Full wwPDB X-ray Structure Validation Report

Jan 31, 2016 – 07:32 PM GMT

PDB ID	:	1FZF
Title	:	CRYSTAL STRUCTURE OF FRAGMENT DOUBLE-D FROM HUMAN FIBRIN WITH THE PEPTIDE LIGAND GLY-HIS-ARG-PRO-AMIDE
Authors	:	Everse, S.J.; Spraggon, G.; Veerapandian, L.; Doolittle, R.F.
Deposited on	:	1998-12-28
Resolution	:	2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

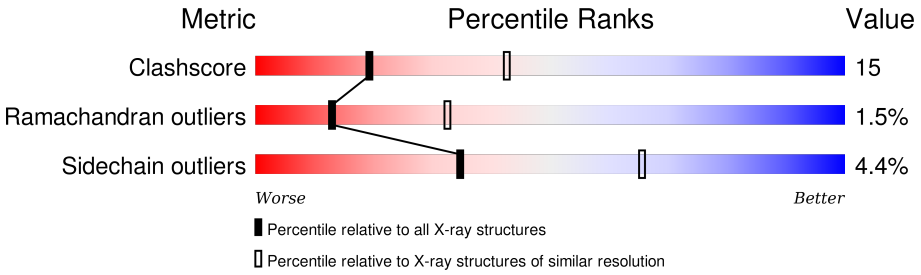
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)

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	47% 26% • 23%
1	D	87	43% 18% • 38%
2	B	328	68% 20% • • 8%
2	E	328	64% 23% • 10%
3	C	319	64% 26% • 8%
3	F	319	62% 24% • 11%
4	M	4	75% 25%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	N	4	50% 25% 25%
4	S	4	75% 25%
4	T	4	75% 25%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10581 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	67	Total	C	N	O	S	0	0	0
			547	337	103	104	3			
1	D	54	Total	C	N	O	S	0	0	0
			441	269	84	85	3			

- Molecule 2 is a protein called FIBRINOGEN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	303	Total	C	N	O	S	0	0	0
			2428	1515	429	462	22			
2	E	296	Total	C	N	O	S	0	0	0
			2377	1484	420	451	22			

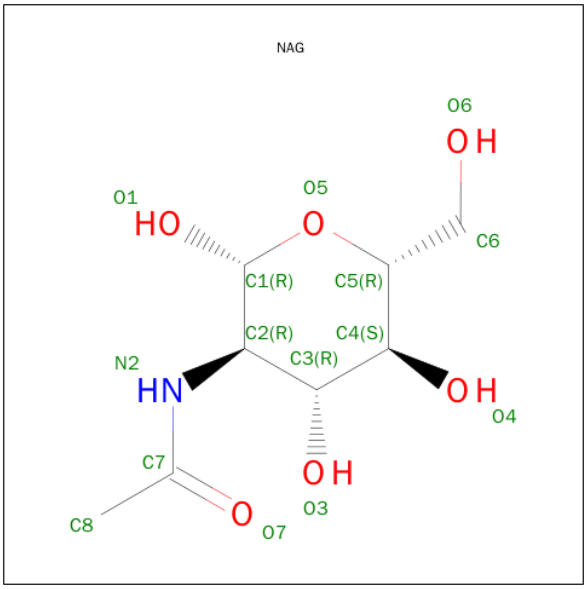
- Molecule 3 is a protein called FIBRINOGEN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	292	Total	C	N	O	S	0	0	0
			2343	1485	396	451	11			
3	F	285	Total	C	N	O	S	0	0	0
			2287	1453	384	439	11			

- Molecule 4 is a protein called FIBRINOGEN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	S	4	Total	C	N	O	0	0	0
			31	19	9	3			
4	T	4	Total	C	N	O	0	0	0
			31	19	9	3			
4	M	4	Total	C	N	O	0	0	0
			31	19	9	3			
4	N	4	Total	C	N	O	0	0	0
			31	19	9	3			

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

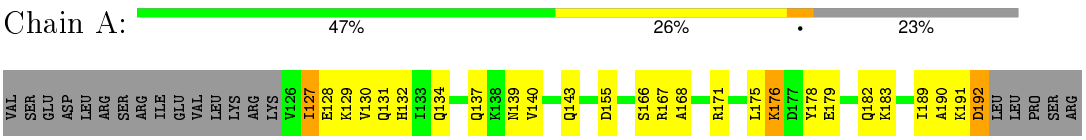
3 Residue-property plots (i)

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.

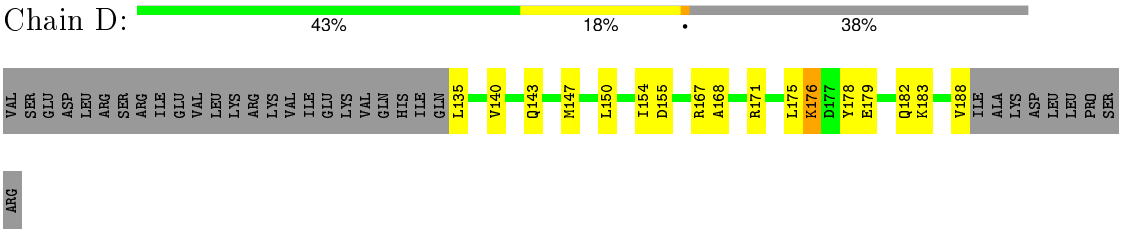
- Molecule 1: FIBRINOGEN

Chain A:



