



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:58 PM GMT

PDB ID : 1RF1  
Title : Crystal Structure of Fragment D of gammaE132A Fibrinogen with the Peptide  
Ligand Gly-His-Arg-Pro-amide  
Authors : Kostelansky, M.S.; Gorkun, O.V.; Lord, S.T.  
Deposited on : 2003-11-07  
Resolution : 2.53 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](mailto: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.

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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) : 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

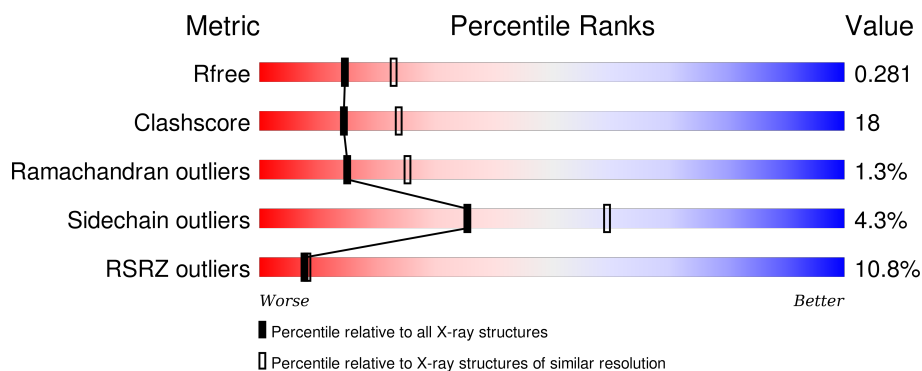
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.53 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	4241 (2.54-2.50)
Clashscore	102246	4968 (2.54-2.50)
Ramachandran outliers	100387	4873 (2.54-2.50)
Sidechain outliers	100360	4875 (2.54-2.50)
RSRZ outliers	91569	4253 (2.54-2.50)

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  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	66	<div> <div>24%</div> <div>53%</div> <div>36%</div> <div>8%</div> <div>.</div> </div>
1	D	66	<div> <div>30%</div> <div>42%</div> <div>39%</div> <div>15%</div> <div>.</div> </div>
2	B	313	<div> <div>7%</div> <div>68%</div> <div>27%</div> <div>.</div> <div>.</div> </div>
2	E	313	<div> <div>5%</div> <div>67%</div> <div>24%</div> <div>6%</div> <div>.</div> </div>
3	C	311	<div> <div>11%</div> <div>65%</div> <div>28%</div> <div>.</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	311	
4	G	4	
4	H	4	
4	I	4	
4	J	4	

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	E	3	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10928 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/alpha-E 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	56	Total	C	N	O	S	0	0	0
			458	280	87	88	3			

- Molecule 2 is a protein called Fibrinogen beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	299	Total	C	N	O	S	0	0	0
			2399	1499	423	455	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	298	Total	C	N	O	S	0	0	0
			2387	1515	402	459	11			
3	F	291	Total	C	N	O	S	0	0	0
			2332	1479	395	447	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	132	ALA	GLU	ENGINEERED	UNP P02679
F	132	ALA	GLU	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	0	0	0
			33	19	9	5			

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

- Molecule 5 is a polymer of unknown type called SUGAR (NAG-NAG-FUC).

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

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

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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	6	Total	O	0	0
			6	6		
7	B	51	Total	O	0	0
			51	51		
7	C	30	Total	O	0	0
			30	30		
7	D	11	Total	O	0	0
			11	11		
7	E	89	Total	O	0	0
			89	89		
7	F	60	Total	O	0	0
			60	60		

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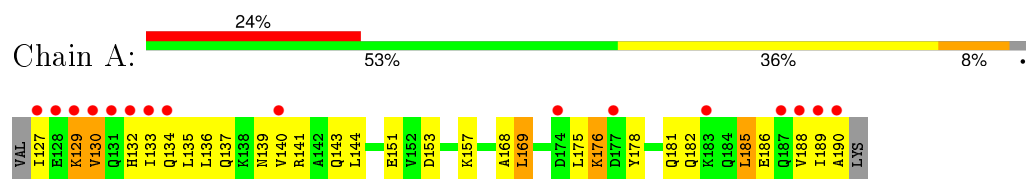
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	J	1	Total	O	0	0
			1	1		

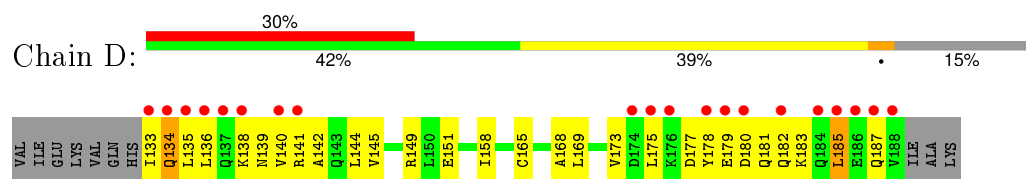
### 3 Residue-property plots [i](#)

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.

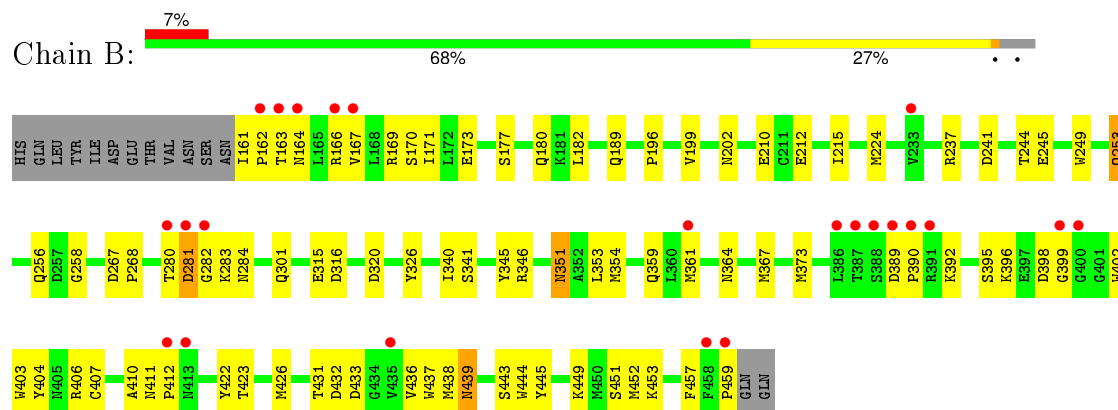
- Molecule 1: Fibrinogen alpha/alpha-E chain



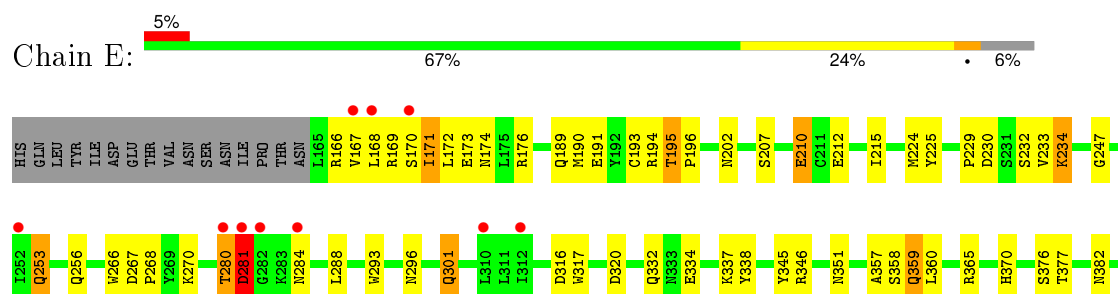
- Molecule 1: Fibrinogen alpha/alpha-E chain



