Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:20 PM GMT

PDB ID	:	1T89
Title	:	CRYSTAL STRUCTURE OF A HUMAN TYPE III FC GAMMA RECEPTOR IN COMPLEX WITH AN FC FRAGMENT OF IGG1 (HEXAGONAL)
Authors	:	Radaev, S.; Motyka, S.; Fridman, W.-H.; Sautes-Fridman, C.; Sun, P.D.
Deposited on	:	2004-05-11
Resolution	:	3.50 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 (i)) were used in the production of this report:

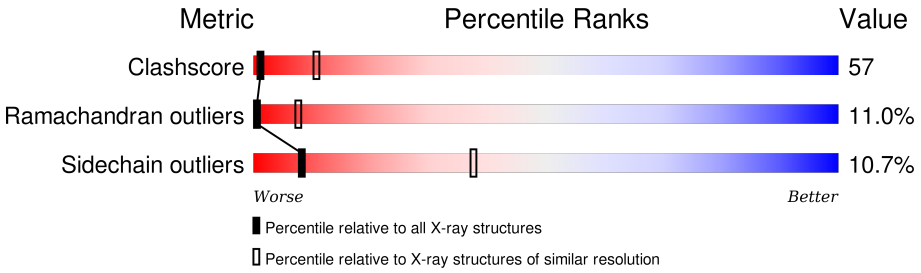
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	224	29% 50% 13% • 6%
1	B	224	22% 55% 15% • 5%
2	C	176	35% 52% 8% 5%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MAN	A	452	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	FUC	B	455	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4919 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 recombinant IgG1 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	210	Total	C	N	O	S	0	0	0
			1677	1067	282	321	7			
1	B	213	Total	C	N	O	S	0	0	0
			1700	1083	285	325	7			

- Molecule 2 is a protein called Low affinity immunoglobulin gamma Fc region receptor III-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	167	Total	C	N	O	S	101	0	0
			1347	856	231	256	4			

- Molecule 3 is a polymer of unknown type called SUGAR (8-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	8	Total	C	N	O	0	0
			96	54	3	39		

- Molecule 4 is a polymer of unknown type called SUGAR (8-MER).

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

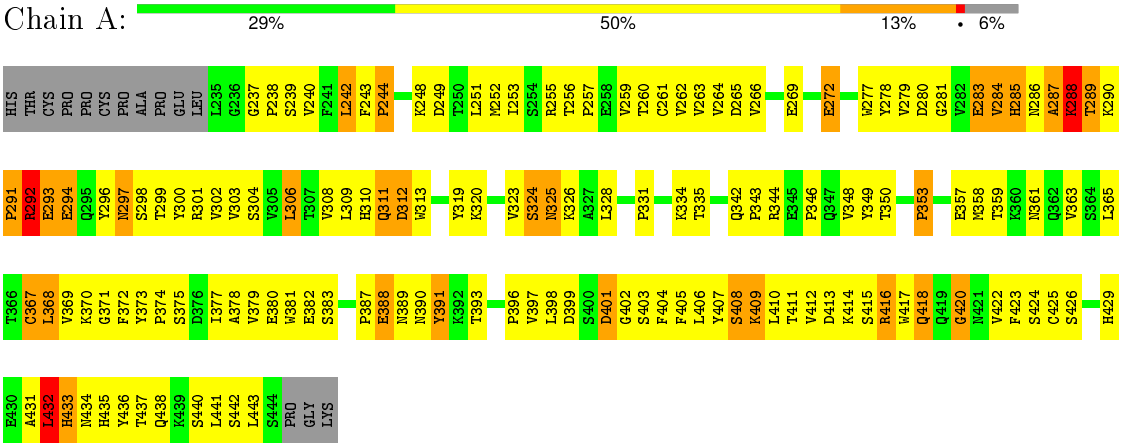
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

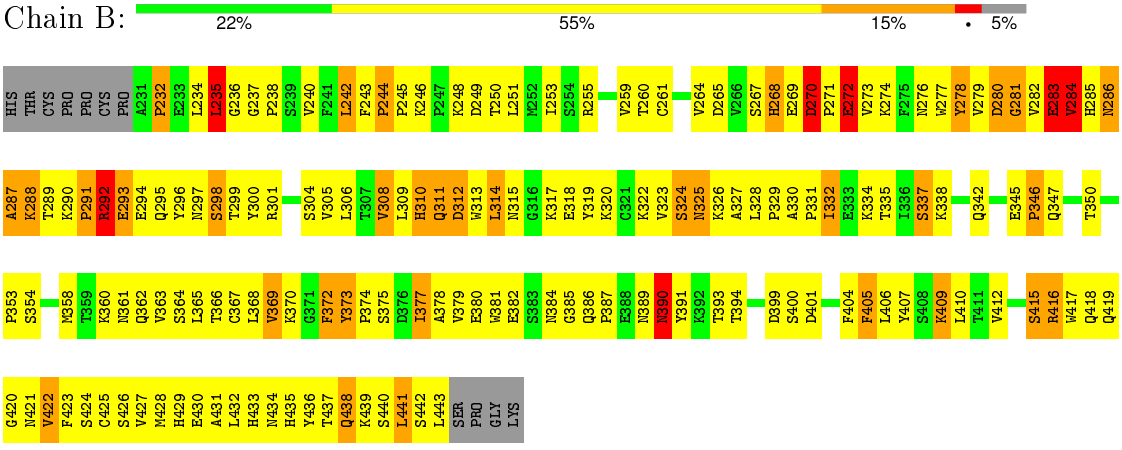
• Molecule 1: recombinant IgG1 heavy chain

Chain A:



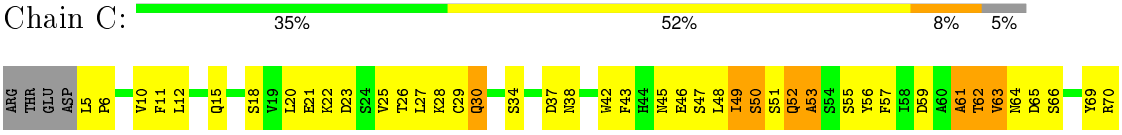
• Molecule 1: recombinant IgG1 heavy chain

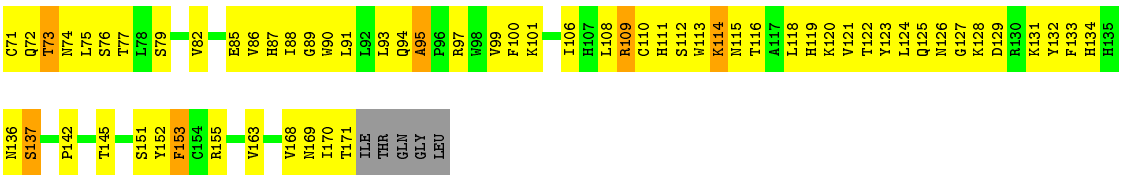
Chain B:



• Molecule 2: Low affinity immunoglobulin gamma Fc region receptor III-B

Chain C:




C71
Q72
T73
N74
L75
S76
T77
L78
S79
V82
E85
V86
H87
I88
G89
W90
L91
L92
L93
Q94
A95
P96
R97
W98
V99
F100
K101
I106
H107
L108
R109
C110
H111
S112
W113
K114
N115
T116
A117
L118
H119
K120
V121
T122
Y123
L124
Q125
N126
G127
K128
D129
K130
K131
Y132
F133
H134
H135
N136
S137
P142
T145
S151
Y152
F153
C154
R155
V163
V168
N169
I170
T171
ILE
THR
GLN
GLY
LEU

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	114.98Å 114.98Å 301.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 3.50	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-3.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.247 , 0.309	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4919	wwPDB-VP
Average B, all atoms (Å^2)	79.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, NDG, GAL, 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	0.61	3/1723 (0.2%)	0.77	0/2346
1	B	0.54	3/1747 (0.2%)	0.71	1/2380 (0.0%)
2	C	0.49	0/1385	0.72	0/1884
All	All	0.55	6/4855 (0.1%)	0.74	1/6610 (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
4	B	1	0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	294	GLU	CD-OE2	7.71	1.34	1.25
1	B	294	GLU	CD-OE2	7.44	1.33	1.25
1	A	283	GLU	CD-OE2	7.35	1.33	1.25
1	A	272	GLU	CD-OE2	7.28	1.33	1.25
1	B	272	GLU	CD-OE2	7.18	1.33	1.25
1	B	283	GLU	CD-OE2	7.00	1.33	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	425	CYS	CA-CB-SG	5.47	123.85	114.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	455	FUC	C1

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	1677	0	1644	210	0
1	B	1700	0	1668	224	0
2	C	1347	0	1288	115	0
3	A	96	0	82	12	0
4	B	99	0	85	11	0
All	All	4919	0	4767	539	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 57.