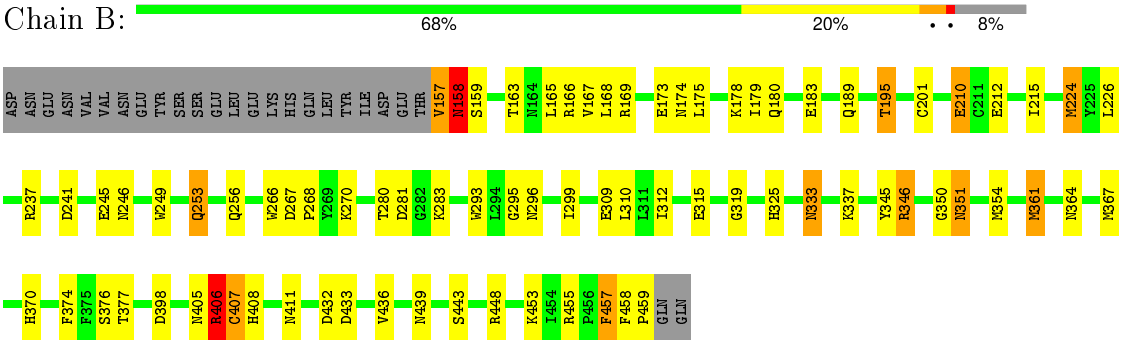
- Molecule 1: FIBRINOGEN

Chain D:



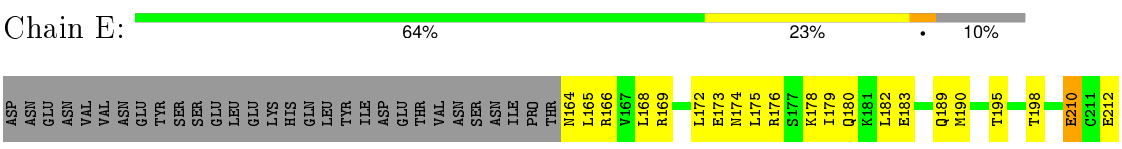
- Molecule 2: FIBRINOGEN

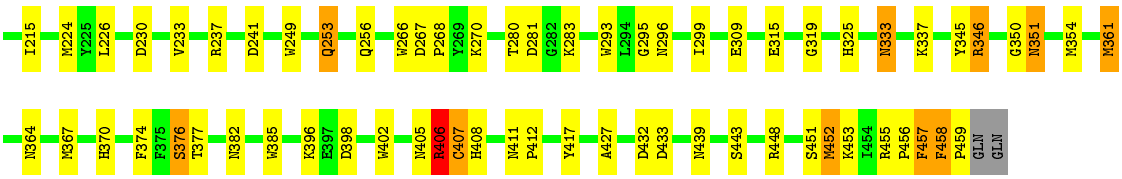
Chain B:



- Molecule 2: FIBRINOGEN

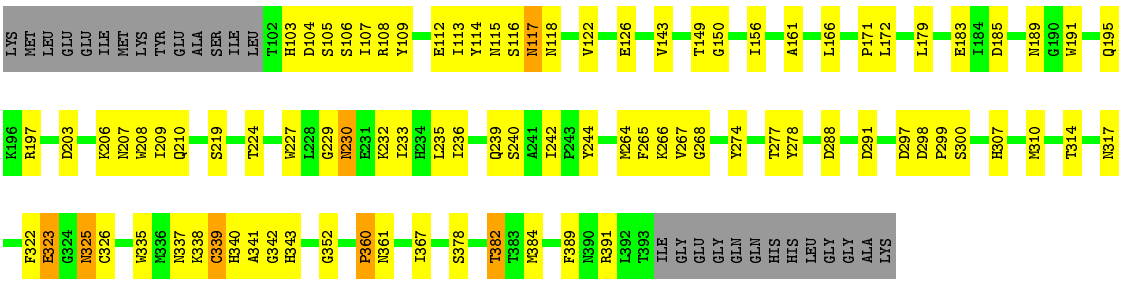
Chain E:





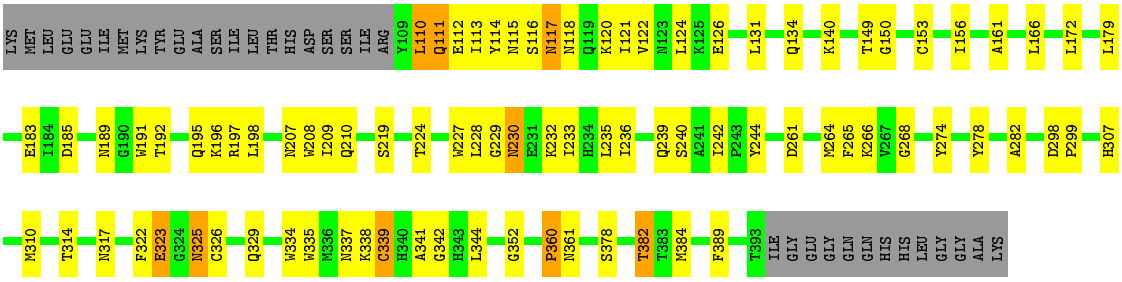
• Molecule 3: FIBRINOGEN

Chain C:



• Molecule 3: FIBRINOGEN

Chain F:



• Molecule 4: FIBRINOGEN

Chain S:

• Molecule 4: FIBRINOGEN

Chain T:

• Molecule 4: FIBRINOGEN

Chain M:

• Molecule 4: FIBRINOGEN

Chain N:

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 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	54.80Å 149.40Å 234.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.70	Depositor
% Data completeness (in resolution range)	88.5 (30.00-2.70)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.233 , 0.302	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10581	wwPDB-VP
Average B, all atoms (Å^2)	49.0	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	0.53	1/548 (0.2%)	0.71	1/731 (0.1%)
1	D	0.33	0/441	0.57	0/587
2	B	0.39	0/2490	0.72	5/3364 (0.1%)
2	E	0.38	0/2438	0.67	3/3291 (0.1%)
3	C	0.40	0/2408	0.62	0/3257
3	F	0.42	0/2351	0.64	0/3180
4	M	0.57	0/32	0.44	0/42
4	N	0.45	0/32	0.47	0/42
4	S	0.36	0/32	0.72	0/42
4	T	0.47	0/32	0.47	0/42
All	All	0.40	1/10804 (0.0%)	0.66	9/14578 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	192	ASP	C-O	-9.73	1.04	1.23

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	157	VAL	N-CA-C	13.26	146.79	111.00
1	A	192	ASP	CA-C-O	-12.26	94.35	120.10
2	B	406	ARG	NE-CZ-NH2	-7.01	116.79	120.30
2	B	157	VAL	CB-CA-C	-6.77	98.54	111.40
2	E	406	ARG	NE-CZ-NH2	-6.42	117.09	120.30
2	E	406	ARG	NE-CZ-NH1	6.30	123.45	120.30
2	B	406	ARG	NE-CZ-NH1	6.26	123.43	120.30
2	E	452	MET	CG-SD-CE	6.12	109.99	100.20
2	B	158	ASN	N-CA-C	-5.99	94.83	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	547	0	573	24	0
1	D	441	0	458	18	0
2	B	2428	0	2296	62	0
2	E	2377	0	2245	86	0
3	C	2343	0	2188	68	0
3	F	2287	0	2136	82	0
4	M	31	0	32	1	0
4	N	31	0	32	2	0
4	S	31	0	32	1	0
4	T	31	0	32	1	0
5	B	14	0	13	6	0
5	E	14	0	13	3	0
6	B	1	0	0	0	0
6	C	2	0	0	0	0
6	E	2	0	0	0	0
6	F	1	0	0	0	0
All	All	10581	0	10050	312	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 15.

