



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:25 PM GMT

PDB ID : 1OW0  
Title : Crystal structure of human FcαRI bound to IgA1-Fc  
Authors : Herr, A.B.; Ballister, E.R.; Bjorkman, P.J.  
Deposited on : 2003-03-27  
Resolution : 3.10 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

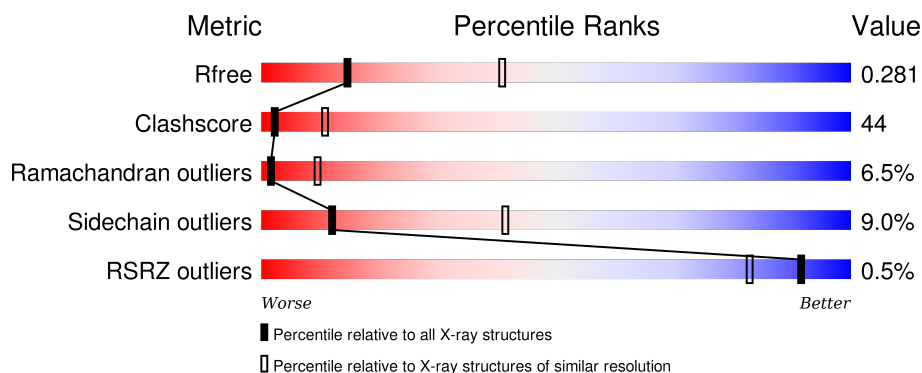
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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	214	
1	B	214	
2	C	207	
2	D	207	

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	NAG	A	500	-	-	-	X
3	NAG	A	505	-	-	X	-
4	NAG	B	600	-	-	-	X
4	FUC	B	601	X	-	-	-
4	NAG	B	605	-	-	X	-

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6280 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 Ig alpha-1 chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	209	Total	C	N	O	S	0	0	0
			1435	913	245	270	7			
1	B	209	Total	C	N	O	S	0	0	0
			1435	913	245	270	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	241	ALA	CYS	ENGINEERED	UNP P01876
B	241	ALA	CYS	ENGINEERED	UNP P01876

- Molecule 2 is a protein called Immunoglobulin alpha Fc receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	190	Total	C	N	O	S	0	0	0
			1414	914	239	255	6			
2	D	190	Total	C	N	O	S	0	0	0
			1414	914	239	255	6			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	196	ALA	-	EXPRESSION TAG	UNP P24071
C	197	ILE	-	EXPRESSION TAG	UNP P24071
C	198	ASP	-	EXPRESSION TAG	UNP P24071
C	199	GLY	-	EXPRESSION TAG	UNP P24071
C	200	ARG	-	EXPRESSION TAG	UNP P24071
C	201	ALA	-	EXPRESSION TAG	UNP P24071
C	202	HIS	-	EXPRESSION TAG	UNP P24071
C	203	HIS	-	EXPRESSION TAG	UNP P24071
C	204	HIS	-	EXPRESSION TAG	UNP P24071
C	205	HIS	-	EXPRESSION TAG	UNP P24071

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Chain	Residue	Modelled	Actual	Comment	Reference
C	206	HIS	-	EXPRESSION TAG	UNP P24071
C	207	HIS	-	EXPRESSION TAG	UNP P24071
D	196	ALA	-	EXPRESSION TAG	UNP P24071
D	197	ILE	-	EXPRESSION TAG	UNP P24071
D	198	ASP	-	EXPRESSION TAG	UNP P24071
D	199	GLY	-	EXPRESSION TAG	UNP P24071
D	200	ARG	-	EXPRESSION TAG	UNP P24071
D	201	ALA	-	EXPRESSION TAG	UNP P24071
D	202	HIS	-	EXPRESSION TAG	UNP P24071
D	203	HIS	-	EXPRESSION TAG	UNP P24071
D	204	HIS	-	EXPRESSION TAG	UNP P24071
D	205	HIS	-	EXPRESSION TAG	UNP P24071
D	206	HIS	-	EXPRESSION TAG	UNP P24071
D	207	HIS	-	EXPRESSION TAG	UNP P24071

- 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
			105	59	4	42		

- 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
			105	59	4	42		

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



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

- Molecule 6 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	5	Total	C	N	O	0	0
			61	34	2	25		
6	D	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 7 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	3	Total	C	N	O	0	0
			39	22	2	15		
7	D	3	Total	C	N	O	0	0
			39	22	2	15		

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	C	6	Total	C	N	O	0	0
			72	40	2	30		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	D	6	Total	C	N	O	0	0
			72	40	2	30		

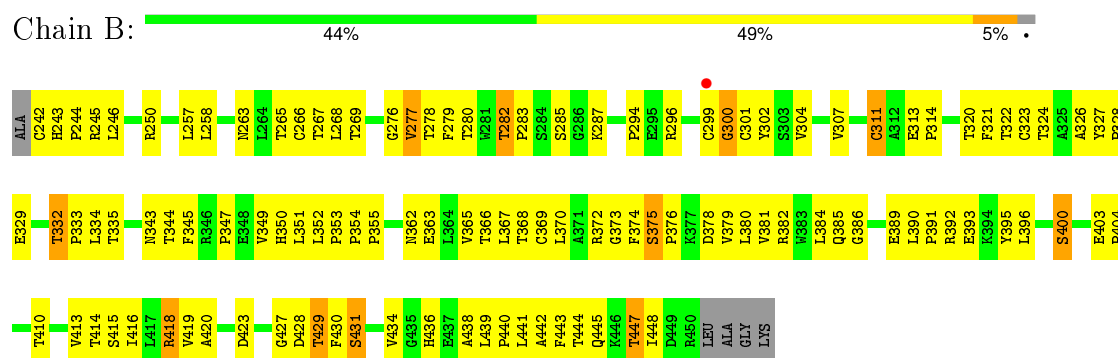
### 3 Residue-property plots

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.

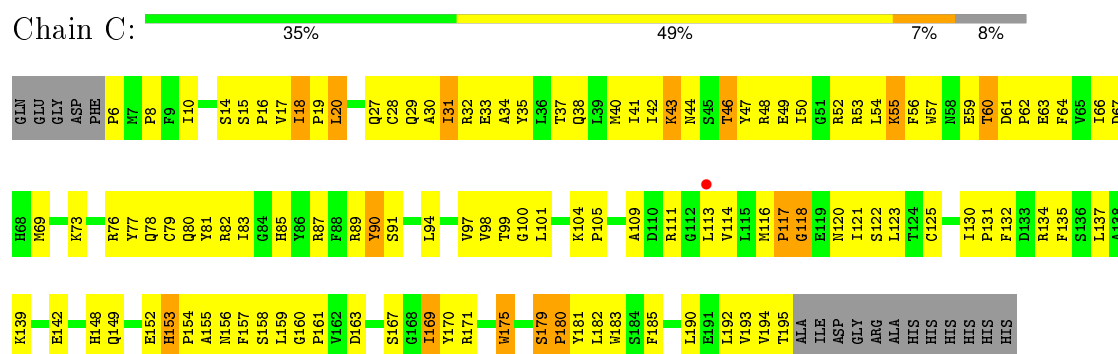
#### • Molecule 1: Ig alpha-1 chain C region



#### • Molecule 1: Ig alpha-1 chain C region

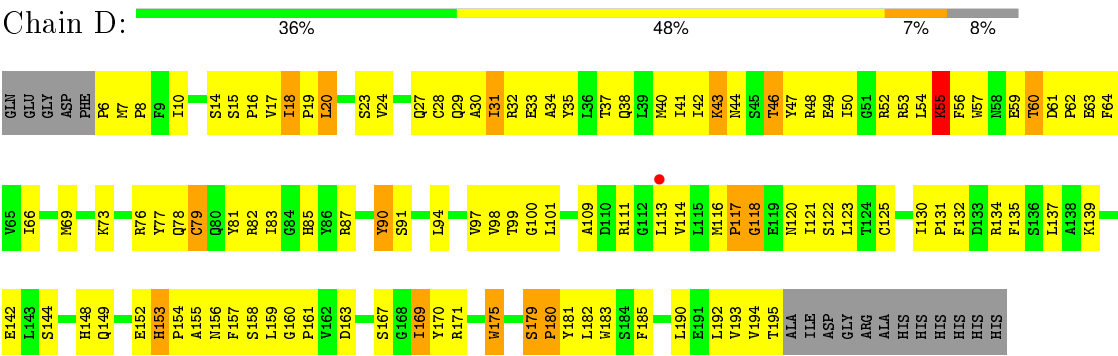


#### • Molecule 2: Immunoglobulin alpha Fc receptor





● Molecule 2: Immunoglobulin alpha Fc receptor



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	142.99 Å   142.99 Å   67.66 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	29.69 – 3.10 29.69 – 3.06	Depositor EDS
% Data completeness (in resolution range)	95.2 (29.69-3.10) 93.7 (29.69-3.06)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.32 (at 3.06 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.252 , 0.284 0.249 , 0.281	Depositor DCC
$R_{free}$ test set	1300 reflections (4.87%)	DCC
Wilson B-factor (Å <sup>2</sup> )	83.2	Xtriage
Anisotropy	0.637	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 68.6	EDS
Estimated twinning fraction	0.027 for -h,-k,l 0.458 for h,-h-k,-l 0.026 for -k,-h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 27262 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6280	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, NDG, SIA, 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	0.47	0/1474	0.74	0/2041
1	B	0.45	0/1474	0.73	0/2041
2	C	0.47	0/1454	0.70	1/1989 (0.1%)
2	D	0.45	0/1454	0.70	1/1989 (0.1%)
All	All	0.46	0/5856	0.72	2/8060 (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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	C	6	PRO	N-CA-CB	6.07	110.59	103.30
2	D	6	PRO	N-CA-CB	6.04	110.55	103.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	601	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	1435	0	1279	130	0
1	B	1435	0	1279	128	0
2	C	1414	0	1295	126	0
2	D	1414	0	1295	125	0
3	A	105	0	89	20	0
4	B	105	0	89	22	0
5	C	14	0	13	2	0
5	D	14	0	13	2	0
6	C	61	0	52	3	0
6	D	61	0	52	3	0
7	C	39	0	34	1	0
7	D	39	0	34	1	0
8	C	72	0	61	2	0
8	D	72	0	61	2	0
All	All	6280	0	5646	523	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 44.

