



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:48 PM GMT

PDB ID : 3S6C  
Title : Structure of human CD1e  
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Deposited on : 2011-05-25  
Resolution : 2.90 Å(reported)

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

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

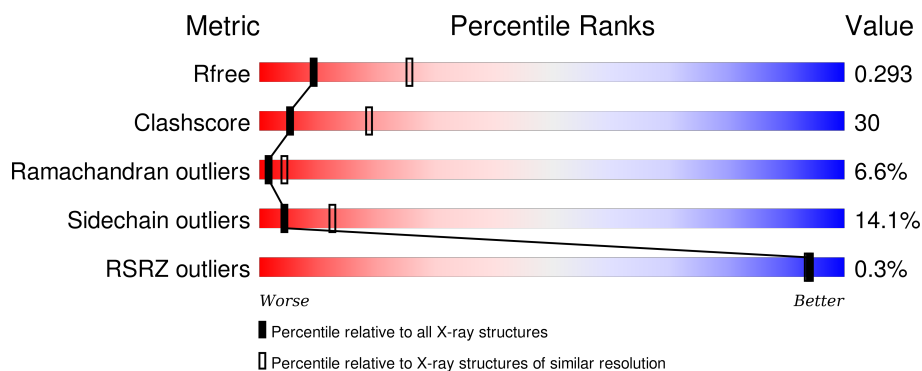
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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	392	<div> <div style="width: 48%; background-color: green;"></div> <div style="width: 36%; background-color: yellow;"></div> <div style="width: 10%; background-color: orange;"></div> <div style="width: 5%; background-color: red;"></div> <div style="width: 1%; background-color: grey;"></div> </div> <div>48% 36% 10% • 5%</div>

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
2	FUC	A	2002	X	-	-	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2897 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 Beta-2-microglobulin, T-cell surface glycoprotein CD1e, membrane-associated.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	372	2867	1822	501	530	14	0	1	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1100	ASP	-	LINKER	UNP P61769
A	1101	ASP	-	LINKER	UNP P61769
A	1102	ASP	-	LINKER	UNP P61769
A	1103	ASP	-	LINKER	UNP P61769
A	1104	LYS	-	LINKER	UNP P61769
A	1105	GLY	-	LINKER	UNP P61769
A	1106	SER	-	LINKER	UNP P61769
A	1107	SER	-	LINKER	UNP P61769
A	1108	SER	-	LINKER	UNP P61769
A	1109	SER	-	LINKER	UNP P61769
A	1110	ASP	-	LINKER	UNP P61769
A	1111	ASP	-	LINKER	UNP P61769
A	1112	ASP	-	LINKER	UNP P61769
A	1113	ASP	-	LINKER	UNP P61769
A	1114	LYS	-	LINKER	UNP P61769
A	75	ARG	GLN	SEE REMARK 999	UNP P15812
A	273	GLU	-	EXPRESSION TAG	UNP P15812
A	274	ASN	-	EXPRESSION TAG	UNP P15812
A	275	LEU	-	EXPRESSION TAG	UNP P15812
A	276	TYR	-	EXPRESSION TAG	UNP P15812
A	277	PHE	-	EXPRESSION TAG	UNP P15812
A	278	GLN	-	EXPRESSION TAG	UNP P15812

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

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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).

