



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2022 – 04:05 PM EDT

PDB ID : 3M1B
Title : Crystal structure of human FcRn with a dimeric peptide inhibitor
Authors : Mezo, A.R.; Sridhar, V.; Badger, J.; Sakorafas, P.; Nienaber, V.
Deposited on : 2010-03-04
Resolution : 3.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

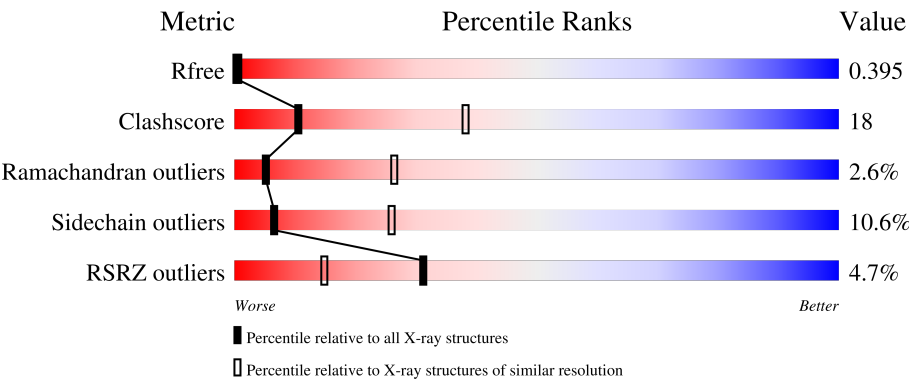
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.28.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.28.1

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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 ≥ 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	267	<div><div>3%</div><div>55%</div><div>38%</div><div>6%</div><div></div></div>
1	C	267	<div><div>4%</div><div>57%</div><div>36%</div><div>6%</div><div></div></div>
1	E	267	<div><div>3%</div><div>56%</div><div>37%</div><div>6%</div><div></div></div>
1	G	267	<div><div>5%</div><div>56%</div><div>39%</div><div></div><div></div></div>
2	B	99	<div><div>7%</div><div>59%</div><div>38%</div><div></div><div></div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	99	<div><div><div></div><div></div><div></div></div><div>4%67%30%</div><div></div></div>
2	F	99	<div><div><div></div><div></div><div></div></div><div>12%60%38%</div><div></div></div>
2	H	99	<div><div><div></div><div></div><div></div></div><div>4%58%39%</div><div></div></div>
3	I	16	<div><div><div></div><div></div><div></div></div><div>19%50%31%</div><div></div></div>
3	J	16	<div><div><div></div><div></div><div></div></div><div>44%25%6%25%</div><div></div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11241 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 IgG receptor FcRn large subunit p51.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	S	0	0	0
			1958	1253	329	368	8			
1	C	263	Total	C	N	O	S	0	0	0
			1958	1253	329	368	8			
1	E	263	Total	C	N	O	S	0	0	0
			1958	1253	329	368	8			
1	G	263	Total	C	N	O	S	0	0	0
			1958	1253	329	368	8			

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	0	0	0
			808	514	135	156	3			
2	D	99	Total	C	N	O	S	0	0	0
			808	514	135	156	3			
2	F	99	Total	C	N	O	S	0	0	0
			808	514	135	156	3			
2	H	99	Total	C	N	O	S	0	0	0
			808	514	135	156	3			

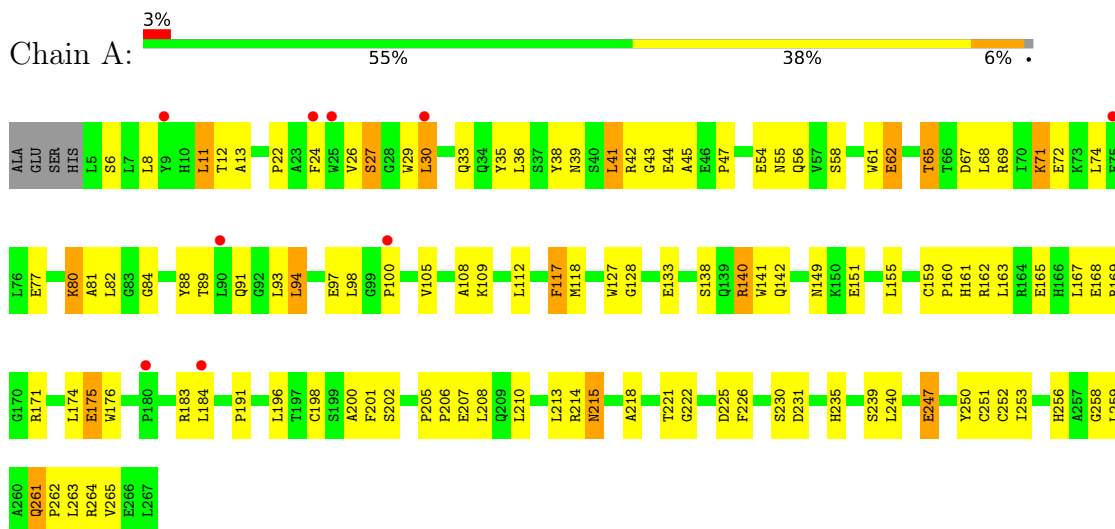
- Molecule 3 is a protein called DIMERIC PEPTIDE INHIBITOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	11	Total	C	N	O	S	0	0	0
			83	55	13	13	2			
3	J	12	Total	C	N	O	S	0	0	0
			94	64	14	14	2			

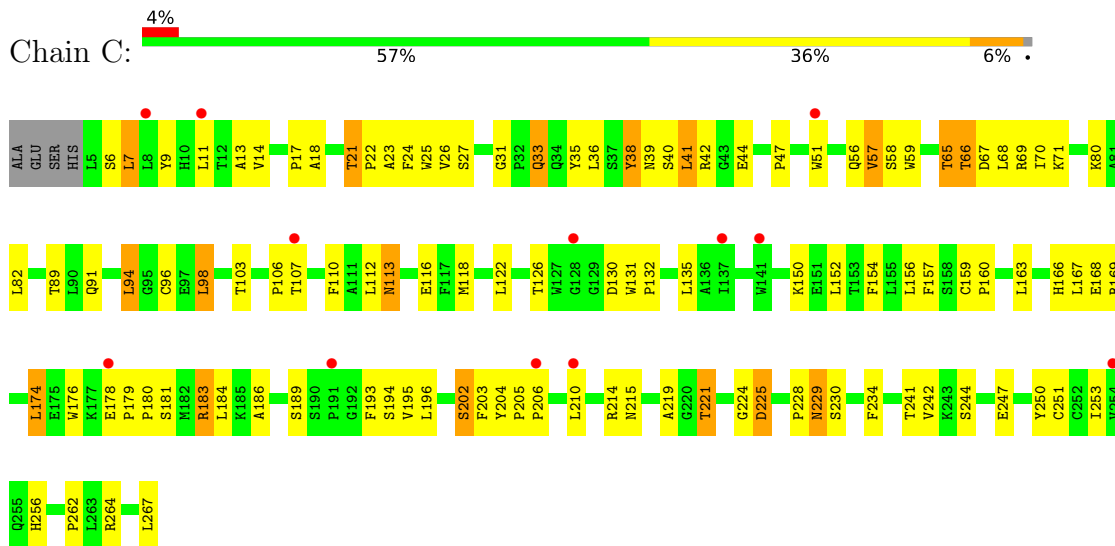
3 Residue-property plots [i](#)

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: IgG receptor FcRn large subunit p51

