E:455:ARG:HG2	2:E:456:PRO:HD2	1.79	0.63
3:F:197:ARG:HA	3:F:225:GLU:HG3	1.79	0.63
3:C:275:ARG:HB2	3:C:311:GLN:HG2	1.80	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:171:ILE:HD13	2:E:172:LEU:N	2.14	0.63
2:B:351:ASN:HD22	2:B:351:ASN:C	2.02	0.63
3:F:337:ASN:C	3:F:339:CYS:H	2.01	0.63
3:C:337:ASN:C	3:C:339:CYS:H	2.02	0.63
3:F:227:TRP:HZ2	3:F:230:ASN:HD21	1.48	0.62
3:C:149:THR:HG23	3:C:168:PHE:O	1.99	0.61
2:E:323:LYS:HE2	2:E:325:HIS:HB2	1.81	0.61
2:B:280:THR:OG1	2:B:283:LYS:HB2	2.00	0.61
3:C:164:SER:HB3	3:C:184:ILE:H	1.64	0.61
2:B:315:GLU:HB3	2:B:449:LYS:HB2	1.83	0.61
3:C:356:LYS:HE3	3:C:376:TRP:HZ2	1.66	0.61
2:E:439:ASN:HD22	2:E:439:ASN:H	1.49	0.60
1:A:191:LYS:HG2	1:A:192:ASP:N	2.15	0.60
3:F:356:LYS:HE3	3:F:376:TRP:HZ2	1.65	0.60
3:C:184:ILE:HA	3:C:189:ASN:O	2.02	0.60
3:C:273:LYS:NZ	3:C:319:ASN:HD21	1.99	0.60
2:E:265:LYS:O	2:E:268:PRO:HD2	2.00	0.60
2:E:203:ILE:HD12	2:E:203:ILE:H	1.67	0.60
1:A:140:VAL:CG1	2:B:171:ILE:HD11	2.29	0.60
2:B:171:ILE:HD13	2:B:172:LEU:N	2.18	0.59
3:F:275:ARG:HB2	3:F:311:GLN:HG2	1.83	0.59
3:C:266:LYS:NZ	3:F:303:PHE:HB3	2.18	0.59
3:C:275:ARG:HA	3:C:311:GLN:HA	1.85	0.59
2:B:252:ILE:HG12	2:B:454:ILE:HD12	1.85	0.58
2:B:351:ASN:HD21	2:B:354:MET:H	1.50	0.58
3:F:151:LYS:HD2	3:F:151:LYS:N	2.18	0.58
3:F:295:PHE:HE1	3:F:305:THR:HG21	1.69	0.58
2:B:394:CYS:SG	2:B:407:CYS:N	2.77	0.58
3:C:365:ASN:HD22	3:C:365:ASN:N	2.01	0.58
1:A:161:CYS:SG	1:A:165:CYS:SG	3.02	0.57
3:F:149:THR:HG23	3:F:168:PHE:O	2.02	0.57
3:F:275:ARG:HA	3:F:311:GLN:HA	1.86	0.57
2:E:351:ASN:HD21	2:E:354:MET:H	1.52	0.57
2:E:367:MET:O	2:E:406:ARG:HB2	2.04	0.57
1:D:141:ARG:HH22	1:D:182:GLN:HG2	1.70	0.57
2:E:212:GLU:HG3	2:E:216:ARG:NH1	2.19	0.57
3:C:227:TRP:HZ2	3:C:230:ASN:ND2	2.01	0.57
2:E:160:ASN:H	2:E:162:PRO:HD2	1.67	0.56
2:E:212:GLU:O	2:E:215:ILE:HG22	2.05	0.56
1:A:168:ALA:HA	2:B:189:GLN:HE22	1.70	0.56
2:B:212:GLU:O	2:B:215:ILE:HG22	2.04	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:470:NAG:H3	4:B:471:NAG:O4	2.05	0.56
2:E:279:ASN:ND2	2:E:286:CYS:SG	2.78	0.56
2:B:276:VAL:HA	2:B:292:TYR:CD1	2.40	0.56
2:B:361:MET:O	2:B:364:ASN:HB2	2.06	0.56
2:B:203:ILE:H	2:B:203:ILE:HD12	1.70	0.56
2:E:394:CYS:SG	2:E:407:CYS:N	2.78	0.56
3:F:250:LEU:HD12	3:F:379:MET:HG3	1.87	0.56
2:B:328:GLY:HA3	2:B:343:ASN:OD1	2.06	0.56
2:E:328:GLY:HA3	2:E:343:ASN:OD1	2.06	0.56
1:D:148:LYS:O	1:D:152:VAL:HG23	2.06	0.55
2:E:300:SER:HA	2:E:331:VAL:HB	1.88	0.55
2:B:367:MET:O	2:B:406:ARG:HB2	2.07	0.55
3:F:164:SER:HB3	3:F:184:ILE:H	1.71	0.55
