



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:02 AM GMT

PDB ID : 2Z6X  
Title : Crystal structure of 22G, the wild-type protein of the photoswitchable GFP-like protein Dronpa  
Authors : Kikuchi, A.; Jeyakanthan, J.; Taka, J.; Shiro, Y.; Mizuno, H.; Miyawaki, A.  
Deposited on : 2007-08-09  
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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

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

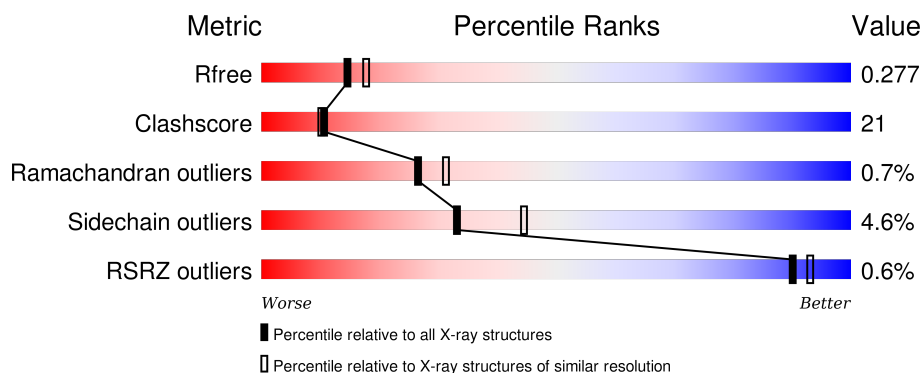
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
$R_{free}$	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (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 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	255	<div> <div>51%</div> <div>30%</div> <div>•</div> <div>15%</div> </div>
1	B	255	<div> <div>51%</div> <div>30%</div> <div>•</div> <div>15%</div> </div>
1	C	255	<div> <div>54%</div> <div>29%</div> <div>•</div> <div>16%</div> </div>
1	D	255	<div> <div>53%</div> <div>30%</div> <div>•</div> <div>16%</div> </div>
1	E	255	<div> <div>49%</div> <div>32%</div> <div>•</div> <div>15%</div> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	F	255	
1	G	255	
1	H	255	

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
1	GYC	A	63	X	-	-	-
1	GYC	B	63	X	-	-	-
1	GYC	C	63	X	-	-	-
1	GYC	D	63	X	-	-	-
1	GYC	E	63	X	-	-	-
1	GYC	F	63	X	-	-	-
1	GYC	G	63	X	-	-	-
1	GYC	H	63	X	-	X	-

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15008 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 photochromic protein Dronpa.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	217	Total	C	N	O	S	0	0	0
			1750	1122	295	323	10			
1	B	216	Total	C	N	O	S	0	0	0
			1743	1117	294	322	10			
1	C	215	Total	C	N	O	S	0	0	0
			1737	1114	293	320	10			
1	D	215	Total	C	N	O	S	0	0	0
			1737	1114	293	320	10			
1	E	216	Total	C	N	O	S	0	0	0
			1743	1117	294	322	10			
1	F	216	Total	C	N	O	S	0	0	0
			1743	1117	294	322	10			
1	G	215	Total	C	N	O	S	0	0	0
			1737	1114	293	320	10			
1	H	215	Total	C	N	O	S	0	0	0
			1737	1114	293	320	10			

- Molecule 2 is water.

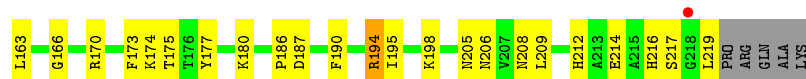
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	113	Total	O	0	0
			113	113		
2	B	140	Total	O	0	0
			140	140		
2	C	157	Total	O	0	0
			157	157		
2	D	139	Total	O	0	0
			139	139		
2	E	148	Total	O	0	0
			148	148		
2	F	145	Total	O	0	0
			145	145		

*Continued on next page...*

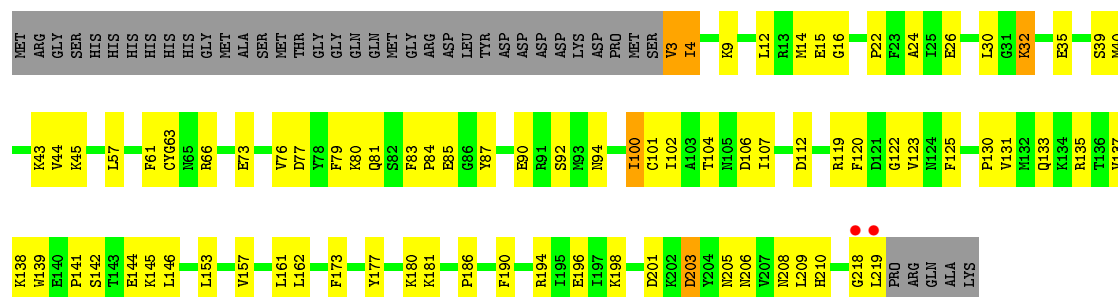
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	128	Total 128	O 128	0	0
2	H	111	Total 111	O 111	0	0

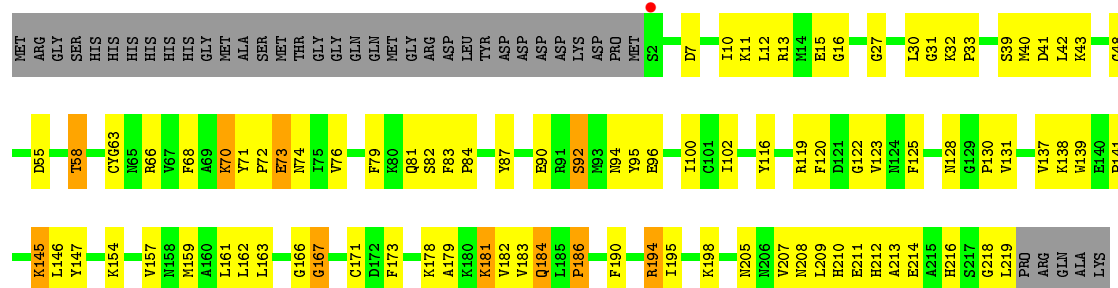




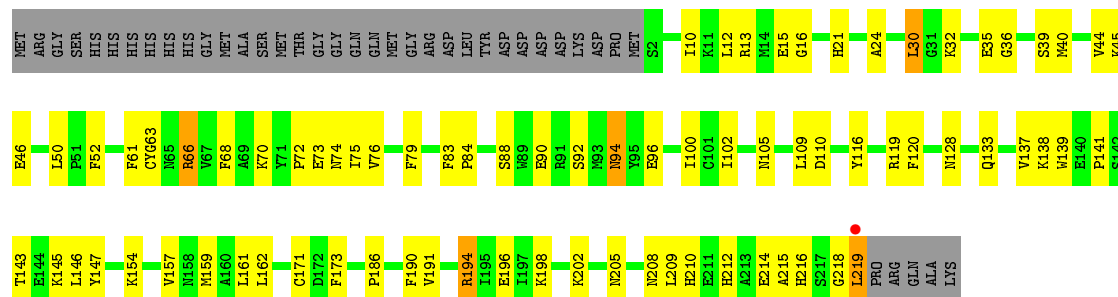
- Molecule 1: photochromic protein Dronpa



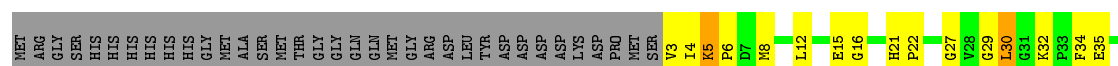
- Molecule 1: photochromic protein Dronpa

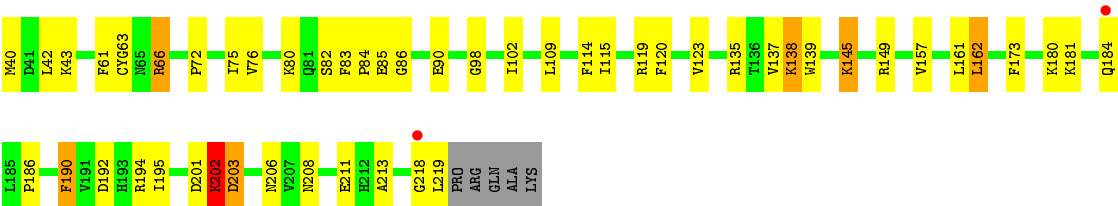


- Molecule 1: photochromic protein Dronpa

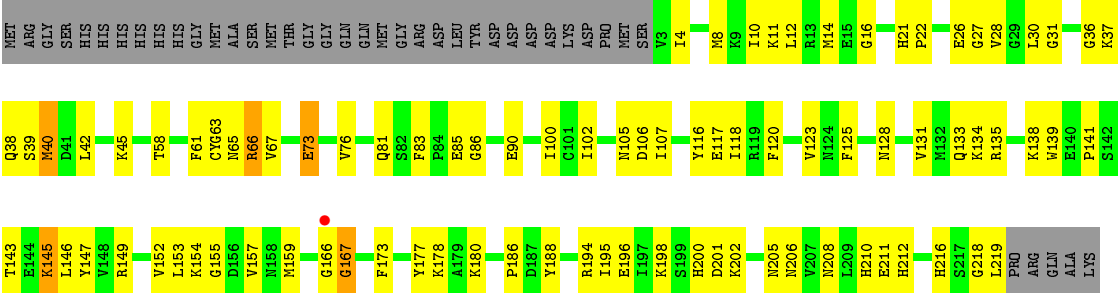


- Molecule 1: photochromic protein Dronpa





● Molecule 1: photochromic protein Dronpa





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	111.68Å 111.68Å 156.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.96 – 2.30 42.10 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.0 (19.96-2.30) 99.1 (42.10-2.30)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.98 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.219 , 0.278 0.219 , 0.277	Depositor DCC
$R_{free}$ test set	4269 reflections (5.08%)	DCC
Wilson B-factor (Å <sup>2</sup> )	24.4	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 9.8	EDS
Estimated twinning fraction	0.310 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.23$	Xtriage
Outliers	0 of 84980 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	15008	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% 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: GYC

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	0.40	0/1774	0.67	0/2394
1	B	0.40	0/1766	0.68	0/2382
1	C	0.43	0/1760	0.71	0/2374
1	D	0.43	0/1760	0.71	0/2374
1	E	0.42	0/1766	0.68	0/2382
1	F	0.45	0/1766	0.70	0/2382
1	G	0.41	0/1760	0.71	0/2374
1	H	0.40	0/1760	0.66	0/2374
All	All	0.42	0/14112	0.69	0/19036

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	1	0
1	B	1	0
1	C	1	0
1	D	1	0
1	E	1	0
1	F	1	0
1	G	1	0
1	H	1	0
All	All	8	0

There are no bond length outliers.