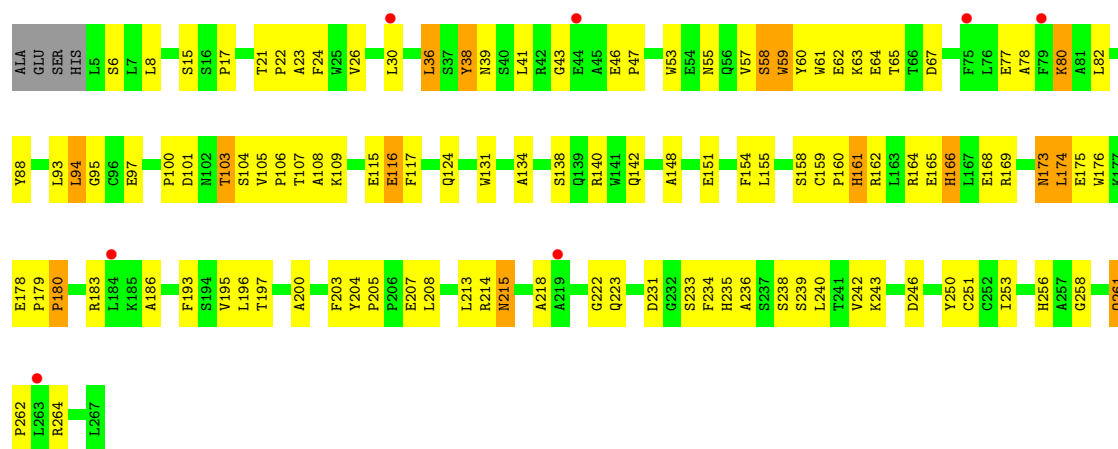


- Molecule 1: IgG receptor FcRn large subunit p51

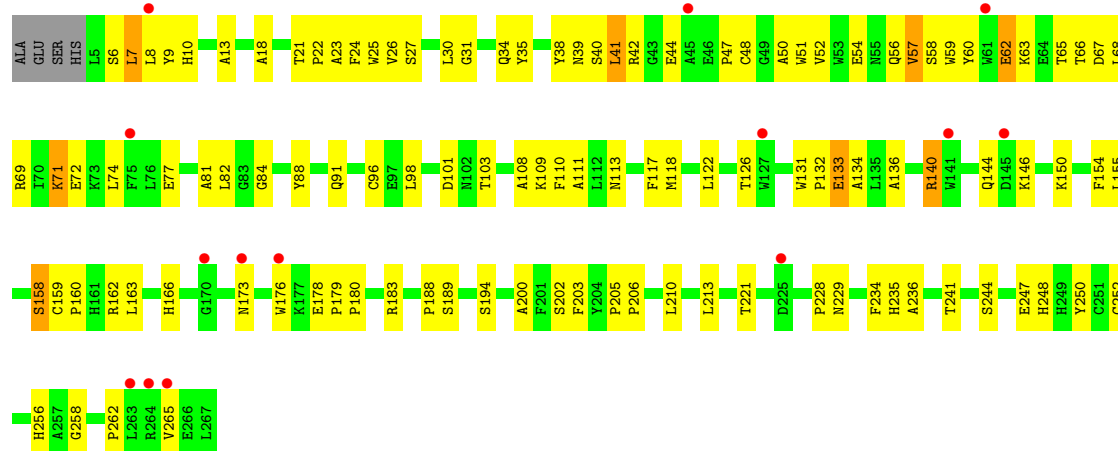


- Molecule 1: IgG receptor FcRn large subunit p51

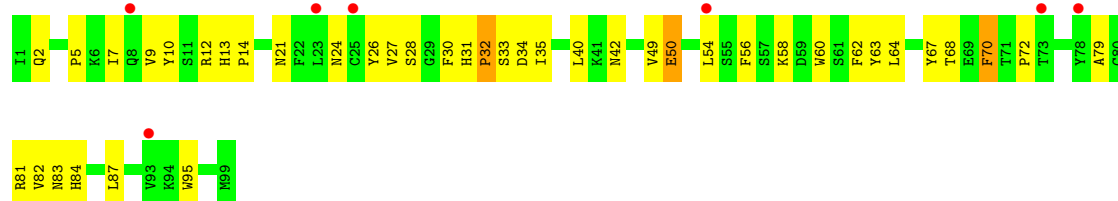




- Molecule 1: IgG receptor FcRn large subunit p51



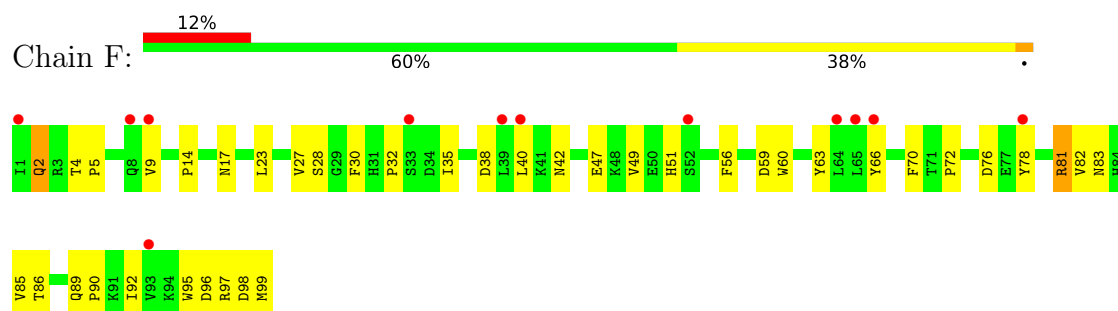
- Molecule 2: Beta-2-microglobulin



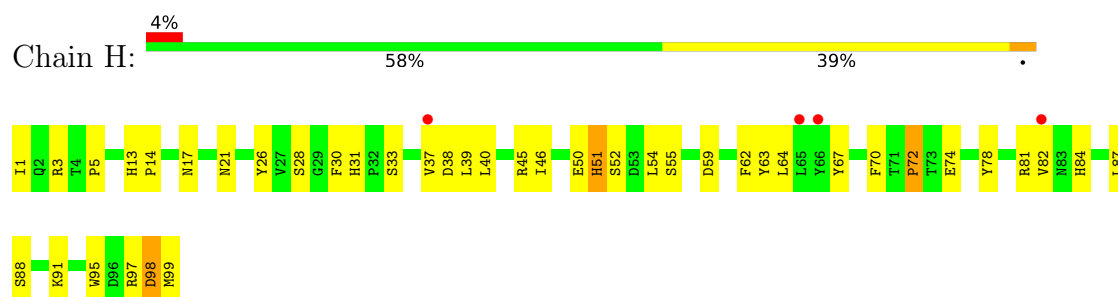
- Molecule 2: Beta-2-microglobulin



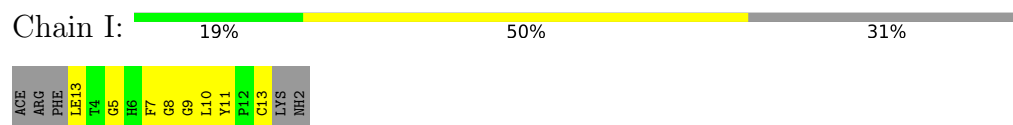
- Molecule 2: Beta-2-microglobulin



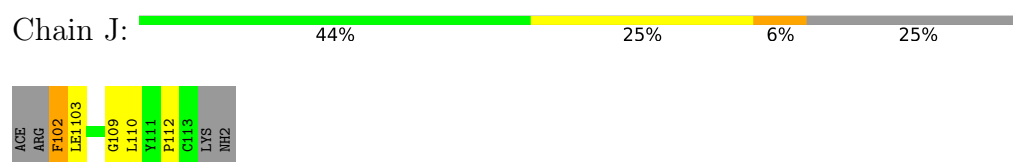
- Molecule 2: Beta-2-microglobulin



- Molecule 3: DIMERIC PEPTIDE INHIBITOR



- Molecule 3: DIMERIC PEPTIDE INHIBITOR



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.05Å 158.43Å 82.54Å 90.00° 90.11° 90.00°	Depositor
Resolution (Å)	37.24 – 3.10 37.22 – 3.08	Depositor EDS
% Data completeness (in resolution range)	100.0 (37.24-3.10) 89.5 (37.22-3.08)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 3.06Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.314 , 0.397 0.306 , 0.395	Depositor DCC
R_{free} test set	1475 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	96.3	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 39.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.390 for h,-k,-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	11241	wwPDB-VP
Average B, all atoms (Å ²)	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MLE, LE1, SAR