2:E:251:VAL:HG22	2:E:453:LYS:HG2	1.88	0.55
2:E:280:THR:OG1	2:E:283:LYS:HB2	2.06	0.55
1:D:161:CYS:HA	3:F:135:CYS:HB3	1.88	0.55
2:E:315:GLU:HB3	2:E:449:LYS:HB2	1.88	0.55
2:B:309:GLU:HB3	2:B:457:PHE:HB2	1.87	0.54
3:C:252:ASP:HB2	3:C:377:TYR:OH	2.06	0.54
2:B:300:SER:OG	2:B:304:ARG:NH1	2.41	0.54
2:B:249:TRP:CZ3	2:B:455:ARG:HB2	2.42	0.54
2:E:241:ASP:HB3	2:E:249:TRP:HB2	1.88	0.54
2:E:267:ASP:HB3	2:E:268:PRO:HD3	1.90	0.54
3:F:197:ARG:HB2	3:F:382:THR:HB	1.89	0.54
1:A:161:CYS:SG	2:B:193:CYS:SG	3.06	0.54
2:B:237:ARG:HG3	2:B:237:ARG:HH11	1.72	0.54
2:E:455:ARG:HG2	2:E:456:PRO:CD	2.38	0.54
2:B:241:ASP:HB3	2:B:249:TRP:HB2	1.90	0.53
2:B:267:ASP:HB3	2:B:268:PRO:HD3	1.90	0.53
3:C:280:TYR:HB3	3:F:275:ARG:NH2	2.23	0.53
3:F:195:GLN:HB3	3:F:384:MET:HB2	1.91	0.53
1:A:119:ILE:HA	1:A:122:LEU:HB3	1.90	0.53
4:E:471:NAG:O7	4:E:471:NAG:H3	2.07	0.53
2:E:309:GLU:HG2	2:E:455:ARG:O	2.09	0.53
2:B:265:LYS:O	2:B:268:PRO:HD2	2.08	0.53
2:E:329:PHE:CE2	2:E:454:ILE:HD11	2.44	0.53
2:E:361:MET:O	2:E:364:ASN:HB2	2.08	0.53
3:C:238:THR:HG22	3:C:266:LYS:HG3	1.90	0.53
3:C:248:VAL:O	3:C:259:THR:HA	2.09	0.53
3:F:248:VAL:O	3:F:259:THR:HA	2.10	0.52
2:B:212:GLU:HG3	2:B:216:ARG:NH1	2.24	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:117:SER:HA	1:D:120:GLU:HB3	1.92	0.52
2:E:420:GLY:HA2	2:E:446:SER:O	2.10	0.52
3:C:295:PHE:HE1	3:C:305:THR:HG21	1.73	0.52
2:B:300:SER:HA	2:B:331:VAL:HB	1.92	0.52
3:C:151:LYS:HD2	3:C:151:LYS:N	2.25	0.52
2:B:253:GLN:HB3	2:B:452:MET:HB2	1.92	0.52
2:B:309:GLU:HG2	2:B:455:ARG:O	2.10	0.52
3:F:227:TRP:HZ2	3:F:230:ASN:ND2	2.08	0.52
1:A:141:ARG:HH22	1:A:182:GLN:HG2	1.73	0.52
2:B:422:TYR:O	2:B:444:TRP:HB3	2.10	0.52
2:B:439:ASN:HD22	2:B:439:ASN:N	2.05	0.52
2:B:199:VAL:O	3:C:141:ASP:HA	2.10	0.52
2:E:237:ARG:HG3	2:E:237:ARG:HH11	1.75	0.52
2:B:303:THR:HB	2:B:330:THR:HA	1.92	0.51
3:F:238:THR:HG22	3:F:266:LYS:HG3	1.92	0.51
1:A:130:VAL:HG22	2:B:161:ILE:HD11	1.92	0.51
1:A:153:ASP:O	1:A:157:LYS:HG2	2.10	0.51
3:C:356:LYS:HG3	3:C:376:TRP:CZ2	2.45	0.51
2:B:270:LYS:HA	2:B:296:ASN:HB2	1.92	0.51
2:B:279:ASN:ND2	2:B:286:CYS:SG	2.83	0.51
2:E:300:SER:OG	2:E:304:ARG:NH1	2.43	0.51
2:B:363:GLU:O	2:B:367:MET:HG2	2.11	0.50
3:C:365:ASN:HD22	3:C:365:ASN:H	1.58	0.50
2:E:279:ASN:HA	2:E:286:CYS:HA	1.94	0.50
2:E:203:ILE:HD12	2:E:203:ILE:N	2.26	0.50
2:E:253:GLN:NE2	2:E:451:SER:HA	2.26	0.50
1:A:117:SER:O	1:A:121:VAL:HG22	2.12	0.50
1:D:141:ARG:NH2	1:D:182:GLN:HG2	2.27	0.50
2:E:325:HIS:HB3	2:E:346:ARG:HG3	1.93	0.50