All (539) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:ARG:NE	1:A:293:GLU:H	1.49	1.10
1:A:292:ARG:HE	1:A:292:ARG:CA	1.63	1.10
1:A:292:ARG:HA	1:A:292:ARG:HE	0.98	1.09
1:B:308:VAL:HG12	1:B:309:LEU:H	1.13	1.08
1:A:350:THR:HB	1:A:441:LEU:HD12	1.39	1.05
1:A:346:PRO:HB3	1:A:372:PHE:HB3	1.41	1.03
1:A:432:LEU:HD13	1:A:437:THR:HG22	1.40	1.02
1:A:288:LYS:HA	1:A:288:LYS:HE3	1.39	1.02
1:B:420:GLY:HA2	1:B:443:LEU:HD13	1.39	1.01
1:A:344:ARG:HH12	1:A:401:ASP:HB3	1.29	0.96
1:A:292:ARG:HA	1:A:292:ARG:NE	1.80	0.95
1:A:292:ARG:NE	1:A:293:GLU:N	2.20	0.90
1:A:409:LYS:HB3	1:B:407:TYR:OH	1.71	0.89
4:B:448:NDG:H4	4:B:455:FUC:H2	1.53	0.89
1:B:308:VAL:HG12	1:B:309:LEU:N	1.89	0.89
1:B:330:ALA:HB1	1:B:331:PRO:HD2	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:PRO:O	1:B:292:ARG:HB2	1.74	0.87
1:A:407:TYR:OH	1:B:409:LYS:HB2	1.73	0.87
1:B:238:PRO:HB3	1:B:265:ASP:O	1.73	0.87
1:A:286:ASN:O	1:A:288:LYS:N	2.06	0.86
1:B:368:LEU:HD12	1:B:369:VAL:H	1.42	0.83
1:A:286:ASN:C	1:A:288:LYS:H	1.82	0.82
1:B:273:VAL:HG11	1:B:323:VAL:CG1	2.09	0.82
1:B:310:HIS:HB2	1:B:311:GLN:OE1	1.80	0.82
1:B:240:VAL:HG23	1:B:332:ILE:HD12	1.62	0.81
1:B:328:LEU:HD21	1:B:332:ILE:HD11	1.62	0.81
1:A:249:ASP:HA	1:A:255:ARG:HD3	1.62	0.81
1:B:308:VAL:CG1	1:B:309:LEU:H	1.94	0.81
1:A:284:VAL:HG12	1:A:287:ALA:HB2	1.62	0.80
1:B:283:GLU:HG2	1:B:284:VAL:H	1.46	0.80
1:B:301:ARG:HH11	4:B:449:NDG:H8C2	1.46	0.80
1:A:297:ASN:HB2	1:A:299:THR:HG22	1.64	0.80
2:C:27:LEU:HD12	2:C:56:TYR:HD2	1.48	0.79
1:A:381:TRP:CZ2	1:A:425:CYS:HB3	2.17	0.79
1:A:286:ASN:C	1:A:288:LYS:N	2.36	0.79
1:A:370:LYS:NZ	1:B:360:LYS:HE3	1.98	0.79
1:B:295:GLN:HE21	1:B:300:TYR:HE1	1.28	0.78
1:A:397:VAL:HG21	1:B:394:THR:HG22	1.63	0.78
1:B:309:LEU:HB3	1:B:312:ASP:HB2	1.66	0.77
1:B:308:VAL:HG11	1:B:313:TRP:HB2	1.65	0.77
1:A:266:VAL:HB	1:A:300:TYR:HB2	1.65	0.77
1:B:382:GLU:HB2	1:B:424:SER:HB2	1.64	0.77
1:A:253:ILE:HA	1:A:310:HIS:CE1	2.18	0.77
2:C:90:TRP:O	2:C:112:SER:HA	1.85	0.77
3:A:448:NDG:H6C1	3:A:449:NAG:H82	1.65	0.77
2:C:91:LEU:HA	2:C:111:HIS:O	1.83	0.76
1:A:370:LYS:HZ3	1:B:360:LYS:HE3	1.49	0.76
1:A:243:PHE:CD2	3:A:453:NDG:H5	2.20	0.76
1:A:292:ARG:NE	1:A:292:ARG:CA	2.42	0.76
1:B:423:PHE:O	1:B:440:SER:HA	1.85	0.76
1:A:346:PRO:CB	1:A:372:PHE:HB3	2.16	0.76
1:A:242:LEU:HD23	1:A:260:THR:O	1.86	0.76
1:A:411:THR:O	1:A:412:VAL:HG13	1.86	0.76
1:B:377:ILE:HD11	1:B:427:VAL:HG13	1.69	0.75
1:A:346:PRO:HB3	1:A:372:PHE:CB	2.17	0.75
1:B:273:VAL:HG13	1:B:324:SER:O	1.87	0.74
1:A:237:GLY:O	2:C:120:LYS:HE2	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:GLU:O	1:B:284:VAL:HG13	1.87	0.74
1:A:422:VAL:HG22	1:A:442:SER:HB2	1.69	0.74
1:B:270:ASP:H	1:B:271:PRO:HD3	1.53	0.74
1:A:344:ARG:NH1	1:A:401:ASP:HB3	2.01	0.74
1:A:325:ASN:ND2	1:A:326:LYS:H	1.86	0.73
1:B:308:VAL:HG13	1:B:319:TYR:CZ	2.24	0.73
1:A:266:VAL:HB	1:A:300:TYR:CB	2.19	0.72
1:A:292:ARG:CZ	1:A:293:GLU:H	2.01	0.72
1:A:379:VAL:HG13	1:A:426:SER:O	1.90	0.72
2:C:27:LEU:HD12	2:C:56:TYR:CD2	2.25	0.72
1:A:243:PHE:CE2	3:A:452:MAN:H2	2.24	0.72
1:B:273:VAL:HG11	1:B:323:VAL:HG13	1.70	0.71
1:B:242:LEU:HD23	1:B:260:THR:O	1.89	0.71
2:C:108:LEU:HD11	2:C:170:ILE:HD11	1.73	0.70
1:B:309:LEU:HD23	1:B:312:ASP:OD1	1.92	0.70
1:A:308:VAL:CG1	1:A:313:TRP:HB2	2.21	0.70
1:B:377:ILE:HG12	1:B:378:ALA:N	2.06	0.70
1:B:382:GLU:O	1:B:424:SER:N	2.24	0.70
1:B:350:THR:HB	1:B:441:LEU:HD12	1.72	0.70
1:A:381:TRP:CH2	1:A:425:CYS:HB3	2.28	0.69
2:C:155:ARG:HB2	2:C:163:VAL:O	1.91	0.69
1:B:311:GLN:C	1:B:315:ASN:HD22	1.94	0.69
2:C:5:LEU:HD22	2:C:75:LEU:O	1.92	0.69
1:B:232:PRO:HD3	1:B:298:SER:OG	1.93	0.68
1:B:405:PHE:HD1	1:B:406:LEU:N	1.91	0.68
1:B:287:ALA:O	1:B:289:THR:N	2.26	0.68
2:C:89:GLY:O	2:C:113:TRP:HB2	1.93	0.68
1:B:276:ASN:HB3	1:B:278:TYR:HE1	1.58	0.68
2:C:43:PHE:HA	2:C:47:SER:O	1.94	0.68
1:B:361:ASN:O	1:B:362:GLN:HG3	1.94	0.67
1:B:273:VAL:HG11	1:B:323:VAL:HG12	1.75	0.67
2:C:97:ARG:HG3	2:C:100:PHE:CE2	2.30	0.67
1:B:353:PRO:HG3	1:B:363:VAL:CG2	2.24	0.67
1:B:246:LYS:O	1:B:250:THR:HG23	1.94	0.67
1:B:328:LEU:HD21	1:B:332:ILE:CD1	2.24	0.66
1:A:240:VAL:HG22	1:A:263:VAL:HG22	1.76	0.66
1:A:414:LYS:HG2	1:A:418:GLN:NE2	2.10	0.66
2:C:99:VAL:HA	2:C:171:THR:O	1.95	0.66
2:C:122:THR:HG21	2:C:129:ASP:OD2	1.97	0.65
1:A:308:VAL:HG13	1:A:319:TYR:CZ	2.32	0.64
2:C:48:LEU:HD12	2:C:48:LEU:N	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:ASN:C	1:B:327:ALA:H	2.01	0.64
2:C:125:GLN:HA	2:C:151:SER:O	1.98	0.64
1:B:261:CYS:HB2	1:B:277:TRP:CH2	2.32	0.64
1:A:432:LEU:HD23	1:A:432:LEU:H	1.61	0.63
1:B:380:GLU:HB2	1:B:426:SER:HB2	1.81	0.63
1:A:238:PRO:HB3	1:A:265:ASP:O	1.97	0.63
1:B:353:PRO:HG3	1:B:363:VAL:HG21	1.79	0.63
1:A:288:LYS:HA	1:A:288:LYS:CE	2.15	0.63
1:A:422:VAL:HG22	1:A:442:SER:CB	2.29	0.63
1:B:311:GLN:CD	1:B:311:GLN:H	2.02	0.63
1:A:383:SER:OG	1:A:388:GLU:HG2	1.99	0.63
2:C:11:PHE:HE1	2:C:30:GLN:HB3	1.64	0.62
1:B:272:GLU:OE1	1:B:272:GLU:HA	1.98	0.62
1:A:367:CYS:HB3	1:A:381:TRP:CZ2	2.33	0.62
1:B:301:ARG:NH1	4:B:449:NDG:H8C2	2.14	0.62
1:A:397:VAL:CG2	1:B:394:THR:HG22	2.30	0.62
1:B:268:HIS:O	1:B:271:PRO:HD3	2.00	0.62
1:B:309:LEU:HD23	1:B:312:ASP:CG	2.20	0.62
1:B:368:LEU:CD1	1:B:369:VAL:H	2.11	0.62
1:A:371:GLY:HA2	1:A:403:SER:OG	2.00	0.62
1:A:374:PRO:O	1:A:429:HIS:HE1	1.81	0.62
1:B:432:LEU:HB2	1:B:435:HIS:HA	1.81	0.62
1:B:250:THR:OG1	1:B:314:LEU:HD21	2.00	0.62
1:A:259:VAL:HG13	1:A:308:VAL:HG21	1.82	0.62
2:C:63:VAL:O	2:C:66:SER:HB2	2.00	0.62
1:A:286:ASN:O	1:A:289:THR:N	2.32	0.61
1:A:266:VAL:O	1:A:300:TYR:HB2	1.99	0.61
3:A:448:NDG:H6C1	3:A:449:NAG:C8	2.30	0.61
1:A:409:LYS:NZ	1:A:409:LYS:HB2	2.15	0.61
1:B:283:GLU:CG	1:B:284:VAL:H	2.13	0.61
2:C:6:PRO:O	2:C:76:SER:HA	2.00	0.61
1:B:313:TRP:CZ3	1:B:338:LYS:N	2.69	0.61
1:B:238:PRO:HG2	1:B:328:LEU:HD11	1.82	0.61
1:A:243:PHE:HE2	3:A:452:MAN:H2	1.66	0.61
1:A:432:LEU:O	1:A:433:HIS:C	2.38	0.60
1:A:286:ASN:O	1:A:289:THR:OG1	2.14	0.60