There are no bond angle outliers.

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	63	GYC	CA1
1	B	63	GYC	CA1
1	C	63	GYC	CA1
1	D	63	GYC	CA1
1	E	63	GYC	CA1
1	F	63	GYC	CA1
1	G	63	GYC	CA1
1	H	63	GYC	CA1

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	1750	0	1693	85	0
1	B	1743	0	1686	81	0
1	C	1737	0	1681	77	0
1	D	1737	0	1681	78	0
1	E	1743	0	1686	82	0
1	F	1743	0	1686	71	0
1	G	1737	0	1681	61	0
1	H	1737	0	1682	80	0
2	A	113	0	0	9	0
2	B	140	0	0	10	0
2	C	157	0	0	10	0
2	D	139	0	0	9	0
2	E	148	0	0	8	0
2	F	145	0	0	6	0
2	G	128	0	0	9	0
2	H	111	0	0	6	0
All	All	15008	0	13476	584	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 21.

All (584) 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:H:63:GYC:HA31	1:H:63:GYC:HN2	1.15	1.08
1:C:138:LYS:HG2	1:C:162:LEU:HD21	1.38	1.05
1:C:187:ASP:HB3	2:C:371:HOH:O	1.59	1.01
1:H:198:LYS:HA	1:H:198:LYS:HE2	1.47	0.97
1:D:198:LYS:HB2	1:D:208:ASN:HD22	1.30	0.94
1:A:198:LYS:HB2	1:A:208:ASN:HD22	1.32	0.92
1:C:162:LEU:HD23	1:C:162:LEU:H	1.35	0.92
1:H:198:LYS:HB2	1:H:208:ASN:HD22	1.34	0.92
1:G:162:LEU:HB2	2:G:235:HOH:O	1.70	0.91
1:E:138:LYS:HG2	1:E:162:LEU:HD21	1.51	0.91
1:A:133:GLN:HG2	1:E:48:GLY:H	1.37	0.90
1:D:198:LYS:HA	1:D:198:LYS:HE2	1.53	0.90
1:B:203:ASP:HB3	2:B:362:HOH:O	1.73	0.87
1:H:146:LEU:HD23	1:H:154:LYS:O	1.75	0.87
1:G:27:GLY:HA3	1:G:42:LEU:HD23	1.57	0.87
1:B:81:GLN:HE22	1:B:184:GLN:H	1.23	0.86
1:C:76:VAL:HB	1:C:186:PRO:HB3	1.56	0.86
1:B:218:GLY:O	1:B:219:LEU:HB2	1.75	0.86
1:F:198:LYS:HB2	1:F:208:ASN:HD22	1.41	0.86
1:B:63:GYC:HA31	1:B:63:GYC:N	1.90	0.85
1:E:63:GYC:HA31	1:E:63:GYC:N	1.92	0.85
1:F:194:ARG:HH12	1:H:219:LEU:HA	1.40	0.85
1:B:40:MET:HE1	1:B:61:PHE:O	1.77	0.85
1:E:102:ILE:HG12	1:F:102:ILE:HD12	1.59	0.83
1:B:73:GLU:H	1:B:73:GLU:CD	1.78	0.83
1:G:5:LYS:H	1:G:5:LYS:HD2	1.42	0.83
1:H:63:GYC:N	1:H:63:GYC:HA31	1.94	0.82
1:E:73:GLU:CD	1:E:73:GLU:H	1.81	0.82
1:G:102:ILE:HD12	1:H:102:ILE:HB	1.61	0.81
1:E:162:LEU:H	1:E:162:LEU:HD23	1.45	0.81
1:F:32:LYS:HB3	1:F:35:GLU:HG3	1.61	0.81
1:F:94:ASN:HB2	2:F:251:HOH:O	1.79	0.80
1:C:43:LYS:HG2	1:C:206:ASN:ND2	1.97	0.80
1:G:76:VAL:HB	1:G:186:PRO:HB3	1.62	0.80
1:C:3:VAL:HA	2:C:319:HOH:O	1.81	0.79
1:H:146:LEU:HD22	1:H:153:LEU:HG	1.63	0.79
1:A:63:GYC:N	1:A:63:GYC:HA31	1.98	0.79
1:B:202:LYS:HB3	2:B:363:HOH:O	1.81	0.79
1:C:32:LYS:HD3	1:C:35:GLU:HG3	1.66	0.78
1:B:58:THR:HB	1:B:195:ILE:HD11	1.66	0.78
1:A:202:LYS:HD3	1:A:202:LYS:O	1.84	0.78
1:G:63:GYC:HA31	1:G:63:GYC:N	1.98	0.78