3:C:251:GLU:HB3	3:C:381:LYS:HB2	1.94	0.49
2:E:178:LYS:O	2:E:181:LYS:HB3	2.12	0.49
3:F:252:ASP:HB2	3:F:377:TYR:OH	2.12	0.49
3:C:307:HIS:HE1	3:C:341:ALA:H	1.59	0.49
2:E:415:ARG:O	2:E:434:GLY:HA2	2.12	0.49
2:B:203:ILE:HD12	2:B:203:ILE:N	2.28	0.49
1:D:117:SER:HA	1:D:120:GLU:CB	2.43	0.49
2:E:312:ILE:HB	2:E:324:ALA:HB3	1.93	0.49
1:A:178:TYR:O	1:A:182:GLN:HG3	2.11	0.49
1:A:158:ILE:HG23	2:B:189:GLN:HE21	1.77	0.49
2:B:171:ILE:O	2:B:174:ASN:HB3	2.13	0.49
3:F:273:LYS:NZ	3:F:319:ASN:HD21	2.10	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:365:ASN:N	3:F:365:ASN:HD22	2.09	0.49
2:B:329:PHE:CE2	2:B:454:ILE:HD11	2.48	0.49
1:D:176:LYS:H	1:D:176:LYS:HD3	1.77	0.49
3:F:387:ILE:HG13	3:F:388:PRO:HD2	1.94	0.49
2:E:270:LYS:HA	2:E:296:ASN:HB2	1.95	0.49
1:A:176:LYS:H	1:A:176:LYS:HD3	1.77	0.48
2:B:178:LYS:O	2:B:181:LYS:HB3	2.12	0.48
3:C:103:HIS:O	3:C:107:ILE:HG12	2.14	0.48
2:E:238:VAL:HG12	2:E:239:TYR:N	2.28	0.48
2:E:253:GLN:HE22	2:E:451:SER:HA	1.77	0.48
2:E:303:THR:HB	2:E:330:THR:HA	1.94	0.48
4:B:470:NAG:C5	4:B:471:NAG:H62	2.40	0.48
2:E:329:PHE:CD2	2:E:454:ILE:HD11	2.49	0.48
3:C:250:LEU:HD12	3:C:379:MET:HG3	1.94	0.48
2:E:244:THR:HG22	2:E:245:GLU:N	2.29	0.48
2:E:266:TRP:CE3	2:E:380:ARG:HG2	2.49	0.48
2:B:420:GLY:HA2	2:B:446:SER:O	2.14	0.48
3:C:236:ILE:O	3:C:239:GLN:HG2	2.13	0.48
3:F:337:ASN:C	3:F:339:CYS:N	2.67	0.48
2:E:253:GLN:HB3	2:E:452:MET:HB2	1.95	0.48
2:B:255:ARG:NH1	2:B:413:ASN:HA	2.29	0.47
2:E:396:LYS:HB2	2:E:429:HIS:CD2	2.49	0.47
3:F:154:GLN:NE2	3:F:387:ILE:HD11	2.29	0.47
3:F:356:LYS:HG3	3:F:376:TRP:CZ2	2.47	0.47
2:B:266:TRP:CE3	2:B:380:ARG:HG2	2.48	0.47
1:D:117:SER:C	1:D:119:ILE:H	2.18	0.47
2:B:239:TYR:HD2	2:B:277:ALA:HB2	1.80	0.47
2:E:363:GLU:O	2:E:367:MET:HG2	2.14	0.47
3:C:118:ASN:O	3:C:122:VAL:HG23	2.15	0.47
2:E:373:MET:SD	2:E:405:ASN:CB	2.98	0.47
2:B:279:ASN:HA	2:B:286:CYS:HA	1.95	0.47
3:F:93:ILE:HB	3:F:95:LYS:HE2	1.97	0.47
2:B:325:HIS:HB3	2:B:346:ARG:HG3	1.97	0.47
2:E:162:PRO:O	2:E:166:ARG:HB2	2.14	0.47
2:E:171:ILE:O	2:E:175:LEU:HG	2.14	0.47
2:E:255:ARG:NH1	2:E:413:ASN:HA	2.29	0.47
2:B:237:ARG:HG3	2:B:237:ARG:NH1	2.30	0.47
2:B:329:PHE:HE2	2:B:454:ILE:HD11	1.79	0.47
4:B:470:NAG:C2	4:B:471:NAG:H4	2.44	0.47
3:C:273:LYS:HZ3	3:C:319:ASN:HD21	1.62	0.47
3:C:374:THR:HG22	3:C:375:ARG:H	1.80	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:325:HIS:O	2:E:345:TYR:HA	2.15	0.47
3:F:118:ASN:O	3:F:122:VAL:HG23	2.15	0.47
3:C:264:MET:O	3:C:278:TYR:HA	2.14	0.47
3:F:251:GLU:HB3	3:F:381:LYS:HB2	1.96	0.47