- Molecule 2: Fibrinogen beta chain

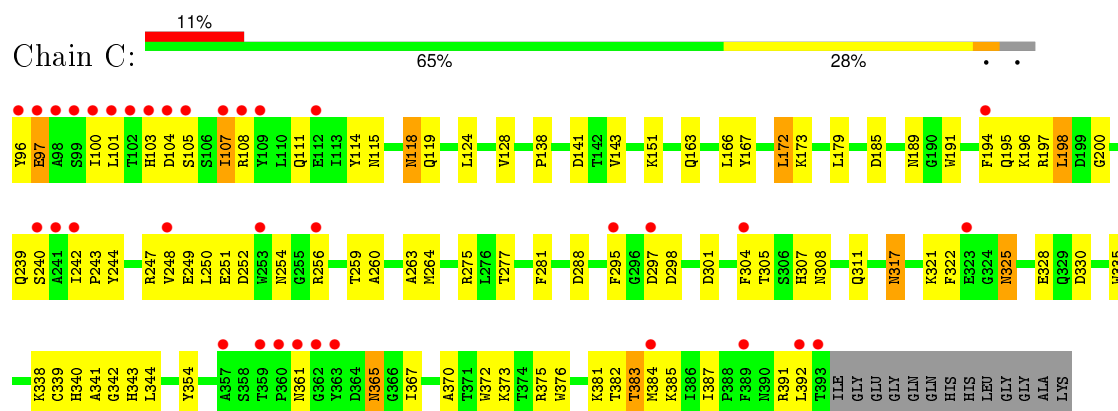


- Molecule 2: Fibrinogen beta chain

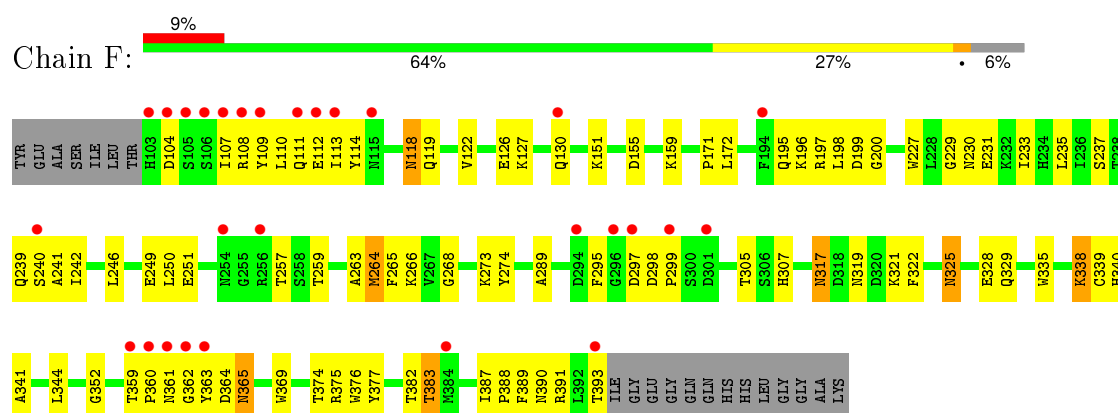




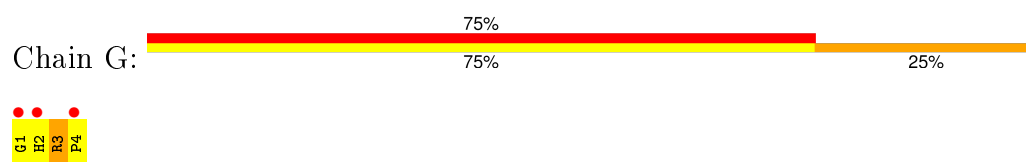
• Molecule 3: Fibrinogen gamma chain



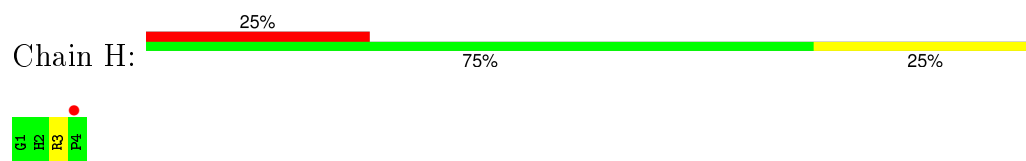
• Molecule 3: Fibrinogen gamma chain



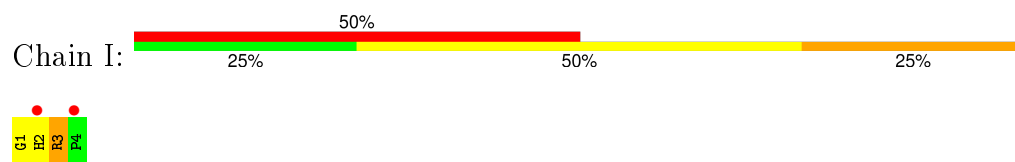
• Molecule 4: GHRP peptide



• Molecule 4: GHRP peptide



• Molecule 4: GHRP peptide





- Molecule 4: GHRP peptide

Chain J:  75% 25%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.71Å 94.68Å 228.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	17.97 – 2.53 35.02 – 2.53	Depositor EDS
% Data completeness (in resolution range)	99.9 (17.97-2.53) 99.7 (35.02-2.53)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.08 (at 2.54Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.234 , 0.281 0.235 , 0.281	Depositor DCC
$R_{free}$ test set	3316 reflections (5.07%)	DCC
Wilson B-factor (Å <sup>2</sup> )	33.2	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 47.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 65588 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	10928	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.33% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 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, 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	0.29	0/524	0.52	0/699
1	D	0.29	0/458	0.50	0/610
2	B	0.36	0/2461	0.61	0/3324
2	E	0.39	0/2430	0.65	1/3280 (0.0%)
3	C	0.36	0/2453	0.56	0/3319
3	F	0.39	0/2397	0.60	0/3242
4	G	0.52	0/34	0.51	0/43
4	H	0.46	0/34	0.52	0/43
4	I	0.47	0/34	0.41	0/43
4	J	0.49	0/34	0.51	0/43
All	All	0.37	0/10859	0.60	1/14646 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	399	GLY	N-CA-C	7.12	130.89	113.10

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	523	0	547	37	0
1	D	458	0	477	30	0
2	B	2399	0	2269	78	0
2	E	2369	0	2238	72	0
3	C	2387	0	2234	88	0
3	F	2332	0	2180	92	0
4	G	33	0	32	5	0
4	H	33	0	32	1	0
4	I	33	0	32	9	0
4	J	33	0	32	1	0
5	B	38	0	34	7	0
5	E	38	0	34	7	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	6	0	0	0	0
7	B	51	0	0	3	0
7	C	30	0	0	2	0
7	D	11	0	0	0	0
7	E	89	0	0	1	0
7	F	60	0	0	2	0
7	J	1	0	0	0	0
All	All	10928	0	10141	375	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 18.