All (523) 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:B:345:PHE:H	1:B:375:SER:HB2	1.16	1.06
1:A:345:PHE:H	1:A:375:SER:HB2	1.14	1.05
1:A:345:PHE:H	1:A:375:SER:CB	1.78	0.96
1:B:345:PHE:H	1:B:375:SER:CB	1.80	0.94
1:B:391:PRO:HA	4:B:606:GAL:H62	1.48	0.94
1:A:282:THR:OG1	1:A:283:PRO:HD3	1.68	0.94
1:B:282:THR:OG1	1:B:283:PRO:HD3	1.68	0.94
2:C:109:ALA:HB2	2:C:123:LEU:HD23	1.49	0.94
1:A:345:PHE:N	1:A:375:SER:HB2	1.83	0.94
1:B:375:SER:CB	1:B:376:PRO:HD3	1.98	0.93
1:A:391:PRO:HA	3:A:506:GAL:H62	1.48	0.93
2:D:109:ALA:HB2	2:D:123:LEU:HD23	1.51	0.93
2:D:179:SER:HB2	2:D:182:LEU:HD12	1.51	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:345:PHE:N	1:B:375:SER:HB2	1.84	0.91
1:B:375:SER:OG	1:B:376:PRO:HD3	1.71	0.90
6:C:722:MAN:H61	6:C:723:BMA:O2	1.70	0.90
1:A:375:SER:CB	1:A:376:PRO:HD3	2.01	0.89
2:C:179:SER:HB2	2:C:182:LEU:HD12	1.53	0.89
1:A:344:THR:HA	1:A:375:SER:OG	1.73	0.89
6:D:822:MAN:H61	6:D:823:BMA:O2	1.70	0.88
1:A:375:SER:OG	1:A:376:PRO:HD3	1.74	0.87
2:C:69:MET:HG3	2:C:98:VAL:HG12	1.56	0.87
2:D:69:MET:HG3	2:D:98:VAL:HG12	1.56	0.86
1:B:344:THR:HA	1:B:375:SER:OG	1.75	0.86
1:B:382:ARG:NH2	4:B:605:NAG:HN2	1.76	0.84
1:A:441:LEU:O	1:A:443:PHE:N	2.14	0.81
1:A:382:ARG:NH2	3:A:505:NAG:HN2	1.78	0.80
1:B:353:PRO:HG3	1:B:448:ILE:HD11	1.63	0.79
2:C:153:HIS:CB	2:C:154:PRO:HD3	2.12	0.78
2:C:169:ILE:HD11	2:C:171:ARG:NH2	1.99	0.78
2:C:101:LEU:HD11	2:C:182:LEU:HD22	1.66	0.77
1:A:353:PRO:HG3	1:A:448:ILE:HD11	1.64	0.77
2:D:153:HIS:CB	2:D:154:PRO:HD3	2.13	0.77
1:A:263:ASN:HB2	3:A:500:NAG:O7	1.85	0.77
1:B:375:SER:HB3	1:B:376:PRO:HD3	1.65	0.76
1:A:375:SER:HB3	1:A:376:PRO:HD3	1.68	0.76
2:D:169:ILE:HD11	2:D:171:ARG:NH2	2.00	0.76
2:C:34:ALA:HB2	2:C:83:ILE:HD13	1.67	0.75
1:B:263:ASN:HB2	4:B:600:NAG:O7	1.86	0.75
1:B:419:VAL:HG11	1:B:430:PHE:CZ	2.22	0.75
1:A:419:VAL:HG11	1:A:430:PHE:CZ	2.22	0.74
2:D:101:LEU:HD11	2:D:182:LEU:HD22	1.67	0.74
2:D:34:ALA:HB2	2:D:83:ILE:HD13	1.69	0.74
2:C:20:LEU:HD21	2:C:101:LEU:HD21	1.70	0.74
2:C:8:PRO:HD2	2:C:91:SER:HA	1.70	0.73
2:D:20:LEU:HD21	2:D:101:LEU:HD21	1.70	0.73
2:D:8:PRO:HD2	2:D:91:SER:HA	1.70	0.73
1:B:441:LEU:O	1:B:443:PHE:N	2.16	0.73
4:B:603:BMA:H4	4:B:605:NAG:H61	1.71	0.73
3:A:503:BMA:H4	3:A:505:NAG:H61	1.70	0.73
3:A:507:SIA:HN5	3:A:507:SIA:H8	1.54	0.72
4:B:607:SIA:H8	4:B:607:SIA:HN5	1.54	0.72
1:A:263:ASN:HB2	3:A:500:NAG:C7	2.20	0.72
2:D:31:ILE:HG23	2:D:31:ILE:O	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:374:PHE:HZ	1:B:413:VAL:HG23	1.55	0.71
1:B:263:ASN:HB2	4:B:600:NAG:C7	2.21	0.70
2:D:60:THR:HG22	2:D:61:ASP:H	1.56	0.70
1:B:375:SER:CB	1:B:376:PRO:CD	2.69	0.70
2:C:158:SER:O	2:C:159:LEU:HD23	1.92	0.70
2:D:43:LYS:O	2:D:46:THR:HG23	1.92	0.69
2:C:101:LEU:HD12	2:C:182:LEU:HB3	1.74	0.69
2:C:43:LYS:O	2:C:46:THR:HG23	1.92	0.69
2:C:31:ILE:O	2:C:31:ILE:HG23	1.91	0.68
1:B:353:PRO:HG3	1:B:448:ILE:CD1	2.24	0.68
2:D:158:SER:O	2:D:159:LEU:HD23	1.93	0.68
1:A:374:PHE:HZ	1:A:413:VAL:HG23	1.59	0.68
2:C:60:THR:HG22	2:C:61:ASP:H	1.58	0.68
2:C:66:ILE:HG23	2:C:73:LYS:HZ3	1.57	0.68
2:D:101:LEU:HD12	2:D:182:LEU:HB3	1.75	0.68
2:C:8:PRO:HA	2:C:29:GLN:OE1	1.94	0.67
1:A:384:LEU:HD23	1:A:389:GLU:HA	1.76	0.67
2:C:33:GLU:O	2:C:83:ILE:HG23	1.95	0.67
1:A:375:SER:CB	1:A:376:PRO:CD	2.73	0.67
2:C:18:ILE:HG22	2:C:19:PRO:HD2	1.75	0.67
1:A:353:PRO:HG3	1:A:448:ILE:CD1	2.24	0.67
2:D:8:PRO:HA	2:D:29:GLN:OE1	1.94	0.67
1:A:314:PRO:HB2	1:A:321:PHE:CZ	2.30	0.67
2:D:18:ILE:HG22	2:D:19:PRO:HD2	1.76	0.67
6:C:720:NAG:O6	6:C:721:NAG:H82	1.96	0.66
1:B:385:GLN:HB3	1:B:390:LEU:HD21	1.78	0.66
1:B:382:ARG:HG2	1:B:382:ARG:HH11	1.60	0.66
2:D:98:VAL:CG2	2:D:182:LEU:HD23	2.26	0.66
1:A:385:GLN:HB3	1:A:390:LEU:HD21	1.76	0.66
1:B:384:LEU:HD23	1:B:389:GLU:HA	1.77	0.66
1:B:418:ARG:HG3	1:B:418:ARG:HH11	1.61	0.66
2:C:117:PRO:HD3	2:C:195:THR:O	1.95	0.66
2:D:8:PRO:O	2:D:91:SER:HB2	1.96	0.65
6:D:820:NAG:O6	6:D:821:NAG:H82	1.97	0.65
2:C:98:VAL:CG2	2:C:182:LEU:HD23	2.25	0.65
1:A:263:ASN:H	3:A:500:NAG:HN2	1.45	0.65
2:D:117:PRO:HD3	2:D:195:THR:O	1.96	0.65
1:B:314:PRO:HB2	1:B:321:PHE:CZ	2.32	0.65
2:C:179:SER:N	2:C:180:PRO:HD3	2.12	0.65
2:D:109:ALA:HB2	2:D:123:LEU:CD2	2.26	0.64
2:C:57:TRP:NE1	2:C:62:PRO:HG3	2.11	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:109:ALA:HB2	2:C:123:LEU:CD2	2.26	0.64
1:A:418:ARG:HH11	1:A:418:ARG:HG3	1.61	0.64
1:B:344:THR:HA	1:B:375:SER:HG	1.63	0.64
2:D:33:GLU:O	2:D:83:ILE:HG23	1.97	0.64
1:B:263:ASN:H	4:B:600:NAG:HN2	1.46	0.64
1:A:391:PRO:HA	3:A:506:GAL:C6	2.26	0.64
2:D:90:TYR:N	2:D:90:TYR:CD1	2.65	0.63
1:B:400:SER:HA	1:B:413:VAL:HG22	1.80	0.63
1:B:418:ARG:NH1	1:B:418:ARG:HG3	2.13	0.63
2:C:122:SER:HA	2:C:157:PHE:O	1.98	0.63
2:D:179:SER:N	2:D:180:PRO:HD3	2.13	0.63
2:C:8:PRO:O	2:C:91:SER:HB2	1.98	0.63
2:C:54:LEU:O	2:C:55:LYS:HB3	1.98	0.63
2:D:122:SER:HA	2:D:157:PHE:O	1.98	0.63
1:A:282:THR:HG23	1:A:322:THR:HB	1.81	0.63
1:A:418:ARG:HG3	1:A:418:ARG:NH1	2.14	0.63
1:A:382:ARG:HH11	1:A:382:ARG:HG2	1.62	0.63
2:C:179:SER:O	2:C:181:TYR:N	2.32	0.63
1:A:431:SER:OG	1:A:447:THR:HG23	1.99	0.62
1:A:282:THR:CB	1:A:283:PRO:HD3	2.29	0.62
1:B:282:THR:CB	1:B:283:PRO:HD3	2.30	0.62
1:B:282:THR:HG23	1:B:322:THR:HB	1.80	0.62
2:D:57:TRP:NE1	2:D:62:PRO:HG3	2.15	0.62
2:D:42:ILE:H	2:D:42:ILE:HD12	1.64	0.62
1:A:345:PHE:H	1:A:375:SER:CA	2.12	0.61
1:A:400:SER:HA	1:A:413:VAL:HG22	1.82	0.61
2:C:90:TYR:N	2:C:90:TYR:CD1	2.65	0.61
2:D:66:ILE:HG23	2:D:73:LYS:HZ3	1.64	0.61
2:D:111:ARG:HG2	2:D:121:ILE:HG13	1.82	0.61
1:B:391:PRO:HA	4:B:606:GAL:C6	2.26	0.61
2:D:43:LYS:O	2:D:44:ASN:HB2	1.99	0.61
2:D:179:SER:O	2:D:181:TYR:N	2.34	0.61
1:A:385:GLN:CB	1:A:390:LEU:HD21	2.31	0.61
2:C:42:ILE:H	2:C:42:ILE:HD12	1.66	0.61
1:B:345:PHE:H	1:B:375:SER:CA	2.13	0.61
1:B:385:GLN:CB	1:B:390:LEU:HD21	2.30	0.60
