



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 11:11 PM UTC

PDB ID : 5I9K / pdb_00005i9k
EMDB ID : EMD-8076
Title : The structure of microsomal glutathione transferase 1
Authors : Kuang, Q.; Purhonen, P.; Jegerschold, C.; Morgenstern, R.; Hebert, H.
Deposited on : 2016-02-20
Resolution : 3.50 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB/EMDB entry.

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

A user guide is available at

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

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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

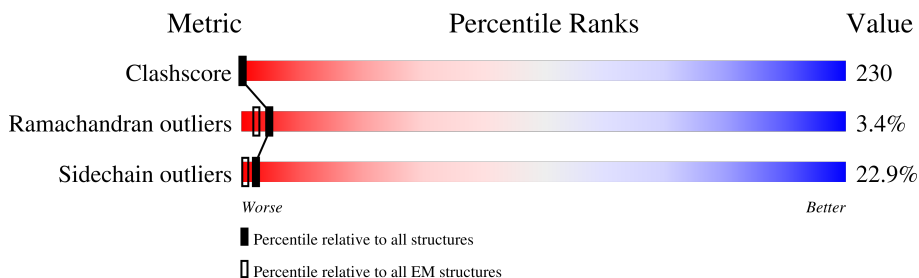
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON CRYSTALLOGRAPHY

The reported resolution of this entry is 3.50 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)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	155	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PC1	A	202	X	-	X	-
3	PC1	A	203	X	-	-	-
4	PLM	A	204	-	-	X	-
4	PLM	A	205	-	-	X	-

2 Entry composition [i](#)

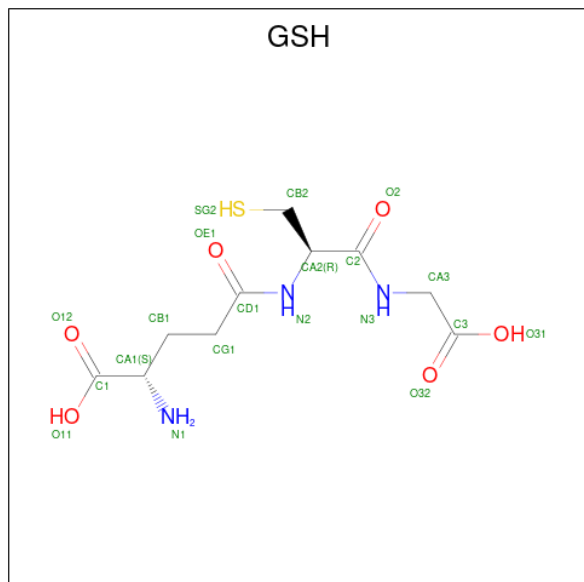
There are 4 unique types of molecules in this entry. The entry contains 1132 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Microsomal glutathione S-transferase 1.

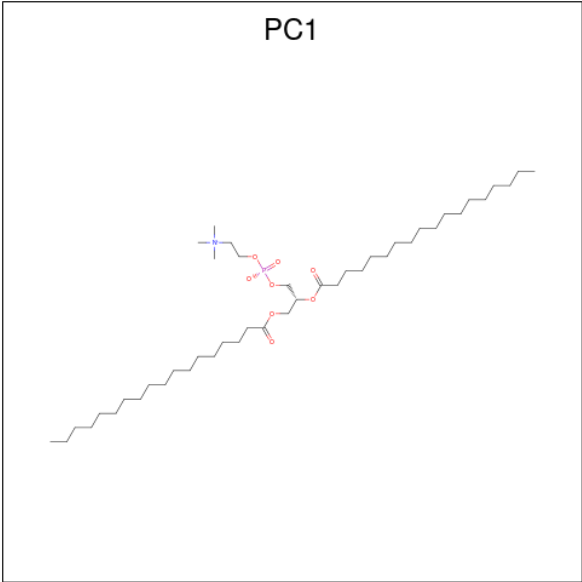
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	123	984	644	169	167	4	0	0

- Molecule 2 is GLUTATHIONE (CCD ID: GSH) (formula: C₁₀H₁₇N₃O₆S).



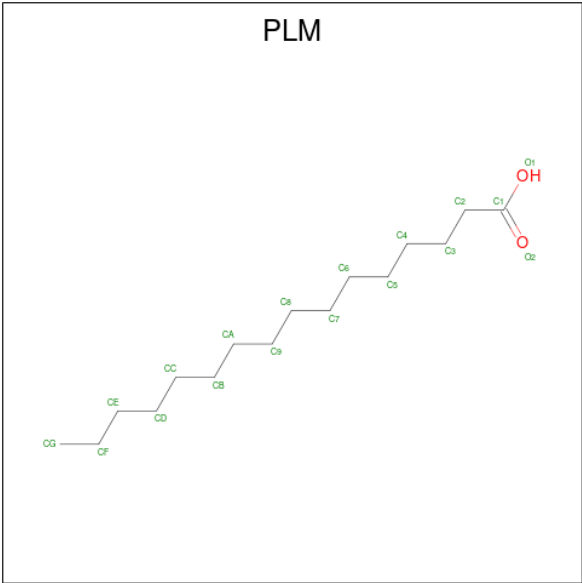
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
2	A	1	20	10	3	6	1	0

- Molecule 3 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: C₄₄H₈₈NO₈P).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			54	44	1	8	1	
3	A	1	Total	C	N	O	P	0
			54	44	1	8	1	

- Molecule 4 is PALMITIC ACID (CCD ID: PLM) (formula: C₁₆H₃₂O₂).



Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	C	0
			10	10	
4	A	1	Total	C	0
			10	10	

3 Residue-property plots

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. 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. 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: Microsomal glutathione S-transferase 1



4 Experimental information

Property	Value	Source
EM reconstruction method	CRYSTALLOGRAPHY	Depositor
Imposed symmetry	2D CRYSTAL, $a=81.8 \text{ \AA}$, $b=81.8 \text{ \AA}$, $c=100.0 \text{ \AA}$, $\gamma=120.0^\circ$, space group=P 6	Depositor
Number of images used	Not provided	
Resolution determination method	DIFFRACTION PATTERN/LAYERLINES	Depositor
CTF correction method	NONE	Depositor
Microscope	JEOL 2100F	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	TVIPS TEMCAM-F415 (4k x 4k)	Depositor

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: PLM, PC1, GSH

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	1.37	5/1005 (0.5%)	1.92	35/1360 (2.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	143	SER	N-CA	6.45	1.53	1.46
1	A	93	TYR	N-CA	6.21	1.54	1.46
1	A	147	ARG	CA-C	5.46	1.60	1.52
1	A	78	ASN	N-CA	5.13	1.52	1.46
1	A	23	ILE	CA-CB	5.04	1.61	1.54

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	12	VAL	N-CA-C	12.36	123.34	110.36
1	A	32	SER	N-CA-C	-10.62	98.85	112.23
1	A	12	VAL	CB-CA-C	-10.29	98.72	111.88
1	A	92	LEU	N-CA-C	10.08	123.70	111.40
1	A	107	PHE	N-CA-C	-9.86	95.21	111.37
1	A	135	PHE	N-CA-C	-8.91	100.35	111.75
1	A	108	ARG	N-CA-C	8.38	121.16	111.11
1	A	13	LEU	N-CA-C	-8.37	102.10	111.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	16	PHE	N-CA-C	7.60	119.20	111.07
1	A	136	VAL	N-CA-C	7.59	117.56	110.42
1	A	89	ILE	CB-CA-C	-7.28	102.48	112.02
1	A	129	ASN	N-CA-C	-6.89	104.07	113.30
1	A	80	LEU	N-CA-C	-6.78	103.97	111.36
1	A	89	ILE	N-CA-C	6.77	116.89	110.53
1	A	150	ARG	N-CA-C	-6.66	104.02	111.28
1	A	24	LEU	N-CA-C	6.41	120.83	112.89
1	A	25	ALA	N-CA-C	-6.37	104.42	111.36
1	A	143	SER	N-CA-C	6.32	117.86	110.97
1	A	154	TYR	N-CA-C	-6.05	105.61	112.87
1	A	23	ILE	CB-CA-C	6.05	121.21	111.29
1	A	72	VAL	N-CA-C	-5.96	105.31	110.74
1	A	11	GLU	CA-C-N	5.87	128.17	120.60
1	A	11	GLU	C-N-CA	5.87	128.17	120.60
1	A	121	TYR	N-CA-C	5.74	123.02	110.80
1	A	77	LEU	N-CA-C	5.69	118.34	111.40
1	A	29	PHE	N-CA-C	-5.59	104.19	111.02
1	A	90	GLY	N-CA-C	-5.58	99.95	113.18
1	A	110	PHE	N-CA-C	-5.57	105.12	111.14
1	A	136	VAL	N-CA-CB	5.54	116.91	110.65
1	A	105	ILE	CB-CA-C	-5.46	102.34	111.29
1	A	22	ILE	N-CA-C	-5.35	98.21	109.34
1	A	75	ALA	N-CA-C	-5.24	105.26	110.97
1	A	31	SER	N-CA-C	5.21	117.75	111.40
1	A	127	GLN	N-CA-C	-5.19	103.05	109.64
1	A	114	ARG	N-CA-C	5.01	116.83	111.36

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	121	TYR	Peptide

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	984	0	1019	545	3
2	A	20	0	15	1	1
3	A	108	0	176	33	2
4	A	20	0	32	48	0
All	All	1132	0	1242	547	3

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 230.