All (312) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:176:ARG:HA	3:F:117:ASN:HB3	1.30	1.06
3:C:310:MET:SD	3:C:337:ASN:HB2	2.16	0.85
3:C:107:ILE:H	3:C:107:ILE:HD12	1.42	0.85
3:F:310:MET:SD	3:F:337:ASN:HB2	2.18	0.84
5:B:470:NAG:H2	5:B:470:NAG:H62	1.61	0.82
3:C:209:ILE:H	3:C:209:ILE:HD12	1.41	0.82
2:B:157:VAL:O	2:B:157:VAL:CG1	2.27	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:209:ILE:HD12	3:F:209:ILE:H	1.44	0.81
2:E:166:ARG:HH22	3:F:110:LEU:HG	1.47	0.78
2:E:189:GLN:HG3	3:F:131:LEU:HD11	1.63	0.78
1:A:131:GLN:HA	1:A:134:GLN:HG2	1.67	0.76
2:E:179:ILE:HG21	3:F:120:LYS:HB3	1.69	0.75
2:E:169:ARG:O	2:E:173:GLU:HG2	1.86	0.74
3:F:307:HIS:HE1	3:F:341:ALA:H	1.35	0.74
2:E:176:ARG:HA	3:F:117:ASN:CB	2.16	0.73
3:C:117:ASN:HD22	3:C:118:ASN:N	1.87	0.73
2:E:182:LEU:HB2	3:F:124:LEU:HD21	1.71	0.72
2:E:333:ASN:ND2	2:E:333:ASN:H	1.87	0.72
1:D:140:VAL:HG12	3:F:114:TYR:CE1	2.24	0.72
2:E:190:MET:HG3	3:F:134:GLN:HE22	1.53	0.72
3:C:322:PHE:HB2	3:C:338:LYS:HA	1.72	0.71
2:E:293:TRP:HZ2	2:E:296:ASN:HD21	1.39	0.71
2:E:179:ILE:HG21	3:F:120:LYS:CB	2.21	0.71
1:D:188:VAL:HG22	2:E:165:LEU:HD13	1.73	0.70
2:B:398:ASP:HA	2:B:433:ASP:HB3	1.73	0.70
2:B:333:ASN:ND2	2:B:333:ASN:H	1.90	0.70
3:C:149:THR:HG22	3:C:150:GLY:H	1.57	0.70
2:B:364:ASN:ND2	5:B:470:NAG:C1	2.55	0.70
2:B:351:ASN:ND2	2:B:354:MET:H	1.90	0.69
2:B:293:TRP:HZ2	2:B:296:ASN:HD21	1.39	0.68
3:F:360:PRO:HG2	3:F:361:ASN:H	1.57	0.68
2:E:412:PRO:HG2	2:E:452:MET:CE	2.24	0.68
2:B:157:VAL:O	2:B:157:VAL:HG13	1.93	0.68
2:E:364:ASN:HD21	5:E:470:NAG:C1	2.06	0.68
2:E:398:ASP:HA	2:E:433:ASP:HB3	1.75	0.67
3:F:117:ASN:HD22	3:F:118:ASN:N	1.93	0.66
2:E:180:GLN:O	2:E:183:GLU:HG2	1.96	0.66
3:C:172:LEU:H	3:C:239:GLN:HE21	1.44	0.65
2:E:351:ASN:ND2	2:E:354:MET:H	1.94	0.65
2:B:405:ASN:C	2:B:407:CYS:H	1.98	0.65
3:F:149:THR:HG22	3:F:150:GLY:H	1.61	0.65
3:C:307:HIS:HE1	3:C:341:ALA:H	1.45	0.65
2:E:367:MET:HB2	2:E:406:ARG:HB3	1.79	0.65
2:B:364:ASN:HD21	5:B:470:NAG:C1	2.09	0.64
3:C:360:PRO:HG2	3:C:361:ASN:H	1.63	0.64
1:A:168:ALA:HA	2:B:189:GLN:HE22	1.61	0.64
3:C:307:HIS:HD2	3:C:335:TRP:O	1.80	0.64
2:B:180:GLN:O	2:B:183:GLU:HG2	1.98	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:405:ASN:C	2:E:407:CYS:H	2.01	0.63
3:F:322:PHE:HB2	3:F:338:LYS:HA	1.80	0.63
3:C:227:TRP:HZ2	3:C:230:ASN:HD21	1.47	0.63
1:D:140:VAL:HG12	3:F:114:TYR:HE1	1.64	0.62
3:F:235:LEU:O	3:F:239:GLN:HB3	2.00	0.62
2:B:166:ARG:C	2:B:168:LEU:H	2.01	0.62
2:E:402:TRP:HH2	2:E:452:MET:HE1	1.64	0.62
2:B:367:MET:HB2	2:B:406:ARG:HB3	1.82	0.61
1:D:155:ASP:HA	1:D:171:ARG:NH1	2.16	0.61
3:F:307:HIS:HD2	3:F:335:TRP:O	1.82	0.61
3:C:264:MET:O	3:C:278:TYR:HA	2.01	0.61
2:E:172:LEU:HD13	3:F:114:TYR:HB2	1.83	0.61
2:E:182:LEU:CB	3:F:124:LEU:HD21	2.30	0.60
3:C:104:ASP:HA	3:C:107:ILE:HD13	1.83	0.60
3:C:235:LEU:O	3:C:239:GLN:HB3	2.02	0.60
3:C:172:LEU:H	3:C:239:GLN:NE2	2.00	0.60
1:A:131:GLN:H	1:A:131:GLN:CD	2.04	0.60
2:B:458:PHE:HB3	2:B:459:PRO:HD3	1.82	0.60
1:D:175:LEU:H	1:D:175:LEU:HD23	1.66	0.60
2:B:210:GLU:OE1	2:B:212:GLU:HB3	2.02	0.59
3:C:240:SER:OG	3:C:242:ILE:HG12	2.02	0.59
2:B:169:ARG:O	2:B:173:GLU:HG2	2.02	0.59
2:E:168:LEU:H	2:E:168:LEU:HD22	1.66	0.59
2:E:210:GLU:OE1	2:E:212:GLU:HB3	2.03	0.59
3:C:107:ILE:H	3:C:107:ILE:CD1	2.15	0.59
3:F:195:GLN:HB3	3:F:384:MET:HB2	1.84	0.59
1:A:155:ASP:HA	1:A:171:ARG:NH1	2.18	0.58
5:B:470:NAG:C6	5:B:470:NAG:H2	2.33	0.58
3:C:195:GLN:HB3	3:C:384:MET:HB2	1.85	0.58
3:C:209:ILE:H	3:C:209:ILE:CD1	2.15	0.58
3:F:307:HIS:CE1	3:F:341:ALA:H	2.18	0.58
