



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 09:16 AM UTC

PDB ID : 1LMW / pdb_00001lmw
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 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)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
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

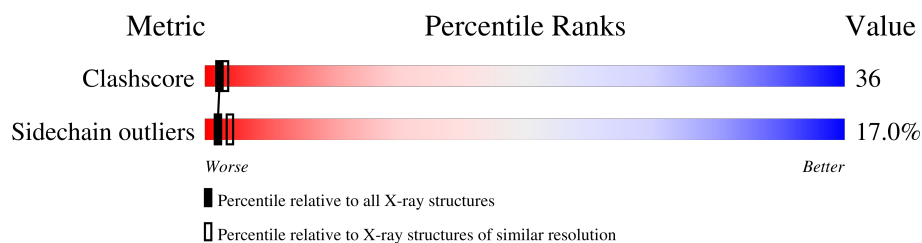
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

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	190562	6492 (2.50-2.50)
Sidechain outliers	187428	6380 (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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	23	
1	C	23	
2	B	253	
2	D	253	

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.

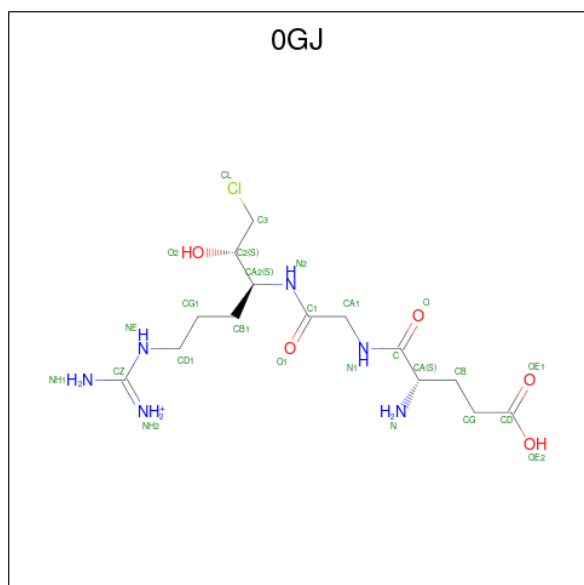
- Molecule 1 is a protein called UROKINASE-TYPE PLASMINOGEN ACTIVATOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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
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 (CCD ID: 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		

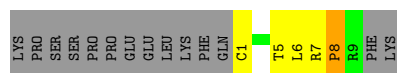
3 Residue-property plots

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.

Note EDS was not executed.

• Molecule 1: UROKINASE-TYPE PLASMINOGEN ACTIVATOR

Chain A: 



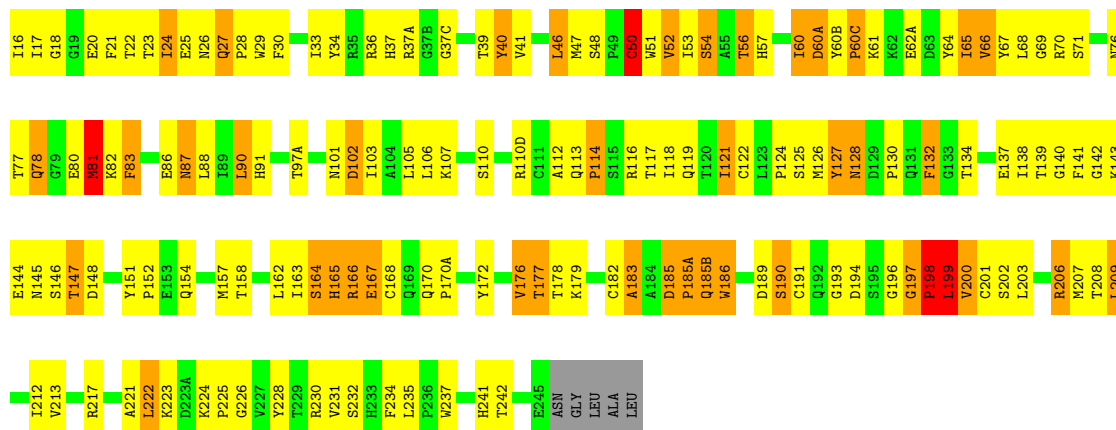
• Molecule 1: UROKINASE-TYPE PLASMINOGEN ACTIVATOR

Chain C: 

