



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 09:23 pm BST

PDB ID : 1LMW
Title : LMW U-PA Structure complexed with EGRCMK (GLU-GLY-ARG Chloromethyl Ketone)
Authors : Spraggon, G.S.; Phillips, C.; Nowak, U.K.; Ponting, C.P.; Saunders, D.; Dobson, C.M.; Stuart, D.I.; Jones, E.Y.
Deposited on : 1995-07-26
Resolution : 2.50 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

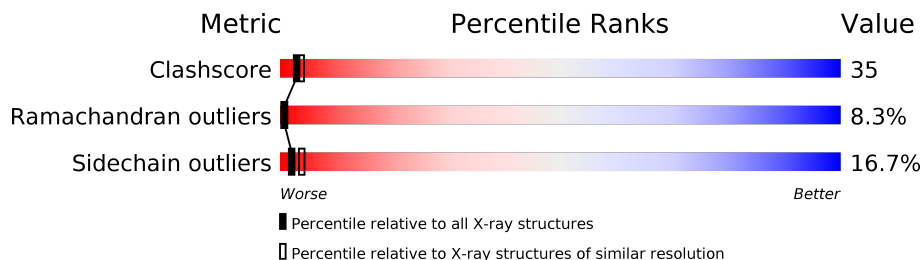
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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 ≥ 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	23	17% 22% 61%
1	C	23	22% 13% 65%
2	B	253	37% 45% 14% ..
2	D	253	37% 50% 10% ..

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4093 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.

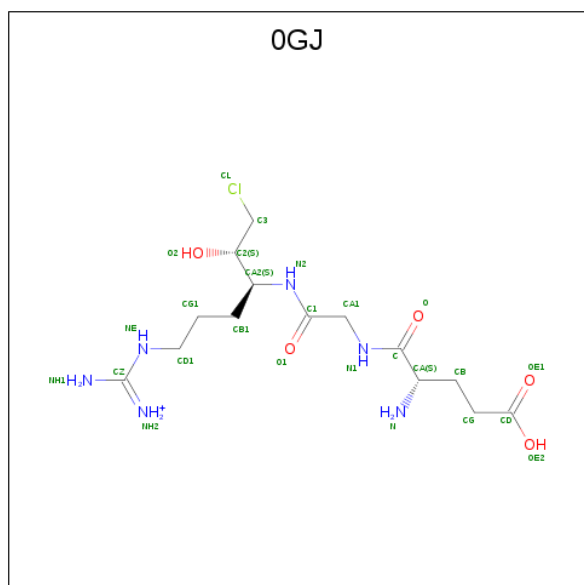
- Molecule 1 is a protein called UROKINASE-TYPE PLASMINOGEN ACTIVATOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	9	Total	C	N	O	S	0	0	1
			62	37	14	10	1			
1	C	8	Total	C	N	O	S	0	0	0
			61	37	13	10	1			

- Molecule 2 is a protein called UROKINASE-TYPE PLASMINOGEN ACTIVATOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	248	Total	C	N	O	S	0	0	0
			1960	1234	342	367	17			
2	D	248	Total	C	N	O	S	0	0	0
			1960	1234	342	367	17			

- Molecule 3 is L-alpha-glutamyl-N-{(1S)-4-[[amino(iminio)methyl]amino]-1-[(1S)-2-chloro-1-hydroxyethyl]butyl}glycinamide (three-letter code: 0GJ) (formula: C₁₄H₂₈ClN₆O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			25	14	6	5		
3	D	1	Total	C	N	O	0	0
			25	14	6	5		

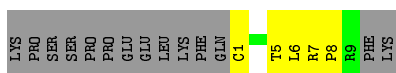
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

Note EDS was not executed.

- Molecule 1: UROKINASE-TYPE PLASMINOGEN ACTIVATOR

Chain A: 



- Molecule 1: UROKINASE-TYPE PLASMINOGEN ACTIVATOR

Chain C: 



- Molecule 2: UROKINASE-TYPE PLASMINOGEN ACTIVATOR

Chain B: 



- Molecule 2: UROKINASE-TYPE PLASMINOGEN ACTIVATOR

Chain D: 



M76	M77	Q78	Q79	E80	M81	K82	F83	M87	L88	L89	L90	H91	K92	D93	Y94	S95	A96	D97	L97A	L97B	A98	H99	H100	H101	D102	I103	A104	L105	L106	K107	I108	E110B	A112	Q113	P114	S115	R116	T117	I118	Q119	T120	C121	C122	L123	M126	Y127	M128	T134	S135	C136	E137	I138	G142
K143	E144	M145	S146	Y149	L150	Y151	P152	E153	K156	M157	T158	V159	V160	I163	S164	H165	R166	Q169	Q170	P170A	H170B	Y171	Y172	E175	V176	K179	A183	A184	D185	P185B	Q185B	W186	K187	T188	D189	S190	C191	Q192	S195	P198	L199	V200	C201	S202	L203	R206	M207	T208	L209				
T210	G211	I212	V213	S214	G216	R217	G218	C220	A221	L222	K223	D223A	Y228	T229	R230	V231	S232	H233	P236	W237	T238	R239	S240	H241	T242	K243	E244	E245	ASN	GLY	LEU	LEU	ALA	LEU																			