1:B:318:GLU:HA	1:B:337:SER:HB3	1.82	0.60
2:C:91:LEU:HD12	2:C:155:ARG:HA	1.83	0.60
1:B:418:GLN:C	1:B:420:GLY:H	2.05	0.60
2:C:113:TRP:O	2:C:116:THR:HG23	2.01	0.60
2:C:49:ILE:O	2:C:51:SER:N	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:THR:HB	1:B:441:LEU:CD1	2.30	0.60
1:A:431:ALA:O	1:A:432:LEU:O	2.20	0.60
1:B:375:SER:HB3	1:B:404:PHE:CE2	2.37	0.60
2:C:10:VAL:HB	2:C:82:VAL:HG21	1.83	0.60
1:A:237:GLY:H	2:C:120:LYS:HE3	1.66	0.60
1:A:278:TYR:HB2	1:A:320:LYS:HB3	1.84	0.60
2:C:52:GLN:O	2:C:53:ALA:C	2.39	0.60
4:B:450:BMA:H61	4:B:452:MAN:H5	1.81	0.60
1:B:313:TRP:HZ3	1:B:337:SER:HA	1.67	0.59
1:B:309:LEU:O	1:B:312:ASP:HB2	2.03	0.59
1:A:432:LEU:HB2	1:A:436:TYR:N	2.18	0.59
1:A:288:LYS:HE2	1:A:290:LYS:NZ	2.17	0.59
1:A:308:VAL:HG11	1:A:313:TRP:HB2	1.82	0.59
1:A:398:LEU:HD12	1:A:403:SER:O	2.02	0.59
2:C:21:GLU:OE2	2:C:63:VAL:HG22	2.03	0.59
1:A:238:PRO:CG	1:A:328:LEU:HD13	2.33	0.59
1:B:308:VAL:HG13	1:B:319:TYR:OH	2.03	0.58
1:A:422:VAL:HG12	1:A:423:PHE:N	2.18	0.58
1:B:368:LEU:HD12	1:B:406:LEU:O	2.02	0.58
2:C:64:ASN:C	2:C:66:SER:H	2.05	0.58
1:A:277:TRP:CD1	1:A:289:THR:HG21	2.39	0.58
1:B:365:LEU:HB2	1:B:410:LEU:HB3	1.85	0.58
1:B:443:LEU:HD12	1:B:443:LEU:N	2.18	0.58
2:C:12:LEU:HD21	2:C:27:LEU:HD23	1.84	0.58
2:C:90:TRP:O	2:C:91:LEU:HD23	2.03	0.58
1:A:288:LYS:HE2	1:A:290:LYS:HZ3	1.68	0.58
1:B:270:ASP:H	1:B:271:PRO:CD	2.17	0.58
1:A:350:THR:HB	1:A:441:LEU:CD1	2.23	0.58
1:A:412:VAL:HG12	1:A:416:ARG:NH1	2.19	0.58
1:B:405:PHE:CD1	1:B:406:LEU:N	2.71	0.58
1:B:432:LEU:HB2	1:B:435:HIS:CA	2.34	0.58
1:A:350:THR:CB	1:A:441:LEU:HD12	2.26	0.58
1:B:251:LEU:CD2	1:B:430:GLU:HA	2.33	0.57
1:A:349:TYR:HE2	1:A:370:LYS:HE3	1.69	0.57
1:B:390:ASN:O	1:B:410:LEU:HD12	2.03	0.57
1:B:269:GLU:O	1:B:270:ASP:HB2	2.04	0.57
1:B:259:VAL:HG23	1:B:308:VAL:HG21	1.85	0.57
1:B:279:VAL:C	1:B:281:GLY:H	2.08	0.57
1:A:379:VAL:HA	1:A:426:SER:O	2.05	0.57
1:A:288:LYS:HG3	1:A:290:LYS:HZ1	1.68	0.56
1:B:377:ILE:HG13	1:B:428:MET:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:CYS:HB2	1:A:277:TRP:CH2	2.40	0.56
1:B:417:TRP:O	1:B:443:LEU:HD11	2.05	0.56
1:A:238:PRO:HD2	1:A:328:LEU:CD1	2.35	0.56
1:A:279:VAL:O	1:A:281:GLY:N	2.38	0.56
1:B:301:ARG:HH11	4:B:449:NDG:C8	2.16	0.56
2:C:12:LEU:HD21	2:C:27:LEU:CD2	2.35	0.56
1:A:237:GLY:HA2	2:C:134:HIS:ND1	2.19	0.56
1:A:424:SER:HB2	1:A:438:GLN:HE21	1.70	0.56
1:B:360:LYS:NZ	1:B:360:LYS:HB3	2.20	0.56
2:C:43:PHE:HE2	2:C:48:LEU:CD1	2.18	0.56
2:C:99:VAL:HG22	2:C:171:THR:HG23	1.88	0.56
2:C:118:LEU:HG	2:C:121:VAL:HG22	1.87	0.56
1:B:234:LEU:O	1:B:236:GLY:N	2.38	0.56
2:C:21:GLU:O	2:C:22:LYS:HB2	2.04	0.56
2:C:100:PHE:CD1	2:C:106:ILE:HG12	2.41	0.56
2:C:18:SER:OG	2:C:87:HIS:HE1	1.87	0.56
1:A:357:GLU:HG2	1:A:357:GLU:O	2.05	0.56
1:A:411:THR:HG22	1:A:412:VAL:H	1.71	0.56
1:A:410:LEU:HD12	1:A:411:THR:N	2.20	0.56
1:A:411:THR:HG22	1:A:412:VAL:N	2.19	0.56
1:B:301:ARG:HD2	4:B:449:NDG:H8C3	1.88	0.56
1:B:345:GLU:HA	1:B:431:ALA:HB3	1.87	0.56
1:B:432:LEU:O	1:B:434:ASN:N	2.39	0.55
1:B:250:THR:O	1:B:314:LEU:HD11	2.06	0.55
2:C:168:VAL:HG12	2:C:169:ASN:N	2.20	0.55
1:A:388:GLU:HA	1:A:388:GLU:OE1	2.06	0.55
1:A:292:ARG:C	1:A:292:ARG:HE	2.09	0.55
1:B:273:VAL:HG12	1:B:274:LYS:N	2.21	0.55
1:B:279:VAL:O	1:B:281:GLY:N	2.39	0.55
2:C:25:VAL:HG12	2:C:26:THR:N	2.21	0.55
1:A:407:TYR:O	1:A:408:SER:HB2	2.06	0.55
1:A:290:LYS:O	1:A:304:SER:HA	2.07	0.55
1:A:420:GLY:HA2	1:A:443:LEU:HD13	1.89	0.55
2:C:126:ASN:O	2:C:128:LYS:N	2.40	0.55
1:A:288:LYS:HG3	1:A:290:LYS:HE2	1.89	0.55
1:B:234:LEU:O	1:B:235:LEU:C	2.45	0.55
1:A:361:ASN:N	1:A:361:ASN:HD22	2.05	0.55
1:A:308:VAL:HG12	1:A:313:TRP:HB2	1.88	0.54
1:B:405:PHE:CD1	1:B:405:PHE:C	2.80	0.54
1:B:268:HIS:HB3	1:B:269:GLU:OE2	2.07	0.54
4:B:452:MAN:H4	4:B:453:NAG:H83	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:273:VAL:HG13	1:B:324:SER:C	2.28	0.54
1:B:377:ILE:CG1	1:B:378:ALA:N	2.71	0.54
2:C:42:TRP:CZ3	2:C:71:CYS:HB3	2.43	0.54
2:C:124:LEU:N	2:C:124:LEU:HD12	2.22	0.54
1:B:296:TYR:CE1	1:B:301:ARG:HD3	2.43	0.54
1:A:357:GLU:C	1:A:359:THR:H	2.11	0.54
1:A:443:LEU:N	1:A:443:LEU:HD12	2.23	0.54
1:A:253:ILE:HG13	1:A:310:HIS:ND1	2.23	0.54
2:C:91:LEU:CD1	2:C:155:ARG:HA	2.37	0.54
1:B:443:LEU:H	1:B:443:LEU:HD12	1.73	0.53
1:A:382:GLU:OE2	1:A:382:GLU:N	2.41	0.53
1:A:436:TYR:CD1	1:A:437:THR:N	2.77	0.53
2:C:113:TRP:O	2:C:115:ASN:N	2.41	0.53
1:A:284:VAL:HG12	1:A:287:ALA:CB	2.33	0.53
2:C:125:GLN:HB2	2:C:152:TYR:CE2	2.44	0.53
1:A:243:PHE:N	1:A:243:PHE:CD1	2.76	0.53
2:C:133:PHE:CD2	2:C:137:SER:HB2	2.44	0.53
1:B:389:ASN:O	1:B:391:TYR:HD1	1.91	0.53
1:B:283:GLU:C	1:B:284:VAL:HG22	2.29	0.53
1:B:277:TRP:HE1	1:B:304:SER:HG	1.56	0.53
1:A:368:LEU:HD12	1:A:368:LEU:O	2.08	0.53
2:C:12:LEU:CD2	2:C:27:LEU:HD23	2.39	0.52
1:B:384:ASN:ND2	1:B:385:GLY:H	2.08	0.52
2:C:126:ASN:O	2:C:128:LYS:HG3	2.10	0.52
1:A:252:MET:HB2	1:A:255:ARG:HD2	1.91	0.52
1:A:311:GLN:O	1:A:312:ASP:C	2.47	0.52
2:C:73:THR:O	2:C:75:LEU:N	2.42	0.52
2:C:57:PHE:CE2	2:C:59:ASP:HB2	2.45	0.52
1:B:365:LEU:HD21	1:B:417:TRP:CE3	2.44	0.52
1:A:396:PRO:HA	1:A:405:PHE:O	2.09	0.52
1:A:238:PRO:HD2	1:A:328:LEU:HD13	1.91	0.52
1:B:249:ASP:HA	1:B:255:ARG:HB3	1.91	0.52
1:B:313:TRP:O	1:B:315:ASN:N	2.42	0.51
1:A:374:PRO:O	1:A:429:HIS:CE1	2.62	0.51
1:A:252:MET:CE	1:A:255:ARG:HE	2.23	0.51
1:A:381:TRP:CE2	1:A:425:CYS:HB3	2.46	0.51
1:A:367:CYS:HB3	1:A:381:TRP:CH2	2.44	0.51
1:B:264:VAL:O	1:B:265:ASP:HB2	2.10	0.51
2:C:152:TYR:CD1	2:C:170:ILE:HD12	2.45	0.51
2:C:94:GLN:O	2:C:95:ALA:HB2	2.10	0.51
1:A:269:GLU:OE2	1:A:269:GLU:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:VAL:HG23	1:B:308:VAL:CG2	2.40	0.51
2:C:123:TYR:C	2:C:124:LEU:HD12	2.31	0.51
2:C:48:LEU:N	2:C:48:LEU:CD1	2.74	0.51
2:C:99:VAL:HG22	2:C:171:THR:CG2	2.40	0.51
1:A:320:LYS:HB2	1:A:335:THR:HG22	1.93	0.51
1:B:311:GLN:O	1:B:315:ASN:ND2	2.43	0.50
1:A:288:LYS:HG3	1:A:290:LYS:NZ	2.25	0.50
1:A:353:PRO:HD3	1:A:365:LEU:HD23	1.92	0.50