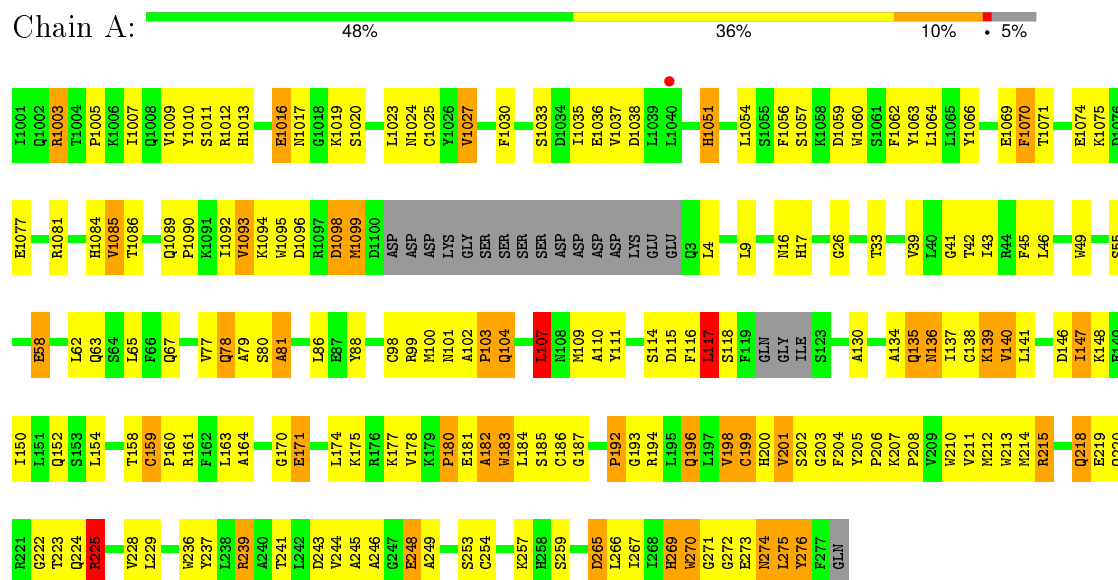


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		

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

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

- Molecule 1: Beta-2-microglobulin, T-cell surface glycoprotein CD1e, membrane-associated



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	206.29Å 45.93Å 65.63Å 90.00° 91.48° 90.00°	Depositor
Resolution (Å)	51.55 – 2.90 51.56 – 2.90	Depositor EDS
% Data completeness (in resolution range)	93.9 (51.55-2.90) 93.9 (51.56-2.90)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.88 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, $R_{free}$	0.241 , 0.296 0.241 , 0.293	Depositor DCC
$R_{free}$ test set	664 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	77.2	Xtriage
Anisotropy	0.462	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 60.2	EDS
Estimated twinning fraction	0.036 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 13125 reflections (0.008%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	2897	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.21% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.83	3/2953 (0.1%)	0.88	5/4015 (0.1%)

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
1	A	0	1
2	A	1	0
All	All	1	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	276	TYR	CD1-CE1	-5.92	1.30	1.39
1	A	182	ALA	CA-CB	5.42	1.63	1.52
1	A	183	TRP	CB-CG	-5.06	1.41	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	201	VAL	CB-CA-C	-6.06	99.89	111.40
1	A	117	LEU	CA-CB-CG	6.03	129.18	115.30
1	A	266	LEU	CA-CB-CG	5.64	128.27	115.30
1	A	225	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	A	198	VAL	CB-CA-C	-5.37	101.19	111.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	2002	FUC	C1

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	274	ASN	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2867	0	2574	167	0
2	A	24	0	22	0	0
3	A	6	0	8	3	0
All	All	2897	0	2604	167	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 30.

