Full wwPDB X-ray Structure Validation Report

Jan 31, 2016 – 07:57 PM GMT

PDB ID	:	1I1A
Title	:	CRYSTAL STRUCTURE OF THE NEONATAL FC RECEPTOR COMPLEXED WITH A HETERODIMERIC FC
Authors	:	Martin, W.L.; West Jr., A.P.; Gan, L.; Bjorkman, P.J.
Deposited on	:	2001-01-31
Resolution	:	2.80 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:

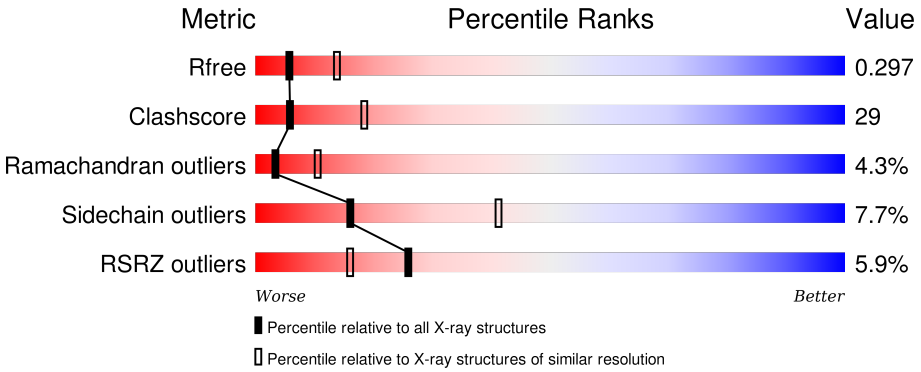
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	269	51% 39% 8%
2	B	99	54% 44%
3	C	225	% 50% 36% 6% 9%
4	D	239	18% 33% 46% 7% 14%

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
11	CYS	A	901	-	-	-	X
6	FUC	D	552	X	-	-	-
6	NAG	D	553	-	-	-	X
8	FUC	A	652	X	-	-	-
9	FUC	A	702	X	-	-	-
9	MAN	A	708	-	-	X	-
9	NDG	A	709	-	-	X	X

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 6526 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 NEONATAL FC RECEPTOR A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	265	Total	C	N	O	S	0	0	0
			2106	1335	363	398	10			

- Molecule 2 is a protein called BETA-2-MICROGLOBULIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	0	0	0
			821	528	137	152	4			

- Molecule 3 is a protein called IG GAMMA-2A CHAIN C REGION.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	205	Total	C	N	O	S	2	0	0
			1634	1038	274	313	9			

- Molecule 4 is a protein called IG GAMMA-2A CHAIN C REGION.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	205	Total	C	N	O	S	0	0	0
			1621	1027	268	317	9			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	252	GLY	THR	ENGINEERED	UNP P20760
D	253	GLY	ILE	ENGINEERED	UNP P20760
D	254	GLY	THR	ENGINEERED	UNP P20760
D	310	GLU	HIS	ENGINEERED	UNP P20760
D	433	GLU	HIS	ENGINEERED	UNP P20760
D	435	GLU	HIS	ENGINEERED	UNP P20760
D	448	GLY	-	CLONING ARTIFACT	UNP P20760
D	449	ILE	-	CLONING ARTIFACT	UNP P20760

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	450	GLU	-	CLONING ARTIFACT	UNP P20760
D	451	GLY	-	CLONING ARTIFACT	UNP P20760
D	452	ARG	-	CLONING ARTIFACT	UNP P20760
D	453	GLY	-	CLONING ARTIFACT	UNP P20760
D	454	SER	-	CLONING ARTIFACT	UNP P20760
D	455	SER	-	CLONING ARTIFACT	UNP P20760
D	456	HIS	-	CLONING ARTIFACT	UNP P20760
D	457	HIS	-	CLONING ARTIFACT	UNP P20760
D	458	HIS	-	CLONING ARTIFACT	UNP P20760
D	459	HIS	-	CLONING ARTIFACT	UNP P20760
D	460	HIS	-	CLONING ARTIFACT	UNP P20760
D	461	HIS	-	CLONING ARTIFACT	UNP P20760

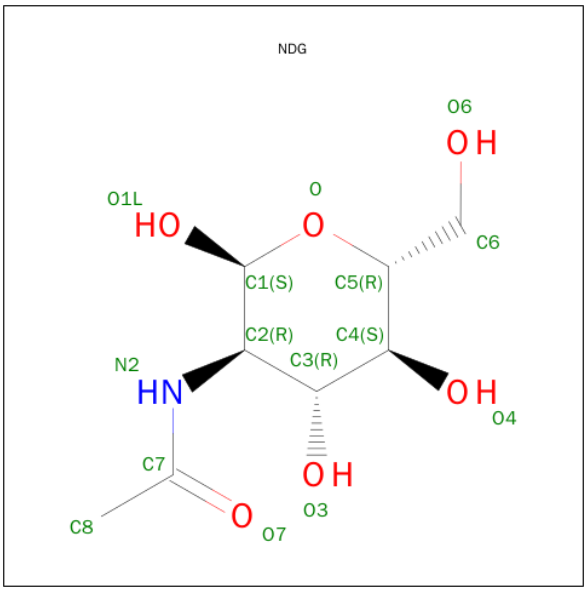
- Molecule 5 is a polymer of unknown type called SUGAR (8-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	C	8	99	56	4	39	0	0

- Molecule 6 is a polymer of unknown type called SUGAR (8-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	D	8	99	56	4	39	0	0

- Molecule 7 is SUGAR (2-(ACETYLAMINO)-2-DEOXY-A-D-GLUCOPYRANOSE) (three-letter code: NDG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			14	8	1	5		

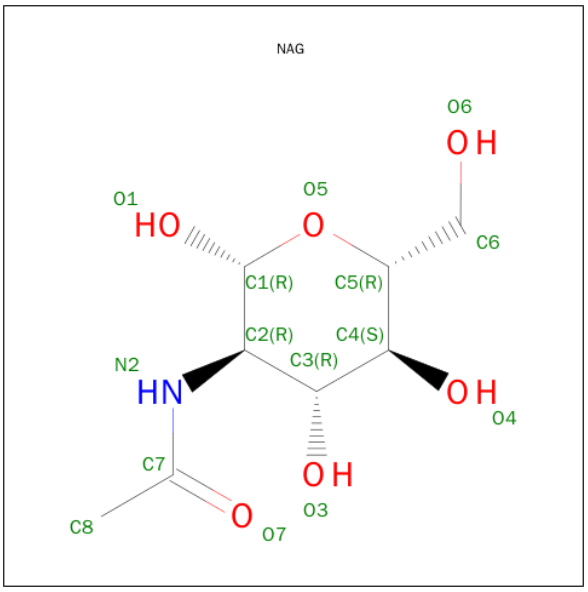
- Molecule 8 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	2	Total	C	N	O	0	0
			24	14	1	9		

- Molecule 9 is a polymer of unknown type called SUGAR (6-MER).

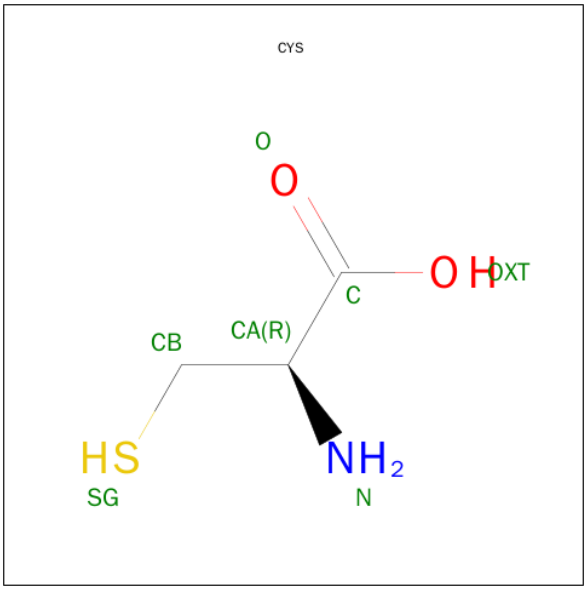
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	6	Total	C	N	O	0	0
			74	42	3	29		

- Molecule 10 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 11 is CYSTEINE (three-letter code: CYS) (formula: $C_3H_7NO_2S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	A	1	Total	C	N	O	S	0	0
			7	3	1	2	1		
11	A	1	Total	C	N	O	S	0	0
			7	3	1	2	1		

- Molecule 12 is water.