All (375) 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:168:LEU:HD23	3:F:110:LEU:HD13	1.45	0.97
2:E:358:SER:HA	2:E:365:ARG:HH12	1.37	0.88
2:E:359:GLN:H	2:E:359:GLN:HE21	1.19	0.88
3:F:151:LYS:HB3	3:F:239:GLN:HE22	1.41	0.85
3:C:172:LEU:H	3:C:172:LEU:HD23	1.44	0.82
1:D:134:GLN:NE2	1:D:134:GLN:H	1.77	0.81
1:A:127:ILE:HG12	1:A:130:VAL:HG23	1.61	0.81
3:F:113:ILE:HD12	3:F:114:TYR:N	1.97	0.79
1:D:139:ASN:HB3	3:F:114:TYR:CZ	2.19	0.78
2:E:359:GLN:H	2:E:359:GLN:NE2	1.82	0.77
2:B:439:ASN:HD22	2:B:439:ASN:H	1.29	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:3:NAG:H61	5:E:5:FUC:H5	1.66	0.76
1:A:143:GLN:HE21	3:C:118:ASN:ND2	1.83	0.76
3:C:249:GLU:HB2	3:C:383:THR:HG23	1.66	0.76
2:B:389:ASP:HB3	2:B:392:LYS:HG3	1.67	0.76
3:C:197:ARG:HB2	3:C:382:THR:HB	1.67	0.75
1:A:140:VAL:HG23	1:A:185:LEU:HD11	1.69	0.75
3:F:249:GLU:HB2	3:F:383:THR:HG23	1.69	0.74
2:E:202:ASN:HD22	2:E:284:ASN:HD22	1.35	0.74
2:B:423:THR:H	2:B:426:MET:HE3	1.53	0.74
2:E:439:ASN:H	2:E:439:ASN:HD22	1.35	0.74
3:C:325:ASN:HD22	3:C:325:ASN:C	1.90	0.73
3:F:249:GLU:HG2	3:F:259:THR:HG22	1.70	0.73
2:B:359:GLN:HE22	2:B:438:MET:HB3	1.54	0.73
2:E:457:PHE:O	2:E:459:PRO:HD3	1.89	0.72
2:E:234:LYS:H	2:E:234:LYS:HD2	1.55	0.72
2:E:172:LEU:HD13	3:F:113:ILE:HD11	1.72	0.71
2:E:423:THR:N	2:E:426:MET:HE3	2.06	0.70
2:E:358:SER:HA	2:E:365:ARG:NH1	2.07	0.70
2:E:406:ARG:NH1	4:J:3:ARG:O	2.25	0.69
2:B:202:ASN:ND2	2:B:284:ASN:HB2	2.07	0.69
3:F:325:ASN:HD22	3:F:325:ASN:C	1.96	0.69
2:E:230:ASP:OD2	2:E:232:SER:HB2	1.93	0.69
3:F:108:ARG:HA	3:F:111:GLN:HE21	1.55	0.69
3:F:365:ASN:HD22	3:F:365:ASN:H	1.41	0.69
2:B:316:ASP:OD2	2:B:320:ASP:HB2	1.92	0.69
3:C:252:ASP:OD2	3:C:256:ARG:HB2	1.92	0.69
3:C:307:HIS:CE1	3:C:341:ALA:H	2.11	0.68
1:D:179:GLU:O	1:D:183:LYS:HG3	1.93	0.68
5:B:3:NAG:H4	5:B:4:NAG:HN2	1.58	0.68
3:C:387:ILE:HD11	3:C:391:ARG:HG2	1.75	0.68
2:B:423:THR:N	2:B:426:MET:HE3	2.09	0.67
2:E:280:THR:HG23	2:E:288:LEU:HG	1.77	0.66
3:F:151:LYS:HD3	3:F:172:LEU:HD21	1.75	0.66
2:B:202:ASN:HD22	2:B:284:ASN:HB2	1.61	0.66
1:D:133:ILE:HD11	3:F:107:ILE:HD12	1.78	0.66
3:F:338:LYS:N	3:F:339:CYS:HA	2.09	0.66
1:A:169:LEU:H	2:B:189:GLN:NE2	1.93	0.66
1:A:169:LEU:H	2:B:189:GLN:HE22	1.43	0.66
2:B:361:MET:HB2	5:B:3:NAG:H81	1.77	0.65
3:F:307:HIS:HE1	3:F:341:ALA:H	1.45	0.65
3:C:101:LEU:HD12	3:C:101:LEU:H	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:172:LEU:H	3:F:239:GLN:HE21	1.45	0.65
3:C:307:HIS:HE1	3:C:341:ALA:H	1.45	0.65
2:E:234:LYS:H	2:E:234:LYS:CD	2.10	0.63
3:C:101:LEU:HD12	3:C:101:LEU:N	2.14	0.63
3:C:195:GLN:OE1	3:C:382:THR:HG22	1.99	0.63
3:F:118:ASN:O	3:F:122:VAL:HG23	1.99	0.63
3:C:295:PHE:HE2	3:C:305:THR:HG21	1.62	0.63
2:B:163:THR:HA	2:B:166:ARG:HD2	1.80	0.62
3:F:325:ASN:ND2	3:F:328:GLU:H	1.97	0.62
2:B:345:TYR:HB2	2:B:354:MET:CE	2.30	0.62
2:E:406:ARG:N	2:E:407:CYS:HA	2.13	0.62
3:C:295:PHE:HB2	3:C:301:ASP:OD2	1.99	0.62
2:E:345:TYR:O	2:E:346:ARG:HG3	1.99	0.62
3:C:105:SER:HA	3:C:108:ARG:HH21	1.63	0.62
2:B:351:ASN:C	2:B:351:ASN:HD22	2.00	0.62
2:E:439:ASN:N	2:E:439:ASN:HD22	1.97	0.62
5:E:3:NAG:H61	5:E:5:FUC:H3	1.80	0.62
3:C:151:LYS:HB3	3:C:239:GLN:HE22	1.65	0.62
3:C:119:GLN:HA	3:C:119:GLN:HE21	1.65	0.61
3:F:240:SER:O	3:F:242:ILE:HG13	2.00	0.61
3:F:307:HIS:HD2	3:F:335:TRP:O	1.82	0.61
2:E:270:LYS:HE2	2:E:334:GLU:OE1	2.00	0.61
2:B:439:ASN:HD22	2:B:439:ASN:N	1.98	0.61
1:D:173:VAL:HG12	1:D:175:LEU:HD22	1.83	0.61
2:B:253:GLN:NE2	2:B:451:SER:HA	2.16	0.60
3:C:251:GLU:HB3	3:C:381:LYS:HB2	1.81	0.60
1:A:188:VAL:HG21	2:B:167:VAL:HG21	1.83	0.60
3:C:104:ASP:O	3:C:107:ILE:HG22	2.01	0.60
5:E:3:NAG:H61	5:E:5:FUC:C5	2.32	0.60
2:B:359:GLN:NE2	2:B:438:MET:HB3	2.17	0.59
1:A:132:HIS:HB3	3:C:107:ILE:HD11	1.84	0.59
1:A:135:LEU:HG	1:A:139:ASN:ND2	2.17	0.59
1:A:185:LEU:HD22	1:A:189:ILE:HD11	1.82	0.59
2:B:351:ASN:ND2	2:B:354:MET:H	2.01	0.59
2:E:210:GLU:OE1	2:E:212:GLU:HB3	2.03	0.59
3:F:321:LYS:O	3:F:338:LYS:HD3	2.02	0.59
1:A:178:TYR:O	1:A:182:GLN:HG3	2.03	0.58
3:C:325:ASN:ND2	3:C:328:GLU:H	2.00	0.58
1:D:169:LEU:H	2:E:189:GLN:HE22	1.49	0.58
2:B:161:ILE:HB	2:B:162:PRO:HD3	1.84	0.58
3:C:108:ARG:HA	3:C:111:GLN:HE21	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:LYS:HE3	3:C:100:ILE:HG23	1.85	0.58
2:E:229:PRO:HB2	2:E:301:GLN:HE22	1.67	0.58
3:C:307:HIS:HE1	3:C:342:GLY:H	1.52	0.58
2:E:212:GLU:O	2:E:215:ILE:HG22	2.04	0.58
3:C:103:HIS:O	3:C:107:ILE:HB	2.04	0.57
3:F:389:PHE:C	3:F:391:ARG:H	2.07	0.57
2:B:457:PHE:O	2:B:459:PRO:HD3	2.04	0.57
3:C:340:HIS:O	4:G:1:GLY:HA2	2.04	0.57
3:F:197:ARG:HB2	3:F:382:THR:HB	1.85	0.57
3:C:295:PHE:CE2	3:C:305:THR:HG21	2.39	0.57
3:C:119:GLN:HA	3:C:119:GLN:NE2	2.19	0.57
2:E:293:TRP:HE1	2:E:296:ASN:ND2	2.03	0.57
3:C:307:HIS:CE1	3:C:342:GLY:H	2.23	0.57
1:D:177:ASP:O	1:D:181:GLN:HG3	2.04	0.56
1:A:188:VAL:CG2	2:B:167:VAL:HG21	2.35	0.56
3:F:200:GLY:HA2	7:F:408:HOH:O	2.05	0.56
3:C:200:GLY:HA2	7:C:408:HOH:O	2.05	0.56
2:B:282:GLY:O	2:B:283:LYS:HG2	2.05	0.56
3:C:281:PHE:HB2	3:C:288:ASP:OD2	2.05	0.56
1:D:169:LEU:H	2:E:189:GLN:NE2	2.04	0.56
3:C:361:ASN:N	3:C:361:ASN:HD22	2.03	0.56
2:B:316:ASP:HB2	2:B:445:TYR:OH	2.06	0.56
3:F:322:PHE:HB2	3:F:338:LYS:HG3	1.88	0.56
3:C:172:LEU:CD2	3:C:172:LEU:H	2.10	0.56
3:C:101:LEU:H	3:C:101:LEU:CD1	2.19	0.56
2:B:345:TYR:CG	2:B:346:ARG:N	2.74	0.55
3:F:322:PHE:CZ	4:I:3:ARG:HG2	2.42	0.55
1:A:168:ALA:HA	2:B:189:GLN:HE22	1.71	0.55
1:A:135:LEU:HG	1:A:139:ASN:HD21	1.72	0.55
1:A:176:LYS:HB2	1:A:176:LYS:NZ	2.22	0.55
1:A:144:LEU:HD13	1:A:182:GLN:HG2	1.89	0.55
3:F:227:TRP:HZ2	3:F:230:ASN:HD21	1.53	0.55
3:F:196:LYS:NZ	3:F:383:THR:HB	2.22	0.54
1:D:133:ILE:HD11	3:F:107:ILE:HG23	1.88	0.54