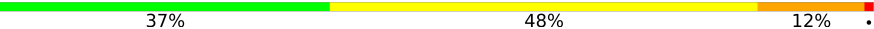


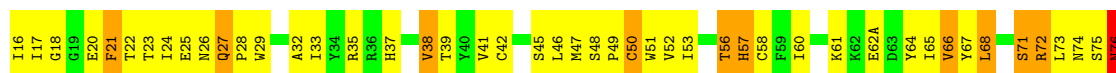
• Molecule 2: UROKINASE-TYPE PLASMINOGEN ACTIVATOR

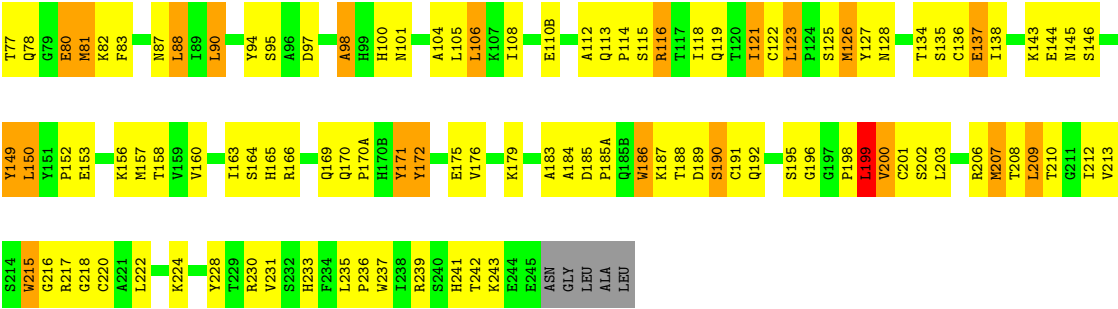
Chain B: 



• Molecule 2: UROKINASE-TYPE PLASMINOGEN ACTIVATOR

Chain D: 





4 Data and refinement statistics

Xtriage (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	176.70 Å 176.70 Å 54.40 Å 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.	Xtriage
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	1.08	1/62 (1.6%)	1.23	0/82
1	C	0.74	0/61	0.74	0/80
2	B	0.80	0/2009	1.33	27/2720 (1.0%)
2	D	0.76	0/2009	1.26	25/2720 (0.9%)
All	All	0.79	1/4141 (0.0%)	1.29	52/5602 (0.9%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	8	PRO	C-N	-5.19	1.26	1.33

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	197	GLY	CA-C-N	14.26	137.67	119.84
2	B	197	GLY	C-N-CA	14.26	137.67	119.84
2	B	199	LEU	N-CA-C	-11.01	90.79	108.73
2	D	199	LEU	N-CA-C	-10.21	93.02	109.76
2	D	66	VAL	N-CA-C	8.19	120.12	108.17
2	D	21	PHE	N-CA-C	-7.84	97.81	109.81
2	D	27	GLN	CA-C-N	7.72	127.39	119.82
2	D	27	GLN	C-N-CA	7.72	127.39	119.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	198	PRO	N-CA-C	7.71	128.36	112.47
2	B	66	VAL	N-CA-C	7.33	118.37	108.11
2	B	200	VAL	N-CA-C	7.26	118.35	107.75
2	D	200	VAL	N-CA-C	7.11	119.19	107.24
2	D	38	VAL	N-CA-C	6.90	118.53	108.53
2	D	76	ASN	N-CA-C	6.66	120.03	110.24
2	D	116	ARG	N-CA-C	6.60	118.56	111.36
2	B	37(C)	GLY	N-CA-C	6.52	128.63	113.18
2	D	224	LYS	CA-C-N	6.42	126.39	120.03
2	D	224	LYS	C-N-CA	6.42	126.39	120.03
2	D	172	TYR	N-CA-C	6.39	120.39	112.59
2	B	193	GLY	N-CA-C	-6.38	105.96	114.25
2	B	165	HIS	N-CA-C	-6.23	104.41	111.14
2	D	215	TRP	N-CA-C	6.22	116.66	107.88
2	B	56	THR	N-CA-C	6.21	118.13	111.36
2	D	98	ALA	N-CA-C	6.20	118.71	110.53
2	B	242	THR	N-CA-C	6.15	118.78	111.71
2	B	226	GLY	N-CA-C	-6.05	100.87	111.46
2	B	50	CYS	N-CA-C	6.01	119.57	112.72
2	B	186	TRP	N-CA-C	5.88	120.26	113.38
2	B	76	ASN	N-CA-C	5.82	119.03	110.30
2	D	196	GLY	N-CA-C	-5.77	108.22	115.08
2	B	67	TYR	N-CA-C	5.77	118.36	109.07
2	B	164	SER	N-CA-C	5.66	118.80	110.59
2	D	126	MET	N-CA-C	5.65	122.84	110.80
2	B	52	VAL	N-CA-C	-5.61	101.32	109.29
2	D	150	LEU	N-CA-C	5.52	118.55	109.72
2	B	27	GLN	CA-C-N	5.50	126.72	119.84
2	B	27	GLN	C-N-CA	5.50	126.72	119.84
2	D	81	MET	N-CA-C	5.50	118.05	108.76
2	B	81	MET	N-CA-C	5.44	117.27	108.41
2	B	128	ASN	N-CA-C	5.42	118.58	107.69
2	D	71	SER	N-CA-C	5.41	120.15	113.50
2	B	33	ILE	N-CA-C	5.39	115.62	107.80
2	B	167	GLU	N-CA-C	5.39	117.01	111.03
2	D	164	SER	N-CA-C	5.27	118.09	110.28
2	B	183	ALA	N-CA-C	5.23	117.70	108.75
2	D	235	LEU	CA-C-N	-5.17	113.38	119.84
2	D	235	LEU	C-N-CA	-5.17	113.38	119.84
2	D	113	GLN	CA-C-N	5.15	126.28	119.84
2	D	113	GLN	C-N-CA	5.15	126.28	119.84
2	D	20	GLU	N-CA-C	5.12	116.45	109.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	40	TYR	N-CA-C	5.05	116.98	109.25
2	B	83	PHE	N-CA-C	5.02	117.30	109.52

