Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:00 AM GMT

PDB ID	:	2OYH
Title	:	Crystal Structure of Fragment D of gammaD298,301A Fibrinogen with the Peptide Ligand Gly-His-Arg-Pro-Amide
Authors	:	Kostelansky, M.S.; Gorkun, O.V.; Lord, S.T.
Deposited on	:	2007-02-22
Resolution	:	2.40 Å(reported)

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

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

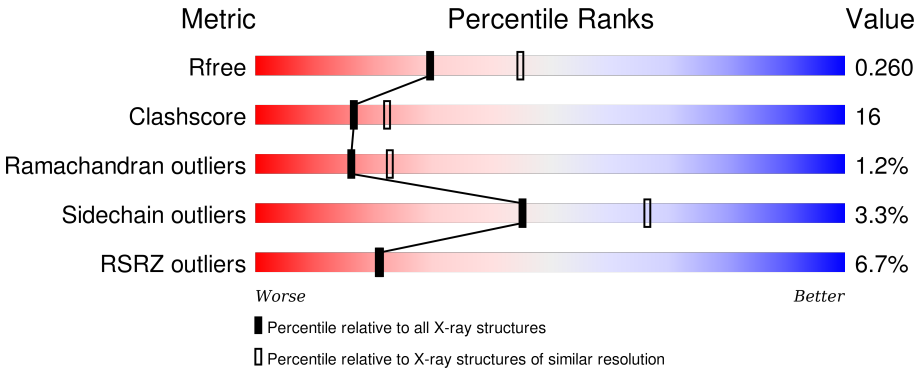
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	66	12% 52% 44%
1	D	66	32% 48% 32% 18%
2	B	313	2% 62% 32% 5%
2	E	313	4% 71% 21% 6%
3	C	311	6% 71% 22%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	311	6% 65% 26% 8%
4	G	4	25% 75% 25%
4	H	4	100%
4	I	4	50% 50% 50%
4	J	4	75% 25%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	B	3	-	-	-	X
5	NAG	E	3	-	-	X	-
5	FUC	E	5	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10847 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 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	64	Total	C	N	O	S	0	0	0
			523	322	99	99	3			
1	D	54	Total	C	N	O	S	0	0	0
			442	270	84	85	3			

- Molecule 2 is a protein called Fibrinogen beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	298	Total	C	N	O	S	0	0	0
			2392	1494	422	454	22			
2	E	295	Total	C	N	O	S	0	0	0
			2369	1480	418	449	22			

- Molecule 3 is a protein called Fibrinogen gamma chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	299	Total	C	N	O	S	0	0	0
			2393	1521	403	458	11			
3	F	285	Total	C	N	O	S	0	0	0
			2277	1448	384	434	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	298	ALA	ASP	ENGINEERED	UNP P02679
C	301	ALA	ASP	ENGINEERED	UNP P02679
F	298	ALA	ASP	ENGINEERED	UNP P02679
F	301	ALA	ASP	ENGINEERED	UNP P02679

- Molecule 4 is a protein called GHRP peptide.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	G	4	Total C N O 33 19 9 5	0	0	0
4	H	4	Total C N O 33 19 9 5	0	0	0
4	I	4	Total C N O 33 19 9 5	0	0	0
4	J	4	Total C N O 33 19 9 5	0	0	0

- Molecule 5 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	3	Total C N O 38 22 2 14	0	0
5	E	3	Total C N O 38 22 2 14	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	1	Total Ca 1 1	0	0
6	F	1	Total Ca 1 1	0	0
6	E	1	Total Ca 1 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	9	Total O 9 9	0	0
7	B	54	Total O 54 54	0	0
7	C	29	Total O 29 29	0	0
7	D	11	Total O 11 11	0	0
7	E	91	Total O 91 91	0	0

Continued on next page...

Continued from previous page...

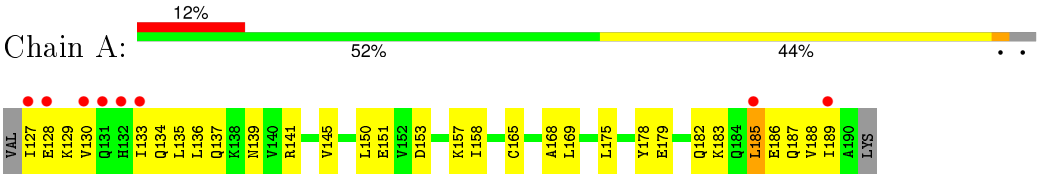
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	F	44	Total O 44 44	0	0
7	J	1	Total O 1 1	0	0

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.

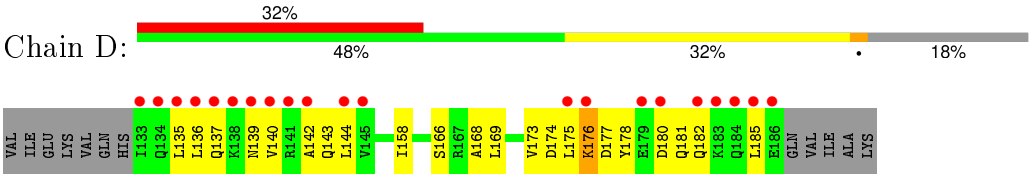
- Molecule 1: Fibrinogen alpha chain

Chain A:



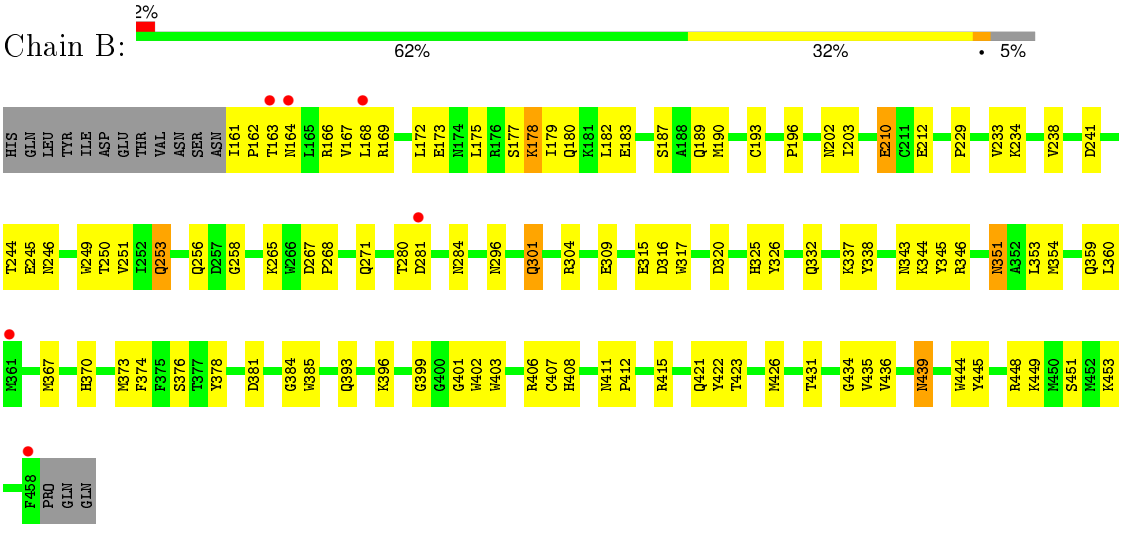
- Molecule 1: Fibrinogen alpha chain

Chain D:



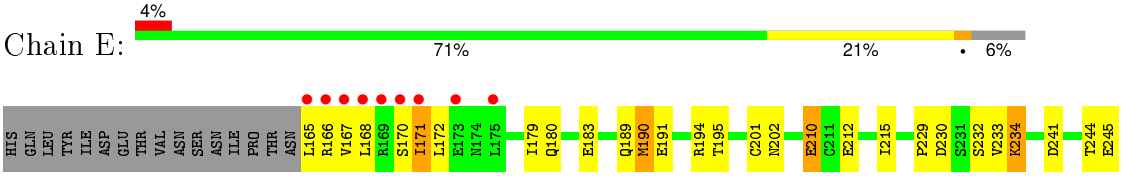
- Molecule 2: Fibrinogen beta chain

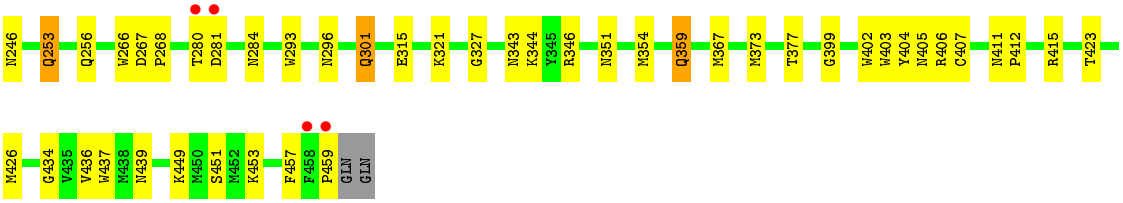
Chain B:



- Molecule 2: Fibrinogen beta chain

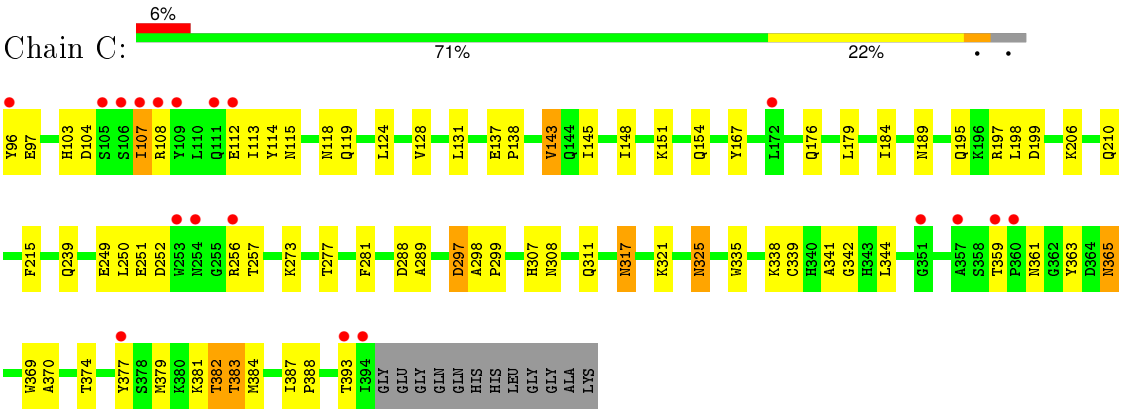
Chain E:





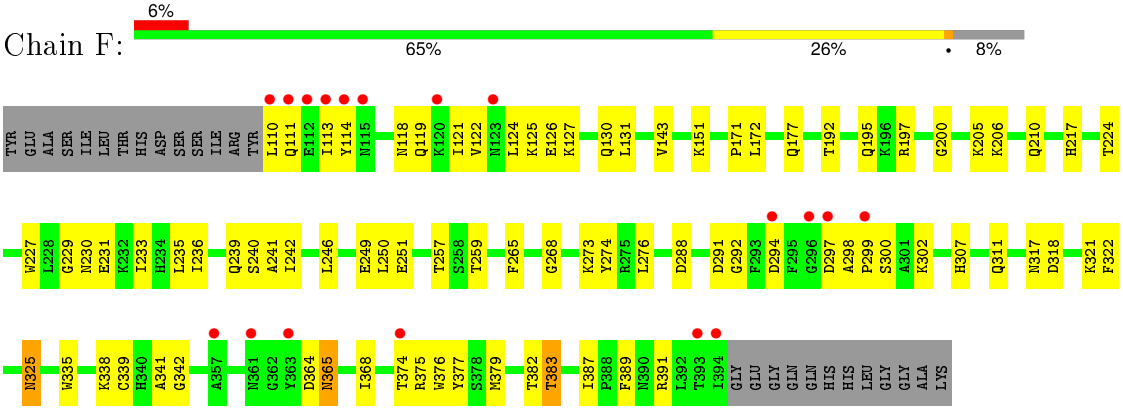
- Molecule 3: Fibrinogen gamma chain

Chain C:



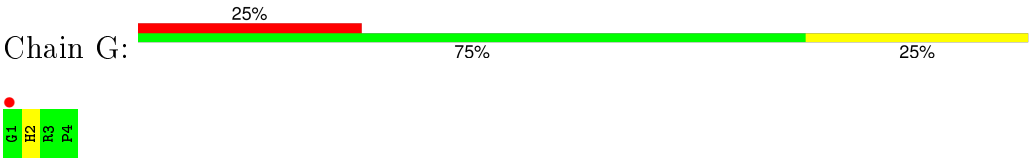
- Molecule 3: Fibrinogen gamma chain

Chain F:



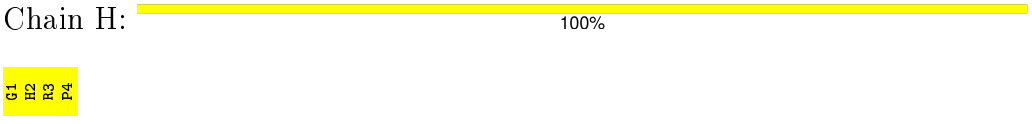
- Molecule 4: GHRP peptide

Chain G:



- Molecule 4: GHRP peptide

Chain H:



- Molecule 4: GHRP peptide

Chain I:

- Molecule 4: GHRP peptide

Chain J:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	89.16Å 94.12Å 226.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	18.00 – 2.40 43.46 – 2.41	Depositor EDS
% Data completeness (in resolution range)	95.5 (18.00-2.40) 95.6 (43.46-2.41)	Depositor EDS
R_{merge}	0.00	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	3.46 (at 2.39Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.220 , 0.259 0.221 , 0.260	Depositor DCC
R_{free} test set	3604 reflections (5.05%)	DCC
Wilson B-factor (Å^2)	40.0	Xtriage
Anisotropy	0.006	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 45.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 71572 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10847	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.94% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.28	0/524	0.51	0/699
1	D	0.29	0/442	0.51	0/588
2	B	0.35	0/2453	0.60	0/3312
2	E	0.38	0/2430	0.65	1/3280 (0.0%)
3	C	0.34	0/2459	0.54	0/3327
3	F	0.36	0/2340	0.60	0/3165
4	G	0.48	0/34	0.46	0/43
4	H	0.46	0/34	0.49	0/43
4	I	0.47	0/34	0.44	0/43
4	J	0.54	0/34	0.53	0/43
All	All	0.36	0/10784	0.59	1/14543 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	399	GLY	N-CA-C	6.85	130.23	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	523	0	547	36	0
1	D	442	0	460	27	0
2	B	2392	0	2262	93	0
2	E	2369	0	2238	73	0
3	C	2393	0	2248	62	0
3	F	2277	0	2140	76	0
4	G	33	0	32	1	0
4	H	33	0	32	3	0
4	I	33	0	32	3	0
4	J	33	0	32	1	0
5	B	38	0	34	2	0
5	E	38	0	34	9	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
7	A	9	0	0	0	0
7	B	54	0	0	3	0
7	C	29	0	0	1	0
7	D	11	0	0	0	0
7	E	91	0	0	1	0
7	F	44	0	0	1	0
7	J	1	0	0	0	0
All	All	10847	0	10091	341	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 16.