1:B:375:SER:HB3	1:B:376:PRO:CD	2.31	0.60
2:D:44:ASN:HA	5:D:810:NAG:H82	1.84	0.60
2:D:101:LEU:CD1	2:D:182:LEU:HD22	2.32	0.60
1:A:300:GLY:O	1:A:302:TYR:N	2.30	0.60
2:C:55:LYS:HD3	2:C:56:PHE:O	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:604:BMA:H3	4:B:605:NAG:O7	2.02	0.60
2:D:100:GLY:HA2	2:D:185:PHE:CD1	2.37	0.60
1:B:300:GLY:O	1:B:302:TYR:N	2.31	0.60
3:A:504:BMA:H3	3:A:505:NAG:O7	2.01	0.59
2:C:44:ASN:HA	5:C:710:NAG:H82	1.84	0.59
1:A:278:THR:HG22	1:A:279:PHE:N	2.17	0.59
1:B:277:VAL:HG12	1:B:327:TYR:HB3	1.84	0.59
1:A:392:ARG:CB	3:A:505:NAG:H83	2.33	0.59
2:C:100:GLY:HA2	2:C:185:PHE:CD1	2.38	0.59
1:B:354:PRO:HG3	1:B:367:LEU:HD23	1.85	0.59
2:C:111:ARG:HG2	2:C:121:ILE:HG13	1.84	0.59
1:B:278:THR:HG22	1:B:279:PHE:H	1.67	0.59
1:B:278:THR:HG22	1:B:279:PHE:N	2.17	0.59
2:C:18:ILE:O	2:C:98:VAL:HA	2.02	0.59
1:A:278:THR:HG22	1:A:279:PHE:H	1.66	0.59
2:D:113:LEU:HD21	2:D:190:LEU:HB3	1.84	0.59
1:A:282:THR:CG2	1:A:322:THR:HB	2.33	0.59
2:C:34:ALA:HB2	2:C:83:ILE:CD1	2.32	0.59
2:C:43:LYS:O	2:C:44:ASN:HB2	2.01	0.59
2:C:101:LEU:CD1	2:C:182:LEU:HD22	2.31	0.59
2:D:54:LEU:O	2:D:55:LYS:HB3	2.03	0.59
2:D:18:ILE:O	2:D:98:VAL:HA	2.03	0.58
1:B:282:THR:CG2	1:B:322:THR:HB	2.34	0.58
1:B:379:VAL:HG21	1:B:413:VAL:HG21	1.84	0.58
2:C:113:LEU:HD21	2:C:190:LEU:HB3	1.84	0.58
1:A:311:CYS:O	1:A:314:PRO:HD2	2.04	0.58
1:A:354:PRO:HG3	1:A:367:LEU:HD23	1.85	0.58
1:B:375:SER:OG	1:B:376:PRO:CD	2.49	0.58
1:B:382:ARG:HG2	1:B:382:ARG:NH1	2.19	0.58
2:C:153:HIS:CB	2:C:154:PRO:CD	2.82	0.58
1:A:386:GLY:HA2	1:A:429:THR:HG23	1.85	0.58
2:C:57:TRP:CE2	2:C:62:PRO:HG3	2.39	0.58
2:D:169:ILE:HD11	2:D:171:ARG:CZ	2.34	0.57
3:A:507:SIA:O1B	3:A:507:SIA:H4	2.04	0.57
2:D:57:TRP:CE2	2:D:62:PRO:HG3	2.39	0.57
2:C:66:ILE:HG23	2:C:73:LYS:NZ	2.19	0.57
2:D:116:MET:O	2:D:118:GLY:N	2.37	0.57
1:B:419:VAL:HG21	1:B:430:PHE:CE2	2.40	0.57
2:C:116:MET:O	2:C:118:GLY:N	2.38	0.57
1:A:277:VAL:HG12	1:A:327:TYR:HB3	1.84	0.57
1:A:263:ASN:ND2	3:A:500:NAG:C1	2.67	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:431:SER:OG	1:B:447:THR:HG23	2.04	0.57
1:B:386:GLY:HA2	1:B:429:THR:HG23	1.85	0.57
2:D:69:MET:HG3	2:D:98:VAL:CG1	2.33	0.57
1:A:379:VAL:HG21	1:A:413:VAL:HG21	1.85	0.57
4:B:607:SIA:H4	4:B:607:SIA:O1B	2.05	0.57
2:D:167:SER:HB2	2:D:194:VAL:H	1.69	0.57
1:A:344:THR:HA	1:A:375:SER:HG	1.67	0.57
2:D:149:GLN:O	2:D:149:GLN:HG3	2.04	0.56
1:B:263:ASN:ND2	4:B:600:NAG:C1	2.68	0.56
1:A:245:ARG:O	1:A:268:LEU:HD12	2.05	0.56
2:C:149:GLN:HG3	2:C:149:GLN:O	2.04	0.56
1:A:375:SER:HB3	1:A:376:PRO:CD	2.33	0.56
2:C:169:ILE:HD11	2:C:171:ARG:CZ	2.34	0.56
2:D:42:ILE:HD12	2:D:42:ILE:N	2.20	0.56
2:C:139:LYS:O	2:C:142:GLU:HG2	2.06	0.56
1:B:392:ARG:CB	4:B:605:NAG:H83	2.36	0.56
1:A:419:VAL:HG21	1:A:430:PHE:CE2	2.41	0.56
1:B:378:ASP:O	1:B:379:VAL:HG13	2.06	0.56
1:B:321:PHE:N	1:B:321:PHE:CD1	2.74	0.56
2:D:15:SER:OG	2:D:17:VAL:HG22	2.06	0.56
2:D:139:LYS:O	2:D:142:GLU:HG2	2.06	0.56
2:D:55:LYS:HD3	2:D:56:PHE:O	2.06	0.55
2:C:42:ILE:N	2:C:42:ILE:HD12	2.22	0.55
1:A:354:PRO:HG3	1:A:367:LEU:CD2	2.37	0.55
1:B:372:ARG:NH1	1:B:403:GLU:OE1	2.38	0.55
2:C:167:SER:HB2	2:C:194:VAL:H	1.70	0.55
1:A:382:ARG:HG2	1:A:382:ARG:NH1	2.20	0.55
1:B:285:SER:C	1:B:287:LYS:H	2.10	0.55
2:D:179:SER:H	2:D:180:PRO:HD3	1.72	0.55
1:A:375:SER:HB3	1:A:436:HIS:NE2	2.21	0.55
1:B:354:PRO:HG3	1:B:367:LEU:CD2	2.37	0.55
2:C:179:SER:H	2:C:180:PRO:HD3	1.70	0.55
1:A:372:ARG:NH1	1:A:403:GLU:OE1	2.41	0.54
1:A:372:ARG:NH1	1:A:372:ARG:HG2	2.22	0.54
2:D:34:ALA:HB2	2:D:83:ILE:CD1	2.35	0.54
1:B:311:CYS:O	1:B:314:PRO:HD2	2.07	0.54
2:C:44:ASN:HD22	5:C:710:NAG:H82	1.73	0.54
1:B:372:ARG:NH1	1:B:372:ARG:HG2	2.21	0.54
2:D:66:ILE:HG23	2:D:73:LYS:NZ	2.22	0.54
2:D:40:MET:CE	2:D:47:TYR:HB3	2.38	0.54
1:A:321:PHE:CD1	1:A:321:PHE:N	2.75	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:PRO:HB2	1:A:321:PHE:HZ	1.70	0.54
1:B:245:ARG:O	1:B:268:LEU:HD12	2.08	0.53
1:B:375:SER:HB3	1:B:436:HIS:NE2	2.24	0.53
1:A:431:SER:CB	1:A:447:THR:HG23	2.38	0.53
2:D:44:ASN:HD22	5:D:810:NAG:H82	1.73	0.53
1:A:285:SER:C	1:A:287:LYS:H	2.11	0.53
1:A:344:THR:CA	1:A:375:SER:OG	2.50	0.53
2:C:15:SER:OG	2:C:17:VAL:HG22	2.08	0.52
1:A:355:PRO:HG3	1:B:352:LEU:HD21	1.91	0.52
2:C:175:TRP:NE1	2:C:183:TRP:NE1	2.58	0.52
2:D:153:HIS:CB	2:D:154:PRO:CD	2.83	0.52
2:C:40:MET:CE	2:C:47:TYR:HB3	2.38	0.52
1:B:395:TYR:HE1	4:B:605:NAG:H81	1.74	0.52
1:B:314:PRO:HB2	1:B:321:PHE:HZ	1.73	0.52
1:A:246:LEU:HD11	1:A:266:CYS:SG	2.50	0.52
2:C:19:PRO:O	2:C:20:LEU:C	2.46	0.52
6:D:822:MAN:C6	6:D:823:BMA:O2	2.52	0.52
1:B:431:SER:CB	1:B:447:THR:HG23	2.40	0.52
2:D:167:SER:OG	2:D:193:VAL:HA	2.10	0.52
2:D:27:GLN:HE21	2:D:63:GLU:HG3	1.74	0.52
1:A:352:LEU:HD21	1:B:355:PRO:HG3	1.92	0.51
1:B:257:LEU:O	1:B:258:LEU:HD23	2.10	0.51
1:A:395:TYR:HE1	3:A:505:NAG:H81	1.74	0.51
2:D:19:PRO:O	2:D:20:LEU:C	2.49	0.51
1:B:366:THR:OG1	1:B:418:ARG:HD3	2.11	0.51
2:D:66:ILE:N	2:D:66:ILE:HD12	2.26	0.51
2:D:179:SER:N	2:D:180:PRO:CD	2.74	0.51
2:C:167:SER:OG	2:C:193:VAL:HA	2.11	0.51
2:C:179:SER:N	2:C:180:PRO:CD	2.73	0.50
2:C:69:MET:HG3	2:C:98:VAL:CG1	2.35	0.50
2:C:27:GLN:HE21	2:C:63:GLU:HG3	1.75	0.50
2:C:35:TYR:OH	2:C:82:ARG:NH1	2.44	0.50
4:B:606:GAL:O2	4:B:607:SIA:H32	2.11	0.50
1:A:242:CYS:SG	1:A:243:HIS:N	2.85	0.50
2:D:98:VAL:HG21	2:D:182:LEU:HD23	1.93	0.50
2:C:41:ILE:HD12	2:C:77:TYR:CZ	2.47	0.50
2:D:41:ILE:HD12	2:D:77:TYR:CZ	2.45	0.50
2:D:28:CYS:O	2:D:62:PRO:HD2	2.11	0.50
3:A:506:GAL:O2	3:A:507:SIA:H32	2.11	0.50
1:B:246:LEU:HD11	1:B:266:CYS:SG	2.51	0.50
2:C:31:ILE:HG23	2:C:34:ALA:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:17:VAL:HG12	2:D:97:VAL:CG2	2.42	0.49
1:B:268:LEU:HD11	1:B:334:LEU:HD12	1.94	0.49
2:D:31:ILE:HG21	2:D:81:TYR:CD2	2.47	0.49