All (167) 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:1016:GLU:H	1:A:1016:GLU:CD	1.47	1.12
1:A:1020:SER:HA	1:A:1071:THR:HG22	1.38	1.00
1:A:1020:SER:CA	1:A:1071:THR:HG22	1.94	0.97
1:A:183:TRP:O	1:A:184:LEU:HD23	1.64	0.96
1:A:1020:SER:HA	1:A:1071:THR:CG2	1.96	0.95
1:A:198:VAL:HG12	1:A:199:CYS:O	1.68	0.94
1:A:1016:GLU:OE2	1:A:1016:GLU:N	2.01	0.92
1:A:1016:GLU:N	1:A:1016:GLU:CD	2.20	0.90
1:A:1020:SER:N	1:A:1071:THR:HG22	1.88	0.89
1:A:171:GLU:H	1:A:174:LEU:HD12	1.43	0.83
1:A:1023:LEU:HD23	1:A:1024:ASN:N	1.95	0.81
1:A:248:GLU:OE1	1:A:248:GLU:HA	1.81	0.80
1:A:1020:SER:CA	1:A:1071:THR:CG2	2.58	0.80
1:A:269:HIS:CD2	1:A:269:HIS:H	2.02	0.77
1:A:253:SER:OG	1:A:254:CYS:N	2.15	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1054:LEU:HA	1:A:1064:LEU:HD21	1.68	0.76
1:A:78:GLN:HE21	1:A:78:GLN:HA	1.49	0.76
1:A:1016:GLU:OE2	1:A:1016:GLU:CA	2.34	0.76
1:A:1010:TYR:CE1	1:A:229:LEU:HD13	2.23	0.74
1:A:225:ARG:HG3	1:A:225:ARG:HH11	1.51	0.74
1:A:147:ILE:HA	1:A:150:ILE:HD12	1.70	0.74
1:A:210:TRP:CZ2	1:A:212:MET:HG3	2.24	0.73
1:A:16:ASN:HA	1:A:88:TYR:CD2	2.24	0.71
1:A:1016:GLU:OE2	1:A:1017:ASN:N	2.25	0.70
1:A:192:PRO:O	1:A:194:ARG:N	2.25	0.69
1:A:1084:HIS:HE1	1:A:1086:THR:HG23	1.57	0.69
1:A:1023:LEU:HD23	1:A:1024:ASN:H	1.56	0.69
1:A:171:GLU:N	1:A:174:LEU:HD12	2.08	0.68
1:A:201:VAL:HG21	1:A:211:VAL:HG21	1.76	0.68
1:A:213:TRP:CE3	1:A:253:SER:O	2.47	0.67
1:A:1016:GLU:OE2	1:A:1016:GLU:C	2.34	0.66
1:A:1012:ARG:HD3	3:A:2003:GOL:O3	1.96	0.66
1:A:210:TRP:CZ2	1:A:212:MET:CG	2.79	0.65
1:A:224:GLN:HB2	1:A:241:THR:HG22	1.79	0.65
1:A:98:CYS:SG	1:A:160:PRO:N	2.70	0.64
1:A:269:HIS:CD2	1:A:269:HIS:N	2.65	0.64
1:A:239:ARG:HD2	1:A:239:ARG:O	1.97	0.64
1:A:117:LEU:HD13	1:A:118:SER:N	2.13	0.63
1:A:1085:VAL:HG23	1:A:1086:THR:H	1.63	0.63
1:A:150:ILE:HG22	1:A:154:LEU:CD1	2.29	0.62
1:A:248:GLU:CA	1:A:248:GLU:OE1	2.48	0.61
1:A:185:SER:OG	1:A:200:HIS:NE2	2.32	0.61
1:A:1009:VAL:HG21	1:A:1093:VAL:HG12	1.83	0.61
1:A:186:CYS:SG	1:A:270:TRP:HH2	2.23	0.61
1:A:271:GLY:O	1:A:274:ASN:CB	2.49	0.61
1:A:33:THR:O	1:A:45:PHE:O	2.19	0.61
1:A:270:TRP:CZ2	1:A:272:GLY:HA3	2.36	0.60
1:A:181:GLU:O	1:A:202:SER:N	2.32	0.59
1:A:276:TYR:CD1	1:A:276:TYR:C	2.76	0.59
1:A:62:LEU:HA	1:A:65:LEU:HD12	1.85	0.59
1:A:269:HIS:H	1:A:269:HIS:HD2	1.51	0.59
1:A:1010:TYR:CD1	1:A:229:LEU:HD13	2.38	0.58
1:A:246:ALA:O	1:A:249:ALA:HB3	2.03	0.58
1:A:107:LEU:HD12	1:A:107:LEU:C	2.25	0.57
1:A:100:MET:HA	1:A:101:ASN:CB	2.34	0.57
1:A:1084:HIS:CE1	1:A:1086:THR:HG23	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:GLN:CG	1:A:243:ASP:HB3	2.35	0.56
1:A:150:ILE:HG22	1:A:154:LEU:HD12	1.88	0.56
1:A:203:GLY:HA3	3:A:2003:GOL:C1	2.36	0.56
1:A:204:PHE:CE2	1:A:236:TRP:HB2	2.40	0.56
1:A:78:GLN:NE2	1:A:88:TYR:OH	2.40	0.55
1:A:183:TRP:HB2	1:A:275:LEU:HD22	1.89	0.55
1:A:86:LEU:N	1:A:86:LEU:CD1	2.70	0.55
1:A:1020:SER:N	1:A:1071:THR:CG2	2.64	0.55
1:A:1020:SER:HA	1:A:1071:THR:HG23	1.84	0.55
1:A:98:CYS:SG	1:A:159:CYS:C	2.87	0.54
1:A:1017:ASN:HD21	1:A:1074:GLU:HB2	1.73	0.53
1:A:224:GLN:HB2	1:A:241:THR:CG2	2.39	0.53
1:A:182:ALA:HA	1:A:200:HIS:O	2.09	0.53
1:A:55:SER:OG	1:A:58:GLU:HB2	2.07	0.53
1:A:265:ASP:OD2	1:A:265:ASP:N	2.43	0.51
1:A:1085:VAL:HG23	1:A:1086:THR:N	2.24	0.51
1:A:210:TRP:CZ2	1:A:212:MET:HG2	2.46	0.50
1:A:114:SER:O	1:A:115:ASP:C	2.50	0.50
1:A:1037:VAL:HG21	1:A:1066:TYR:CE1	2.46	0.50
1:A:154:LEU:O	1:A:158:THR:HB	2.12	0.50
1:A:1054:LEU:HA	1:A:1064:LEU:CD2	2.41	0.49
1:A:186:CYS:HG	1:A:270:TRP:HH2	1.58	0.49
1:A:1051:HIS:HD1	1:A:1051:HIS:C	2.15	0.49
1:A:1098:ASP:N	1:A:1098:ASP:OD1	2.44	0.49
1:A:146:ASP:OD1	1:A:147:ILE:N	2.46	0.49
1:A:78:GLN:NE2	1:A:78:GLN:HA	2.24	0.49
1:A:1009:VAL:HG12	1:A:1095:TRP:HD1	1.78	0.48
1:A:170:GLY:HA3	1:A:174:LEU:HD12	1.95	0.48