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 ⓘ

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	154	8
2	D	1960	0	1901	134	8
3	B	25	0	24	1	0
3	D	25	0	24	0	0
All	All	4093	0	3986	293	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 36.

All (293) 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:24:ILE:HG13	2:B:71:SER:HB3	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:27:GLN:HG3	2:B:139:THR:HG21	1.60	0.82
2:B:191:CYS:O	2:B:194:ASP:HB2	1.82	0.78
2:D:202:SER:HB3	2:D:207:MET:HE3	1.65	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
2:D:27:GLN:OE1	2:D:157:MET:HE3	1.89	0.73
2:D:27:GLN:HG3	2:D:29:TRP:NE1	2.03	0.73
2:D:126:MET:HE1	2:D:236:PRO:HG3	1.71	0.71
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:21:PHE:HD2	2:B:154:GLN:HB3	1.55	0.70
2:B:130:PRO:HG3	2:B:203:LEU:HD21	1.73	0.70
2:B:202:SER:HB3	2:B:207:MET:HE3	1.73	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:23:THR:H	2:B:26:ASN:HD22	1.40	0.69
2:B:91:HIS:HD2	2:B:101:ASN:HB3	1.57	0.69
2:D:170:GLN:CD	2:D:170(A):PRO:HD2	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:112:ALA:C	2:B:114:PRO:HD3	2.20	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:B:26:ASN:HB3	2:B:157:MET:HE1	1.80	0.63
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
2:D:106:LEU:HD12	2:D:106:LEU:N	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:56:THR:CG2	2:D:90:LEU:HB3	2.30	0.61
2:D:122:CYS:O	2:D:208:THR:HG22	2.00	0.61
2:D:23:THR:C	2:D:25:GLU:H	2.08	0.61
2:B:37:HIS:HB3	2:B:37(A):ARG:HH12	1.65	0.61
2:B:17:ILE:HG22	2:B:17:ILE:O	2.00	0.60
2:D:239:ARG:HH11	2:D:243:LYS:HZ1	1.48	0.60
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:B:81:MET:HE3	2:B:82:LYS:H	1.66	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:60:ILE:O	2:B:60(C):PRO:HD3	2.02	0.59
2:B:138:ILE:HG22	2:B:198:PRO:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:185:ASP:CG	2:D:185(A):PRO:HD2	2.28	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:HG2	2:B:217:ARG:HH11	1.68	0.58
2:D:166:ARG:HH11	2:D:166:ARG:HG2	1.70	0.57
2:D:41:VAL:CG1	2:D:58:CYS:HB3	2.35	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: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
2:B:78:GLN:H	2:B:78:GLN:CD	2.13	0.55
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:112:ALA:C	2:D:114:PRO:HD3	2.32	0.54
2:D:27:GLN:NE2	2:D:200:VAL:HG21	2.22	0.54
2:B:47:MET:HE2	2:B:53:ILE:HG21	1.90	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: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
2:B:97(A):THR:HA	2:D:60:ILE:CD1	2.39	0.53
1:C:4:LYS:HE3	2:D:29:TRP:HH2	1.74	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:D:186:TRP:C	2:D:187:LYS:HD2	2.34	0.53
2:B:27:GLN:CG	2:B:139:THR:HG21	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:17:ILE:HG22	2:D:17:ILE:O	2.10	0.52
2:D:128:ASN:HD21	2:D:203:LEU:HD13	1.75	0.52
2:D:23:THR:H	2:D:26:ASN:HD22	1.56	0.52
2:D:41:VAL:HG21	2:D:64:TYR:HE1	1.75	0.51
2:B:116:ARG:HH11	2:B:116:ARG:CB	2.23	0.51
2:B:37(A):ARG:H	2:B:37(A):ARG:CZ	2.24	0.51
2:D:123:LEU:HD12	2:D:123:LEU:H	1.76	0.51
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:D:202:SER:CB	2:D:207:MET:HE3	2.37	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
2:D:215:TRP:HE3	2:D:216:GLY:N	2.10	0.50
2:B:106:LEU:HD12	2:B:106:LEU:N	2.27	0.49
2:B:69:GLY:O	2:B:80:GLU:HB3	2.12	0.49
2:B:116:ARG:HB2	2:B:116:ARG:HH11	1.75	0.49
2:B:20:GLU:O	2:B:21:PHE:C	2.53	0.49
2:B:90:LEU:HD12	2:B:90:LEU:H	1.77	0.49
2:B:86:GLU:HG3	2:B:86:GLU:O	2.12	0.49
2:B:69:GLY:O	2:B:80:GLU:CB	2.61	0.48
2:B:138:ILE:HG22	2:B:199:LEU:HA	1.93	0.48
2:D:171:TYR:N	2:D:171:TYR:CD1	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:16:ILE:HG22	2:D:18:GLY:H	1.78	0.48
2:D:105:LEU:HD12	2:D:237:TRP:CH2	2.48	0.48