4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	176.70Å 176.70Å 54.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (30.00-2.50)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.224 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	4093	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

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: 0GJ

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	0.80	0/62	0.84	0/82
1	C	0.50	0/61	0.70	0/80
2	B	0.64	0/2009	0.90	4/2720 (0.1%)
2	D	0.63	0/2009	0.88	1/2720 (0.0%)
All	All	0.64	0/4141	0.89	5/5602 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	B	199	LEU	N-CA-C	-7.49	90.79	111.00
2	D	199	LEU	N-CA-C	-6.66	93.02	111.00
2	B	198	PRO	N-CA-C	6.25	128.36	112.10
2	B	37(C)	GLY	N-CA-C	6.21	128.63	113.10
2	B	150	LEU	CA-CB-CG	6.10	129.32	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	57	HIS	Sidechain

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	62	0	68	9	0
1	C	61	0	68	3	0
2	B	1960	0	1901	148	8
2	D	1960	0	1901	127	8
3	B	25	0	24	1	0
3	D	25	0	24	0	0
All	All	4093	0	3986	280	9

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 35.

All (280) 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)
2:B:121:ILE:HD13	2:B:209:LEU:HB2	1.49	0.95
2:B:145:ASN:HB3	2:B:148:ASP:HB2	1.52	0.91
2:B:202:SER:HA	2:B:207:MET:HA	1.55	0.88
2:B:37:HIS:HE1	2:B:39:THR:HG23	1.39	0.86
2:B:22:THR:HG21	2:B:157:MET:SD	2.16	0.85
2:D:72:ARG:HH21	2:D:74:ASN:H	1.24	0.84
2:B:144:GLU:HG3	2:B:152:PRO:HG3	1.62	0.82
2:B:27:GLN:HG3	2:B:139:THR:HG21	1.60	0.82
2:B:24:ILE:HG13	2:B:71:SER:HB3	1.61	0.82
2:B:191:CYS:O	2:B:194:ASP:HB2	1.82	0.78
1:A:6:LEU:HG	1:A:8:PRO:HD3	1.66	0.77
2:D:56:THR:HG23	2:D:104:ALA:HB2	1.66	0.77
1:A:7:ARG:HH22	2:B:116:ARG:HE	1.31	0.76
2:B:145:ASN:HB3	2:B:148:ASP:CB	2.15	0.75
2:B:37:HIS:CE1	2:B:39:THR:HG23	2.19	0.75
2:B:60:ILE:HG22	2:B:60(A):ASP:N	2.01	0.75
2:D:146:SER:HB3	2:D:220:CYS:HB2	1.69	0.75
2:B:66:VAL:HG13	2:B:83:PHE:HB2	1.69	0.74
2:D:88:LEU:HD12	2:D:106:LEU:HG	1.70	0.74
2:B:36:ARG:HE	2:B:65:ILE:HD13	1.52	0.74
2:B:197:GLY:O	2:B:213:VAL:HG23	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:27:GLN:HG3	2:D:29:TRP:NE1	2.03	0.73
2:B:46:LEU:HD22	2:B:48:SER:O	1.90	0.71
2:D:45:SER:OG	2:D:198:PRO:HG3	1.90	0.71
2:B:130:PRO:HG3	2:B:203:LEU:HD21	1.73	0.70
2:B:21:PHE:HD2	2:B:154:GLN:HB3	1.55	0.70
2:D:29:TRP:HA	2:D:119:GLN:O	1.92	0.70
2:D:45:SER:HB2	2:D:53:ILE:HG22	1.72	0.70
2:D:77:THR:O	2:D:80:GLU:HB3	1.91	0.70
2:D:18:GLY:HA3	2:D:158:THR:HB	1.73	0.70
2:B:88:LEU:HD12	2:B:106:LEU:HG	1.74	0.69
2:D:72:ARG:HE	2:D:74:ASN:N	1.90	0.69
2:B:91:HIS:HD2	2:B:101:ASN:HB3	1.57	0.69