2:E:402:TRP:CH2	2:E:452:MET:HE1	2.38	0.58
2:B:201:CYS:O	3:C:143:VAL:HG21	2.05	0.57
2:E:190:MET:CG	3:F:134:GLN:HE22	2.17	0.57
1:A:175:LEU:HD23	1:A:175:LEU:H	1.69	0.57
2:E:432:ASP:OD2	2:E:443:SER:HB2	2.04	0.57
3:C:107:ILE:N	3:C:107:ILE:HD12	2.18	0.57
2:E:183:GLU:HA	3:F:124:LEU:CD1	2.35	0.57
3:C:149:THR:HG22	3:C:150:GLY:N	2.21	0.56
2:B:295:GLY:O	2:B:299:ILE:HG13	2.05	0.56
1:D:147:MET:SD	3:F:121:ILE:HD11	2.46	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:175:LEU:H	1:D:175:LEU:CD2	2.19	0.56
3:F:172:LEU:H	3:F:239:GLN:NE2	2.04	0.56
2:E:212:GLU:O	2:E:215:ILE:HG22	2.06	0.56
2:E:402:TRP:CH2	2:E:452:MET:CE	2.89	0.56
3:C:227:TRP:HZ2	3:C:230:ASN:ND2	2.04	0.55
1:A:129:LYS:HE2	3:C:104:ASP:HB2	1.88	0.55
3:C:108:ARG:O	3:C:112:GLU:HG3	2.07	0.55
3:F:323:GLU:H	3:F:323:GLU:CD	2.10	0.55
2:E:241:ASP:HB3	2:E:249:TRP:HB2	1.89	0.55
3:F:307:HIS:CE1	3:F:342:GLY:H	2.25	0.55
3:F:227:TRP:HZ2	3:F:230:ASN:HD21	1.55	0.55
3:F:264:MET:O	3:F:278:TYR:HA	2.07	0.54
2:E:367:MET:HG3	4:N:2:HIS:HB2	1.90	0.54
3:F:307:HIS:HE1	3:F:342:GLY:H	1.56	0.54
2:E:319:GLY:HA2	2:E:448:ARG:HH22	1.73	0.54
2:B:351:ASN:C	2:B:351:ASN:HD22	2.10	0.54
2:E:333:ASN:H	2:E:333:ASN:HD22	1.53	0.54
3:F:149:THR:HG22	3:F:150:GLY:N	2.23	0.54
1:A:175:LEU:CD2	1:A:175:LEU:H	2.21	0.54
2:E:325:HIS:HB3	2:E:346:ARG:HG3	1.89	0.54
3:F:172:LEU:H	3:F:239:GLN:HE21	1.56	0.54
2:E:224:MET:CE	2:E:237:ARG:HD3	2.39	0.53
2:B:175:LEU:O	2:B:179:ILE:HG12	2.09	0.53
2:E:175:LEU:O	2:E:179:ILE:HG12	2.09	0.53
2:E:361:MET:O	2:E:364:ASN:HB2	2.08	0.53
2:E:351:ASN:C	2:E:351:ASN:HD22	2.12	0.53
2:B:224:MET:CE	2:B:237:ARG:HD3	2.38	0.53
3:F:240:SER:OG	3:F:242:ILE:HG12	2.09	0.53
2:B:157:VAL:O	2:B:157:VAL:HG12	2.03	0.53
2:E:337:LYS:HB2	2:E:374:PHE:CD1	2.44	0.53
3:C:326:CYS:SG	3:C:339:CYS:N	2.82	0.52
3:F:219:SER:OG	3:F:224:THR:HG22	2.09	0.52
3:C:391:ARG:HG2	3:C:391:ARG:HH11	1.74	0.52
2:E:350:GLY:HA3	2:E:439:ASN:HB3	1.90	0.52
2:E:190:MET:SD	3:F:134:GLN:NE2	2.82	0.52
2:E:270:LYS:HA	2:E:296:ASN:HB2	1.92	0.52
3:F:122:VAL:O	3:F:126:GLU:HG2	2.10	0.52
3:F:232:LYS:O	3:F:236:ILE:HG13	2.10	0.52
1:A:139:ASN:HB3	3:C:114:TYR:CE1	2.44	0.52
2:B:319:GLY:HA2	2:B:448:ARG:HH22	1.74	0.52
2:B:241:ASP:HB3	2:B:249:TRP:HB2	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:325:HIS:HB3	2:B:346:ARG:HG3	1.90	0.52
3:F:166:LEU:HD13	3:F:179:LEU:HD21	1.92	0.52
2:B:163:THR:O	2:B:166:ARG:HG2	2.10	0.52
2:B:212:GLU:O	2:B:215:ILE:HG22	2.09	0.52
3:F:268:GLY:O	3:F:274:TYR:HA	2.09	0.51
3:F:115:ASN:HA	3:F:118:ASN:HB3	1.92	0.51
2:E:398:ASP:HA	2:E:433:ASP:CB	2.40	0.51
3:F:229:GLY:O	3:F:233:ILE:HG13	2.10	0.51
3:F:242:ILE:HG13	3:F:242:ILE:O	2.10	0.51
3:C:166:LEU:HD13	3:C:179:LEU:HD21	1.93	0.50
2:B:266:TRP:HA	2:B:377:THR:HG21	1.92	0.50
3:C:323:GLU:H	3:C:323:GLU:CD	2.14	0.50
3:F:156:ILE:HG22	3:F:161:ALA:HB2	1.93	0.50
1:D:154:ILE:HD12	2:E:182:LEU:HD13	1.92	0.50
1:D:175:LEU:O	1:D:178:TYR:HB2	2.11	0.50
2:B:367:MET:HB2	2:B:406:ARG:CB	2.42	0.50
2:B:309:GLU:HG2	2:B:455:ARG:O	2.12	0.50
3:C:122:VAL:O	3:C:126:GLU:HG2	2.12	0.50
2:E:402:TRP:CZ3	2:E:452:MET:HE3	2.46	0.50
3:F:265:PHE:C	3:F:266:LYS:HD2	2.33	0.50
3:C:113:ILE:O	3:C:116:SER:HB3	2.12	0.50
2:E:325:HIS:O	2:E:345:TYR:HA	2.12	0.49
3:F:326:CYS:SG	3:F:339:CYS:N	2.85	0.49
2:E:183:GLU:HA	3:F:124:LEU:HD11	1.95	0.49
2:B:270:LYS:HA	2:B:296:ASN:HB2	1.94	0.49
1:A:128:GLU:O	1:A:132:HIS:HB2	2.12	0.49
2:B:337:LYS:HB2	2:B:374:PHE:CD1	2.47	0.49
3:C:207:ASN:OD1	3:C:210:GLN:HG3	2.13	0.49
1:A:179:GLU:HA	1:A:182:GLN:NE2	2.27	0.49