2:B:171:ILE:HA	2:B:174:ASN:HB3	1.96	0.47
3:C:337:ASN:C	3:C:339:CYS:N	2.68	0.46
1:D:176:LYS:H	1:D:176:LYS:CD	2.28	0.46
2:E:151:LEU:C	2:E:153:ILE:H	2.18	0.46
3:C:307:HIS:CE1	3:C:341:ALA:H	2.33	0.46
2:E:238:VAL:HG11	2:E:250:THR:HG23	1.98	0.46
2:B:244:THR:HG22	2:B:245:GLU:N	2.31	0.46
2:E:309:GLU:HB3	2:E:457:PHE:HB2	1.97	0.46
3:F:300:SER:O	3:F:304:PHE:HB2	2.15	0.46
1:D:140:VAL:CG1	2:E:171:ILE:HD11	2.45	0.46
2:E:239:TYR:HD2	2:E:277:ALA:HB2	1.80	0.46
3:F:193:VAL:HG22	3:F:385:LYS:HB3	1.98	0.46
3:F:264:MET:O	3:F:278:TYR:HA	2.16	0.46
3:F:307:HIS:HD2	3:F:335:TRP:O	1.99	0.46
3:C:197:ARG:HD3	3:C:204:PHE:CZ	2.51	0.46
3:F:239:GLN:O	3:F:242:ILE:HG12	2.16	0.46
2:E:171:ILE:HA	2:E:174:ASN:HB3	1.98	0.46
3:C:197:ARG:HB2	3:C:382:THR:HB	1.97	0.46
1:A:141:ARG:HH22	1:A:182:GLN:HE21	1.62	0.46
3:C:96:TYR:C	3:C:98:ALA:H	2.19	0.46
1:A:141:ARG:NH2	1:A:182:GLN:HG2	2.30	0.45
2:B:238:VAL:HG12	2:B:239:TYR:N	2.31	0.45
1:D:161:CYS:SG	2:E:193:CYS:SG	3.15	0.45
3:C:239:GLN:O	3:C:242:ILE:HG12	2.16	0.45
2:E:439:ASN:HD22	2:E:439:ASN:N	2.13	0.45
1:A:148:LYS:O	1:A:152:VAL:HG23	2.15	0.45
3:F:156:ILE:HD11	3:F:169:ILE:HG22	1.98	0.45
1:A:139:ASN:HB3	3:C:114:TYR:CZ	2.51	0.45
2:E:237:ARG:HG3	2:E:237:ARG:NH1	2.32	0.45
2:B:168:LEU:O	2:B:172:LEU:HB2	2.16	0.45
3:C:374:THR:HG22	3:C:375:ARG:N	2.31	0.45
2:E:168:LEU:O	2:E:172:LEU:HB2	2.17	0.45
3:F:334:TRP:CH2	3:F:344:LEU:HB2	2.52	0.45
2:B:424:TRP:HA	2:B:444:TRP:CH2	2.52	0.45
1:D:178:TYR:O	1:D:182:GLN:HG3	2.17	0.45
2:E:358:SER:HA	2:E:365:ARG:HH12	1.80	0.45
3:F:94:MET:C	3:F:96:TYR:H	2.19	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:103:HIS:O	3:F:107:ILE:HG12	2.17	0.45
3:F:155:ASP:O	3:F:159:LYS:HG3	2.17	0.45
3:F:207:ASN:ND2	3:F:209:ILE:H	2.14	0.45
1:A:165:CYS:HB3	2:B:193:CYS:HA	1.98	0.45
3:F:374:THR:HG22	3:F:375:ARG:N	2.32	0.45
2:B:171:ILE:O	2:B:175:LEU:HG	2.16	0.44
2:B:345:TYR:CD2	2:B:351:ASN:HB2	2.52	0.44
3:F:197:ARG:HD3	3:F:204:PHE:CZ	2.53	0.44
3:C:154:GLN:NE2	3:C:190:GLY:H	2.15	0.44
3:C:154:GLN:NE2	3:C:387:ILE:HD11	2.32	0.44
1:D:180:ASP:HB3	1:D:184:GLN:NE2	2.33	0.44
2:E:424:TRP:HA	2:E:444:TRP:CH2	2.52	0.44
3:F:236:ILE:O	3:F:239:GLN:HG2	2.17	0.44
3:F:246:LEU:HD12	3:F:385:LYS:O	2.16	0.44
2:B:312:ILE:HB	2:B:324:ALA:HB3	2.00	0.44
3:C:196:LYS:HD3	3:C:383:THR:HB	2.00	0.44
3:F:273:LYS:HB2	3:F:311:GLN:HB3	2.00	0.44
2:B:405:ASN:C	2:B:407:CYS:N	2.71	0.44
3:C:334:TRP:CH2	3:C:344:LEU:HB2	2.53	0.44
2:E:249:TRP:CE3	2:E:455:ARG:HB2	2.52	0.44
2:B:161:ILE:N	2:B:162:PRO:CD	2.81	0.44