2:B:23:THR:H	2:B:26:ASN:HD22	1.40	0.69
2:B:183:ALA:HB3	2:B:228:TYR:HE1	1.57	0.69
2:B:143:LYS:HG2	2:B:145:ASN:O	1.92	0.69
2:B:21:PHE:CD2	2:B:154:GLN:HB3	2.27	0.69
2:D:230:ARG:HD2	2:D:233:HIS:HD2	1.57	0.69
2:B:116:ARG:HB2	2:B:116:ARG:NH1	2.08	0.68
2:D:35:ARG:NH2	2:D:37:HIS:HE1	1.92	0.68
2:D:72:ARG:NH2	2:D:74:ASN:H	1.92	0.67
1:A:7:ARG:HH22	2:B:116:ARG:NE	1.92	0.67
2:B:134:THR:O	2:B:162:LEU:HD13	1.95	0.67
2:D:144:GLU:OE2	2:D:152:PRO:HB3	1.95	0.67
2:D:61:LYS:NZ	2:D:62(A):GLU:HB2	2.09	0.67
2:D:212:ILE:O	2:D:228:TYR:HB3	1.95	0.67
2:D:165:HIS:HE1	2:D:169:GLN:HE22	1.43	0.66
2:B:172:TYR:HE1	2:B:224:LYS:HD2	1.61	0.66
2:B:172:TYR:CE1	2:B:224:LYS:HD2	2.30	0.66
2:B:209:LEU:HD22	2:B:231:VAL:HG21	1.77	0.66
2:B:40:TYR:CZ	2:B:141:PHE:HD2	2.14	0.66
2:B:56:THR:HG22	2:B:90:LEU:HB3	1.76	0.65
2:D:170:GLN:CD	2:D:170(A):PRO:HD2	2.16	0.65
2:D:230:ARG:HD2	2:D:233:HIS:CD2	2.31	0.65
2:B:183:ALA:HB3	2:B:228:TYR:CE1	2.31	0.65
2:B:57:HIS:HA	2:B:60:ILE:HG12	1.76	0.64
2:B:66:VAL:CG1	2:B:83:PHE:HB2	2.26	0.64
2:D:27:GLN:HG3	2:D:29:TRP:HE1	1.62	0.64
2:B:122:CYS:HB2	2:B:208:THR:HG22	1.80	0.64
2:D:61:LYS:HZ3	2:D:62(A):GLU:HB2	1.63	0.64
2:D:42:CYS:HB3	2:D:195:SER:O	1.98	0.63
2:B:212:ILE:O	2:B:228:TYR:HA	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:17:ILE:HG22	2:B:17:ILE:O	2.00	0.62
2:D:106:LEU:N	2:D:106:LEU:HD12	2.14	0.62
2:B:230:ARG:CG	2:B:232:SER:HB2	2.29	0.61
2:D:213:VAL:HG22	2:D:228:TYR:CE2	2.35	0.61
2:D:122:CYS:O	2:D:208:THR:HG22	2.00	0.61
2:D:56:THR:CG2	2:D:90:LEU:HB3	2.30	0.61
2:B:112:ALA:C	2:B:114:PRO:HD3	2.20	0.61
2:B:37:HIS:HB3	2:B:37(A):ARG:HH12	1.65	0.61
2:D:239:ARG:HH11	2:D:243:LYS:HZ1	1.48	0.61
2:B:16:ILE:HG22	2:B:18:GLY:H	1.66	0.60
2:B:24:ILE:HG21	2:B:70:ARG:N	2.17	0.60
2:B:114:PRO:HA	2:B:118:ILE:HG22	1.82	0.60
2:D:72:ARG:HG2	2:D:153:GLU:O	2.02	0.60
2:D:122:CYS:HB2	2:D:207:MET:O	2.02	0.60
2:B:138:ILE:HG22	2:B:198:PRO:O	2.02	0.59
2:B:60:ILE:O	2:B:60(C):PRO:HD3	2.02	0.59
2:D:56:THR:HG22	2:D:90:LEU:HB3	1.83	0.59
2:B:29:TRP:HA	2:B:119:GLN:O	2.01	0.59
2:B:132:PHE:CD2	2:B:164:SER:HB3	2.37	0.59
2:D:22:THR:HG21	2:D:157:MET:SD	2.43	0.59
2:B:90:LEU:N	2:B:90:LEU:HD12	2.16	0.59
2:B:20:GLU:O	2:B:22:THR:HG23	2.02	0.59
2:D:48:SER:HB2	2:D:49:PRO:HD3	1.85	0.58
2:B:144:GLU:CG	2:B:152:PRO:HG3	2.33	0.58
2:B:176:VAL:HG11	2:B:182:CYS:SG	2.43	0.58
2:D:165:HIS:CE1	2:D:169:GLN:HE22	2.22	0.58
2:D:41:VAL:HG12	2:D:58:CYS:HB3	1.85	0.58
2:B:170:GLN:HB3	2:B:170(A):PRO:HD2	1.86	0.58
2:B:217:ARG:HH11	2:B:217:ARG:HG2	1.68	0.58
2:D:166:ARG:HG2	2:D:166:ARG:HH11	1.70	0.57
2:D:41:VAL:CG1	2:D:58:CYS:HB3	2.35	0.57
2:D:201:CYS:CB	2:D:210:THR:HG1	2.18	0.57