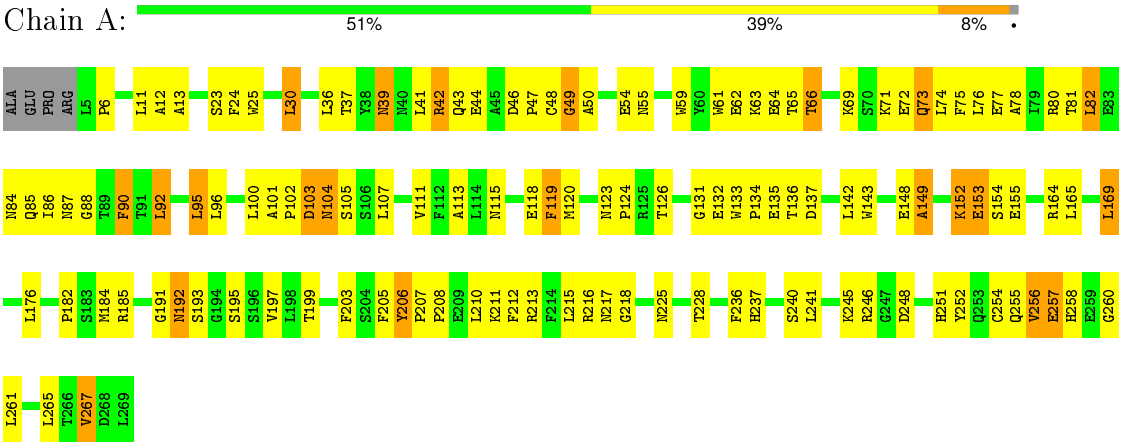
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	3	Total O 3 3	0	0
12	B	2	Total O 2 2	0	0
12	C	1	Total O 1 1	0	0

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.

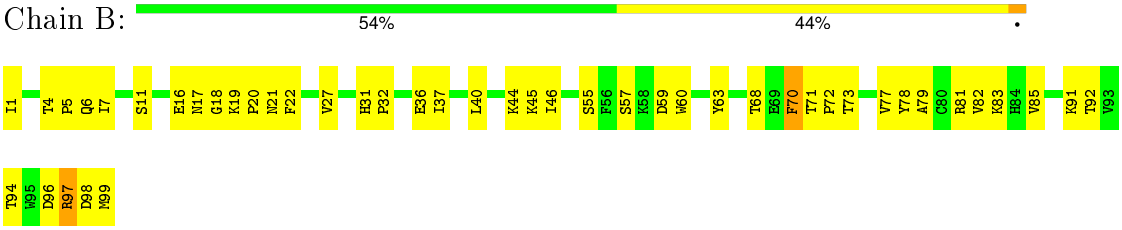
- Molecule 1: NEONATAL FC RECEPTOR A

Chain A:



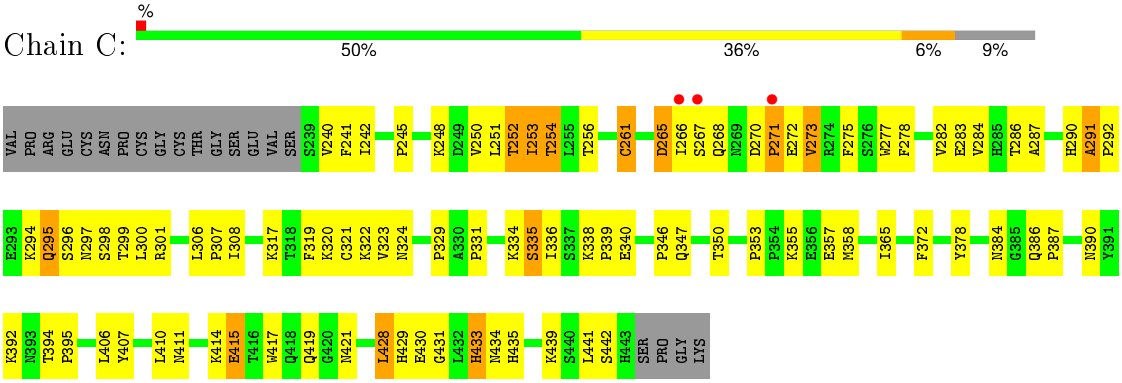
- Molecule 2: BETA-2-MICROGLOBULIN

Chain B:



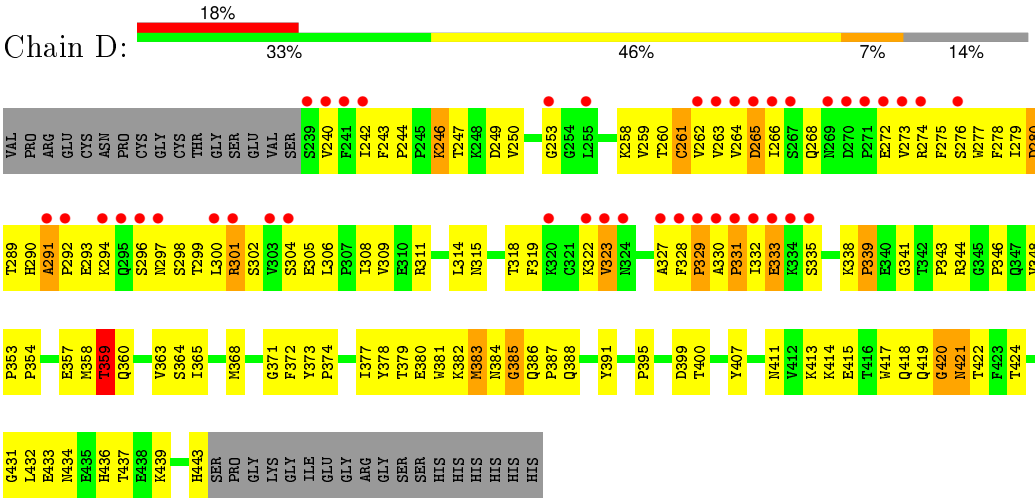
- Molecule 3: IG GAMMA-2A CHAIN C REGION

Chain C:



- Molecule 4: IG GAMMA-2A CHAIN C REGION

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	68.36Å 74.21Å 196.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.95 – 2.80 29.60 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.6 (19.95-2.80) 98.7 (29.60-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	4.11 (at 2.80Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.222 , 0.292 0.232 , 0.297	Depositor DCC
R_{free} test set	1195 reflections (4.78%)	DCC
Wilson B-factor (Å^2)	61.1	Xtriage
Anisotropy	0.135	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 73.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 25054 reflections (0.004%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6526	wwPDB-VP
Average B, all atoms (Å^2)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.20% 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: BMA, NAG, NDG, FUC, FUL, MAN

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	0.51	0/2167	0.76	2/2946 (0.1%)
2	B	0.48	0/846	0.73	0/1149
3	C	0.50	0/1682	0.75	0/2292
4	D	0.43	0/1666	0.66	0/2267
All	All	0.48	0/6361	0.73	2/8654 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
6	D	1	0
8	A	1	0
9	A	1	0
All	All	3	0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	30	LEU	N-CA-C	-5.38	96.46	111.00
1	A	107	LEU	N-CA-C	-5.18	97.02	111.00

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	A	652	FUC	C1
9	A	702	FUC	C1
6	D	552	FUC	C1

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	2106	0	1993	110	0
2	B	821	0	807	32	0
3	C	1634	0	1589	73	0
4	D	1621	0	1570	144	0
5	C	99	0	85	7	0
6	D	99	0	85	8	0
7	A	14	0	13	1	0
8	A	24	0	22	1	0
9	A	74	0	64	20	0
10	A	14	0	13	1	0
11	A	14	0	6	2	0
12	A	3	0	0	0	0
12	B	2	0	0	1	0
12	C	1	0	0	0	0
All	All	6526	0	6247	368	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 29.