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	0.41	0/2020	0.57	0/2764
1	C	0.40	0/2020	0.58	0/2764
1	E	0.42	0/2020	0.60	1/2764 (0.0%)
1	G	0.39	0/2020	0.55	0/2764
2	B	0.38	0/831	0.56	0/1130
2	D	0.41	0/831	0.57	0/1130
2	F	0.39	0/831	0.57	0/1130
2	H	0.45	0/831	0.60	0/1130
3	I	0.48	0/63	0.43	0/83
3	J	0.50	0/74	0.39	0/96
All	All	0.41	0/11541	0.57	1/15755 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	I	0	3
3	J	0	2
All	All	0	5

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	30	LEU	CA-CB-CG	5.54	128.04	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	I	3	LE1	Mainchain,Peptide
3	I	8	GLY	Peptide
3	J	102	PHE	Mainchain
3	J	103	LE1	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1958	0	1753	79	0
1	C	1958	0	1753	80	0
1	E	1958	0	1753	72	0
1	G	1958	0	1753	73	0
2	B	808	0	741	27	0
2	D	808	0	741	25	0
2	F	808	0	741	25	0
2	H	808	0	741	23	0
3	I	83	0	75	3	0
3	J	94	0	82	2	0
All	All	11241	0	10133	395	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 (395) 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:G:84:GLY:HA3	1:G:88:TYR:OH	1.53	1.07
1:C:150:LYS:O	1:C:154:PHE:HB2	1.57	1.03
2:H:84:HIS:H	2:H:87:LEU:HD12	1.33	0.91
1:A:6:SER:CB	1:A:97:GLU:HB3	2.00	0.91
2:H:17:ASN:ND2	2:H:74:GLU:OE1	2.05	0.90
1:A:6:SER:HB3	1:A:97:GLU:HB3	1.54	0.86
1:A:22:PRO:HB3	1:A:39:ASN:HB2	1.60	0.81
1:G:146:LYS:O	1:G:150:LYS:HG3	1.81	0.80
1:A:252:CYS:HB3	1:A:265:VAL:HB	1.63	0.80
2:D:26:TYR:HB2	2:D:65:LEU:HD13	1.64	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:CYS:HB3	1:A:160:PRO:HD3	1.64	0.80
1:A:84:GLY:HA3	1:A:88:TYR:OH	1.82	0.79
1:E:6:SER:HB3	1:E:97:GLU:HB3	1.64	0.78
1:A:67:ASP:OD2	1:A:162:ARG:NH2	2.15	0.78
1:C:247:GLU:CD	1:C:247:GLU:H	1.86	0.78
2:F:96:ASP:HB3	2:F:99:MET:HB2	1.66	0.78
1:A:12:THR:HG23	1:A:91:GLN:HG2	1.66	0.77
2:D:40:LEU:HB3	2:D:43:GLY:HA2	1.65	0.77
1:E:94:LEU:HD12	1:E:108:ALA:HA	1.66	0.77
1:C:94:LEU:HA	1:C:107:THR:O	1.85	0.76
1:G:213:LEU:O	1:G:250:TYR:HA	1.86	0.75
1:C:24:PHE:HB3	1:C:40:SER:HB3	1.66	0.75
1:A:38:TYR:OH	1:A:69:ARG:HG3	1.86	0.74
1:C:159:CYS:HB3	1:C:160:PRO:HD3	1.68	0.74
2:F:2:GLN:HG2	2:F:32:PRO:HD3	1.69	0.74
2:F:49:VAL:HG12	2:F:66:TYR:HD2	1.52	0.74
1:E:261:GLN:HG3	1:E:262:PRO:HD2	1.70	0.73
2:D:81:ARG:HD3	2:D:90:PRO:HB2	1.69	0.73
1:G:42:ARG:HH21	1:G:44:GLU:HB3	1.54	0.70
1:E:6:SER:CB	1:E:97:GLU:HB3	2.21	0.70
1:C:35:TYR:O	1:C:47:PRO:HA	1.92	0.69
1:C:22:PRO:HA	1:C:41:LEU:HD13	1.74	0.69
2:B:7:ILE:HG23	2:B:27:VAL:HG22	1.75	0.68
1:G:133:GLU:HA	1:G:136:ALA:HB3	1.74	0.68
1:A:167:LEU:O	1:A:171:ARG:HB2	1.94	0.68
2:B:13:HIS:HB2	2:B:21:ASN:HD21	1.59	0.67
1:A:77:GLU:HG3	1:A:140:ARG:HE	1.58	0.67
1:A:196:LEU:O	1:A:239:SER:HA	1.95	0.66
1:G:71:LYS:HA	1:G:74:LEU:HD12	1.77	0.66
2:D:54:LEU:HD12	2:D:64:LEU:HD12	1.78	0.65
1:G:110:PHE:HB2	1:G:118:MET:HB2	1.77	0.65
1:E:205:PRO:O	1:E:256:HIS:CE1	2.50	0.64
1:A:261:GLN:HG3	1:A:262:PRO:HD2	1.79	0.64
1:C:203:PHE:HB2	1:C:256:HIS:CE1	2.33	0.64
2:D:30:PHE:CE2	2:D:62:PHE:HB2	2.33	0.64
1:A:45:ALA:H	1:A:65:THR:HG23	1.63	0.64
1:E:253:ILE:HD13	1:E:264:ARG:HA	1.78	0.64
1:E:159:CYS:HB3	1:E:160:PRO:HD3	1.78	0.64
1:C:22:PRO:HB3	1:C:39:ASN:HB2	1.79	0.64
1:C:57:VAL:O	1:C:59:TRP:N	2.30	0.63
1:C:160:PRO:HA	1:C:163:LEU:HB3	1.81	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:162:ARG:O	1:E:166:HIS:CD2	2.52	0.63
2:F:2:GLN:NE2	2:F:86:THR:HG23	2.14	0.63
1:G:98:LEU:HG	1:G:163:LEU:HD23	1.80	0.62
1:G:57:VAL:O	1:G:59:TRP:N	2.32	0.62
2:H:78:TYR:HB2	2:H:95:TRP:HE3	1.64	0.62
1:A:149:ASN:C	1:A:151:GLU:H	2.03	0.61
1:E:196:LEU:O	1:E:239:SER:HA	2.01	0.61
1:C:110:PHE:HB2	1:C:118:MET:HB2	1.81	0.61
1:G:256:HIS:HD2	1:G:258:GLY:H	1.49	0.61
1:C:22:PRO:CB	1:C:39:ASN:HB2	2.30	0.60
1:G:91:GLN:HB2	1:G:111:ALA:HB3	1.82	0.60
1:G:122:LEU:HD12	1:G:122:LEU:H	1.65	0.60
1:A:247:GLU:O	1:A:250:TYR:HB2	2.01	0.60
1:E:77:GLU:HG3	1:E:140:ARG:HE	1.66	0.60
1:G:65:THR:HA	1:G:68:LEU:HD12	1.84	0.60
1:A:256:HIS:CD2	1:A:258:GLY:H	2.20	0.60
2:F:23:LEU:HB2	2:F:70:PHE:CE1	2.37	0.60
1:C:11:LEU:HD21	1:C:71:LYS:HG2	1.84	0.60
1:G:101:ASP:HB2	1:G:103:THR:OG1	2.02	0.60
1:E:196:LEU:HD12	1:E:242:VAL:HG11	1.84	0.59
2:F:27:VAL:HG21	2:F:82:VAL:HG21	1.83	0.59
1:A:213:LEU:CD2	1:A:218:ALA:HA	2.33	0.59
1:C:25:TRP:HZ2	2:D:54:LEU:HD22	1.66	0.59
1:C:157:PHE:O	1:C:160:PRO:HD2	2.02	0.59
1:A:222:GLY:HA3	1:A:239:SER:O	2.02	0.59
1:G:144:GLN:HA	1:G:144:GLN:OE1	2.01	0.59
1:A:11:LEU:HG	1:A:26:VAL:HG13	1.85	0.59
1:E:104:SER:O	1:E:106:PRO:HD3	2.03	0.59
2:F:81:ARG:HD3	2:F:90:PRO:HB2	1.84	0.59
1:C:183:ARG:HG2	2:D:98:ASP:OD1	2.02	0.59
1:C:178:GLU:O	1:C:203:PHE:HA	2.02	0.58
1:G:84:GLY:HA3	1:G:88:TYR:HH	1.65	0.58
2:B:56:PHE:HA	2:B:62:PHE:HA	1.85	0.58
1:C:189:SER:H	1:C:194:SER:HA	1.68	0.58
1:C:24:PHE:O	1:C:40:SER:N	2.36	0.57
1:E:22:PRO:HB2	1:E:24:PHE:O	2.03	0.57
1:G:244:SER:HA	1:G:247:GLU:OE1	2.04	0.57
1:A:222:GLY:HA2	1:A:240:LEU:HD13	1.86	0.57
1:A:184:LEU:HD22	1:A:252:CYS:HB2	1.86	0.57
1:E:148:ALA:O	1:E:151:GLU:HB2	2.05	0.57
2:H:50:GLU:HB3	2:H:67:TYR:CZ	2.40	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:59:TRP:HA	1:E:62:GLU:OE1	2.05	0.57
1:A:56:GLN:C	1:A:169:ARG:HH21	2.07	0.56
1:C:25:TRP:CZ2	2:D:54:LEU:HD22	2.38	0.56
1:G:7:LEU:HD21	1:G:9:TYR:HE1	1.70	0.56
2:B:5:PRO:HB3	2:B:30:PHE:HB3	1.88	0.56
1:C:68:LEU:O	1:C:71:LYS:N	2.38	0.56
1:A:205:PRO:O	1:A:256:HIS:HE1	1.89	0.56
1:G:159:CYS:HB3	1:G:160:PRO:HD3	1.88	0.56
1:G:160:PRO:HA	1:G:163:LEU:HB3	1.88	0.56
1:C:196:LEU:HD12	1:C:242:VAL:HG11	1.87	0.56
1:C:98:LEU:HG	1:C:163:LEU:HD21	1.86	0.56
1:E:117:PHE:HD2	1:E:134:ALA:HB2	1.71	0.56
2:B:5:PRO:HB2	2:B:27:VAL:HG12	1.88	0.56
2:B:27:VAL:HG21	2:B:82:VAL:HG21	1.87	0.55
1:G:30:LEU:CD2	1:G:35:TYR:HB3	2.37	0.55
1:C:154:PHE:O	1:C:159:CYS:HB2	2.06	0.55
1:G:25:TRP:HB2	1:G:38:TYR:O	2.06	0.55
2:F:42:ASN:HD21	2:F:76:ASP:HA	1.71	0.55
1:C:131:TRP:HB3	1:C:132:PRO:CD	2.37	0.55
1:G:24:PHE:HB3	1:G:40:SER:HB3	1.87	0.55
2:D:54:LEU:HD21	2:D:62:PHE:CD1	2.42	0.55
1:A:71:LYS:HA	1:A:74:LEU:HD12	1.89	0.54
2:F:5:PRO:HA	2:F:30:PHE:HB3	1.88	0.54
1:A:94:LEU:HD12	1:A:108:ALA:HA	1.89	0.54
1:G:256:HIS:CD2	1:G:258:GLY:H	2.23	0.54
