



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 3, 2023 – 03:32 AM EDT

PDB ID : 3RMY  
Title : Crystal structure of HCR/D W1238A mutant  
Authors : Fu, Z.; Karalewitz, A.; Kroken, A.; Kim, J.-J.P.; Barbieri, J.T.  
Deposited on : 2011-04-21  
Resolution : 2.30 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35

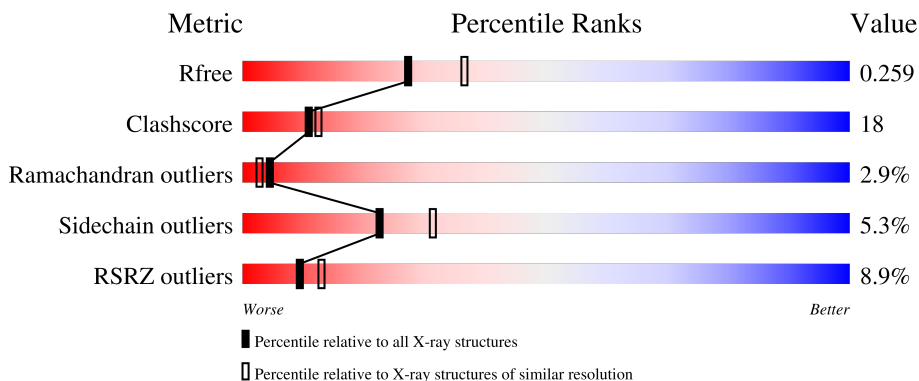
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


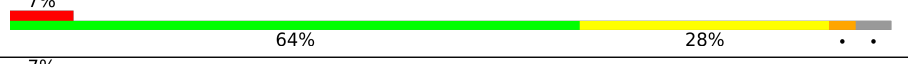


The reported resolution of this entry is 2.30 Å.

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))
$R_{free}$	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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	415	
1	B	415	
1	C	415	
1	D	415	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13352 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 Botulinum neurotoxin type D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	401	3284	2097	541	636	10	0	0	0
1	B	398	3263	2082	538	633	10	0	0	0
1	C	403	3286	2093	545	638	10	0	0	0
1	D	404	3294	2099	546	639	10	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1238	ALA	TRP	engineered mutation	UNP P19321
B	1238	ALA	TRP	engineered mutation	UNP P19321
C	1238	ALA	TRP	engineered mutation	UNP P19321
D	1238	ALA	TRP	engineered mutation	UNP P19321

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

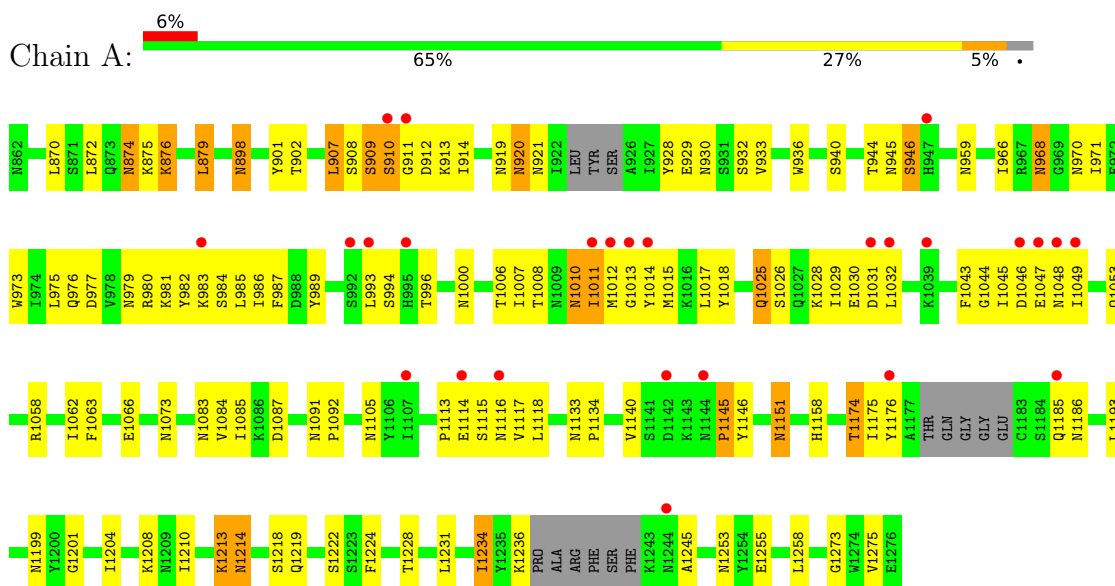
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	55	Total O 55 55	0	0
3	B	60	Total O 60 60	0	0
3	C	51	Total O 51 51	0	0
3	D	41	Total O 41 41	0	0

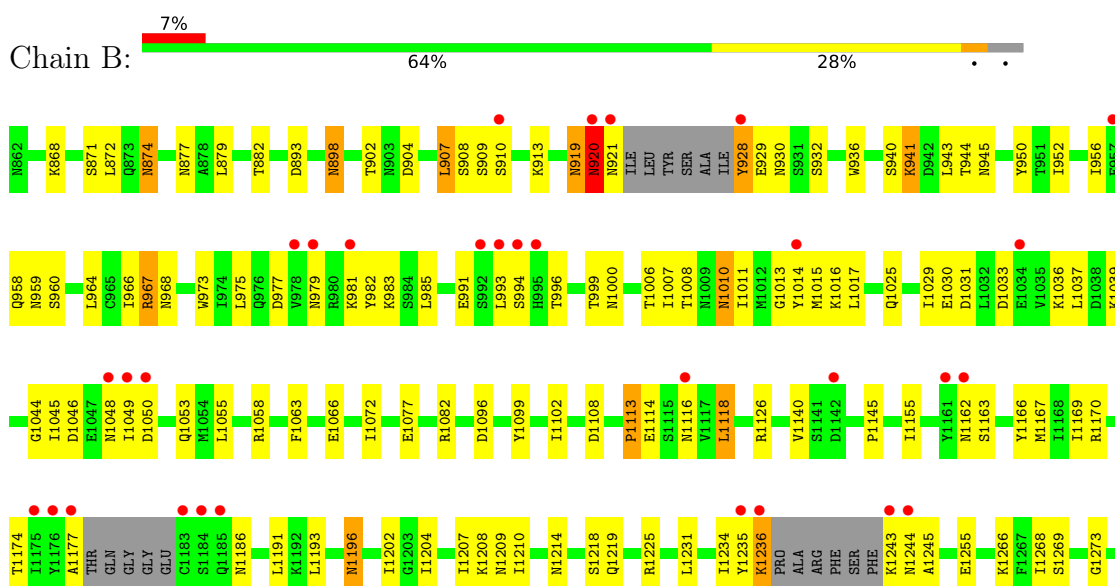
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: Botulinum neurotoxin type D