2:B:199:VAL:HG23	3:C:141:ASP:HA	1.99	0.44
2:B:325:HIS:O	2:B:345:TYR:HA	2.18	0.43
3:C:352:GLY:HA2	3:C:378:SER:O	2.17	0.43
3:C:364:ASP:OD1	3:C:364:ASP:N	2.48	0.43
1:D:156:ILE:O	1:D:159:ARG:HG2	2.18	0.43
1:A:156:ILE:O	1:A:159:ARG:HG2	2.18	0.43
1:A:178:TYR:OH	2:B:178:LYS:HG2	2.17	0.43
2:B:162:PRO:O	2:B:166:ARG:HB2	2.17	0.43
2:B:375:PHE:CE1	2:B:402:TRP:HA	2.53	0.43
3:C:387:ILE:HG13	3:C:388:PRO:HD2	2.00	0.43
3:C:390:ASN:HD22	3:C:391:ARG:N	2.17	0.43
2:E:190:MET:SD	3:F:131:LEU:HD13	2.58	0.43
3:F:307:HIS:HE1	3:F:341:ALA:H	1.65	0.43
4:B:471:NAG:O7	4:B:471:NAG:C1	2.65	0.43
4:B:470:NAG:H5	4:B:471:NAG:O4	2.18	0.43
2:E:176:ARG:HH12	3:F:113:ILE:HD12	1.83	0.43
2:E:224:MET:SD	2:E:237:ARG:HD3	2.58	0.43
3:C:100:ILE:O	3:C:104:ASP:N	2.48	0.43
3:C:207:ASN:ND2	3:C:209:ILE:H	2.16	0.43
3:C:227:TRP:CZ2	3:C:230:ASN:ND2	2.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:332:GLN:HB3	2:E:336:ASN:HB2	2.01	0.43
2:E:402:TRP:CG	2:E:403:TRP:N	2.86	0.43
1:A:174:ASP:HA	1:A:176:LYS:HZ3	1.83	0.43
2:B:238:VAL:HG11	2:B:250:THR:HG23	2.00	0.43
2:B:406:ARG:HD2	2:B:406:ARG:HA	1.88	0.43
1:D:153:ASP:O	1:D:157:LYS:HG2	2.19	0.43
3:C:307:HIS:HD2	3:C:335:TRP:O	2.01	0.43
2:E:214:ILE:HG22	2:E:219:GLY:HA3	1.99	0.43
3:F:251:GLU:HB2	3:F:257:THR:HG22	2.01	0.43
2:B:247:GLY:C	2:B:249:TRP:H	2.22	0.43
1:A:180:ASP:HB2	1:A:181:GLN:HE21	1.84	0.42
2:E:247:GLY:C	2:E:249:TRP:H	2.23	0.42
2:B:190:MET:HG2	3:C:131:LEU:HD13	2.01	0.42
1:D:141:ARG:HH22	1:D:182:GLN:HE21	1.65	0.42
2:E:330:THR:OG1	2:E:341:SER:HB3	2.19	0.42
2:E:406:ARG:HD2	2:E:406:ARG:HA	1.87	0.42
3:F:374:THR:HG22	3:F:375:ARG:H	1.83	0.42
2:B:264:ARG:NH1	2:B:273:PHE:HB2	2.35	0.42
3:C:365:ASN:H	3:C:365:ASN:ND2	2.16	0.42
2:E:405:ASN:C	2:E:407:CYS:N	2.71	0.42
2:B:239:TYR:CZ	2:B:289:PRO:HD3	2.55	0.42
3:C:166:LEU:HB3	3:C:179:LEU:HD11	2.01	0.42
3:C:195:GLN:HB3	3:C:384:MET:HB2	2.01	0.42
3:F:313:SER:OG	3:F:319:ASN:HB2	2.19	0.42
2:E:190:MET:HG2	3:F:131:LEU:HD13	2.01	0.42
1:A:125:LYS:O	1:A:128:GLU:HB3	2.19	0.42
2:B:249:TRP:CE3	2:B:455:ARG:HB2	2.55	0.42
2:B:343:ASN:HA	2:B:354:MET:CE	2.50	0.42
2:E:242:MET:HA	2:E:247:GLY:O	2.20	0.42
2:E:375:PHE:CE1	2:E:402:TRP:HA	2.55	0.42
3:F:125:LYS:O	3:F:128:VAL:HG22	2.20	0.42
2:B:162:PRO:HG3	3:C:103:HIS:NE2	2.35	0.41
2:E:248:GLY:O	2:E:455:ARG:HG3	2.19	0.41
3:F:307:HIS:CE1	3:F:341:ALA:H	2.38	0.41
2:B:200:SER:HA	3:C:141:ASP:OD1	2.20	0.41
1:D:123:LYS:O	1:D:127:ILE:HG13	2.19	0.41
2:E:252:ILE:HG13	2:E:299:ILE:HG12	2.02	0.41
2:E:351:ASN:ND2	2:E:351:ASN:C	2.72	0.41