2:H:5:PRO:HG3	2:H:84:HIS:HB2	1.89	0.54
2:H:40:LEU:HD23	2:H:45:ARG:HA	1.90	0.54
1:C:194:SER:O	1:C:242:VAL:HG22	2.08	0.54
1:E:138:SER:O	1:E:142:GLN:HG2	2.08	0.54
1:A:127:TRP:CZ3	1:A:141:TRP:HB3	2.43	0.54
2:H:30:PHE:HE2	2:H:33:SER:HA	1.73	0.54
1:E:55:ASN:O	1:E:169:ARG:NE	2.38	0.54
1:E:162:ARG:O	1:E:166:HIS:HD2	1.90	0.54
2:F:9:VAL:HG11	2:F:95:TRP:HB2	1.89	0.54
1:A:43:GLY:O	1:A:69:ARG:NH2	2.30	0.54
1:E:106:PRO:HB3	1:E:155:LEU:HD22	1.88	0.53
1:E:155:LEU:O	1:E:160:PRO:HD3	2.08	0.53
1:E:205:PRO:HB2	1:E:207:GLU:OE2	2.07	0.53
1:G:200:ALA:HB3	1:G:236:ALA:HB3	1.89	0.53
2:B:13:HIS:HB2	2:B:21:ASN:ND2	2.22	0.53
1:E:180:PRO:HB3	1:E:203:PHE:HB3	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:26:TYR:OH	2:H:28:SER:HB3	2.09	0.53
1:G:117:PHE:HD2	1:G:134:ALA:HB2	1.74	0.53
1:C:180:PRO:HB3	1:C:203:PHE:HD1	1.74	0.53
1:G:108:ALA:O	1:G:109:LYS:HG3	2.08	0.53
2:H:51:HIS:CG	2:H:51:HIS:O	2.61	0.53
1:A:205:PRO:HB2	1:A:206:PRO:HD2	1.91	0.53
1:C:36:LEU:HD23	1:C:36:LEU:C	2.29	0.53
1:G:22:PRO:HA	1:G:41:LEU:HD13	1.90	0.53
1:C:184:LEU:HB3	1:C:267:LEU:HA	1.91	0.53
1:A:6:SER:HB2	1:A:97:GLU:HB3	1.89	0.52
1:A:80:LYS:HB3	1:A:140:ARG:NH2	2.24	0.52
2:B:40:LEU:HD12	2:B:79:ALA:HB3	1.91	0.52
1:E:222:GLY:HA2	1:E:240:LEU:HD13	1.91	0.52
1:G:81:ALA:HB2	1:G:140:ARG:HD2	1.91	0.52
1:G:162:ARG:O	1:G:166:HIS:HD2	1.93	0.52
1:E:58:SER:C	1:E:60:TYR:H	2.13	0.52
2:H:81:ARG:HA	2:H:91:LYS:O	2.09	0.52
1:E:93:LEU:HD13	2:F:56:PHE:CE1	2.45	0.52
1:A:161:HIS:ND1	1:A:165:GLU:OE2	2.43	0.52
1:C:6:SER:O	1:C:31:GLY:N	2.42	0.52
1:A:210:LEU:O	1:A:221:THR:HG22	2.10	0.52
2:D:6:LYS:HB3	2:D:28:SER:O	2.10	0.51
1:A:39:ASN:O	1:A:43:GLY:HA2	2.11	0.51
1:C:180:PRO:HB3	1:C:203:PHE:CD1	2.46	0.51
2:B:31:HIS:HA	2:B:32:PRO:O	2.10	0.51
1:E:178:GLU:N	1:E:204:TYR:O	2.43	0.51
1:A:253:ILE:CD1	1:A:264:ARG:HG2	2.41	0.51
1:E:64:GLU:OE1	1:E:162:ARG:HD3	2.11	0.51
1:C:7:LEU:HD23	1:C:163:LEU:HB2	1.93	0.50
1:C:229:ASN:HD22	1:C:229:ASN:N	2.09	0.50
1:C:42:ARG:HH21	1:C:44:GLU:HB3	1.77	0.50
2:F:5:PRO:HD3	2:F:86:THR:OG1	2.11	0.50
1:G:13:ALA:HA	1:G:23:ALA:O	2.11	0.50
2:H:1:ILE:HD13	2:H:3:ARG:HG3	1.93	0.50
2:H:17:ASN:HA	2:H:72:PRO:HB2	1.92	0.50
1:E:6:SER:CA	1:E:97:GLU:HB3	2.41	0.50
2:F:2:GLN:HE21	2:F:86:THR:HG23	1.76	0.50
1:C:22:PRO:HD3	1:C:41:LEU:HD22	1.92	0.50
1:G:47:PRO:HG2	1:G:52:VAL:HG13	1.94	0.50
1:A:93:LEU:HB3	1:A:109:LYS:HB2	1.94	0.50
1:A:231:ASP:H	2:B:12:ARG:HH21	1.60	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:51:HIS:CG	2:D:51:HIS:O	2.64	0.50
2:F:51:HIS:HB3	2:F:66:TYR:CZ	2.47	0.50
1:G:205:PRO:HB2	1:G:206:PRO:HD2	1.94	0.50
2:H:97:ARG:O	2:H:98:ASP:HB2	2.11	0.50
1:E:39:ASN:O	1:E:43:GLY:N	2.42	0.50
1:G:229:ASN:HD21	1:G:235:HIS:HB2	1.76	0.50
1:G:22:PRO:CB	1:G:39:ASN:HB2	2.42	0.50
1:A:69:ARG:O	1:A:72:GLU:HB3	2.11	0.50
1:C:56:GLN:OE1	1:C:56:GLN:HA	2.12	0.49
1:E:205:PRO:O	1:E:256:HIS:HE1	1.94	0.49
2:F:96:ASP:C	2:F:98:ASP:H	2.15	0.49
1:E:67:ASP:HB3	1:E:154:PHE:HE2	1.76	0.49
2:B:5:PRO:HB2	2:B:27:VAL:CG1	2.43	0.49
1:C:96:CYS:HA	1:C:106:PRO:HA	1.95	0.49
1:E:197:THR:HG21	2:F:99:MET:HA	1.95	0.49
1:C:26:VAL:HG12	1:C:27:SER:N	2.28	0.48
2:D:17:ASN:HD21	2:D:74:GLU:HB2	1.78	0.48
2:D:55:SER:O	2:D:62:PHE:HA	2.13	0.48
2:B:83:ASN:HA	2:B:87:LEU:HD12	1.94	0.48
1:E:97:GLU:O	1:E:104:SER:HA	2.12	0.48
2:F:5:PRO:CA	2:F:30:PHE:HB3	2.43	0.48
1:A:127:TRP:CD2	1:A:141:TRP:HE3	2.31	0.48
1:A:171:ARG:HD2	1:A:175:GLU:HB2	1.96	0.48
2:D:26:TYR:CZ	2:D:28:SER:HB3	2.49	0.48
2:D:42:ASN:HD21	2:D:76:ASP:HA	1.79	0.48
1:E:57:VAL:O	1:E:59:TRP:CD1	2.67	0.48
1:A:47:PRO:HB3	1:A:61:TRP:CZ2	2.49	0.48
2:D:40:LEU:HB3	2:D:43:GLY:CA	2.40	0.48
2:F:40:LEU:O	2:F:78:TYR:HA	2.13	0.48
1:G:59:TRP:HA	1:G:62:GLU:OE1	2.14	0.48
1:G:22:PRO:HB3	1:G:39:ASN:HB2	1.95	0.48
3:I:9:SAR:HA3	3:I:10:MLE:HN1	1.57	0.48
1:A:30:LEU:HD22	1:A:35:TYR:CE1	2.49	0.48
1:E:222:GLY:HA2	1:E:240:LEU:CD1	2.44	0.47
1:G:71:LYS:O	1:G:74:LEU:HB2	2.14	0.47
1:A:26:VAL:HG12	1:A:27:SER:N	2.29	0.47
1:C:14:VAL:HG12	1:C:89:THR:HG23	1.95	0.47
1:C:203:PHE:HE2	1:C:206:PRO:HA	1.79	0.47
1:E:160:PRO:O	1:E:164:ARG:N	2.43	0.47
1:G:74:LEU:O	1:G:77:GLU:HB3	2.14	0.47
1:A:82:LEU:HA	3:I:11:TYR:OH	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:SER:OG	2:B:12:ARG:NH2	2.47	0.47
1:C:98:LEU:HG	1:C:163:LEU:CD2	2.44	0.47
2:H:38:ASP:OD2	2:H:81:ARG:NH1	2.47	0.47
1:A:26:VAL:HG21	1:A:68:LEU:HD22	1.97	0.47
1:C:33:GLN:OE1	1:C:51:TRP:HZ2	1.97	0.47
2:D:39:LEU:HB3	2:D:46:ILE:HD12	1.96	0.47
1:E:22:PRO:HD3	1:E:41:LEU:HD22	1.95	0.47
2:H:78:TYR:CB	2:H:95:TRP:HE3	2.28	0.47
1:G:38:TYR:OH	1:G:69:ARG:HG3	2.14	0.47
1:E:101:ASP:C	1:E:103:THR:H	2.19	0.46
2:F:59:ASP:O	2:F:60:TRP:HB2	2.14	0.46
3:J:102:PHE:HA	3:J:112:PRO:HA	1.97	0.46
1:A:253:ILE:HD13	1:A:264:ARG:HA	1.96	0.46
1:E:94:LEU:HA	1:E:107:THR:O	2.16	0.46
2:H:54:LEU:HD21	2:H:62:PHE:CD1	2.49	0.46
1:A:174:LEU:O	1:A:176:TRP:N	2.48	0.46
1:E:203:PHE:CE2	1:E:234:PHE:HB3	2.51	0.46
2:B:49:VAL:HG22	2:B:68:THR:HB	1.97	0.46
1:E:38:TYR:C	1:E:38:TYR:CD2	2.89	0.46
1:G:229:ASN:H	1:G:229:ASN:HD22	1.63	0.46
1:A:62:GLU:HA	1:A:65:THR:OG1	2.15	0.46
2:H:26:TYR:CE1	2:H:63:TYR:HB2	2.51	0.46
1:A:56:GLN:HG2	1:A:61:TRP:NE1	2.31	0.46
1:C:179:PRO:HA	1:C:256:HIS:CD2	2.51	0.46
1:E:117:PHE:CD2	1:E:134:ALA:HB2	2.51	0.46
1:C:210:LEU:O	1:C:221:THR:HG23	2.16	0.46
1:E:115:GLU:O	1:E:116:GLU:C	2.54	0.46
1:A:159:CYS:HB3	1:A:160:PRO:CD	2.42	0.46
1:C:180:PRO:HA	1:C:202:SER:O	2.15	0.45
1:C:186:ALA:HB2	1:C:196:LEU:HD21	1.99	0.45
1:E:174:LEU:O	1:E:176:TRP:N	2.49	0.45
2:F:83:ASN:HB2	2:F:90:PRO:HB3	1.98	0.45
1:G:162:ARG:O	1:G:166:HIS:CD2	2.69	0.45
1:E:59:TRP:O	1:E:63:LYS:HB2	2.16	0.45
1:G:60:TYR:C	1:G:62:GLU:H	2.19	0.45
1:G:188:PRO:HA	1:G:194:SER:HA	1.99	0.45
1:G:228:PRO:HA	1:G:234:PHE:HA	1.97	0.45
1:C:112:LEU:O	1:C:113:ASN:C	2.55	0.45
1:E:46:GLU:HA	1:E:47:PRO:HD2	1.69	0.45
1:G:229:ASN:HD22	1:G:229:ASN:N	2.15	0.45
1:A:81:ALA:HB2	1:A:140:ARG:HD2	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:ALA:HB2	1:C:24:PHE:HD1	1.80	0.45
1:E:15:SER:HG	1:E:88:TYR:H	1.62	0.45
1:C:159:CYS:HB3	1:C:160:PRO:CD	2.44	0.45
1:C:203:PHE:HB2	1:C:256:HIS:NE2	2.32	0.45