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:26:GLU:HG3	1:C:45:LYS:HG3	1.63	0.78
1:E:184:GLN:HG3	2:E:243:HOH:O	1.84	0.77
1:F:198:LYS:HE3	1:F:210:HIS:ND1	2.01	0.76
1:F:63:GYC:N	1:F:63:GYC:HA31	1.99	0.76
1:D:3:VAL:HA	2:D:349:HOH:O	1.85	0.75
1:B:137:VAL:HB	1:B:162:LEU:CD2	2.16	0.75
1:C:63:GYC:HA31	1:C:63:GYC:N	2.01	0.75
1:A:128:ASN:HA	1:A:133:GLN:HE22	1.52	0.75
1:D:63:GYC:N	1:D:63:GYC:HA31	2.01	0.74
1:F:218:GLY:O	1:F:219:LEU:HB2	1.86	0.74
1:G:66:ARG:HA	1:G:66:ARG:HH11	1.52	0.74
1:D:196:GLU:HG3	1:D:198:LYS:HE3	1.69	0.74
1:E:58:THR:HG21	2:E:235:HOH:O	1.87	0.73
1:A:202:LYS:HD2	2:A:276:HOH:O	1.87	0.73
1:A:198:LYS:HB2	1:A:208:ASN:ND2	2.03	0.72
1:H:157:VAL:CG1	1:H:173:PHE:HB2	2.19	0.72
1:F:73:GLU:HG3	2:F:325:HOH:O	1.89	0.72
2:G:267:HOH:O	1:H:178:LYS:HD3	1.88	0.72
1:B:198:LYS:HB2	1:B:208:ASN:HD22	1.54	0.72
1:F:70:LYS:HE3	1:F:214:GLU:HG2	1.72	0.71
1:C:70:LYS:HB3	1:C:214:GLU:HG2	1.72	0.71
1:F:105:ASN:OD1	1:F:116:TYR:HB3	1.90	0.71
1:A:220:PRO:HD3	2:A:333:HOH:O	1.89	0.71
1:B:138:LYS:HG2	1:B:162:LEU:HD22	1.73	0.71
1:A:100:ILE:HD12	1:B:92:SER:OG	1.91	0.70
1:E:70:LYS:HB3	1:E:214:GLU:HG2	1.73	0.70
1:B:9:LYS:HD2	2:B:358:HOH:O	1.90	0.70
1:C:138:LYS:CG	1:C:162:LEU:HD21	2.21	0.70
1:A:128:ASN:HA	1:A:133:GLN:NE2	2.06	0.69
1:C:194:ARG:HA	1:C:194:ARG:HE	1.55	0.69
1:G:102:ILE:HD11	1:H:100:ILE:HG13	1.74	0.69
1:E:82:SER:HA	1:E:181:LYS:HE2	1.73	0.69
1:B:137:VAL:HB	1:B:162:LEU:HD21	1.73	0.69
1:E:219:LEU:O	1:E:219:LEU:HD23	1.92	0.69
1:F:109:LEU:HD12	1:F:110:ASP:H	1.57	0.69
1:D:198:LYS:CA	1:D:198:LYS:HE2	2.22	0.69
1:C:130:PRO:HD2	2:C:227:HOH:O	1.92	0.68
1:G:137:VAL:HB	1:G:162:LEU:CD2	2.24	0.68
1:B:43:LYS:HA	1:B:205:ASN:O	1.94	0.68
1:A:219:LEU:HD11	1:C:212:HIS:CD2	2.28	0.68
1:B:58:THR:HB	1:B:195:ILE:CD1	2.24	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:198:LYS:HB2	1:E:208:ASN:HD22	1.59	0.67
1:H:141:PRO:HG3	1:H:194:ARG:NH2	2.09	0.67
1:A:102:ILE:HG21	2:B:239:HOH:O	1.93	0.67
1:B:66:ARG:HH11	1:B:66:ARG:HA	1.59	0.67
2:F:330:HOH:O	1:H:219:LEU:HD23	1.94	0.66
1:G:123:VAL:HG22	1:H:102:ILE:HD13	1.76	0.66
1:B:202:LYS:CB	2:B:363:HOH:O	2.42	0.66
1:H:157:VAL:HG12	1:H:173:PHE:HB2	1.76	0.66
1:H:125:PHE:CE1	1:H:131:VAL:HG21	2.30	0.66
1:A:36:GLY:O	1:A:212:HIS:HA	1.95	0.66
1:C:43:LYS:HG2	1:C:206:ASN:HD22	1.60	0.66
1:H:14:MET:HG3	1:H:118:ILE:HG22	1.78	0.66
1:D:76:VAL:HB	1:D:186:PRO:HB3	1.78	0.66
1:F:109:LEU:HD12	1:F:110:ASP:N	2.11	0.66
1:G:40:MET:HE1	1:G:61:PHE:O	1.96	0.66
1:A:92:SER:OG	1:B:100:ILE:HD12	1.96	0.65
1:E:16:GLY:HA3	1:E:120:PHE:O	1.96	0.65
1:G:138:LYS:HG3	1:G:162:LEU:CD2	2.26	0.65
1:F:137:VAL:HB	1:F:162:LEU:CD2	2.26	0.65
1:F:76:VAL:HB	1:F:186:PRO:HB3	1.77	0.65
1:A:82:SER:O	1:A:181:LYS:HE2	1.97	0.65
1:E:139:TRP:CZ3	1:E:161:LEU:HG	2.32	0.65
1:G:180:LYS:HB3	2:G:350:HOH:O	1.97	0.64
1:C:194:ARG:CA	1:C:194:ARG:HE	2.11	0.64
1:B:12:LEU:HD12	1:B:12:LEU:C	2.18	0.64
2:A:226:HOH:O	1:C:194:ARG:HD2	1.97	0.64
1:B:76:VAL:HB	1:B:186:PRO:HB3	1.79	0.64
1:C:5:LYS:HB2	1:C:8:MET:HE3	1.79	0.63
1:B:26:GLU:OE1	1:B:45:LYS:HE3	1.97	0.63
1:H:63:GYC:CA3	1:H:63:GYC:HN2	2.00	0.63
1:D:40:MET:HE1	1:D:61:PHE:O	1.98	0.63
1:G:29:GLY:C	1:G:30:LEU:HD23	2.18	0.63
1:F:137:VAL:HB	1:F:162:LEU:HD21	1.80	0.62
1:E:92:SER:OG	1:F:100:ILE:HD12	2.00	0.62
1:E:128:ASN:HB2	2:E:276:HOH:O	1.98	0.62
1:H:105:ASN:ND2	1:H:107:ILE:HD11	2.15	0.62
1:C:123:VAL:HB	1:D:90:GLU:HB3	1.82	0.62
1:B:87:TYR:CZ	1:B:107:ILE:HD12	2.35	0.62
1:H:26:GLU:OE1	1:H:45:LYS:HE3	1.99	0.62
1:H:138:LYS:NZ	1:H:194:ARG:HH12	1.97	0.61
1:A:199:SER:O	1:A:200:HIS:HB3	2.00	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:83:PHE:HB3	1:G:84:PRO:HA	1.82	0.61
1:B:81:GLN:NE2	1:B:184:GLN:H	1.95	0.61
1:G:203:ASP:N	1:G:203:ASP:OD1	2.34	0.61
1:H:138:LYS:HZ1	1:H:194:ARG:HH12	1.49	0.60
1:A:137:VAL:HG12	1:A:138:LYS:HG3	1.83	0.60
1:G:137:VAL:O	1:G:138:LYS:HB3	2.00	0.60
1:F:72:PRO:HB2	1:F:74:ASN:OD1	2.00	0.60
1:H:146:LEU:HD21	1:H:177:TYR:CE2	2.37	0.60
1:A:12:LEU:C	1:A:12:LEU:HD12	2.22	0.60
1:E:162:LEU:N	1:E:162:LEU:HD23	2.14	0.60
1:C:130:PRO:HB3	1:C:163:LEU:HD22	1.84	0.60
1:D:146:LEU:HD12	1:D:146:LEU:N	2.17	0.60
1:D:139:TRP:CZ3	1:D:161:LEU:HG	2.37	0.60
1:H:40:MET:HE1	1:H:61:PHE:O	2.02	0.60
1:C:125:PHE:CE1	1:C:131:VAL:HG21	2.37	0.59
1:C:133:GLN:OE1	1:C:135:ARG:NE	2.25	0.59
1:B:138:LYS:HG2	1:B:162:LEU:CD2	2.32	0.59
1:F:138:LYS:HG2	1:F:162:LEU:CD2	2.32	0.59
1:E:27:GLY:HA3	1:E:42:LEU:HD23	1.83	0.59
1:F:141:PRO:HG3	1:F:194:ARG:CD	2.33	0.59
1:H:10:ILE:O	1:H:28:VAL:HA	2.02	0.59
1:F:16:GLY:HA3	1:F:120:PHE:O	2.02	0.59
1:D:133:GLN:HG2	2:D:234:HOH:O	2.03	0.59
1:E:218:GLY:O	1:E:219:LEU:HB3	2.02	0.59
1:H:200:HIS:HA	1:H:206:ASN:O	2.02	0.59
1:G:15:GLU:O	1:G:119:ARG:HD2	2.03	0.59
1:D:100:ILE:HD13	1:D:123:VAL:HG23	1.85	0.58
1:E:81:GLN:OE1	1:E:183:VAL:HB	2.03	0.58
1:F:138:LYS:HG2	1:F:162:LEU:HD21	1.84	0.58
1:E:166:GLY:O	1:E:167:GLY:O	2.22	0.58
1:D:130:PRO:HG3	1:D:135:ARG:HH12	1.68	0.58
1:H:65:ASN:OD1	1:H:67:VAL:HB	2.04	0.58
1:D:83:PHE:HB3	1:D:84:PRO:HA	1.86	0.57
1:E:145:LYS:HG3	1:E:190:PHE:CE2	2.39	0.57
1:A:27:GLY:HA3	1:A:42:LEU:HD23	1.84	0.57
1:E:15:GLU:O	1:E:119:ARG:HD2	2.04	0.57
1:H:4:ILE:HG23	1:H:8:MET:SD	2.45	0.57
1:G:5:LYS:HD2	1:G:5:LYS:N	2.15	0.57
1:C:157:VAL:HG13	1:C:173:PHE:HB2	1.87	0.57
1:F:45:LYS:O	1:F:46:GLU:HG3	2.05	0.57
1:B:170:ARG:NH1	1:B:170:ARG:HB3	2.20	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:157:VAL:HG13	1:H:173:PHE:HB2	1.87	0.57
1:C:162:LEU:HD23	1:C:162:LEU:N	2.13	0.57
1:D:157:VAL:HG13	1:D:173:PHE:HB2	1.86	0.57
1:B:98:GLY:O	1:B:100:ILE:HG13	2.04	0.56
1:D:138:LYS:HG3	1:D:162:LEU:CD2	2.35	0.56
1:D:12:LEU:C	1:D:12:LEU:HD12	2.26	0.56
1:B:195:ILE:HD11	1:B:209:LEU:HD11	1.87	0.56
1:F:94:ASN:ND2	2:F:260:HOH:O	2.31	0.56
1:C:216:HIS:HD2	1:C:217:SER:O	1.87	0.56
1:D:85:GLU:CD	1:D:181:LYS:HD3	2.26	0.56
1:D:198:LYS:HG3	1:D:210:HIS:CE1	2.41	0.56
1:A:135:ARG:HD3	1:E:48:GLY:O	2.06	0.56
1:A:85:GLU:OE1	1:A:181:LYS:NZ	2.32	0.56
1:E:87:TYR:HB3	1:E:179:ALA:HA	1.86	0.56
1:E:87:TYR:CB	1:E:179:ALA:HA	2.35	0.56
1:H:16:GLY:HA3	1:H:120:PHE:O	2.06	0.56
1:C:63:GYC:HE1	1:C:195:ILE:HB	1.87	0.56
1:B:60:VAL:HG21	1:B:120:PHE:CD1	2.41	0.56
1:A:73:GLU:H	1:A:73:GLU:CD	2.10	0.55
1:C:30:LEU:C	1:C:30:LEU:HD12	2.27	0.55
1:C:67:VAL:HA	2:C:233:HOH:O	2.06	0.55
1:A:10:ILE:HD11	1:A:68:PHE:CZ	2.41	0.55
1:G:109:LEU:HD13	1:G:114:PHE:CD2	2.41	0.55
1:D:125:PHE:CE1	1:D:131:VAL:HG21	2.42	0.55
1:G:66:ARG:CA	1:G:66:ARG:HH11	2.20	0.55
1:G:135:ARG:HG2	2:G:265:HOH:O	2.06	0.55
1:A:125:PHE:CE1	1:A:131:VAL:HG21	2.41	0.55
1:C:219:LEU:C	1:C:219:LEU:HD13	2.27	0.55
1:B:198:LYS:HB2	1:B:208:ASN:ND2	2.21	0.55
1:C:100:ILE:CG2	1:D:102:ILE:HD11	2.37	0.55
1:C:198:LYS:HB2	1:C:208:ASN:HD22	1.72	0.55
1:H:198:LYS:CB	1:H:208:ASN:HD22	2.15	0.55
1:E:58:THR:HB	1:E:195:ILE:HD13	1.88	0.55
1:F:146:LEU:N	1:F:146:LEU:HD12	2.21	0.55
1:G:12:LEU:HD12	1:G:12:LEU:C	2.28	0.54
1:C:8:MET:HG3	1:C:33:PRO:HG2	1.89	0.54
1:D:141:PRO:HG3	1:D:194:ARG:HD2	1.87	0.54
1:A:157:VAL:CG1	1:A:173:PHE:HB2	2.37	0.54
1:H:198:LYS:CA	1:H:198:LYS:HE2	2.31	0.54
1:F:190:PHE:HB2	1:F:216:HIS:CE1	2.42	0.54
1:H:139:TRP:CZ3	1:H:159:MET:HB3	2.42	0.54