1:A:268:LEU:HD11	1:A:334:LEU:HD12	1.94	0.49
1:A:418:ARG:HH11	1:A:418:ARG:CG	2.24	0.49
2:D:37:THR:HB	2:D:53:ARG:HB2	1.94	0.49
2:D:76:ARG:HA	2:D:94:LEU:O	2.13	0.49
1:B:324:THR:HG22	1:B:335:THR:OG1	2.12	0.49
1:B:391:PRO:O	1:B:392:ARG:C	2.49	0.49
2:C:66:ILE:N	2:C:66:ILE:HD12	2.28	0.49
1:B:347:PRO:HG3	1:B:374:PHE:CB	2.43	0.49
2:D:42:ILE:HG22	2:D:43:LYS:N	2.27	0.49
2:D:121:ILE:HG12	2:D:122:SER:N	2.27	0.49
2:D:38:GLN:NE2	2:D:49:GLU:OE1	2.32	0.49
2:C:37:THR:HB	2:C:53:ARG:HB2	1.95	0.49
1:A:371:ALA:O	1:A:374:PHE:HE2	1.96	0.49
2:C:98:VAL:HG21	2:C:182:LEU:HD23	1.92	0.49
1:B:418:ARG:CG	1:B:418:ARG:HH11	2.25	0.49
1:B:344:THR:CA	1:B:375:SER:OG	2.53	0.49
1:A:436:HIS:HD2	1:A:438:ALA:HB3	1.76	0.49
1:A:245:ARG:N	1:A:269:THR:O	2.44	0.49
1:B:242:CYS:SG	1:B:243:HIS:N	2.85	0.49
2:C:137:LEU:HD11	2:C:170:TYR:HB3	1.95	0.48
1:A:404:PRO:HD3	1:B:396:LEU:HB2	1.95	0.48
2:C:10:ILE:O	2:C:10:ILE:HG23	2.13	0.48
1:A:347:PRO:HG3	1:A:374:PHE:CB	2.42	0.48
1:B:282:THR:HG1	1:B:283:PRO:HD3	1.76	0.48
2:C:18:ILE:HG22	2:C:19:PRO:CD	2.42	0.48
1:B:263:ASN:HB2	4:B:600:NAG:N2	2.29	0.48
1:B:419:VAL:CG1	1:B:420:ALA:N	2.76	0.48
2:C:42:ILE:HG22	2:C:43:LYS:N	2.28	0.48
1:B:321:PHE:HD1	1:B:321:PHE:H	1.60	0.48
1:A:327:TYR:HB2	1:A:328:PRO:HD2	1.95	0.48
2:C:40:MET:HE2	2:C:47:TYR:HB3	1.95	0.48
2:D:175:TRP:NE1	2:D:183:TRP:NE1	2.61	0.48
2:D:137:LEU:HD11	2:D:170:TYR:HB3	1.95	0.48
1:B:322:THR:HG22	1:B:323:CYS:N	2.27	0.48
1:A:419:VAL:CG1	1:A:420:ALA:N	2.76	0.48
1:A:257:LEU:O	1:A:258:LEU:HD23	2.13	0.48
2:C:76:ARG:HA	2:C:94:LEU:O	2.13	0.48
1:B:245:ARG:N	1:B:269:THR:O	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:PHE:HD1	1:A:321:PHE:H	1.61	0.48
8:D:844:BMA:H62	8:D:845:BMA:O5	2.13	0.48
2:D:31:ILE:HG23	2:D:34:ALA:HB3	1.95	0.48
1:B:391:PRO:C	1:B:393:GLU:N	2.65	0.48
2:D:15:SER:OG	2:D:17:VAL:CG2	2.61	0.48
2:C:15:SER:OG	2:C:17:VAL:CG2	2.62	0.48
2:D:130:ILE:HA	2:D:131:PRO:HD3	1.62	0.48
1:B:368:THR:HG23	1:B:416:ILE:HD11	1.96	0.48
2:D:10:ILE:HG23	2:D:10:ILE:O	2.14	0.48
8:C:744:BMA:H62	8:C:745:BMA:O5	2.14	0.48
1:A:263:ASN:HB2	3:A:500:NAG:N2	2.28	0.47
2:D:130:ILE:HG21	2:D:132:PHE:CZ	2.49	0.47
1:B:327:TYR:HB2	1:B:328:PRO:HD2	1.95	0.47
2:C:90:TYR:HD1	2:C:90:TYR:N	2.11	0.47
2:D:179:SER:CB	2:D:182:LEU:HD12	2.33	0.47
1:B:395:TYR:HE1	4:B:605:NAG:C8	2.28	0.47
1:A:391:PRO:O	1:A:392:ARG:C	2.53	0.47
1:A:372:ARG:HH11	1:A:372:ARG:HG2	1.79	0.47
1:B:372:ARG:HH11	1:B:372:ARG:HG2	1.79	0.47
2:D:18:ILE:HG22	2:D:19:PRO:CD	2.43	0.47
1:A:324:THR:HG22	1:A:335:THR:OG1	2.15	0.47
1:B:380:LEU:O	1:B:434:VAL:HA	2.15	0.47
1:A:378:ASP:O	1:A:379:VAL:HG13	2.15	0.47
1:B:392:ARG:CB	4:B:605:NAG:O3	2.63	0.46
2:C:17:VAL:HG12	2:C:97:VAL:CG2	2.44	0.46
8:D:843:MAN:O3	8:D:844:BMA:C1	2.63	0.46
1:B:350:HIS:HB2	1:B:370:LEU:HB3	1.97	0.46
1:A:380:LEU:O	1:A:434:VAL:HA	2.15	0.46
1:A:392:ARG:CB	3:A:505:NAG:O3	2.63	0.46
1:B:313:GLU:CB	1:B:314:PRO:HD3	2.46	0.46
1:B:277:VAL:CG2	1:B:304:VAL:HG11	2.46	0.46
2:C:125:CYS:SG	2:C:135:PHE:CD2	3.09	0.46
2:D:90:TYR:N	2:D:90:TYR:HD1	2.12	0.46
2:C:121:ILE:HG12	2:C:122:SER:N	2.30	0.46
1:A:277:VAL:CG2	1:A:304:VAL:HG11	2.45	0.46
2:C:18:ILE:HA	2:C:19:PRO:HD3	1.64	0.46
2:D:152:GLU:O	2:D:153:HIS:C	2.54	0.46
8:C:743:MAN:O3	8:C:744:BMA:C1	2.63	0.46
2:C:120:ASN:HB2	7:C:730:NAG:H83	1.98	0.46
6:C:722:MAN:C6	6:C:723:BMA:O2	2.51	0.46
2:D:149:GLN:O	2:D:149:GLN:CG	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:149:GLN:O	2:C:149:GLN:CG	2.63	0.46
2:D:41:ILE:HG23	2:D:41:ILE:O	2.15	0.46
1:B:430:PHE:O	1:B:447:THR:HG22	2.16	0.46
1:A:430:PHE:O	1:A:447:THR:HG22	2.16	0.46
2:D:17:VAL:HA	2:D:97:VAL:HG23	1.97	0.46
2:D:40:MET:HE2	2:D:47:TYR:HB3	1.96	0.46
2:D:35:TYR:OH	2:D:82:ARG:NH1	2.48	0.46
1:B:296:ARG:HA	1:B:302:TYR:HA	1.98	0.46
1:A:366:THR:OG1	1:A:418:ARG:HD3	2.16	0.46
2:D:135:PHE:O	2:D:149:GLN:HA	2.15	0.46
2:C:125:CYS:SG	2:C:135:PHE:HD2	2.37	0.46
2:C:137:LEU:HB3	2:C:148:HIS:HB2	1.98	0.46
2:D:120:ASN:HB2	7:D:830:NAG:H83	1.97	0.46
1:A:324:THR:HA	1:A:334:LEU:O	2.16	0.46
2:C:14:SER:OG	2:C:15:SER:N	2.48	0.46
3:A:507:SIA:H113	3:A:507:SIA:H4	1.98	0.45
1:B:419:VAL:HG12	1:B:420:ALA:N	2.30	0.45
1:A:368:THR:HG23	1:A:416:ILE:HD11	1.98	0.45
1:B:324:THR:HA	1:B:334:LEU:O	2.16	0.45
2:C:152:GLU:O	2:C:153:HIS:C	2.54	0.45
1:A:313:GLU:CB	1:A:314:PRO:HD3	2.46	0.45
1:A:395:TYR:HE1	3:A:505:NAG:C8	2.28	0.45
1:A:419:VAL:HG12	1:A:420:ALA:N	2.31	0.45
2:D:14:SER:OG	2:D:15:SER:N	2.48	0.45
2:C:52:ARG:O	2:C:53:ARG:NH1	2.44	0.45
1:A:375:SER:OG	1:A:376:PRO:CD	2.54	0.45
1:A:392:ARG:HA	1:A:395:TYR:CZ	2.52	0.45
1:B:344:THR:HA	1:B:375:SER:CB	2.46	0.45
1:B:352:LEU:HA	1:B:353:PRO:HD3	1.74	0.45
1:A:352:LEU:HA	1:A:353:PRO:HD3	1.75	0.45
2:C:31:ILE:HG21	2:C:81:TYR:CD2	2.51	0.45
2:C:41:ILE:HG23	2:C:41:ILE:O	2.15	0.45
2:D:52:ARG:N	2:D:64:PHE:HE2	2.14	0.45
1:A:344:THR:HA	1:A:375:SER:CB	2.47	0.45
1:B:322:THR:CG2	1:B:323:CYS:N	2.80	0.45
2:D:109:ALA:CB	2:D:123:LEU:HD23	2.36	0.45
2:C:52:ARG:N	2:C:64:PHE:HE2	2.15	0.45
4:B:607:SIA:H113	4:B:607:SIA:H4	1.98	0.45
1:A:391:PRO:C	1:A:393:GLU:N	2.65	0.45
2:C:31:ILE:HD11	2:C:89:ARG:NH2	2.31	0.45
2:D:50:ILE:HD11	2:D:77:TYR:HE2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:370:LEU:HD13	1:B:414:THR:HG22	1.99	0.45
1:A:373:GLY:HA2	1:A:410:THR:HB	1.99	0.45
2:C:50:ILE:HD11	2:C:77:TYR:HE2	1.81	0.45
2:C:130:ILE:HG21	2:C:132:PHE:CZ	2.51	0.45
2:D:31:ILE:CG2	2:D:31:ILE:O	2.63	0.45
1:A:277:VAL:HG21	1:A:304:VAL:HG11	1.99	0.45
2:D:137:LEU:HB3	2:D:148:HIS:HB2	1.99	0.45
1:B:436:HIS:HD2	1:B:438:ALA:HB3	1.81	0.44
2:C:28:CYS:O	2:C:62:PRO:HD2	2.17	0.44
2:D:41:ILE:HD12	2:D:77:TYR:CE1	2.52	0.44
2:C:80:GLN:HG3	2:C:90:TYR:CZ	2.52	0.44
1:A:296:ARG:HA	1:A:302:TYR:HA	1.98	0.44
2:D:15:SER:HA	2:D:16:PRO:HD3	1.68	0.44
2:C:17:VAL:HA	2:C:97:VAL:HG23	1.98	0.44