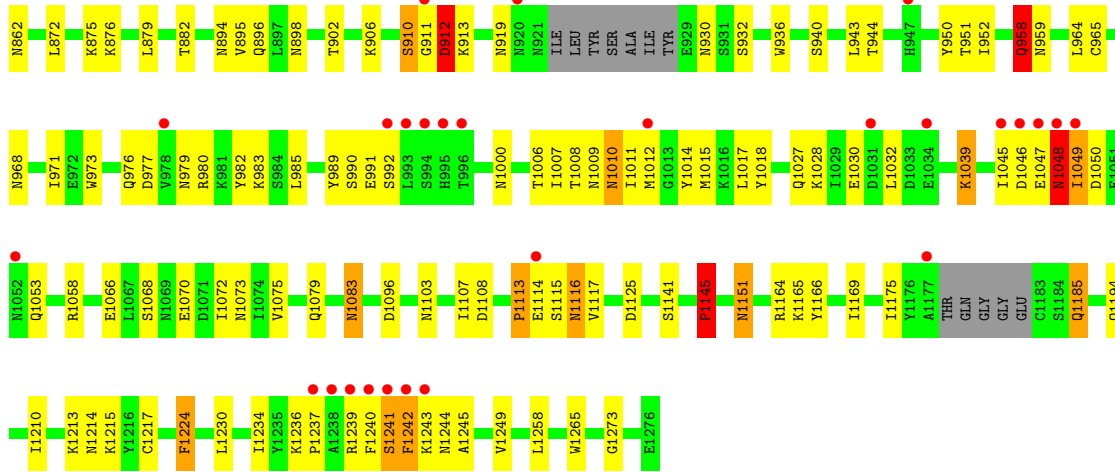


- Molecule 1: Botulinum neurotoxin type D

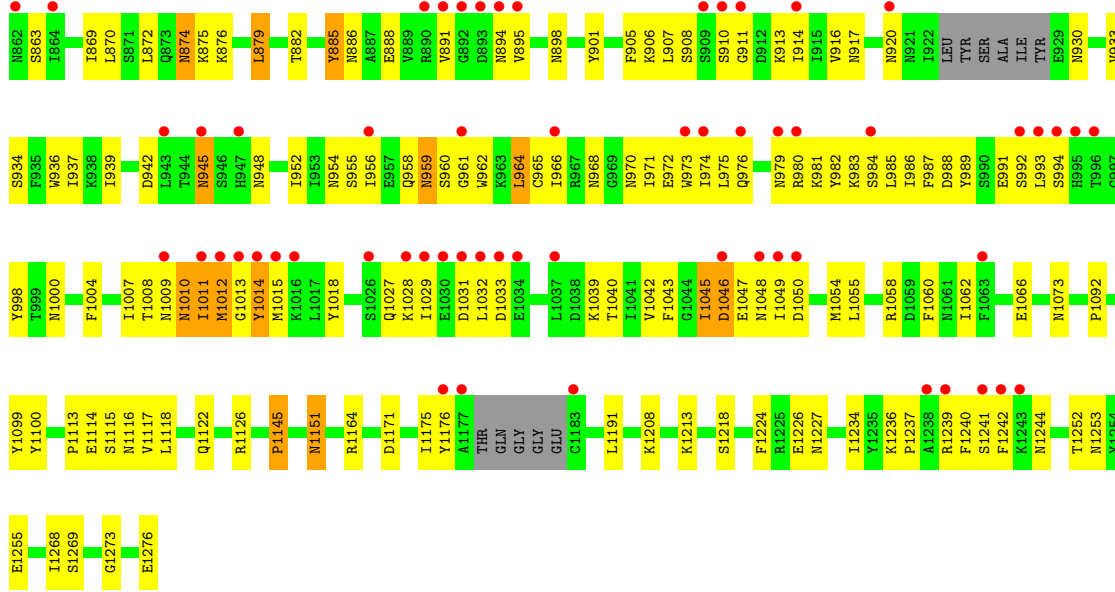


E1276

• Molecule 1: Botulinum neurotoxin type D



• Molecule 1: Botulinum neurotoxin type D



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.52Å 115.62Å 107.18Å 90.00° 91.90° 90.00°	Depositor
Resolution (Å)	36.60 – 2.30 36.59 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.6 (36.60-2.30) 95.6 (36.59-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.75 (at 2.29Å)	Xtrriage
Refinement program	CNS 1.3	Depositor
R, $R_{free}$	0.232 , 0.269 0.224 , 0.259	Depositor DCC
$R_{free}$ test set	4914 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.2	Xtrriage
Anisotropy	0.167	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 41.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.024 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	13352	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% 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, 0.333 respectively for untwinned datasets, and 0.375, 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

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	0.38	0/3347	0.61	0/4529
1	B	0.39	0/3326	0.62	0/4500
1	C	0.38	0/3350	0.63	0/4536
1	D	0.35	0/3358	0.57	0/4547
All	All	0.38	0/13381	0.61	0/18112

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3284	0	3237	125	0
1	B	3263	0	3212	116	0
1	C	3286	0	3225	98	0
1	D	3294	0	3236	138	0
2	A	6	0	8	0	0
2	C	6	0	8	0	0
2	D	6	0	8	1	0
3	A	55	0	0	2	0
3	B	60	0	0	0	0

*Continued on next page...*



Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	51	0	0	1	0
3	D	41	0	0	0	0
All	All	13352	0	12934	475	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (475) 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:920:ASN:HA	1:B:1039:LYS:HZ3	1.18	1.06
1:B:991:GLU:HB3	1:B:994:SER:HB3	1.44	1.00
1:C:983:LYS:HE3	1:C:1030:GLU:H	1.26	0.99
1:B:944:THR:HG21	1:B:999:THR:HG23	1.43	0.97
1:A:1010:ASN:ND2	1:A:1014:TYR:H	1.61	0.96
1:A:1011:ILE:HD13	1:A:1011:ILE:H	1.30	0.93
1:C:976:GLN:HB3	1:C:982:TYR:HB3	1.50	0.93
1:C:910:SER:HB2	1:C:1048:ASN:HA	1.50	0.92
1:D:958:GLN:HE21	1:D:960:SER:H	1.16	0.91
1:C:1234:ILE:HD11	1:C:1244:ASN:HB3	1.52	0.89
1:C:958:GLN:HG2	1:C:959:ASN:H	1.35	0.89
1:A:1010:ASN:HD21	1:A:1014:TYR:H	1.17	0.88
1:B:983:LYS:HE2	1:B:1029:ILE:HA	1.56	0.86
1:B:868:LYS:HE3	1:B:871:SER:HB2	1.56	0.86
1:C:944:THR:HG22	1:C:989:TYR:OH	1.78	0.84
1:C:983:LYS:HE2	1:C:1032:LEU:HD13	1.59	0.83
1:C:1175:ILE:HG12	1:C:1237:PRO:HB3	1.61	0.83
1:C:1236:LYS:HG2	1:C:1244:ASN:ND2	1.93	0.82
1:B:1010:ASN:HD21	1:B:1014:TYR:H	1.26	0.81
1:B:920:ASN:HA	1:B:1039:LYS:NZ	1.96	0.81
1:B:910:SER:HB2	1:B:1048:ASN:HA	1.62	0.80
1:D:952:ILE:HD11	1:D:964:LEU:HD22	1.64	0.79
1:C:936:TRP:HB2	1:C:1058:ARG:HG2	1.65	0.78
1:A:1210:ILE:HD11	1:A:1219:GLN:HG3	1.66	0.77
1:D:991:GLU:HB2	1:D:994:SER:HB3	1.67	0.77
1:A:911:GLY:O	1:A:913:LYS:HG3	1.84	0.77
1:D:972:GLU:HG3	1:D:974:ILE:HD11	1.66	0.76
1:D:980:ARG:NH2	1:D:980:ARG:HB3	2.01	0.76
1:D:1011:ILE:HD13	1:D:1011:ILE:H	1.50	0.76
1:A:1010:ASN:HD21	1:A:1014:TYR:N	1.83	0.76
1:A:940:SER:O	1:A:944:THR:HG23	1.85	0.76