1:A:1027:VAL:HG23	1:A:1064:LEU:HB2	1.96	0.47
1:A:130:ALA:HB1	1:A:134:ALA:HB2	1.96	0.47
1:A:270:TRP:CZ2	1:A:272:GLY:CA	2.98	0.47
1:A:98:CYS:SG	1:A:160:PRO:HD3	2.55	0.47
1:A:26:GLY:O	1:A:33:THR:OG1	2.33	0.47
1:A:41:GLY:O	1:A:42:THR:HG23	2.14	0.47
1:A:100:MET:CA	1:A:101:ASN:CB	2.93	0.47
1:A:270:TRP:CD1	1:A:270:TRP:C	2.88	0.47
1:A:245:ALA:O	1:A:248:GLU:N	2.47	0.46
1:A:147:ILE:CG2	1:A:148:LYS:N	2.78	0.46
1:A:214:MET:O	1:A:215:ARG:HB2	2.14	0.46
1:A:147:ILE:HG22	1:A:148:LYS:N	2.31	0.46
1:A:196:GLN:HG2	1:A:243:ASP:HB3	1.95	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1056:PHE:CZ	1:A:9:LEU:HB3	2.50	0.46
1:A:222:GLY:O	1:A:223:THR:C	2.52	0.46
1:A:1037:VAL:HG12	1:A:1038:ASP:N	2.29	0.46
1:A:181:GLU:HG2	1:A:183:TRP:HZ3	1.79	0.46
1:A:213:TRP:HE3	1:A:253:SER:O	1.97	0.46
1:A:1016:GLU:OE1	1:A:1019:LYS:HB2	2.15	0.46
1:A:137:ILE:O	1:A:141:LEU:HD13	2.15	0.46
1:A:1084:HIS:O	1:A:1086:THR:N	2.49	0.46
1:A:178:VAL:HG12	1:A:204:PHE:HA	1.96	0.46
1:A:207:LYS:O	1:A:208:PRO:C	2.55	0.45
1:A:80:SER:O	1:A:81:ALA:C	2.54	0.45
1:A:204:PHE:CZ	1:A:236:TRP:HB2	2.52	0.45
1:A:86:LEU:HD12	1:A:86:LEU:N	2.31	0.45
1:A:244:VAL:HG22	1:A:248:GLU:HB2	1.97	0.45
1:A:210:TRP:CE3	1:A:257:LYS:HD2	2.52	0.45
1:A:1007:ILE:HG23	1:A:1025:CYS:SG	2.57	0.45
1:A:98:CYS:SG	1:A:160:PRO:CD	3.05	0.45
1:A:1003:ARG:O	1:A:1030:PHE:HA	2.17	0.45
1:A:210:TRP:CH2	1:A:212:MET:HG3	2.51	0.44
1:A:117:LEU:HD22	1:A:138:CYS:SG	2.58	0.44
1:A:1033:SER:HB3	1:A:1062:PHE:CE2	2.52	0.44
1:A:117:LEU:C	1:A:117:LEU:CD1	2.86	0.44
1:A:163:LEU:O	1:A:164:ALA:C	2.56	0.44
1:A:1016:GLU:HG2	1:A:1019:LYS:HG3	2.00	0.44
1:A:196:GLN:HG3	1:A:243:ASP:HB3	2.00	0.44
1:A:1051:HIS:HD2	1:A:1066:TYR:CE2	2.36	0.44
1:A:180:PRO:HG3	1:A:204:PHE:HB3	1.99	0.44
1:A:275:LEU:C	1:A:275:LEU:HD12	2.38	0.43
1:A:1037:VAL:CG2	1:A:1066:TYR:CE1	3.01	0.43
1:A:1060:TRP:CE2	1:A:110:ALA:HB2	2.54	0.43
1:A:41:GLY:C	1:A:42:THR:HG23	2.39	0.43
1:A:43:ILE:HG22	1:A:43:ILE:O	2.17	0.43
1:A:207:LYS:N	1:A:208:PRO:HD2	2.33	0.43
1:A:117:LEU:CD1	1:A:118:SER:N	2.82	0.43
1:A:241:THR:O	1:A:241:THR:HG23	2.19	0.43
1:A:275:LEU:HG	1:A:275:LEU:O	2.19	0.42
1:A:55:SER:OG	1:A:58:GLU:N	2.39	0.42
1:A:134:ALA:O	1:A:135:GLN:C	2.58	0.42
1:A:177:LYS:HD3	1:A:206:PRO:HD3	2.00	0.42
1:A:228:VAL:O	1:A:228:VAL:HG12	2.18	0.42
1:A:1063:TYR:CD1	1:A:1063:TYR:C	2.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:ASN:CA	1:A:88:TYR:CD2	3.01	0.41
1:A:185:SER:HG	1:A:200:HIS:CD2	2.38	0.41
1:A:1059:ASP:O	1:A:1060:TRP:HB2	2.20	0.41
1:A:1099:MET:HE2	1:A:239:ARG:HG3	2.02	0.41
1:A:203:GLY:HA3	3:A:2003:GOL:H11	2.02	0.41
1:A:139:LYS:O	1:A:140:VAL:C	2.59	0.41
1:A:253:SER:OG	1:A:267:ILE:HG22	2.21	0.41
1:A:1099:MET:HE2	1:A:237:TYR:OH	2.21	0.41
1:A:1035:ILE:HG12	1:A:1036:GLU:N	2.34	0.41
1:A:77:VAL:O	1:A:78:GLN:C	2.59	0.41
1:A:1016:GLU:HG2	1:A:1019:LYS:CG	2.50	0.41
1:A:225:ARG:CG	1:A:225:ARG:HH11	2.29	0.41
1:A:1099:MET:CE	1:A:237:TYR:OH	2.69	0.41
1:A:1051:HIS:C	1:A:1051:HIS:ND1	2.74	0.41
1:A:1009:VAL:HG23	1:A:1093:VAL:HG11	2.02	0.41
1:A:214:MET:SD	1:A:219:GLU:HA	2.61	0.41
1:A:161:ARG:O	1:A:164:ALA:HB3	2.20	0.41
1:A:109:MET:O	1:A:116:PHE:HB3	2.21	0.41
1:A:136:ASN:N	1:A:136:ASN:HD22	2.18	0.41
1:A:213:TRP:HB2	1:A:223:THR:OG1	2.21	0.41
1:A:1005:PRO:HA	1:A:1030:PHE:HB3	2.01	0.41
1:A:205:TYR:CD2	1:A:206:PRO:HA	2.56	0.41
1:A:257:LYS:HE2	1:A:265:ASP:OD1	2.21	0.41
1:A:1016:GLU:CD	1:A:1019:LYS:HG2	2.42	0.40
1:A:1069:GLU:O	1:A:1070:PHE:HB3	2.21	0.40
1:A:1037:VAL:HB	1:A:1066:TYR:CZ	2.56	0.40
1:A:1089:GLN:O	1:A:1090:PRO:C	2.60	0.40
1:A:103:PRO:O	1:A:104:GLN:CB	2.69	0.40
1:A:1011:SER:OG	1:A:1013:HIS:O	2.32	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	367/392 (94%)	284 (77%)	59 (16%)	24 (6%)	<b>1</b> <b>4</b>