1:B:349:VAL:HA	1:B:370:LEU:O	2.16	0.44
1:A:349:VAL:HA	1:A:370:LEU:O	2.17	0.44
1:A:396:LEU:HB2	1:B:404:PRO:HD3	1.99	0.44
1:B:381:VAL:HG11	1:B:415:SER:HB2	1.98	0.44
1:B:277:VAL:HG21	1:B:304:VAL:HG11	2.00	0.44
2:D:125:CYS:SG	2:D:135:PHE:HD2	2.40	0.44
2:C:53:ARG:HG2	2:C:53:ARG:HH11	1.83	0.44
1:A:350:HIS:HB2	1:A:370:LEU:HB3	2.00	0.44
1:A:439:LEU:HD13	1:A:444:THR:OG1	2.18	0.44
1:B:280:THR:O	1:B:323:CYS:HA	2.17	0.44
1:A:372:ARG:NE	1:B:418:ARG:NH2	2.65	0.44
1:A:418:ARG:NH2	1:B:372:ARG:NE	2.66	0.44
2:C:49:GLU:OE2	2:C:52:ARG:NE	2.50	0.44
1:A:280:THR:O	1:A:323:CYS:HA	2.18	0.44
1:A:322:THR:HG22	1:A:323:CYS:N	2.32	0.44
1:A:311:CYS:C	1:A:314:PRO:HD2	2.38	0.44
1:A:354:PRO:HB3	1:A:365:VAL:HB	2.00	0.44
2:D:53:ARG:HH11	2:D:53:ARG:HG2	1.83	0.44
2:C:94:LEU:HA	2:C:94:LEU:HD12	1.69	0.44
1:B:354:PRO:HB3	1:B:365:VAL:HB	2.00	0.44
2:C:8:PRO:HD2	2:C:90:TYR:O	2.18	0.44
2:C:61:ASP:HA	2:C:62:PRO:HD3	1.80	0.44
1:A:278:THR:HB	1:A:326:ALA:HB3	2.00	0.44
2:C:175:TRP:CD1	2:C:183:TRP:NE1	2.86	0.44
2:C:41:ILE:HD12	2:C:77:TYR:CE1	2.53	0.44
2:C:130:ILE:HA	2:C:131:PRO:HD3	1.61	0.44
2:D:167:SER:HA	2:D:192:LEU:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:83:ILE:HB	2:D:87:ARG:CB	2.48	0.43
2:C:167:SER:HA	2:C:192:LEU:O	2.18	0.43
4:B:602:NAG:H4	4:B:603:BMA:O2	2.17	0.43
1:A:263:ASN:ND2	3:A:500:NAG:C2	2.81	0.43
1:B:263:ASN:ND2	4:B:600:NAG:C2	2.81	0.43
1:A:347:PRO:HG3	1:A:374:PHE:HB3	2.00	0.43
1:B:347:PRO:HG3	1:B:374:PHE:HB3	2.01	0.43
1:B:257:LEU:HD21	2:D:85:HIS:ND1	2.33	0.43
3:A:502:NAG:H4	3:A:503:BMA:O2	2.18	0.43
1:B:278:THR:HB	1:B:326:ALA:HB3	2.00	0.43
2:D:125:CYS:SG	2:D:135:PHE:CD2	3.11	0.43
2:D:130:ILE:HG21	2:D:132:PHE:CE2	2.54	0.43
2:D:131:PRO:O	2:D:132:PHE:C	2.56	0.43
2:D:8:PRO:HD2	2:D:90:TYR:O	2.18	0.43
1:A:384:LEU:HD12	1:A:445:GLN:NE2	2.34	0.43
2:D:134:ARG:O	2:D:175:TRP:CB	2.66	0.43
1:B:416:ILE:HA	1:B:416:ILE:HD13	1.77	0.43
2:C:83:ILE:HB	2:C:87:ARG:CB	2.48	0.43
2:D:61:ASP:HA	2:D:62:PRO:HD3	1.80	0.43
1:A:370:LEU:HD13	1:A:414:THR:HG22	2.00	0.43
2:C:135:PHE:O	2:C:149:GLN:HA	2.19	0.43
1:B:351:LEU:HA	1:B:351:LEU:HD12	1.83	0.43
1:B:427:GLY:O	1:B:428:ASP:C	2.57	0.43
2:C:131:PRO:O	2:C:132:PHE:C	2.57	0.42
1:A:332:THR:HA	1:A:333:PRO:HD3	1.71	0.42
1:A:436:HIS:CD2	1:A:438:ALA:HB3	2.54	0.42
2:C:18:ILE:O	2:C:99:THR:N	2.53	0.42
1:B:384:LEU:HD12	1:B:445:GLN:NE2	2.33	0.42
2:D:52:ARG:O	2:D:53:ARG:NH1	2.47	0.42
1:B:439:LEU:HA	1:B:440:PRO:HD3	1.80	0.42
1:B:311:CYS:C	1:B:314:PRO:HD2	2.39	0.42
1:A:324:THR:HG22	1:A:335:THR:HG23	2.01	0.42
1:A:327:TYR:HE2	1:A:334:LEU:HG	1.84	0.42
2:C:134:ARG:O	2:C:175:TRP:CB	2.67	0.42
2:C:38:GLN:NE2	2:C:49:GLU:OE1	2.33	0.42
1:A:347:PRO:HD3	1:A:436:HIS:CD2	2.54	0.42
2:C:113:LEU:HG	2:C:192:LEU:HA	2.02	0.42
2:D:60:THR:CG2	2:D:61:ASP:H	2.24	0.42
4:B:607:SIA:H91	4:B:607:SIA:H6	1.94	0.42
2:D:18:ILE:O	2:D:99:THR:N	2.51	0.42
2:D:40:MET:HE3	2:D:47:TYR:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:CYS:O	1:A:414:THR:HA	2.20	0.42
2:C:31:ILE:HD11	2:C:89:ARG:CZ	2.50	0.42
1:B:379:VAL:CG2	1:B:413:VAL:HG21	2.49	0.42
1:B:332:THR:HA	1:B:333:PRO:HD3	1.72	0.42
2:C:15:SER:HA	2:C:16:PRO:HD3	1.68	0.42
2:D:48:ARG:O	2:D:50:ILE:HG23	2.20	0.42
1:B:323:CYS:O	1:B:335:THR:HA	2.20	0.42
1:B:445:GLN:HE22	2:D:55:LYS:HB2	1.84	0.42
2:C:17:VAL:O	2:C:17:VAL:HG23	2.20	0.42
1:A:427:GLY:O	1:A:428:ASP:C	2.57	0.42
2:C:57:TRP:CD1	2:C:62:PRO:HG3	2.55	0.41
1:B:382:ARG:CZ	4:B:605:NAG:HN2	2.33	0.41
2:C:48:ARG:O	2:C:50:ILE:HG23	2.20	0.41
1:A:257:LEU:HD21	2:C:85:HIS:ND1	2.35	0.41
1:A:264:LEU:C	1:A:264:LEU:HD23	2.41	0.41
1:A:322:THR:CG2	1:A:323:CYS:N	2.84	0.41
1:B:324:THR:HG22	1:B:335:THR:HG23	2.02	0.41
2:C:163:ASP:O	2:C:194:VAL:HG11	2.20	0.41
2:D:17:VAL:O	2:D:17:VAL:HG23	2.21	0.41
1:A:364:LEU:HD23	1:A:364:LEU:HA	1.86	0.41
1:A:293:PRO:HA	1:A:294:PRO:HD3	1.86	0.41
1:A:282:THR:HG1	1:A:283:PRO:HD3	1.80	0.41
2:C:40:MET:HE3	2:C:47:TYR:HB3	2.03	0.41
1:A:381:VAL:HG11	1:A:415:SER:HB2	2.01	0.41
1:B:392:ARG:HA	1:B:395:TYR:CZ	2.55	0.41
2:D:57:TRP:CD1	2:D:62:PRO:HG3	2.55	0.41
1:B:369:CYS:O	1:B:414:THR:HA	2.21	0.41
2:C:19:PRO:O	2:C:20:LEU:O	2.38	0.41
1:B:373:GLY:HA2	1:B:410:THR:HB	2.03	0.41
2:D:23:SER:O	2:D:24:VAL:HG13	2.21	0.41
2:C:67:ASP:O	2:C:73:LYS:NZ	2.54	0.41
2:C:125:CYS:HB3	2:C:155:ALA:HB3	2.02	0.41
1:B:439:LEU:HD13	1:B:444:THR:OG1	2.20	0.41
2:C:78:GLN:HG2	2:C:79:CYS:N	2.36	0.41
1:A:270:GLY:O	1:A:272:ARG:N	2.53	0.41
2:C:179:SER:CB	2:C:182:LEU:HD12	2.35	0.41
1:A:445:GLN:HE22	2:C:55:LYS:HB2	1.86	0.41
2:D:163:ASP:O	2:D:194:VAL:HG11	2.21	0.41
2:C:78:GLN:CG	2:C:79:CYS:N	2.84	0.41
2:D:111:ARG:CG	2:D:121:ILE:HG13	2.50	0.41
2:D:125:CYS:HB3	2:D:155:ALA:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:49:GLU:OE2	2:D:52:ARG:NE	2.52	0.41
2:D:78:GLN:CG	2:D:79:CYS:N	2.84	0.41
2:C:31:ILE:O	2:C:31:ILE:CG2	2.63	0.40
1:A:242:CYS:O	1:A:244:PRO:HD3	2.21	0.40
2:D:53:ARG:NH1	2:D:53:ARG:HG2	2.36	0.40
1:A:416:ILE:HD13	1:A:416:ILE:HA	1.76	0.40
2:D:7:MET:HA	2:D:8:PRO:HD3	1.87	0.40
1:B:257:LEU:HD21	2:D:85:HIS:CE1	2.56	0.40
2:D:179:SER:HB2	2:D:182:LEU:CD1	2.36	0.40
1:B:354:PRO:HA	1:B:355:PRO:HD3	1.94	0.40
1:A:328:PRO:C	1:A:330:SER:H	2.25	0.40
2:C:53:ARG:NH1	2:C:53:ARG:HG2	2.36	0.40
2:D:132:PHE:HB3	2:D:175:TRP:H	1.86	0.40
2:C:104:LYS:HA	2:C:105:PRO:HD3	1.81	0.40
2:D:94:LEU:HD12	2:D:94:LEU:HA	1.71	0.40
1:B:242:CYS:O	1:B:244:PRO:HD3	2.22	0.40
2:C:130:ILE:HG21	2:C:132:PHE:CE2	2.57	0.40
2:D:78:GLN:HG2	2:D:79:CYS:N	2.36	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	207/214 (97%)	173 (84%)	22 (11%)	12 (6%)	2	12
1	B	207/214 (97%)	174 (84%)	21 (10%)	12 (6%)	2	12
2	C	188/207 (91%)	143 (76%)	32 (17%)	13 (7%)	1	8
2	D	188/207 (91%)	143 (76%)	31 (16%)	14 (7%)	1	7
All	All	790/842 (94%)	633 (80%)	106 (13%)	51 (6%)	1	9