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:GLN:HB3	2:B:337:HOH:O	2.07	0.54
1:C:80:LYS:HG3	2:C:233:HOH:O	2.08	0.54
1:H:128:ASN:HA	1:H:133:GLN:NE2	2.22	0.54
1:F:72:PRO:HD2	1:F:75:ILE:HG13	1.90	0.54
1:E:7:ASP:OD1	1:E:32:LYS:NZ	2.35	0.54
1:G:5:LYS:HB3	1:G:5:LYS:NZ	2.23	0.54
1:A:195:ILE:O	1:A:196:GLU:HG3	2.07	0.54
1:E:63:GYC:HE1	1:E:195:ILE:HB	1.90	0.54
1:H:76:VAL:HB	1:H:186:PRO:HB3	1.90	0.54
1:A:220:PRO:CD	2:A:333:HOH:O	2.50	0.54
1:A:138:LYS:C	1:A:138:LYS:HD3	2.29	0.54
1:D:32:LYS:HE3	2:D:283:HOH:O	2.07	0.54
1:D:4:ILE:HD11	1:D:80:LYS:HE3	1.90	0.53
1:A:102:ILE:HG13	2:B:239:HOH:O	2.08	0.53
1:F:83:PHE:HB3	1:F:84:PRO:HA	1.90	0.53
1:E:13:ARG:HH11	1:E:13:ARG:HG3	1.73	0.53
1:A:76:VAL:HB	1:A:186:PRO:HB3	1.90	0.53
1:D:100:ILE:CD1	1:D:123:VAL:HG23	2.37	0.53
1:A:87:TYR:HA	1:A:180:LYS:HG3	1.91	0.53
1:D:133:GLN:HB2	1:D:135:ARG:HG3	1.91	0.53
1:E:162:LEU:CD2	1:E:162:LEU:H	2.18	0.53
1:E:81:GLN:OE1	1:E:184:GLN:HG2	2.08	0.53
1:B:191:VAL:HG22	1:B:215:ALA:HB2	1.91	0.53
1:H:73:GLU:HA	1:H:73:GLU:OE1	2.07	0.53
1:G:4:ILE:HD12	1:G:80:LYS:HB3	1.90	0.53
1:C:43:LYS:HA	1:C:205:ASN:O	2.09	0.53
1:A:12:LEU:HD12	1:A:12:LEU:O	2.09	0.53
1:F:50:LEU:HD13	1:F:52:PHE:CZ	2.44	0.53
1:C:174:LYS:HE2	2:C:294:HOH:O	2.08	0.53
1:H:133:GLN:HG2	2:H:297:HOH:O	2.08	0.53
1:B:137:VAL:HB	1:B:162:LEU:HD23	1.89	0.53
1:E:100:ILE:HD12	1:F:92:SER:OG	2.09	0.52
1:G:145:LYS:HD2	1:G:145:LYS:N	2.24	0.52
1:G:83:PHE:HA	1:G:86:GLY:H	1.74	0.52
1:C:100:ILE:HG22	1:D:102:ILE:HD11	1.92	0.52
1:G:90:GLU:HB3	1:H:123:VAL:HB	1.91	0.52
1:E:70:LYS:CB	1:E:214:GLU:HG2	2.39	0.52
1:D:77:ASP:O	1:D:81:GLN:HG3	2.09	0.52
1:C:8:MET:HE2	1:C:112:ASP:HB2	1.91	0.52
1:A:4:ILE:HD11	1:A:83:PHE:HB2	1.92	0.52
1:C:76:VAL:HB	1:C:186:PRO:CB	2.34	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:ASP:OD2	1:B:206:ASN:N	2.41	0.52
1:H:206:ASN:ND2	2:H:291:HOH:O	2.42	0.52
1:A:190:PHE:HB2	1:A:216:HIS:CE1	2.44	0.52
1:F:137:VAL:O	1:F:138:LYS:HB3	2.09	0.52
1:E:125:PHE:CE1	1:E:131:VAL:HG21	2.45	0.52
1:F:128:ASN:HA	1:F:133:GLN:NE2	2.25	0.52
1:H:83:PHE:HA	1:H:86:GLY:H	1.75	0.52
1:E:90:GLU:OE2	1:E:178:LYS:HE3	2.09	0.52
1:A:141:PRO:HG3	1:A:194:ARG:CZ	2.40	0.52
1:B:73:GLU:CD	1:B:73:GLU:N	2.57	0.52
1:B:198:LYS:HG3	1:B:210:HIS:CE1	2.44	0.52
1:H:138:LYS:NZ	1:H:194:ARG:NH1	2.58	0.52
1:G:4:ILE:HG23	1:G:8:MET:SD	2.49	0.52
1:E:10:ILE:HD12	1:E:116:TYR:OH	2.10	0.52
1:A:220:PRO:CG	2:A:333:HOH:O	2.57	0.51
1:B:81:GLN:HE21	1:B:183:VAL:HB	1.75	0.51
1:H:11:LYS:HG3	1:H:28:VAL:HG12	1.91	0.51
1:F:13:ARG:NE	1:F:15:GLU:OE2	2.41	0.51
1:E:137:VAL:O	1:E:138:LYS:HB3	2.09	0.51
1:G:123:VAL:HB	1:H:90:GLU:HB3	1.92	0.51
1:D:196:GLU:O	1:D:209:LEU:HD12	2.10	0.51
1:A:139:TRP:CZ3	1:A:159:MET:HB3	2.45	0.51
1:B:139:TRP:CE2	1:B:161:LEU:HD21	2.45	0.51
1:D:30:LEU:HD12	1:D:30:LEU:C	2.31	0.51
1:B:40:MET:SD	1:B:42:LEU:HD21	2.50	0.51
1:E:81:GLN:O	1:E:181:LYS:HE2	2.11	0.51
1:G:43:LYS:HG2	1:G:206:ASN:ND2	2.25	0.51
1:A:202:LYS:C	1:A:202:LYS:HD3	2.31	0.51
1:B:149:ARG:O	1:B:150:ASP:HB2	2.11	0.51
1:G:32:LYS:HB2	1:G:35:GLU:HB2	1.93	0.51
1:H:85:GLU:O	1:H:180:LYS:HG3	2.10	0.51
1:H:39:SER:O	1:H:40:MET:HB3	2.11	0.51
1:H:12:LEU:HD12	1:H:12:LEU:C	2.31	0.51
1:C:30:LEU:O	1:C:30:LEU:HD12	2.12	0.50
1:A:180:LYS:HE2	2:A:302:HOH:O	2.10	0.50
1:B:50:LEU:HD22	1:B:52:PHE:CZ	2.45	0.50
1:D:198:LYS:HB2	1:D:208:ASN:ND2	2.12	0.50
1:B:195:ILE:CG1	1:B:209:LEU:HD11	2.41	0.50
1:D:130:PRO:HG3	1:D:135:ARG:NH1	2.26	0.50
1:B:144:GLU:HA	1:B:157:VAL:HB	1.92	0.50
1:D:43:LYS:HD3	1:D:45:LYS:HZ1	1.76	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:106:ASP:HB2	2:D:278:HOH:O	2.12	0.50
1:E:76:VAL:HB	1:E:186:PRO:HB3	1.94	0.50
1:A:135:ARG:HD2	2:E:236:HOH:O	2.12	0.50
1:A:32:LYS:HD3	1:A:35:GLU:OE2	2.12	0.50
1:H:65:ASN:C	1:H:67:VAL:H	2.15	0.50
1:D:138:LYS:CG	1:D:162:LEU:HD21	2.42	0.50
1:F:32:LYS:CB	1:F:35:GLU:HG3	2.37	0.49
1:F:139:TRP:CZ3	1:F:161:LEU:HG	2.47	0.49
1:E:145:LYS:HG3	1:E:190:PHE:CD2	2.48	0.49
1:E:146:LEU:HA	1:E:154:LYS:O	2.12	0.49
1:E:159:MET:HA	2:E:240:HOH:O	2.13	0.49
1:E:70:LYS:HE3	1:E:70:LYS:C	2.33	0.49
1:E:83:PHE:HB3	1:E:84:PRO:HA	1.94	0.49
1:F:128:ASN:HA	1:F:133:GLN:HE21	1.77	0.49
1:H:14:MET:HG3	1:H:118:ILE:CG2	2.42	0.49
1:E:159:MET:HG3	1:E:173:PHE:CZ	2.47	0.49
1:B:53:ALA:O	1:B:56:ILE:HG12	2.12	0.49
1:G:137:VAL:HB	1:G:162:LEU:HD21	1.94	0.49
1:C:100:ILE:HD12	1:D:92:SER:OG	2.13	0.49
1:F:40:MET:HE1	1:F:61:PHE:O	2.13	0.49
1:G:138:LYS:HG3	1:G:162:LEU:HD22	1.94	0.49
1:E:195:ILE:HG12	1:E:209:LEU:HD11	1.94	0.49
1:G:102:ILE:HD12	1:H:102:ILE:CB	2.40	0.49
1:H:146:LEU:HD22	1:H:153:LEU:CG	2.38	0.48
1:E:58:THR:HB	1:E:195:ILE:CD1	2.43	0.48
1:A:9:LYS:O	1:A:10:ILE:HD13	2.14	0.48
1:D:194:ARG:HD3	2:D:225:HOH:O	2.13	0.48
1:H:27:GLY:HA3	1:H:42:LEU:HD23	1.95	0.48
1:G:208:ASN:ND2	2:G:256:HOH:O	2.46	0.48
1:A:190:PHE:N	1:A:190:PHE:CD1	2.82	0.48
1:D:201:ASP:OD2	1:D:206:ASN:HB2	2.14	0.48
1:G:114:PHE:C	1:G:115:ILE:HD12	2.33	0.48
1:A:157:VAL:HG12	1:A:173:PHE:HB2	1.95	0.48
1:B:30:LEU:N	1:B:30:LEU:CD2	2.77	0.48
1:A:94:ASN:HD22	1:A:95:TYR:N	2.12	0.48
1:B:92:SER:HB3	1:B:174:LYS:HB2	1.95	0.48
1:C:129:GLY:O	1:C:133:GLN:HB2	2.13	0.48
1:D:87:TYR:HA	1:D:180:LYS:HG3	1.96	0.48
1:F:12:LEU:C	1:F:12:LEU:HD12	2.34	0.48
1:A:44:VAL:HG23	2:A:255:HOH:O	2.14	0.48
1:F:10:ILE:HD11	1:F:68:PHE:CZ	2.49	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:TYR:N	1:A:204:TYR:CD1	2.82	0.47
1:A:133:GLN:HG2	1:E:48:GLY:N	2.18	0.47
1:B:195:ILE:HG23	1:B:195:ILE:O	2.14	0.47
1:E:63:GYC:CA3	1:E:63:GYC:N	2.67	0.47
1:G:123:VAL:HG22	1:H:102:ILE:CD1	2.43	0.47
1:E:10:ILE:HD11	1:E:68:PHE:CE1	2.49	0.47