3:F:364:ASP:OD1	3:F:364:ASP:N	2.48	0.41
3:F:387:ILE:CG1	3:F:388:PRO:HD2	2.50	0.41
2:E:373:MET:HB3	2:E:373:MET:HE2	1.93	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:422:TYR:O	2:E:444:TRP:HB3	2.20	0.41
1:A:176:LYS:H	1:A:176:LYS:CD	2.27	0.41
2:B:378:TYR:HB3	2:B:396:LYS:O	2.20	0.41
2:B:402:TRP:CG	2:B:403:TRP:N	2.88	0.41
3:C:228:LEU:HG	3:C:232:LYS:HD2	2.03	0.41
2:B:453:LYS:O	2:B:454:ILE:HG13	2.21	0.41
3:C:273:LYS:HZ2	3:C:319:ASN:HD21	1.67	0.41
2:E:161:ILE:N	2:E:162:PRO:CD	2.84	0.41
3:F:354:TYR:CE1	3:F:376:TRP:HA	2.55	0.41
2:B:424:TRP:HA	2:B:444:TRP:CZ3	2.55	0.41
3:C:365:ASN:N	3:C:365:ASN:ND2	2.67	0.41
3:F:154:GLN:NE2	3:F:190:GLY:H	2.18	0.41
2:B:160:ASN:N	2:B:162:PRO:HD2	2.32	0.41
2:B:164:ASN:N	2:B:164:ASN:HD22	2.18	0.41
2:B:167:VAL:HG13	2:B:168:LEU:N	2.36	0.41
2:B:458:PHE:HA	2:B:459:PRO:HD3	1.87	0.41
1:A:123:LYS:O	1:A:127:ILE:HG13	2.21	0.41
1:A:131:GLN:HA	1:A:134:GLN:HG3	2.01	0.41
1:A:180:ASP:HB3	1:A:184:GLN:NE2	2.36	0.41
3:C:246:LEU:O	3:C:261:ASP:HA	2.21	0.41
3:C:307:HIS:HE1	3:C:341:ALA:N	2.18	0.41
3:C:354:TYR:CE2	3:C:376:TRP:HD1	2.39	0.41
3:C:354:TYR:CE1	3:C:376:TRP:HA	2.56	0.41
1:D:115:LEU:HA	1:D:118:ARG:HH11	1.86	0.41
1:D:159:ARG:O	2:E:259:SER:HA	2.21	0.41
2:E:311:LEU:CD1	2:E:323:LYS:HE3	2.51	0.41
1:A:127:ILE:O	1:A:131:GLN:HG3	2.21	0.41
2:B:310:LEU:HD12	2:B:453:LYS:O	2.21	0.41
3:C:273:LYS:HB2	3:C:311:GLN:HB3	2.03	0.41
3:C:164:SER:HB2	3:C:182:CYS:O	2.21	0.40
3:C:167:TYR:O	3:C:179:LEU:HD12	2.21	0.40
1:D:178:TYR:OH	2:E:178:LYS:HG2	2.21	0.40
3:F:365:ASN:HD22	3:F:365:ASN:H	1.69	0.40
2:B:229:PRO:HD2	2:B:233:VAL:HG21	2.03	0.40
2:B:343:ASN:HD21	2:B:344:LYS:NZ	2.19	0.40
3:C:356:LYS:HE3	3:C:376:TRP:CZ2	2.51	0.40
3:F:141:ASP:CG	3:F:143:VAL:HG22	2.41	0.40
3:F:273:LYS:HZ3	3:F:319:ASN:HD21	1.68	0.40
2:B:295:GLY:O	2:B:299:ILE:HG13	2.21	0.40
3:F:352:GLY:HA2	3:F:378:SER:O	2.21	0.40
1:D:158:ILE:HG23	2:E:189:GLN:HE21	1.86	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:249:TRP:CZ2	2:B:455:ARG:NH2	2.90	0.40
3:C:304:PHE:HD1	3:C:304:PHE:HA	1.76	0.40

All (29) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:391:ARG:NH2	3:F:126:GLU:CB[2_656]	0.22	1.98
3:C:123:ASN:OD1	2:E:390:PRO:CB[2_656]	0.83	1.37
2:B:390:PRO:C	3:F:130:GLN:OE1[2_656]	1.06	1.14
2:B:390:PRO:CA	3:F:130:GLN:OE1[2_656]	1.15	1.05
2:B:390:PRO:CB	3:F:130:GLN:CD[2_656]	1.36	0.84
2:B:391:ARG:N	3:F:130:GLN:OE1[2_656]	1.37	0.83
2:B:390:PRO:CB	3:F:130:GLN:CG[2_656]	1.43	0.77
2:B:391:ARG:CZ	3:F:126:GLU:CB[2_656]	1.44	0.76