2:D:27:GLN:NE2	2:D:29:TRP:HZ2	2.03	0.56
1:C:1:CYS:O	1:C:3:GLN:HG3	2.05	0.56
2:D:23:THR:C	2:D:25:GLU:H	2.08	0.56
2:B:230:ARG:HG2	2:B:232:SER:HB2	1.86	0.56
2:D:138:ILE:HG23	2:D:199:LEU:HD23	1.86	0.56
2:B:24:ILE:HG13	2:B:71:SER:CB	2.32	0.56
2:B:18:GLY:HA3	2:B:158:THR:HB	1.88	0.56
1:A:6:LEU:HG	1:A:8:PRO:CD	2.35	0.55
2:D:172:TYR:HB2	2:D:176:VAL:HG23	1.86	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:202:SER:HA	2:D:207:MET:HA	1.87	0.55
2:D:32:ALA:O	2:D:66:VAL:HG23	2.05	0.55
2:D:137:GLU:HG2	2:D:200:VAL:HB	1.89	0.55
2:D:27:GLN:NE2	2:D:200:VAL:HG21	2.22	0.54
2:D:218:GLY:HA3	2:D:222:LEU:HD12	1.89	0.54
2:B:124:PRO:O	2:B:235:LEU:HD11	2.07	0.54
2:D:61:LYS:CE	2:D:62(A):GLU:HB2	2.38	0.54
2:D:185:ASP:CG	2:D:185(A):PRO:HD2	2.28	0.54
2:D:88:LEU:CD1	2:D:106:LEU:HG	2.37	0.54
2:B:132:PHE:HD2	2:B:164:SER:HB3	1.71	0.53
2:B:37:HIS:HB3	2:B:37(A):ARG:NH1	2.24	0.53
2:B:18:GLY:HA3	2:B:158:THR:CB	2.39	0.53
2:D:172:TYR:O	2:D:175:GLU:HB2	2.08	0.53
2:D:23:THR:O	2:D:25:GLU:N	2.40	0.53
1:C:4:LYS:HE3	2:D:29:TRP:HH2	1.74	0.53
2:B:97(A):THR:HA	2:D:60:ILE:CD1	2.39	0.53
2:B:24:ILE:HG21	2:B:70:ARG:H	1.73	0.53
2:D:94:TYR:HA	2:D:101:ASN:HB2	1.91	0.53
2:B:27:GLN:CG	2:B:139:THR:HG21	2.35	0.52
2:D:215:TRP:HE3	2:D:216:GLY:CA	2.22	0.52
2:B:52:VAL:HG12	2:B:53:ILE:N	2.24	0.52
2:D:163:ILE:HG13	2:D:183:ALA:HA	1.92	0.52
2:B:202:SER:HB3	2:B:207:MET:HG2	1.91	0.52
2:D:128:ASN:HD21	2:D:203:LEU:HD13	1.75	0.52
2:D:17:ILE:HG22	2:D:17:ILE:O	2.10	0.52
2:D:23:THR:H	2:D:26:ASN:HD22	1.56	0.52
2:B:47:MET:HE2	2:B:53:ILE:HG21	1.92	0.52
2:D:41:VAL:HG21	2:D:64:TYR:HE1	1.75	0.51
2:B:116:ARG:CB	2:B:116:ARG:HH11	2.23	0.51
2:B:37(A):ARG:CZ	2:B:37(A):ARG:H	2.24	0.51
2:D:123:LEU:H	2:D:123:LEU:HD12	1.76	0.51
2:B:78:GLN:H	2:B:78:GLN:CD	2.13	0.50
2:D:149:TYR:N	2:D:149:TYR:CD1	2.79	0.50
2:B:27:GLN:N	2:B:28:PRO:CD	2.74	0.50
2:D:48:SER:HB2	2:D:49:PRO:CD	2.41	0.50
2:B:110:SER:HB3	2:B:110(D):ARG:H	1.75	0.50
2:D:61:LYS:HE2	2:D:62(A):GLU:HB2	1.93	0.50
2:D:121:ILE:HD13	2:D:209:LEU:HD12	1.94	0.50
2:D:188:THR:O	2:D:189:ASP:HB2	2.11	0.50
2:D:90:LEU:N	2:D:90:LEU:HD12	2.26	0.50
2:B:91:HIS:CD2	2:B:101:ASN:HB3	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:112:ALA:C	2:D:114:PRO:HD3	2.32	0.50
2:D:215:TRP:HE3	2:D:216:GLY:N	2.10	0.50
2:B:106:LEU:N	2:B:106:LEU:HD12	2.27	0.49
2:B:116:ARG:HB2	2:B:116:ARG:HH11	1.75	0.49
2:B:69:GLY:O	2:B:80:GLU:HB3	2.12	0.49
2:B:90:LEU:H	2:B:90:LEU:HD12	1.77	0.49
2:B:86:GLU:O	2:B:86:GLU:HG3	2.12	0.49
2:B:138:ILE:HG22	2:B:199:LEU:HA	1.93	0.48
2:B:69:GLY:O	2:B:80:GLU:CB	2.61	0.48
2:D:171:TYR:CD1	2:D:171:TYR:N	2.80	0.48
2:D:213:VAL:HG22	2:D:228:TYR:HE2	1.76	0.48
2:B:132:PHE:HD2	2:B:164:SER:CB	2.27	0.48