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:985:LEU:HD21	1:D:1015:MET:HG3	1.67	0.76
1:B:991:GLU:HB3	1:B:994:SER:CB	2.17	0.75
1:A:910:SER:HB3	1:A:1047:GLU:O	1.86	0.74
1:C:958:GLN:CG	1:C:959:ASN:H	2.01	0.73
1:D:991:GLU:HB2	1:D:994:SER:CB	2.18	0.72
1:C:1236:LYS:HG2	1:C:1244:ASN:HD21	1.54	0.72
1:D:958:GLN:HE21	1:D:960:SER:N	1.87	0.72
1:A:1010:ASN:C	1:A:1010:ASN:HD22	1.91	0.72
1:D:970:ASN:ND2	1:D:988:ASP:HB3	2.05	0.71
1:D:980:ARG:HB3	1:D:980:ARG:HH21	1.53	0.71
1:D:1009:ASN:ND2	1:D:1015:MET:HB3	2.06	0.71
1:D:958:GLN:HG2	1:D:959:ASN:H	1.56	0.70
1:B:1207:ILE:HD11	1:B:1218:SER:OG	1.90	0.70
1:B:907:LEU:HG	1:B:1044:GLY:HA2	1.73	0.69
1:C:940:SER:O	1:C:944:THR:HG23	1.92	0.69
1:A:1140:VAL:HG13	1:A:1199:ASN:OD1	1.92	0.69
1:D:913:LYS:NZ	1:D:1046:ASP:H	1.91	0.69
1:A:1011:ILE:H	1:A:1011:ILE:CD1	2.03	0.68
1:D:971:ILE:HG22	1:D:987:PHE:O	1.92	0.68
1:B:1207:ILE:HD11	1:B:1218:SER:CB	2.23	0.68
1:B:977:ASP:OD2	1:B:981:LYS:HB3	1.94	0.68
1:B:1050:ASP:HB2	1:B:1053:GLN:HG3	1.75	0.68
1:B:983:LYS:HD2	1:B:1029:ILE:HG23	1.75	0.67
1:A:1011:ILE:HD13	1:A:1011:ILE:N	2.08	0.67
1:C:910:SER:HB2	1:C:1048:ASN:CA	2.23	0.67
1:D:1008:THR:HB	1:D:1066:GLU:HG3	1.77	0.67
1:B:1236:LYS:HD2	1:B:1236:LYS:N	2.10	0.66
1:D:983:LYS:HB2	1:D:1027:GLN:HE22	1.59	0.66
1:A:932:SER:HB2	1:A:1063:PHE:HB2	1.78	0.66
1:B:930:ASN:HD22	1:B:1010:ASN:HA	1.59	0.66
1:B:940:SER:O	1:B:944:THR:HG22	1.95	0.66
1:B:967:ARG:HG3	1:B:967:ARG:HH11	1.61	0.66
1:D:1045:ILE:N	1:D:1045:ILE:HD13	2.11	0.65
1:D:958:GLN:CD	1:D:958:GLN:H	1.99	0.65
1:B:985:LEU:HD11	1:B:1015:MET:HG2	1.77	0.65
1:B:1207:ILE:HD11	1:B:1218:SER:HB2	1.79	0.65
1:A:1255:GLU:HA	1:A:1258:LEU:HD23	1.76	0.65
1:D:936:TRP:HB2	1:D:1058:ARG:HG2	1.79	0.65
1:A:1000:ASN:ND2	1:A:1273:GLY:HA3	2.11	0.65
1:C:1011:ILE:HG13	1:C:1012:MET:H	1.62	0.64
1:B:1050:ASP:H	1:B:1053:GLN:HE21	1.46	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:974:ILE:HA	1:D:984:SER:HB3	1.79	0.64
1:C:1039:LYS:HD2	1:C:1039:LYS:N	2.13	0.64
1:B:983:LYS:CE	1:B:1029:ILE:HA	2.29	0.63
1:C:958:GLN:H	1:C:958:GLN:CD	2.02	0.63
1:D:1009:ASN:HD21	1:D:1015:MET:HB3	1.61	0.63
1:B:1209:ASN:HA	1:B:1218:SER:HB3	1.79	0.63
1:A:1029:ILE:HG23	1:A:1032:LEU:HB3	1.79	0.63
1:C:1113:PRO:O	1:C:1114:GLU:HG2	1.98	0.63
1:B:981:LYS:NZ	1:B:1031:ASP:HB3	2.13	0.63
1:D:1073:ASN:HD21	1:D:1213:LYS:NZ	1.97	0.63
1:B:1010:ASN:HD21	1:B:1014:TYR:N	1.97	0.62
1:C:898:ASN:OD1	1:C:902:THR:HA	1.99	0.62
1:A:910:SER:HA	1:A:1045:ILE:O	2.00	0.62
1:B:985:LEU:HA	1:B:1025:GLN:NE2	2.14	0.62
1:D:971:ILE:HG23	1:D:971:ILE:O	2.00	0.62
1:D:970:ASN:HA	1:D:988:ASP:HA	1.80	0.62
1:C:973:TRP:CD2	1:C:1007:ILE:HD13	2.35	0.62
1:A:1208:LYS:O	1:A:1218:SER:HB2	2.00	0.62
1:B:958:GLN:HG3	1:B:959:ASN:H	1.64	0.62
1:A:983:LYS:HD3	1:A:1032:LEU:HD13	1.82	0.62
1:A:1030:GLU:C	1:A:1032:LEU:H	2.03	0.61
1:A:933:VAL:CG2	1:A:1007:ILE:HB	2.29	0.61
1:A:959:ASN:O	1:A:976:GLN:HG3	2.00	0.61
1:A:1210:ILE:HD13	1:A:1218:SER:HA	1.82	0.61
1:C:894:ASN:HD22	1:C:912:ASP:HA	1.66	0.60
1:A:986:ILE:HG22	1:A:1025:GLN:HE22	1.66	0.60
1:C:983:LYS:HE3	1:C:1030:GLU:N	2.08	0.60
1:B:928:TYR:N	1:B:1011:ILE:HA	2.16	0.60
1:C:1107:ILE:HD12	1:C:1108:ASP:N	2.16	0.60
1:D:933:VAL:CG1	1:D:1007:ILE:HB	2.32	0.60
1:A:910:SER:OG	1:A:1048:ASN:HA	2.01	0.60
1:C:983:LYS:HG3	1:C:1032:LEU:CD1	2.32	0.60
1:C:990:SER:O	1:C:992:SER:N	2.35	0.59
1:B:882:THR:O	1:C:1224:PHE:O	2.21	0.59
1:A:936:TRP:HB2	1:A:1058:ARG:HG2	1.82	0.59
1:D:960:SER:HA	1:D:976:GLN:O	2.02	0.59
1:A:1025:GLN:O	1:A:1026:SER:HB3	2.02	0.59
1:B:1010:ASN:C	1:B:1010:ASN:HD22	2.06	0.58
1:A:1000:ASN:HD21	1:A:1273:GLY:HA3	1.68	0.58
1:D:885:TYR:N	1:D:885:TYR:CD1	2.71	0.58
1:B:1096:ASP:OD2	1:B:1145:PRO:O	2.21	0.58

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1210:ILE:HD12	1:B:1218:SER:HA	1.86	0.58
1:C:1169:ILE:HD13	1:C:1194:GLN:OE1	2.04	0.58
1:D:874:ASN:HD22	1:D:875:LYS:N	2.01	0.58
1:A:929:GLU:HG2	1:A:1011:ILE:HA	1.86	0.57
1:B:1099:TYR:CE1	1:B:1269:SER:HB3	2.39	0.57
1:B:1210:ILE:HD12	1:B:1218:SER:CA	2.35	0.57
1:B:950:TYR:HB2	1:B:966:ILE:HG12	1.86	0.57
1:D:981:LYS:HE2	1:D:1031:ASP:HB3	1.86	0.57
1:D:958:GLN:HG2	1:D:959:ASN:N	2.18	0.57
1:B:936:TRP:HB2	1:B:1058:ARG:HG2	1.86	0.57
1:C:1010:ASN:C	1:C:1010:ASN:HD22	2.08	0.57
1:D:875:LYS:HD3	1:D:882:THR:HG21	1.85	0.57
1:D:974:ILE:N	1:D:974:ILE:HD12	2.20	0.56
1:D:989:TYR:HB2	1:D:998:TYR:HB2	1.87	0.56
1:A:1049:ILE:HB	1:A:1053:GLN:HB2	1.87	0.56
1:A:1174:THR:HG23	1:A:1176:TYR:H	1.70	0.56
1:C:1234:ILE:CD1	1:C:1244:ASN:HB3	2.31	0.56
1:D:870:LEU:HB3	1:D:1062:ILE:HB	1.87	0.56
1:D:888:GLU:O	1:D:916:VAL:HA	2.05	0.56
1:A:909:SER:O	1:A:911:GLY:N	2.39	0.56
1:B:994:SER:OG	1:B:996:THR:HG22	2.06	0.56
1:D:981:LYS:CE	1:D:1031:ASP:HB3	2.36	0.56
1:D:1113:PRO:O	1:D:1117:VAL:O	2.24	0.55
1:B:868:LYS:HE3	1:B:871:SER:CB	2.33	0.55
1:D:1122:GLN:NE2	1:D:1126:ARG:HH11	2.02	0.55
1:B:1055:LEU:HD12	1:B:1055:LEU:C	2.27	0.55
1:A:870:LEU:HB3	1:A:1062:ILE:HB	1.88	0.55
1:D:983:LYS:HB2	1:D:1027:GLN:NE2	2.22	0.55
1:D:1008:THR:O	1:D:1015:MET:HA	2.06	0.55
1:D:1011:ILE:H	1:D:1011:ILE:CD1	2.19	0.55
1:C:1107:ILE:HD12	1:C:1107:ILE:C	2.26	0.55
1:C:1113:PRO:HG2	1:C:1114:GLU:H	1.72	0.55
1:D:1073:ASN:HD21	1:D:1213:LYS:HZ3	1.53	0.55
1:C:1010:ASN:HD21	1:C:1014:TYR:H	1.53	0.54
1:D:895:VAL:HG11	1:D:914:ILE:HD11	1.89	0.54
1:B:1235:TYR:C	1:B:1236:LYS:HD2	2.28	0.54
1:D:1011:ILE:HD13	1:D:1011:ILE:N	2.19	0.54
1:D:1276:GLU:O	2:D:1402:GOL:H32	2.08	0.54
1:A:1010:ASN:ND2	1:A:1010:ASN:C	2.60	0.54
1:A:1175:ILE:HG23	1:A:1176:TYR:CD2	2.43	0.54
1:B:1037:LEU:N	1:B:1037:LEU:HD12	2.23	0.54