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1085	VAL
1	A	99	ARG
1	A	104	GLN
1	A	171	GLU
1	A	193	GLY
1	A	79	ALA
1	A	81	ALA
1	A	102	ALA
1	A	196	GLN
1	A	215	ARG
1	A	1075	LYS
1	A	46	LEU
1	A	107	LEU
1	A	1070	PHE
1	A	39	VAL
1	A	180	PRO
1	A	192	PRO
1	A	218	GLN
1	A	4	LEU
1	A	49	TRP
1	A	175	LYS
1	A	140	VAL
1	A	187	GLY
1	A	103	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	278/340 (82%)	239 (86%)	39 (14%)	<b>4</b> <b>12</b>

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1003	ARG
1	A	1016	GLU
1	A	1027	VAL
1	A	1051	HIS
1	A	1057	SER
1	A	1077	GLU
1	A	1081	ARG
1	A	1092	ILE
1	A	1093	VAL
1	A	1094	LYS
1	A	1096	ASP
1	A	1098	ASP
1	A	1099	MET
1	A	17	HIS
1	A	58	GLU
1	A	63	GLN
1	A	67	GLN
1	A	78	GLN
1	A	107	LEU
1	A	111	TYR
1	A	117	LEU
1	A	135	GLN
1	A	136	ASN
1	A	139	LYS
1	A	147	ILE
1	A	152	GLN
1	A	159	CYS
1	A	199	CYS
1	A	218	GLN
1	A	220	GLN
1	A	225	ARG
1	A	239	ARG
1	A	248	GLU
1	A	259	SER
1	A	265	ASP
1	A	269	HIS
1	A	270	TRP
1	A	273	GLU
1	A	275	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	17	HIS
1	A	57	GLN
1	A	61	ASN
1	A	63	GLN
1	A	67	GLN
1	A	78	GLN
1	A	136	ASN
1	A	269	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 ⓘ