2:E:191:GLU:HA	2:E:194:ARG:HD3	1.89	0.54
3:C:307:HIS:HD2	3:C:335:TRP:O	1.90	0.54
1:A:176:LYS:HB2	1:A:176:LYS:HZ3	1.73	0.54
2:B:267:ASP:HB3	2:B:268:PRO:HD3	1.88	0.54
3:C:96:TYR:CG	3:C:97:GLU:N	2.76	0.54
3:F:344:LEU:HB3	3:F:382:THR:HG21	1.89	0.54
2:E:195:THR:HG22	2:E:196:PRO:HD2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:365:ASN:N	3:F:365:ASN:HD22	2.03	0.53
3:C:305:THR:HB	3:C:341:ALA:HB2	1.91	0.53
3:F:195:GLN:OE1	3:F:382:THR:HG22	2.08	0.53
1:A:136:LEU:HD21	3:C:111:GLN:HG2	1.91	0.53
1:D:140:VAL:HG23	1:D:141:ARG:N	2.24	0.53
1:D:140:VAL:HG23	1:D:141:ARG:H	1.74	0.53
2:E:337:LYS:HG2	2:E:382:ASN:ND2	2.24	0.53
2:E:171:ILE:HG13	2:E:172:LEU:N	2.24	0.53
5:B:3:NAG:C4	5:B:4:NAG:HN2	2.22	0.53
3:F:172:LEU:HD22	3:F:172:LEU:H	1.75	0.52
3:C:338:LYS:N	3:C:339:CYS:HA	2.23	0.52
3:F:307:HIS:CE1	3:F:341:ALA:H	2.26	0.52
3:F:119:GLN:HA	3:F:119:GLN:NE2	2.23	0.52
2:E:357:ALA:O	2:E:365:ARG:HG3	2.09	0.52
3:C:107:ILE:O	3:C:107:ILE:HD13	2.10	0.52
2:B:253:GLN:HE22	2:B:451:SER:HA	1.75	0.52
2:B:432:ASP:OD2	2:B:443:SER:HB2	2.08	0.52
3:F:171:PRO:HA	3:F:239:GLN:NE2	2.25	0.52
3:F:340:HIS:O	4:I:1:GLY:HA3	2.10	0.52
1:D:151:GLU:HG2	1:D:173:VAL:HG13	1.92	0.52
3:F:229:GLY:O	3:F:233:ILE:HG13	2.10	0.52
2:B:373:MET:HE2	2:B:404:TYR:O	2.10	0.51
5:E:3:NAG:H61	5:E:5:FUC:C3	2.40	0.51
1:A:175:LEU:HD22	1:A:175:LEU:H	1.76	0.51
2:B:432:ASP:N	2:B:432:ASP:OD1	2.43	0.51
2:B:410:ALA:C	2:B:412:PRO:HD3	2.31	0.51
5:E:3:NAG:C6	5:E:5:FUC:H5	2.36	0.51
2:B:244:THR:HG22	2:B:245:GLU:HG3	1.92	0.51
1:D:144:LEU:HD13	1:D:182:GLN:HG2	1.93	0.51
3:F:352:GLY:O	3:F:377:TYR:HA	2.10	0.51
3:C:259:THR:HG22	3:C:260:ALA:N	2.26	0.51
2:E:436:VAL:HG12	2:E:437:TRP:N	2.25	0.51
1:D:178:TYR:O	1:D:182:GLN:HG3	2.11	0.51
2:E:415:ARG:HD3	7:E:484:HOH:O	2.11	0.51
1:A:181:GLN:NE2	2:B:171:ILE:HG23	2.27	0.50
3:C:243:PRO:HG2	7:C:435:HOH:O	2.11	0.50
2:E:253:GLN:HB3	2:E:452:MET:HB2	1.93	0.50
2:B:361:MET:HB2	5:B:3:NAG:C8	2.41	0.50
2:B:367:MET:HB2	2:B:406:ARG:HB3	1.93	0.50
2:B:163:THR:HG22	2:B:166:ARG:NH1	2.26	0.50
2:E:172:LEU:HB3	3:F:113:ILE:CD1	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:423:THR:H	2:E:426:MET:HE3	1.75	0.50
2:B:457:PHE:CE2	2:B:459:PRO:HG3	2.46	0.50
2:B:436:VAL:HG12	2:B:437:TRP:N	2.27	0.50
3:C:108:ARG:HA	3:C:111:GLN:NE2	2.27	0.50
2:B:258:GLY:HA2	7:B:463:HOH:O	2.10	0.50
3:F:108:ARG:O	3:F:111:GLN:HG2	2.12	0.50
3:F:389:PHE:O	3:F:391:ARG:N	2.45	0.50
3:F:249:GLU:O	3:F:250:LEU:HD13	2.12	0.50
2:E:253:GLN:NE2	2:E:451:SER:HA	2.27	0.50
3:C:344:LEU:HA	3:C:367:ILE:HG23	1.94	0.49
3:F:389:PHE:C	3:F:391:ARG:N	2.66	0.49
2:E:436:VAL:CG1	2:E:437:TRP:N	2.74	0.49
3:C:365:ASN:HD22	3:C:365:ASN:H	1.60	0.49
2:B:167:VAL:O	2:B:170:SER:HB3	2.12	0.49
1:D:185:LEU:HD13	1:D:185:LEU:O	2.12	0.49
1:D:168:ALA:HA	2:E:189:GLN:HE22	1.77	0.49
2:E:316:ASP:OD2	2:E:320:ASP:HB2	2.12	0.49
2:E:172:LEU:HD22	3:F:113:ILE:CD1	2.43	0.49
1:D:133:ILE:HD11	3:F:107:ILE:CG2	2.43	0.49
3:C:166:LEU:HB3	3:C:179:LEU:HD11	1.94	0.49
4:G:2:HIS:CD2	4:G:4:PRO:HD3	2.47	0.49
3:C:249:GLU:CB	3:C:383:THR:HG23	2.40	0.49
2:E:266:TRP:HA	2:E:377:THR:HG21	1.95	0.49
3:F:273:LYS:HE3	3:F:319:ASN:HD21	1.78	0.49
3:F:339:CYS:HB2	4:I:1:GLY:O	2.13	0.49
2:B:224:MET:CE	2:B:237:ARG:HD3	2.43	0.49
2:B:326:TYR:CE2	2:B:353:LEU:HD12	2.48	0.49
3:C:240:SER:O	3:C:242:ILE:HG13	2.12	0.49
3:C:107:ILE:O	3:C:111:GLN:HG3	2.14	0.48
1:A:175:LEU:HD22	1:A:175:LEU:N	2.29	0.48
3:C:361:ASN:N	3:C:361:ASN:ND2	2.60	0.48
5:E:3:NAG:C6	5:E:4:NAG:H2	2.43	0.48
2:B:351:ASN:ND2	2:B:354:MET:HB2	2.28	0.48
3:C:263:ALA:HB1	3:C:264:MET:CE	2.44	0.48
2:B:364:ASN:HD22	5:B:3:NAG:H82	1.79	0.48
2:B:280:THR:O	2:B:281:ASP:C	2.52	0.48
2:E:317:TRP:CE3	2:E:448:ARG:HD3	2.48	0.48
3:F:151:LYS:HD3	3:F:172:LEU:CD2	2.44	0.48
3:C:325:ASN:ND2	3:C:325:ASN:C	2.63	0.48
5:B:3:NAG:H4	5:B:5:FUC:H5	1.95	0.48
2:B:326:TYR:HE1	2:B:354:MET:HE2	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:175:LEU:N	1:D:175:LEU:HD22	2.29	0.48
2:B:406:ARG:N	2:B:407:CYS:HA	2.26	0.48
3:C:297:ASP:HB3	4:G:2:HIS:NE2	2.28	0.48
3:F:375:ARG:HH22	4:I:2:HIS:CD2	2.31	0.48
3:C:321:LYS:O	3:C:338:LYS:HD3	2.14	0.48
3:F:127:LYS:HA	3:F:130:GLN:NE2	2.28	0.48
1:D:135:LEU:HD13	1:D:139:ASN:ND2	2.29	0.47
2:E:171:ILE:HG13	2:E:172:LEU:H	1.79	0.47
1:A:129:LYS:NZ	1:A:129:LYS:HB3	2.29	0.47
2:B:439:ASN:ND2	2:B:439:ASN:N	2.61	0.47
2:E:234:LYS:HD2	2:E:234:LYS:N	2.26	0.47
3:F:237:SER:HB2	3:F:266:LYS:HA	1.96	0.47
3:F:365:ASN:ND2	3:F:365:ASN:H	2.11	0.47
1:A:182:GLN:O	1:A:186:GLU:HG2	2.14	0.47
3:F:359:THR:HG21	3:F:363:TYR:O	2.14	0.47
3:F:196:LYS:HD2	3:F:383:THR:HB	1.96	0.47
3:C:317:ASN:HD22	3:C:317:ASN:C	2.18	0.47
3:C:322:PHE:CZ	4:G:3:ARG:HG2	2.50	0.47
3:C:247:ARG:NH2	3:C:392:LEU:HD11	2.30	0.47
3:F:155:ASP:O	3:F:159:LYS:HG3	2.15	0.47
2:E:439:ASN:N	2:E:439:ASN:ND2	2.61	0.47
2:E:411:ASN:N	2:E:412:PRO:HD3	2.29	0.47
3:C:275:ARG:HA	3:C:311:GLN:HA	1.97	0.47
3:C:195:GLN:HB3	3:C:384:MET:HB2	1.96	0.46
2:B:351:ASN:HD21	2:B:354:MET:HB2	1.80	0.46
1:A:136:LEU:O	1:A:140:VAL:HG22	2.14	0.46
1:A:133:ILE:O	1:A:137:GLN:HG3	2.14	0.46
1:D:158:ILE:HG23	2:E:189:GLN:HE21	1.80	0.46
5:B:4:NAG:C7	5:B:4:NAG:O3	2.63	0.46
2:B:406:ARG:O	2:B:406:ARG:HG2	2.16	0.46
1:D:140:VAL:HG12	2:E:172:LEU:HD21	1.96	0.46
3:C:254:ASN:HB2	3:C:256:ARG:NH1	2.29	0.46
3:F:339:CYS:N	4:I:1:GLY:O	2.45	0.46
3:F:295:PHE:HE2	3:F:305:THR:HG21	1.80	0.46
2:B:402:TRP:CG	2:B:403:TRP:N	2.83	0.46
1:D:136:LEU:O	1:D:140:VAL:HG22	2.16	0.46
2:B:390:PRO:O	2:B:396:LYS:HE3	2.16	0.46
2:E:191:GLU:HG2	2:E:194:ARG:HH11	1.81	0.46
3:C:304:PHE:CD1	3:C:338:LYS:HE3	2.51	0.46
3:C:124:LEU:O	3:C:128:VAL:HG23	2.15	0.46