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:911:GLY:N	1:D:1046:ASP:HA	2.23	0.54
1:A:1214:ASN:C	1:A:1214:ASN:HD22	2.11	0.54
1:D:958:GLN:CG	1:D:959:ASN:H	2.20	0.54
1:C:958:GLN:N	1:C:958:GLN:OE1	2.41	0.53
1:D:933:VAL:HG11	1:D:973:TRP:CH2	2.43	0.53
1:B:1234:ILE:HD11	1:B:1244:ASN:HB3	1.90	0.53
1:C:1011:ILE:HG13	1:C:1012:MET:SD	2.48	0.53
1:D:917:ASN:OD1	1:D:1040:THR:HG22	2.08	0.53
1:C:1117:VAL:HG21	1:C:1239:ARG:HD2	1.90	0.53
1:D:983:LYS:NZ	1:D:1032:LEU:HG	2.24	0.53
1:C:1083:ASN:CG	1:C:1151:ASN:HD21	2.11	0.53
1:A:986:ILE:H	1:A:1025:GLN:NE2	2.06	0.53
1:B:1045:ILE:HG13	1:B:1045:ILE:O	2.09	0.53
1:C:911:GLY:O	1:C:913:LYS:HG3	2.08	0.53
1:D:1234:ILE:HD11	1:D:1244:ASN:HB3	1.91	0.53
1:A:945:ASN:OD1	1:A:993:LEU:HD11	2.07	0.53
1:C:958:GLN:CG	1:C:959:ASN:N	2.71	0.52
1:C:983:LYS:HB3	1:C:1027:GLN:NE2	2.24	0.52
1:D:980:ARG:HH21	1:D:980:ARG:CB	2.22	0.52
1:A:944:THR:HG22	1:A:989:TYR:OH	2.08	0.52
1:D:930:ASN:ND2	1:D:1010:ASN:HA	2.24	0.52
1:B:1207:ILE:HD12	1:B:1219:GLN:O	2.09	0.52
1:A:966:ILE:HA	1:A:970:ASN:O	2.09	0.52
1:B:945:ASN:OD1	1:B:993:LEU:HD21	2.09	0.52
1:A:879:LEU:HD12	1:A:914:ILE:HD13	1.92	0.52
1:D:955:SER:HB3	1:D:962:TRP:O	2.10	0.52
1:C:1151:ASN:N	1:C:1151:ASN:HD22	2.07	0.52
1:C:958:GLN:HG2	1:C:959:ASN:N	2.16	0.52
1:C:1164:ARG:HD3	1:C:1166:TYR:CZ	2.45	0.52
1:D:913:LYS:HZ1	1:D:1046:ASP:H	1.58	0.52
1:A:910:SER:CB	1:A:1048:ASN:HA	2.40	0.52
1:C:1175:ILE:CG1	1:C:1237:PRO:HB3	2.36	0.52
1:A:908:SER:C	1:A:1049:ILE:HD11	2.30	0.52
1:B:1007:ILE:HD12	1:B:1007:ILE:N	2.25	0.52
1:C:1114:GLU:HG3	1:C:1115:SER:N	2.25	0.52
1:A:987:PHE:HB2	1:A:1017:LEU:HD21	1.92	0.51
1:B:983:LYS:NZ	1:B:1031:ASP:H	2.08	0.51
1:D:964:LEU:HD21	1:D:971:ILE:CG1	2.41	0.51
1:A:1073:ASN:HD21	1:A:1213:LYS:HZ1	1.58	0.51
1:A:1073:ASN:HD21	1:A:1213:LYS:NZ	2.09	0.51
1:C:1050:ASP:OD1	1:C:1053:GLN:HG3	2.10	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:991:GLU:HB2	1:D:994:SER:HB2	1.92	0.51
1:D:1208:LYS:O	1:D:1218:SER:HB2	2.10	0.51
1:A:1008:THR:O	1:A:1015:MET:HA	2.10	0.51
1:D:1055:LEU:HD12	1:D:1055:LEU:C	2.31	0.51
1:A:1013:GLY:O	1:A:1028:LYS:HA	2.10	0.51
1:A:1140:VAL:CG2	1:A:1204:ILE:HD12	2.40	0.51
1:B:967:ARG:HD2	1:B:968:ASN:HB2	1.93	0.51
1:B:1243:LYS:HE2	1:B:1245:ALA:HB2	1.93	0.51
1:D:1176:TYR:HE2	1:D:1236:LYS:HG3	1.76	0.51
1:A:1210:ILE:HD11	1:A:1219:GLN:CG	2.37	0.51
1:C:983:LYS:HG3	1:C:1032:LEU:HD13	1.93	0.51
1:D:1049:ILE:HD12	1:D:1049:ILE:O	2.10	0.51
1:B:1210:ILE:HD11	1:B:1219:GLN:HG3	1.93	0.51
1:D:1236:LYS:HB3	1:D:1244:ASN:ND2	2.25	0.51
1:A:983:LYS:O	1:A:984:SER:HB2	2.10	0.50
1:A:901:TYR:CZ	1:A:1092:PRO:HD3	2.45	0.50
1:C:1010:ASN:C	1:C:1010:ASN:ND2	2.64	0.50
1:D:930:ASN:HA	1:D:1009:ASN:O	2.11	0.50
1:D:1099:TYR:CE1	1:D:1269:SER:HB3	2.46	0.50
1:D:964:LEU:HD21	1:D:971:ILE:HG13	1.92	0.50
1:A:930:ASN:ND2	1:A:1010:ASN:HA	2.27	0.50
1:D:917:ASN:HA	1:D:1039:LYS:O	2.12	0.50
1:B:1140:VAL:CG2	1:B:1204:ILE:HD12	2.41	0.50
1:C:1210:ILE:HG21	1:C:1217:CYS:SG	2.51	0.50
1:D:948:ASN:N	1:D:948:ASN:HD22	2.08	0.50
1:B:920:ASN:HA	1:B:1039:LYS:CE	2.42	0.50
1:B:920:ASN:CA	1:B:1039:LYS:HZ3	2.08	0.50
1:D:961:GLY:O	1:D:975:LEU:HD12	2.12	0.50
1:D:1011:ILE:HG12	1:D:1012:MET:N	2.27	0.49
1:C:911:GLY:O	1:C:912:ASP:C	2.50	0.49
1:D:992:SER:O	1:D:993:LEU:HB2	2.11	0.49
1:A:910:SER:HB2	1:A:1046:ASP:O	2.12	0.49
1:A:959:ASN:O	1:A:976:GLN:NE2	2.45	0.49
1:B:868:LYS:HG3	1:B:1063:PHE:CE1	2.47	0.49
1:D:1010:ASN:HD22	1:D:1010:ASN:H	1.59	0.49
1:A:1176:TYR:OH	1:A:1236:LYS:HA	2.11	0.49
1:C:1006:THR:HB	1:C:1018:TYR:HB2	1.95	0.49
1:C:1000:ASN:ND2	1:C:1273:GLY:HA3	2.26	0.49
1:A:1234:ILE:HD13	1:A:1245:ALA:H	1.77	0.49
1:C:1114:GLU:CG	1:C:1115:SER:N	2.75	0.49
1:C:1096:ASP:OD2	1:C:1145:PRO:O	2.31	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1151:ASN:N	1:D:1151:ASN:ND2	2.61	0.49
1:B:1255:GLU:H	1:B:1255:GLU:CD	2.16	0.49
1:A:1013:GLY:O	1:A:1028:LYS:HG3	2.12	0.49
1:B:1207:ILE:CD1	1:B:1218:SER:HB2	2.41	0.49
1:C:973:TRP:CG	1:C:1007:ILE:HD13	2.48	0.49
1:C:1164:ARG:HD3	1:C:1166:TYR:OH	2.13	0.49
1:A:1006:THR:HB	1:A:1018:TYR:HB2	1.95	0.49
1:C:930:ASN:HA	1:C:1009:ASN:O	2.13	0.49
1:C:1028:LYS:NZ	1:C:1030:GLU:HG2	2.28	0.48
1:D:1151:ASN:N	1:D:1151:ASN:HD22	2.10	0.48
1:A:1030:GLU:O	1:A:1032:LEU:N	2.46	0.48
1:B:1167:MET:O	1:B:1169:ILE:HG23	2.13	0.48
1:D:982:TYR:CD1	1:D:982:TYR:C	2.86	0.48
1:D:956:ILE:O	1:D:956:ILE:HG13	2.14	0.48
1:A:1185:GLN:O	1:A:1186:ASN:C	2.52	0.48
1:C:958:GLN:CD	1:C:958:GLN:N	2.67	0.48
1:D:970:ASN:HB3	1:D:986:ILE:HD11	1.95	0.48
1:D:1171:ASP:OD1	1:D:1239:ARG:NH2	2.47	0.48
1:A:1186:ASN:H	1:A:1253:ASN:HD22	1.61	0.48
1:B:909:SER:HA	1:B:1049:ILE:HD11	1.96	0.48
1:A:898:ASN:ND2	1:A:902:THR:HA	2.29	0.48
1:C:896:GLN:NE2	1:C:906:LYS:HD2	2.29	0.48
1:C:983:LYS:HG3	1:C:1032:LEU:HD11	1.96	0.48
1:D:913:LYS:HZ3	1:D:1046:ASP:HB3	1.79	0.48
1:D:1007:ILE:HD12	1:D:1007:ILE:N	2.28	0.48
1:A:930:ASN:HD21	1:A:1011:ILE:H	1.62	0.47
1:B:1000:ASN:ND2	1:B:1273:GLY:HA3	2.29	0.47
1:B:1166:TYR:HB3	1:B:1193:LEU:HB3	1.95	0.47
1:C:1115:SER:O	1:C:1116:ASN:HB3	2.14	0.47
1:C:1240:PHE:O	1:C:1242:PHE:N	2.46	0.47
1:D:954:ASN:HB3	1:D:1042:VAL:HB	1.95	0.47
1:D:885:TYR:N	1:D:885:TYR:HD1	2.10	0.47
1:A:908:SER:O	1:A:909:SER:C	2.52	0.47
1:C:1230:LEU:HA	1:C:1249:VAL:O	2.15	0.47
1:A:1011:ILE:HG12	1:A:1012:MET:N	2.29	0.47
1:A:959:ASN:HB3	1:A:980:ARG:HG2	1.96	0.47
1:B:930:ASN:ND2	1:B:1010:ASN:HA	2.29	0.47
1:A:945:ASN:O	1:A:946:SER:C	2.53	0.47
1:B:928:TYR:CD2	1:B:929:GLU:N	2.83	0.47
1:D:948:ASN:N	1:D:948:ASN:ND2	2.63	0.47
1:D:972:GLU:HB3	1:D:986:ILE:CD1	2.44	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:952:ILE:HG21	1:B:1055:LEU:HD21	1.97	0.47
1:C:875:LYS:HE3	1:C:875:LYS:HA	1.96	0.47
1:D:1164:ARG:NH2	1:D:1164:ARG:HB2	2.29	0.47
1:A:1029:ILE:HD12	1:A:1029:ILE:N	2.30	0.47
1:B:1055:LEU:HD12	1:B:1055:LEU:O	2.16	0.46
1:A:930:ASN:N	1:A:930:ASN:HD22	2.13	0.46
1:A:994:SER:C	1:A:996:THR:H	2.18	0.46
1:B:1140:VAL:HG22	1:B:1204:ILE:HD12	1.97	0.46
1:D:974:ILE:HD12	1:D:974:ILE:H	1.80	0.46
1:D:1000:ASN:ND2	1:D:1273:GLY:HA3	2.30	0.46
1:A:1013:GLY:C	1:A:1029:ILE:HD13	2.35	0.46
1:D:942:ASP:HA	1:D:945:ASN:HD21	1.80	0.46
1:A:979:ASN:O	1:A:980:ARG:HB2	2.16	0.46
1:B:1010:ASN:C	1:B:1010:ASN:ND2	2.69	0.46
1:B:1049:ILE:HB	1:B:1053:GLN:HB2	1.97	0.46
1:A:983:LYS:CE	1:A:1032:LEU:HB2	2.46	0.46
1:A:1105:ASN:O	1:B:1163:SER:HA	2.15	0.46
1:B:950:TYR:HB2	1:B:966:ILE:CG1	2.46	0.46
1:A:1010:ASN:HB3	1:A:1066:GLU:OE2	2.16	0.46
1:D:964:LEU:HD23	1:D:965:CYS:N	2.31	0.46
1:A:1113:PRO:O	1:A:1115:SER:N	2.49	0.46
1:A:1151:ASN:HB2	1:A:1208:LYS:HA	1.98	0.46
1:C:950:TYR:OH	1:C:1049:ILE:HG21	2.16	0.46
1:C:1049:ILE:HB	1:C:1050:ASP:H	1.59	0.46
1:A:1007:ILE:N	1:A:1007:ILE:HD12	2.31	0.45
1:B:898:ASN:ND2	1:B:902:THR:HA	2.31	0.45
1:B:1155:ILE:HD12	1:B:1155:ILE:C	2.36	0.45
1:B:1170:ARG:O	1:B:1202:ILE:HD11	2.16	0.45
1:D:1237:PRO:HG2	1:D:1240:PHE:CB	2.45	0.45
1:A:874:ASN:C	1:A:874:ASN:HD22	2.19	0.45
1:A:968:ASN:HD22	1:A:968:ASN:HA	1.55	0.45
1:D:966:ILE:O	1:D:966:ILE:HG13	2.16	0.45
1:A:914:ILE:HB	1:A:1043:PHE:HB2	1.98	0.45
1:A:919:ASN:HD22	1:A:921:ASN:CG	2.20	0.45
1:D:934:SER:HB2	1:D:1004:PHE:CE1	2.52	0.45
1:A:1201:GLY:HA2	1:A:1204:ILE:HG12	1.98	0.45
1:C:977:ASP:OD2	1:C:1032:LEU:HA	2.16	0.45
1:B:919:ASN:O	1:B:921:ASN:N	2.49	0.45
1:C:1075:VAL:O	1:C:1079:GLN:HG3	2.17	0.45
1:D:958:GLN:CD	1:D:958:GLN:N	2.67	0.45