2 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	$\# Z  > 2$
2	NAG	A	2001	1,2	14,14,15	0.93	0	15,19,21	1.78	5 (33%)
2	FUC	A	2002	2	10,10,11	0.84	0	14,14,16	1.53	3 (21%)

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
2	NAG	A	2001	1,2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FUC	A	2002	2	1/1/4/5	0/0/17/20	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2001	NAG	O7-C7-C8	-2.52	117.44	122.06
2	A	2001	NAG	O7-C7-N2	2.02	125.99	121.86
2	A	2002	FUC	O4-C4-C5	2.71	116.21	109.84
2	A	2002	FUC	C1-C2-C3	2.84	112.89	109.54
2	A	2001	NAG	C3-C4-C5	2.93	115.31	110.20
2	A	2001	NAG	C2-N2-C7	3.00	126.90	123.04
2	A	2001	NAG	C4-C3-C2	3.15	116.12	111.23
2	A	2002	FUC	O5-C5-C6	3.27	111.53	106.13

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	2002	FUC	C1

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.6 Ligand geometry [i](#)

1 ligand is 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	GOL	A	2003	-	5,5,5	0.59	0	5,5,5	1.27	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	GOL	A	2003	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2003	GOL	3	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	372/392 (94%)	-0.14	1 (0%) 94 94	44, 86, 132, 153	2 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1040	LEU	2.4

### 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
2	NAG	A	2001	14/15	0.85	0.20	0.94	70,78,81,85	0
2	FUC	A	2002	10/11	0.88	0.15	-	88,91,91,92	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
3	GOL	A	2003	6/6	0.94	0.15	-0.85	63,65,67,69	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.