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	375	SER
1	A	442	ALA
1	B	375	SER
1	B	442	ALA
2	C	31	ILE
2	C	117	PRO
2	D	31	ILE
2	D	117	PRO
1	A	277	VAL
1	A	301	CYS
1	A	329	GLU
1	A	362	ASN
1	B	277	VAL
1	B	301	CYS
1	B	329	GLU
1	B	362	ASN
2	C	20	LEU
2	C	43	LYS
2	C	153	HIS
2	C	160	GLY
2	C	179	SER
2	C	180	PRO
2	D	20	LEU
2	D	43	LYS
2	D	153	HIS
2	D	160	GLY
2	D	179	SER
2	D	180	PRO
1	A	299	CYS
1	B	299	CYS
2	C	32	ARG
2	D	32	ARG
1	A	363	GLU
1	B	363	GLU
2	C	30	ALA
2	D	114	VAL
1	A	294	PRO
1	A	311	CYS
1	B	294	PRO
1	B	311	CYS
2	C	114	VAL
1	A	276	GLY
1	B	276	GLY

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Mol	Chain	Res	Type
2	D	30	ALA
2	D	55	LYS
2	C	118	GLY
2	D	118	GLY
1	A	300	GLY
1	B	300	GLY
2	D	161	PRO
2	C	161	PRO