1:B:920:ASN:O	1:B:920:ASN:ND2	2.50	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:901:TYR:CZ	1:D:1092:PRO:HD3	2.51	0.45
1:D:908:SER:HB3	1:D:1054:MET:HB3	1.99	0.45
1:A:1275:VAL:HG22	3:A:102:HOH:O	2.15	0.45
1:C:913:LYS:HZ1	1:C:1046:ASP:HB3	1.82	0.45
1:C:950:TYR:O	1:C:965:CYS:HA	2.17	0.45
1:C:1073:ASN:HD21	1:C:1213:LYS:NZ	2.15	0.45
1:A:875:LYS:O	1:A:876:LYS:O	2.34	0.45
1:A:1140:VAL:HG21	1:A:1204:ILE:HD12	1.98	0.45
1:B:943:LEU:HG	1:B:966:ILE:HD12	1.99	0.45
1:C:951:THR:O	1:C:1045:ILE:HG22	2.16	0.45
1:C:1068:SER:O	1:C:1072:ILE:HG13	2.17	0.45
1:D:1029:ILE:CG2	1:D:1032:LEU:HB2	2.47	0.45
1:B:941:LYS:NZ	1:B:941:LYS:HB3	2.32	0.44
1:D:1010:ASN:H	1:D:1010:ASN:ND2	2.15	0.44
1:B:952:ILE:HG21	1:B:1055:LEU:CD2	2.47	0.44
1:D:966:ILE:HA	1:D:970:ASN:O	2.16	0.44
1:C:1045:ILE:HB	1:C:1047:GLU:OE2	2.18	0.44
1:C:1215:LYS:HG2	3:C:200:HOH:O	2.17	0.44
1:D:869:ILE:HD11	1:D:1062:ILE:CG2	2.48	0.44
1:A:920:ASN:HD22	1:A:920:ASN:HA	1.59	0.44
1:A:933:VAL:HG12	1:A:1062:ILE:HG12	2.00	0.44
1:A:1030:GLU:C	1:A:1032:LEU:N	2.70	0.44
1:C:1151:ASN:N	1:C:1151:ASN:ND2	2.65	0.44
1:D:1226:GLU:HG3	1:D:1227:ASN:N	2.32	0.44
1:C:1115:SER:C	1:C:1117:VAL:H	2.21	0.44
1:C:1117:VAL:CG2	1:C:1239:ARG:HD2	2.47	0.44
1:D:939:ILE:HD12	1:D:939:ILE:N	2.32	0.44
1:A:1255:GLU:CA	1:A:1258:LEU:HD23	2.46	0.44
1:A:976:GLN:HA	1:A:981:LYS:O	2.18	0.44
1:A:994:SER:C	1:A:996:THR:N	2.71	0.44
1:D:958:GLN:CG	1:D:959:ASN:N	2.80	0.44
1:D:1100:TYR:HB2	1:D:1268:ILE:HB	2.00	0.44
1:A:982:TYR:CD1	1:A:982:TYR:C	2.91	0.44
1:C:964:LEU:HD11	1:C:971:ILE:CG1	2.48	0.44
1:C:1045:ILE:O	1:C:1045:ILE:HG13	2.18	0.44
1:A:985:LEU:HG	1:A:1015:MET:CE	2.48	0.43
1:B:1008:THR:HB	1:B:1066:GLU:HG3	2.00	0.43
1:C:1011:ILE:HG13	1:C:1012:MET:N	2.29	0.43
1:D:958:GLN:NE2	1:D:960:SER:HB3	2.33	0.43
1:D:1049:ILE:HD12	1:D:1049:ILE:C	2.37	0.43
1:B:983:LYS:HZ1	1:B:1031:ASP:H	1.65	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1103:ASN:HB2	1:C:1265:TRP:CZ3	2.53	0.43
1:D:1175:ILE:CG1	1:D:1237:PRO:HB3	2.47	0.43
1:A:1010:ASN:ND2	1:A:1013:GLY:H	2.16	0.43
1:B:981:LYS:HD3	1:B:1031:ASP:O	2.18	0.43
1:A:910:SER:HB3	1:A:1047:GLU:C	2.37	0.43
1:B:908:SER:O	1:B:1049:ILE:HD11	2.17	0.43
1:B:1174:THR:HG23	1:B:1177:ALA:H	1.83	0.43
1:B:930:ASN:HD21	1:B:1011:ILE:H	1.65	0.43
1:B:943:LEU:HD13	1:B:1053:GLN:HB3	2.00	0.43
1:C:932:SER:OG	1:C:1008:THR:HG22	2.19	0.43
1:C:979:ASN:O	1:C:980:ARG:HB2	2.17	0.43
1:D:985:LEU:N	1:D:985:LEU:HD22	2.32	0.43
1:A:1210:ILE:CD1	1:A:1218:SER:HA	2.48	0.43
1:B:964:LEU:HD13	1:B:973:TRP:HE3	1.82	0.43
1:C:952:ILE:HG22	1:C:1045:ILE:CG2	2.48	0.43
1:C:1185:GLN:HE21	1:C:1185:GLN:HB2	1.63	0.43
1:D:972:GLU:HG3	1:D:974:ILE:CD1	2.42	0.43
1:D:879:LEU:HD11	1:D:905:PHE:CD2	2.54	0.43
1:A:985:LEU:HG	1:A:1015:MET:HE2	2.01	0.43
1:A:1011:ILE:HG12	1:A:1012:MET:H	1.84	0.43
1:D:952:ILE:HD11	1:D:964:LEU:HD13	2.01	0.43
1:D:979:ASN:O	1:D:980:ARG:HB2	2.18	0.43
1:D:983:LYS:HZ3	1:D:1032:LEU:HG	1.84	0.43
1:D:1028:LYS:HG2	1:D:1029:ILE:N	2.34	0.43
1:A:1133:ASN:HA	1:A:1134:PRO:HD2	1.91	0.43
1:B:1196:ASN:H	1:B:1196:ASN:ND2	2.16	0.43
1:A:907:LEU:HG	1:A:1044:GLY:HA2	2.01	0.42
1:A:973:TRP:O	1:A:984:SER:HA	2.19	0.42
1:B:1208:LYS:O	1:B:1218:SER:HB2	2.18	0.42
1:B:1231:LEU:C	1:B:1231:LEU:HD12	2.39	0.42
1:A:977:ASP:OD2	1:A:981:LYS:HB3	2.19	0.42
1:B:1113:PRO:HA	1:B:1118:LEU:HD12	1.99	0.42
1:C:1175:ILE:HG12	1:C:1237:PRO:CB	2.40	0.42
1:A:1118:LEU:HD11	1:A:1193:LEU:HG	2.00	0.42
1:B:932:SER:HB2	1:B:1063:PHE:HB2	2.00	0.42
1:B:1102:ILE:HD13	1:B:1268:ILE:HD11	2.01	0.42
1:A:1084:VAL:HG11	1:A:1092:PRO:HB3	2.02	0.42
1:B:1208:LYS:O	1:B:1218:SER:CB	2.67	0.42
1:D:983:LYS:HZ1	1:D:1031:ASP:HB2	1.85	0.42
1:D:1010:ASN:HD22	1:D:1010:ASN:N	2.15	0.42
1:D:1175:ILE:HG12	1:D:1237:PRO:HB3	2.01	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:908:SER:O	1:A:1049:ILE:HD11	2.20	0.42
1:A:919:ASN:CG	1:A:920:ASN:H	2.22	0.42
1:A:933:VAL:HG23	1:A:1007:ILE:HB	2.00	0.42
1:B:1207:ILE:HD12	1:B:1208:LYS:H	1.85	0.42
1:C:913:LYS:NZ	1:C:1046:ASP:HB3	2.35	0.42
1:C:973:TRP:CD1	1:C:1015:MET:HE1	2.55	0.42
1:C:1125:ASP:OD1	1:C:1125:ASP:C	2.58	0.42
1:A:1174:THR:HG22	1:A:1176:TYR:O	2.20	0.42
1:D:894:ASN:N	1:D:894:ASN:HD22	2.18	0.42
1:A:1085:ILE:HD11	1:A:1151:ASN:HA	2.01	0.42
1:B:874:ASN:HD21	1:B:877:ASN:HA	1.84	0.42
1:B:1207:ILE:HD11	1:B:1218:SER:HG	1.82	0.42
1:A:1151:ASN:CB	1:A:1208:LYS:HA	2.50	0.42
1:D:914:ILE:HB	1:D:1043:PHE:HB2	2.02	0.42
1:D:1113:PRO:O	1:D:1115:SER:N	2.53	0.42
1:B:1108:ASP:OD2	1:B:1126:ARG:NE	2.53	0.41
1:D:1014:TYR:HA	1:D:1027:GLN:O	2.19	0.41
1:A:930:ASN:HD21	1:A:1011:ILE:N	2.17	0.41
1:A:1140:VAL:HG22	1:A:1204:ILE:HD12	2.02	0.41
1:B:904:ASP:OD2	1:B:904:ASP:C	2.58	0.41
1:B:920:ASN:HD22	1:B:1039:LYS:NZ	2.17	0.41
1:D:911:GLY:H	1:D:1046:ASP:HA	1.84	0.41
1:B:1008:THR:OG1	1:B:1016:LYS:HB2	2.20	0.41
1:D:869:ILE:HD11	1:D:1062:ILE:HG22	2.02	0.41
1:D:976:GLN:HB2	1:D:982:TYR:HB3	2.03	0.41
1:A:875:LYS:HA	1:A:875:LYS:HE3	2.01	0.41
1:A:1087:ASP:OD1	1:A:1091:ASN:HB2	2.21	0.41
1:B:991:GLU:O	1:B:994:SER:HB2	2.20	0.41
1:B:1011:ILE:C	1:B:1013:GLY:N	2.74	0.41
1:B:1234:ILE:HD12	1:B:1245:ALA:C	2.41	0.41
1:C:985:LEU:HD13	1:C:1017:LEU:HB2	2.02	0.41
1:C:1015:MET:O	1:C:1015:MET:HG3	2.20	0.41
1:D:870:LEU:HD23	1:D:1062:ILE:HD12	2.02	0.41
1:D:885:TYR:HD1	1:D:885:TYR:H	1.67	0.41
1:D:905:PHE:HD1	1:D:907:LEU:HD11	1.85	0.41
1:A:1115:SER:C	1:A:1117:VAL:H	2.23	0.41
1:B:1000:ASN:HD21	1:B:1273:GLY:HA3	1.85	0.41
1:B:1236:LYS:HE2	1:B:1244:ASN:OD1	2.20	0.41
1:D:1011:ILE:C	1:D:1013:GLY:H	2.23	0.41
1:B:1006:THR:HG21	1:B:1072:ILE:HG12	2.03	0.41
1:C:943:LEU:O	1:C:943:LEU:HD12	2.21	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1234:ILE:HD12	1:C:1245:ALA:C	2.40	0.41
1:D:945:ASN:H	1:D:945:ASN:ND2	2.18	0.41
1:C:875:LYS:HD3	1:C:882:THR:HG21	2.02	0.41
1:C:983:LYS:CE	1:C:1032:LEU:HD13	2.40	0.41
1:C:1210:ILE:HD12	1:C:1210:ILE:HA	1.89	0.41
1:A:919:ASN:CG	1:A:920:ASN:N	2.74	0.41
1:B:913:LYS:HE2	1:B:1046:ASP:HB3	2.02	0.41
1:D:1252:THR:O	1:D:1253:ASN:C	2.58	0.41
1:A:971:ILE:HG22	1:A:987:PHE:HB3	2.03	0.41
1:A:983:LYS:CD	1:A:1032:LEU:HD13	2.49	0.41
1:B:952:ILE:CG2	1:B:1055:LEU:HD21	2.51	0.41
1:B:975:LEU:HB2	1:B:1015:MET:HE1	2.03	0.41
1:B:1077:GLU:OE1	1:B:1082:ARG:NH1	2.52	0.41
1:D:872:LEU:HB2	1:D:1060:PHE:HB3	2.03	0.41
1:D:891:VAL:CG1	1:D:895:VAL:HB	2.51	0.41
1:D:988:ASP:O	1:D:988:ASP:CG	2.58	0.41
1:D:1029:ILE:HG23	1:D:1032:LEU:HB2	2.03	0.41
1:D:1175:ILE:HD11	1:D:1237:PRO:HB3	2.03	0.41
1:B:956:ILE:HG23	1:B:960:SER:O	2.21	0.41
1:D:1073:ASN:ND2	1:D:1213:LYS:NZ	2.67	0.41
1:B:982:TYR:CD1	1:B:982:TYR:C	2.95	0.40
1:A:1222:SER:HB3	1:A:1228:THR:OG1	2.21	0.40
1:B:977:ASP:OD1	1:B:979:ASN:N	2.52	0.40
1:A:975:LEU:O	1:A:982:TYR:HA	2.22	0.40
1:A:1158:HIS:HD2	3:A:13:HOH:O	2.04	0.40
1:B:967:ARG:HH11	1:B:967:ARG:CG	2.30	0.40
1:C:1010:ASN:HB3	1:C:1066:GLU:CD	2.41	0.40
1:D:906:LYS:C	1:D:907:LEU:HD12	2.42	0.40
1:B:958:GLN:NE2	1:B:1036:LYS:NZ	2.70	0.40
1:B:985:LEU:HD13	1:B:1017:LEU:HB2	2.03	0.40
1:D:1255:GLU:OE2	1:D:1255:GLU:HA	2.21	0.40
1:A:1085:ILE:HD11	1:A:1151:ASN:CA	2.52	0.40
1:A:1231:LEU:C	1:A:1231:LEU:HD12	2.42	0.40
1:D:937:ILE:CD1	1:D:939:ILE:HD11	2.52	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	393/415 (95%)	345 (88%)	38 (10%)	10 (2%)	5 4
1	B	390/415 (94%)	357 (92%)	26 (7%)	7 (2%)	8 7
1	C	397/415 (96%)	348 (88%)	32 (8%)	17 (4%)	2 1
1	D	398/415 (96%)	344 (86%)	42 (11%)	12 (3%)	4 2
All	All	1578/1660 (95%)	1394 (88%)	138 (9%)	46 (3%)	4 3