All (341) 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:F:374:THR:HG22	3:F:376:TRP:H	1.23	1.02
3:C:148:ILE:H	3:C:148:ILE:HD12	1.33	0.92
2:E:234:LYS:H	2:E:234:LYS:HD2	1.33	0.92
1:A:128:GLU:HG2	1:A:129:LYS:H	1.35	0.90
3:C:249:GLU:HB2	3:C:383:THR:HG23	1.51	0.90
3:F:151:LYS:HB3	3:F:239:GLN:HE22	1.37	0.88
1:A:127:ILE:HG22	1:A:130:VAL:HG23	1.55	0.86
1:D:185:LEU:HD23	2:E:171:ILE:HD11	1.61	0.83
2:E:373:MET:HE1	2:E:405:ASN:HA	1.60	0.82
3:F:307:HIS:HE1	3:F:341:ALA:H	1.27	0.81
1:A:130:VAL:O	1:A:134:GLN:HG3	1.81	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:136:LEU:HD11	3:F:111:GLN:HB2	1.62	0.80
3:F:197:ARG:HB2	3:F:382:THR:HB	1.64	0.79
2:B:367:MET:SD	2:B:406:ARG:HD3	2.22	0.79
2:E:423:THR:N	2:E:426:MET:HE3	1.98	0.79
1:A:135:LEU:HG	1:A:139:ASN:HD21	1.46	0.79
5:E:3:NAG:H61	5:E:5:FUC:H3	1.66	0.78
2:E:165:LEU:HD11	2:E:168:LEU:HD22	1.64	0.77
3:F:249:GLU:HB2	3:F:383:THR:HG23	1.67	0.76
2:B:316:ASP:HB2	2:B:445:TYR:OH	1.86	0.76
3:C:151:LYS:HB3	3:C:239:GLN:HE22	1.51	0.76
2:B:202:ASN:HD22	2:B:284:ASN:HD22	1.31	0.75
2:B:423:THR:N	2:B:426:MET:HE3	2.01	0.75
1:D:136:LEU:HD21	3:F:111:GLN:HG3	1.68	0.75
2:B:163:THR:HB	2:B:166:ARG:HD2	1.69	0.74
4:H:2:HIS:CD2	4:H:4:PRO:HD3	2.22	0.74
1:A:127:ILE:HG12	1:A:128:GLU:H	1.53	0.73
3:C:108:ARG:O	3:C:112:GLU:HG3	1.88	0.73
2:B:439:ASN:HD22	2:B:439:ASN:H	1.37	0.73
2:E:439:ASN:H	2:E:439:ASN:HD22	1.38	0.72
1:A:153:ASP:O	1:A:157:LYS:HG2	1.88	0.72
2:E:359:GLN:H	2:E:359:GLN:HE21	1.36	0.71
5:E:3:NAG:H61	5:E:5:FUC:H5	1.72	0.71
2:E:230:ASP:HB3	2:E:233:VAL:HG12	1.72	0.71
1:A:127:ILE:HG22	1:A:130:VAL:CG2	2.21	0.70
1:D:166:SER:HB3	2:E:195:THR:HG22	1.73	0.70
3:F:307:HIS:CE1	3:F:341:ALA:H	2.08	0.70
5:E:3:NAG:H62	5:E:4:NAG:H2	1.72	0.70
2:B:423:THR:H	2:B:426:MET:HE3	1.54	0.69
2:B:351:ASN:HD21	2:B:354:MET:H	1.40	0.69
1:D:144:LEU:HD21	1:D:182:GLN:HG2	1.75	0.69
2:E:234:LYS:H	2:E:234:LYS:CD	2.06	0.68
2:E:415:ARG:O	2:E:434:GLY:HA2	1.93	0.68
3:F:200:GLY:HA2	7:F:409:HOH:O	1.93	0.68
2:E:373:MET:CE	2:E:405:ASN:HA	2.23	0.68
1:D:139:ASN:HB3	3:F:114:TYR:CZ	2.30	0.67
2:B:351:ASN:ND2	2:B:354:MET:H	1.93	0.66
2:B:202:ASN:ND2	2:B:284:ASN:HB2	2.10	0.66
3:F:276:LEU:HD23	3:F:276:LEU:C	2.15	0.66
2:E:202:ASN:HD22	2:E:284:ASN:HD22	1.42	0.66
1:A:128:GLU:HG2	1:A:129:LYS:N	2.08	0.66
3:C:307:HIS:HE1	3:C:341:ALA:H	1.44	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:251:GLU:HB3	3:C:381:LYS:HB2	1.78	0.65
3:C:252:ASP:OD2	3:C:256:ARG:HB2	1.95	0.65
1:A:182:GLN:O	1:A:186:GLU:HG2	1.96	0.65
1:A:168:ALA:HA	2:B:189:GLN:HE22	1.62	0.65
2:B:351:ASN:OD1	2:B:354:MET:HB2	1.96	0.65
2:B:367:MET:HB2	2:B:406:ARG:HB3	1.78	0.65
5:E:3:NAG:H4	5:E:4:NAG:N2	2.10	0.65
3:C:148:ILE:CD1	3:C:148:ILE:H	2.08	0.64
2:B:439:ASN:HD22	2:B:439:ASN:N	1.95	0.64
1:A:188:VAL:HG21	2:B:167:VAL:HG21	1.79	0.64
2:E:202:ASN:ND2	2:E:284:ASN:HB2	2.13	0.64
3:F:338:LYS:N	3:F:339:CYS:HA	2.11	0.64
2:B:415:ARG:O	2:B:434:GLY:HA2	1.98	0.63
1:A:185:LEU:HD22	1:A:189:ILE:HD11	1.80	0.63
1:D:136:LEU:HD21	3:F:111:GLN:CG	2.28	0.63
3:C:197:ARG:HB2	3:C:382:THR:HB	1.79	0.63
1:A:127:ILE:HG23	1:A:128:GLU:N	2.13	0.63
5:E:3:NAG:H61	5:E:5:FUC:C3	2.29	0.62
3:F:249:GLU:HG2	3:F:259:THR:HG22	1.79	0.62
2:E:201:CYS:O	3:F:143:VAL:HG21	1.98	0.62
1:A:178:TYR:O	1:A:182:GLN:HG3	1.99	0.62
1:A:183:LYS:O	1:A:187:GLN:HG3	1.99	0.62
1:A:135:LEU:HG	1:A:139:ASN:ND2	2.13	0.62
2:E:406:ARG:NH1	4:J:3:ARG:O	2.33	0.61
2:B:343:ASN:OD1	2:B:344:LYS:HE2	2.01	0.61
1:D:178:TYR:O	1:D:182:GLN:HG3	2.00	0.61
3:F:118:ASN:O	3:F:122:VAL:HG23	2.00	0.61
1:A:169:LEU:H	2:B:189:GLN:NE2	1.98	0.60
2:B:161:ILE:N	2:B:162:PRO:HD2	2.17	0.60
3:C:307:HIS:CE1	3:C:341:ALA:H	2.20	0.60
1:A:139:ASN:HB3	3:C:114:TYR:CZ	2.37	0.60
2:E:172:LEU:HD23	2:E:172:LEU:O	2.02	0.59
3:C:148:ILE:N	3:C:148:ILE:HD12	2.12	0.59
2:E:168:LEU:HD21	3:F:110:LEU:HB3	1.84	0.59
3:C:325:ASN:HD22	3:C:325:ASN:C	2.07	0.58
1:A:133:ILE:O	1:A:137:GLN:HG3	2.03	0.58
2:E:423:THR:H	2:E:426:MET:HE3	1.67	0.58
1:D:169:LEU:H	2:E:189:GLN:HE22	1.50	0.58
1:A:127:ILE:N	1:A:130:VAL:HB	2.18	0.58
2:E:212:GLU:O	2:E:215:ILE:HG22	2.04	0.58
3:F:195:GLN:OE1	3:F:382:THR:HG22	2.04	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:3:NAG:H4	5:B:4:NAG:HN2	1.69	0.58
2:E:253:GLN:NE2	2:E:451:SER:HA	2.19	0.58
3:C:251:GLU:HG3	3:C:257:THR:HG22	1.85	0.58
1:D:185:LEU:HD13	1:D:185:LEU:O	2.03	0.57
2:B:210:GLU:OE1	2:B:212:GLU:HB3	2.03	0.57
1:D:144:LEU:CD2	1:D:182:GLN:HE21	2.17	0.57
3:F:288:ASP:OD2	3:F:291:ASP:HB2	2.05	0.57
2:B:233:VAL:HG12	2:B:234:LYS:N	2.19	0.57
2:E:367:MET:HB2	2:E:406:ARG:HB3	1.85	0.57
2:B:251:VAL:HG22	2:B:453:LYS:HE2	1.87	0.57
1:D:136:LEU:O	1:D:140:VAL:HG22	2.04	0.56
2:B:315:GLU:HB3	2:B:449:LYS:HB2	1.88	0.56
2:B:229:PRO:HB3	2:B:301:GLN:HE22	1.71	0.56
1:A:151:GLU:OE2	2:B:182:LEU:HD21	2.06	0.56
3:F:374:THR:HG22	3:F:376:TRP:N	2.08	0.56
5:E:3:NAG:H61	5:E:5:FUC:C5	2.36	0.56
1:D:158:ILE:HG23	2:E:189:GLN:HE21	1.71	0.56
3:F:297:ASP:OD2	4:I:2:HIS:HB3	2.05	0.56
1:A:127:ILE:HG12	1:A:128:GLU:OE2	2.05	0.56
3:F:119:GLN:HA	3:F:119:GLN:NE2	2.20	0.56
2:B:253:GLN:NE2	2:B:451:SER:HA	2.21	0.56
2:B:316:ASP:OD2	2:B:320:ASP:HB2	2.06	0.56
2:B:326:TYR:CE2	2:B:353:LEU:HD12	2.41	0.55