All (368) 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)
4:D:323:VAL:HG11	4:D:332:ILE:HG13	1.30	1.06
4:D:258:LYS:HD3	4:D:305:GLU:HB3	1.37	1.06
3:C:320:LYS:HG2	3:C:335:SER:HB2	1.39	1.05
9:A:702:FUC:H4	3:C:434:ASN:HD21	1.22	1.04
1:A:131:GLY:HA3	1:A:136:THR:HG21	1.44	0.98
2:B:20:PRO:HA	2:B:71:THR:HG22	1.43	0.98
1:A:210:LEU:O	11:A:951:CYS:HA	1.63	0.96
1:A:206:TYR:HB3	1:A:207:PRO:HD3	1.50	0.93
4:D:260:THR:HG22	4:D:261:CYS:H	1.31	0.92
4:D:294:LYS:HG2	4:D:300:LEU:HD23	1.51	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:266:ILE:HB	3:C:300:LEU:HB3	1.53	0.90
4:D:240:VAL:HB	4:D:332:ILE:HG21	1.56	0.87
4:D:247:THR:HA	4:D:250:VAL:HG12	1.57	0.87
4:D:384:ASN:HA	4:D:422:THR:HB	1.57	0.86
4:D:273:VAL:HG13	4:D:323:VAL:HG21	1.56	0.86
4:D:329:PRO:O	4:D:331:PRO:HD3	1.77	0.84
4:D:432:LEU:HD13	4:D:437:THR:HG22	1.59	0.82
1:A:137:ASP:OD1	9:A:702:FUC:H3	1.80	0.80
1:A:192:ASN:CG	1:A:193:SER:H	1.86	0.79
1:A:86:ILE:HG21	3:C:254:THR:HG21	1.65	0.79
3:C:301:ARG:HH21	5:C:503:NAG:H81	1.46	0.79
4:D:301:ARG:HH22	6:D:553:NAG:H81	1.46	0.78
1:A:39:ASN:HD21	1:A:42:ARG:HB2	1.46	0.78
3:C:242:ILE:HG12	3:C:336:ILE:HG23	1.65	0.78
2:B:17:ASN:HD21	2:B:97:ARG:HH12	1.31	0.77
9:A:702:FUC:H4	3:C:434:ASN:ND2	1.99	0.77
1:A:199:THR:HG23	1:A:241:LEU:CD2	2.14	0.77
1:A:101:ALA:O	1:A:103:ASP:N	2.18	0.77
4:D:260:THR:HG22	4:D:261:CYS:N	1.99	0.76
4:D:266:ILE:HD12	4:D:300:LEU:HD12	1.67	0.75
3:C:346:PRO:HG3	3:C:372:PHE:HB3	1.67	0.75
1:A:77:GLU:HA	1:A:80:ARG:HH11	1.51	0.75
4:D:353:PRO:HG3	4:D:364:SER:O	1.87	0.75
3:C:320:LYS:HG2	3:C:335:SER:CB	2.17	0.75
1:A:59:TRP:HA	1:A:62:GLU:HG3	1.67	0.74
3:C:301:ARG:NH2	5:C:503:NAG:H81	2.02	0.74
4:D:359:THR:HG23	4:D:360:GLN:H	1.52	0.74
1:A:131:GLY:CA	1:A:136:THR:HG21	2.17	0.73
4:D:277:TRP:O	4:D:283:GLU:HA	1.88	0.73
3:C:248:LYS:O	3:C:252:THR:HG23	1.88	0.73
3:C:320:LYS:CG	3:C:335:SER:HB2	2.16	0.72
1:A:135:GLU:OE2	3:C:254:THR:HB	1.90	0.72
4:D:266:ILE:O	4:D:299:THR:HA	1.89	0.72
4:D:240:VAL:HB	4:D:332:ILE:CG2	2.20	0.71
9:A:701:NDG:C6	9:A:703:NAG:HN2	2.04	0.71
2:B:11:SER:HB2	2:B:21:ASN:ND2	2.06	0.71
4:D:263:VAL:HG11	4:D:273:VAL:HG21	1.71	0.70
2:B:11:SER:HB2	2:B:21:ASN:HD21	1.55	0.70
3:C:271:PRO:C	3:C:273:VAL:H	1.94	0.70
4:D:314:LEU:HD23	4:D:338:LYS:HD2	1.73	0.70
4:D:309:VAL:HG12	4:D:311:ARG:HG2	1.73	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:383:MET:C	4:D:385:GLY:H	1.96	0.69
9:A:701:NDG:H6C1	9:A:703:NAG:HN2	1.57	0.69
1:A:77:GLU:HA	1:A:80:ARG:NH1	2.08	0.68
4:D:323:VAL:CG1	4:D:332:ILE:HG13	2.16	0.68
4:D:351:MET:HE2	4:D:368:MET:HB2	1.75	0.67
4:D:377:ILE:HG12	4:D:378:TYR:N	2.09	0.67
4:D:359:THR:HG23	4:D:360:GLN:N	2.10	0.66
4:D:276:SER:HB3	4:D:283:GLU:OE1	1.95	0.66
3:C:429:HIS:CD2	3:C:431:GLY:H	2.13	0.66
4:D:378:TYR:HB3	4:D:428:LEU:HB2	1.77	0.65
7:A:601:NDG:O4	7:A:601:NDG:H8C1	1.96	0.65
1:A:208:PRO:HG3	1:A:236:PHE:CE1	2.32	0.65
2:B:55:SER:HB3	2:B:63:TYR:CE1	2.31	0.65
2:B:21:ASN:ND2	2:B:22:PHE:H	1.94	0.65
4:D:240:VAL:HG13	4:D:262:VAL:O	1.96	0.65
2:B:17:ASN:HD21	2:B:97:ARG:NH1	1.95	0.65
1:A:245:LYS:HG3	1:A:248:ASP:HB2	1.79	0.64
3:C:365:ILE:HG13	3:C:410:LEU:HD23	1.78	0.64
4:D:263:VAL:HG21	4:D:273:VAL:HG11	1.78	0.63
4:D:242:ILE:HG21	4:D:335:SER:O	1.98	0.63
9:A:708:MAN:H2	9:A:709:NDG:H3	1.81	0.63
1:A:192:ASN:ND2	1:A:193:SER:H	1.97	0.63
1:A:36:LEU:HD23	1:A:37:THR:N	2.13	0.63
4:D:383:MET:HB2	4:D:388:GLN:NE2	2.13	0.63
1:A:71:LYS:NZ	1:A:153:GLU:OE1	2.31	0.63
4:D:301:ARG:NH2	6:D:553:NAG:H81	2.12	0.63
4:D:246:LYS:HD3	4:D:249:ASP:OD2	1.98	0.63
2:B:19:LYS:N	2:B:19:LYS:HD3	2.13	0.63
6:D:553:NAG:O7	6:D:555:MAN:H3	2.00	0.62
1:A:39:ASN:HD22	1:A:39:ASN:C	2.02	0.62
4:D:373:TYR:CD1	4:D:374:PRO:HA	2.35	0.62
9:A:704:BMA:H2	9:A:708:MAN:H5	1.81	0.61
5:C:503:NAG:O7	5:C:505:MAN:H3	2.00	0.61
4:D:346:PRO:HB3	4:D:372:PHE:HB3	1.82	0.61
4:D:260:THR:CG2	4:D:261:CYS:H	2.08	0.61
4:D:436:HIS:ND1	4:D:437:THR:N	2.49	0.61
1:A:62:GLU:O	1:A:66:THR:HG22	2.00	0.61
1:A:101:ALA:C	1:A:103:ASP:H	2.03	0.61
4:D:294:LYS:HG2	4:D:300:LEU:CD2	2.28	0.60
4:D:240:VAL:CB	4:D:332:ILE:HG21	2.29	0.60
4:D:247:THR:HA	4:D:250:VAL:CG1	2.30	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:ASN:CG	1:A:193:SER:N	2.54	0.60
4:D:332:ILE:O	4:D:333:GLU:HB2	2.01	0.60
2:B:20:PRO:CA	2:B:71:THR:HG22	2.25	0.60
1:A:206:TYR:HB3	1:A:207:PRO:CD	2.28	0.60
1:A:216:ARG:HD2	1:A:252:TYR:CZ	2.37	0.60
1:A:206:TYR:O	1:A:207:PRO:C	2.41	0.59
1:A:73:GLN:O	1:A:77:GLU:HG3	2.01	0.59
1:A:131:GLY:HA3	1:A:136:THR:CG2	2.25	0.59
4:D:242:ILE:HG13	4:D:243:PHE:N	2.17	0.59
4:D:360:GLN:HE21	4:D:360:GLN:HA	1.66	0.59
4:D:301:ARG:HD3	4:D:301:ARG:O	2.02	0.59
3:C:415:GLU:O	3:C:419:GLN:HG3	2.01	0.59
4:D:279:ILE:O	4:D:280:ASP:HB2	2.03	0.59
4:D:272:GLU:CD	4:D:327:ALA:HB3	2.23	0.58
4:D:343:PRO:HB3	4:D:430:GLU:O	2.04	0.58
3:C:384:ASN:HD21	3:C:421:ASN:HD22	1.52	0.58
3:C:271:PRO:HA	3:C:273:VAL:HG23	1.84	0.58
9:A:704:BMA:C2	9:A:708:MAN:H5	2.34	0.58
1:A:215:LEU:HD22	1:A:218:GLY:O	2.03	0.58
4:D:266:ILE:HG12	4:D:328:PHE:CE1	2.39	0.57
4:D:246:LYS:H	4:D:246:LYS:CD	2.17	0.57
2:B:36:GLU:HB2	2:B:83:LYS:HB2	1.87	0.57
4:D:263:VAL:H	4:D:302:SER:HB2	1.69	0.57
1:A:256:VAL:HG23	1:A:265:LEU:HB3	1.87	0.57
4:D:433:GLU:O	4:D:434:ASN:HB2	2.04	0.57
9:A:709:NDG:O4	3:C:439:LYS:HE3	2.06	0.56
2:B:7:ILE:HD12	2:B:91:LYS:HD2	1.85	0.56
2:B:81:ARG:HG3	2:B:92:THR:OG1	2.04	0.56
3:C:334:LYS:HD2	5:C:509:NAG:H81	1.88	0.56
1:A:206:TYR:CB	1:A:207:PRO:HD3	2.31	0.56
4:D:377:ILE:CG1	4:D:378:TYR:H	2.19	0.56