1:F:66:ARG:HH11	1:F:66:ARG:HA	1.78	0.47
1:A:211:GLU:HG2	1:A:212:HIS:N	2.30	0.47
1:A:212:HIS:CE1	1:C:219:LEU:HD11	2.50	0.47
1:G:6:PRO:O	1:G:32:LYS:HA	2.14	0.47
1:B:145:LYS:NZ	1:D:142:SER:HB2	2.29	0.47
1:H:216:HIS:HD2	1:H:218:GLY:H	1.63	0.47
1:F:196:GLU:O	1:F:209:LEU:HD12	2.15	0.47
1:C:10:ILE:HD11	1:C:68:PHE:CZ	2.50	0.47
1:H:63:GYC:HB2	1:H:66:ARG:NH2	2.29	0.47
1:B:66:ARG:NH1	1:B:66:ARG:HA	2.29	0.47
1:E:157:VAL:HG12	1:E:173:PHE:HB2	1.97	0.47
1:A:70:LYS:HB3	1:A:214:GLU:HG3	1.96	0.47
1:D:104:THR:HB	2:D:259:HOH:O	2.15	0.47
1:E:157:VAL:CG1	1:E:173:PHE:HB2	2.45	0.47
1:A:95:TYR:CD2	1:A:171:CYS:HB2	2.50	0.47
1:G:82:SER:O	1:G:181:LYS:HE2	2.14	0.47
1:H:36:GLY:O	1:H:212:HIS:HA	2.15	0.47
1:B:3:VAL:HG11	1:B:84:PRO:HB3	1.96	0.46
1:F:76:VAL:HB	1:F:186:PRO:CB	2.43	0.46
1:A:191:VAL:HA	1:A:215:ALA:HA	1.97	0.46
1:B:73:GLU:HG3	2:B:249:HOH:O	2.15	0.46
1:G:157:VAL:HG12	1:G:173:PHE:HB2	1.97	0.46
1:C:137:VAL:HB	1:C:162:LEU:HG	1.97	0.46
1:F:141:PRO:HG3	1:F:194:ARG:HD3	1.97	0.46
1:C:133:GLN:HB3	1:C:135:ARG:HG3	1.97	0.46
1:G:157:VAL:CG1	1:G:173:PHE:HB2	2.45	0.46
1:A:133:GLN:HB2	1:A:133:GLN:HE21	1.54	0.46
1:G:76:VAL:HB	1:G:186:PRO:CB	2.38	0.46
1:D:100:ILE:O	1:D:122:GLY:HA2	2.16	0.46
1:B:85:GLU:N	1:B:85:GLU:OE2	2.44	0.46
1:D:32:LYS:CB	1:D:35:GLU:HB2	2.45	0.46
1:F:50:LEU:HD13	1:F:52:PHE:CE1	2.49	0.46
1:A:83:PHE:N	1:A:83:PHE:CD1	2.82	0.46
1:B:65:ASN:CG	1:B:67:VAL:HG12	2.36	0.46
1:A:10:ILE:HD11	1:A:68:PHE:HZ	1.80	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:72:PRO:HB2	1:E:74:ASN:OD1	2.16	0.46
1:D:16:GLY:O	1:D:22:PRO:HA	2.15	0.46
1:C:85:GLU:O	1:C:180:LYS:HD2	2.15	0.46
1:A:105:ASN:OD1	1:A:116:TYR:HB3	2.16	0.46
1:H:146:LEU:HD21	1:H:177:TYR:HE2	1.78	0.46
1:D:107:ILE:O	1:D:180:LYS:NZ	2.46	0.46
1:B:30:LEU:O	1:B:30:LEU:HD23	2.15	0.46
1:H:21:HIS:HA	1:H:22:PRO:HD2	1.84	0.46
1:H:63:GYC:HB2	1:H:66:ARG:HH22	1.80	0.46
1:F:39:SER:HB2	1:F:210:HIS:CD2	2.51	0.46
1:E:73:GLU:CD	1:E:73:GLU:N	2.61	0.46
1:D:144:GLU:HG2	1:D:146:LEU:HD11	1.97	0.46
1:D:66:ARG:HG2	1:D:79:PHE:CE2	2.50	0.46
1:C:58:THR:HG21	2:C:230:HOH:O	2.15	0.46
1:E:58:THR:HG22	1:E:209:LEU:HD13	1.97	0.45
1:F:36:GLY:O	1:F:212:HIS:HA	2.15	0.45
1:C:12:LEU:HD12	1:C:12:LEU:C	2.37	0.45
1:H:58:THR:O	1:H:63:GYC:HB11	2.16	0.45
1:C:30:LEU:C	1:C:30:LEU:CD1	2.84	0.45
1:B:85:GLU:CD	1:B:181:LYS:HD3	2.36	0.45
1:H:152:VAL:HG11	1:H:178:LYS:HG2	1.99	0.45
1:E:66:ARG:HG2	1:E:79:PHE:CE2	2.51	0.45
1:G:192:ASP:O	1:G:213:ALA:HA	2.17	0.45
1:E:58:THR:HG22	1:E:209:LEU:CD1	2.46	0.45
1:F:32:LYS:HD3	1:F:35:GLU:OE1	2.16	0.45
1:C:9:LYS:C	1:C:10:ILE:HG13	2.36	0.45
1:D:44:VAL:CG2	1:D:205:ASN:HA	2.47	0.45
1:D:43:LYS:HD3	1:D:45:LYS:NZ	2.31	0.45
1:D:40:MET:CE	1:D:61:PHE:O	2.64	0.45
1:D:87:TYR:N	1:D:180:LYS:HZ2	2.15	0.45
1:D:32:LYS:HB3	1:D:35:GLU:HB2	1.99	0.45
1:A:79:PHE:HB2	2:A:261:HOH:O	2.17	0.45
1:D:138:LYS:HG3	1:D:162:LEU:HD21	1.97	0.45
1:G:16:GLY:CA	1:G:120:PHE:O	2.65	0.45
1:E:96:GLU:OE1	1:G:149:ARG:NH2	2.45	0.45
1:F:157:VAL:HG13	1:F:173:PHE:HB2	1.98	0.45
1:C:157:VAL:CG1	1:C:173:PHE:HB2	2.46	0.45
1:B:104:THR:OG1	1:B:119:ARG:HB3	2.17	0.45
1:H:76:VAL:HG13	1:H:81:GLN:NE2	2.32	0.45
1:F:190:PHE:O	1:F:215:ALA:HA	2.17	0.44
1:F:30:LEU:HD12	1:F:30:LEU:O	2.16	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:63:GYC:HE1	1:H:195:ILE:HB	1.99	0.44
1:E:55:ASP:O	1:E:58:THR:OG1	2.34	0.44
1:F:159:MET:HG3	1:F:173:PHE:CE1	2.52	0.44
1:H:147:TYR:HB3	1:H:188:TYR:CD1	2.53	0.44
1:G:98:GLY:HA3	2:G:289:HOH:O	2.17	0.44
1:G:162:LEU:HD12	2:G:235:HOH:O	2.16	0.44
1:A:102:ILE:HB	1:B:102:ILE:HD12	1.99	0.44
1:B:60:VAL:HG21	1:B:120:PHE:HD1	1.80	0.44
1:D:44:VAL:HG23	1:D:205:ASN:HA	1.99	0.44
1:B:2:SER:O	1:B:5:LYS:HD2	2.16	0.44
1:E:12:LEU:HD12	1:E:12:LEU:C	2.37	0.44
1:G:190:PHE:N	1:G:190:PHE:CD1	2.85	0.44
1:A:102:ILE:HD12	1:B:123:VAL:CG2	2.48	0.44
1:E:41:ASP:HA	1:E:207:VAL:O	2.17	0.44
1:G:21:HIS:HA	1:G:22:PRO:HD2	1.83	0.44
1:C:39:SER:HA	1:C:209:LEU:O	2.17	0.44
1:E:123:VAL:HB	1:F:90:GLU:HB3	2.00	0.44
1:A:38:GLN:CD	1:A:63:GYC:HG1	2.21	0.44
1:D:157:VAL:CG1	1:D:173:PHE:HB2	2.48	0.44
1:A:66:ARG:HB3	1:A:79:PHE:CD1	2.53	0.44
1:C:16:GLY:HA3	1:C:120:PHE:O	2.18	0.44
1:H:196:GLU:HA	2:H:275:HOH:O	2.17	0.44
1:D:3:VAL:HB	1:D:4:ILE:H	1.72	0.44
1:F:218:GLY:O	1:F:219:LEU:CB	2.63	0.44
1:D:144:GLU:HG2	1:D:146:LEU:CD1	2.48	0.44
1:G:138:LYS:HD2	1:G:139:TRP:O	2.18	0.44
1:F:145:LYS:NZ	1:H:143:THR:H	2.16	0.44
1:B:203:ASP:O	1:B:204:TYR:HB2	2.18	0.43
1:A:93:MET:HG2	1:A:173:PHE:CE1	2.53	0.43
1:E:11:LYS:HD3	2:E:336:HOH:O	2.18	0.43
1:B:63:GYC:HE1	1:B:195:ILE:CG2	2.48	0.43
1:F:147:TYR:O	1:F:154:LYS:HB2	2.18	0.43
1:A:146:LEU:HD22	1:A:189:HIS:NE2	2.32	0.43
1:C:190:PHE:CD1	1:C:190:PHE:N	2.87	0.43
1:F:21:HIS:HD2	2:F:316:HOH:O	2.01	0.43
1:H:134:LYS:NZ	2:H:290:HOH:O	2.47	0.43
1:H:66:ARG:HA	1:H:66:ARG:HD3	1.92	0.43
1:C:94:ASN:ND2	1:C:100:ILE:HG12	2.33	0.43
1:A:6:PRO:HA	2:A:231:HOH:O	2.18	0.43
1:C:83:PHE:HB3	1:C:84:PRO:HA	2.01	0.43
1:E:147:TYR:N	1:E:147:TYR:CD1	2.86	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:ARG:HH11	1:C:135:ARG:CB	2.31	0.43
1:E:100:ILE:O	1:E:122:GLY:HA2	2.19	0.43
1:D:15:GLU:O	1:D:119:ARG:HD2	2.19	0.43
1:E:30:LEU:HD12	1:E:30:LEU:C	2.39	0.43
1:D:63:GYC:N	1:D:63:GYC:CA3	2.75	0.43
1:D:137:VAL:HB	1:D:162:LEU:CD2	2.49	0.43
1:C:12:LEU:HB2	1:C:116:TYR:HB2	2.01	0.43
1:C:132:MET:HG2	2:C:268:HOH:O	2.19	0.43
1:E:190:PHE:HB2	1:E:216:HIS:CE1	2.54	0.43
1:A:6:PRO:O	1:A:32:LYS:HA	2.19	0.43
1:G:139:TRP:CZ3	1:G:161:LEU:HG	2.53	0.42
1:D:4:ILE:CD1	1:D:80:LYS:HE3	2.48	0.42
1:G:34:PHE:HB2	2:G:323:HOH:O	2.18	0.42
1:E:130:PRO:HB3	1:E:163:LEU:HD22	2.01	0.42