All (547) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:PHE:CZ	1:A:94:SER:HA	1.37	1.55
1:A:122:LEU:CA	4:A:204:PLM:H21	1.51	1.40
1:A:34:THR:HB	1:A:72:VAL:CG1	1.53	1.37
1:A:27:MET:CE	1:A:83:ILE:HG21	1.58	1.32
1:A:91:LEU:O	1:A:94:SER:HB3	1.32	1.30
1:A:81:GLU:O	1:A:85:PRO:HD2	1.25	1.29
1:A:104:LEU:HA	1:A:107:PHE:CD2	1.66	1.29
1:A:108:ARG:O	1:A:111:VAL:HG12	1.36	1.24
1:A:106:HIS:HB3	1:A:144:MET:SD	1.77	1.23
1:A:122:LEU:HA	4:A:204:PLM:C2	1.68	1.23
1:A:114:ARG:HA	1:A:117:HIS:CD2	1.73	1.23
1:A:67:GLU:CG	1:A:125:LEU:HG	1.69	1.23
1:A:23:ILE:HD13	1:A:86:PHE:HE1	1.00	1.17
1:A:118:THR:HB	4:A:204:PLM:H51	1.19	1.17
1:A:37:GLN:O	1:A:40:THR:HG22	1.46	1.15
1:A:34:THR:HB	1:A:72:VAL:HG13	1.16	1.14
1:A:136:VAL:HG11	3:A:202:PC1:C3I	1.77	1.13
1:A:67:GLU:HG3	1:A:125:LEU:CG	1.77	1.13
1:A:67:GLU:HA	1:A:125:LEU:HD11	1.17	1.12
1:A:23:ILE:CD1	1:A:86:PHE:HE1	1.61	1.12
1:A:119:ILE:HG13	4:A:204:PLM:H62	1.29	1.12
1:A:89:ILE:CG1	4:A:205:PLM:H52	1.79	1.12
1:A:123:THR:H	1:A:124:PRO:HD2	1.12	1.12
1:A:121:TYR:CE1	1:A:129:ASN:HA	1.84	1.11
1:A:16:PHE:CZ	1:A:94:SER:CA	2.34	1.10
1:A:89:ILE:HG13	4:A:205:PLM:H52	1.11	1.10
1:A:122:LEU:HA	4:A:204:PLM:H21	1.13	1.08
1:A:91:LEU:O	1:A:94:SER:CB	2.00	1.07
1:A:136:VAL:CG1	3:A:202:PC1:H3I3	1.83	1.07
1:A:67:GLU:HG3	1:A:125:LEU:HG	1.26	1.07