1:A:324:SER:HB3	1:A:331:PRO:HB3	1.94	0.50
1:A:350:THR:HB	1:A:441:LEU:HB2	1.92	0.50
1:B:372:PHE:CE2	1:B:404:PHE:HB3	2.47	0.50
2:C:42:TRP:HB3	2:C:49:ILE:HD11	1.92	0.50
1:B:317:LYS:HB3	1:B:319:TYR:HE1	1.77	0.50
1:A:243:PHE:CE2	3:A:453:NDG:H5	2.46	0.50
1:B:309:LEU:HB3	1:B:312:ASP:CB	2.39	0.50
1:A:363:VAL:HG13	1:A:412:VAL:HG23	1.94	0.50
1:A:372:PHE:HZ	1:A:406:LEU:HD23	1.77	0.50
1:A:348:VAL:HG22	1:A:369:VAL:HG13	1.94	0.50
1:A:243:PHE:HE2	3:A:452:MAN:C2	2.24	0.50
1:B:244:PRO:HB2	1:B:245:PRO:HD2	1.93	0.50
1:B:279:VAL:HG23	1:B:284:VAL:HG21	1.93	0.50
1:A:238:PRO:HG2	1:A:328:LEU:HD13	1.94	0.50
1:A:262:VAL:HG11	1:A:301:ARG:HE	1.77	0.50
1:B:240:VAL:CG2	1:B:332:ILE:HD12	2.38	0.50
1:A:441:LEU:C	1:A:441:LEU:HD23	2.32	0.50
1:B:325:ASN:HB3	1:B:328:LEU:HD13	1.94	0.49
1:B:301:ARG:NH1	4:B:449:NDG:C8	2.75	0.49
2:C:113:TRP:C	2:C:115:ASN:N	2.66	0.49
1:A:391:TYR:HB3	1:A:410:LEU:HD13	1.95	0.49
1:B:283:GLU:HG2	1:B:284:VAL:N	2.19	0.49
1:B:379:VAL:HA	1:B:426:SER:O	2.12	0.49
1:A:406:LEU:C	1:A:406:LEU:HD12	2.33	0.49
1:B:248:LYS:O	1:B:251:LEU:N	2.46	0.49
2:C:91:LEU:HD13	2:C:110:CYS:SG	2.52	0.49
1:A:265:ASP:O	2:C:134:HIS:HE1	1.95	0.49
2:C:48:LEU:O	2:C:49:ILE:HG23	2.12	0.49
2:C:71:CYS:O	2:C:79:SER:HB3	2.11	0.49
1:A:396:PRO:HA	1:A:406:LEU:HB3	1.92	0.49
1:A:291:PRO:HA	1:A:303:VAL:O	2.12	0.49
1:B:325:ASN:C	1:B:327:ALA:N	2.66	0.49
1:A:349:TYR:HB3	1:B:354:SER:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:TRP:C	1:B:315:ASN:H	2.16	0.49
1:A:415:SER:HA	1:A:418:GLN:HE21	1.77	0.49
1:B:253:ILE:C	1:B:253:ILE:HD12	2.33	0.49
1:A:263:VAL:HG21	1:A:323:VAL:HG11	1.94	0.49
4:B:448:NDG:C4	4:B:455:FUC:H2	2.36	0.49
1:A:297:ASN:HD22	1:A:299:THR:CG2	2.25	0.49
2:C:120:LYS:HA	2:C:133:PHE:O	2.13	0.49
2:C:124:LEU:O	2:C:152:TYR:HA	2.13	0.49
1:A:244:PRO:HA	1:A:259:VAL:HG12	1.95	0.49
1:A:409:LYS:HD3	1:B:405:PHE:CE2	2.48	0.48
2:C:100:PHE:O	2:C:101:LYS:HG3	2.13	0.48
1:B:386:GLN:HA	1:B:387:PRO:HD3	1.62	0.48
1:B:317:LYS:HB3	1:B:319:TYR:CE1	2.47	0.48
1:B:237:GLY:O	1:B:238:PRO:C	2.50	0.48
2:C:38:ASN:CG	2:C:38:ASN:O	2.51	0.48
2:C:48:LEU:C	2:C:49:ILE:HG12	2.33	0.48
1:B:297:ASN:OD1	1:B:298:SER:N	2.46	0.48
1:B:317:LYS:CB	1:B:319:TYR:HE1	2.27	0.48
1:A:414:LYS:O	1:A:415:SER:C	2.51	0.48
2:C:120:LYS:HG2	2:C:132:TYR:OH	2.13	0.48
2:C:152:TYR:O	2:C:153:PHE:HB3	2.13	0.48
2:C:72:GLN:HG3	2:C:73:THR:H	1.78	0.48
2:C:73:THR:C	2:C:75:LEU:H	2.17	0.48
2:C:48:LEU:O	2:C:49:ILE:HG12	2.13	0.48
4:B:450:BMA:H61	4:B:452:MAN:C5	2.43	0.48
1:A:237:GLY:H	2:C:120:LYS:CE	2.26	0.48
1:B:243:PHE:CD2	4:B:453:NAG:H5	2.49	0.48
1:B:240:VAL:O	1:B:334:LYS:HE3	2.14	0.48
1:B:372:PHE:O	1:B:404:PHE:HB2	2.14	0.48
1:B:270:ASP:N	1:B:271:PRO:CD	2.76	0.48
2:C:113:TRP:C	2:C:115:ASN:H	2.16	0.47
2:C:21:GLU:HG3	2:C:88:ILE:HD13	1.96	0.47
1:B:235:LEU:CD2	1:B:235:LEU:N	2.76	0.47
1:A:257:PRO:HG2	1:A:310:HIS:CD2	2.49	0.47
2:C:64:ASN:C	2:C:66:SER:N	2.67	0.47
1:A:263:VAL:CG2	1:A:323:VAL:HG21	2.44	0.47
1:B:309:LEU:O	1:B:310:HIS:C	2.52	0.47
1:B:365:LEU:HD21	1:B:417:TRP:CZ3	2.49	0.47
1:A:417:TRP:O	1:A:443:LEU:HD11	2.15	0.47
1:B:293:GLU:OE2	1:B:300:TYR:CE2	2.68	0.47
1:A:432:LEU:O	1:A:435:HIS:N	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:GLN:HA	1:A:343:PRO:HD3	1.74	0.47
1:A:393:THR:HA	1:A:408:SER:HA	1.95	0.47
1:A:288:LYS:HG3	1:A:290:LYS:CE	2.44	0.47
1:B:330:ALA:HB1	1:B:331:PRO:CD	2.34	0.47
1:A:312:ASP:HB3	1:A:319:TYR:OH	2.15	0.47
1:A:409:LYS:HD3	1:B:405:PHE:CD2	2.49	0.47
1:A:361:ASN:ND2	1:A:361:ASN:N	2.63	0.47
1:A:292:ARG:HE	1:A:293:GLU:N	2.02	0.47
1:B:311:GLN:N	1:B:311:GLN:OE1	2.39	0.47
1:A:373:TYR:HA	1:A:374:PRO:HA	1.67	0.47
1:B:420:GLY:HA2	1:B:443:LEU:CD1	2.28	0.47
1:B:372:PHE:CE1	1:B:377:ILE:HG21	2.50	0.47
1:B:235:LEU:HD23	1:B:235:LEU:N	2.28	0.47
1:A:292:ARG:CD	1:A:293:GLU:H	2.23	0.47
1:B:375:SER:HB3	1:B:404:PHE:CZ	2.50	0.47
2:C:73:THR:HG23	2:C:76:SER:HB2	1.96	0.47
1:B:245:PRO:HD3	1:B:259:VAL:HG22	1.97	0.46
1:A:391:TYR:CB	1:A:410:LEU:HD13	2.45	0.46
2:C:49:ILE:O	2:C:50:SER:C	2.53	0.46
1:B:423:PHE:O	1:B:441:LEU:N	2.44	0.46
2:C:99:VAL:HA	2:C:171:THR:HG23	1.96	0.46
1:B:422:VAL:CG2	1:B:442:SER:HB3	2.46	0.46
1:B:363:VAL:HG23	1:B:364:SER:N	2.29	0.46
1:A:289:THR:C	1:A:290:LYS:HD2	2.35	0.46
1:B:382:GLU:HG3	1:B:426:SER:OG	2.15	0.46
3:A:452:MAN:HO3	3:A:453:NDG:C1	2.28	0.46
1:B:295:GLN:O	1:B:296:TYR:CD1	2.69	0.46
1:B:290:LYS:HB3	1:B:305:VAL:HB	1.96	0.46
1:B:320:LYS:HG3	1:B:335:THR:HG22	1.98	0.46
1:B:368:LEU:CG	1:B:369:VAL:N	2.79	0.46
2:C:21:GLU:C	2:C:23:ASP:H	2.18	0.46
2:C:20:LEU:O	2:C:23:ASP:HB2	2.16	0.46
1:B:276:ASN:HB2	1:B:322:LYS:HB3	1.97	0.46
1:B:346:PRO:CG	1:B:432:LEU:HD21	2.46	0.46
1:A:325:ASN:ND2	1:A:326:LYS:N	2.60	0.46
2:C:52:GLN:O	2:C:53:ALA:O	2.33	0.46
1:A:238:PRO:HA	1:A:265:ASP:HB2	1.97	0.46
1:A:407:TYR:HE2	1:B:366:THR:HG21	1.80	0.46
1:B:249:ASP:HA	1:B:255:ARG:CB	2.46	0.46
1:A:346:PRO:CA	1:A:372:PHE:HB3	2.45	0.45
1:A:291:PRO:HG3	1:A:304:SER:OG	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:282:VAL:HG22	1:B:283:GLU:N	2.31	0.45
1:A:283:GLU:HG2	1:A:285:HIS:H	1.81	0.45
1:B:350:THR:HB	1:B:441:LEU:CG	2.46	0.45
2:C:29:CYS:HB2	2:C:42:TRP:CZ2	2.51	0.45
1:A:369:VAL:O	1:A:405:PHE:HA	2.16	0.45
2:C:11:PHE:CE1	2:C:30:GLN:HB3	2.48	0.45
1:A:309:LEU:O	1:A:312:ASP:HB2	2.16	0.45
1:A:286:ASN:O	1:A:287:ALA:C	2.55	0.45
1:B:282:VAL:CG2	1:B:283:GLU:N	2.79	0.45
1:B:267:SER:HB2	1:B:270:ASP:HB3	1.98	0.45
1:B:251:LEU:HD22	1:B:430:GLU:HA	1.99	0.45
2:C:12:LEU:HA	2:C:12:LEU:HD23	1.56	0.45
1:B:436:TYR:CD1	1:B:437:THR:N	2.85	0.45
1:B:311:GLN:O	1:B:315:ASN:N	2.50	0.45
1:B:368:LEU:HD12	1:B:369:VAL:N	2.22	0.45
1:B:406:LEU:N	1:B:406:LEU:HD23	2.31	0.45
3:A:452:MAN:O3	3:A:453:NDG:C1	2.64	0.45
1:A:346:PRO:CG	1:A:432:LEU:HD21	2.46	0.45
1:B:439:LYS:HD2	1:B:439:LYS:HA	1.82	0.45
1:A:391:TYR:CG	1:A:391:TYR:O	2.70	0.44
1:A:346:PRO:HG2	1:A:432:LEU:HD21	1.99	0.44
1:B:308:VAL:CG1	1:B:309:LEU:N	2.61	0.44