2:F:56:PHE:C	2:F:63:TYR:HE2	2.21	0.45
1:A:200:ALA:O	1:A:235:HIS:ND1	2.50	0.44
1:E:174:LEU:H	1:E:174:LEU:HD22	1.81	0.44
1:A:98:LEU:HG	1:A:163:LEU:HD23	1.99	0.44
1:E:17:PRO:HG3	1:E:23:ALA:HB2	2.00	0.44
1:E:200:ALA:HB3	1:E:236:ALA:HB3	1.98	0.44
1:A:36:LEU:HD23	1:A:36:LEU:C	2.38	0.44
1:A:42:ARG:NH2	1:A:44:GLU:HB3	2.32	0.44
1:C:65:THR:HG22	1:C:69:ARG:NE	2.32	0.44
1:G:18:ALA:O	1:G:21:THR:HB	2.17	0.44
1:G:66:THR:HA	1:G:69:ARG:HD2	1.99	0.44
1:E:64:GLU:OE1	1:E:162:ARG:NH1	2.49	0.44
1:G:6:SER:O	1:G:31:GLY:N	2.51	0.44
2:B:26:TYR:CE1	2:B:63:TYR:HB2	2.52	0.44
2:H:31:HIS:HD2	2:H:62:PHE:CE2	2.36	0.44
1:A:201:PHE:CD1	2:B:14:PRO:HG3	2.52	0.44
1:A:253:ILE:HA	1:A:263:LEU:O	2.17	0.44
2:B:32:PRO:HB2	2:B:33:SER:H	1.63	0.44
1:C:7:LEU:HD11	1:C:9:TYR:CE1	2.51	0.44
1:C:244:SER:HA	1:C:247:GLU:OE1	2.17	0.44
1:E:178:GLU:HA	1:E:179:PRO:HD3	1.90	0.44
1:A:13:ALA:HB2	1:A:24:PHE:HD1	1.83	0.44
1:C:253:ILE:HD12	1:C:264:ARG:HG2	2.00	0.44
2:D:83:ASN:HA	2:D:87:LEU:HD12	1.99	0.44
1:G:10:HIS:O	1:G:26:VAL:HA	2.18	0.44
1:C:193:PHE:HA	1:C:242:VAL:O	2.18	0.43
1:E:242:VAL:HB	1:E:250:TYR:CE1	2.53	0.43
1:G:50:ALA:O	1:G:52:VAL:N	2.51	0.43
1:G:67:ASP:OD2	1:G:162:ARG:NH2	2.51	0.43
1:C:228:PRO:HA	1:C:234:PHE:HA	1.99	0.43
1:E:109:LYS:HA	1:E:109:LYS:HD3	1.74	0.43
1:G:178:GLU:HA	1:G:179:PRO:HD2	1.87	0.43
2:H:21:ASN:N	2:H:70:PHE:O	2.50	0.43
1:A:29:TRP:HA	1:A:33:GLN:O	2.18	0.43
1:A:54:GLU:O	1:A:56:GLN:N	2.51	0.43
2:B:70:PHE:CE2	2:B:72:PRO:HB3	2.54	0.43
1:E:243:LYS:O	1:E:246:ASP:HB3	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:132:PRO:O	1:G:136:ALA:N	2.51	0.43
1:A:112:LEU:HB2	1:A:117:PHE:CZ	2.53	0.43
2:B:58:LYS:C	2:B:60:TRP:H	2.21	0.43
1:C:17:PRO:HG3	1:C:23:ALA:HB2	2.00	0.43
1:A:93:LEU:HD13	2:B:56:PHE:HE1	1.84	0.43
1:C:224:GLY:O	1:C:225:ASP:HB2	2.18	0.43
1:A:89:THR:O	1:A:112:LEU:HD12	2.18	0.43
2:B:31:HIS:O	2:B:84:HIS:HE1	2.01	0.43
1:E:8:LEU:HD23	1:E:95:GLY:HA3	2.00	0.43
1:E:214:ARG:O	1:E:215:ASN:C	2.57	0.43
1:G:98:LEU:HG	1:G:163:LEU:CD2	2.48	0.43
1:G:210:LEU:HD22	1:G:252:CYS:SG	2.59	0.43
1:E:223:GLN:O	1:E:238:SER:HA	2.19	0.43
2:D:84:HIS:H	2:D:87:LEU:HD12	1.84	0.43
1:G:117:PHE:CD2	1:G:134:ALA:HB2	2.54	0.43
1:C:169:ARG:H	1:C:169:ARG:HG3	1.66	0.43
1:A:214:ARG:O	1:A:215:ASN:C	2.57	0.42
2:D:17:ASN:ND2	2:D:74:GLU:HB2	2.34	0.42
1:E:256:HIS:CD2	1:E:258:GLY:H	2.36	0.42
1:G:133:GLU:HA	1:G:136:ALA:CB	2.46	0.42
1:C:247:GLU:CD	1:C:247:GLU:N	2.62	0.42
1:A:165:GLU:O	1:A:168:GLU:N	2.52	0.42
1:C:167:LEU:HG	1:C:167:LEU:O	2.20	0.42
1:C:186:ALA:HB2	1:C:196:LEU:CD2	2.49	0.42
1:E:77:GLU:HG3	1:E:140:ARG:HH21	1.83	0.42
2:F:56:PHE:C	2:F:63:TYR:CE2	2.93	0.42
1:A:201:PHE:HB3	2:B:12:ARG:O	2.19	0.42
1:A:206:PRO:O	1:A:208:LEU:N	2.52	0.42
1:G:203:PHE:HB2	1:G:256:HIS:CE1	2.54	0.42
2:H:13:HIS:HB3	2:H:14:PRO:HD2	2.01	0.42
1:A:47:PRO:HG3	1:A:61:TRP:CE2	2.54	0.42
2:B:31:HIS:ND1	2:B:32:PRO:HA	2.35	0.42
1:C:174:LEU:C	1:C:176:TRP:H	2.23	0.42
1:E:231:ASP:OD1	1:E:233:SER:OG	2.34	0.42
1:G:59:TRP:O	1:G:63:LYS:HB2	2.20	0.42
1:G:155:LEU:O	1:G:159:CYS:HB3	2.19	0.42
1:A:159:CYS:CB	1:A:160:PRO:HD3	2.43	0.42
2:B:9:VAL:HG11	2:B:95:TRP:HB2	2.02	0.42
1:C:42:ARG:C	1:C:44:GLU:H	2.22	0.42
1:E:53:TRP:HA	1:E:53:TRP:CE3	2.54	0.42
2:F:27:VAL:CG2	2:F:82:VAL:HG21	2.50	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:56:GLN:HE21	1:C:166:HIS:CE1	2.38	0.42
1:C:68:LEU:O	1:C:71:LYS:HB2	2.20	0.42
1:A:22:PRO:HA	1:A:41:LEU:HD13	2.02	0.41
1:C:11:LEU:HD11	1:C:94:LEU:HD22	2.01	0.41
1:C:66:THR:O	1:C:70:ILE:HG13	2.20	0.41
1:A:65:THR:H	1:A:65:THR:HG1	1.53	0.41
1:G:154:PHE:HA	1:G:158:SER:OG	2.20	0.41
1:G:180:PRO:HB3	1:G:203:PHE:HB3	2.03	0.41
1:A:8:LEU:HD23	1:A:94:LEU:O	2.21	0.41
2:B:84:HIS:HB3	2:B:87:LEU:HG	2.02	0.41
1:C:33:GLN:OE1	1:C:51:TRP:CZ2	2.73	0.41
1:G:38:TYR:OH	1:G:69:ARG:CG	2.69	0.41
1:C:135:LEU:HD23	1:C:135:LEU:HA	1.90	0.41
1:C:152:LEU:O	1:C:156:LEU:HB2	2.20	0.41
2:D:44:GLU:O	2:D:45:ARG:C	2.59	0.41
3:I:5:GLY:C	3:I:7:PHE:N	2.73	0.41
1:A:171:ARG:HA	1:A:174:LEU:HD23	2.02	0.41
1:C:38:TYR:CD2	1:C:38:TYR:C	2.94	0.41
1:C:110:PHE:N	1:C:110:PHE:CD1	2.88	0.41
2:H:39:LEU:HB3	2:H:46:ILE:HD12	2.02	0.41
1:E:161:HIS:ND1	1:E:165:GLU:OE2	2.53	0.41
1:E:213:LEU:HD23	1:E:218:ALA:HA	2.03	0.41
1:A:118:MET:HA	1:A:128:GLY:O	2.21	0.41
1:E:93:LEU:HD13	2:F:56:PHE:HE1	1.85	0.41
1:G:96:CYS:SG	1:G:160:PRO:HD3	2.61	0.41
1:A:138:SER:O	1:A:142:GLN:HG2	2.21	0.41
2:D:21:ASN:CG	2:D:22:PHE:H	2.24	0.41
1:E:173:ASN:O	1:E:176:TRP:HB3	2.21	0.41
1:G:54:GLU:OE1	1:G:56:GLN:NE2	2.54	0.41
1:C:18:ALA:O	1:C:21:THR:HB	2.20	0.41
1:E:78:ALA:C	1:E:80:LYS:H	2.24	0.41
2:F:17:ASN:HA	2:F:72:PRO:O	2.21	0.41
1:G:252:CYS:HB3	1:G:265:VAL:HB	2.03	0.41
2:H:37:VAL:HG13	2:H:82:VAL:HG22	2.02	0.41
2:D:97:ARG:O	2:D:98:ASP:HB2	2.21	0.41
1:G:72:GLU:C	1:G:74:LEU:N	2.75	0.41
1:C:91:GLN:NE2	2:D:60:TRP:HB3	2.36	0.40
1:E:6:SER:HA	1:E:97:GLU:HB3	2.03	0.40
1:E:36:LEU:HD12	1:E:61:TRP:HZ3	1.86	0.40
2:H:59:ASP:OD1	2:H:59:ASP:C	2.60	0.40
1:A:205:PRO:CB	1:A:206:PRO:HD2	2.51	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:204:TYR:CD2	1:C:205:PRO:HA	2.56	0.40
1:E:235:HIS:CG	1:E:236:ALA:N	2.89	0.40
2:B:50:GLU:HB3	2:B:67:TYR:CZ	2.57	0.40
1:G:203:PHE:HD2	1:G:256:HIS:HE1	1.69	0.40
1:A:149:ASN:C	1:A:151:GLU:N	2.72	0.40
1:A:174:LEU:C	1:A:176:TRP:N	2.75	0.40
2:B:10:TYR:CE2	2:B:24:ASN:HB2	2.57	0.40
1:C:122:LEU:HD12	1:C:122:LEU:H	1.86	0.40
1:E:186:ALA:HA	1:E:195:VAL:O	2.22	0.40
1:G:56:GLN:HA	1:G:56:GLN:OE1	2.21	0.40
3:J:109:SAR:HA3	3:J:110:MLE:HN1	1.78	0.40
1:C:116:GLU:HB2	2:D:60:TRP:HE1	1.86	0.40
1:C:214:ARG:HA	1:C:250:TYR:HA	2.03	0.40
1:G:50:ALA:C	1:G:52:VAL:H	2.25	0.40
1:G:77:GLU:OE2	1:G:140:ARG:NH2	2.54	0.40
1:G:173:ASN:O	1:G:176:TRP:HB3	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	261/267 (98%)	215 (82%)	39 (15%)	7 (3%)	5	25
1	C	261/267 (98%)	213 (82%)	38 (15%)	10 (4%)	3	19
1	E	261/267 (98%)	219 (84%)	33 (13%)	9 (3%)	3	21
1	G	261/267 (98%)	224 (86%)	30 (12%)	7 (3%)	5	25
2	B	97/99 (98%)	84 (87%)	12 (12%)	1 (1%)	15	49
2	D	97/99 (98%)	82 (84%)	14 (14%)	1 (1%)	15	49
2	F	97/99 (98%)	84 (87%)	12 (12%)	1 (1%)	15	49