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:LEU:CA	1:A:107:PHE:HD2	1.67	1.07
1:A:27:MET:HE1	1:A:83:ILE:HG21	1.07	1.06
1:A:34:THR:CB	1:A:72:VAL:HG13	1.83	1.06
1:A:81:GLU:O	1:A:85:PRO:CD	2.02	1.06
1:A:130:ARG:HA	1:A:134:PHE:CE1	1.91	1.06
1:A:104:LEU:HA	1:A:107:PHE:HD2	0.94	1.05
1:A:23:ILE:HD13	1:A:86:PHE:CE1	1.90	1.05
1:A:127:GLN:HG2	1:A:129:ASN:HD21	1.20	1.04
1:A:114:ARG:CA	1:A:117:HIS:HD2	1.70	1.04
1:A:136:VAL:HG12	3:A:202:PC1:H3G1	1.03	1.03
1:A:67:GLU:CA	1:A:125:LEU:HD11	1.89	1.02
1:A:26:LYS:O	1:A:30:LEU:HG	1.56	1.02
1:A:106:HIS:HB3	1:A:144:MET:CG	1.89	1.02
1:A:149:LEU:O	1:A:153:LEU:HG	1.58	1.01
1:A:114:ARG:HA	1:A:117:HIS:HD2	0.86	1.01
1:A:23:ILE:O	1:A:26:LYS:HB3	1.60	1.00
1:A:83:ILE:HD11	1:A:87:LEU:HD21	1.44	1.00
1:A:114:ARG:NH1	1:A:138:TYR:HD2	1.60	0.99
1:A:136:VAL:HG12	3:A:202:PC1:C3G	1.92	0.99
1:A:37:GLN:C	1:A:40:THR:HG22	1.87	0.99
1:A:118:THR:CB	4:A:204:PLM:H51	1.93	0.99
1:A:144:MET:O	1:A:148:LEU:HG	1.61	0.99
1:A:145:ALA:O	1:A:149:LEU:HG	1.63	0.99
1:A:67:GLU:HG3	1:A:125:LEU:CD1	1.90	0.98
1:A:93:TYR:CE2	1:A:149:LEU:HD22	1.97	0.98
1:A:141:THR:O	1:A:145:ALA:CB	2.11	0.98
1:A:136:VAL:CG1	3:A:202:PC1:H3G1	1.92	0.98
1:A:99:ASP:OD2	1:A:101:SER:N	1.97	0.98
1:A:34:THR:CB	1:A:72:VAL:CG1	2.41	0.98
1:A:71:ARG:CZ	1:A:123:THR:HB	1.95	0.97
1:A:71:ARG:HG3	1:A:125:LEU:HD21	1.46	0.97
1:A:142:LEU:O	1:A:146:TYR:HD1	1.47	0.96
1:A:16:PHE:CE1	1:A:94:SER:HA	2.00	0.96
1:A:121:TYR:HB3	4:A:204:PLM:H22	1.47	0.96
1:A:33:ALA:C	1:A:37:GLN:HE21	1.74	0.95
1:A:79:ASP:HA	1:A:82:ASN:ND2	1.82	0.95
1:A:37:GLN:HA	1:A:40:THR:CG2	1.97	0.95
1:A:116:TYR:CD1	3:A:203:PC1:H281	2.02	0.94
1:A:67:GLU:HG2	1:A:125:LEU:HG	1.49	0.94
1:A:34:THR:HB	1:A:72:VAL:HG12	1.46	0.94
1:A:37:GLN:CA	1:A:40:THR:HG22	1.98	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:ILE:HG13	4:A:205:PLM:C5	1.97	0.94
1:A:93:TYR:CZ	1:A:149:LEU:HA	2.02	0.94
1:A:38:ARG:HE	1:A:72:VAL:HG12	1.32	0.94
1:A:37:GLN:HA	1:A:40:THR:HG22	1.47	0.93
1:A:136:VAL:HG11	3:A:202:PC1:H3I3	0.95	0.93
1:A:150:ARG:O	1:A:154:TYR:HD1	1.50	0.93
1:A:106:HIS:CB	1:A:144:MET:SD	2.56	0.93
1:A:130:ARG:HA	1:A:134:PHE:CD1	2.05	0.92
1:A:140:VAL:CG2	3:A:202:PC1:H3D1	2.00	0.92
1:A:121:TYR:CZ	1:A:129:ASN:HA	2.05	0.91
1:A:30:LEU:O	1:A:34:THR:HG23	1.69	0.91
1:A:27:MET:CE	1:A:83:ILE:CG2	2.47	0.91
1:A:23:ILE:CD1	1:A:86:PHE:CE1	2.52	0.91
1:A:114:ARG:CA	1:A:117:HIS:CD2	2.51	0.90
1:A:119:ILE:CG1	4:A:204:PLM:H62	2.02	0.90
1:A:67:GLU:HA	1:A:125:LEU:CD1	2.02	0.89
1:A:118:THR:HB	4:A:204:PLM:C5	2.01	0.89
1:A:127:GLN:HG2	1:A:129:ASN:ND2	1.88	0.89
1:A:122:LEU:CB	4:A:204:PLM:H21	2.02	0.89
1:A:123:THR:H	1:A:124:PRO:CD	1.86	0.89
1:A:141:THR:O	1:A:145:ALA:HB2	1.70	0.88
1:A:18:SER:O	1:A:22:ILE:HG13	1.72	0.88
1:A:117:HIS:CE1	1:A:134:PHE:CE2	2.62	0.88
1:A:88:GLY:O	1:A:92:LEU:CD1	2.21	0.88
1:A:149:LEU:HD13	4:A:205:PLM:H61	1.56	0.87
1:A:142:LEU:O	1:A:146:TYR:CD1	2.26	0.87
1:A:38:ARG:NH2	1:A:73:ARG:HA	1.90	0.87
1:A:33:ALA:O	1:A:37:GLN:HG3	1.74	0.87
1:A:122:LEU:C	4:A:204:PLM:H21	1.99	0.87
1:A:38:ARG:HG3	1:A:72:VAL:HG11	1.57	0.86
1:A:121:TYR:CE1	1:A:129:ASN:CA	2.56	0.86
1:A:23:ILE:CG2	1:A:83:ILE:HD13	2.06	0.86
1:A:27:MET:SD	1:A:83:ILE:HG12	2.15	0.86
1:A:140:VAL:HG21	3:A:202:PC1:H3D1	1.56	0.86
1:A:27:MET:SD	1:A:83:ILE:CB	2.63	0.86
1:A:37:GLN:O	1:A:40:THR:CG2	2.24	0.85
1:A:142:LEU:HB3	1:A:146:TYR:HE1	1.41	0.85
1:A:106:HIS:CD2	1:A:148:LEU:CD2	2.60	0.85
1:A:106:HIS:HB3	1:A:144:MET:HG3	1.58	0.84
1:A:27:MET:SD	1:A:83:ILE:HB	2.17	0.84
1:A:38:ARG:HH22	1:A:73:ARG:HA	1.41	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:HIS:CE1	1:A:134:PHE:HE2	1.96	0.83
1:A:104:LEU:CA	1:A:107:PHE:CD2	2.52	0.83
1:A:119:ILE:HG13	4:A:204:PLM:C6	2.07	0.83
1:A:82:ASN:OD1	1:A:114:ARG:NH2	2.10	0.83
1:A:105:ILE:O	1:A:109:ILE:HG13	1.77	0.83
1:A:150:ARG:O	1:A:154:TYR:CD1	2.31	0.83
1:A:103:ALA:HA	1:A:106:HIS:CE1	2.13	0.83
1:A:111:VAL:O	1:A:115:ILE:HG12	1.78	0.83
1:A:142:LEU:C	1:A:146:TYR:HD1	1.87	0.83
1:A:140:VAL:CG2	3:A:202:PC1:C3D	2.57	0.83
1:A:150:ARG:HB3	1:A:154:TYR:CE1	2.12	0.82
1:A:114:ARG:HH12	1:A:138:TYR:HD2	0.83	0.82
1:A:16:PHE:HZ	1:A:94:SER:HA	1.35	0.82
1:A:150:ARG:HA	1:A:153:LEU:CD1	2.09	0.82
1:A:79:ASP:HA	1:A:82:ASN:CG	2.05	0.82
1:A:30:LEU:HD11	4:A:204:PLM:H92	1.60	0.82
1:A:118:THR:OG1	4:A:204:PLM:H71	1.78	0.82
1:A:42:LYS:HD2	1:A:69:VAL:HG23	1.62	0.81
1:A:130:ARG:HA	1:A:134:PHE:HE1	1.45	0.81
1:A:119:ILE:O	1:A:122:LEU:HB3	1.81	0.81
1:A:106:HIS:CB	1:A:144:MET:CG	2.59	0.81
1:A:114:ARG:NH1	1:A:138:TYR:N	2.28	0.80
1:A:114:ARG:NH1	1:A:138:TYR:HA	1.96	0.80
1:A:150:ARG:HA	1:A:153:LEU:HD12	1.64	0.80
1:A:12:VAL:O	1:A:16:PHE:HD2	1.65	0.80
1:A:41:ASN:HB3	1:A:68:LYS:HG3	1.64	0.79
1:A:38:ARG:HE	1:A:72:VAL:CG1	1.94	0.79
1:A:93:TYR:OH	1:A:153:LEU:HD21	1.81	0.79
1:A:106:HIS:O	1:A:107:PHE:C	2.24	0.79
1:A:15:ALA:CB	1:A:19:TYR:OH	2.30	0.79
1:A:108:ARG:O	1:A:111:VAL:CG1	2.27	0.79
1:A:67:GLU:CG	1:A:125:LEU:CG	2.47	0.79
1:A:114:ARG:O	1:A:117:HIS:CD2	2.36	0.79
1:A:22:ILE:O	1:A:23:ILE:C	2.26	0.79
1:A:140:VAL:HB	3:A:202:PC1:C3E	2.13	0.78
1:A:144:MET:O	1:A:148:LEU:CG	2.32	0.78
1:A:34:THR:OG1	1:A:76:HIS:NE2	2.15	0.78
1:A:90:GLY:O	1:A:91:LEU:C	2.24	0.78
1:A:138:TYR:O	1:A:142:LEU:HG	1.83	0.78
1:A:121:TYR:HB3	4:A:204:PLM:C2	2.14	0.77
1:A:12:VAL:O	1:A:16:PHE:CD2	2.37	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:MET:SD	1:A:83:ILE:CG1	2.73	0.77
1:A:104:LEU:O	1:A:108:ARG:HG3	1.84	0.77
1:A:106:HIS:HD2	1:A:148:LEU:CD2	1.96	0.77
1:A:133:ALA:O	1:A:136:VAL:HG23	1.83	0.77
1:A:140:VAL:HB	3:A:202:PC1:C3D	2.14	0.77