2:B:191:GLU:OE2	2:E:194:ARG:NH2[2_646]	1.45	0.75
2:B:191:GLU:CD	2:E:194:ARG:NH2[2_646]	1.57	0.63
2:B:391:ARG:NH2	3:F:126:GLU:CA[2_656]	1.58	0.62
2:B:391:ARG:NH2	3:F:126:GLU:CG[2_656]	1.62	0.58
2:B:390:PRO:CG	2:E:190:MET:CE[2_656]	1.65	0.55
2:B:390:PRO:CA	3:F:130:GLN:CD[2_656]	1.70	0.50
2:B:390:PRO:N	3:F:130:GLN:OE1[2_656]	1.70	0.50
1:A:116:ARG:NH2	1:D:121:VAL:CG1[2_656]	1.82	0.38
1:A:116:ARG:NH2	1:D:121:VAL:CB[2_656]	1.90	0.30
3:C:123:ASN:CG	2:E:390:PRO:CB[2_656]	1.92	0.28
2:B:390:PRO:C	3:F:130:GLN:CD[2_656]	1.93	0.27
2:B:390:PRO:CB	3:F:130:GLN:OE1[2_656]	2.00	0.20
3:C:123:ASN:OD1	2:E:390:PRO:CG[2_656]	2.05	0.15
2:B:391:ARG:N	3:F:130:GLN:CD[2_656]	2.06	0.14
3:C:119:GLN:NE2	2:E:391:ARG:NE[2_656]	2.07	0.13
2:B:191:GLU:OE1	2:E:194:ARG:NH2[2_646]	2.09	0.11
1:A:117:SER:OG	1:D:121:VAL:CG1[2_656]	2.11	0.09
3:C:119:GLN:CD	2:E:391:ARG:CG[2_656]	2.12	0.08
1:A:116:ARG:NH2	1:D:121:VAL:CG2[2_656]	2.13	0.07
3:C:123:ASN:OD1	2:E:390:PRO:CA[2_656]	2.16	0.04
2:B:390:PRO:CB	3:F:130:GLN:NE2[2_656]	2.17	0.03

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	79/87 (91%)	71 (90%)	8 (10%)	0	100	100
1	D	78/87 (90%)	72 (92%)	5 (6%)	1 (1%)	12	45
2	B	307/328 (94%)	271 (88%)	31 (10%)	5 (2%)	9	40
2	E	306/328 (93%)	272 (89%)	29 (10%)	5 (2%)	9	40
3	C	301/319 (94%)	260 (86%)	36 (12%)	5 (2%)	9	39
3	F	300/319 (94%)	261 (87%)	37 (12%)	2 (1%)	22	60
All	All	1371/1468 (93%)	1207 (88%)	146 (11%)	18 (1%)	12	45

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	244	THR
3	C	339	CYS
3	C	393	THR
2	E	244	THR
3	F	339	CYS
2	B	407	CYS
3	C	390	ASN
1	D	119	ILE
2	E	407	CYS
2	B	158	ASN
3	C	198	LEU
2	B	160	ASN
2	E	158	ASN
3	F	198	LEU
2	B	157	VAL
2	E	160	ASN
2	E	245	GLU
3	C	362	GLY

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	76/82 (93%)	68 (90%)	8 (10%)	7 27
1	D	75/82 (92%)	69 (92%)	6 (8%)	12 40
2	B	267/286 (93%)	252 (94%)	15 (6%)	21 56
2	E	266/286 (93%)	253 (95%)	13 (5%)	25 61
3	C	256/267 (96%)	241 (94%)	15 (6%)	19 54
3	F	255/267 (96%)	240 (94%)	15 (6%)	19 54
All	All	1195/1270 (94%)	1123 (94%)	72 (6%)	19 53

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	125	LYS
1	A	150	LEU
1	A	161	CYS
1	A	169	LEU
1	A	171	ARG
1	A	176	LYS
1	A	186	GLU
1	A	192	ASP
2	B	151	LEU
2	B	152	TYR
2	B	161	ILE
2	B	171	ILE
2	B	199	VAL
2	B	210	GLU
2	B	253	GLN
2	B	281	ASP
2	B	346	ARG
2	B	351	ASN
2	B	363	GLU
2	B	385	TRP
2	B	398	ASP
2	B	439	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	455	ARG
3	C	117	ASN