2:D:171:TYR:N	2:D:171:TYR:HD1	2.11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:16:ILE:CG2	2:B:18:GLY:H	2.27	0.47
2:B:40:TYR:CE2	2:B:141:PHE:HB2	2.49	0.47
2:B:51:TRP:CE3	2:B:105:LEU:HB3	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:140:GLY:C	2:B:142:GLY:H	2.23	0.47
2:B:145:ASN:OD1	2:B:147:THR:HG23	2.14	0.47
2:D:66:VAL:HG13	2:D:83:PHE:HB2	1.95	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:B:237:TRP:NE1	2:B:241:HIS:NE2	2.63	0.47
2:D:242:THR:O	2:D:242:THR:HG22	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:O	2:D:53:ILE:HG23	2.14	0.46
1:A:5:THR:CG2	1:A:6:LEU:N	2.78	0.46
2:D:46:LEU:HD11	2:D:68:LEU:HD21	1.96	0.46
2:D:143:LYS:HB3	2:D:145:ASN:O	2.15	0.46
2:D:23:THR:C	2:D:25:GLU:N	2.74	0.46
2:D:27:GLN:N	2:D:28:PRO:CD	2.78	0.46
2:D:126:MET:HE1	2:D:236:PRO:CG	2.43	0.46
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
1:A:1:CYS:C	2:B:122:CYS:SG	3.00	0.45
2:B:23:THR:C	2:B:25:GLU:H	2.24	0.45
2:B:54:SER:OG	2:B:196:GLY:HA3	2.17	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: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:HG23	2:B:103:ILE:O	2.15	0.45
2:D:17:ILE:HG12	2:D:144:GLU:C	2.42	0.45
2:D:160:VAL:HG23	2:D:184:ALA:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:17:ILE:O	2:B:17:ILE:CG2	2.64	0.45
2:B:77:THR:O	2:B:77:THR:HG22	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:46:LEU:HD23	2:B:46:LEU:HA	1.86	0.44
2:B:53:ILE:HG23	2:B:53:ILE:O	2.17	0.44
2:B:61:LYS:O	2:B:64:TYR:HD1	1.99	0.44
2:D:45:SER:O	2:D:52:VAL:HA	2.17	0.44
2:D:112:ALA:O	2:D:114:PRO:HD3	2.18	0.44
2:B:56:THR:OG1	2:B:102:ASP:HA	2.17	0.44
2:B:172:TYR:HB2	2:B:176:VAL:HG22	2.00	0.44
2:D:48:SER:CB	2:D:49:PRO:CD	2.96	0.44
2:D:50:CYS:HA	2:D:108:ILE:CG1	2.48	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:D:185:ASP:O	2:D:185(A):PRO:C	2.61	0.44
2:B:126:MET:O	2:B:128:ASN:N	2.50	0.44
2:D:97:ASP:OD1	2:D:98:ALA:N	2.50	0.44
2:D:191:CYS:SG	2:D:192:GLN:N	2.87	0.44
2:B:217:ARG:HG2	2:B:217:ARG:NH1	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
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:B:30:PHE:CD1	2:B:30:PHE:C	2.95	0.43
2:D:136:CYS:HB3	2:D:200:VAL:O	2.19	0.43
2:B:185:ASP:O	2:B:185(A):PRO:C	2.61	0.43
2:D:94:TYR:CD1	2:D:95:SER:N	2.87	0.43
2:B:27:GLN:HG3	2:B:139:THR:CG2	2.41	0.43
2:B:112:ALA:O	2:B:114:PRO:HD3	2.17	0.43
2:B:113:GLN:O	2:B:114:PRO:C	2.61	0.43
2:B:234:PHE:CD1	2:B:234:PHE:N	2.87	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:189:ASP:HB2	2:B:221:ALA:HB2	2.01	0.42
2:B:124:PRO:HD3	2:B:209:LEU:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:197:GLY:HA2	2:B:198:PRO:HD3	1.64	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:138:ILE:CG2	2:B:199:LEU:HD23	2.49	0.42
2:B:143:LYS:NZ	2:B:146:SER:O	2.50	0.42
2:D:57:HIS:CD2	2:D:57:HIS:C	2.98	0.42
2:D:165:HIS:CE1	2:D:169:GLN:OE1	2.73	0.42
2:B:60:ILE:HD13	2:B:60:ILE:HA	1.83	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: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:41:VAL:HG21	2:D:64:TYR:CE1	2.53	0.41
2:D:165:HIS:ND1	2:D:169:GLN:OE1	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:61:LYS:CE	2:B:62(A):GLU:HB2	2.50	0.41
2:B:217:ARG:HG2	3:B:1:0GJ:OE2	2.21	0.41
2:B:116:ARG:NH1	2:B:116:ARG:CB	2.80	0.41
2:B:57:HIS:C	2:B:57:HIS:CD2	2.97	0.41
2:D:47:MET:SD	2:D:121:ILE:HD11	2.61	0.41
2:D:53:ILE:O	2:D:53:ILE:CG2	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
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:33:ILE:HD13	2:D:66:VAL:HG23	2.03	0.40
2:D:228:TYR:N	2:D:228:TYR:CD1	2.89	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:67:TYR:OH	2:D:82:LYS:HE3	2.21	0.40
2:D:166:ARG:HH11	2:D:166:ARG:CG	2.32	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](#)