2:D:72:ARG:NE	2:D:74:ASN:N	2.60	0.48
2:B:34:TYR:CE1	2:B:40:TYR:HB2	2.49	0.48
2:D:105:LEU:HD12	2:D:237:TRP:CH2	2.48	0.48
2:D:171:TYR:HD1	2:D:171:TYR:N	2.11	0.48
2:D:16:ILE:HG22	2:D:18:GLY:H	1.78	0.48
2:B:50:CYS:O	2:B:107:LYS:HA	2.14	0.48
2:D:27:GLN:NE2	2:D:29:TRP:CZ2	2.80	0.48
2:D:21:PHE:HA	2:D:156:LYS:HA	1.96	0.48
2:B:16:ILE:CG2	2:B:18:GLY:H	2.27	0.47
2:D:186:TRP:C	2:D:187:LYS:HD2	2.34	0.47
2:B:51:TRP:CE3	2:B:105:LEU:HB3	2.49	0.47
2:B:40:TYR:CE2	2:B:141:PHE:HB2	2.49	0.47
2:B:60:ILE:CG2	2:B:60(A):ASP:N	2.71	0.47
2:B:37(A):ARG:HH11	2:B:37(A):ARG:HG2	1.78	0.47
2:B:52:VAL:HG12	2:B:53:ILE:H	1.79	0.47
2:D:137:GLU:O	2:D:200:VAL:N	2.47	0.47
2:B:145:ASN:OD1	2:B:147:THR:HG23	2.14	0.47
2:D:201:CYS:SG	2:D:210:THR:HG21	2.55	0.47
2:D:215:TRP:CE3	2:D:216:GLY:HA2	2.50	0.47
2:D:66:VAL:HG13	2:D:83:PHE:HB2	1.95	0.47
2:B:237:TRP:NE1	2:B:241:HIS:NE2	2.63	0.47
2:D:242:THR:HG22	2:D:242:THR:O	2.15	0.47
2:B:213:VAL:HG22	2:B:228:TYR:CE2	2.50	0.47
2:B:177:THR:OG1	2:B:179:LYS:HG2	2.15	0.47
2:D:53:ILE:HG23	2:D:53:ILE:O	2.14	0.46
1:A:5:THR:CG2	1:A:6:LEU:N	2.78	0.46
2:D:143:LYS:HB3	2:D:145:ASN:O	2.15	0.46
2:D:46:LEU:HD11	2:D:68:LEU:HD21	1.96	0.46
2:D:27:GLN:N	2:D:28:PRO:CD	2.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:24:ILE:HG13	2:D:71:SER:HB3	1.97	0.46
2:D:237:TRP:NE1	2:D:241:HIS:NE2	2.64	0.46
2:D:47:MET:SD	2:D:121:ILE:CD1	3.03	0.46
2:D:170:GLN:CG	2:D:170(A):PRO:HD2	2.46	0.46
2:D:190:SER:O	2:D:191:CYS:HB2	2.16	0.46
2:B:27:GLN:HA	2:B:27:GLN:OE1	2.16	0.45
1:A:7:ARG:N	1:A:8:PRO:HD3	2.30	0.45
2:B:163:ILE:HG23	2:B:167:GLU:HB2	1.97	0.45
2:B:185(B):GLN:CG	2:B:223:LYS:HG2	2.46	0.45
2:B:54:SER:OG	2:B:196:GLY:HA3	2.17	0.45
2:B:34:TYR:HE1	2:B:40:TYR:HB2	1.82	0.45
2:D:134:THR:HG22	2:D:135:SER:N	2.32	0.45
2:D:165:HIS:CE1	2:D:169:GLN:NE2	2.84	0.45
2:B:103:ILE:O	2:B:103:ILE:HG23	2.15	0.45
2:D:160:VAL:HG23	2:D:184:ALA:O	2.17	0.45
2:B:17:ILE:CG2	2:B:17:ILE:O	2.64	0.45
2:B:77:THR:HG22	2:B:77:THR:O	2.17	0.45
2:B:206:ARG:H	2:B:206:ARG:HD2	1.81	0.45
2:D:94:TYR:HD1	2:D:100:HIS:O	2.00	0.45
2:D:115:SER:H	2:D:118:ILE:HB	1.83	0.44
1:A:7:ARG:NH2	2:B:116:ARG:HE	2.08	0.44
2:B:122:CYS:CB	2:B:208:THR:HG22	2.45	0.44
2:B:20:GLU:O	2:B:21:PHE:C	2.53	0.44
2:B:46:LEU:HA	2:B:46:LEU:HD23	1.86	0.44
2:B:53:ILE:HG23	2:B:53:ILE:O	2.17	0.44
2:B:202:SER:HB3	2:B:207:MET:CE	2.48	0.44
2:B:61:LYS:O	2:B:64:TYR:HD1	1.99	0.44
2:D:112:ALA:O	2:D:114:PRO:HD3	2.18	0.44
2:D:45:SER:O	2:D:52:VAL:HA	2.17	0.44
2:B:172:TYR:HB2	2:B:176:VAL:HG22	2.00	0.44
2:B:56:THR:OG1	2:B:102:ASP:HA	2.17	0.44
2:D:50:CYS:HA	2:D:108:ILE:CG1	2.48	0.44
2:D:48:SER:CB	2:D:49:PRO:CD	2.96	0.44