3:C:240:VAL:O	3:C:334:LYS:NZ	2.39	0.56
4:D:280:ASP:O	4:D:282:VAL:HG23	2.05	0.56
1:A:75:PHE:CD2	1:A:92:LEU:HD13	2.41	0.56
4:D:377:ILE:HG12	4:D:378:TYR:H	1.69	0.55
4:D:384:ASN:CA	4:D:422:THR:HB	2.32	0.55
2:B:40:LEU:HA	2:B:44:LYS:O	2.06	0.55
4:D:377:ILE:CG1	4:D:378:TYR:N	2.69	0.55
4:D:357:GLU:HG2	4:D:363:VAL:HG12	1.89	0.55
4:D:318:THR:HG22	4:D:319:PHE:N	2.22	0.55
4:D:291:ALA:O	4:D:293:GLU:N	2.39	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:341:GLY:HA3	4:D:373:TYR:HE2	1.72	0.55
4:D:268:GLN:HG2	4:D:268:GLN:O	2.07	0.55
1:A:44:GLU:HA	1:A:65:THR:HG23	1.88	0.55
3:C:322:LYS:O	3:C:322:LYS:HD3	2.07	0.54
1:A:36:LEU:C	1:A:36:LEU:HD23	2.28	0.54
4:D:246:LYS:H	4:D:246:LYS:HD2	1.73	0.54
9:A:709:NDG:O3	3:C:439:LYS:HE3	2.08	0.54
9:A:704:BMA:H2	9:A:708:MAN:C5	2.38	0.54
4:D:243:PHE:HE1	6:D:555:MAN:H2	1.70	0.54
4:D:348:VAL:HG21	4:D:427:VAL:HG21	1.88	0.54
4:D:296:SER:C	4:D:298:SER:H	2.11	0.54
3:C:378:TYR:HB3	3:C:428:LEU:HB2	1.89	0.54
1:A:86:ILE:HG22	1:A:87:ASN:N	2.21	0.54
4:D:318:THR:HG22	4:D:319:PHE:H	1.73	0.53
9:A:708:MAN:O3	9:A:709:NDG:H5	2.09	0.53
2:B:72:PRO:O	2:B:73:THR:HG23	2.09	0.53
4:D:264:VAL:O	4:D:265:ASP:HB2	2.09	0.53
3:C:394:THR:HG23	3:C:407:TYR:O	2.09	0.53
3:C:433:HIS:O	3:C:434:ASN:HB2	2.08	0.53
1:A:100:LEU:HG	1:A:165:LEU:HD23	1.91	0.52
1:A:213:ARG:HH11	1:A:213:ARG:CB	2.22	0.52
1:A:215:LEU:O	1:A:252:TYR:HA	2.09	0.52
9:A:709:NDG:C6	3:C:347:GLN:HA	2.40	0.52
4:D:243:PHE:CE1	6:D:555:MAN:H2	2.44	0.52
4:D:368:MET:HG3	4:D:407:TYR:CE2	2.45	0.52
1:A:111:VAL:CG1	1:A:118:GLU:HG3	2.39	0.52
1:A:208:PRO:HG3	1:A:236:PHE:CD1	2.45	0.51
1:A:104:ASN:O	1:A:105:SER:HB2	2.10	0.51
1:A:90:PHE:CD1	1:A:90:PHE:N	2.78	0.51
4:D:259:VAL:HG23	4:D:308:ILE:HD13	1.93	0.51
1:A:213:ARG:HB2	1:A:213:ARG:NH1	2.25	0.51
1:A:13:ALA:HA	1:A:23:SER:O	2.10	0.51
4:D:273:VAL:CG1	4:D:323:VAL:HG21	2.34	0.51
4:D:278:PHE:CE1	4:D:322:LYS:HD3	2.45	0.51
1:A:54:GLU:HG2	1:A:55:ASN:N	2.26	0.51
4:D:383:MET:HA	4:D:422:THR:O	2.11	0.51
3:C:350:THR:OG1	3:C:441:LEU:HD13	2.10	0.51
3:C:290:HIS:O	3:C:291:ALA:C	2.49	0.51
2:B:31:HIS:ND1	2:B:32:PRO:HA	2.25	0.51
4:D:264:VAL:HG11	6:D:553:NAG:H82	1.93	0.51
1:A:184:MET:HB2	1:A:267:VAL:HG11	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:331:PRO:O	4:D:332:ILE:HG23	2.11	0.50
1:A:199:THR:HG23	1:A:241:LEU:HD21	1.92	0.50
1:A:184:MET:O	1:A:185:ARG:HG2	2.11	0.50
4:D:413:LYS:HB3	4:D:415:GLU:OE2	2.11	0.50
4:D:290:HIS:O	4:D:291:ALA:O	2.29	0.50
4:D:354:PRO:HG2	4:D:357:GLU:HB2	1.92	0.50
1:A:210:LEU:HD11	1:A:256:VAL:CG1	2.42	0.49
4:D:242:ILE:HG22	6:D:559:NAG:H82	1.94	0.49
9:A:701:NDG:C5	9:A:703:NAG:HN2	2.25	0.49
1:A:225:ASN:ND2	10:A:751:NAG:H82	2.27	0.49
4:D:301:ARG:C	4:D:301:ARG:HD3	2.33	0.49
3:C:248:LYS:O	3:C:252:THR:CG2	2.58	0.49
1:A:261:LEU:HD13	1:A:265:LEU:HB2	1.94	0.49
3:C:271:PRO:C	3:C:273:VAL:N	2.61	0.49
1:A:132:GLU:O	1:A:132:GLU:HG2	2.12	0.49
2:B:99:MET:CE	12:B:985:HOH:O	2.60	0.49
4:D:358:MET:HE3	4:D:414:LYS:HE3	1.94	0.49
2:B:16:GLU:O	2:B:19:LYS:HG2	2.12	0.49
4:D:274:ARG:O	4:D:323:VAL:HG23	2.12	0.49
1:A:206:TYR:CB	1:A:207:PRO:CD	2.89	0.49
1:A:86:ILE:CG2	1:A:87:ASN:N	2.76	0.49
3:C:301:ARG:HE	5:C:503:NAG:C8	2.25	0.49
1:A:101:ALA:C	1:A:103:ASP:N	2.65	0.49
1:A:74:LEU:HD22	1:A:143:TRP:CD1	2.48	0.49
3:C:278:PHE:HA	3:C:282:VAL:O	2.12	0.49
2:B:17:ASN:ND2	2:B:97:ARG:HH12	2.04	0.48
4:D:351:MET:CE	4:D:368:MET:HB2	2.41	0.48
2:B:70:PHE:HD2	2:B:78:TYR:CZ	2.31	0.48
4:D:413:LYS:O	4:D:414:LYS:C	2.51	0.48
3:C:294:LYS:HE2	3:C:298:SER:HA	1.95	0.48
1:A:75:PHE:CE2	1:A:92:LEU:HD22	2.48	0.48
3:C:270:ASP:O	3:C:272:GLU:N	2.46	0.48
4:D:399:ASP:OD1	4:D:400:THR:N	2.46	0.48
4:D:365:ILE:HG22	4:D:381:TRP:CH2	2.49	0.48
3:C:346:PRO:HG3	3:C:372:PHE:CB	2.40	0.48
4:D:359:THR:CG2	4:D:360:GLN:H	2.23	0.48
4:D:291:ALA:O	4:D:293:GLU:HG3	2.13	0.48
3:C:353:PRO:HB3	3:C:357:GLU:OE1	2.14	0.48
3:C:261:CYS:HB2	3:C:277:TRP:CZ2	2.49	0.48
3:C:322:LYS:HE2	3:C:331:PRO:HB3	1.96	0.48
3:C:319:PHE:CD1	3:C:319:PHE:N	2.82	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:309:VAL:CG1	4:D:311:ARG:HG2	2.41	0.48
2:B:1:ILE:HD11	3:C:307:PRO:HB2	1.96	0.48
3:C:242:ILE:O	3:C:242:ILE:HG23	2.13	0.47
4:D:277:TRP:CE3	4:D:306:LEU:HD22	2.50	0.47
2:B:27:VAL:HG21	2:B:37:ILE:HD13	1.97	0.47
4:D:383:MET:C	4:D:385:GLY:N	2.66	0.47
1:A:81:THR:HG21	1:A:142:LEU:HD22	1.96	0.47
1:A:182:PRO:HB3	1:A:205:PHE:HB3	1.96	0.47
3:C:275:PHE:CE1	3:C:323:VAL:HG22	2.50	0.47
1:A:210:LEU:HD11	1:A:256:VAL:HG12	1.96	0.47
1:A:88:GLY:O	1:A:90:PHE:CZ	2.67	0.47
4:D:417:TRP:O	4:D:418:GLN:C	2.52	0.47
4:D:240:VAL:CG2	4:D:332:ILE:HG21	2.44	0.47
4:D:432:LEU:HD22	4:D:437:THR:HG21	1.97	0.47
1:A:43:GLN:OE1	1:A:69:LYS:HE2	2.15	0.47
4:D:296:SER:O	4:D:298:SER:N	2.43	0.47
1:A:255:GLN:HA	1:A:265:LEU:O	2.15	0.46
4:D:383:MET:O	4:D:385:GLY:N	2.45	0.46
3:C:294:LYS:CE	3:C:298:SER:HA	2.44	0.46
3:C:386:GLN:O	3:C:387:PRO:C	2.53	0.46
1:A:72:GLU:HG2	1:A:76:LEU:HD12	1.97	0.46
4:D:419:GLN:O	4:D:420:GLY:O	2.34	0.46
4:D:311:ARG:O	4:D:315:ASN:ND2	2.49	0.46
1:A:25:TRP:HA	1:A:39:ASN:HA	1.97	0.46
3:C:242:ILE:HG12	3:C:336:ILE:CG2	2.39	0.46
4:D:278:PHE:CE2	4:D:283:GLU:HB2	2.51	0.46
4:D:274:ARG:HG2	4:D:275:PHE:H	1.81	0.46
4:D:301:ARG:HA	4:D:301:ARG:HH11	1.80	0.46
1:A:44:GLU:OE2	1:A:46:ASP:OD1	2.33	0.46
1:A:81:THR:HG22	1:A:81:THR:O	2.15	0.46
1:A:47:PRO:HB3	1:A:61:TRP:CZ2	2.51	0.46
1:A:44:GLU:HA	1:A:65:THR:CG2	2.45	0.45
1:A:123:ASN:HB3	1:A:126:THR:OG1	2.16	0.45