2:E:357:ALA:HB3	2:E:360:LEU:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:259:THR:CG2	3:C:260:ALA:N	2.79	0.45
2:E:172:LEU:HB3	3:F:113:ILE:HD13	1.97	0.45
3:F:365:ASN:ND2	3:F:365:ASN:N	2.64	0.45
1:A:151:GLU:OE2	2:B:182:LEU:HD21	2.16	0.45
3:C:101:LEU:N	3:C:101:LEU:CD1	2.79	0.45
3:C:185:ASP:OD2	3:C:189:ASN:HB2	2.15	0.45
3:C:151:LYS:HB3	3:C:239:GLN:NE2	2.29	0.45
3:F:387:ILE:HD11	3:F:391:ARG:HG2	1.97	0.45
1:D:181:GLN:HE22	2:E:174:ASN:HD21	1.64	0.45
1:D:135:LEU:C	1:D:135:LEU:HD13	2.37	0.45
2:E:202:ASN:ND2	2:E:284:ASN:HB2	2.32	0.45
2:B:395:SER:HA	2:B:404:TYR:CE2	2.51	0.45
2:B:241:ASP:HB3	2:B:249:TRP:HB2	1.99	0.45
2:E:233:VAL:HG22	2:E:234:LYS:HD2	1.99	0.45
1:A:153:ASP:O	1:A:157:LYS:HG2	2.16	0.45
1:D:139:ASN:O	1:D:142:ALA:HB3	2.15	0.45
1:A:127:ILE:HG12	1:A:130:VAL:CG2	2.40	0.45
5:E:3:NAG:H62	5:E:4:NAG:H2	1.98	0.45
2:E:281:ASP:OD2	2:E:281:ASP:N	2.50	0.45
3:C:196:LYS:O	3:C:197:ARG:HD2	2.17	0.45
2:B:169:ARG:O	2:B:173:GLU:HG3	2.17	0.45
3:C:354:TYR:CE1	3:C:376:TRP:HA	2.51	0.45
3:F:268:GLY:O	3:F:274:TYR:HA	2.17	0.45
2:B:161:ILE:N	2:B:162:PRO:HD2	2.32	0.44
2:E:207:SER:HB3	7:F:461:HOH:O	2.16	0.44
3:C:340:HIS:N	4:G:1:GLY:O	2.45	0.44
1:A:127:ILE:HD11	1:A:129:LYS:HG2	1.99	0.44
1:D:141:ARG:O	1:D:145:VAL:HG23	2.17	0.44
2:B:411:ASN:N	2:B:412:PRO:HD3	2.33	0.44
3:F:246:LEU:HD22	3:F:265:PHE:CE1	2.52	0.44
3:F:325:ASN:ND2	3:F:325:ASN:C	2.66	0.44
2:B:177:SER:O	2:B:180:GLN:HB3	2.17	0.44
2:B:199:VAL:HG23	3:C:141:ASP:HA	1.99	0.44
2:B:351:ASN:C	2:B:351:ASN:ND2	2.71	0.44
3:F:329:GLN:OE1	4:I:3:ARG:HD3	2.18	0.44
3:F:393:THR:HG22	3:F:393:THR:O	2.18	0.44
1:A:188:VAL:C	1:A:190:ALA:H	2.21	0.44
3:C:248:VAL:HG12	3:C:250:LEU:CD2	2.48	0.44
3:F:196:LYS:HZ2	3:F:383:THR:CG2	2.32	0.43
2:B:422:TYR:CE1	2:B:444:TRP:HA	2.53	0.43
3:F:375:ARG:NH2	4:I:2:HIS:CD2	2.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:354:TYR:O	3:C:376:TRP:HB3	2.18	0.43
3:C:194:PHE:C	3:C:194:PHE:CD1	2.92	0.43
3:F:263:ALA:HB1	3:F:264:MET:CE	2.48	0.43
3:C:167:TYR:O	3:C:179:LEU:HD12	2.18	0.43
1:A:134:GLN:HA	1:A:137:GLN:OE1	2.17	0.43
2:E:332:GLN:O	2:E:338:TYR:HA	2.19	0.43
3:F:172:LEU:CD2	3:F:239:GLN:NE2	2.81	0.43
2:E:169:ARG:HH12	3:F:109:TYR:HE2	1.61	0.43
2:E:173:GLU:HG2	2:E:176:ARG:NH2	2.33	0.43
3:F:231:GLU:O	3:F:235:LEU:HG	2.18	0.43
1:A:129:LYS:HE3	3:C:100:ILE:CG2	2.49	0.43
2:B:253:GLN:HB3	2:B:452:MET:HB2	2.01	0.43
3:F:374:THR:HG22	3:F:376:TRP:H	1.83	0.43
2:B:351:ASN:O	2:B:351:ASN:ND2	2.51	0.43
7:B:506:HOH:O	3:C:138:PRO:HG3	2.18	0.43
2:E:253:GLN:HE21	2:E:253:GLN:C	2.23	0.42
3:F:297:ASP:HB3	4:I:2:HIS:CE1	2.54	0.42
3:C:114:TYR:CD2	3:C:115:ASN:ND2	2.87	0.42
3:F:109:TYR:C	3:F:111:GLN:H	2.22	0.42
2:B:315:GLU:HB3	2:B:449:LYS:HB2	2.00	0.42
3:F:298:ASP:HA	3:F:299:PRO:HD3	1.89	0.42
2:B:163:THR:HA	2:B:166:ARG:CD	2.47	0.42
2:B:162:PRO:C	2:B:164:ASN:N	2.72	0.42
2:B:212:GLU:O	2:B:215:ILE:HG22	2.19	0.42
3:C:173:LYS:HE3	3:C:173:LYS:HB2	1.80	0.42
3:F:289:ALA:HB3	3:F:369:TRP:CE2	2.54	0.42
3:C:365:ASN:ND2	3:C:365:ASN:H	2.17	0.42
3:C:250:LEU:N	3:C:250:LEU:HD22	2.35	0.42
1:A:140:VAL:HG23	1:A:141:ARG:N	2.34	0.42
2:B:315:GLU:HA	2:B:320:ASP:O	2.20	0.42
3:F:340:HIS:CE1	4:I:1:GLY:HA2	2.54	0.42
2:B:345:TYR:O	2:B:346:ARG:HB3	2.20	0.42
3:F:172:LEU:HD22	3:F:239:GLN:NE2	2.34	0.42
3:F:251:GLU:HG3	3:F:257:THR:HG22	2.00	0.42
2:E:422:TYR:HA	2:E:426:MET:CE	2.49	0.42
3:F:172:LEU:HD22	3:F:239:GLN:HE21	1.85	0.41
3:F:387:ILE:HG12	3:F:388:PRO:HD2	2.01	0.41
2:E:166:ARG:O	2:E:168:LEU:N	2.53	0.41
2:B:453:LYS:HG3	7:B:467:HOH:O	2.19	0.41
1:D:165:CYS:HB3	2:E:193:CYS:HA	2.03	0.41
2:E:224:MET:HG2	2:E:225:TYR:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:134:GLN:O	1:D:138:LYS:HE2	2.19	0.41
3:C:191:TRP:CE3	3:C:385:LYS:HG3	2.55	0.41
3:C:172:LEU:CD2	3:C:239:GLN:HE21	2.33	0.41
3:F:364:ASP:OD1	3:F:375:ARG:HB2	2.20	0.41
2:E:402:TRP:CG	2:E:403:TRP:N	2.89	0.41
1:D:149:ARG:HH21	2:E:425:ASP:HA	1.83	0.41
2:B:398:ASP:HA	2:B:433:ASP:HB3	2.02	0.41
3:F:113:ILE:C	3:F:113:ILE:HD12	2.39	0.41
2:B:431:THR:HG21	4:H:3:ARG:NH2	2.36	0.41
3:F:239:GLN:O	3:F:240:SER:C	2.58	0.41
3:F:104:ASP:O	3:F:108:ARG:HG3	2.19	0.41
1:A:169:LEU:N	2:B:189:GLN:HE22	2.14	0.41
3:C:263:ALA:HB1	3:C:264:MET:HE1	2.03	0.41
2:E:376:SER:O	2:E:401:GLY:HA2	2.21	0.41
3:C:372:TRP:C	3:C:373:LYS:HG2	2.41	0.41
3:F:198:LEU:HD12	3:F:199:ASP:N	2.36	0.41
1:A:136:LEU:O	1:A:140:VAL:HG13	2.21	0.41
3:F:317:ASN:ND2	3:F:319:ASN:OD1	2.53	0.41
3:F:359:THR:OG1	3:F:362:GLY:HA2	2.21	0.41
2:E:172:LEU:HD22	3:F:113:ILE:HD11	2.03	0.41
3:F:122:VAL:O	3:F:126:GLU:HG3	2.21	0.41
2:E:346:ARG:HG3	2:E:346:ARG:HH11	1.84	0.41
3:C:343:HIS:O	3:C:367:ILE:HA	2.20	0.41
3:F:295:PHE:CE2	3:F:305:THR:HG21	2.55	0.41
1:A:127:ILE:N	1:A:130:VAL:HB	2.36	0.40
3:C:295:PHE:CD1	3:C:375:ARG:HD2	2.56	0.40
1:D:181:GLN:HE22	2:E:174:ASN:ND2	2.19	0.40
2:B:436:VAL:CG1	2:B:437:TRP:N	2.83	0.40
2:E:370:HIS:CE1	2:E:408:HIS:HB2	2.56	0.40
2:B:340:ILE:HG12	2:B:341:SER:N	2.36	0.40
3:F:387:ILE:CD1	3:F:391:ARG:HG2	2.51	0.40
3:C:96:TYR:O	3:C:97:GLU:HB2	2.20	0.40
3:C:277:THR:HA	3:C:308:ASN:OD1	2.22	0.40
2:B:389:ASP:HA	2:B:390:PRO:HD2	1.96	0.40
1:A:189:ILE:O	1:A:189:ILE:HG22	2.22	0.40
2:E:267:ASP:HB3	2:E:268:PRO:HD3	2.03	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	62/66 (94%)	54 (87%)	7 (11%)	1 (2%)	12	20
1	D	54/66 (82%)	51 (94%)	3 (6%)	0	100	100
2	B	297/313 (95%)	266 (90%)	28 (9%)	3 (1%)	19	33
2	E	293/313 (94%)	269 (92%)	18 (6%)	6 (2%)	9	14
3	C	296/311 (95%)	273 (92%)	20 (7%)	3 (1%)	19	33
3	F	289/311 (93%)	264 (91%)	21 (7%)	4 (1%)	14	23
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	1299/1396 (93%)	1185 (91%)	97 (8%)	17 (1%)	15	25