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	97/99 (98%)	81 (84%)	14 (14%)	2 (2%)	7	30
3	I	7/16 (44%)	6 (86%)	1 (14%)	0	100	100
3	J	7/16 (44%)	5 (71%)	2 (29%)	0	100	100
All	All	1446/1496 (97%)	1213 (84%)	195 (14%)	38 (3%)	5	26

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	ASN
1	C	58	SER
1	C	215	ASN
1	G	58	SER
1	G	202	SER
1	A	100	PRO
1	A	207	GLU
1	C	202	SER
1	C	225	ASP
1	E	59	TRP
1	E	100	PRO
1	E	166	HIS
1	E	175	GLU
1	E	193	PHE
1	G	189	SER
2	H	98	ASP
1	A	175	GLU
1	A	191	PRO
1	C	65	THR
1	C	113	ASN
2	D	45	ARG
1	E	58	SER
1	E	215	ASN
1	G	51	TRP
1	G	113	ASN
1	A	58	SER
1	A	215	ASN
1	C	38	TYR
1	C	57	VAL
1	C	219	ALA
1	E	116	GLU
2	F	14	PRO
2	B	32	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	262	PRO
1	G	57	VAL
1	G	262	PRO
1	E	180	PRO
2	H	72	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	186/220 (84%)	163 (88%)	23 (12%)	4	19
1	C	186/220 (84%)	163 (88%)	23 (12%)	4	19
1	E	186/220 (84%)	165 (89%)	21 (11%)	6	23
1	G	186/220 (84%)	168 (90%)	18 (10%)	8	30
2	B	88/94 (94%)	78 (89%)	10 (11%)	5	23
2	D	88/94 (94%)	83 (94%)	5 (6%)	20	52
2	F	88/94 (94%)	77 (88%)	11 (12%)	4	18
2	H	88/94 (94%)	82 (93%)	6 (7%)	16	45
3	I	6/9 (67%)	5 (83%)	1 (17%)	2	9
3	J	7/9 (78%)	7 (100%)	0	100	100
All	All	1109/1274 (87%)	991 (89%)	118 (11%)	6	26