1:B:130:PRO:HD2	2:B:238:HOH:O	2.17	0.42
1:E:141:PRO:HG3	1:E:194:ARG:CZ	2.49	0.42
1:E:137:VAL:HB	1:E:162:LEU:HG	2.01	0.42
1:B:81:GLN:NE2	1:B:183:VAL:HB	2.34	0.42
1:F:191:VAL:HA	1:F:215:ALA:HA	2.01	0.42
1:H:107:ILE:HG12	1:H:116:TYR:CD1	2.54	0.42
1:H:26:GLU:HG3	1:H:45:LYS:HG3	2.00	0.42
1:C:100:ILE:O	1:C:122:GLY:HA2	2.19	0.42
1:D:219:LEU:HA	2:D:245:HOH:O	2.19	0.42
1:G:219:LEU:HD12	2:G:321:HOH:O	2.19	0.42
1:C:128:ASN:HD22	1:C:128:ASN:H	1.66	0.42
1:C:170:ARG:NH1	1:C:170:ARG:HB3	2.34	0.42
1:G:76:VAL:HG11	1:G:184:GLN:O	2.19	0.42
1:G:63:GYC:HE1	1:G:195:ILE:HB	2.01	0.42
1:E:171:CYS:HG	1:E:173:PHE:HE1	1.65	0.42
1:D:162:LEU:H	1:D:162:LEU:HD23	1.84	0.42
1:D:218:GLY:O	1:D:219:LEU:O	2.36	0.42
1:D:194:ARG:CD	2:D:225:HOH:O	2.66	0.42
1:A:216:HIS:CD2	1:A:217:SER:O	2.72	0.42
1:A:21:HIS:HA	1:A:22:PRO:HD2	1.87	0.42
1:H:37:LYS:HE3	2:H:319:HOH:O	2.18	0.42
1:C:162:LEU:CD2	1:C:162:LEU:H	2.18	0.42
1:F:100:ILE:HG12	2:F:260:HOH:O	2.19	0.42
1:H:125:PHE:CD1	1:H:131:VAL:HG21	2.54	0.42
1:D:57:LEU:HD23	1:D:120:PHE:CE2	2.54	0.42
1:A:145:LYS:O	1:A:155:GLY:HA2	2.20	0.42
1:D:85:GLU:OE2	1:D:181:LYS:HD3	2.20	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:PRO:CG	1:A:194:ARG:CZ	2.97	0.42
1:B:30:LEU:N	1:B:30:LEU:HD23	2.35	0.42
1:C:146:LEU:HB3	1:C:153:LEU:HD11	2.00	0.42
1:H:201:ASP:OD1	1:H:205:ASN:N	2.52	0.42
1:E:31:GLY:O	1:E:33:PRO:HD3	2.19	0.42
1:F:198:LYS:HG3	1:F:210:HIS:CE1	2.55	0.42
1:G:15:GLU:O	1:G:119:ARG:HA	2.19	0.42
1:F:171:CYS:SG	1:F:173:PHE:HE1	2.42	0.42
1:C:83:PHE:HA	1:C:86:GLY:H	1.85	0.42
1:H:166:GLY:O	1:H:167:GLY:O	2.37	0.42
1:B:109:LEU:HD13	1:B:114:PHE:CE2	2.55	0.42
1:C:27:GLY:HA3	1:C:42:LEU:HD23	2.01	0.42
1:D:205:ASN:ND2	2:D:232:HOH:O	2.52	0.42
1:E:95:TYR:CD2	1:E:171:CYS:HB2	2.55	0.42
1:D:153:LEU:HB3	1:D:177:TYR:HB2	2.01	0.42
1:B:146:LEU:HA	1:B:154:LYS:O	2.19	0.42
1:D:14:MET:O	1:D:24:ALA:HA	2.19	0.42
1:D:203:ASP:N	1:D:203:ASP:OD1	2.52	0.42
1:B:195:ILE:CD1	1:B:209:LEU:HD11	2.48	0.42
1:B:58:THR:O	1:B:63:GYC:HB11	2.20	0.42
1:E:71:TYR:HA	1:E:72:PRO:HD2	1.96	0.42
1:B:91:ARG:NE	1:B:175:THR:OG1	2.51	0.42
1:B:83:PHE:HB3	1:B:84:PRO:HA	2.01	0.41
1:B:119:ARG:HA	1:B:119:ARG:HD2	1.89	0.41
1:G:72:PRO:CG	1:G:75:ILE:HD12	2.50	0.41
1:E:138:LYS:HG2	1:E:162:LEU:CD2	2.36	0.41
1:A:102:ILE:HD12	1:B:123:VAL:HG22	2.02	0.41
1:E:139:TRP:CE3	1:E:161:LEU:HG	2.55	0.41
1:A:87:TYR:HB3	1:A:179:ALA:HA	2.03	0.41
1:B:84:PRO:O	1:B:85:GLU:C	2.58	0.41
1:A:211:GLU:OE2	1:A:213:ALA:HB2	2.21	0.41
1:A:76:VAL:HG11	1:A:184:GLN:HB3	2.02	0.41
1:F:40:MET:CE	1:F:61:PHE:O	2.68	0.41
1:A:94:ASN:C	1:A:94:ASN:HD22	2.23	0.41
1:F:171:CYS:SG	1:F:173:PHE:CE1	3.13	0.41
1:H:31:GLY:HA2	1:H:38:GLN:HA	2.02	0.41
1:B:194:ARG:NH2	2:B:292:HOH:O	2.46	0.41
1:H:149:ARG:NH1	2:H:261:HOH:O	2.52	0.41
1:F:76:VAL:CB	1:F:186:PRO:HB3	2.47	0.41
1:A:200:HIS:HA	1:A:206:ASN:O	2.19	0.41
1:B:109:LEU:HD13	1:B:114:PHE:CD2	2.56	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:39:SER:CB	1:E:210:HIS:CD2	3.04	0.41
1:C:166:GLY:HA3	2:C:311:HOH:O	2.20	0.41
1:D:9:LYS:HE2	1:D:112:ASP:OD1	2.20	0.41
1:A:145:LYS:HD2	1:A:145:LYS:N	2.35	0.41
1:A:31:GLY:O	1:A:33:PRO:HD3	2.21	0.41
1:H:106:ASP:HB3	1:H:117:GLU:HB3	2.03	0.41
1:E:40:MET:O	1:E:208:ASN:HA	2.21	0.41
1:H:39:SER:HG	1:H:210:HIS:CE1	2.39	0.41
1:F:24:ALA:HB3	1:F:46:GLU:HB2	2.03	0.41
1:A:4:ILE:HG22	1:A:34:PHE:CE1	2.56	0.41
1:D:43:LYS:HA	1:D:205:ASN:O	2.21	0.41
1:F:44:VAL:HB	1:F:205:ASN:HD22	1.86	0.41
1:A:40:MET:SD	1:A:61:PHE:HB3	2.61	0.41
1:G:201:ASP:O	1:G:202:LYS:C	2.59	0.41
1:A:197:ILE:HG23	1:A:207:VAL:HG13	2.01	0.41
1:B:190:PHE:CD1	1:B:190:PHE:N	2.89	0.41
1:C:76:VAL:HG23	2:C:270:HOH:O	2.21	0.41
1:C:32:LYS:HB3	1:C:35:GLU:HG3	2.03	0.41
1:E:198:LYS:HE3	1:E:210:HIS:ND1	2.35	0.41
1:B:139:TRP:CD2	1:B:161:LEU:HD21	2.56	0.41
1:F:66:ARG:HG2	1:F:79:PHE:CE2	2.56	0.41
1:D:39:SER:HA	1:D:209:LEU:O	2.21	0.40
1:A:128:ASN:CA	1:A:133:GLN:HE22	2.30	0.40
1:C:3:VAL:HG22	1:C:4:ILE:N	2.37	0.40
1:C:195:ILE:HG23	1:C:195:ILE:O	2.20	0.40
1:F:216:HIS:HD2	1:F:218:GLY:H	1.69	0.40
1:A:141:PRO:HG3	1:A:194:ARG:NE	2.36	0.40
1:C:31:GLY:HA3	1:C:68:PHE:CE2	2.56	0.40
1:C:146:LEU:HA	1:C:154:LYS:O	2.20	0.40
1:F:96:GLU:OE2	1:H:149:ARG:NH2	2.53	0.40
1:D:73:GLU:HG3	1:D:73:GLU:O	2.19	0.40
1:B:42:LEU:O	1:B:206:ASN:HA	2.21	0.40
1:D:85:GLU:O	1:D:180:LYS:HD2	2.21	0.40
1:A:18:VAL:C	1:A:20:GLY:N	2.75	0.40
1:C:36:GLY:O	1:C:212:HIS:HA	2.21	0.40
1:D:101:CYS:O	1:D:102:ILE:HG13	2.21	0.40
1:F:44:VAL:CG2	1:F:205:ASN:HA	2.52	0.40
1:E:212:HIS:CD2	1:E:213:ALA:N	2.90	0.40
1:A:135:ARG:CD	2:E:236:HOH:O	2.69	0.40
1:C:40:MET:O	1:C:208:ASN:HA	2.21	0.40
1:E:43:LYS:HA	1:E:205:ASN:O	2.21	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:175:THR:HG21	1:C:177:TYR:CZ	2.57	0.40
1:F:143:THR:H	1:H:145:LYS:NZ	2.19	0.40
1:G:85:GLU:OE2	1:G:85:GLU:N	2.41	0.40
1:C:145:LYS:HD2	1:C:145:LYS:N	2.37	0.40
1:F:119:ARG:HA	1:F:119:ARG:HD2	1.95	0.40
1:B:71:TYR:HA	1:B:72:PRO:HD3	1.86	0.40
2:E:357:HOH:O	1:G:149:ARG:HD3	2.21	0.40
1:H:145:LYS:O	1:H:155:GLY:HA2	2.21	0.40
1:B:16:GLY:O	1:B:22:PRO:HA	2.21	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	214/255 (84%)	199 (93%)	13 (6%)	2 (1%)	21	24
1	B	213/255 (84%)	196 (92%)	16 (8%)	1 (0%)	34	41
1	C	212/255 (83%)	198 (93%)	14 (7%)	0	100	100
1	D	212/255 (83%)	202 (95%)	10 (5%)	0	100	100
1	E	213/255 (84%)	203 (95%)	9 (4%)	1 (0%)	34	41
1	F	213/255 (84%)	204 (96%)	8 (4%)	1 (0%)	34	41
1	G	212/255 (83%)	202 (95%)	7 (3%)	3 (1%)	14	13
1	H	212/255 (83%)	195 (92%)	13 (6%)	4 (2%)	10	8
All	All	1701/2040 (83%)	1599 (94%)	90 (5%)	12 (1%)	26	31