3:F:337:ASN:C	3:F:339:CYS:N	2.66	0.49
2:E:267:ASP:HB2	2:E:268:PRO:HD3	1.94	0.49
2:B:432:ASP:OD2	2:B:443:SER:HB2	2.12	0.49
3:F:197:ARG:HB2	3:F:382:THR:HB	1.95	0.48
2:B:361:MET:O	2:B:364:ASN:HB2	2.12	0.48
3:C:229:GLY:O	3:C:233:ILE:HG13	2.14	0.48
2:B:350:GLY:HA3	2:B:439:ASN:HB3	1.95	0.48
3:C:197:ARG:HB2	3:C:382:THR:HB	1.94	0.48
3:F:113:ILE:O	3:F:116:SER:HB3	2.13	0.48
3:C:219:SER:OG	3:C:224:THR:HG22	2.14	0.48
3:F:207:ASN:OD1	3:F:210:GLN:HG3	2.13	0.48
2:E:295:GLY:O	2:E:299:ILE:HG13	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:351:ASN:ND2	2:B:354:MET:HB2	2.29	0.48
2:B:163:THR:C	2:B:165:LEU:H	2.16	0.48
5:B:470:NAG:C6	5:B:470:NAG:C2	2.85	0.48
2:B:405:ASN:C	2:B:407:CYS:N	2.65	0.48
3:C:195:GLN:OE1	3:C:382:THR:HG22	2.14	0.47
3:F:227:TRP:HZ2	3:F:230:ASN:ND2	2.11	0.47
3:C:244:TYR:H	3:C:266:LYS:NZ	2.11	0.47
2:E:280:THR:HB	2:E:283:LYS:HB2	1.96	0.47
2:B:333:ASN:HD22	2:B:333:ASN:H	1.58	0.47
3:C:268:GLY:O	3:C:274:TYR:HA	2.15	0.47
2:E:458:PHE:H	2:E:459:PRO:HD2	1.80	0.47
2:E:412:PRO:HG2	2:E:452:MET:HE2	1.97	0.47
2:B:309:GLU:HB2	2:B:325:HIS:HE1	1.79	0.47
2:B:398:ASP:HA	2:B:433:ASP:CB	2.43	0.47
3:F:352:GLY:HA2	3:F:378:SER:O	2.15	0.47
1:A:137:GLN:O	1:A:140:VAL:HG22	2.14	0.46
2:B:253:GLN:C	2:B:253:GLN:HE21	2.19	0.46
3:C:352:GLY:HA2	3:C:378:SER:O	2.16	0.46
3:F:298:ASP:OD1	3:F:299:PRO:HD2	2.15	0.46
3:C:156:ILE:HG22	3:C:161:ALA:HB2	1.97	0.46
1:A:175:LEU:HD23	1:A:175:LEU:N	2.31	0.46
3:C:265:PHE:C	3:C:266:LYS:HD2	2.36	0.46
3:F:195:GLN:OE1	3:F:382:THR:HG22	2.15	0.46
1:A:139:ASN:HB3	3:C:114:TYR:CZ	2.50	0.46
2:E:293:TRP:HZ2	2:E:296:ASN:ND2	2.09	0.46
2:E:364:ASN:ND2	5:E:470:NAG:H2	2.30	0.46
3:F:209:ILE:H	3:F:209:ILE:CD1	2.18	0.46
3:C:340:HIS:ND1	3:C:343:HIS:HB2	2.31	0.46
3:F:208:TRP:HA	3:F:314:THR:HG21	1.97	0.46
2:B:370:HIS:HE1	2:B:408:HIS:HB2	1.81	0.46
3:C:298:ASP:OD1	3:C:299:PRO:HD2	2.16	0.46
3:F:156:ILE:HG22	3:F:161:ALA:CB	2.46	0.46
2:E:183:GLU:HA	3:F:124:LEU:HD13	1.97	0.45
1:D:175:LEU:HD23	1:D:175:LEU:N	2.30	0.45
2:B:280:THR:HB	2:B:283:LYS:HB2	1.99	0.45
3:F:228:LEU:HG	3:F:232:LYS:HD2	1.98	0.45
2:B:315:GLU:HG2	2:B:448:ARG:HH21	1.81	0.45
1:D:179:GLU:HA	1:D:182:GLN:HG2	1.98	0.45
2:E:266:TRP:HA	2:E:377:THR:HG21	1.98	0.45
3:F:244:TYR:H	3:F:266:LYS:NZ	2.14	0.45
3:C:106:SER:HA	3:C:109:TYR:CD2	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:309:GLU:HB2	2:E:325:HIS:HE1	1.82	0.45
2:B:325:HIS:O	2:B:345:TYR:HA	2.17	0.45
1:D:179:GLU:HA	1:D:182:GLN:NE2	2.31	0.45
1:D:179:GLU:O	1:D:182:GLN:HG2	2.16	0.45
2:E:230:ASP:O	2:E:233:VAL:HG22	2.17	0.45
1:D:176:LYS:HA	1:D:176:LYS:HZ2	1.81	0.45
2:E:179:ILE:HG13	3:F:117:ASN:HB2	1.97	0.45
1:A:129:LYS:HD2	1:A:129:LYS:N	2.32	0.45
3:C:105:SER:HB2	3:C:109:TYR:OH	2.17	0.45
3:C:232:LYS:O	3:C:236:ILE:HG13	2.16	0.45
3:F:244:TYR:H	3:F:266:LYS:HZ3	1.65	0.44
1:A:179:GLU:HA	1:A:182:GLN:HG2	1.99	0.44
2:E:253:GLN:NE2	2:E:451:SER:HA	2.32	0.44
3:F:261:ASP:O	3:F:282:ALA:N	2.49	0.44
1:A:166:SER:HB3	2:B:195:THR:HG23	1.98	0.44
3:C:337:ASN:C	3:C:339:CYS:N	2.69	0.44
3:C:242:ILE:O	3:C:242:ILE:HG13	2.17	0.44
2:E:345:TYR:CG	2:E:346:ARG:N	2.85	0.44
3:C:391:ARG:HG2	3:C:391:ARG:NH1	2.32	0.44
3:C:185:ASP:OD2	3:C:189:ASN:HB2	2.17	0.44
3:C:325:ASN:HD22	3:C:325:ASN:C	2.20	0.44
3:C:307:HIS:CE1	3:C:342:GLY:H	2.36	0.44
2:B:224:MET:HE2	2:B:237:ARG:HD3	1.98	0.44
1:A:179:GLU:O	1:A:182:GLN:HG2	2.17	0.44
2:B:267:ASP:HB2	2:B:268:PRO:HD3	2.00	0.44
3:C:115:ASN:HA	3:C:118:ASN:HB3	2.00	0.44
2:E:367:MET:HB2	2:E:406:ARG:CB	2.47	0.44
2:E:249:TRP:HB3	2:E:453:LYS:HB3	2.00	0.44