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	27	SER
1	A	30	LEU
1	A	41	LEU
1	A	62	GLU
1	A	65	THR
1	A	71	LYS
1	A	80	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	94	LEU
1	A	105	VAL
1	A	117	PHE
1	A	133	GLU
1	A	140	ARG
1	A	155	LEU
1	A	183	ARG
1	A	198	CYS
1	A	202	SER
1	A	225	ASP
1	A	226	PHE
1	A	247	GLU
1	A	251	CYS
1	A	259	LEU
1	A	261	GLN
2	B	2	GLN
2	B	28	SER
2	B	34	ASP
2	B	35	ILE
2	B	42	ASN
2	B	50	GLU
2	B	54	LEU
2	B	64	LEU
2	B	70	PHE
2	B	81	ARG
1	C	7	LEU
1	C	21	THR
1	C	33	GLN
1	C	41	LEU
1	C	66	THR
1	C	67	ASP
1	C	80	LYS
1	C	82	LEU
1	C	94	LEU
1	C	98	LEU
1	C	103	THR
1	C	126	THR
1	C	130	ASP
1	C	168	GLU
1	C	174	LEU
1	C	181	SER
1	C	183	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	195	VAL
1	C	221	THR
1	C	229	ASN
1	C	230	SER
1	C	241	THR
1	C	251	CYS
2	D	33	SER
2	D	55	SER
2	D	61	SER
2	D	64	LEU
2	D	92	ILE
1	E	21	THR
1	E	26	VAL
1	E	36	LEU
1	E	38	TYR
1	E	65	THR
1	E	80	LYS
1	E	82	LEU
1	E	94	LEU
1	E	103	THR
1	E	105	VAL
1	E	124	GLN
1	E	131	TRP
1	E	158	SER
1	E	161	HIS
1	E	168	GLU
1	E	173	ASN
1	E	174	LEU
1	E	183	ARG
1	E	208	LEU
1	E	251	CYS
1	E	261	GLN
2	F	2	GLN
2	F	4	THR
2	F	28	SER
2	F	35	ILE
2	F	38	ASP
2	F	47	GLU
2	F	81	ARG
2	F	85	VAL
2	F	89	GLN
2	F	92	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	97	ARG
1	G	7	LEU
1	G	8	LEU
1	G	27	SER
1	G	34	GLN
1	G	41	LEU
1	G	48	CYS
1	G	62	GLU
1	G	71	LYS
1	G	82	LEU
1	G	126	THR
1	G	131	TRP
1	G	133	GLU
1	G	140	ARG
1	G	158	SER
1	G	183	ARG
1	G	221	THR
1	G	241	THR
1	G	248	HIS
2	H	51	HIS
2	H	52	SER
2	H	55	SER
2	H	64	LEU
2	H	88	SER
2	H	99	MET
3	I	13	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	HIS
1	A	173	ASN
1	A	229	ASN
1	A	256	HIS
2	B	24	ASN
1	C	91	GLN
1	C	173	ASN
1	C	256	HIS
2	D	42	ASN
1	E	34	GLN
1	E	139	GLN
1	E	142	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	256	HIS
2	F	2	GLN
2	F	8	GLN
2	F	42	ASN
2	F	89	GLN
1	G	139	GLN
1	G	229	ASN
2	H	31	HIS
3	J	106	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 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	$\# Z > 2$
3	MLE	I	10	3	7,8,9	0.49	0	6,9,11	1.22	0
3	LE1	I	3	3	3,7,8	0.84	0	3,10,12	1.55	0
3	SAR	J	109	3	4,4,5	0.65	0	1,3,5	1.80	0
3	SAR	I	9	3	4,4,5	0.56	0	1,3,5	1.95	0
3	MLE	J	110	3	7,8,9	0.49	0	6,9,11	1.20	0
3	LE1	J	103	3	3,7,8	0.78	0	3,10,12	1.22	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MLE	I	10	3	-	4/5/8/10	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LE1	I	3	3	-	0/4/8/10	-
3	SAR	J	109	3	-	1/1/2/3	-
3	SAR	I	9	3	-	1/1/2/3	-
3	MLE	J	110	3	-	1/5/8/10	-
3	LE1	J	103	3	-	3/4/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	9	SAR	C-CA-N-CN
3	J	103	LE1	C-CA-CB-C9
3	J	103	LE1	C-CA-CB-C8
3	J	103	LE1	N-CA-CB-C9
3	J	109	SAR	C-CA-N-CN
3	J	110	MLE	O-C-CA-CB
3	I	10	MLE	C-CA-CB-CG
3	I	10	MLE	CA-CB-CG-CD1
3	I	10	MLE	N-CA-CB-CG
3	I	10	MLE	CA-CB-CG-CD2