2:B:18:GLY:O	2:B:71:THR:HB	2.17	0.45
3:C:241:PHE:O	3:C:261:CYS:HA	2.16	0.45
2:B:6:GLN:HA	2:B:6:GLN:OE1	2.17	0.45
4:D:250:VAL:HG22	4:D:250:VAL:O	2.16	0.45
3:C:301:ARG:CZ	5:C:503:NAG:H81	2.47	0.45
1:A:39:ASN:ND2	1:A:39:ASN:C	2.67	0.45
4:D:259:VAL:HG11	4:D:319:PHE:HB2	1.99	0.45
3:C:338:LYS:HG3	3:C:339:PRO:HD2	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:ASN:OD1	1:A:251:HIS:HB3	2.16	0.45
4:D:414:LYS:HD2	4:D:418:GLN:HE22	1.82	0.45
2:B:46:ILE:HG21	2:B:68:THR:HG21	1.99	0.45
3:C:392:LYS:HE2	4:D:400:THR:HG22	1.98	0.45
1:A:213:ARG:HH11	1:A:213:ARG:HB2	1.81	0.45
3:C:295:GLN:CD	3:C:296:SER:H	2.20	0.45
1:A:191:GLY:HA3	1:A:197:VAL:HG23	1.98	0.45
4:D:278:PHE:HA	4:D:283:GLU:HA	1.99	0.44
1:A:12:ALA:O	1:A:24:PHE:HA	2.17	0.44
1:A:39:ASN:ND2	1:A:42:ARG:H	2.15	0.44
9:A:709:NDG:H6C2	3:C:347:GLN:HA	1.99	0.44
4:D:263:VAL:HB	4:D:302:SER:CB	2.47	0.44
4:D:259:VAL:HB	4:D:306:LEU:HD23	1.98	0.44
4:D:339:PRO:HG2	4:D:374:PRO:HB3	1.99	0.44
2:B:57:SER:HB2	2:B:59:ASP:OD1	2.17	0.44
1:A:95:LEU:C	1:A:96:LEU:HD22	2.38	0.44
1:A:192:ASN:ND2	1:A:193:SER:N	2.65	0.44
1:A:118:GLU:HG2	1:A:119:PHE:N	2.31	0.44
4:D:421:ASN:HA	4:D:421:ASN:HD22	1.58	0.44
4:D:289:THR:HA	4:D:304:SER:HA	2.00	0.44
4:D:359:THR:HG23	4:D:360:GLN:HG2	1.99	0.44
4:D:383:MET:N	4:D:386:GLN:O	2.44	0.44
3:C:265:ASP:HA	3:C:299:THR:HB	2.00	0.44
1:A:124:PRO:O	1:A:154:SER:OG	2.33	0.44
1:A:210:LEU:HD12	1:A:257:GLU:O	2.17	0.43
1:A:90:PHE:HA	1:A:115:ASN:OD1	2.17	0.43
1:A:133:TRP:CE2	3:C:253:ILE:HD12	2.53	0.43
9:A:708:MAN:H2	9:A:709:NDG:H5	1.99	0.43
1:A:195:SER:O	1:A:246:ARG:NH1	2.51	0.43
3:C:270:ASP:C	3:C:272:GLU:H	2.21	0.43
4:D:391:TYR:C	4:D:391:TYR:CD1	2.91	0.43
1:A:30:LEU:HA	1:A:30:LEU:HD23	1.87	0.43
4:D:382:LYS:HG2	4:D:385:GLY:C	2.39	0.43
3:C:277:TRP:CE3	3:C:306:LEU:HD22	2.53	0.43
9:A:701:NDG:H5	9:A:703:NAG:HN2	1.81	0.43
1:A:113:ALA:HB2	2:B:60:TRP:CE2	2.54	0.43
4:D:419:GLN:O	4:D:420:GLY:C	2.57	0.43
9:A:701:NDG:H6C1	9:A:703:NAG:N2	2.30	0.43
4:D:299:THR:HG21	6:D:551:NAG:HN2	1.83	0.43
1:A:41:LEU:N	1:A:41:LEU:HD23	2.34	0.43
1:A:258:HIS:CD2	1:A:260:GLY:H	2.37	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:LYS:O	1:A:155:GLU:N	2.52	0.43
3:C:267:SER:O	3:C:268:GLN:HB2	2.19	0.42
4:D:290:HIS:O	4:D:291:ALA:C	2.57	0.42
1:A:84:ASN:HD22	1:A:84:ASN:HA	1.62	0.42
1:A:73:GLN:HG3	1:A:74:LEU:N	2.35	0.42
4:D:272:GLU:OE2	4:D:327:ALA:HB3	2.19	0.42
4:D:358:MET:CE	4:D:418:GLN:NE2	2.82	0.42
2:B:4:THR:HA	2:B:5:PRO:HD3	1.85	0.42
2:B:79:ALA:CB	2:B:94:THR:HA	2.49	0.42
3:C:395:PRO:HD2	4:D:395:PRO:HD2	2.02	0.42
4:D:308:ILE:HG21	4:D:319:PHE:CE2	2.55	0.42
4:D:414:LYS:O	4:D:417:TRP:HB3	2.20	0.42
3:C:317:LYS:O	3:C:319:PHE:CE1	2.73	0.42
3:C:277:TRP:O	3:C:283:GLU:HA	2.19	0.42
4:D:349:TYR:N	4:D:349:TYR:CD2	2.87	0.42
1:A:48:CYS:O	1:A:49:GLY:C	2.57	0.42
1:A:211:LYS:HG2	11:A:951:CYS:OXT	2.20	0.42
4:D:338:LYS:HE2	4:D:430:GLU:OE1	2.19	0.42
9:A:708:MAN:H2	9:A:709:NDG:C3	2.48	0.42
1:A:133:TRP:O	3:C:434:ASN:OD1	2.37	0.42
4:D:382:LYS:HG3	4:D:387:PRO:HA	2.02	0.42
1:A:39:ASN:HD21	1:A:42:ARG:H	1.67	0.42
1:A:81:THR:O	1:A:85:GLN:HG3	2.20	0.42
2:B:96:ASP:O	2:B:98:ASP:N	2.53	0.42
1:A:78:ALA:O	1:A:82:LEU:HB2	2.19	0.42
4:D:278:PHE:HA	4:D:282:VAL:O	2.20	0.42
4:D:259:VAL:CG2	4:D:308:ILE:HD13	2.50	0.42
3:C:322:LYS:HE2	3:C:324:ASN:HB2	2.02	0.42
3:C:322:LYS:NZ	3:C:324:ASN:HB2	2.34	0.42
4:D:414:LYS:CD	4:D:418:GLN:HE22	2.33	0.42
1:A:203:PHE:CE2	1:A:237:HIS:HE1	2.38	0.42
1:A:169:LEU:HD12	1:A:169:LEU:HA	1.76	0.42
4:D:240:VAL:HG21	4:D:332:ILE:HD13	2.01	0.41
1:A:206:TYR:CG	1:A:207:PRO:N	2.85	0.41
4:D:384:ASN:HA	4:D:422:THR:CB	2.38	0.41
4:D:309:VAL:C	4:D:311:ARG:N	2.73	0.41
1:A:81:THR:OG1	1:A:142:LEU:HD21	2.19	0.41
3:C:251:LEU:HD21	3:C:430:GLU:HB3	2.02	0.41
1:A:120:MET:HE2	1:A:136:THR:HA	2.02	0.41
1:A:254:CYS:HB3	1:A:267:VAL:HG23	2.01	0.41
2:B:45:LYS:O	2:B:46:ILE:C	2.57	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:GLU:O	1:A:149:ALA:C	2.58	0.41
1:A:212:PHE:CD2	1:A:240:SER:HB2	2.55	0.41
4:D:424:THR:HG23	4:D:439:LYS:O	2.20	0.41
3:C:256:THR:HG22	3:C:256:THR:O	2.20	0.41
3:C:245:PRO:HB2	3:C:250:VAL:HG23	2.02	0.41
4:D:374:PRO:O	4:D:429:HIS:HE1	2.04	0.41
2:B:21:ASN:ND2	2:B:22:PHE:N	2.65	0.41
3:C:297:ASN:O	3:C:298:SER:HB2	2.21	0.41
2:B:20:PRO:HA	2:B:71:THR:CG2	2.31	0.41
4:D:330:ALA:O	4:D:331:PRO:O	2.39	0.41
1:A:206:TYR:O	1:A:208:PRO:N	2.54	0.41
4:D:264:VAL:O	4:D:265:ASP:CB	2.68	0.41
3:C:428:LEU:HA	3:C:435:HIS:O	2.21	0.41
4:D:415:GLU:C	4:D:417:TRP:N	2.73	0.41
4:D:240:VAL:HG11	4:D:332:ILE:HD12	2.02	0.40
1:A:245:LYS:HG2	1:A:245:LYS:H	1.64	0.40
4:D:379:THR:HG22	4:D:380:GLU:N	2.36	0.40
4:D:279:ILE:HG12	4:D:319:PHE:CD2	2.56	0.40
9:A:708:MAN:C2	9:A:709:NDG:H5	2.51	0.40
3:C:286:THR:HG22	3:C:307:PRO:HG2	2.03	0.40
3:C:266:ILE:C	3:C:268:GLN:H	2.24	0.40
4:D:436:HIS:CG	4:D:437:THR:N	2.89	0.40
4:D:368:MET:HG3	4:D:407:TYR:CZ	2.56	0.40
1:A:64:GLU:HA	1:A:164:ARG:HH12	1.86	0.40
4:D:359:THR:CG2	4:D:360:GLN:N	2.79	0.40
1:A:96:LEU:HD22	1:A:96:LEU:N	2.35	0.40
3:C:241:PHE:CE2	5:C:503:NAG:H4	2.57	0.40
1:A:11:LEU:HD11	1:A:71:LYS:HD2	2.04	0.40
3:C:414:LYS:O	3:C:417:TRP:HB3	2.22	0.40
8:A:651:NDG:O6	8:A:652:FUC:H63	2.21	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	263/269 (98%)	228 (87%)	26 (10%)	9 (3%)	5 16
2	B	97/99 (98%)	88 (91%)	8 (8%)	1 (1%)	19 52
3	C	203/225 (90%)	173 (85%)	22 (11%)	8 (4%)	4 12
4	D	203/239 (85%)	144 (71%)	44 (22%)	15 (7%)	1 3
All	All	766/832 (92%)	633 (83%)	100 (13%)	33 (4%)	3 10