3:C:244:TYR:H	3:C:266:LYS:HZ3	1.65	0.44
3:C:208:TRP:HA	3:C:314:THR:HG21	1.99	0.44
2:B:345:TYR:CG	2:B:346:ARG:N	2.85	0.44
3:C:203:ASP:O	3:C:206:LYS:HE2	2.18	0.44
3:F:111:GLN:NE2	3:F:112:GLU:HG3	2.33	0.43
2:B:293:TRP:HZ2	2:B:296:ASN:ND2	2.12	0.43
3:C:265:PHE:CZ	3:C:267:VAL:HG23	2.54	0.43
1:D:179:GLU:HB3	1:D:183:LYS:HE3	2.00	0.43
2:E:293:TRP:CZ2	2:E:296:ASN:ND2	2.86	0.43
3:C:298:ASP:OD2	3:C:300:SER:HB2	2.18	0.43
3:F:111:GLN:CD	3:F:111:GLN:H	2.21	0.43
2:E:179:ILE:HG21	3:F:120:LYS:HB2	1.96	0.43
3:C:307:HIS:HE1	3:C:342:GLY:H	1.66	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:196:LYS:HD2	3:F:198:LEU:HD21	2.00	0.43
3:F:153:CYS:SG	3:F:192:THR:HA	2.59	0.43
2:B:174:ASN:O	2:B:178:LYS:HG2	2.18	0.43
2:E:376:SER:HB3	2:E:382:ASN:H	1.84	0.42
3:F:325:ASN:HD22	3:F:325:ASN:C	2.23	0.42
3:F:185:ASP:OD2	3:F:189:ASN:HB2	2.19	0.42
2:E:166:ARG:NH2	3:F:110:LEU:HG	2.25	0.42
3:C:209:ILE:N	3:C:209:ILE:HD12	2.21	0.42
2:B:310:LEU:HD12	2:B:453:LYS:O	2.19	0.42
2:E:457:PHE:HB3	2:E:458:PHE:H	1.49	0.42
1:A:134:GLN:HA	1:A:137:GLN:NE2	2.35	0.42
2:B:436:VAL:HG11	2:B:443:SER:HA	2.02	0.42
3:C:156:ILE:HG22	3:C:161:ALA:CB	2.50	0.42
3:F:183:GLU:HB3	3:F:191:TRP:HB2	2.02	0.42
1:A:179:GLU:HB3	1:A:183:LYS:HE3	2.01	0.42
3:C:343:HIS:O	3:C:367:ILE:HA	2.20	0.41
2:E:385:TRP:CH2	4:N:3:ARG:HD2	2.55	0.41
2:E:455:ARG:HA	2:E:456:PRO:HD3	1.83	0.41
3:C:339:CYS:SG	4:S:3:ARG:CZ	3.09	0.41
5:B:470:NAG:H62	5:B:470:NAG:C2	2.37	0.41
2:E:333:ASN:ND2	2:E:333:ASN:N	2.61	0.41
2:E:370:HIS:HE1	2:E:408:HIS:HB2	1.85	0.41
1:A:127:ILE:HB	1:A:130:VAL:HG21	2.02	0.41
2:E:458:PHE:N	2:E:459:PRO:HD2	2.35	0.41
2:B:310:LEU:HD21	2:B:312:ILE:HD11	2.02	0.41
2:E:417:TYR:OH	2:E:427:ALA:HA	2.21	0.41
2:E:179:ILE:HD12	3:F:121:ILE:HG12	2.01	0.41
2:E:405:ASN:C	2:E:407:CYS:N	2.69	0.41
3:F:344:LEU:HD12	3:F:384:MET:SD	2.60	0.41
2:E:315:GLU:HG2	2:E:448:ARG:HH21	1.84	0.41
1:A:127:ILE:HB	1:A:130:VAL:CG2	2.50	0.41
1:D:135:LEU:HD22	1:D:135:LEU:N	2.36	0.41
1:D:150:LEU:HD12	1:D:150:LEU:HA	1.87	0.41
1:A:128:GLU:C	1:A:129:LYS:HD2	2.41	0.41
2:E:364:ASN:ND2	5:E:470:NAG:C2	2.84	0.41
2:B:408:HIS:CD2	2:B:411:ASN:HB2	2.56	0.41
2:B:408:HIS:O	4:M:1:GLY:HA2	2.20	0.41
3:C:288:ASP:OD2	3:C:291:ASP:HB2	2.20	0.41
3:C:183:GLU:HB3	3:C:191:TRP:HB2	2.03	0.41
2:E:226:LEU:HD12	2:E:226:LEU:HA	1.91	0.41
2:B:158:ASN:ND2	2:B:159:SER:H	2.18	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:198:THR:HG22	3:F:140:LYS:HB2	2.03	0.41
3:F:322:PHE:HE2	3:F:329:GLN:HE22	1.69	0.41
2:E:408:HIS:CD2	2:E:411:ASN:HB2	2.56	0.41
2:B:226:LEU:HD12	2:B:226:LEU:HA	1.97	0.41
1:A:176:LYS:HZ2	1:A:176:LYS:HA	1.86	0.41
3:F:339:CYS:SG	4:T:3:ARG:CZ	3.09	0.41
3:F:209:ILE:HD12	3:F:209:ILE:N	2.25	0.40
3:C:171:PRO:HA	3:C:239:GLN:NE2	2.36	0.40
2:B:245:GLU:O	2:B:246:ASN:HB2	2.21	0.40
2:B:166:ARG:C	2:B:168:LEU:N	2.72	0.40
3:F:334:TRP:CH2	3:F:344:LEU:HB2	2.56	0.40
1:A:175:LEU:O	1:A:178:TYR:HB2	2.22	0.40
2:E:396:LYS:HD2	2:E:396:LYS:HA	1.88	0.40
3:F:337:ASN:O	3:F:338:LYS:C	2.59	0.40
2:E:370:HIS:CE1	2:E:402:TRP:HE1	2.40	0.40
2:B:166:ARG:HD3	2:B:166:ARG:HA	1.80	0.40
2:E:174:ASN:O	2:E:178:LYS:HG2	2.22	0.40
1:D:168:ALA:HA	2:E:189:GLN:HE22	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	65/87 (75%)	58 (89%)	3 (5%)	4 (6%)	2 2
1	D	52/87 (60%)	50 (96%)	2 (4%)	0	100 100
2	B	301/328 (92%)	271 (90%)	25 (8%)	5 (2%)	11 29
2	E	294/328 (90%)	267 (91%)	23 (8%)	4 (1%)	14 35
3	C	290/319 (91%)	265 (91%)	22 (8%)	3 (1%)	19 45
3	F	283/319 (89%)	257 (91%)	23 (8%)	3 (1%)	17 42