2:D:67:TYR:CE1	2:D:82:LYS:HB2	2.53	0.44
2:D:74:ASN:O	2:D:75:SER:HB2	2.18	0.44
2:B:126:MET:O	2:B:128:ASN:N	2.50	0.44
2:D:191:CYS:SG	2:D:192:GLN:N	2.87	0.44
2:D:97:ASP:OD1	2:D:98:ALA:N	2.50	0.44
2:B:217:ARG:NH1	2:B:217:ARG:HG2	2.32	0.43
1:C:4:LYS:CE	2:D:29:TRP:HH2	2.31	0.43
1:A:5:THR:HG22	1:A:6:LEU:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:190:SER:O	2:B:191:CYS:HB2	2.18	0.43
2:B:125:SER:H	2:B:128:ASN:HD21	1.66	0.43
2:D:76:ASN:OD1	2:D:76:ASN:N	2.51	0.43
2:D:136:CYS:HB3	2:D:200:VAL:O	2.19	0.43
2:D:94:TYR:CD1	2:D:95:SER:N	2.87	0.43
2:B:112:ALA:O	2:B:114:PRO:HD3	2.17	0.43
2:B:234:PHE:N	2:B:234:PHE:CD1	2.87	0.43
2:B:27:GLN:HG3	2:B:139:THR:CG2	2.41	0.43
2:B:27:GLN:HG2	2:B:157:MET:CE	2.48	0.43
2:D:27:GLN:HE21	2:D:29:TRP:HE1	1.67	0.43
2:B:132:PHE:CD1	2:B:132:PHE:O	2.72	0.42
2:B:140:GLY:C	2:B:142:GLY:H	2.23	0.42
2:B:189:ASP:HB2	2:B:221:ALA:HB2	2.01	0.42
2:B:197:GLY:HA2	2:B:198:PRO:HD3	1.64	0.42
2:B:124:PRO:HD3	2:B:209:LEU:O	2.19	0.42
2:B:60:ILE:HG22	2:B:60(A):ASP:H	1.81	0.42
2:B:217:ARG:NH2	2:B:222:LEU:HD11	2.35	0.42
2:B:230:ARG:CD	2:B:232:SER:HB2	2.49	0.42
2:D:165:HIS:HE1	2:D:169:GLN:NE2	2.14	0.42
2:B:143:LYS:NZ	2:B:146:SER:O	2.50	0.42
2:B:138:ILE:CG2	2:B:199:LEU:HD23	2.49	0.42
2:D:165:HIS:CE1	2:D:169:GLN:OE1	2.73	0.42
2:B:121:ILE:H	2:B:121:ILE:HG13	1.71	0.42
2:B:143:LYS:HE3	2:B:145:ASN:O	2.20	0.42
2:B:60:ILE:HD13	2:B:60:ILE:HA	1.83	0.42
2:B:137:GLU:O	2:B:200:VAL:HB	2.20	0.42
2:D:51:TRP:NE1	2:D:242:THR:HG23	2.35	0.41
2:B:143:LYS:HD2	2:B:148:ASP:O	2.19	0.41
2:B:151:TYR:HA	2:B:152:PRO:HD2	1.83	0.41
2:D:165:HIS:ND1	2:D:169:GLN:OE1	2.53	0.41
2:D:41:VAL:HG21	2:D:64:TYR:CE1	2.53	0.41
2:B:87:ASN:HB3	2:B:107:LYS:HB3	2.03	0.41
2:D:203:LEU:HA	2:D:203:LEU:HD23	1.69	0.41
2:D:215:TRP:HE3	2:D:216:GLY:HA2	1.85	0.41
2:B:217:ARG:HG2	3:B:1:0GJ:OE2	2.21	0.41
2:B:61:LYS:CE	2:B:62(A):GLU:HB2	2.50	0.41
2:B:116:ARG:CB	2:B:116:ARG:NH1	2.80	0.41
2:D:47:MET:SD	2:D:121:ILE:HD11	2.61	0.41
2:D:53:ILE:CG2	2:D:53:ILE:O	2.69	0.41
2:B:172:TYR:CE1	2:B:224:LYS:CD	3.02	0.41
2:D:215:TRP:CE3	2:D:216:GLY:N	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:CYS:C	2:B:122:CYS:SG	3.00	0.40
2:B:23:THR:C	2:B:25:GLU:H	2.24	0.40
2:B:88:LEU:HD23	2:B:90:LEU:HD11	2.02	0.40
2:B:185(A):PRO:O	2:B:185(B):GLN:HB2	2.21	0.40
2:D:228:TYR:N	2:D:228:TYR:CD1	2.89	0.40
2:D:33:ILE:HD13	2:D:66:VAL:HG23	2.03	0.40
2:B:166:ARG:O	2:B:170:GLN:HG3	2.21	0.40
2:B:167:GLU:HA	2:B:170:GLN:OE1	2.21	0.40
2:D:17:ILE:HG12	2:D:144:GLU:C	2.42	0.40
2:D:166:ARG:HH11	2:D:166:ARG:CG	2.32	0.40
2:D:67:TYR:OH	2:D:82:LYS:HE3	2.21	0.40
2:B:163:ILE:HG23	2:B:167:GLU:CB	2.52	0.40
2:D:172:TYR:HB2	2:D:176:VAL:CG2	2.52	0.40