There are no ring outliers.

4 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	10	MLE	1	0
3	J	109	SAR	1	0
3	I	9	SAR	1	0
3	J	110	MLE	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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 ²)	Q < 0.9
1	A	263/267 (98%)	0.03	9 (3%)	45	24	93, 107, 114, 120	0
1	C	263/267 (98%)	0.13	12 (4%)	32	16	84, 110, 127, 132	0
1	E	263/267 (98%)	0.03	7 (2%)	54	31	87, 105, 115, 119	0
1	G	263/267 (98%)	0.11	14 (5%)	26	12	86, 112, 125, 131	0
2	B	99/99 (100%)	0.25	7 (7%)	16	6	112, 126, 145, 148	0
2	D	99/99 (100%)	0.22	4 (4%)	38	19	102, 114, 136, 147	0
2	F	99/99 (100%)	0.44	12 (12%)	4	1	110, 124, 141, 142	0
2	H	99/99 (100%)	0.13	4 (4%)	38	19	94, 111, 120, 127	0
3	I	8/16 (50%)	0.33	0	100	100	97, 99, 107, 109	0
3	J	9/16 (56%)	-0.10	0	100	100	102, 107, 111, 112	0
All	All	1465/1496 (97%)	0.13	69 (4%)	31	15	84, 110, 130, 148	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	75	PHE	5.2
1	G	264	ARG	4.8
1	C	128	GLY	4.4
2	H	82	VAL	4.3
2	F	9	VAL	4.2
2	B	78	TYR	4.2
2	F	65	LEU	3.9
1	G	45	ALA	3.8
1	E	30	LEU	3.8
2	F	64	LEU	3.8
2	F	1	ILE	3.7
2	B	23	LEU	3.5
1	G	145	ASP	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	170	GLY	3.3
2	B	8	GLN	3.3
2	B	25	CYS	3.2
1	E	44	GLU	3.2
2	F	33	SER	3.2
1	G	141	TRP	3.0
1	C	107	THR	3.0
1	C	178	GLU	3.0
2	F	78	TYR	2.9
1	G	61	TRP	2.9
2	D	39	LEU	2.8
1	E	75	PHE	2.8
2	D	5	PRO	2.8
1	A	24	PHE	2.8
1	C	141	TRP	2.7
1	A	90	LEU	2.7
1	C	191	PRO	2.7
1	A	25	TRP	2.7
2	D	15	ALA	2.7
1	E	79	PHE	2.7
2	D	86	THR	2.6
1	A	180	PRO	2.6
2	B	54	LEU	2.6
2	F	8	GLN	2.6
2	H	37	VAL	2.6
1	A	75	PHE	2.5
2	F	39	LEU	2.5
1	E	263	LEU	2.4
2	H	65	LEU	2.4
1	G	263	LEU	2.3
2	H	66	TYR	2.3
1	G	265	VAL	2.3
1	G	225	ASP	2.3
1	G	176	TRP	2.2
1	A	9	TYR	2.2
1	A	100	PRO	2.2
1	C	206	PRO	2.2
2	F	66	TYR	2.2
2	F	52	SER	2.2
1	C	210	LEU	2.2
2	F	40	LEU	2.2
1	E	184	LEU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	137	ILE	2.1
2	B	73	THR	2.1
1	A	184	LEU	2.1
1	C	51	TRP	2.1
1	G	8	LEU	2.1
1	C	254	VAL	2.1
1	C	11	LEU	2.0
1	E	219	ALA	2.0
1	C	8	LEU	2.0
2	B	93	VAL	2.0
2	F	93	VAL	2.0
1	G	127	TRP	2.0
1	A	30	LEU	2.0
1	G	173	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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, 95th 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(\AA^2)	Q<0.9
3	LE1	I	3	8/9	0.87	0.26	104,105,106,108	0
3	MLE	J	110	9/10	0.93	0.28	109,110,110,110	0
3	SAR	J	109	5/6	0.94	0.26	108,108,109,109	0
3	LE1	J	103	8/9	0.94	0.20	108,109,109,112	0
3	MLE	I	10	9/10	0.96	0.32	103,103,104,105	0
3	SAR	I	9	5/6	0.98	0.24	100,100,102,102	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.