1:A:106:HIS:CD2	1:A:148:LEU:HD21	2.18	0.77
1:A:116:TYR:HD1	3:A:203:PC1:H281	1.50	0.77
1:A:81:GLU:HA	1:A:84:VAL:HB	1.67	0.77
1:A:15:ALA:CA	1:A:19:TYR:CZ	2.68	0.77
1:A:149:LEU:HD23	1:A:149:LEU:N	1.98	0.76
1:A:150:ARG:HA	1:A:154:TYR:HE1	1.50	0.76
1:A:15:ALA:HB1	1:A:19:TYR:CE2	2.19	0.76
1:A:71:ARG:NH1	1:A:123:THR:HB	2.00	0.76
1:A:106:HIS:CG	1:A:144:MET:SD	2.78	0.75
1:A:116:TYR:HE1	3:A:203:PC1:H262	1.49	0.75
1:A:117:HIS:ND1	1:A:134:PHE:CE2	2.55	0.75
1:A:33:ALA:C	1:A:37:GLN:NE2	2.44	0.75
1:A:24:LEU:O	1:A:28:MET:HB2	1.86	0.75
1:A:15:ALA:HA	1:A:19:TYR:CZ	2.21	0.75
1:A:106:HIS:CD2	1:A:148:LEU:HD22	2.22	0.75
1:A:106:HIS:HD2	1:A:148:LEU:HD21	1.52	0.74
1:A:119:ILE:HD11	4:A:204:PLM:H82	1.69	0.74
1:A:114:ARG:HH11	1:A:137:GLY:C	1.94	0.74
1:A:70:GLU:OE2	1:A:125:LEU:HD13	1.87	0.74
1:A:88:GLY:O	1:A:92:LEU:HD12	1.87	0.73
1:A:83:ILE:CD1	1:A:87:LEU:HD21	2.17	0.73
1:A:88:GLY:O	1:A:92:LEU:HG	1.88	0.73
1:A:142:LEU:HB3	1:A:146:TYR:CE1	2.23	0.73
1:A:15:ALA:HB1	1:A:19:TYR:OH	1.89	0.73
1:A:113:ALA:CB	1:A:140:VAL:HG11	2.20	0.72
1:A:71:ARG:HG3	1:A:125:LEU:CD2	2.19	0.72
1:A:107:PHE:HA	1:A:110:PHE:CE2	2.25	0.71
1:A:80:LEU:O	1:A:83:ILE:HG22	1.90	0.71
1:A:80:LEU:O	1:A:80:LEU:HD23	1.90	0.71
1:A:136:VAL:O	1:A:140:VAL:HG12	1.91	0.71
1:A:34:THR:O	1:A:38:ARG:HG3	1.89	0.71
1:A:140:VAL:HB	3:A:202:PC1:H3E1	1.71	0.71
1:A:20:ALA:O	1:A:24:LEU:N	2.20	0.71
1:A:78:ASN:ND2	1:A:117:HIS:HE1	1.89	0.71
1:A:149:LEU:O	1:A:153:LEU:CG	2.37	0.71
1:A:80:LEU:O	1:A:83:ILE:CG2	2.39	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:ILE:CD1	4:A:204:PLM:H82	2.21	0.71
1:A:125:LEU:N	1:A:126:PRO:HD2	2.05	0.71
1:A:38:ARG:CG	1:A:72:VAL:HG11	2.21	0.70
1:A:114:ARG:HH22	1:A:138:TYR:HE2	1.37	0.70
1:A:114:ARG:NH1	1:A:138:TYR:CA	2.54	0.70
1:A:76:HIS:HB3	1:A:77:LEU:HD12	1.73	0.70
1:A:16:PHE:CE1	1:A:94:SER:CA	2.70	0.70
1:A:93:TYR:CE1	1:A:149:LEU:O	2.45	0.69
1:A:144:MET:O	1:A:148:LEU:CD1	2.39	0.69
1:A:15:ALA:HA	1:A:19:TYR:OH	1.91	0.69
1:A:27:MET:HE1	1:A:83:ILE:CG2	2.03	0.69
1:A:42:LYS:CG	1:A:66:ASP:HB3	2.23	0.69
1:A:82:ASN:CG	1:A:114:ARG:HH21	2.01	0.69
1:A:90:GLY:O	1:A:92:LEU:N	2.25	0.69
1:A:119:ILE:O	1:A:122:LEU:HD22	1.92	0.69
1:A:123:THR:N	1:A:124:PRO:HD2	1.98	0.69
1:A:114:ARG:HH11	1:A:138:TYR:N	1.88	0.68
1:A:38:ARG:O	1:A:41:ASN:O	2.11	0.68
1:A:106:HIS:O	1:A:107:PHE:O	2.11	0.68
1:A:146:TYR:O	1:A:150:ARG:HD2	1.93	0.67
1:A:121:TYR:O	1:A:124:PRO:CG	2.42	0.67
1:A:153:LEU:HD12	1:A:154:TYR:CE1	2.30	0.67
1:A:99:ASP:OD2	1:A:99:ASP:C	2.36	0.67
1:A:121:TYR:HE1	1:A:129:ASN:CA	2.08	0.67
1:A:37:GLN:HA	1:A:40:THR:HG21	1.77	0.67
1:A:72:VAL:O	1:A:73:ARG:C	2.38	0.67
1:A:15:ALA:HB1	1:A:19:TYR:CZ	2.29	0.67
1:A:78:ASN:O	1:A:82:ASN:OD1	2.13	0.67
1:A:85:PRO:O	1:A:86:PHE:C	2.33	0.67
1:A:106:HIS:CB	1:A:144:MET:HG3	2.21	0.67
1:A:41:ASN:OD1	1:A:68:LYS:NZ	2.19	0.67
1:A:38:ARG:NH2	1:A:73:ARG:CA	2.58	0.67
1:A:83:ILE:HD11	1:A:87:LEU:CD2	2.23	0.67
1:A:32:SER:O	1:A:35:ALA:HB3	1.95	0.66
1:A:96:SER:O	1:A:152:ARG:HB3	1.95	0.66
1:A:15:ALA:C	1:A:19:TYR:CE2	2.74	0.66
1:A:82:ASN:HB3	1:A:114:ARG:HE	1.60	0.66
1:A:67:GLU:CG	1:A:125:LEU:CD1	2.71	0.66
1:A:121:TYR:HB3	1:A:122:LEU:HA	1.76	0.66
1:A:140:VAL:HG23	3:A:202:PC1:H3D2	1.78	0.66
1:A:11:GLU:O	1:A:14:MET:HB3	1.95	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:MET:SD	1:A:83:ILE:HG21	2.35	0.66
1:A:70:GLU:O	1:A:74:ARG:N	2.26	0.65
1:A:67:GLU:O	1:A:125:LEU:HD21	1.97	0.65
1:A:34:THR:O	1:A:35:ALA:C	2.40	0.65
1:A:143:SER:OG	1:A:144:MET:HE2	1.98	0.64
1:A:15:ALA:CA	1:A:19:TYR:OH	2.45	0.64
1:A:67:GLU:HG3	1:A:125:LEU:HD12	1.78	0.64
1:A:76:HIS:O	1:A:80:LEU:N	2.30	0.64
1:A:83:ILE:O	1:A:87:LEU:HG	1.98	0.64
1:A:70:GLU:O	1:A:74:ARG:HB2	1.97	0.64
1:A:38:ARG:NE	1:A:72:VAL:HG12	2.10	0.64
1:A:136:VAL:HG11	3:A:202:PC1:C3H	2.28	0.64
1:A:41:ASN:O	1:A:42:LYS:CB	2.46	0.63
1:A:89:ILE:O	1:A:93:TYR:HD2	1.81	0.63
1:A:121:TYR:HD2	4:A:204:PLM:C1	2.11	0.63
1:A:88:GLY:O	1:A:92:LEU:CG	2.45	0.63
1:A:122:LEU:HB2	4:A:204:PLM:C4	2.29	0.63
1:A:140:VAL:CB	3:A:202:PC1:C3D	2.76	0.63
1:A:87:LEU:O	1:A:91:LEU:HB2	1.98	0.63
1:A:122:LEU:HA	4:A:204:PLM:H22	1.72	0.63
1:A:40:THR:HG23	1:A:41:ASN:N	2.13	0.63
1:A:26:LYS:HE3	1:A:115:ILE:CG2	2.28	0.63
1:A:122:LEU:CA	4:A:204:PLM:C2	2.38	0.63
1:A:80:LEU:HD23	1:A:80:LEU:C	2.24	0.62
1:A:34:THR:HG1	1:A:76:HIS:CE1	2.17	0.62
1:A:150:ARG:CB	1:A:154:TYR:CE1	2.81	0.62
1:A:114:ARG:C	1:A:117:HIS:CD2	2.78	0.62
1:A:93:TYR:CE1	1:A:153:LEU:HD23	2.35	0.62
1:A:113:ALA:HB3	1:A:140:VAL:HG11	1.81	0.61
1:A:24:LEU:O	1:A:28:MET:CB	2.48	0.61
1:A:114:ARG:HH12	1:A:138:TYR:CA	2.12	0.61
1:A:140:VAL:CG2	3:A:202:PC1:H3D2	2.29	0.61
1:A:122:LEU:O	1:A:122:LEU:HD12	2.00	0.61
1:A:93:TYR:HE2	1:A:149:LEU:HD22	1.63	0.61
1:A:140:VAL:HG23	3:A:202:PC1:C3D	2.30	0.61
1:A:114:ARG:HH12	1:A:138:TYR:HA	1.59	0.61
1:A:42:LYS:HZ3	1:A:69:VAL:HG22	1.65	0.60
1:A:83:ILE:O	1:A:84:VAL:C	2.42	0.60
1:A:150:ARG:CA	1:A:154:TYR:CE1	2.84	0.60
1:A:86:PHE:CZ	1:A:110:PHE:HZ	2.19	0.60
1:A:93:TYR:HE1	1:A:153:LEU:HD23	1.64	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:LEU:O	1:A:107:PHE:HB2	2.01	0.60
1:A:115:ILE:HG13	1:A:116:TYR:H	1.67	0.60
1:A:141:THR:O	1:A:145:ALA:HB3	1.97	0.60
1:A:140:VAL:O	1:A:141:THR:C	2.45	0.60
1:A:29:PHE:O	1:A:33:ALA:HB2	2.01	0.60
1:A:142:LEU:C	1:A:146:TYR:CD1	2.74	0.60
1:A:30:LEU:CD1	4:A:204:PLM:H92	2.29	0.59
1:A:119:ILE:O	1:A:122:LEU:CD2	2.51	0.59
1:A:129:ASN:O	1:A:134:PHE:CE1	2.55	0.59
1:A:136:VAL:CG1	3:A:202:PC1:C3G	2.68	0.59
1:A:38:ARG:NE	1:A:72:VAL:CG1	2.65	0.59
1:A:127:GLN:HA	1:A:129:ASN:OD1	2.02	0.59
1:A:15:ALA:O	1:A:18:SER:OG	2.19	0.59