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	M	2/4 (50%)	2 (100%)	0	0	100	100
4	N	2/4 (50%)	1 (50%)	1 (50%)	0	100	100
4	S	2/4 (50%)	2 (100%)	0	0	100	100
4	T	2/4 (50%)	2 (100%)	0	0	100	100
All	All	1293/1484 (87%)	1175 (91%)	99 (8%)	19 (2%)	13	32

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	191	LYS
2	B	407	CYS
3	C	339	CYS
2	E	407	CYS
3	F	110	LEU
2	B	281	ASP
2	E	281	ASP
2	E	458	PHE
3	F	339	CYS
1	A	190	ALA
2	B	256	GLN
2	B	457	PHE
3	C	360	PRO
3	F	360	PRO
3	C	297	ASP
2	B	167	VAL
2	E	256	GLN
1	A	127	ILE
1	A	189	ILE

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	62/82 (76%)	58 (94%)	4 (6%)	21	46

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	50/82 (61%)	47 (94%)	3 (6%)	24 50
2	B	261/286 (91%)	249 (95%)	12 (5%)	33 64
2	E	254/286 (89%)	243 (96%)	11 (4%)	35 66
3	C	246/267 (92%)	237 (96%)	9 (4%)	41 72
3	F	239/267 (90%)	231 (97%)	8 (3%)	45 76
4	M	3/3 (100%)	3 (100%)	0	100 100
4	N	3/3 (100%)	2 (67%)	1 (33%)	0 0
4	S	3/3 (100%)	2 (67%)	1 (33%)	0 0
4	T	3/3 (100%)	3 (100%)	0	100 100
All	All	1124/1282 (88%)	1075 (96%)	49 (4%)	35 65

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	143	GLN
1	A	167	ARG
1	A	176	LYS
1	A	192	ASP
2	B	158	ASN
2	B	195	THR
2	B	210	GLU
2	B	224	MET
2	B	253	GLN
2	B	333	ASN
2	B	346	ARG
2	B	351	ASN
2	B	361	MET
2	B	376	SER
2	B	406	ARG
2	B	457	PHE
3	C	103	HIS
3	C	117	ASN
3	C	230	ASN
3	C	277	THR
3	C	317	ASN
3	C	323	GLU
3	C	325	ASN
3	C	382	THR
3	C	389	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	143	GLN
1	D	167	ARG
1	D	176	LYS
2	E	164	ASN
2	E	195	THR
2	E	210	GLU
2	E	253	GLN
2	E	333	ASN
2	E	346	ARG
2	E	351	ASN
2	E	361	MET
2	E	376	SER
2	E	406	ARG
2	E	457	PHE
3	F	111	GLN
3	F	117	ASN
3	F	230	ASN
3	F	317	ASN
3	F	323	GLU
3	F	325	ASN
3	F	382	THR
3	F	389	PHE
4	S	3	ARG
4	N	3	ARG

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

Mol	Chain	Res	Type
1	A	131	GLN
1	A	134	GLN
1	A	143	GLN
1	A	181	GLN
1	A	182	GLN
2	B	160	ASN
2	B	164	ASN
2	B	174	ASN
2	B	189	GLN
2	B	253	GLN
2	B	254	ASN
2	B	256	GLN
2	B	296	ASN
2	B	333	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	339	GLN
2	B	351	ASN
2	B	364	ASN
2	B	408	HIS
2	B	439	ASN
3	C	117	ASN
3	C	130	GLN
3	C	163	GLN
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	325	ASN
1	D	181	GLN
2	E	164	ASN
2	E	174	ASN
2	E	189	GLN
2	E	253	GLN
2	E	256	GLN
2	E	296	ASN
2	E	333	ASN
2	E	339	GLN
2	E	351	ASN
2	E	364	ASN
2	E	408	HIS
2	E	439	ASN
3	F	111	GLN
3	F	130	GLN
3	F	134	GLN
3	F	163	GLN
3	F	177	GLN
3	F	230	ASN
3	F	239	GLN
3	F	307	HIS
3	F	317	ASN
3	F	325	ASN
3	F	390	ASN
4	N	2	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 6 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	$\#\|Z\| > 2$
5	NAG	B	470	-	14,14,15	0.50	0	15,19,21	0.89	1 (6%)
5	NAG	E	470	-	14,14,15	0.48	0	15,19,21	0.71	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
5	NAG	B	470	-	-	0/6/23/26	0/1/1/1
5	NAG	E	470	-	-	0/6/23/26	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})
5	B	470	NAG	C2-N2-C7	-2.37	119.99	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	470	NAG	6	0
5	E	470	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.