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	876	LYS
1	A	910	SER
1	A	1145	PRO
1	A	1224	PHE
1	C	876	LYS
1	C	991	GLU
1	C	1048	ASN
1	C	1145	PRO
1	C	1241	SER
1	D	1145	PRO
1	D	1224	PHE
1	A	909	SER
1	A	1031	ASP
1	A	1114	GLU
1	B	920	ASN
1	C	895	VAL
1	C	910	SER
1	C	958	GLN
1	C	1224	PHE
1	D	863	SER
1	D	886	ASN
1	D	910	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	968	ASN
1	D	1242	PHE
1	B	1033	ASP
1	B	1186	ASN
1	C	912	ASP
1	C	1113	PRO
1	D	1047	GLU
1	A	912	ASP
1	A	946	SER
1	B	1030	GLU
1	B	1114	GLU
1	C	919	ASN
1	C	968	ASN
1	C	1049	ILE
1	D	1046	ASP
1	B	1225	ARG
1	C	1141	SER
1	C	1242	PHE
1	C	1243	LYS
1	D	959	ASN
1	D	1012	MET
1	D	1114	GLU
1	A	1146	TYR
1	B	1113	PRO

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	375/386 (97%)	356 (95%)	19 (5%)	24	33
1	B	373/386 (97%)	353 (95%)	20 (5%)	22	30
1	C	374/386 (97%)	356 (95%)	18 (5%)	25	36
1	D	375/386 (97%)	353 (94%)	22 (6%)	19	27
All	All	1497/1544 (97%)	1418 (95%)	79 (5%)	22	31