1:A:114:ARG:HG2	1:A:137:GLY:HA3	1.84	0.59
1:A:121:TYR:CD2	4:A:204:PLM:C1	2.86	0.59
1:A:133:ALA:O	1:A:136:VAL:CG2	2.50	0.59
1:A:114:ARG:HG2	1:A:137:GLY:CA	2.33	0.59
1:A:91:LEU:O	1:A:94:SER:HB2	1.97	0.59
1:A:27:MET:SD	1:A:83:ILE:CG2	2.90	0.58
1:A:150:ARG:CA	1:A:154:TYR:HE1	2.14	0.58
1:A:151:SER:O	1:A:155:LEU:HG	2.03	0.58
1:A:104:LEU:HD12	1:A:105:ILE:N	2.19	0.58
1:A:150:ARG:HA	1:A:154:TYR:CE1	2.34	0.58
1:A:23:ILE:O	1:A:26:LYS:CB	2.46	0.58
1:A:34:THR:CA	1:A:72:VAL:HG13	2.34	0.58
1:A:106:HIS:ND1	1:A:106:HIS:N	2.51	0.58
1:A:145:ALA:C	1:A:149:LEU:HG	2.29	0.58
1:A:78:ASN:HD21	1:A:117:HIS:HE1	1.50	0.57
1:A:119:ILE:CG1	4:A:204:PLM:H82	2.34	0.57
1:A:71:ARG:NE	1:A:123:THR:O	2.37	0.57
1:A:41:ASN:O	1:A:42:LYS:HB2	2.02	0.57
1:A:119:ILE:HA	4:A:204:PLM:H42	1.86	0.57
1:A:78:ASN:HD21	1:A:117:HIS:CE1	2.22	0.57
1:A:15:ALA:CB	1:A:19:TYR:CZ	2.88	0.56
1:A:136:VAL:CG1	3:A:202:PC1:C3I	2.61	0.56
1:A:122:LEU:HB2	4:A:204:PLM:H21	1.84	0.56
1:A:136:VAL:CG1	3:A:202:PC1:C3H	2.83	0.56
1:A:105:ILE:HD11	3:A:202:PC1:H251	1.88	0.56
1:A:116:TYR:CE1	3:A:203:PC1:H281	2.40	0.56
1:A:117:HIS:CE1	1:A:134:PHE:CD2	2.93	0.56
1:A:142:LEU:CB	1:A:146:TYR:HE1	2.16	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:GLU:OE1	1:A:74:ARG:NH2	2.38	0.56
1:A:105:ILE:CG2	1:A:109:ILE:HD11	2.35	0.56
1:A:23:ILE:HG12	1:A:86:PHE:CD1	2.40	0.56
1:A:122:LEU:HB2	4:A:204:PLM:H42	1.87	0.56
1:A:29:PHE:O	1:A:33:ALA:CB	2.54	0.56
1:A:26:LYS:HE3	1:A:115:ILE:HG22	1.87	0.56
1:A:76:HIS:CB	1:A:77:LEU:HD12	2.36	0.56
1:A:93:TYR:HE1	1:A:153:LEU:CD2	2.19	0.55
1:A:74:ARG:NH2	1:A:125:LEU:O	2.39	0.55
1:A:122:LEU:CD1	1:A:123:THR:HG23	2.36	0.55
1:A:23:ILE:HG23	1:A:83:ILE:HD13	1.84	0.55
1:A:23:ILE:HG21	1:A:83:ILE:HD13	1.84	0.55
1:A:119:ILE:HG13	4:A:204:PLM:H82	1.87	0.55
1:A:121:TYR:O	1:A:124:PRO:HG2	2.06	0.55
1:A:66:ASP:O	1:A:67:GLU:C	2.49	0.55
1:A:121:TYR:CE1	1:A:129:ASN:C	2.84	0.55
1:A:22:ILE:O	1:A:24:LEU:N	2.40	0.55
1:A:30:LEU:O	1:A:34:THR:CG2	2.48	0.55
1:A:117:HIS:ND1	1:A:134:PHE:CD2	2.75	0.55
1:A:41:ASN:O	1:A:42:LYS:CG	2.55	0.55
1:A:105:ILE:HD11	3:A:202:PC1:C25	2.36	0.55
1:A:150:ARG:HA	1:A:153:LEU:HD11	1.89	0.55
1:A:106:HIS:HB2	1:A:144:MET:HB3	1.89	0.54
1:A:93:TYR:CE1	1:A:153:LEU:CD2	2.90	0.54
1:A:93:TYR:HE1	1:A:149:LEU:O	1.91	0.54
1:A:117:HIS:ND1	1:A:118:THR:N	2.55	0.54
1:A:33:ALA:HB1	1:A:37:GLN:NE2	2.22	0.54
1:A:104:LEU:C	1:A:108:ARG:HG3	2.32	0.54
1:A:77:LEU:HD11	2:A:201:GSH:O11	2.08	0.54
1:A:86:PHE:C	1:A:86:PHE:CD2	2.86	0.54
1:A:143:SER:O	1:A:147:ARG:HG2	2.08	0.54
1:A:89:ILE:O	1:A:93:TYR:CD2	2.61	0.54
1:A:16:PHE:CE1	1:A:94:SER:CB	2.91	0.53
1:A:86:PHE:CE1	1:A:110:PHE:HZ	2.26	0.53
1:A:66:ASP:O	1:A:69:VAL:N	2.25	0.53
1:A:70:GLU:CD	1:A:125:LEU:HD22	2.32	0.53
1:A:77:LEU:O	1:A:81:GLU:HG2	2.08	0.53
1:A:34:THR:CA	1:A:72:VAL:CG1	2.86	0.53
1:A:70:GLU:O	1:A:74:ARG:CB	2.56	0.53
1:A:81:GLU:O	1:A:82:ASN:C	2.52	0.53
1:A:40:THR:CG2	1:A:41:ASN:N	2.70	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:ASN:O	1:A:42:LYS:HG3	2.08	0.53
1:A:111:VAL:CG1	1:A:112:GLY:N	2.71	0.53
1:A:118:THR:O	4:A:204:PLM:H22	2.07	0.53
1:A:42:LYS:HD2	1:A:66:ASP:HB3	1.90	0.53
1:A:121:TYR:OH	1:A:128:PRO:O	2.21	0.53
1:A:19:TYR:O	1:A:23:ILE:HD12	2.09	0.53
1:A:121:TYR:CE1	1:A:128:PRO:O	2.61	0.53
1:A:70:GLU:CD	1:A:125:LEU:HD13	2.34	0.52
1:A:83:ILE:HG13	1:A:87:LEU:HD11	1.92	0.52
1:A:117:HIS:HE1	1:A:134:PHE:HE2	1.50	0.52
1:A:80:LEU:HD23	1:A:84:VAL:HG23	1.91	0.52
1:A:121:TYR:CE2	1:A:124:PRO:O	2.63	0.52
1:A:78:ASN:ND2	1:A:117:HIS:CE1	2.76	0.52
1:A:42:LYS:NZ	1:A:69:VAL:HG22	2.24	0.52
1:A:100:LEU:HD12	1:A:100:LEU:O	2.10	0.52
1:A:23:ILE:HG21	1:A:83:ILE:CD1	2.40	0.52
1:A:75:ALA:O	1:A:76:HIS:C	2.53	0.52
1:A:104:LEU:O	1:A:108:ARG:CG	2.54	0.52
1:A:149:LEU:CD1	4:A:205:PLM:H61	2.37	0.52
1:A:153:LEU:HD12	1:A:154:TYR:HE1	1.73	0.52
1:A:15:ALA:HB1	1:A:19:TYR:HE2	1.72	0.51
1:A:122:LEU:CB	4:A:204:PLM:C2	2.82	0.51
1:A:15:ALA:C	1:A:19:TYR:CZ	2.88	0.51
1:A:103:ALA:O	1:A:106:HIS:CE1	2.63	0.51
1:A:148:LEU:N	1:A:148:LEU:HD23	2.26	0.51
1:A:117:HIS:CG	1:A:118:THR:N	2.78	0.51
1:A:42:LYS:NZ	1:A:69:VAL:CG2	2.74	0.51
1:A:106:HIS:NE2	1:A:148:LEU:HD22	2.25	0.51
1:A:41:ASN:CB	1:A:68:LYS:HG3	2.38	0.51
1:A:80:LEU:C	1:A:83:ILE:HG22	2.34	0.51
1:A:66:ASP:O	1:A:69:VAL:HB	2.11	0.51
1:A:130:ARG:NH2	1:A:138:TYR:CE1	2.79	0.51
1:A:141:THR:HB	1:A:142:LEU:HD23	1.92	0.51
1:A:105:ILE:O	1:A:108:ARG:HB2	2.10	0.50
1:A:125:LEU:N	1:A:126:PRO:CD	2.73	0.50
1:A:20:ALA:HA	1:A:23:ILE:HB	1.93	0.50
1:A:114:ARG:HG3	1:A:137:GLY:HA2	1.93	0.50
1:A:16:PHE:CE1	1:A:94:SER:HB2	2.47	0.50
1:A:116:TYR:CE1	3:A:203:PC1:H262	2.38	0.50
1:A:134:PHE:C	1:A:136:VAL:N	2.64	0.50
1:A:113:ALA:O	1:A:117:HIS:HB3	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:ARG:CG	1:A:137:GLY:CA	2.90	0.50
1:A:118:THR:O	1:A:121:TYR:N	2.43	0.50
1:A:142:LEU:O	1:A:146:TYR:N	2.33	0.50
1:A:112:GLY:HA2	1:A:115:ILE:HD11	1.93	0.50
1:A:83:ILE:HG23	1:A:84:VAL:N	2.27	0.50
1:A:10:ASN:HA	1:A:13:LEU:HD12	1.93	0.50
1:A:10:ASN:O	1:A:14:MET:N	2.38	0.49
1:A:19:TYR:HA	1:A:22:ILE:HD12	1.95	0.49
1:A:142:LEU:O	1:A:145:ALA:HB3	2.12	0.49
1:A:148:LEU:O	1:A:149:LEU:C	2.52	0.49
1:A:80:LEU:O	1:A:83:ILE:HG23	2.12	0.49
1:A:86:PHE:CE1	1:A:110:PHE:CZ	3.01	0.49
1:A:89:ILE:HG23	1:A:149:LEU:HD21	1.93	0.49
1:A:106:HIS:O	1:A:110:PHE:CD2	2.65	0.49
1:A:129:ASN:O	1:A:134:PHE:HE1	1.93	0.49
1:A:42:LYS:HD2	1:A:69:VAL:CG2	2.40	0.49
1:A:117:HIS:ND1	1:A:117:HIS:C	2.70	0.49
1:A:97:GLY:O	1:A:152:ARG:NH1	2.45	0.49
1:A:141:THR:O	1:A:145:ALA:N	2.44	0.49
1:A:121:TYR:OH	1:A:129:ASN:HA	2.12	0.49
1:A:68:LYS:HA	1:A:71:ARG:HD2	1.94	0.48