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	97	GLU
2	E	170	SER
2	E	281	ASP
2	B	281	ASP
3	C	198	LEU
3	F	241	ALA
3	F	360	PRO
3	F	390	ASN
2	E	167	VAL
2	B	256	GLN
3	C	370	ALA
2	E	256	GLN
3	F	338	LYS
2	E	171	ILE

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Mol	Chain	Res	Type
2	B	399	GLY
1	A	130	VAL
2	E	247	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	59/61 (97%)	55 (93%)	4 (7%)	20	35
1	D	52/61 (85%)	48 (92%)	4 (8%)	16	29
2	B	257/271 (95%)	251 (98%)	6 (2%)	58	83
2	E	253/271 (93%)	242 (96%)	11 (4%)	35	59
3	C	250/258 (97%)	237 (95%)	13 (5%)	29	49
3	F	244/258 (95%)	236 (97%)	8 (3%)	45	71
4	G	3/3 (100%)	2 (67%)	1 (33%)	0	0
4	H	3/3 (100%)	3 (100%)	0	100	100
4	I	3/3 (100%)	2 (67%)	1 (33%)	0	0
4	J	3/3 (100%)	3 (100%)	0	100	100
All	All	1127/1192 (94%)	1079 (96%)	48 (4%)	35	59

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	129	LYS
1	A	169	LEU
1	A	176	LYS
1	A	185	LEU
2	B	196	PRO
2	B	210	GLU
2	B	253	GLN
2	B	301	GLN
2	B	351	ASN
2	B	439	ASN