All (9) 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)
2:D:110(B):GLU:OE2	2:D:206:ARG:NH2[5_655]	1.72	0.48
2:B:127:TYR:O	2:D:166:ARG:NE[6_675]	1.76	0.44
2:B:127:TYR:CB	2:D:166:ARG:NH2[6_675]	1.96	0.24
2:B:127:TYR:CB	2:D:166:ARG:CZ[6_675]	1.97	0.23
2:B:127:TYR:CA	2:D:166:ARG:NH2[6_675]	1.98	0.22
2:B:127:TYR:CB	2:D:166:ARG:NE[6_675]	1.98	0.22
2:B:127:TYR:O	2:D:166:ARG:CD[6_675]	2.11	0.09
2:B:37:HIS:CD2	2:B:116:ARG:NH2[3_675]	2.17	0.03
2:B:127:TYR:C	2:D:166:ARG:NE[6_675]	2.18	0.02

5.3 Torsion angles [\(i\)](#)

5.3.1 Protein backbone [\(i\)](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	7/23 (30%)	5 (71%)	2 (29%)	0	100	100
1	C	6/23 (26%)	6 (100%)	0	0	100	100
2	B	246/253 (97%)	179 (73%)	42 (17%)	25 (10%)	0	0
2	D	246/253 (97%)	181 (74%)	48 (20%)	17 (7%)	1	1
All	All	505/552 (92%)	371 (74%)	92 (18%)	42 (8%)	1	1

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	37(C)	GLY
2	B	60	ILE
2	B	92	LYS
2	B	127	TYR
2	D	24	ILE
2	D	48	SER
2	D	73	LEU
2	D	75	SER
2	D	126	MET
2	B	73	LEU
2	D	92	LYS
2	D	114	PRO
2	D	142	GLY
2	B	20	GLU
2	B	114	PRO
2	B	116	ARG
2	B	133	GLY
2	B	152	PRO
2	B	221	ALA
2	D	102	ASP
2	B	18	GLY
2	B	37(D)	SER
2	B	97(B)	LEU
2	B	198	PRO
2	D	184	ALA
2	D	189	ASP
2	D	221	ALA
2	B	24	ILE
2	B	185(B)	GLN
2	D	49	PRO
2	B	28	PRO
2	B	48	SER
2	B	130	PRO

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Mol	Chain	Res	Type
2	B	195	SER
2	D	27	GLN
2	D	41	VAL
2	D	185(A)	PRO
2	B	19	GLY
2	B	225	PRO
2	B	103	ILE
2	B	185(A)	PRO
2	D	236	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	7/22 (32%)	7 (100%)	0	100	100
1	C	7/22 (32%)	7 (100%)	0	100	100
2	B	217/220 (99%)	179 (82%)	38 (18%)	2	3
2	D	217/220 (99%)	180 (83%)	37 (17%)	2	3
All	All	448/484 (93%)	373 (83%)	75 (17%)	2	4

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	24	ILE
2	B	37(A)	ARG
2	B	46	LEU
2	B	50	CYS
2	B	54	SER
2	B	60(B)	TYR
2	B	61	LYS
2	B	65	ILE
2	B	68	LEU
2	B	78	GLN
2	B	81	MET
2	B	87	ASN

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Mol	Chain	Res	Type
2	B	88	LEU
2	B	90	LEU
2	B	97(B)	LEU
2	B	102	ASP
2	B	117	THR
2	B	121	ILE
2	B	127	TYR
2	B	132	PHE
2	B	147	THR
2	B	165	HIS
2	B	168	CYS
2	B	169	GLN
2	B	176	VAL
2	B	177	THR
2	B	178	THR
2	B	185	ASP
2	B	185(A)	PRO
2	B	186	TRP
2	B	190	SER
2	B	198	PRO
2	B	199	LEU
2	B	206	ARG
2	B	209	LEU
2	B	217	ARG
2	B	222	LEU
2	B	225	PRO
2	D	24	ILE
2	D	37(A)	ARG
2	D	38	VAL
2	D	50	CYS
2	D	56	THR
2	D	60(B)	TYR
2	D	72	ARG
2	D	73	LEU
2	D	76	ASN
2	D	78	GLN
2	D	80	GLU
2	D	81	MET
2	D	87	ASN
2	D	90	LEU
2	D	97(A)	THR
2	D	97(B)	LEU

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Mol	Chain	Res	Type
2	D	102	ASP
2	D	106	LEU
2	D	113	GLN
2	D	116	ARG
2	D	121	ILE
2	D	123	LEU
2	D	127	TYR
2	D	149	TYR
2	D	150	LEU
2	D	171	TYR
2	D	179	LYS
2	D	185(A)	PRO
2	D	186	TRP
2	D	187	LYS
2	D	190	SER
2	D	199	LEU
2	D	207	MET
2	D	209	LEU
2	D	217	ARG
2	D	223(A)	ASP
2	D	231	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	26	ASN
2	B	37	HIS
2	B	78	GLN
2	B	87	ASN
2	B	91	HIS
2	B	204	GLN
2	D	26	ASN
2	D	87	ASN
2	D	128	ASN
2	D	165	HIS
2	D	170	GLN
2	D	185(B)	GLN
2	D	204	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

2 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
3	0GJ	B	1	2	20,24,25	0.73	1 (5%)	23,30,31	0.94	2 (8%)
3	0GJ	D	1	2	20,24,25	0.58	0	23,30,31	0.82	1 (4%)

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	0GJ	B	1	2	-	6/27/29/31	-
3	0GJ	D	1	2	-	5/27/29/31	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1	0GJ	C3-C2	2.84	1.60	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1	0GJ	O2-C2-C3	-2.83	101.37	109.74
3	B	1	0GJ	O2-C2-C3	-2.82	101.39	109.74
3	B	1	0GJ	CB1-CA2-C2	2.19	116.31	112.51

There are no chirality outliers.