1:A:99:ASP:O	1:A:152:ARG:NH1	2.35	0.48
1:A:119:ILE:HG13	4:A:204:PLM:C7	2.43	0.48
1:A:23:ILE:CG1	1:A:86:PHE:CE1	2.96	0.48
1:A:42:LYS:CD	1:A:66:ASP:HB3	2.43	0.48
1:A:69:VAL:HG12	1:A:70:GLU:N	2.27	0.48
1:A:114:ARG:O	1:A:117:HIS:CG	2.66	0.48
1:A:140:VAL:CB	3:A:202:PC1:H3D1	2.44	0.48
1:A:14:MET:O	1:A:18:SER:OG	2.32	0.48
1:A:140:VAL:HB	3:A:202:PC1:H3D2	1.94	0.48
1:A:15:ALA:CB	1:A:19:TYR:CE2	2.94	0.47
1:A:121:TYR:CB	1:A:122:LEU:HA	2.44	0.47
1:A:145:ALA:O	1:A:146:TYR:C	2.56	0.47
1:A:142:LEU:HD23	1:A:142:LEU:N	2.30	0.47
1:A:110:PHE:CD1	1:A:110:PHE:C	2.91	0.47
1:A:37:GLN:O	1:A:41:ASN:N	2.29	0.47
1:A:130:ARG:HA	1:A:134:PHE:HD1	1.72	0.47
1:A:68:LYS:O	1:A:72:VAL:HG23	2.14	0.47
1:A:117:HIS:O	1:A:118:THR:C	2.56	0.47
1:A:89:ILE:HG23	1:A:149:LEU:CD2	2.45	0.47
1:A:82:ASN:CB	1:A:114:ARG:HE	2.27	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:PHE:C	1:A:86:PHE:HD2	2.23	0.47
1:A:85:PRO:HB3	4:A:205:PLM:H32	1.98	0.46
1:A:114:ARG:NH1	1:A:138:TYR:CD2	2.51	0.46
1:A:130:ARG:CA	1:A:134:PHE:CD1	2.88	0.46
1:A:81:GLU:O	1:A:85:PRO:HD3	2.06	0.46
1:A:83:ILE:CD1	1:A:87:LEU:CD2	2.87	0.46
1:A:86:PHE:CZ	1:A:110:PHE:CZ	3.02	0.46
1:A:96:SER:O	1:A:152:ARG:CB	2.63	0.46
1:A:28:MET:O	1:A:29:PHE:C	2.56	0.46
1:A:124:PRO:C	1:A:126:PRO:HD2	2.41	0.46
1:A:122:LEU:O	4:A:204:PLM:H21	2.14	0.46
1:A:93:TYR:CZ	1:A:149:LEU:CA	2.87	0.46
1:A:138:TYR:O	1:A:142:LEU:CG	2.59	0.46
1:A:148:LEU:CD2	1:A:148:LEU:H	2.28	0.46
1:A:33:ALA:O	1:A:37:GLN:CG	2.57	0.46
1:A:105:ILE:HG23	1:A:109:ILE:HD11	1.97	0.46
1:A:89:ILE:CG2	1:A:149:LEU:HD21	2.46	0.46
1:A:103:ALA:CA	1:A:106:HIS:CE1	2.92	0.46
1:A:38:ARG:NH2	1:A:73:ARG:N	2.64	0.45
1:A:70:GLU:O	1:A:71:ARG:C	2.59	0.45
1:A:85:PRO:HB3	4:A:205:PLM:C1	2.46	0.45
1:A:93:TYR:CZ	1:A:149:LEU:HD22	2.49	0.45
1:A:71:ARG:O	1:A:74:ARG:HB2	2.17	0.45
1:A:27:MET:HE3	1:A:83:ILE:HG21	1.79	0.45
1:A:122:LEU:N	1:A:124:PRO:HD2	2.31	0.45
1:A:153:LEU:C	1:A:155:LEU:N	2.74	0.45
1:A:23:ILE:HG12	1:A:86:PHE:HD1	1.80	0.45
1:A:34:THR:C	1:A:72:VAL:HG11	2.42	0.45
1:A:119:ILE:HA	4:A:204:PLM:C4	2.46	0.45
1:A:148:LEU:HD23	1:A:148:LEU:H	1.82	0.45
1:A:109:ILE:C	1:A:112:GLY:H	2.24	0.45
1:A:138:TYR:O	1:A:142:LEU:CD2	2.64	0.45
1:A:67:GLU:C	1:A:125:LEU:HD11	2.39	0.45
1:A:31:SER:HA	1:A:76:HIS:HE2	1.82	0.44
1:A:107:PHE:HA	1:A:110:PHE:HE2	1.76	0.44
1:A:109:ILE:O	1:A:113:ALA:N	2.27	0.44
1:A:139:GLY:O	1:A:142:LEU:HB2	2.17	0.44
1:A:34:THR:HG1	1:A:76:HIS:CD2	2.33	0.44
1:A:78:ASN:O	1:A:82:ASN:N	2.42	0.44
1:A:83:ILE:HG13	1:A:87:LEU:CG	2.47	0.44
1:A:140:VAL:CB	3:A:202:PC1:H3D2	2.45	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:PHE:HA	1:A:19:TYR:CD2	2.53	0.44
1:A:33:ALA:HB1	1:A:37:GLN:HE21	1.83	0.44
1:A:122:LEU:HB2	4:A:204:PLM:C2	2.48	0.44
1:A:119:ILE:HA	4:A:204:PLM:H62	1.99	0.43
3:A:203:PC1:H3E1	3:A:203:PC1:H3H2	1.66	0.43
1:A:31:SER:HA	1:A:76:HIS:NE2	2.33	0.43
1:A:90:GLY:C	1:A:92:LEU:N	2.74	0.43
1:A:92:LEU:HD13	4:A:205:PLM:H91	2.01	0.43
1:A:93:TYR:HD1	1:A:152:ARG:HB2	1.84	0.43
1:A:116:TYR:O	1:A:120:ALA:N	2.46	0.43
1:A:118:THR:C	4:A:204:PLM:H51	2.43	0.43
1:A:86:PHE:CE2	1:A:110:PHE:HZ	2.35	0.43
1:A:121:TYR:CE2	1:A:124:PRO:HG2	2.53	0.43
1:A:117:HIS:HB2	1:A:133:ALA:O	2.18	0.43
3:A:202:PC1:H3C1	3:A:202:PC1:H3F1	1.68	0.43
1:A:127:GLN:HG2	1:A:129:ASN:CG	2.41	0.43
1:A:12:VAL:H	1:A:12:VAL:HG23	1.50	0.43
1:A:96:SER:C	1:A:98:PRO:HD3	2.44	0.43
1:A:38:ARG:CG	1:A:72:VAL:CG1	2.95	0.43
1:A:99:ASP:OD1	1:A:152:ARG:CZ	2.67	0.43
1:A:130:ARG:NH2	1:A:138:TYR:CZ	2.85	0.42
1:A:26:LYS:HE3	1:A:115:ILE:HG23	1.98	0.42
1:A:146:TYR:C	1:A:150:ARG:HD2	2.44	0.42
1:A:92:LEU:C	1:A:94:SER:N	2.76	0.42
1:A:99:ASP:OD2	1:A:101:SER:CA	2.64	0.42
1:A:145:ALA:O	1:A:149:LEU:CG	2.51	0.42
1:A:31:SER:HA	1:A:76:HIS:CD2	2.55	0.42
1:A:40:THR:CG2	1:A:41:ASN:H	2.32	0.42
1:A:121:TYR:HB3	4:A:204:PLM:C1	2.50	0.42
1:A:72:VAL:C	1:A:74:ARG:N	2.77	0.42
1:A:137:GLY:O	1:A:140:VAL:HG12	2.20	0.42
1:A:89:ILE:HG12	4:A:205:PLM:H52	1.89	0.42
1:A:119:ILE:O	1:A:122:LEU:CB	2.59	0.42
1:A:27:MET:HG2	1:A:79:ASP:OD2	2.20	0.42
1:A:33:ALA:CB	1:A:37:GLN:HE21	2.32	0.42
1:A:42:LYS:HG2	1:A:66:ASP:HB3	2.01	0.42
1:A:114:ARG:CB	1:A:117:HIS:CD2	3.02	0.42
1:A:23:ILE:HG12	1:A:86:PHE:CE1	2.54	0.41
1:A:121:TYR:HE2	1:A:124:PRO:O	2.03	0.41
1:A:83:ILE:HG13	1:A:87:LEU:CD1	2.49	0.41
1:A:98:PRO:O	1:A:99:ASP:C	2.63	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:LEU:N	1:A:107:PHE:CD2	2.88	0.41
1:A:26:LYS:CE	1:A:115:ILE:HG23	2.50	0.41
1:A:16:PHE:CE2	1:A:94:SER:HA	2.28	0.41
1:A:79:ASP:O	1:A:83:ILE:HG22	2.20	0.41
1:A:92:LEU:C	1:A:94:SER:H	2.27	0.41
1:A:103:ALA:O	1:A:106:HIS:CG	2.74	0.41
1:A:144:MET:O	1:A:148:LEU:HD11	2.20	0.41
1:A:148:LEU:HA	1:A:151:SER:OG	2.21	0.41
1:A:84:VAL:HG12	1:A:85:PRO:HD3	2.02	0.41
1:A:93:TYR:CE1	1:A:149:LEU:HA	2.54	0.41
1:A:23:ILE:CG2	1:A:83:ILE:CD1	2.86	0.41
1:A:147:ARG:O	1:A:148:LEU:C	2.64	0.41
1:A:106:HIS:C	1:A:108:ARG:N	2.74	0.41
1:A:110:PHE:O	1:A:111:VAL:C	2.64	0.41
1:A:120:ALA:HB1	3:A:203:PC1:H222	2.02	0.41
1:A:132:LEU:HA	1:A:135:PHE:HB2	2.02	0.41
1:A:144:MET:HB3	1:A:148:LEU:HD11	2.03	0.41
1:A:84:VAL:HG12	1:A:85:PRO:CD	2.50	0.41
1:A:93:TYR:OH	4:A:205:PLM:H81	2.20	0.41
1:A:106:HIS:HB2	1:A:144:MET:CG	2.48	0.40
1:A:149:LEU:O	1:A:153:LEU:CD2	2.69	0.40
1:A:20:ALA:O	1:A:21:THR:C	2.64	0.40
1:A:85:PRO:O	1:A:86:PHE:O	2.37	0.40
1:A:93:TYR:CZ	4:A:205:PLM:CA	3.04	0.40
1:A:76:HIS:CB	1:A:77:LEU:CD1	2.98	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:PHE:CZ	3:A:203:PC1:C36[4_665]	1.97	0.23
1:A:130:ARG:NH2	2:A:201:GSH:SG2[2_655]	2.04	0.16
1:A:36:PHE:CE2	3:A:203:PC1:C36[4_665]	2.10	0.10