3	C	135	CYS
3	C	152	ASP
3	C	175	ASN
3	C	198	LEU
3	C	207	ASN
3	C	264	MET
3	C	277	THR
3	C	317	ASN
3	C	325	ASN
3	C	338	LYS
3	C	365	ASN
3	C	383	THR
3	C	390	ASN
3	C	391	ARG
1	D	125	LYS
1	D	150	LEU
1	D	169	LEU
1	D	171	ARG
1	D	176	LYS
1	D	186	GLU
2	E	155	GLU
2	E	171	ILE
2	E	199	VAL
2	E	210	GLU
2	E	253	GLN
2	E	281	ASP
2	E	322	VAL
2	E	346	ARG
2	E	351	ASN
2	E	363	GLU
2	E	385	TRP
2	E	398	ASP
2	E	454	ILE
3	F	117	ASN
3	F	135	CYS
3	F	152	ASP
3	F	175	ASN
3	F	198	LEU
3	F	207	ASN
3	F	264	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	F	277	THR
3	F	304	PHE
3	F	317	ASN
3	F	325	ASN
3	F	338	LYS
3	F	365	ASN
3	F	383	THR
3	F	390	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	143	GLN
2	B	164	ASN
2	B	174	ASN
2	B	189	GLN
2	B	202	ASN
2	B	246	ASN
2	B	253	GLN
2	B	256	GLN
2	B	271	GLN
2	B	336	ASN
2	B	343	ASN
2	B	351	ASN
2	B	421	GLN
2	B	439	ASN
3	C	111	GLN
3	C	117	ASN
3	C	123	ASN
3	C	130	GLN
3	C	136	GLN
3	C	154	GLN
3	C	175	ASN
3	C	177	GLN
3	C	230	ASN
3	C	239	GLN
3	C	307	HIS
3	C	317	ASN
3	C	319	ASN
3	C	365	ASN
3	C	390	ASN
1	D	184	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	164	ASN
2	E	174	ASN
2	E	189	GLN
2	E	202	ASN
2	E	246	ASN
2	E	253	GLN
2	E	256	GLN
2	E	271	GLN
2	E	351	ASN
2	E	421	GLN
2	E	439	ASN
3	F	111	GLN
3	F	117	ASN
3	F	123	ASN
3	F	130	GLN
3	F	136	GLN
3	F	154	GLN
3	F	177	GLN
3	F	230	ASN
3	F	239	GLN
3	F	307	HIS
3	F	317	ASN
3	F	319	ASN
3	F	365	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 6 are monoatomic - leaving 4 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	E	470	-	14,14,15	0.43	0	17,19,21	0.70	1 (5%)
4	NAG	E	471	-	14,14,15	0.42	0	17,19,21	0.64	0
4	NAG	B	471	-	14,14,15	0.44	0	17,19,21	0.52	0
4	NAG	B	470	-	14,14,15	0.44	0	17,19,21	0.69	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	E	470	-	-	2/6/23/26	0/1/1/1
4	NAG	E	471	-	-	3/6/23/26	0/1/1/1
4	NAG	B	471	-	-	3/6/23/26	0/1/1/1
4	NAG	B	470	-	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	470	NAG	C2-N2-C7	-2.02	120.03	122.90

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	471	NAG	O5-C5-C6-O6
4	B	471	NAG	C4-C5-C6-O6
4	E	471	NAG	O5-C5-C6-O6
4	E	470	NAG	O5-C5-C6-O6
4	E	471	NAG	C4-C5-C6-O6
4	B	471	NAG	C1-C2-N2-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	E	470	NAG	C4-C5-C6-O6
4	B	470	NAG	O5-C5-C6-O6
4	B	470	NAG	C4-C5-C6-O6
4	E	471	NAG	C3-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	471	NAG	1	0
4	B	471	NAG	10	0
4	B	470	NAG	9	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.