### 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	134/181 (74%)	119 (89%)	15 (11%)	7	29
1	B	134/181 (74%)	120 (90%)	14 (10%)	9	32
2	C	138/180 (77%)	129 (94%)	9 (6%)	21	57
2	D	138/180 (77%)	127 (92%)	11 (8%)	15	48
All	All	544/722 (75%)	495 (91%)	49 (9%)	12	41

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

Mol	Chain	Res	Type
1	A	250	ARG
1	A	265	THR
1	A	267	THR
1	A	282	THR
1	A	307	VAL
1	A	320	THR
1	A	332	THR
1	A	343	ASN
1	A	378	ASP
1	A	400	SER
1	A	418	ARG
1	A	423	ASP
1	A	429	THR

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Mol	Chain	Res	Type
1	A	431	SER
1	A	447	THR
1	B	250	ARG
1	B	265	THR
1	B	267	THR
1	B	282	THR
1	B	307	VAL
1	B	320	THR
1	B	332	THR
1	B	343	ASN
1	B	400	SER
1	B	418	ARG
1	B	423	ASP
1	B	429	THR
1	B	431	SER
1	B	447	THR
2	C	18	ILE
2	C	46	THR
2	C	55	LYS
2	C	59	GLU
2	C	60	THR
2	C	90	TYR
2	C	156	ASN
2	C	169	ILE
2	C	175	TRP
2	D	18	ILE
2	D	46	THR
2	D	55	LYS
2	D	59	GLU
2	D	60	THR
2	D	79	CYS
2	D	90	TYR
2	D	144	SER
2	D	156	ASN
2	D	169	ILE
2	D	175	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	263	ASN
1	A	436	HIS

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Mol	Chain	Res	Type
1	B	263	ASN
1	B	436	HIS
2	C	27	GLN
2	C	80	GLN
2	C	149	GLN
2	C	177	ASN
2	D	27	GLN
2	D	80	GLN
2	D	149	GLN
2	D	177	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 ⓘ

44 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	NAG	A	500	3	14,14,15	0.61	0	15,19,21	0.72	1 (6%)
3	FUL	A	501	3	10,10,11	0.52	0	14,14,16	0.97	1 (7%)
3	NAG	A	502	3	14,14,15	0.72	0	15,19,21	0.67	0
3	BMA	A	503	3	11,11,12	0.62	0	14,15,17	0.46	0
3	BMA	A	504	3	11,11,12	1.10	1 (9%)	14,15,17	0.95	1 (7%)
3	NAG	A	505	3	14,14,15	0.79	0	15,19,21	1.08	2 (13%)
3	GAL	A	506	3	11,11,12	0.80	0	14,15,17	0.78	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SIA	A	507	3	16,20,21	0.55	0	18,28,31	0.88	1 (5%)
4	NAG	B	600	4	14,14,15	0.60	0	15,19,21	0.73	1 (6%)
4	FUC	B	601	4	10,10,11	0.52	0	14,14,16	0.97	1 (7%)
4	NAG	B	602	4	14,14,15	0.73	0	15,19,21	0.68	0
4	BMA	B	603	4	11,11,12	0.60	0	14,15,17	0.49	0
4	BMA	B	604	4	11,11,12	1.10	1 (9%)	14,15,17	0.96	1 (7%)
4	NAG	B	605	4	14,14,15	0.77	0	15,19,21	1.08	2 (13%)
4	GAL	B	606	4	11,11,12	0.80	0	14,15,17	0.79	0
4	SIA	B	607	4	16,20,21	0.56	0	18,28,31	0.88	1 (5%)
6	NAG	C	720	2,6	14,14,15	0.58	0	15,19,21	0.72	1 (6%)
6	NAG	C	721	6	14,14,15	0.82	1 (7%)	15,19,21	0.59	0
6	MAN	C	722	6	11,11,12	0.74	0	14,15,17	0.97	1 (7%)
6	BMA	C	723	6	11,11,12	0.52	0	14,15,17	0.57	0
6	MAN	C	727	6	11,11,12	0.59	0	14,15,17	0.86	2 (14%)
7	NAG	C	730	2,7	14,14,15	0.72	0	15,19,21	0.76	1 (6%)
7	NDG	C	731	7	14,14,15	0.86	1 (7%)	15,19,21	1.17	1 (6%)
7	BMA	C	732	7	11,11,12	0.51	0	14,15,17	0.46	0
8	NAG	C	740	8,2	14,14,15	0.86	1 (7%)	15,19,21	0.93	0
8	NAG	C	741	8	14,14,15	0.69	0	15,19,21	1.13	2 (13%)
8	BMA	C	742	8	11,11,12	0.58	0	14,15,17	0.44	0
8	MAN	C	743	8	11,11,12	0.83	0	14,15,17	0.84	1 (7%)
8	BMA	C	744	8	11,11,12	0.72	0	14,15,17	0.51	0
8	BMA	C	745	8	11,11,12	0.69	0	14,15,17	0.30	0
6	NAG	D	820	2,6	14,14,15	0.58	0	15,19,21	0.72	1 (6%)
6	NAG	D	821	6	14,14,15	0.83	1 (7%)	15,19,21	0.59	0
6	MAN	D	822	6	11,11,12	0.75	0	14,15,17	0.97	1 (7%)
6	BMA	D	823	6	11,11,12	0.57	0	14,15,17	0.56	0
6	MAN	D	827	6	11,11,12	0.59	0	14,15,17	0.84	1 (7%)
7	NAG	D	830	2,7	14,14,15	0.74	0	15,19,21	0.76	1 (6%)
7	NDG	D	831	7	14,14,15	0.87	1 (7%)	15,19,21	1.17	1 (6%)
7	BMA	D	832	7	11,11,12	0.50	0	14,15,17	0.46	0
8	NAG	D	840	8,2	14,14,15	0.85	1 (7%)	15,19,21	0.95	0
8	NAG	D	841	8	14,14,15	0.69	0	15,19,21	1.13	2 (13%)
8	BMA	D	842	8	11,11,12	0.58	0	14,15,17	0.45	0
8	MAN	D	843	8	11,11,12	0.83	0	14,15,17	0.83	1 (7%)
8	BMA	D	844	8	11,11,12	0.73	0	14,15,17	0.51	0
8	BMA	D	845	8	11,11,12	0.66	0	14,15,17	0.31	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	NAG	A	500	3	-	0/6/23/26	0/1/1/1
3	FUL	A	501	3	-	0/0/17/20	0/1/1/1
3	NAG	A	502	3	-	0/6/23/26	0/1/1/1
3	BMA	A	503	3	-	0/2/19/22	0/1/1/1
3	BMA	A	504	3	-	0/2/19/22	0/1/1/1
3	NAG	A	505	3	-	1/6/23/26	0/1/1/1
3	GAL	A	506	3	-	0/2/19/22	0/1/1/1
3	SIA	A	507	3	-	0/14/34/38	0/1/1/1
4	NAG	B	600	4	-	0/6/23/26	0/1/1/1
4	FUC	B	601	4	1/1/4/5	0/0/17/20	0/1/1/1
4	NAG	B	602	4	-	0/6/23/26	0/1/1/1
4	BMA	B	603	4	-	0/2/19/22	0/1/1/1
4	BMA	B	604	4	-	0/2/19/22	0/1/1/1
4	NAG	B	605	4	-	1/6/23/26	0/1/1/1
4	GAL	B	606	4	-	0/2/19/22	0/1/1/1
4	SIA	B	607	4	-	0/14/34/38	0/1/1/1
6	NAG	C	720	2,6	-	0/6/23/26	0/1/1/1
6	NAG	C	721	6	-	0/6/23/26	0/1/1/1
6	MAN	C	722	6	-	0/2/19/22	0/1/1/1
6	BMA	C	723	6	-	0/2/19/22	0/1/1/1
6	MAN	C	727	6	-	0/2/19/22	0/1/1/1
7	NAG	C	730	2,7	-	0/6/23/26	0/1/1/1
7	NDG	C	731	7	-	0/6/23/26	0/1/1/1
7	BMA	C	732	7	-	0/2/19/22	0/1/1/1
8	NAG	C	740	8,2	-	0/6/23/26	0/1/1/1
8	NAG	C	741	8	-	0/6/23/26	0/1/1/1
8	BMA	C	742	8	-	0/2/19/22	0/1/1/1
8	MAN	C	743	8	-	0/2/19/22	1/1/1/1
8	BMA	C	744	8	-	0/2/19/22	0/1/1/1
8	BMA	C	745	8	-	0/2/19/22	0/1/1/1
6	NAG	D	820	2,6	-	0/6/23/26	0/1/1/1
6	NAG	D	821	6	-	0/6/23/26	0/1/1/1
6	MAN	D	822	6	-	0/2/19/22	0/1/1/1
6	BMA	D	823	6	-	0/2/19/22	0/1/1/1
6	MAN	D	827	6	-	0/2/19/22	0/1/1/1
7	NAG	D	830	2,7	-	0/6/23/26	0/1/1/1
7	NDG	D	831	7	-	0/6/23/26	0/1/1/1
7	BMA	D	832	7	-	0/2/19/22	0/1/1/1
8	NAG	D	840	8,2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	D	841	8	-	0/6/23/26	0/1/1/1
8	BMA	D	842	8	-	0/2/19/22	0/1/1/1
8	MAN	D	843	8	-	0/2/19/22	1/1/1/1
8	BMA	D	844	8	-	0/2/19/22	0/1/1/1
8	BMA	D	845	8	-	0/2/19/22	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	721	NAG	C1-C2	2.10	1.55	1.52
6	D	821	NAG	C1-C2	2.12	1.55	1.52
7	D	831	NDG	C1-C2	2.22	1.55	1.52
7	C	731	NDG	C1-C2	2.22	1.55	1.52
8	C	740	NAG	C1-C2	2.34	1.55	1.52
8	D	840	NAG	C1-C2	2.34	1.55	1.52
3	A	504	BMA	C2-C3	2.47	1.55	1.52
4	B	604	BMA	C2-C3	2.50	1.55	1.52