1:A:365:LEU:HB2	1:A:410:LEU:O	2.17	0.44
1:A:369:VAL:HB	1:A:372:PHE:HE2	1.82	0.44
1:B:410:LEU:HG	1:B:412:VAL:HG13	1.97	0.44
1:B:237:GLY:HA2	1:B:238:PRO:HD2	1.88	0.44
1:A:252:MET:HE1	1:A:255:ARG:HE	1.81	0.44
1:B:278:TYR:CD1	1:B:278:TYR:N	2.84	0.44
1:B:311:GLN:O	1:B:312:ASP:C	2.56	0.44
1:B:415:SER:O	1:B:416:ARG:C	2.55	0.44
2:C:18:SER:OG	2:C:87:HIS:CE1	2.69	0.44
1:A:377:ILE:CG2	1:A:378:ALA:N	2.80	0.44
1:B:373:TYR:CD2	1:B:373:TYR:C	2.91	0.44
1:B:313:TRP:C	1:B:315:ASN:N	2.70	0.44
1:A:407:TYR:CE2	1:B:366:THR:HG21	2.52	0.44
1:A:302:VAL:HG12	1:A:303:VAL:N	2.32	0.44
1:A:238:PRO:CD	1:A:328:LEU:HD13	2.47	0.44
1:B:261:CYS:HB2	1:B:277:TRP:CZ2	2.53	0.44
1:B:437:THR:HG23	1:B:438:GLN:N	2.33	0.44
1:B:390:ASN:HD22	1:B:390:ASN:HA	1.57	0.44
1:A:368:LEU:C	1:A:368:LEU:HD12	2.37	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:TRP:CG	1:A:410:LEU:HD22	2.52	0.44
2:C:28:LYS:HG3	2:C:55:SER:OG	2.17	0.44
1:B:306:LEU:O	1:B:306:LEU:HD23	2.17	0.44
1:B:369:VAL:HB	1:B:406:LEU:CD2	2.48	0.44
1:A:398:LEU:HD13	1:A:404:PHE:CE1	2.53	0.44
1:B:289:THR:O	1:B:290:LYS:HB2	2.18	0.44
2:C:100:PHE:HD1	2:C:106:ILE:HG12	1.82	0.44
1:A:409:LYS:HG3	1:A:409:LYS:O	2.18	0.44
1:A:424:SER:OG	1:A:440:SER:HA	2.18	0.44
1:B:309:LEU:O	1:B:312:ASP:N	2.51	0.44
1:B:283:GLU:CG	1:B:284:VAL:N	2.79	0.44
1:A:349:TYR:OH	1:B:360:LYS:HD2	2.18	0.43
2:C:34:SER:HA	2:C:75:LEU:HD12	2.00	0.43
1:B:347:GLN:OE1	1:B:370:LYS:HG3	2.18	0.43
1:A:326:LYS:C	1:A:328:LEU:H	2.21	0.43
2:C:94:GLN:OE1	2:C:109:ARG:CD	2.66	0.43
1:B:242:LEU:HD23	1:B:260:THR:C	2.38	0.43
1:B:325:ASN:O	1:B:327:ALA:N	2.51	0.43
1:A:255:ARG:HG2	1:A:255:ARG:HH11	1.82	0.43
1:B:308:VAL:HG13	1:B:319:TYR:CE2	2.52	0.43
1:A:290:LYS:HA	1:A:291:PRO:HD3	1.72	0.43
1:B:405:PHE:O	1:B:406:LEU:HB3	2.19	0.43
1:B:367:CYS:SG	1:B:381:TRP:CH2	3.12	0.43
1:B:313:TRP:CH2	1:B:338:LYS:N	2.86	0.43
1:A:441:LEU:HD23	1:A:442:SER:N	2.34	0.43
2:C:5:LEU:HA	2:C:5:LEU:HD23	1.82	0.43
1:B:235:LEU:O	1:B:235:LEU:HG	2.18	0.43
1:B:389:ASN:O	1:B:391:TYR:N	2.51	0.43
1:A:284:VAL:HG11	1:A:306:LEU:HD11	2.01	0.43
1:B:372:PHE:HE1	1:B:377:ILE:HG21	1.83	0.43
1:A:415:SER:O	1:A:416:ARG:C	2.57	0.43
1:A:434:ASN:C	1:A:436:TYR:N	2.72	0.43
1:B:329:PRO:HG2	2:C:90:TRP:CD2	2.53	0.43
2:C:21:GLU:HA	2:C:61:ALA:O	2.18	0.43
2:C:45:ASN:C	2:C:46:GLU:HG3	2.39	0.43
1:A:248:LYS:NZ	1:A:248:LYS:HB3	2.34	0.43
1:A:288:LYS:HE3	1:A:288:LYS:CA	2.29	0.43
2:C:94:GLN:OE1	2:C:109:ARG:HD2	2.18	0.43
1:A:239:SER:HB2	1:A:264:VAL:HG23	2.00	0.43
1:A:297:ASN:HD22	1:A:299:THR:HG22	1.84	0.42
3:A:453:NDG:C7	3:A:453:NDG:HB	2.31	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:5:LEU:HD21	2:C:75:LEU:HD22	2.00	0.42
2:C:73:THR:HG23	2:C:76:SER:CB	2.48	0.42
1:A:372:PHE:CE1	1:A:404:PHE:HB2	2.53	0.42
2:C:118:LEU:O	2:C:119:HIS:HD2	2.02	0.42
1:B:415:SER:O	1:B:418:GLN:N	2.52	0.42
2:C:125:GLN:NE2	2:C:152:TYR:OH	2.53	0.42
2:C:43:PHE:HD2	2:C:47:SER:O	2.02	0.42
1:B:368:LEU:HG	1:B:369:VAL:N	2.33	0.42
1:A:424:SER:HB3	1:A:438:GLN:HG3	2.00	0.42
1:A:365:LEU:O	1:A:409:LYS:HA	2.20	0.42
1:A:443:LEU:HD12	1:A:443:LEU:H	1.84	0.42
2:C:71:CYS:N	2:C:79:SER:OG	2.32	0.42
2:C:62:THR:C	2:C:86:VAL:HG11	2.40	0.42
2:C:114:LYS:HG3	2:C:114:LYS:O	2.20	0.42
1:B:418:GLN:O	1:B:420:GLY:N	2.53	0.42
1:B:373:TYR:CD2	1:B:374:PRO:N	2.87	0.42
1:B:286:ASN:O	1:B:288:LYS:N	2.52	0.42
1:B:280:ASP:HB2	1:B:317:LYS:HD3	2.02	0.42
1:B:358:MET:HE1	1:B:417:TRP:HD1	1.85	0.42
2:C:72:GLN:CG	2:C:73:THR:N	2.83	0.42
1:B:277:TRP:HZ2	1:B:304:SER:HG	1.65	0.42
1:A:292:ARG:CD	1:A:293:GLU:N	2.83	0.42
1:A:422:VAL:CG1	1:A:423:PHE:N	2.83	0.42
1:A:242:LEU:HD12	1:A:334:LYS:O	2.20	0.42
2:C:48:LEU:HB3	2:C:49:ILE:H	1.55	0.42
1:B:399:ASP:O	1:B:401:ASP:N	2.52	0.42
1:B:242:LEU:HD21	1:B:259:VAL:HG12	2.00	0.42
1:A:442:SER:OG	1:A:443:LEU:N	2.52	0.42
1:B:279:VAL:C	1:B:281:GLY:N	2.73	0.42
2:C:5:LEU:HD11	2:C:75:LEU:HD23	2.02	0.42
1:B:418:GLN:C	1:B:420:GLY:N	2.71	0.41
1:B:350:THR:HB	1:B:441:LEU:HG	2.02	0.41
1:A:325:ASN:HD22	1:A:326:LYS:H	1.64	0.41
1:A:251:LEU:HD22	1:A:435:HIS:ND1	2.35	0.41
1:B:415:SER:O	1:B:417:TRP:N	2.52	0.41
1:A:415:SER:HA	1:A:418:GLN:NE2	2.35	0.41
1:A:429:HIS:C	1:A:431:ALA:H	2.23	0.41
1:B:251:LEU:HD21	1:B:430:GLU:CA	2.50	0.41
1:A:239:SER:HB2	1:A:264:VAL:CG2	2.51	0.41
1:B:423:PHE:O	1:B:440:SER:CA	2.63	0.41
1:A:242:LEU:HA	1:A:242:LEU:HD23	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:GLU:OE1	2:C:131:LYS:NZ	2.52	0.41
1:B:278:TYR:N	1:B:278:TYR:HD1	2.18	0.41
1:B:436:TYR:HD1	1:B:437:THR:N	2.17	0.41
1:B:393:THR:CG2	1:B:406:LEU:HD12	2.51	0.41
1:A:294:GLU:O	1:A:300:TYR:HD1	2.04	0.41
1:B:429:HIS:H	1:B:432:LEU:HD12	1.86	0.41
1:B:312:ASP:O	1:B:313:TRP:C	2.59	0.41
1:A:417:TRP:O	1:A:418:GLN:C	2.58	0.41
1:B:296:TYR:HB3	1:B:297:ASN:H	1.44	0.41
1:B:360:LYS:HZ2	1:B:360:LYS:HB3	1.86	0.41
1:A:243:PHE:CZ	3:A:452:MAN:H2	2.54	0.41
2:C:125:GLN:O	2:C:126:ASN:HB2	2.20	0.41
2:C:43:PHE:HB2	2:C:70:ARG:HB2	2.03	0.41
1:B:277:TRP:HA	1:B:320:LYS:O	2.20	0.41
1:A:243:PHE:CZ	3:A:450:BMA:H62	2.55	0.41
2:C:131:LYS:CG	2:C:133:PHE:HE1	2.34	0.41
1:A:311:GLN:OE1	1:A:311:GLN:HA	2.21	0.41
2:C:43:PHE:HE2	2:C:48:LEU:HD11	1.85	0.41
1:B:235:LEU:O	1:B:235:LEU:CG	2.68	0.41
2:C:65:ASP:O	2:C:69:TYR:HE1	2.04	0.41
1:A:406:LEU:HD12	1:A:407:TYR:O	2.21	0.41
1:A:415:SER:O	1:A:418:GLN:HB3	2.20	0.40
2:C:108:LEU:HD11	2:C:170:ILE:CD1	2.45	0.40
1:B:267:SER:O	1:B:268:HIS:C	2.59	0.40
2:C:151:SER:HA	2:C:168:VAL:O	2.22	0.40
1:A:407:TYR:HH	1:B:409:LYS:HB2	1.78	0.40
2:C:21:GLU:HB2	2:C:113:TRP:HZ3	1.87	0.40
1:B:312:ASP:O	1:B:315:ASN:HB2	2.21	0.40
1:B:346:PRO:HA	1:B:372:PHE:HB3	2.03	0.40
2:C:85:GLU:HG2	2:C:87:HIS:NE2	2.37	0.40
2:C:121:VAL:HG21	2:C:136:ASN:HA	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	208/224 (93%)	160 (77%)	24 (12%)	24 (12%)	0 7
1	B	211/224 (94%)	147 (70%)	35 (17%)	29 (14%)	0 4
2	C	165/176 (94%)	134 (81%)	20 (12%)	11 (7%)	1 19
All	All	584/624 (94%)	441 (76%)	79 (14%)	64 (11%)	0 8