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	167	GLY

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type
1	H	202	LYS
1	A	200	HIS
1	G	218	GLY
1	H	167	GLY
1	F	202	LYS
1	G	138	LYS
1	G	202	LYS
1	H	66	ARG
1	A	138	LYS
1	H	40	MET
1	B	84	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	186/217 (86%)	177 (95%)	9 (5%)	31	42
1	B	185/217 (85%)	173 (94%)	12 (6%)	21	27
1	C	184/217 (85%)	180 (98%)	4 (2%)	60	77
1	D	184/217 (85%)	175 (95%)	9 (5%)	31	41
1	E	185/217 (85%)	173 (94%)	12 (6%)	21	27
1	F	185/217 (85%)	179 (97%)	6 (3%)	46	62
1	G	184/217 (85%)	173 (94%)	11 (6%)	24	31
1	H	184/217 (85%)	179 (97%)	5 (3%)	52	70
All	All	1477/1736 (85%)	1409 (95%)	68 (5%)	33	44

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	66	ARG
1	A	90	GLU
1	A	94	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	133	GLN
1	A	138	LYS
1	A	145	LYS
1	A	194	ARG
1	A	219	LEU
1	B	3	VAL
1	B	9	LYS
1	B	30	LEU
1	B	94	ASN
1	B	102	ILE
1	B	112	ASP
1	B	133	GLN
1	B	162	LEU
1	B	190	PHE
1	B	194	ARG
1	B	203	ASP
1	B	212	HIS
1	C	30	LEU
1	C	128	ASN
1	C	145	LYS
1	C	194	ARG
1	D	3	VAL
1	D	4	ILE
1	D	26	GLU
1	D	32	LYS
1	D	94	ASN
1	D	100	ILE
1	D	145	LYS
1	D	190	PHE
1	D	203	ASP
1	E	58	THR
1	E	70	LYS
1	E	73	GLU
1	E	92	SER
1	E	94	ASN
1	E	145	LYS
1	E	181	LYS
1	E	182	VAL
1	E	184	GLN
1	E	186	PRO
1	E	194	ARG
1	E	211	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	F	30	LEU
1	F	66	ARG
1	F	88	SER
1	F	94	ASN
1	F	194	ARG
1	F	219	LEU
1	G	3	VAL
1	G	5	LYS
1	G	30	LEU
1	G	66	ARG
1	G	145	LYS
1	G	162	LEU
1	G	190	PHE
1	G	194	ARG
1	G	202	LYS
1	G	203	ASP
1	G	211	GLU
1	H	30	LEU
1	H	73	GLU
1	H	135	ARG
1	H	145	LYS
1	H	211	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	HIS
1	A	94	ASN
1	A	133	GLN
1	A	158	ASN
1	A	208	ASN
1	A	216	HIS
1	B	81	GLN
1	B	94	ASN
1	B	205	ASN
1	B	208	ASN
1	B	216	HIS
1	C	21	HIS
1	C	81	GLN
1	C	94	ASN
1	C	128	ASN
1	C	205	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	206	ASN
1	C	208	ASN
1	C	210	HIS
1	C	212	HIS
1	C	216	HIS
1	D	38	GLN
1	D	94	ASN
1	D	205	ASN
1	D	206	ASN
1	D	216	HIS
1	E	21	HIS
1	E	38	GLN
1	E	94	ASN
1	E	158	ASN
1	E	205	ASN
1	E	208	ASN
1	E	212	HIS
1	E	216	HIS
1	F	81	GLN
1	F	94	ASN
1	F	205	ASN
1	F	208	ASN
1	F	216	HIS
1	G	21	HIS
1	G	205	ASN
1	G	206	ASN
1	G	208	ASN
1	G	210	HIS
1	G	216	HIS
1	H	21	HIS
1	H	38	GLN
1	H	158	ASN
1	H	206	ASN
1	H	208	ASN
1	H	216	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

8 non-standard protein/DNA/RNA residues 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
1	GYC	A	63	1	22,22,23	4.29	11 (50%)	27,30,32	3.13	6 (22%)
1	GYC	B	63	1	22,22,23	4.18	11 (50%)	27,30,32	3.17	6 (22%)
1	GYC	C	63	1	22,22,23	4.21	11 (50%)	27,30,32	3.03	7 (25%)
1	GYC	D	63	1	22,22,23	4.24	11 (50%)	27,30,32	3.17	6 (22%)
1	GYC	E	63	1	22,22,23	4.43	10 (45%)	27,30,32	3.00	6 (22%)
1	GYC	F	63	1	22,22,23	4.31	12 (54%)	27,30,32	3.10	6 (22%)
1	GYC	G	63	1	22,22,23	4.38	10 (45%)	27,30,32	3.00	6 (22%)
1	GYC	H	63	1	22,22,23	4.36	10 (45%)	27,30,32	3.08	7 (25%)

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
1	GYC	A	63	1	1/1/5/7	0/8/29/30	0/2/2/2
1	GYC	B	63	1	1/1/5/7	0/8/29/30	0/2/2/2
1	GYC	C	63	1	1/1/5/7	0/8/29/30	0/2/2/2
1	GYC	D	63	1	1/1/5/7	0/8/29/30	0/2/2/2
1	GYC	E	63	1	1/1/5/7	0/8/29/30	0/2/2/2
1	GYC	F	63	1	1/1/5/7	0/8/29/30	0/2/2/2
1	GYC	G	63	1	1/1/5/7	0/8/29/30	0/2/2/2
1	GYC	H	63	1	1/1/5/7	0/8/29/30	0/2/2/2

All (86) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	63	GYC	CA1-C1	-16.67	1.26	1.51
1	H	63	GYC	CA1-C1	-15.88	1.28	1.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	63	GYC	CA1-C1	-15.74	1.28	1.51
1	D	63	GYC	CA1-C1	-15.68	1.28	1.51
1	A	63	GYC	CA1-C1	-15.26	1.28	1.51
1	B	63	GYC	CA1-C1	-15.25	1.28	1.51
1	F	63	GYC	CA1-C1	-15.20	1.29	1.51
1	C	63	GYC	CA1-C1	-14.88	1.29	1.51
1	A	63	GYC	CA2-C2	-7.66	1.40	1.48
1	C	63	GYC	CA2-C2	-7.45	1.40	1.48
1	D	63	GYC	CA2-C2	-6.96	1.41	1.48
1	F	63	GYC	CA2-C2	-6.79	1.41	1.48
1	H	63	GYC	CA2-C2	-6.76	1.41	1.48
1	E	63	GYC	CA2-C2	-6.40	1.41	1.48
1	B	63	GYC	CA2-C2	-6.29	1.41	1.48
1	G	63	GYC	CA2-C2	-5.97	1.42	1.48
1	D	63	GYC	OH-CZ	-4.63	1.26	1.37
1	F	63	GYC	OH-CZ	-4.63	1.26	1.37
1	C	63	GYC	OH-CZ	-4.58	1.26	1.37
1	H	63	GYC	OH-CZ	-4.58	1.26	1.37
1	E	63	GYC	OH-CZ	-4.36	1.26	1.37
1	B	63	GYC	OH-CZ	-4.32	1.26	1.37
1	G	63	GYC	OH-CZ	-4.23	1.27	1.37
1	A	63	GYC	OH-CZ	-4.11	1.27	1.37
1	F	63	GYC	CA3-N3	-3.91	1.40	1.47
1	A	63	GYC	CA3-N3	-3.85	1.40	1.47
1	G	63	GYC	CA3-N3	-3.64	1.41	1.47
1	H	63	GYC	CA3-N3	-3.61	1.41	1.47
1	D	63	GYC	CG2-CB2	-3.52	1.39	1.46
1	C	63	GYC	CG2-CB2	-3.32	1.40	1.46
1	D	63	GYC	CA3-N3	-3.30	1.41	1.47
1	C	63	GYC	CA3-N3	-3.25	1.41	1.47
1	H	63	GYC	CG2-CB2	-3.19	1.40	1.46
1	B	63	GYC	CA3-N3	-2.85	1.42	1.47
1	A	63	GYC	CG2-CB2	-2.74	1.41	1.46
1	F	63	GYC	CG2-CB2	-2.73	1.41	1.46
1	B	63	GYC	CG2-CB2	-2.65	1.41	1.46
1	E	63	GYC	CA3-N3	-2.49	1.43	1.47
1	E	63	GYC	CG2-CB2	-2.23	1.42	1.46
1	A	63	GYC	CE1-CZ	2.00	1.42	1.38
1	D	63	GYC	CD1-CG2	2.03	1.43	1.39
1	A	63	GYC	CD1-CG2	2.06	1.43	1.39
1	B	63	GYC	CB1-SG1	2.09	1.86	1.81
1	E	63	GYC	CB1-CA1	2.09	1.55	1.52