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 PDB entries followed by that with respect to all EM

entries.

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	119/155 (77%)	80 (67%)	35 (29%)	4 (3%)	3	23

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	THR
1	A	22	ILE
1	A	124	PRO
1	A	23	ILE

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 PDB entries followed by that with respect to all EM entries.

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	105/130 (81%)	81 (77%)	24 (23%)	1	5

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	MET
1	A	21	THR
1	A	23	ILE
1	A	30	LEU
1	A	32	SER
1	A	39	LEU
1	A	70	GLU
1	A	84	VAL
1	A	92	LEU
1	A	95	LEU
1	A	99	ASP
1	A	100	LEU
1	A	106	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	108	ARG
1	A	111	VAL
1	A	116	TYR
1	A	117	HIS
1	A	122	LEU
1	A	141	THR
1	A	142	LEU
1	A	147	ARG
1	A	148	LEU
1	A	153	LEU
1	A	154	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	78	ASN
1	A	117	HIS

5.3.3 RNA [i](#)

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 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
4	PLM	A	204	-	9,9,17	0.32	0	8,8,17	0.84	0
2	GSH	A	201	-	18,19,19	2.16	3 (16%)	21,24,24	0.90	0
3	PC1	A	202	-	53,53,53	1.23	2 (3%)	59,61,61	1.09	4 (6%)
3	PC1	A	203	-	53,53,53	1.27	3 (5%)	59,61,61	1.56	12 (20%)
4	PLM	A	205	-	9,9,17	0.83	0	8,8,17	0.62	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
4	PLM	A	204	-	-	2/7/7/15	-
2	GSH	A	201	-	-	0/24/24/24	-
3	PC1	A	202	-	1/1/5/5	34/57/57/57	-
3	PC1	A	203	-	1/1/5/5	24/57/57/57	-
4	PLM	A	205	-	-	3/7/7/15	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	202	PC1	O31-C31	5.80	1.50	1.33
2	A	201	GSH	O2-C2	5.79	1.34	1.23
2	A	201	GSH	OE1-CD1	5.66	1.34	1.23
3	A	203	PC1	O31-C31	5.41	1.49	1.33
3	A	203	PC1	O21-C21	4.58	1.47	1.34
3	A	202	PC1	O21-C21	4.40	1.46	1.34
3	A	203	PC1	C3C-C3B	-2.80	1.37	1.51
2	A	201	GSH	O32-C3	2.79	1.31	1.22

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	203	PC1	O21-C21-C22	4.65	121.55	111.48
3	A	203	PC1	C3F-C3E-C3D	-4.11	93.61	114.37
3	A	202	PC1	O21-C21-C22	3.76	119.61	111.48
3	A	203	PC1	O31-C31-C32	3.48	122.46	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	202	PC1	O31-C31-C32	3.26	121.77	111.83
3	A	203	PC1	C3D-C3C-C3B	-2.93	99.58	114.37
3	A	202	PC1	C23-C22-C21	-2.89	103.09	113.69
3	A	203	PC1	C3E-C3D-C3C	-2.79	100.26	114.37
3	A	203	PC1	O31-C31-O32	-2.77	116.69	123.63
3	A	203	PC1	C39-C38-C37	2.77	128.36	114.37
3	A	203	PC1	C3B-C3A-C39	-2.70	100.71	114.37
3	A	203	PC1	C2-O21-C21	-2.54	111.72	117.80
3	A	203	PC1	O21-C21-O22	-2.37	118.16	123.70
3	A	203	PC1	C3A-C39-C38	-2.33	102.58	114.37
3	A	202	PC1	O31-C31-O32	-2.25	118.00	123.63
3	A	203	PC1	C3-O31-C31	2.23	125.27	117.12

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	202	PC1	C2
3	A	203	PC1	C2

All (63) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	202	PC1	C11-O13-P-O11
3	A	202	PC1	C1-O11-P-O14
3	A	202	PC1	C1-O11-P-O13
3	A	202	PC1	O13-C11-C12-N
3	A	203	PC1	C1-O11-P-O12
3	A	203	PC1	C1-O11-P-O13
3	A	203	PC1	O32-C31-O31-C3
3	A	203	PC1	C32-C31-O31-C3
3	A	202	PC1	C11-C12-N-C14
3	A	202	PC1	C3C-C3D-C3E-C3F
3	A	203	PC1	C21-C22-C23-C24
3	A	203	PC1	C3E-C3F-C3G-C3H
3	A	202	PC1	C32-C31-O31-C3
3	A	202	PC1	C31-C32-C33-C34
3	A	202	PC1	C11-C12-N-C13
3	A	202	PC1	C11-C12-N-C15
3	A	203	PC1	C22-C21-O21-C2
3	A	203	PC1	O22-C21-O21-C2
3	A	202	PC1	C22-C21-O21-C2
3	A	202	PC1	C23-C24-C25-C26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	202	PC1	O22-C21-O21-C2
3	A	202	PC1	O32-C31-O31-C3
3	A	203	PC1	C35-C36-C37-C38
3	A	202	PC1	C2B-C2C-C2D-C2E
3	A	203	PC1	C25-C26-C27-C28
3	A	202	PC1	C32-C33-C34-C35
3	A	203	PC1	C2A-C2B-C2C-C2D
3	A	203	PC1	C33-C34-C35-C36
3	A	203	PC1	C3C-C3D-C3E-C3F
4	A	204	PLM	C2-C3-C4-C5
3	A	202	PC1	C24-C25-C26-C27
3	A	203	PC1	C34-C35-C36-C37
3	A	203	PC1	C1-C2-C3-O31
3	A	202	PC1	C35-C36-C37-C38
3	A	203	PC1	C3F-C3G-C3H-C3I
3	A	203	PC1	C36-C37-C38-C39
3	A	202	PC1	C3B-C3C-C3D-C3E
3	A	202	PC1	C2A-C2B-C2C-C2D
4	A	205	PLM	C7-C8-C9-CA
3	A	203	PC1	O11-C1-C2-C3
3	A	202	PC1	C28-C29-C2A-C2B
3	A	202	PC1	C2-C1-O11-P
3	A	203	PC1	C3B-C3C-C3D-C3E
3	A	202	PC1	C3A-C3B-C3C-C3D
4	A	205	PLM	C2-C3-C4-C5
3	A	202	PC1	C3D-C3E-C3F-C3G
3	A	202	PC1	C29-C2A-C2B-C2C
3	A	202	PC1	O11-C1-C2-O21
3	A	203	PC1	O21-C2-C3-O31
3	A	202	PC1	C27-C28-C29-C2A
3	A	202	PC1	C2E-C2F-C2G-C2H
3	A	202	PC1	C21-C22-C23-C24
3	A	203	PC1	C2F-C2G-C2H-C2I
3	A	202	PC1	C2C-C2D-C2E-C2F
3	A	202	PC1	C11-O13-P-O14
3	A	203	PC1	O11-C1-C2-O21
4	A	205	PLM	C5-C6-C7-C8
3	A	202	PC1	C2D-C2E-C2F-C2G
4	A	204	PLM	C3-C4-C5-C6
3	A	202	PC1	O11-C1-C2-C3
3	A	203	PC1	C3A-C3B-C3C-C3D
3	A	203	PC1	C2B-C2C-C2D-C2E

Continued on next page...

Continued from previous page...

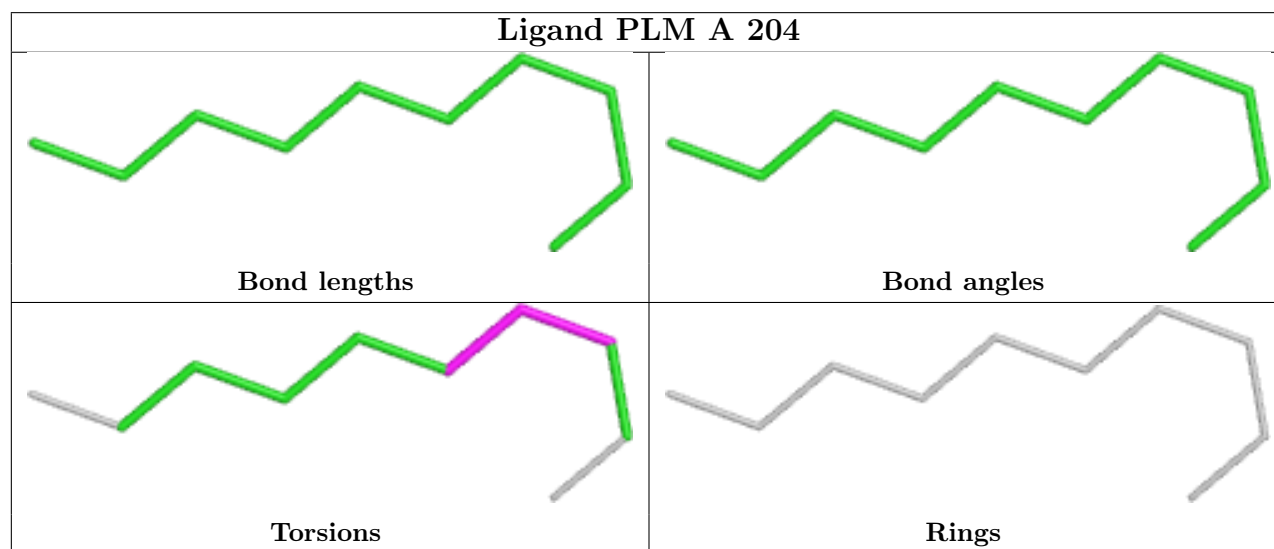
Mol	Chain	Res	Type	Atoms
3	A	202	PC1	C34-C35-C36-C37