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Mol	Chain	Res	Type
3	C	107	ILE
3	C	118	ASN
3	C	143	VAL
3	C	163	GLN
3	C	172	LEU
3	C	198	LEU
3	C	244	TYR
3	C	298	ASP
3	C	317	ASN
3	C	325	ASN
3	C	330	ASP
3	C	365	ASN
3	C	383	THR
1	D	134	GLN
1	D	180	ASP
1	D	185	LEU
1	D	187	GLN
2	E	190	MET
2	E	195	THR
2	E	210	GLU
2	E	234	LYS
2	E	253	GLN
2	E	280	THR
2	E	281	ASP
2	E	301	GLN
2	E	351	ASN
2	E	359	GLN
2	E	439	ASN
3	F	112	GLU
3	F	118	ASN
3	F	264	MET
3	F	317	ASN
3	F	325	ASN
3	F	361	ASN
3	F	365	ASN
3	F	383	THR
4	G	3	ARG
4	I	3	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:



Mol	Chain	Res	Type
1	A	131	GLN
1	A	139	ASN
1	A	187	GLN
2	B	164	ASN
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	339	GLN
2	B	351	ASN
2	B	359	GLN
2	B	408	HIS
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	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
3	C	350	GLN
3	C	361	ASN
3	C	365	ASN
1	D	134	GLN
1	D	139	ASN
1	D	181	GLN
1	D	184	GLN
2	E	174	ASN
2	E	189	GLN
2	E	202	ASN
2	E	243	ASN
2	E	253	GLN
2	E	271	GLN

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Mol	Chain	Res	Type
2	E	296	ASN
2	E	301	GLN
2	E	339	GLN
2	E	351	ASN
2	E	359	GLN
2	E	408	HIS
2	E	421	GLN
2	E	439	ASN
3	F	103	HIS
3	F	111	GLN
3	F	117	ASN
3	F	119	GLN
3	F	123	ASN
3	F	130	GLN
3	F	176	GLN
3	F	230	ASN
3	F	239	GLN
3	F	307	HIS
3	F	317	ASN
3	F	319	ASN
3	F	325	ASN
3	F	350	GLN
3	F	365	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

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	0.98	1 (6%)
5	NAG	B	4	5	14,14,15	0.54	0	15,19,21	0.63	0
5	FUC	B	5	5	10,10,11	0.54	0	14,14,16	0.60	0
5	NAG	E	3	2,5	14,14,15	0.62	0	15,19,21	1.22	3 (20%)
5	NAG	E	4	5	14,14,15	0.47	0	15,19,21	0.71	1 (6%)
5	FUC	E	5	5	10,10,11	0.57	0	14,14,16	0.93	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	-	1/6/23/26	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 (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	3	NAG	C2-N2-C7	-3.02	119.15	123.04
5	E	3	NAG	C2-N2-C7	-2.20	120.21	123.04
5	E	4	NAG	C2-N2-C7	-2.04	120.42	123.04
5	E	3	NAG	C4-C3-C2	2.07	114.44	111.23
5	E	3	NAG	C3-C4-C5	2.14	113.92	110.20
5	E	5	FUC	C1-C2-C3	2.22	112.17	109.54
5	E	5	FUC	C1-O5-C5	2.27	115.88	112.38

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	3	NAG	O7-C7-N2-C2

There are no ring outliers.