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	104	ASN
1	A	149	ALA
1	A	206	TYR
3	C	273	VAL
4	D	291	ALA
4	D	329	PRO
4	D	331	PRO
4	D	333	GLU
1	A	49	GLY
1	A	50	ALA
1	A	103	ASP
1	A	192	ASN
2	B	97	ARG
3	C	271	PRO
3	C	287	ALA
3	C	329	PRO
4	D	261	CYS
4	D	265	ASP
4	D	292	PRO
4	D	297	ASN
4	D	371	GLY
4	D	420	GLY
3	C	358	MET
4	D	359	THR
4	D	431	GLY
1	A	152	LYS
3	C	265	ASP
3	C	292	PRO
4	D	253	GLY
4	D	339	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	385	GLY
3	C	291	ALA
1	A	102	PRO

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	224/227 (99%)	205 (92%)	19 (8%)	13	36
2	B	95/95 (100%)	91 (96%)	4 (4%)	36	71
3	C	191/208 (92%)	173 (91%)	18 (9%)	11	31
4	D	188/216 (87%)	176 (94%)	12 (6%)	22	52
All	All	698/746 (94%)	645 (92%)	53 (8%)	16	42

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	PRO
1	A	39	ASN
1	A	42	ARG
1	A	63	LYS
1	A	66	THR
1	A	73	GLN
1	A	82	LEU
1	A	90	PHE
1	A	92	LEU
1	A	95	LEU
1	A	119	PHE
1	A	134	PRO
1	A	153	GLU
1	A	169	LEU
1	A	176	LEU
1	A	228	THR
1	A	256	VAL
1	A	257	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	267	VAL
2	B	70	PHE
2	B	77	VAL
2	B	82	VAL
2	B	85	VAL
3	C	252	THR
3	C	253	ILE
3	C	254	THR
3	C	261	CYS
3	C	284	VAL
3	C	295	GLN
3	C	308	ILE
3	C	321	CYS
3	C	335	SER
3	C	340	GLU
3	C	355	LYS
3	C	390	ASN
3	C	406	LEU
3	C	411	ASN
3	C	415	GLU
3	C	428	LEU
3	C	433	HIS
3	C	442	SER
4	D	244	PRO
4	D	246	LYS
4	D	280	ASP
4	D	301	ARG
4	D	323	VAL
4	D	344	ARG
4	D	349	TYR
4	D	359	THR
4	D	383	MET
4	D	411	ASN
4	D	421	ASN
4	D	443	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	34	GLN
1	A	39	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	73	GLN
1	A	84	ASN
1	A	93	GLN
1	A	146	GLN
1	A	192	ASN
1	A	237	HIS
1	A	258	HIS
2	B	2	GLN
2	B	17	ASN
2	B	21	ASN
3	C	285	HIS
3	C	288	GLN
3	C	315	ASN
3	C	347	GLN
3	C	360	GLN
3	C	362	GLN
3	C	390	ASN
3	C	411	ASN
3	C	421	ASN
3	C	429	HIS
3	C	434	ASN
4	D	268	GLN
4	D	288	GLN
4	D	315	ASN
4	D	347	GLN
4	D	360	GLN
4	D	384	ASN
4	D	418	GLN
4	D	421	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