2:E:373:MET:HE2	2:E:404:TYR:O	2.06	0.55
3:F:389:PHE:C	3:F:391:ARG:H	2.10	0.55
3:C:365:ASN:H	3:C:365:ASN:HD22	1.55	0.54
2:E:172:LEU:HD22	3:F:113:ILE:HD11	1.90	0.54
3:F:297:ASP:HB2	4:I:2:HIS:HD2	1.72	0.54
2:B:337:LYS:HE2	2:B:374:PHE:CD1	2.43	0.54
2:E:359:GLN:H	2:E:359:GLN:NE2	2.03	0.54
2:B:345:TYR:CG	2:B:346:ARG:N	2.76	0.54
3:F:325:ASN:HD22	3:F:325:ASN:C	2.11	0.54
1:D:169:LEU:H	2:E:189:GLN:NE2	2.05	0.54
5:E:3:NAG:H4	5:E:4:NAG:HN2	1.73	0.54
3:F:121:ILE:O	3:F:125:LYS:HG3	2.07	0.54
2:B:265:LYS:O	2:B:268:PRO:HD2	2.08	0.54
1:A:158:ILE:HG23	2:B:189:GLN:HE21	1.72	0.53
2:B:258:GLY:HA2	7:B:462:HOH:O	2.08	0.53
3:F:307:HIS:HD2	3:F:335:TRP:O	1.91	0.53
3:F:292:GLY:C	3:F:302:LYS:HD2	2.28	0.53
1:A:150:LEU:HD21	3:C:124:LEU:HD23	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:338:LYS:N	3:C:339:CYS:HA	2.21	0.53
2:E:165:LEU:O	2:E:165:LEU:HG	2.08	0.53
1:D:135:LEU:O	1:D:135:LEU:HD13	2.09	0.53
2:E:457:PHE:O	2:E:459:PRO:HD3	2.07	0.53
1:A:169:LEU:H	2:B:189:GLN:HE22	1.54	0.53
3:F:205:LYS:HB3	3:F:205:LYS:NZ	2.23	0.53
2:E:267:ASP:HB3	2:E:268:PRO:HD3	1.91	0.53
2:B:163:THR:HG22	2:B:166:ARG:CZ	2.39	0.53
3:F:365:ASN:HD22	3:F:365:ASN:H	1.55	0.53
3:C:103:HIS:O	3:C:107:ILE:HB	2.09	0.52
1:A:139:ASN:HB3	3:C:114:TYR:CE1	2.44	0.52
2:E:210:GLU:OE1	2:E:212:GLU:HB3	2.09	0.52
3:F:387:ILE:HD11	3:F:391:ARG:HG2	1.92	0.52
3:C:307:HIS:HD2	3:C:335:TRP:O	1.93	0.52
2:E:423:THR:HG23	2:E:426:MET:HE3	1.92	0.52
2:B:202:ASN:HD22	2:B:284:ASN:ND2	2.06	0.52
3:F:251:GLU:HG3	3:F:257:THR:HG22	1.91	0.52
3:C:195:GLN:OE1	3:C:382:THR:HG22	2.09	0.52
3:C:281:PHE:HB2	3:C:288:ASP:OD2	2.10	0.52
1:D:143:GLN:NE2	3:F:118:ASN:OD1	2.43	0.51
3:F:124:LEU:O	3:F:127:LYS:HB3	2.10	0.51
2:B:359:GLN:O	2:B:360:LEU:HD23	2.11	0.51
2:E:315:GLU:HB3	2:E:449:LYS:HB2	1.92	0.51
2:E:179:ILE:O	2:E:183:GLU:HG3	2.10	0.51
2:B:202:ASN:ND2	2:B:284:ASN:HD22	2.05	0.51
1:D:173:VAL:HG12	1:D:175:LEU:HD22	1.93	0.51
3:F:172:LEU:H	3:F:239:GLN:HE21	1.58	0.50
2:B:453:LYS:HE3	7:B:469:HOH:O	2.11	0.50
1:D:174:ASP:OD2	1:D:177:ASP:HB2	2.11	0.50
1:A:185:LEU:HD22	1:A:189:ILE:CD1	2.40	0.50
2:E:190:MET:HE1	3:F:131:LEU:HA	1.93	0.50
2:B:439:ASN:ND2	2:B:439:ASN:N	2.59	0.50
1:A:175:LEU:HD22	1:A:175:LEU:H	1.77	0.50
1:D:144:LEU:HD21	1:D:182:GLN:HE21	1.75	0.50
3:F:322:PHE:CZ	4:I:3:ARG:HG2	2.47	0.50
1:D:168:ALA:HA	2:E:189:GLN:HE22	1.77	0.50
2:B:332:GLN:O	2:B:338:TYR:HA	2.12	0.50
3:F:240:SER:O	3:F:242:ILE:HG13	2.11	0.49
3:F:119:GLN:HA	3:F:119:GLN:HE21	1.78	0.49
1:A:141:ARG:O	1:A:145:VAL:HG23	2.13	0.49
2:E:266:TRP:HA	2:E:377:THR:HG21	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:406:ARG:N	2:E:407:CYS:HA	2.27	0.48
3:F:273:LYS:HB2	3:F:311:GLN:HB3	1.95	0.48
2:B:244:THR:HG22	2:B:245:GLU:HG3	1.94	0.48
2:B:384:GLY:O	2:B:406:ARG:HB2	2.13	0.48
3:F:368:ILE:HG22	3:F:377:TYR:O	2.13	0.48
2:B:385:TRP:HD1	2:B:406:ARG:NH1	2.11	0.48
2:E:439:ASN:H	2:E:439:ASN:ND2	2.09	0.48
7:B:503:HOH:O	3:C:138:PRO:HG3	2.13	0.48
3:C:359:THR:HG21	3:C:363:TYR:O	2.13	0.48
1:A:130:VAL:O	1:A:133:ILE:HG22	2.13	0.47
3:F:298:ALA:C	3:F:300:SER:H	2.17	0.47
2:E:293:TRP:HE1	2:E:296:ASN:ND2	2.12	0.47
3:F:307:HIS:CE1	3:F:342:GLY:H	2.32	0.47
2:E:166:ARG:C	2:E:168:LEU:H	2.18	0.47
3:C:167:TYR:O	3:C:179:LEU:HD12	2.14	0.47
2:E:343:ASN:HA	2:E:354:MET:CE	2.45	0.47
3:F:171:PRO:HA	3:F:239:GLN:NE2	2.30	0.47
2:B:202:ASN:HD22	2:B:284:ASN:HB2	1.78	0.47
2:B:253:GLN:HE22	2:B:451:SER:HA	1.79	0.47
3:C:361:ASN:HD22	3:C:361:ASN:N	2.11	0.47
3:F:250:LEU:HD12	3:F:379:MET:HG3	1.97	0.47
3:F:206:LYS:HD2	3:F:210:GLN:OE1	2.13	0.47
3:F:246:LEU:HD22	3:F:265:PHE:CE1	2.49	0.47
3:C:307:HIS:HE1	3:C:342:GLY:H	1.62	0.47
3:F:321:LYS:O	3:F:338:LYS:HD3	2.14	0.47
3:F:365:ASN:ND2	3:F:365:ASN:H	2.12	0.47
3:C:289:ALA:HB3	3:C:369:TRP:CE2	2.49	0.47
2:B:271:GLN:HE21	2:B:271:GLN:HA	1.80	0.47
3:C:307:HIS:CE1	3:C:342:GLY:H	2.33	0.47
3:C:252:ASP:HB2	3:C:377:TYR:OH	2.13	0.47
3:C:154:GLN:OE1	3:C:387:ILE:HD11	2.15	0.47
2:E:229:PRO:HB2	2:E:301:GLN:HE22	1.80	0.47
2:B:343:ASN:HA	2:B:354:MET:SD	2.55	0.47
2:B:351:ASN:C	2:B:351:ASN:HD22	2.17	0.47
2:B:253:GLN:HE21	2:B:253:GLN:C	2.17	0.46
2:B:267:ASP:HB3	2:B:268:PRO:HD3	1.97	0.46
2:B:178:LYS:HA	2:B:178:LYS:NZ	2.30	0.46
2:B:280:THR:O	2:B:280:THR:HG22	2.16	0.46
2:E:165:LEU:CD1	2:E:168:LEU:HD22	2.41	0.46
3:C:250:LEU:HD11	3:C:344:LEU:HD21	1.98	0.46
5:E:3:NAG:C6	5:E:5:FUC:H5	2.44	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:365:ASN:ND2	3:C:365:ASN:H	2.13	0.46
2:B:370:HIS:O	2:B:373:MET:HG2	2.16	0.46
2:B:161:ILE:N	2:B:162:PRO:CD	2.78	0.46
3:F:365:ASN:N	3:F:365:ASN:HD22	2.12	0.46
2:B:351:ASN:C	2:B:351:ASN:ND2	2.70	0.46
2:B:434:GLY:O	2:B:436:VAL:N	2.48	0.46
3:F:126:GLU:O	3:F:130:GLN:HG3	2.16	0.46
3:C:321:LYS:O	3:C:338:LYS:HD3	2.15	0.46
3:C:119:GLN:HA	3:C:119:GLN:HE21	1.81	0.46
2:B:411:ASN:N	2:B:412:PRO:HD3	2.31	0.46
3:C:321:LYS:O	3:C:338:LYS:HB2	2.16	0.45
2:E:190:MET:HE3	3:F:131:LEU:CD1	2.47	0.45
3:C:297:ASP:HB2	4:G:2:HIS:HD2	1.82	0.45
2:B:315:GLU:HA	2:B:320:ASP:O	2.16	0.45
3:F:318:ASP:OD2	3:F:325:ASN:HA	2.16	0.45
3:F:231:GLU:O	3:F:235:LEU:HG	2.16	0.45
2:E:190:MET:CE	3:F:131:LEU:HA	2.46	0.45
3:F:268:GLY:O	3:F:274:TYR:HA	2.16	0.45
1:D:176:LYS:O	1:D:180:ASP:N	2.49	0.45