There are no protein backbone outliers to report in this entry.

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%)	177 (82%)	40 (18%)	1	3
2	D	198/220 (90%)	165 (83%)	33 (17%)	2	4
All	All	429/484 (89%)	356 (83%)	73 (17%)	2	4

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	24	ILE
2	B	41	VAL
2	B	46	LEU
2	B	50	CYS
2	B	54	SER

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Mol	Chain	Res	Type
2	B	60	ILE
2	B	60(A)	ASP
2	B	60(B)	TYR
2	B	60(C)	PRO
2	B	65	ILE
2	B	68	LEU
2	B	78	GLN
2	B	81	MET
2	B	87	ASN
2	B	90	LEU
2	B	102	ASP
2	B	114	PRO
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	166	ARG
2	B	168	CYS
2	B	176	VAL
2	B	177	THR
2	B	178	THR
2	B	185	ASP
2	B	185(A)	PRO
2	B	185(B)	GLN
2	B	186	TRP
2	B	190	SER
2	B	198	PRO
2	B	199	LEU
2	B	201	CYS
2	B	206	ARG
2	B	209	LEU
2	B	222	LEU
2	B	225	PRO
2	D	38	VAL
2	D	39	THR
2	D	50	CYS
2	D	56	THR
2	D	65	ILE
2	D	68	LEU
2	D	72	ARG