24 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	$\#\|Z\| > 2$
8	NDG	A	651	1,8	14,14,15	0.53	0	15,19,21	0.75	1 (6%)
8	FUC	A	652	8	10,10,11	0.51	0	14,14,16	0.85	1 (7%)
9	NDG	A	701	1,9	14,14,15	0.79	0	15,19,21	1.10	2 (13%)
9	FUC	A	702	9	10,10,11	0.61	0	14,14,16	0.90	1 (7%)
9	NAG	A	703	9	14,14,15	0.52	0	15,19,21	0.60	0
9	BMA	A	704	9	11,11,12	0.64	0	14,15,17	0.78	0
9	MAN	A	708	9	11,11,12	0.59	0	14,15,17	0.73	1 (7%)
9	NDG	A	709	9	14,14,15	0.76	1 (7%)	15,19,21	0.82	0
5	NAG	C	501	3,5	14,14,15	0.64	0	15,19,21	0.76	1 (6%)
5	FUL	C	502	5	10,10,11	0.54	0	14,14,16	0.59	0
5	NAG	C	503	5	14,14,15	0.60	0	15,19,21	0.77	1 (6%)
5	BMA	C	504	5	11,11,12	0.57	0	14,15,17	0.49	0
5	MAN	C	505	5	11,11,12	0.40	0	14,15,17	0.65	0
5	NAG	C	506	5	14,14,15	0.54	0	15,19,21	0.71	1 (6%)
5	MAN	C	508	5	11,11,12	0.47	0	14,15,17	0.66	0
5	NAG	C	509	5	14,14,15	0.57	0	15,19,21	0.63	0
6	NAG	D	551	4,6	14,14,15	0.66	0	15,19,21	0.75	1 (6%)
6	FUC	D	552	6	10,10,11	0.60	0	14,14,16	0.62	0
6	NAG	D	553	6	14,14,15	0.54	0	15,19,21	0.77	1 (6%)
6	BMA	D	554	6	11,11,12	0.54	0	14,15,17	0.46	0
6	MAN	D	555	6	11,11,12	0.49	0	14,15,17	0.66	0
6	NAG	D	556	6	14,14,15	0.50	0	15,19,21	0.72	1 (6%)
6	MAN	D	558	6	11,11,12	0.52	0	14,15,17	0.68	0
6	NAG	D	559	6	14,14,15	0.56	0	15,19,21	0.63	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
8	NDG	A	651	1,8	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	FUC	A	652	8	1/1/4/5	0/0/17/20	0/1/1/1
9	NDG	A	701	1,9	-	0/6/23/26	0/1/1/1
9	FUC	A	702	9	1/1/4/5	0/0/17/20	0/1/1/1
9	NAG	A	703	9	-	0/6/23/26	0/1/1/1
9	BMA	A	704	9	-	0/2/19/22	0/1/1/1
9	MAN	A	708	9	-	0/2/19/22	0/1/1/1
9	NDG	A	709	9	-	1/6/23/26	0/1/1/1
5	NAG	C	501	3,5	-	1/6/23/26	0/1/1/1
5	FUL	C	502	5	-	0/0/17/20	0/1/1/1
5	NAG	C	503	5	-	0/6/23/26	0/1/1/1
5	BMA	C	504	5	-	0/2/19/22	0/1/1/1
5	MAN	C	505	5	-	0/2/19/22	0/1/1/1
5	NAG	C	506	5	-	0/6/23/26	0/1/1/1
5	MAN	C	508	5	-	0/2/19/22	0/1/1/1
5	NAG	C	509	5	-	0/6/23/26	0/1/1/1
6	NAG	D	551	4,6	-	1/6/23/26	0/1/1/1
6	FUC	D	552	6	1/1/4/5	0/0/17/20	0/1/1/1
6	NAG	D	553	6	-	0/6/23/26	0/1/1/1
6	BMA	D	554	6	-	0/2/19/22	0/1/1/1
6	MAN	D	555	6	-	0/2/19/22	0/1/1/1
6	NAG	D	556	6	-	0/6/23/26	0/1/1/1
6	MAN	D	558	6	-	0/2/19/22	0/1/1/1
6	NAG	D	559	6	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	709	NDG	C1-C2	2.28	1.55	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	503	NAG	C2-N2-C7	-2.56	119.75	123.04
6	D	553	NAG	C2-N2-C7	-2.51	119.81	123.04
9	A	701	NDG	C2-N2-C7	-2.35	120.02	123.04
5	C	501	NAG	C2-N2-C7	-2.24	120.16	123.04
6	D	556	NAG	C2-N2-C7	-2.24	120.16	123.04
5	C	506	NAG	C2-N2-C7	-2.23	120.17	123.04
6	D	551	NAG	C2-N2-C7	-2.19	120.23	123.04
8	A	651	NDG	C2-N2-C7	-2.08	120.37	123.04
9	A	701	NDG	C1-O-C5	2.18	115.02	112.25
8	A	652	FUC	C1-O5-C5	2.36	116.02	112.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	708	MAN	C1-O5-C5	2.39	115.28	112.25
9	A	702	FUC	C1-C2-C3	2.47	112.47	109.54