3:C:298:ALA:HB1	3:C:299:PRO:CD	2.46	0.45
2:E:191:GLU:HG2	2:E:194:ARG:HH11	1.82	0.45
3:F:172:LEU:HD22	3:F:239:GLN:HE21	1.82	0.45
2:B:178:LYS:HA	2:B:178:LYS:HZ3	1.81	0.45
2:E:402:TRP:CH2	2:E:412:PRO:HG2	2.52	0.45
1:D:176:LYS:HB2	1:D:176:LYS:HZ3	1.82	0.44
2:B:422:TYR:O	2:B:444:TRP:HB3	2.17	0.44
2:E:453:LYS:HG3	7:E:475:HOH:O	2.17	0.44
1:D:166:SER:HB3	2:E:195:THR:CG2	2.43	0.44
2:B:229:PRO:CB	2:B:301:GLN:HE22	2.30	0.44
3:C:387:ILE:HG12	3:C:388:PRO:HD2	1.98	0.44
2:E:436:VAL:CG1	2:E:437:TRP:N	2.80	0.44
1:D:181:GLN:OE1	2:E:171:ILE:HB	2.16	0.44
2:B:402:TRP:CG	2:B:403:TRP:N	2.86	0.44
2:B:172:LEU:HB3	3:C:113:ILE:CD1	2.48	0.44
2:E:415:ARG:N	2:E:434:GLY:HA2	2.32	0.44
3:F:389:PHE:C	3:F:391:ARG:N	2.71	0.44
3:F:239:GLN:O	3:F:240:SER:C	2.56	0.44
2:B:406:ARG:N	2:B:407:CYS:HA	2.32	0.44
2:B:370:HIS:HE1	2:B:408:HIS:HB2	1.82	0.44
2:B:203:ILE:CD1	3:C:145:ILE:HD11	2.48	0.44
3:C:361:ASN:N	3:C:361:ASN:ND2	2.66	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:195:GLN:HE22	3:C:382:THR:HG21	1.83	0.43
3:F:294:ASP:OD1	3:F:302:LYS:HB2	2.18	0.43
2:E:230:ASP:OD2	2:E:232:SER:HB2	2.18	0.43
2:E:191:GLU:HA	2:E:194:ARG:HD3	1.99	0.43
5:B:4:NAG:O3	5:B:4:NAG:C7	2.66	0.43
2:B:381:ASP:HB2	2:B:393:GLN:OE1	2.19	0.43
2:B:378:TYR:HB2	2:B:396:LYS:HG2	2.00	0.43
1:A:136:LEU:HB3	2:B:168:LEU:HD21	2.00	0.43
2:E:230:ASP:HB3	2:E:233:VAL:CG1	2.46	0.43
2:E:402:TRP:CG	2:E:403:TRP:N	2.87	0.43
1:A:165:CYS:HB3	2:B:193:CYS:HA	2.00	0.43
3:F:364:ASP:HB3	3:F:375:ARG:HG3	1.99	0.43
3:F:307:HIS:HE1	3:F:342:GLY:H	1.65	0.43
2:E:423:THR:HG23	2:E:426:MET:CE	2.48	0.43
2:B:345:TYR:HB2	2:B:354:MET:HE2	2.00	0.43
2:B:175:LEU:O	2:B:179:ILE:HG13	2.19	0.43
2:B:325:HIS:O	2:B:345:TYR:HA	2.19	0.43
3:C:317:ASN:HD22	3:C:317:ASN:C	2.22	0.43
3:C:365:ASN:N	3:C:365:ASN:HD22	2.13	0.43
2:B:376:SER:O	2:B:401:GLY:HA2	2.19	0.43
1:D:136:LEU:HG	3:F:111:GLN:NE2	2.34	0.43
2:B:431:THR:HG21	4:H:3:ARG:NH2	2.34	0.43
3:F:229:GLY:O	3:F:233:ILE:HG13	2.19	0.43
2:B:164:ASN:C	2:B:166:ARG:N	2.72	0.43
3:F:227:TRP:HZ2	3:F:230:ASN:HD21	1.65	0.43
2:B:177:SER:O	2:B:180:GLN:HB3	2.18	0.42
3:F:217:HIS:O	3:F:224:THR:HG23	2.19	0.42
2:B:169:ARG:O	2:B:173:GLU:HG3	2.19	0.42
3:C:251:GLU:HA	3:C:256:ARG:O	2.19	0.42
1:D:142:ALA:C	1:D:144:LEU:H	2.22	0.42
3:F:276:LEU:CD2	3:F:276:LEU:C	2.88	0.42
3:C:143:VAL:O	3:C:143:VAL:HG22	2.19	0.42
2:B:190:MET:HG2	3:C:131:LEU:HD13	2.01	0.42
2:B:241:ASP:HB3	2:B:249:TRP:HB2	2.02	0.42
3:C:114:TYR:CD2	3:C:115:ASN:ND2	2.88	0.42
3:F:143:VAL:HG23	3:F:143:VAL:O	2.19	0.42
5:E:3:NAG:C6	5:E:5:FUC:H3	2.41	0.42
2:B:345:TYR:CD2	2:B:351:ASN:HB2	2.54	0.42
3:C:96:TYR:O	3:C:97:GLU:HB3	2.20	0.42
2:E:439:ASN:N	2:E:439:ASN:ND2	2.65	0.42
3:C:195:GLN:OE1	3:C:382:THR:CG2	2.67	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:LEU:HD22	1:A:175:LEU:N	2.34	0.42
2:B:203:ILE:HD13	3:C:145:ILE:HD11	2.02	0.42
3:F:122:VAL:O	3:F:126:GLU:HG3	2.20	0.42
3:F:192:THR:HG21	3:F:236:ILE:HD13	2.02	0.42
1:D:135:LEU:C	1:D:135:LEU:HD13	2.40	0.42
2:E:190:MET:HE3	3:F:131:LEU:HD12	2.01	0.42
3:F:298:ALA:O	3:F:300:SER:N	2.53	0.42
3:C:137:GLU:HA	3:C:138:PRO:HD3	1.87	0.42
3:C:250:LEU:HD12	3:C:379:MET:HG3	2.01	0.42
2:E:327:GLY:HA3	2:E:344:LYS:HE2	2.01	0.42
2:E:241:ASP:OD2	2:E:453:LYS:NZ	2.51	0.41
3:C:195:GLN:HB3	3:C:384:MET:HB2	2.01	0.41
2:B:233:VAL:CG1	2:B:234:LYS:N	2.82	0.41
3:C:338:LYS:HG2	3:C:338:LYS:O	2.20	0.41
1:A:175:LEU:O	1:A:179:GLU:HG3	2.20	0.41
3:C:273:LYS:HB2	3:C:311:GLN:HB3	2.03	0.41
2:E:439:ASN:N	2:E:439:ASN:HD22	2.10	0.41
1:A:188:VAL:CG2	2:B:167:VAL:HG21	2.48	0.41
2:B:296:ASN:HB3	2:B:338:TYR:CE1	2.56	0.41
3:C:277:THR:HA	3:C:308:ASN:OD1	2.21	0.41
3:F:291:ASP:O	3:F:302:LYS:HE2	2.21	0.41
2:E:180:GLN:HA	2:E:183:GLU:OE1	2.20	0.41
1:A:130:VAL:C	1:A:133:ILE:HG22	2.42	0.41
2:B:385:TRP:CD1	2:B:406:ARG:NH1	2.89	0.41
2:E:168:LEU:HD23	3:F:110:LEU:HD13	2.02	0.41
2:E:411:ASN:N	2:E:412:PRO:HD3	2.36	0.41
2:B:183:GLU:O	2:B:187:SER:HB2	2.21	0.41
2:E:245:GLU:O	2:E:246:ASN:HB2	2.21	0.41
2:B:309:GLU:OE1	2:B:325:HIS:HE1	2.04	0.41
2:E:415:ARG:H	2:E:434:GLY:H	1.69	0.41
2:B:408:HIS:O	4:H:1:GLY:N	2.53	0.41
2:E:321:LYS:HB3	2:E:321:LYS:HE2	1.89	0.40
2:B:238:VAL:HG21	2:B:250:THR:HG23	2.04	0.40
2:E:170:SER:OG	2:E:171:ILE:N	2.53	0.40
2:E:229:PRO:HG2	2:E:230:ASP:H	1.85	0.40
3:C:124:LEU:O	3:C:128:VAL:HG23	2.20	0.40
2:B:245:GLU:O	2:B:246:ASN:HB2	2.22	0.40
3:F:387:ILE:CD1	3:F:391:ARG:HG2	2.50	0.40
2:B:317:TRP:CE3	2:B:448:ARG:HD3	2.57	0.40
3:C:215:PHE:HA	7:C:408:HOH:O	2.20	0.40
2:E:244:THR:O	2:E:245:GLU:C	2.59	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:184:ILE:HA	3:C:189:ASN:O	2.22	0.40
3:C:206:LYS:HB3	3:C:210:GLN:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	62/66 (94%)	58 (94%)	4 (6%)	0	100	100
1	D	52/66 (79%)	46 (88%)	5 (10%)	1 (2%)	10	12
2	B	296/313 (95%)	265 (90%)	27 (9%)	4 (1%)	14	19
2	E	293/313 (94%)	275 (94%)	14 (5%)	4 (1%)	14	19
3	C	297/311 (96%)	274 (92%)	19 (6%)	4 (1%)	15	21
3	F	283/311 (91%)	264 (93%)	17 (6%)	2 (1%)	26	38
4	G	2/4 (50%)	2 (100%)	0	0	100	100
4	H	2/4 (50%)	2 (100%)	0	0	100	100
4	I	2/4 (50%)	2 (100%)	0	0	100	100
4	J	2/4 (50%)	2 (100%)	0	0	100	100
All	All	1291/1396 (92%)	1190 (92%)	86 (7%)	15 (1%)	16	23