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	872	LEU
1	A	874	ASN
1	A	879	LEU
1	A	898	ASN
1	A	907	LEU
1	A	920	ASN
1	A	928	TYR
1	A	968	ASN
1	A	1010	ASN
1	A	1011	ILE
1	A	1025	GLN
1	A	1083	ASN
1	A	1116	ASN
1	A	1145	PRO
1	A	1151	ASN
1	A	1174	THR
1	A	1213	LYS
1	A	1214	ASN
1	A	1234	ILE
1	B	872	LEU
1	B	874	ASN
1	B	879	LEU
1	B	893	ASP
1	B	898	ASN
1	B	907	LEU
1	B	919	ASN
1	B	920	ASN
1	B	928	TYR
1	B	941	LYS
1	B	967	ARG
1	B	1010	ASN
1	B	1116	ASN
1	B	1118	LEU
1	B	1162	ASN
1	B	1191	LEU
1	B	1196	ASN
1	B	1214	ASN
1	B	1236	LYS
1	B	1266	LYS
1	C	862	ASN
1	C	872	LEU
1	C	879	LEU

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	912	ASP
1	C	958	GLN
1	C	1010	ASN
1	C	1039	LYS
1	C	1048	ASN
1	C	1070	GLU
1	C	1083	ASN
1	C	1116	ASN
1	C	1145	PRO
1	C	1151	ASN
1	C	1165	LYS
1	C	1185	GLN
1	C	1214	ASN
1	C	1241	SER
1	C	1258	LEU
1	D	874	ASN
1	D	876	LYS
1	D	879	LEU
1	D	885	TYR
1	D	898	ASN
1	D	920	ASN
1	D	945	ASN
1	D	964	LEU
1	D	1010	ASN
1	D	1011	ILE
1	D	1014	TYR
1	D	1018	TYR
1	D	1033	ASP
1	D	1045	ILE
1	D	1048	ASN
1	D	1050	ASP
1	D	1116	ASN
1	D	1118	LEU
1	D	1145	PRO
1	D	1151	ASN
1	D	1191	LEU
1	D	1241	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	874	ASN