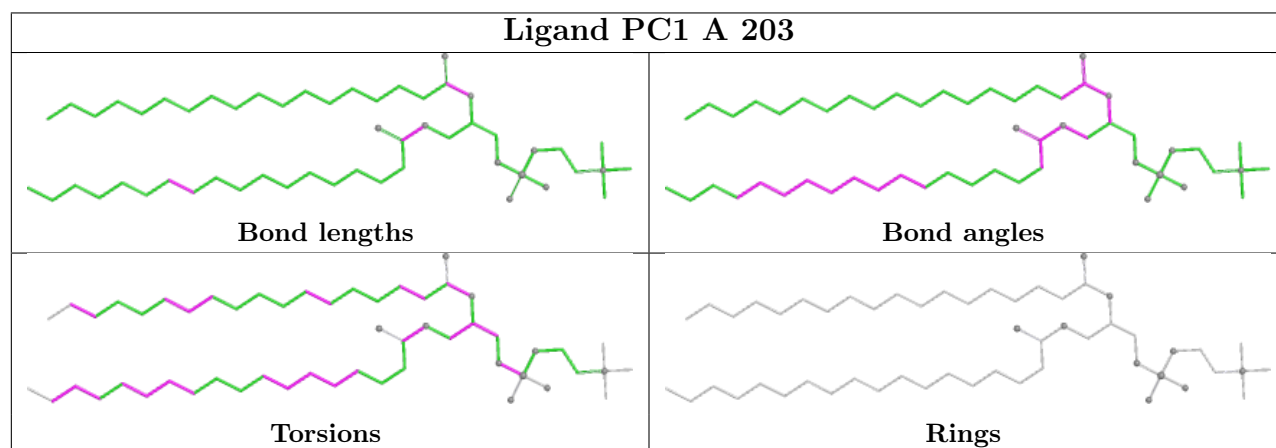
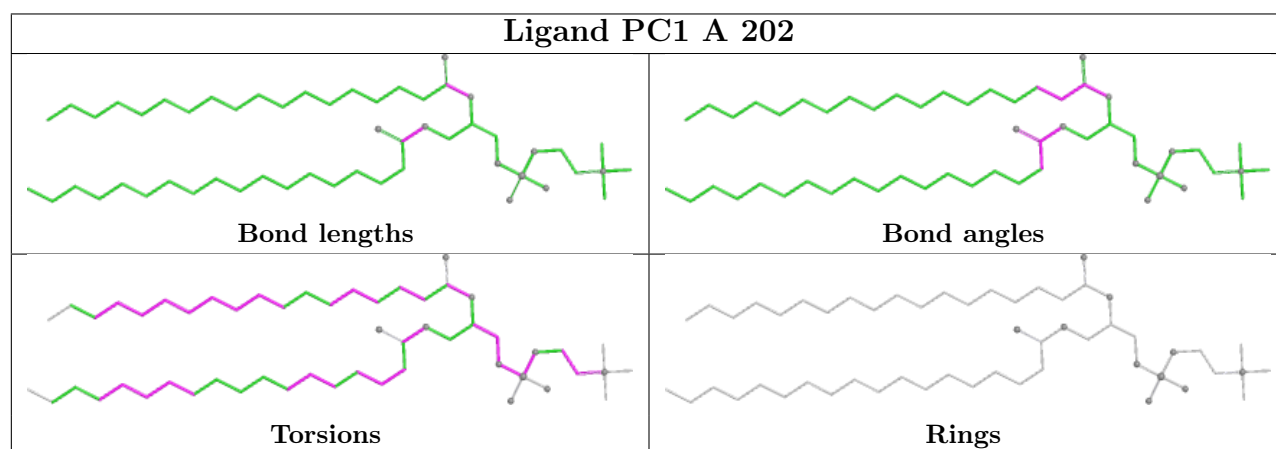
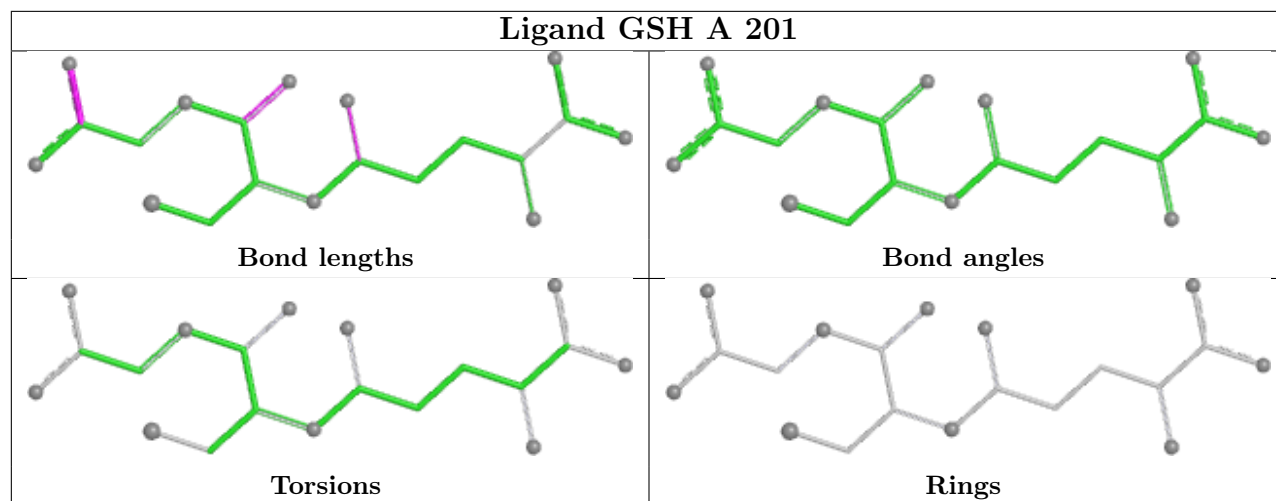
There are no ring outliers.

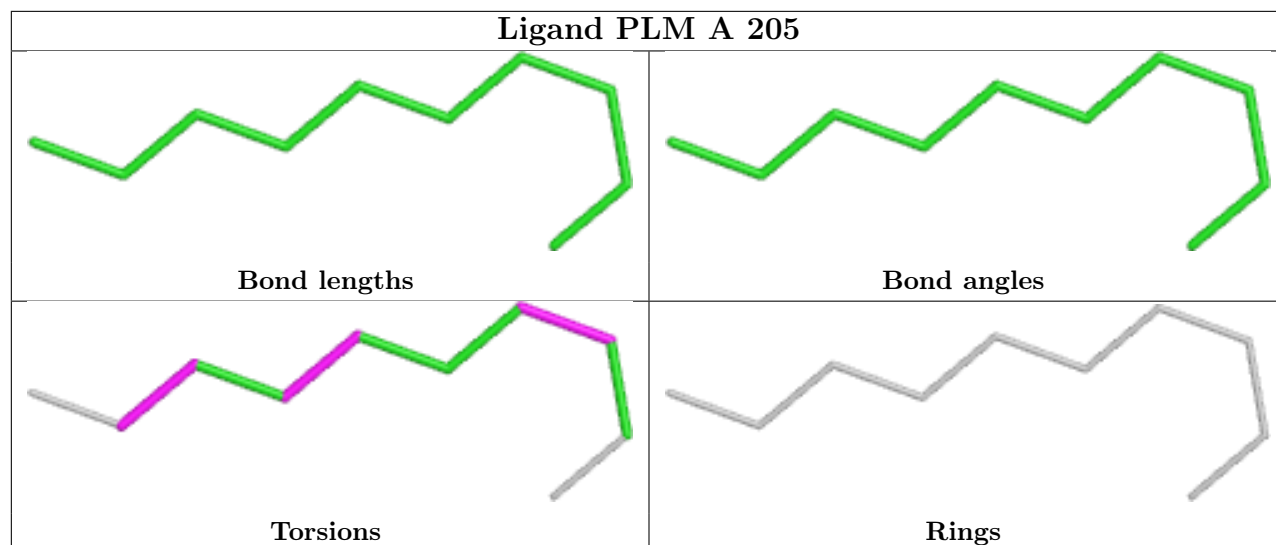
5 monomers are involved in 85 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	204	PLM	37	0
2	A	201	GSH	1	1
3	A	202	PC1	26	0
3	A	203	PC1	7	2
4	A	205	PLM	11	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







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.