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	281	ASP
2	B	399	GLY
3	C	393	THR
2	E	167	VAL
2	E	281	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	F	241	ALA
2	B	256	GLN
3	C	370	ALA
3	C	198	LEU
1	D	137	GLN
2	E	256	GLN
3	C	199	ASP
3	F	299	PRO
2	B	435	VAL
2	E	171	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	59/61 (97%)	58 (98%)	1 (2%)	68 85
1	D	50/61 (82%)	49 (98%)	1 (2%)	63 81
2	B	256/271 (94%)	247 (96%)	9 (4%)	43 64
2	E	253/271 (93%)	244 (96%)	9 (4%)	42 63
3	C	250/257 (97%)	238 (95%)	12 (5%)	31 49
3	F	237/257 (92%)	232 (98%)	5 (2%)	61 80
4	G	3/3 (100%)	3 (100%)	0	100 100
4	H	3/3 (100%)	3 (100%)	0	100 100
4	I	3/3 (100%)	3 (100%)	0	100 100
4	J	3/3 (100%)	3 (100%)	0	100 100
All	All	1117/1190 (94%)	1080 (97%)	37 (3%)	45 66

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	185	LEU
2	B	178	LYS
2	B	196	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	210	GLU
2	B	253	GLN
2	B	301	GLN
2	B	304	ARG
2	B	351	ASN
2	B	421	GLN
2	B	439	ASN
3	C	104	ASP
3	C	107	ILE
3	C	118	ASN
3	C	143	VAL
3	C	176	GLN
3	C	297	ASP
3	C	317	ASN
3	C	325	ASN
3	C	365	ASN
3	C	374	THR
3	C	382	THR
3	C	383	THR
1	D	176	LYS
2	E	190	MET
2	E	210	GLU
2	E	234	LYS
2	E	253	GLN
2	E	280	THR
2	E	301	GLN
2	E	346	ARG
2	E	351	ASN
2	E	359	GLN
3	F	177	GLN
3	F	317	ASN
3	F	325	ASN
3	F	365	ASN
3	F	383	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	GLN
1	A	139	ASN
1	A	184	GLN
1	A	187	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	189	GLN
2	B	202	ASN
2	B	253	GLN
2	B	271	GLN
2	B	296	ASN
2	B	301	GLN
2	B	325	HIS
2	B	339	GLN
2	B	351	ASN
2	B	421	GLN
2	B	439	ASN
3	C	111	GLN
3	C	115	ASN
3	C	117	ASN
3	C	118	ASN
3	C	119	GLN
3	C	134	GLN
3	C	136	GLN
3	C	163	GLN
3	C	176	GLN
3	C	177	GLN
3	C	230	ASN
3	C	239	GLN
3	C	254	ASN
3	C	307	HIS
3	C	317	ASN
3	C	319	ASN
3	C	325	ASN
3	C	350	GLN
3	C	361	ASN
3	C	365	ASN
1	D	143	GLN
1	D	182	GLN
1	D	184	GLN
2	E	189	GLN
2	E	202	ASN
2	E	253	GLN
2	E	271	GLN
2	E	296	ASN
2	E	301	GLN
2	E	339	GLN
2	E	351	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	359	GLN
2	E	408	HIS
2	E	421	GLN
2	E	439	ASN
3	F	111	GLN
3	F	115	ASN
3	F	117	ASN
3	F	118	ASN
3	F	119	GLN
3	F	123	ASN
3	F	130	GLN
3	F	144	GLN
3	F	176	GLN
3	F	230	ASN
3	F	239	GLN
3	F	254	ASN
3	F	307	HIS
3	F	317	ASN
3	F	319	ASN
3	F	325	ASN
3	F	350	GLN
3	F	365	ASN
4	G	2	HIS
4	I	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