All (64) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	280	ASP
1	A	287	ALA
1	A	291	PRO
1	A	408	SER
1	A	432	LEU
1	B	270	ASP
1	B	284	VAL
1	B	287	ALA
1	B	288	LYS
1	B	292	ARG
1	B	298	SER
1	B	390	ASN
1	B	433	HIS
2	C	49	ILE
2	C	50	SER
2	C	142	PRO
1	A	292	ARG
1	A	298	SER
1	A	388	GLU
1	A	390	ASN
1	A	416	ARG
1	A	420	GLY
1	A	433	HIS
1	B	235	LEU
1	B	272	GLU
1	B	283	GLU
1	B	291	PRO
1	B	293	GLU
1	B	312	ASP
1	B	369	VAL
1	B	377	ILE

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Mol	Chain	Res	Type
1	B	416	ARG
1	B	419	GLN
2	C	52	GLN
2	C	53	ALA
2	C	74	ASN
2	C	127	GLY
1	A	288	LYS
1	A	375	SER
1	A	389	ASN
1	A	401	ASP
1	B	280	ASP
1	B	310	HIS
1	B	314	LEU
1	B	326	LYS
1	B	346	PRO
1	B	400	SER
2	C	61	ALA
2	C	114	LYS
1	A	312	ASP
1	B	232	PRO
1	B	415	SER
2	C	37	ASP
1	A	297	ASN
1	A	311	GLN
1	A	402	GLY
1	B	281	GLY
2	C	95	ALA
1	A	358	MET
1	A	387	PRO
1	A	418	GLN
1	A	353	PRO
1	B	244	PRO
1	B	308	VAL