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	741	NAG	C2-N2-C7	-2.74	119.52	123.04
8	D	841	NAG	C2-N2-C7	-2.68	119.60	123.04
4	B	607	SIA	C7-C6-C5	-2.67	110.27	114.32
3	A	507	SIA	C7-C6-C5	-2.66	110.30	114.32
7	D	831	NDG	C2-N2-C7	-2.60	119.70	123.04
7	C	731	NDG	C2-N2-C7	-2.59	119.71	123.04
8	D	841	NAG	C4-C3-C2	-2.58	107.22	111.23
8	C	741	NAG	C4-C3-C2	-2.54	107.27	111.23
3	A	505	NAG	C3-C4-C5	-2.39	106.03	110.20
4	B	605	NAG	C3-C4-C5	-2.38	106.05	110.20
7	C	730	NAG	C2-N2-C7	-2.32	120.06	123.04
7	D	830	NAG	C2-N2-C7	-2.31	120.07	123.04
3	A	500	NAG	C2-N2-C7	-2.14	120.29	123.04
4	B	600	NAG	C2-N2-C7	-2.13	120.30	123.04
3	A	505	NAG	C2-N2-C7	-2.11	120.32	123.04
4	B	605	NAG	C2-N2-C7	-2.08	120.37	123.04
6	C	720	NAG	C2-N2-C7	-2.05	120.41	123.04
6	D	820	NAG	C2-N2-C7	-2.00	120.47	123.04
6	C	727	MAN	C1-C2-C3	2.02	111.93	109.54
6	C	727	MAN	C1-O5-C5	2.22	115.07	112.25
6	D	827	MAN	C1-O5-C5	2.23	115.07	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	504	BMA	C1-C2-C3	2.24	112.19	109.54
4	B	604	BMA	C1-C2-C3	2.25	112.20	109.54
3	A	501	FUL	C1-O5-C5	2.54	116.30	112.38
4	B	601	FUC	C1-O5-C5	2.56	116.33	112.38
6	D	822	MAN	C6-C5-C4	2.77	119.84	113.02
8	D	843	MAN	C1-O5-C5	2.78	115.77	112.25
6	C	722	MAN	C6-C5-C4	2.80	119.92	113.02
8	C	743	MAN	C1-O5-C5	2.81	115.81	112.25

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	601	FUC	C1

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	505	NAG	O7-C7-N2-C2
4	B	605	NAG	O7-C7-N2-C2

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	743	MAN	C1-C2-C3-C4-C5-O5
8	D	843	MAN	C1-C2-C3-C4-C5-O5

30 monomers are involved in 54 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	500	NAG	6	0
3	A	502	NAG	1	0
3	A	503	BMA	2	0
3	A	504	BMA	1	0
3	A	505	NAG	7	0
3	A	506	GAL	3	0
3	A	507	SIA	4	0
4	B	600	NAG	6	0
4	B	602	NAG	1	0
4	B	603	BMA	2	0
4	B	604	BMA	1	0
4	B	605	NAG	8	0
4	B	606	GAL	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	607	SIA	5	0
6	C	720	NAG	1	0
6	C	721	NAG	1	0
6	C	722	MAN	2	0
6	C	723	BMA	2	0
7	C	730	NAG	1	0
8	C	743	MAN	1	0
8	C	744	BMA	2	0
8	C	745	BMA	1	0
6	D	820	NAG	1	0
6	D	821	NAG	1	0
6	D	822	MAN	2	0
6	D	823	BMA	2	0
7	D	830	NAG	1	0
8	D	843	MAN	1	0
8	D	844	BMA	2	0
8	D	845	BMA	1	0

## 5.6 Ligand geometry

2 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$
5	NAG	C	710	2	14,14,15	0.56	0	15,19,21	0.68	0
5	NAG	D	810	2	14,14,15	0.58	0	15,19,21	0.69	1 (6%)

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	C	710	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	D	810	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	810	NAG	C2-N2-C7	-2.04	120.42	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	710	NAG	2	0
5	D	810	NAG	2	0

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	209/214 (97%)	0.08	1 (0%) 91 83	41, 86, 142, 201	0
1	B	209/214 (97%)	0.06	1 (0%) 91 83	41, 86, 142, 201	0
2	C	190/207 (91%)	0.07	1 (0%) 91 83	54, 88, 128, 153	0
2	D	190/207 (91%)	0.06	1 (0%) 91 83	54, 88, 128, 153	0
All	All	798/842 (94%)	0.06	4 (0%) 91 83	41, 87, 140, 201	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	113	LEU	4.1
2	C	113	LEU	3.6
1	A	299	CYS	3.3
1	B	299	CYS	3.3

### 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
4	NAG	B	600	14/15	0.66	0.46	3.49	178,193,200,200	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	A	500	14/15	0.67	0.44	3.17	178,193,200,200	0
8	NAG	D	841	14/15	0.90	0.21	-0.41	146,146,146,146	0
3	GAL	A	506	11/12	0.74	0.22	-0.47	143,151,157,173	0
8	NAG	C	741	14/15	0.89	0.20	-0.51	146,146,146,146	0
3	BMA	A	504	11/12	0.77	0.23	-0.51	146,159,165,173	0
4	GAL	B	606	11/12	0.76	0.20	-0.55	143,151,157,173	0
6	BMA	D	823	11/12	0.83	0.17	-0.78	116,120,132,133	0
8	NAG	D	840	14/15	0.67	0.19	-0.83	138,138,138,138	0
8	NAG	C	740	14/15	0.72	0.18	-0.85	138,138,138,138	0
6	BMA	C	723	11/12	0.84	0.18	-0.91	116,120,132,133	0
4	BMA	B	604	11/12	0.80	0.20	-0.97	146,159,165,173	0
3	NAG	A	502	14/15	0.53	0.43	-	189,197,200,200	0
7	NAG	C	730	14/15	0.67	0.21	-	196,196,196,196	0
8	BMA	C	745	11/12	0.37	0.24	-	177,177,177,177	0
6	NAG	D	820	14/15	0.68	0.72	-	184,199,200,200	0
8	MAN	C	743	11/12	0.72	0.29	-	195,200,200,200	0
4	FUC	B	601	10/11	0.81	0.23	-	200,200,200,200	0
6	NAG	C	720	14/15	0.69	0.75	-	184,199,200,200	0
8	BMA	C	742	11/12	0.78	0.18	-	163,163,163,163	0
4	BMA	B	603	11/12	0.66	0.26	-	197,200,200,200	0
8	BMA	D	842	11/12	0.81	0.20	-	163,163,163,163	0
4	SIA	B	607	20/21	0.77	0.19	-	177,198,200,200	0
6	MAN	D	822	11/12	0.64	0.34	-	200,200,200,200	0
7	BMA	C	732	11/12	0.80	0.41	-	183,191,198,198	0
8	BMA	D	844	11/12	0.81	0.37	-	200,200,200,200	0
8	MAN	D	843	11/12	0.65	0.33	-	195,200,200,200	0
8	BMA	C	744	11/12	0.83	0.39	-	200,200,200,200	0
7	BMA	D	832	11/12	0.88	0.45	-	183,191,198,198	0
4	NAG	B	602	14/15	0.45	0.56	-	189,197,200,200	0
7	NDG	C	731	14/15	0.88	0.26	-	194,200,200,200	0
3	SIA	A	507	20/21	0.76	0.19	-	177,198,200,200	0
6	MAN	C	722	11/12	0.55	0.31	-	200,200,200,200	0
3	BMA	A	503	11/12	0.64	0.30	-	197,200,200,200	0
7	NDG	D	831	14/15	0.87	0.29	-	194,200,200,200	0
3	FUL	A	501	10/11	0.80	0.23	-	200,200,200,200	0
7	NAG	D	830	14/15	0.71	0.22	-	196,196,196,196	0
6	MAN	D	827	11/12	0.69	0.48	-	189,197,200,200	0
4	NAG	B	605	14/15	0.74	0.57	-	200,200,200,200	0
6	MAN	C	727	11/12	0.62	0.47	-	189,197,200,200	0
6	NAG	C	721	14/15	0.30	0.72	-	200,200,200,200	0
8	BMA	D	845	11/12	0.33	0.22	-	177,177,177,177	0
6	NAG	D	821	14/15	0.36	0.73	-	200,200,200,200	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	A	505	14/15	0.78	0.65	-	200,200,200,200	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( $\text{\AA}^2$ )	Q<0.9
5	NAG	C	710	14/15	0.84	0.13	-	151,162,167,167	0
5	NAG	D	810	14/15	0.82	0.12	-	151,162,167,167	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.