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	63	GYC	CE2-CD2	2.12	1.42	1.38
1	A	63	GYC	CB1-CA1	2.14	1.55	1.52
1	F	63	GYC	CD2-CG2	2.17	1.43	1.39
1	B	63	GYC	CE2-CD2	2.22	1.42	1.38
1	B	63	GYC	CB1-CA1	2.23	1.55	1.52
1	B	63	GYC	CD1-CG2	2.24	1.43	1.39
1	G	63	GYC	CD2-CG2	2.25	1.43	1.39
1	D	63	GYC	CB1-SG1	2.27	1.86	1.81
1	C	63	GYC	CB1-SG1	2.28	1.86	1.81
1	H	63	GYC	CB1-SG1	2.30	1.86	1.81
1	H	63	GYC	CE1-CD1	2.31	1.42	1.38
1	D	63	GYC	CE2-CD2	2.32	1.42	1.38
1	C	63	GYC	CD1-CG2	2.35	1.43	1.39
1	G	63	GYC	CD1-CG2	2.35	1.43	1.39
1	A	63	GYC	CE1-CD1	2.39	1.43	1.38
1	D	63	GYC	CB1-CA1	2.41	1.55	1.52
1	H	63	GYC	CD1-CG2	2.42	1.44	1.39
1	F	63	GYC	CB1-SG1	2.43	1.86	1.81
1	G	63	GYC	CB1-CA1	2.43	1.55	1.52
1	H	63	GYC	CB1-CA1	2.48	1.55	1.52
1	E	63	GYC	CD1-CG2	2.50	1.44	1.39
1	A	63	GYC	CE2-CD2	2.52	1.43	1.38
1	C	63	GYC	CE1-CD1	2.53	1.43	1.38
1	E	63	GYC	CE2-CD2	2.54	1.43	1.38
1	E	63	GYC	CE1-CD1	2.56	1.43	1.38
1	F	63	GYC	CE1-CD1	2.60	1.43	1.38
1	D	63	GYC	CE1-CD1	2.61	1.43	1.38
1	G	63	GYC	CE2-CD2	2.61	1.43	1.38
1	F	63	GYC	CB1-CA1	2.64	1.56	1.52
1	F	63	GYC	CE2-CD2	2.67	1.43	1.38
1	F	63	GYC	CD1-CG2	2.68	1.44	1.39
1	B	63	GYC	CE1-CD1	2.75	1.43	1.38
1	G	63	GYC	CE1-CD1	2.80	1.43	1.38
1	C	63	GYC	CB1-CA1	3.09	1.56	1.52
1	D	63	GYC	CB2-CA2	4.27	1.38	1.35
1	C	63	GYC	CB2-CA2	5.35	1.39	1.35
1	A	63	GYC	CB2-CA2	6.09	1.40	1.35
1	H	63	GYC	CB2-CA2	6.35	1.40	1.35
1	F	63	GYC	CB2-CA2	6.40	1.40	1.35
1	B	63	GYC	CB2-CA2	6.49	1.40	1.35
1	E	63	GYC	CB2-CA2	6.87	1.41	1.35
1	G	63	GYC	CB2-CA2	7.85	1.42	1.35

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	63	GYC	CA3-N3-C2	-5.24	115.47	123.99
1	A	63	GYC	CA3-N3-C2	-5.20	115.53	123.99
1	G	63	GYC	CA3-N3-C2	-5.20	115.53	123.99
1	C	63	GYC	CA3-N3-C2	-5.12	115.65	123.99
1	F	63	GYC	CA3-N3-C2	-5.06	115.75	123.99
1	H	63	GYC	CA3-N3-C2	-4.82	116.14	123.99
1	E	63	GYC	CA3-N3-C2	-4.35	116.91	123.99
1	B	63	GYC	CA3-N3-C2	-4.28	117.02	123.99
1	B	63	GYC	CA2-C2-N3	-3.23	101.78	103.40
1	F	63	GYC	CA2-C2-N3	-2.86	101.97	103.40
1	C	63	GYC	CA2-C2-N3	-2.71	102.04	103.40
1	D	63	GYC	CA2-C2-N3	-2.63	102.08	103.40
1	E	63	GYC	CA2-C2-N3	-2.62	102.08	103.40
1	G	63	GYC	CA2-C2-N3	-2.54	102.12	103.40
1	H	63	GYC	CA2-C2-N3	-2.54	102.13	103.40
1	A	63	GYC	O2-C2-CA2	-2.35	129.68	130.95
1	H	63	GYC	O2-C2-CA2	-2.18	129.77	130.95
1	C	63	GYC	O2-C2-CA2	-2.06	129.84	130.95
1	G	63	GYC	C2-CA2-N2	3.64	111.81	108.91
1	A	63	GYC	C2-CA2-N2	3.90	112.02	108.91
1	E	63	GYC	C2-CA2-N2	4.18	112.25	108.91
1	H	63	GYC	C2-CA2-N2	4.36	112.39	108.91
1	F	63	GYC	C2-CA2-N2	4.40	112.42	108.91
1	C	63	GYC	C2-CA2-N2	4.50	112.50	108.91
1	B	63	GYC	C2-CA2-N2	4.72	112.67	108.91
1	D	63	GYC	C2-CA2-N2	5.04	112.93	108.91
1	H	63	GYC	C-CA3-N3	5.61	125.28	113.00
1	B	63	GYC	CA3-N3-C1	5.63	133.90	127.36
1	A	63	GYC	C-CA3-N3	5.78	125.67	113.00
1	G	63	GYC	C-CA3-N3	5.84	125.78	113.00
1	D	63	GYC	C-CA3-N3	5.87	125.86	113.00
1	E	63	GYC	CA3-N3-C1	5.96	134.28	127.36
1	C	63	GYC	C-CA3-N3	6.08	126.32	113.00
1	F	63	GYC	C-CA3-N3	6.35	126.90	113.00
1	H	63	GYC	CA3-N3-C1	6.42	134.81	127.36
1	F	63	GYC	CA3-N3-C1	6.51	134.91	127.36
1	C	63	GYC	CA3-N3-C1	6.65	135.08	127.36
1	G	63	GYC	CA3-N3-C1	6.68	135.12	127.36
1	D	63	GYC	CA3-N3-C1	6.89	135.36	127.36
1	A	63	GYC	CA3-N3-C1	7.08	135.58	127.36
1	E	63	GYC	C-CA3-N3	7.10	128.55	113.00
1	B	63	GYC	C-CA3-N3	7.28	128.93	113.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	63	GYC	CB1-CA1-C1	9.65	126.48	110.12
1	E	63	GYC	CB1-CA1-C1	10.10	127.25	110.12
1	G	63	GYC	CB1-CA1-C1	10.25	127.50	110.12
1	F	63	GYC	CB1-CA1-C1	10.35	127.66	110.12
1	D	63	GYC	CB1-CA1-C1	10.62	128.12	110.12
1	H	63	GYC	CB1-CA1-C1	10.91	128.61	110.12
1	B	63	GYC	CB1-CA1-C1	11.01	128.79	110.12
1	A	63	GYC	CB1-CA1-C1	11.06	128.88	110.12

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	D	63	GYC	CA1
1	G	63	GYC	CA1
1	A	63	GYC	CA1
1	C	63	GYC	CA1
1	F	63	GYC	CA1
1	H	63	GYC	CA1
1	B	63	GYC	CA1
1	E	63	GYC	CA1

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	63	GYC	2	0
1	B	63	GYC	3	0
1	C	63	GYC	2	0
1	D	63	GYC	2	0
1	E	63	GYC	3	0
1	F	63	GYC	1	0
1	G	63	GYC	2	0
1	H	63	GYC	7	0

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	216/255 (84%)	-0.28	1 (0%) 91 94	15, 27, 40, 53	0
1	B	215/255 (84%)	-0.17	1 (0%) 91 94	16, 29, 42, 58	0
1	C	214/255 (83%)	-0.49	1 (0%) 91 94	8, 19, 30, 41	0
1	D	214/255 (83%)	-0.40	2 (0%) 85 89	12, 21, 35, 50	0
1	E	215/255 (84%)	-0.37	1 (0%) 91 94	13, 24, 35, 56	0
1	F	215/255 (84%)	-0.42	1 (0%) 91 94	11, 22, 35, 50	0
1	G	214/255 (83%)	-0.39	2 (0%) 85 89	12, 23, 38, 51	0
1	H	214/255 (83%)	-0.26	1 (0%) 91 94	14, 29, 44, 56	0
All	All	1717/2040 (84%)	-0.35	10 (0%) 90 93	8, 24, 39, 58	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	SER	4.7
1	G	218	GLY	4.7
1	D	219	LEU	3.0
1	F	219	LEU	2.8
1	E	2	SER	2.7
1	C	218	GLY	2.6
1	H	166	GLY	2.1
1	B	219	LEU	2.1
1	G	184	GLN	2.0
1	D	218	GLY	2.0

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

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
1	GYC	D	63	21/22	0.94	0.12	-	16,21,25,28	0
1	GYC	G	63	21/22	0.91	0.13	-	26,27,29,35	0
1	GYC	A	63	21/22	0.91	0.13	-	26,34,35,46	0
1	GYC	C	63	21/22	0.94	0.12	-	15,19,22,25	0
1	GYC	F	63	21/22	0.92	0.13	-	19,25,29,32	0
1	GYC	H	63	21/22	0.91	0.13	-	23,30,33,34	0
1	GYC	B	63	21/22	0.93	0.11	-	26,32,33,39	0
1	GYC	E	63	21/22	0.95	0.11	-	23,26,28,29	0

### 6.3 Carbohydrates

There are no carbohydrates in this entry.

### 6.4 Ligands

There are no ligands in this entry.

### 6.5 Other polymers

There are no such residues in this entry.