*Continued on next page...*



*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	896	GLN
1	A	898	ASN
1	A	919	ASN
1	A	920	ASN
1	A	921	ASN
1	A	930	ASN
1	A	968	ASN
1	A	970	ASN
1	A	979	ASN
1	A	1000	ASN
1	A	1010	ASN
1	A	1025	GLN
1	A	1027	GLN
1	A	1073	ASN
1	A	1116	ASN
1	A	1151	ASN
1	A	1158	HIS
1	A	1214	ASN
1	A	1219	GLN
1	A	1253	ASN
1	B	874	ASN
1	B	898	ASN
1	B	920	ASN
1	B	921	ASN
1	B	930	ASN
1	B	948	ASN
1	B	958	GLN
1	B	970	ASN
1	B	976	GLN
1	B	1000	ASN
1	B	1010	ASN
1	B	1025	GLN
1	B	1027	GLN
1	B	1053	GLN
1	B	1073	ASN
1	B	1116	ASN
1	B	1194	GLN
1	B	1196	ASN
1	B	1199	ASN
1	B	1219	GLN
1	C	865	ASN
1	C	874	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	894	ASN
1	C	896	GLN
1	C	970	ASN
1	C	1000	ASN
1	C	1010	ASN
1	C	1025	GLN
1	C	1027	GLN
1	C	1048	ASN
1	C	1073	ASN
1	C	1116	ASN
1	C	1151	ASN
1	C	1185	GLN
1	C	1199	ASN
1	C	1219	GLN
1	C	1244	ASN
1	D	865	ASN
1	D	874	ASN
1	D	894	ASN
1	D	898	ASN
1	D	920	ASN
1	D	930	ASN
1	D	945	ASN
1	D	948	ASN
1	D	958	GLN
1	D	970	ASN
1	D	1000	ASN
1	D	1010	ASN
1	D	1027	GLN
1	D	1048	ASN
1	D	1053	GLN
1	D	1073	ASN
1	D	1122	GLN
1	D	1151	ASN
1	D	1158	HIS
1	D	1186	ASN
1	D	1199	ASN
1	D	1219	GLN
1	D	1244	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

3 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	$\# Z  > 2$
2	GOL	D	1402	-	5,5,5	0.56	0	5,5,5	0.64	0
2	GOL	A	1400	-	5,5,5	0.62	0	5,5,5	0.61	0
2	GOL	C	1401	-	5,5,5	0.56	0	5,5,5	0.55	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
2	GOL	D	1402	-	-	2/4/4/4	-
2	GOL	A	1400	-	-	2/4/4/4	-
2	GOL	C	1401	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1400	GOL	O1-C1-C2-O2
2	A	1400	GOL	O1-C1-C2-C3
2	C	1401	GOL	O1-C1-C2-O2
2	C	1401	GOL	O1-C1-C2-C3
2	D	1402	GOL	O1-C1-C2-O2
2	D	1402	GOL	O1-C1-C2-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1402	GOL	1	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

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	401/415 (96%)	0.30	26 (6%) 18 24	33, 55, 95, 112	0
1	B	398/415 (95%)	0.41	31 (7%) 13 17	29, 55, 96, 106	0
1	C	403/415 (97%)	0.34	27 (6%) 17 23	34, 55, 93, 106	0
1	D	404/415 (97%)	0.73	59 (14%) 2 3	34, 66, 112, 128	0
All	All	1606/1660 (96%)	0.44	143 (8%) 9 13	29, 57, 101, 128	0

All (143) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1049	ILE	7.5
1	D	1012	MET	7.2
1	D	1014	TYR	7.2
1	D	1013	GLY	7.1
1	D	1049	ILE	7.1
1	D	1032	LEU	6.7
1	C	992	SER	6.6
1	B	995	HIS	5.8
1	B	928	TYR	5.7
1	A	1012	MET	5.6
1	D	1048	ASN	5.3
1	D	910	SER	5.3
1	B	921	ASN	5.2
1	D	1011	ILE	5.2
1	C	1177	ALA	5.1
1	D	1177	ALA	5.0
1	B	993	LEU	5.0
1	D	1241	SER	5.0
1	D	992	SER	5.0
1	A	1011	ILE	5.0
1	D	911	GLY	4.8

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	1009	ASN	4.8
1	B	1162	ASN	4.8
1	C	996	THR	4.8
1	D	1046	ASP	4.8
1	B	920	ASN	4.7
1	D	895	VAL	4.6
1	B	992	SER	4.6
1	D	1238	ALA	4.5
1	D	1050	ASP	4.4
1	A	1114	GLU	4.4
1	D	1030	GLU	4.4
1	C	993	LEU	4.4
1	B	1177	ALA	4.4
1	D	1026	SER	4.4
1	A	992	SER	4.3
1	D	864	ILE	4.2
1	A	1185	GLN	4.2
1	C	1238	ALA	4.1
1	D	973	TRP	4.0
1	A	1048	ASN	4.0
1	C	1012	MET	3.9
1	B	1243	LYS	3.9
1	D	996	THR	3.9
1	A	947	HIS	3.9
1	D	1028	LYS	3.9
1	B	1048	ASN	3.8
1	C	1242	PHE	3.7
1	C	995	HIS	3.7
1	C	1047	GLU	3.7
1	D	979	ASN	3.7
1	A	910	SER	3.7
1	D	1037	LEU	3.7
1	B	1236	LYS	3.6
1	C	1239	ARG	3.6
1	B	1176	TYR	3.6
1	A	1047	GLU	3.6
1	C	1240	PHE	3.5
1	C	1241	SER	3.5
1	D	1033	ASP	3.5
1	A	1046	ASP	3.5
1	D	993	LEU	3.4
1	C	1046	ASP	3.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	862	ASN	3.3
1	C	920	ASN	3.3
1	A	1013	GLY	3.2
1	A	995	HIS	3.2
1	B	1161	TYR	3.2
1	A	911	GLY	3.2
1	A	1142	ASP	3.2
1	B	957	GLU	3.2
1	B	1034	GLU	3.1
1	A	1031	ASP	3.1
1	A	1176	TYR	3.1
1	A	1032	LEU	3.1
1	B	1244	ASN	3.1
1	A	983	LYS	3.1
1	D	894	ASN	3.0
1	B	1235	TYR	3.0
1	D	893	ASP	3.0
1	B	1183	CYS	3.0
1	D	890	ARG	3.0
1	C	1114	GLU	2.9
1	B	1185	GLN	2.9
1	B	1142	ASP	2.9
1	C	1052	ASN	2.9
1	B	1050	ASP	2.9
1	C	994	SER	2.8
1	C	947	HIS	2.8
1	C	1031	ASP	2.8
1	A	1039	LYS	2.8
1	D	891	VAL	2.8
1	B	994	SER	2.8
1	D	947	HIS	2.8
1	C	1048	ASN	2.8
1	D	1015	MET	2.7
1	D	1063	PHE	2.7
1	D	1029	ILE	2.7
1	C	911	GLY	2.6
1	D	1243	LYS	2.6
1	D	1176	TYR	2.6
1	A	1116	ASN	2.6
1	D	966	ILE	2.6
1	D	1242	PHE	2.5
1	B	910	SER	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	1049	ILE	2.5
1	D	994	SER	2.5
1	D	995	HIS	2.4
1	A	993	LEU	2.4
1	C	978	VAL	2.4
1	B	1175	ILE	2.4
1	C	1049	ILE	2.4
1	D	961	GLY	2.4
1	D	1239	ARG	2.4
1	C	1045	ILE	2.4
1	D	909	SER	2.4
1	A	1244	ASN	2.4
1	D	920	ASN	2.4
1	D	980	ARG	2.3
1	D	974	ILE	2.3
1	B	1116	ASN	2.3
1	B	978	VAL	2.3
1	D	892	GLY	2.3
1	A	1144	ASN	2.3
1	C	1237	PRO	2.3
1	B	1014	TYR	2.3
1	B	979	ASN	2.3
1	D	984	SER	2.2
1	A	1014	TYR	2.2
1	A	1107	ILE	2.2
1	B	1184	SER	2.2
1	D	1031	ASP	2.2
1	D	1016	LYS	2.1
1	C	1034	GLU	2.1
1	B	981	LYS	2.1
1	D	914	ILE	2.1
1	D	943	LEU	2.1
1	D	1034	GLU	2.1
1	D	976	GLN	2.1
1	C	1243	LYS	2.1
1	D	1183	CYS	2.0
1	D	945	ASN	2.0
1	D	956	ILE	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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



### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GOL	C	1401	6/6	0.77	0.28	82,83,83,84	0
2	GOL	D	1402	6/6	0.80	0.25	78,80,80,81	0
2	GOL	A	1400	6/6	0.91	0.13	65,71,71,72	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.