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	195/207 (94%)	173 (89%)	22 (11%)	7 34
1	B	197/207 (95%)	172 (87%)	25 (13%)	5 28
2	C	152/160 (95%)	141 (93%)	11 (7%)	18 57
All	All	544/574 (95%)	486 (89%)	58 (11%)	8 37

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	242	LEU
1	A	244	PRO
1	A	256	THR
1	A	272	GLU
1	A	284	VAL
1	A	285	HIS
1	A	288	LYS
1	A	289	THR
1	A	292	ARG
1	A	293	GLU
1	A	296	TYR
1	A	306	LEU
1	A	324	SER
1	A	325	ASN
1	A	367	CYS
1	A	368	LEU
1	A	380	GLU
1	A	391	TYR
1	A	399	ASP
1	A	409	LYS
1	A	413	ASP
1	A	432	LEU
1	B	235	LEU
1	B	242	LEU
1	B	268	HIS
1	B	270	ASP
1	B	278	TYR
1	B	284	VAL
1	B	285	HIS
1	B	286	ASN
1	B	292	ARG
1	B	299	THR
1	B	311	GLN
1	B	324	SER

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Mol	Chain	Res	Type
1	B	325	ASN
1	B	332	ILE
1	B	337	SER
1	B	342	GLN
1	B	372	PHE
1	B	373	TYR
1	B	390	ASN
1	B	405	PHE
1	B	409	LYS
1	B	421	ASN
1	B	422	VAL
1	B	438	GLN
1	B	441	LEU
2	C	15	GLN
2	C	30	GLN
2	C	62	THR
2	C	63	VAL
2	C	73	THR
2	C	77	THR
2	C	93	LEU
2	C	109	ARG
2	C	137	SER
2	C	145	THR
2	C	153	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	295	GLN
1	A	325	ASN
1	A	361	ASN
1	A	384	ASN
1	A	386	GLN
1	A	389	ASN
1	A	418	GLN
1	A	421	ASN
1	A	434	ASN
1	A	438	GLN
1	B	268	HIS
1	B	276	ASN
1	B	286	ASN
1	B	295	GLN