6 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	3	NAG	6	0
5	B	4	NAG	3	0
5	B	5	FUC	1	0
5	E	3	NAG	7	0
5	E	4	NAG	2	0
5	E	5	FUC	5	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	64/66 (96%)	1.04	16 (25%) <b>1</b> <b>1</b>	21, 55, 95, 100	0
1	D	56/66 (84%)	1.07	20 (35%) <b>0</b> <b>0</b>	20, 55, 109, 113	0
2	B	299/313 (95%)	0.41	23 (7%) <b>16</b> <b>18</b>	16, 33, 62, 94	0
2	E	295/313 (94%)	0.24	15 (5%) <b>32</b> <b>37</b>	10, 23, 57, 98	0
3	C	298/311 (95%)	0.69	35 (11%) <b>6</b> <b>6</b>	20, 39, 84, 101	0
3	F	291/311 (93%)	0.54	28 (9%) <b>10</b> <b>11</b>	10, 31, 70, 121	0
4	G	4/4 (100%)	2.92	3 (75%) <b>0</b> <b>0</b>	90, 93, 94, 95	0
4	H	4/4 (100%)	1.19	1 (25%) <b>1</b> <b>1</b>	50, 55, 55, 58	0
4	I	4/4 (100%)	3.11	2 (50%) <b>0</b> <b>0</b>	73, 75, 77, 82	0
4	J	4/4 (100%)	0.17	0 <b>100</b> <b>100</b>	28, 29, 31, 40	0
All	All	1319/1396 (94%)	0.54	143 (10%) <b>8</b> <b>8</b>	10, 33, 87, 121	0

All (143) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	106	SER	8.0
4	I	4	PRO	6.6
3	F	107	ILE	6.5
3	F	393	THR	6.0
3	C	360	PRO	5.9
3	C	362	GLY	5.8
2	B	281	ASP	5.6
3	F	105	SER	5.6
3	F	104	ASP	5.5
3	C	100	ILE	5.4
2	B	459	PRO	5.3
1	D	187	GLN	5.2
1	A	130	VAL	5.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	E	459	PRO	5.0
3	C	96	TYR	5.0
4	G	4	PRO	4.7
2	E	458	PHE	4.7
3	F	108	ARG	4.6
3	C	392	LEU	4.5
3	F	109	TYR	4.4
3	C	241	ALA	4.4
3	F	362	GLY	4.3
3	F	103	HIS	4.3
3	C	101	LEU	4.3
2	B	162	PRO	4.2
3	F	361	ASN	4.1
1	D	185	LEU	4.1
3	C	361	ASN	4.1
2	B	458	PHE	3.9
1	A	128	GLU	3.9
3	C	105	SER	3.9
2	B	388	SER	3.9
3	C	107	ILE	3.9
3	C	297	ASP	3.8
3	F	112	GLU	3.8
1	D	140	VAL	3.7
1	A	131	GLN	3.7
3	C	108	ARG	3.7
2	B	164	ASN	3.6
1	D	135	LEU	3.6
4	G	1	GLY	3.6
1	A	129	LYS	3.6
3	F	296	GLY	3.5
3	F	363	TYR	3.5
2	E	167	VAL	3.5
2	B	282	GLY	3.5
1	A	127	ILE	3.4
2	E	168	LEU	3.4
1	D	184	GLN	3.4
1	A	189	ILE	3.4
1	D	133	ILE	3.2
1	A	133	ILE	3.2
3	C	242	ILE	3.2
3	C	359	THR	3.2
1	A	140	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
3	F	360	PRO	3.2
2	E	281	ASP	3.2
2	E	282	GLY	3.2
3	C	99	SER	3.2
2	B	389	ASP	3.1
1	A	183	LYS	3.1
3	C	240	SER	3.1
3	F	254	ASN	3.1
3	F	297	ASP	3.1
4	I	2	HIS	3.0
1	D	138	LYS	3.0
2	E	170	SER	3.0
2	B	387	THR	2.9
1	A	190	ALA	2.9
2	B	361	MET	2.9
2	B	233	VAL	2.9
1	D	175	LEU	2.9
3	C	389	PHE	2.9
1	D	186	GLU	2.8
3	C	363	TYR	2.8
1	D	137	GLN	2.8
2	B	163	THR	2.8
3	C	98	ALA	2.8
1	A	134	GLN	2.7
2	B	166	ARG	2.7
2	E	280	THR	2.7
2	B	280	THR	2.7
3	C	97	GLU	2.7
1	D	188	VAL	2.7
1	D	136	LEU	2.6
1	D	180	ASP	2.6
3	F	256	ARG	2.6
3	C	104	ASP	2.6
3	C	357	ALA	2.5
3	C	109	TYR	2.5
1	D	179	GLU	2.5
2	E	284	ASN	2.5
2	B	391	ARG	2.5
4	G	2	HIS	2.5
2	B	435	VAL	2.5
3	C	103	HIS	2.5
1	D	176	LYS	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	132	HIS	2.4
3	F	384	MET	2.4
1	D	134	GLN	2.4
3	C	102	THR	2.4
2	B	399	GLY	2.3
3	C	112	GLU	2.3
3	C	393	THR	2.3
3	C	323	GLU	2.3
1	A	188	VAL	2.3
1	D	182	GLN	2.3
1	D	178	TYR	2.3
3	C	384	MET	2.3
3	C	256	ARG	2.3
3	F	359	THR	2.3
2	E	435	VAL	2.3
4	H	4	PRO	2.2
1	D	174	ASP	2.2
2	B	413	ASN	2.2
1	A	177	ASP	2.2
3	F	113	ILE	2.2
3	C	253	TRP	2.2
3	F	115	ASN	2.2
3	F	240	SER	2.1
2	B	412	PRO	2.1
2	B	386	LEU	2.1
1	A	187	GLN	2.1
2	E	312	ILE	2.1
2	B	390	PRO	2.1
3	F	130	GLN	2.1
3	F	294	ASP	2.1
3	F	111	GLN	2.1
2	E	412	PRO	2.1
1	D	141	ARG	2.1
3	C	304	PHE	2.1
3	F	301	ASP	2.1
3	C	248	VAL	2.1
1	A	174	ASP	2.1
2	E	391	ARG	2.0
3	C	295	PHE	2.0
2	B	167	VAL	2.0
2	E	310	LEU	2.0
3	F	299	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	400	GLY	2.0
2	E	252	ILE	2.0
3	C	194	PHE	2.0
3	F	194	PHE	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
5	NAG	E	3	14/15	0.82	0.26	1.00	48,54,61,63	0
5	FUC	B	5	10/11	0.75	0.43	-	87,88,88,89	0
5	FUC	E	5	10/11	0.80	0.37	-	63,63,64,64	0
5	NAG	B	4	14/15	0.65	0.56	-	95,98,100,100	0
5	NAG	B	3	14/15	0.56	0.40	-	79,82,87,91	0
5	NAG	E	4	14/15	0.75	0.45	-	66,68,70,70	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
6	CA	C	407	1/1	0.94	0.12	-1.62	37,37,37,37	0
6	CA	E	462	1/1	0.98	0.06	-1.96	25,25,25,25	0
6	CA	B	462	1/1	0.96	0.05	-2.43	47,47,47,47	0
6	CA	F	407	1/1	0.96	0.05	-3.82	29,29,29,29	0

## 6.5 Other polymers

There are no such residues in this entry.