All (11) torsion outliers are listed below:

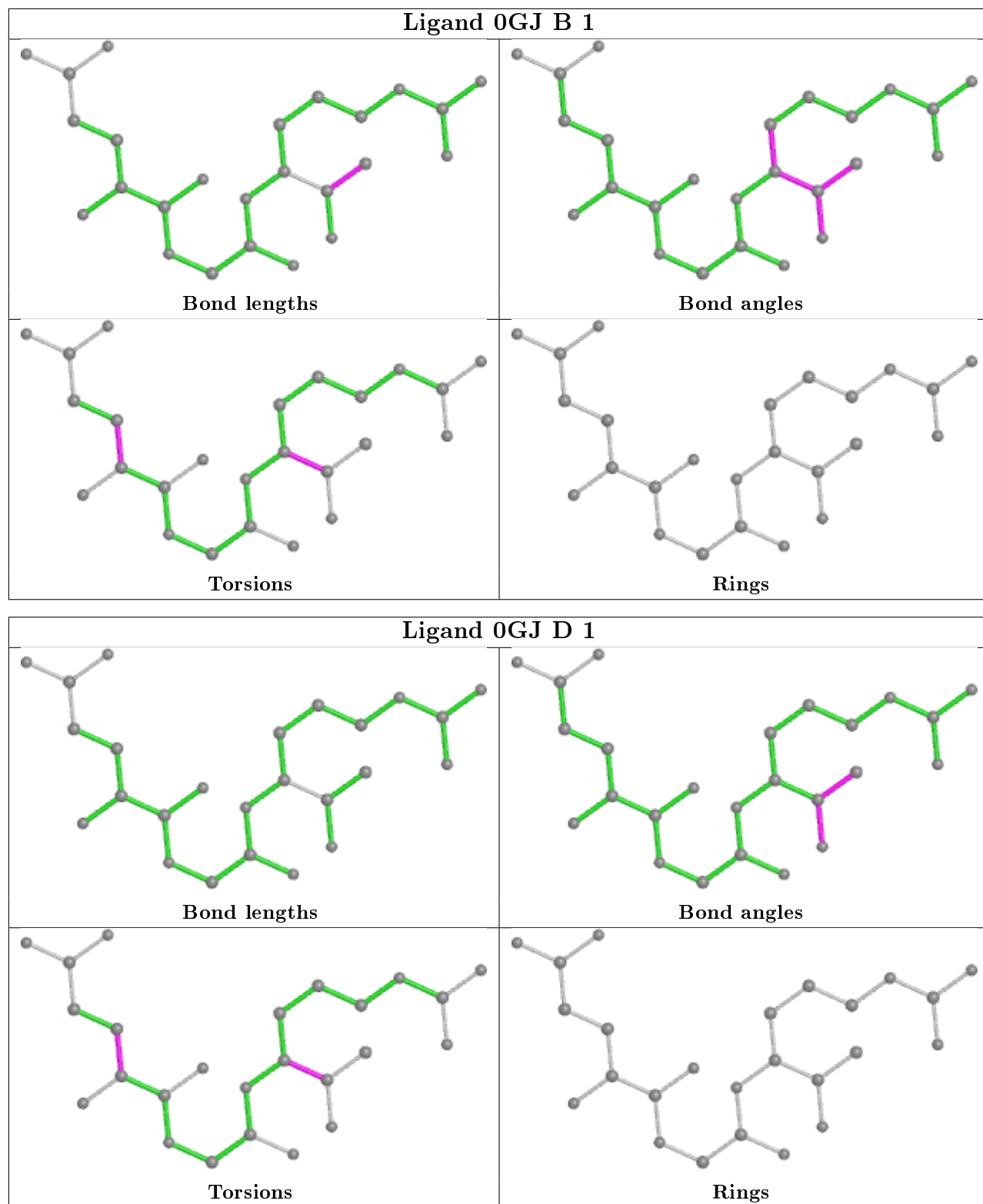
Mol	Chain	Res	Type	Atoms
3	B	1	0GJ	N-CA-CB-CG
3	B	1	0GJ	O2-C2-CA2-CB1
3	D	1	0GJ	N-CA-CB-CG
3	D	1	0GJ	O2-C2-CA2-CB1
3	B	1	0GJ	C-CA-CB-CG
3	B	1	0GJ	O2-C2-CA2-N2
3	B	1	0GJ	C3-C2-CA2-N2
3	D	1	0GJ	O2-C2-CA2-N2
3	D	1	0GJ	C3-C2-CA2-N2
3	B	1	0GJ	C3-C2-CA2-CB1
3	D	1	0GJ	C-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1	0GJ	1	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

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.