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	D	552	FUC	C1
8	A	652	FUC	C1
9	A	702	FUC	C1

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	551	NAG	O7-C7-N2-C2
5	C	501	NAG	O7-C7-N2-C2
9	A	709	NDG	O7-C7-N2-C2

There are no ring outliers.

15 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	651	NDG	1	0
8	A	652	FUC	1	0
9	A	701	NDG	5	0
9	A	702	FUC	3	0
9	A	703	NAG	5	0
9	A	704	BMA	3	0
9	A	708	MAN	8	0
9	A	709	NDG	9	0
5	C	503	NAG	6	0
5	C	505	MAN	1	0
5	C	509	NAG	1	0
6	D	551	NAG	1	0
6	D	553	NAG	4	0
6	D	555	MAN	3	0
6	D	559	NAG	1	0

5.6 Ligand geometry (i)

4 ligands 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	$\#\|Z\| > 2$
7	NDG	A	601	1	14,14,15	0.67	0	15,19,21	0.81	1 (6%)
10	NAG	A	751	1	14,14,15	0.66	0	15,19,21	0.77	0
11	CYS	A	901	1	3,6,6	0.64	0	1,7,7	1.30	0
11	CYS	A	951	1	3,6,6	0.52	0	1,7,7	0.47	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
7	NDG	A	601	1	-	0/6/23/26	0/1/1/1
10	NAG	A	751	1	-	0/6/23/26	0/1/1/1
11	CYS	A	901	1	-	0/2/6/6	0/0/0/0
11	CYS	A	951	1	-	0/2/6/6	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	601	NDG	C2-N2-C7	-2.29	120.10	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	601	NDG	1	0
10	A	751	NAG	1	0
11	A	951	CYS	2	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

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	265/269 (98%)	-0.48	0 100 100	27, 54, 96, 136	0
2	B	99/99 (100%)	-0.53	0 100 100	22, 56, 93, 129	0
3	C	205/225 (91%)	-0.36	3 (1%) 76 68	31, 55, 156, 199	1 (0%)
4	D	205/239 (85%)	0.86	43 (20%) 1 1	35, 92, 194, 202	0
All	All	774/832 (93%)	-0.10	46 (5%) 26 16	22, 61, 168, 202	1 (0%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	271	PRO	10.8
4	D	272	GLU	8.8
4	D	262	VAL	7.4
4	D	332	ILE	7.1
4	D	323	VAL	7.0
4	D	322	LYS	7.0
4	D	265	ASP	5.7
4	D	334	LYS	5.6
4	D	276	SER	5.5
4	D	300	LEU	4.9
4	D	303	VAL	4.8
4	D	331	PRO	4.7
4	D	263	VAL	4.7
4	D	264	VAL	4.5
4	D	270	ASP	4.4
4	D	241	PHE	4.3
4	D	274	ARG	4.3
4	D	329	PRO	4.2
4	D	240	VAL	4.1
4	D	304	SER	3.9
4	D	320	LYS	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	D	242	ILE	3.7
4	D	267	SER	3.7
4	D	273	VAL	3.7
4	D	239	SER	3.6
4	D	266	ILE	3.5
3	C	266	ILE	3.5
4	D	291	ALA	3.4
4	D	281	ASP	3.2
3	C	267	SER	3.1
4	D	333	GLU	3.1
4	D	330	ALA	3.0
4	D	301	ARG	2.9
4	D	328	PHE	2.9
4	D	327	ALA	2.9
4	D	324	ASN	2.8
3	C	271	PRO	2.6
4	D	255	LEU	2.5
4	D	297	ASN	2.5
4	D	295	GLN	2.4
4	D	269	ASN	2.4
4	D	296	SER	2.4
4	D	335	SER	2.3
4	D	253	GLY	2.1
4	D	292	PRO	2.1
4	D	294	LYS	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
9	NDG	A	709	14/15	0.59	0.50	7.55	173,179,179,179	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
9	NAG	A	703	14/15	0.81	0.22	1.85	108,123,128,138	0
9	FUC	A	702	10/11	0.93	0.17	1.54	79,88,92,92	0
6	NAG	D	556	14/15	0.72	0.39	0.02	167,192,202,202	0
5	NAG	C	506	14/15	0.90	0.14	-0.74	76,91,115,116	0
6	NAG	D	553	14/15	0.71	0.45	-0.77	202,202,202,202	0
6	MAN	D	558	11/12	0.81	0.29	-	191,196,199,202	0
9	NDG	A	701	14/15	0.89	0.19	-	91,101,104,105	0
6	BMA	D	554	11/12	0.54	0.31	-	202,202,202,202	0
5	NAG	C	509	14/15	0.68	0.30	-	145,150,153,153	0
6	NAG	D	551	14/15	0.71	0.46	-	202,202,202,202	0
5	MAN	C	505	11/12	0.92	0.15	-	96,98,102,105	0
6	MAN	D	555	11/12	0.80	0.45	-	202,202,202,202	0
6	NAG	D	559	14/15	0.73	0.31	-	188,199,202,202	0
5	MAN	C	508	11/12	0.87	0.13	-	119,127,133,153	0
5	NAG	C	503	14/15	0.90	0.18	-	102,112,116,117	0
9	MAN	A	708	11/12	0.68	0.35	-	189,191,191,191	0
5	BMA	C	504	11/12	0.91	0.12	-	88,92,99,105	0
5	NAG	C	501	14/15	0.88	0.17	-	128,139,144,145	0
8	FUC	A	652	10/11	0.80	0.31	-	171,171,171,171	0
9	BMA	A	704	11/12	0.83	0.21	-	69,103,111,131	0
6	FUC	D	552	10/11	0.76	0.34	-	202,202,202,202	0
5	FUL	C	502	10/11	0.87	0.27	-	142,143,146,147	0
8	NDG	A	651	14/15	0.83	0.27	-	144,149,162,170	0

6.4 Ligands

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
11	CYS	A	901	7/7	0.77	0.36	7.37	89,99,115,120	0
11	CYS	A	951	7/7	0.76	0.25	-	89,154,202,202	0
7	NDG	A	601	14/15	0.44	0.55	-	201,201,201,201	0
10	NAG	A	751	14/15	0.74	0.30	-	101,122,128,129	0

6.5 Other polymers (i)

There are no such residues in this entry.