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Mol	Chain	Res	Type
1	B	315	ASN
1	B	325	ASN
1	B	384	ASN
1	B	386	GLN
1	B	390	ASN
1	B	418	GLN
1	B	419	GLN
1	B	438	GLN
2	C	15	GLN
2	C	72	GLN
2	C	74	ASN
2	C	87	HIS
2	C	107	HIS
2	C	119	HIS
2	C	125	GLN
2	C	140	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

16 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	$\#\|Z\| > 2$
3	NDG	A	448	1,3	14,14,15	0.57	0	15,19,21	1.35	3 (20%)
3	NAG	A	449	3	14,14,15	0.60	0	15,19,21	0.93	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	BMA	A	450	3	11,11,12	0.71	0	14,15,17	0.76	0
3	BMA	A	451	3	11,11,12	0.47	0	14,15,17	0.89	0
3	MAN	A	452	3	11,11,12	0.79	0	14,15,17	0.94	1 (7%)
3	NDG	A	453	3	14,14,15	0.77	0	15,19,21	1.10	2 (13%)
3	GAL	A	454	3	11,11,12	0.67	0	14,15,17	0.57	0
3	FUL	A	455	3	10,10,11	0.64	0	14,14,16	0.74	0
4	NDG	B	448	1,4	14,14,15	1.13	1 (7%)	15,19,21	1.43	3 (20%)
4	NDG	B	449	4	14,14,15	0.65	0	15,19,21	1.20	1 (6%)
4	BMA	B	450	4	11,11,12	0.53	0	14,15,17	0.56	0
4	MAN	B	451	4	11,11,12	0.63	0	14,15,17	0.75	0
4	MAN	B	452	4	11,11,12	0.57	0	14,15,17	0.58	0
4	NAG	B	453	4	14,14,15	0.79	0	15,19,21	1.57	2 (13%)
4	NAG	B	454	4	14,14,15	0.54	0	15,19,21	0.88	1 (6%)
4	FUC	B	455	4	10,10,11	0.61	0	14,14,16	0.72	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
3	NDG	A	448	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	449	3	-	0/6/23/26	0/1/1/1
3	BMA	A	450	3	-	0/2/19/22	0/1/1/1
3	BMA	A	451	3	-	0/2/19/22	0/1/1/1
3	MAN	A	452	3	-	0/2/19/22	0/1/1/1
3	NDG	A	453	3	-	0/6/23/26	0/1/1/1
3	GAL	A	454	3	-	0/2/19/22	0/1/1/1
3	FUL	A	455	3	-	0/0/17/20	0/1/1/1
4	NDG	B	448	1,4	-	0/6/23/26	0/1/1/1
4	NDG	B	449	4	-	0/6/23/26	0/1/1/1
4	BMA	B	450	4	-	0/2/19/22	0/1/1/1
4	MAN	B	451	4	-	0/2/19/22	0/1/1/1
4	MAN	B	452	4	-	0/2/19/22	0/1/1/1
4	NAG	B	453	4	-	2/6/23/26	0/1/1/1
4	NAG	B	454	4	-	0/6/23/26	0/1/1/1
4	FUC	B	455	4	1/1/4/5	0/0/17/20	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	448	NDG	C1-C2	2.72	1.56	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	453	NAG	C4-C3-C2	-4.09	104.88	111.23
4	B	453	NAG	C2-N2-C7	-3.79	118.17	123.04
4	B	449	NDG	C2-N2-C7	-3.33	118.76	123.04
3	A	448	NDG	C2-N2-C7	-2.90	119.32	123.04
4	B	448	NDG	C4-C3-C2	-2.82	106.85	111.23
4	B	454	NAG	C2-N2-C7	-2.68	119.60	123.04
3	A	453	NDG	C2-N2-C7	-2.62	119.68	123.04
3	A	449	NAG	C2-N2-C7	-2.48	119.86	123.04
4	B	448	NDG	C2-N2-C7	-2.36	120.01	123.04
3	A	448	NDG	C4-C3-C2	-2.04	108.05	111.23
3	A	453	NDG	C1-O-C5	2.11	114.92	112.25
3	A	452	MAN	C1-O5-C5	2.15	114.98	112.25
4	B	448	NDG	C1-O-C5	2.87	115.89	112.25
3	A	448	NDG	C1-O-C5	2.94	115.98	112.25

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	455	FUC	C1

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	453	NAG	O7-C7-N2-C2
4	B	453	NAG	C8-C7-N2-C2

There are no ring outliers.

11 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	448	NDG	2	0
3	A	449	NAG	2	0
3	A	450	BMA	1	0
3	A	452	MAN	6	0
3	A	453	NDG	5	0
4	B	448	NDG	2	0
4	B	449	NDG	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	450	BMA	2	0
4	B	452	MAN	3	0
4	B	453	NAG	2	0
4	B	455	FUC	2	0

5.6 Ligand geometry (i)

There are no ligands in this entry.

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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.