6 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length

(or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	B	3	2,5	14,14,15	0.65	0	15,19,21	0.78	1 (6%)
5	NAG	B	4	5	14,14,15	0.62	0	15,19,21	0.70	0
5	FUC	B	5	5	10,10,11	0.53	0	14,14,16	0.65	0
5	NAG	E	3	2,5	14,14,15	0.63	0	15,19,21	1.25	2 (13%)
5	NAG	E	4	5	14,14,15	0.62	0	15,19,21	0.91	1 (6%)
5	FUC	E	5	5	10,10,11	0.59	0	14,14,16	0.89	2 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	B	3	2,5	-	0/6/23/26	0/1/1/1
5	NAG	B	4	5	-	0/6/23/26	0/1/1/1
5	FUC	B	5	5	-	0/0/17/20	0/1/1/1
5	NAG	E	3	2,5	-	0/6/23/26	0/1/1/1
5	NAG	E	4	5	-	0/6/23/26	0/1/1/1
5	FUC	E	5	5	-	0/0/17/20	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	4	NAG	C2-N2-C7	-2.52	119.80	123.04
5	B	3	NAG	C2-N2-C7	-2.44	119.91	123.04
5	E	3	NAG	C2-N2-C7	-2.42	119.92	123.04
5	E	5	FUC	C1-C2-C3	2.03	111.94	109.54
5	E	5	FUC	C1-O5-C5	2.21	115.80	112.38
5	E	3	NAG	C3-C4-C5	2.71	114.92	110.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	3	NAG	1	0
5	B	4	NAG	2	0
5	E	3	NAG	9	0
5	E	4	NAG	3	0
5	E	5	FUC	6	0

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	64/66 (96%)	0.73	8 (12%) 5 5	25, 65, 100, 107	0
1	D	54/66 (81%)	1.44	21 (38%) 0 0	29, 62, 112, 120	0
2	B	298/313 (95%)	0.03	6 (2%) 68 68	24, 42, 75, 105	0
2	E	295/313 (94%)	0.01	13 (4%) 38 39	18, 32, 70, 112	0
3	C	299/311 (96%)	0.32	19 (6%) 23 23	28, 47, 88, 104	0
3	F	285/311 (91%)	0.19	18 (6%) 23 24	23, 39, 79, 114	0
4	G	4/4 (100%)	1.73	1 (25%) 1 1	95, 98, 98, 99	0
4	H	4/4 (100%)	0.92	0 100 100	75, 78, 78, 82	0
4	I	4/4 (100%)	3.03	2 (50%) 0 0	82, 82, 85, 88	0
4	J	4/4 (100%)	0.03	0 100 100	40, 41, 41, 50	0
All	All	1311/1396 (93%)	0.24	88 (6%) 21 21	18, 41, 91, 120	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	394	ILE	7.2
1	D	140	VAL	6.6
4	I	4	PRO	6.5
3	F	393	THR	6.0
3	F	297	ASP	5.3
1	D	185	LEU	5.3
1	D	180	ASP	5.1
2	E	459	PRO	4.8
3	C	360	PRO	4.6
1	D	139	ASN	4.6
1	D	136	LEU	4.6
3	F	299	PRO	4.5
3	F	110	LEU	4.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	138	LYS	4.5
3	C	107	ILE	4.3
3	F	113	ILE	4.3
1	D	135	LEU	4.3
1	D	182	GLN	4.1
1	D	142	ALA	4.1
1	D	133	ILE	4.0
3	C	108	ARG	3.9
4	G	1	GLY	3.9
1	D	184	GLN	3.8
2	E	168	LEU	3.8
3	C	96	TYR	3.8
3	F	394	ILE	3.7
1	D	179	GLU	3.7
3	C	393	THR	3.6
2	E	169	ARG	3.6
1	A	127	ILE	3.4
1	D	176	LYS	3.4
1	D	141	ARG	3.4
1	D	186	GLU	3.2
3	F	363	TYR	3.2
2	B	163	THR	3.1
1	A	128	GLU	3.1
3	C	253	TRP	3.0
3	F	115	ASN	3.0
2	E	167	VAL	2.9
2	E	170	SER	2.9
3	C	357	ALA	2.9
1	A	189	ILE	2.9
1	D	183	LYS	2.9
3	C	172	LEU	2.8
4	I	2	HIS	2.8
1	D	137	GLN	2.8
1	A	133	ILE	2.8
3	C	254	ASN	2.8
2	E	166	ARG	2.8
3	F	111	GLN	2.8
2	B	458	PHE	2.7
2	B	281	ASP	2.7
2	B	168	LEU	2.7
1	A	185	LEU	2.6
3	F	114	TYR	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	E	171	ILE	2.6
1	D	175	LEU	2.6
2	E	458	PHE	2.6
1	A	131	GLN	2.6
3	F	361	ASN	2.6
2	E	175	LEU	2.5
3	C	105	SER	2.5
3	F	374	THR	2.4
1	D	134	GLN	2.4
3	F	296	GLY	2.4
1	A	130	VAL	2.4
1	A	132	HIS	2.4
3	C	106	SER	2.3
3	F	112	GLU	2.3
1	D	145	VAL	2.3
3	C	111	GLN	2.3
2	E	281	ASP	2.3
2	B	164	ASN	2.3
2	E	280	THR	2.2
3	C	109	TYR	2.2
3	F	357	ALA	2.2
2	E	173	GLU	2.2
3	C	359	THR	2.2
3	C	256	ARG	2.2
3	F	120	LYS	2.2
1	D	144	LEU	2.2
2	E	165	LEU	2.2
3	F	294	ASP	2.1
3	C	112	GLU	2.1
3	C	351	GLY	2.1
2	B	361	MET	2.1
3	C	377	TYR	2.1
3	F	123	ASN	2.0

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

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

6.3 Carbohydrates (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	NAG	B	3	14/15	0.76	0.30	2.87	89,94,100,103	0
5	NAG	E	3	14/15	0.87	0.20	0.39	60,64,73,77	0
5	FUC	E	5	10/11	0.91	0.24	-	72,73,74,74	0
5	NAG	B	4	14/15	0.74	0.41	-	106,108,108,109	0
5	FUC	B	5	10/11	0.77	0.34	-	101,101,102,102	0
5	NAG	E	4	14/15	0.70	0.34	-	80,83,86,87	0

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	CA	C	1	1/1	0.96	0.14	-0.36	49,49,49,49	0
6	CA	F	1	1/1	0.96	0.10	-1.58	40,40,40,40	0
6	CA	B	2	1/1	0.95	0.16	-	57,57,57,57	0
6	CA	E	2	1/1	0.91	0.15	-	40,40,40,40	0

6.5 Other polymers (i)

There are no such residues in this entry.