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Mol	Chain	Res	Type
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	88	LEU
2	D	90	LEU
2	D	106	LEU
2	D	116	ARG
2	D	121	ILE
2	D	123	LEU
2	D	125	SER
2	D	127	TYR
2	D	137	GLU
2	D	149	TYR
2	D	150	LEU
2	D	171	TYR
2	D	179	LYS
2	D	186	TRP
2	D	190	SER
2	D	199	LEU
2	D	207	MET
2	D	209	LEU
2	D	217	ARG
2	D	231	VAL

Sometimes 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	113	GLN
2	D	119	GLN
2	D	128	ASN
2	D	165	HIS
2	D	170	GLN
2	D	185(B)	GLN

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Mol	Chain	Res	Type
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 oligosaccharides 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	23,24,25	0.82	1 (4%)	26,30,31	0.87	1 (3%)
3	0GJ	D	1	2	23,24,25	0.69	0	26,30,31	0.92	2 (7%)

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	-	6/29/29/31	-
3	0GJ	D	1	2	-	6/29/29/31	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1	0GJ	C3-C2	2.94	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	-2.78	101.37	109.68
3	B	1	0GJ	O2-C2-C3	-2.77	101.39	109.68
3	D	1	0GJ	C2-CA2-N2	-2.14	107.01	110.90

There are no chirality outliers.

All (12) 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
3	D	1	0GJ	C3-C2-CA2-CB1

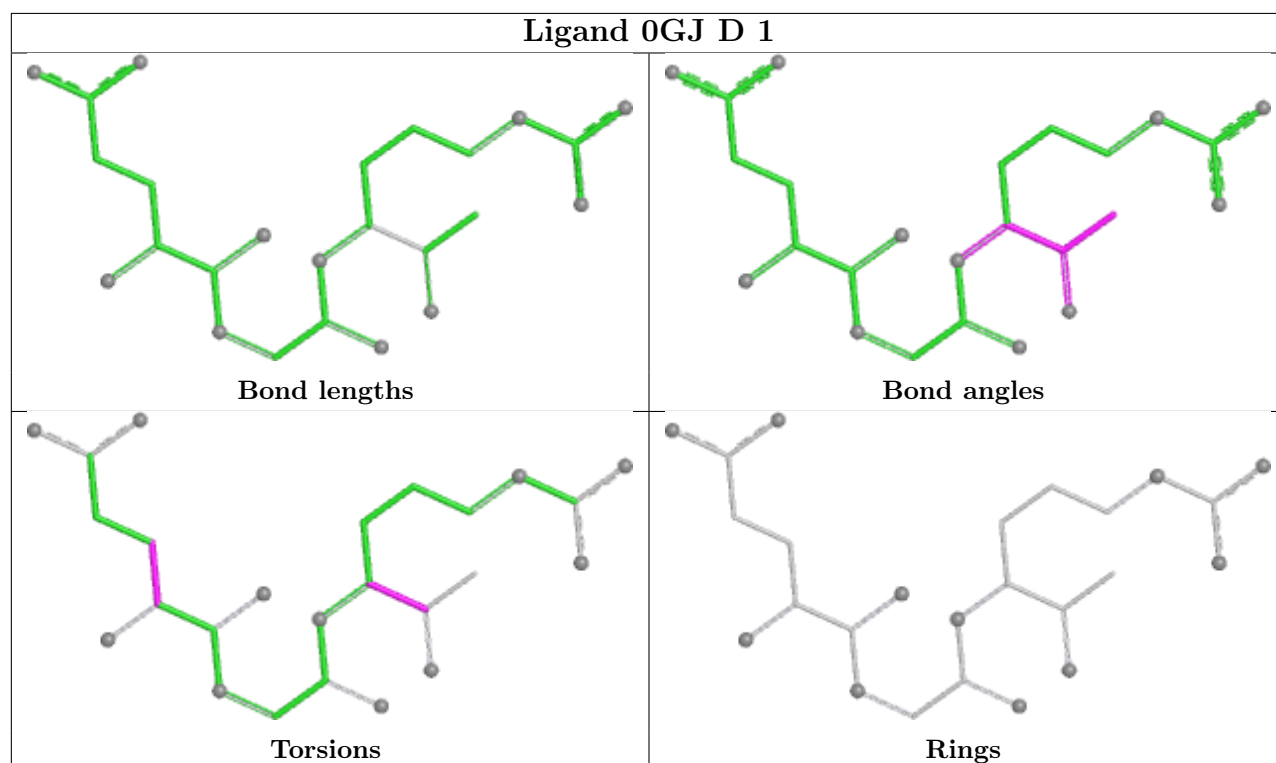
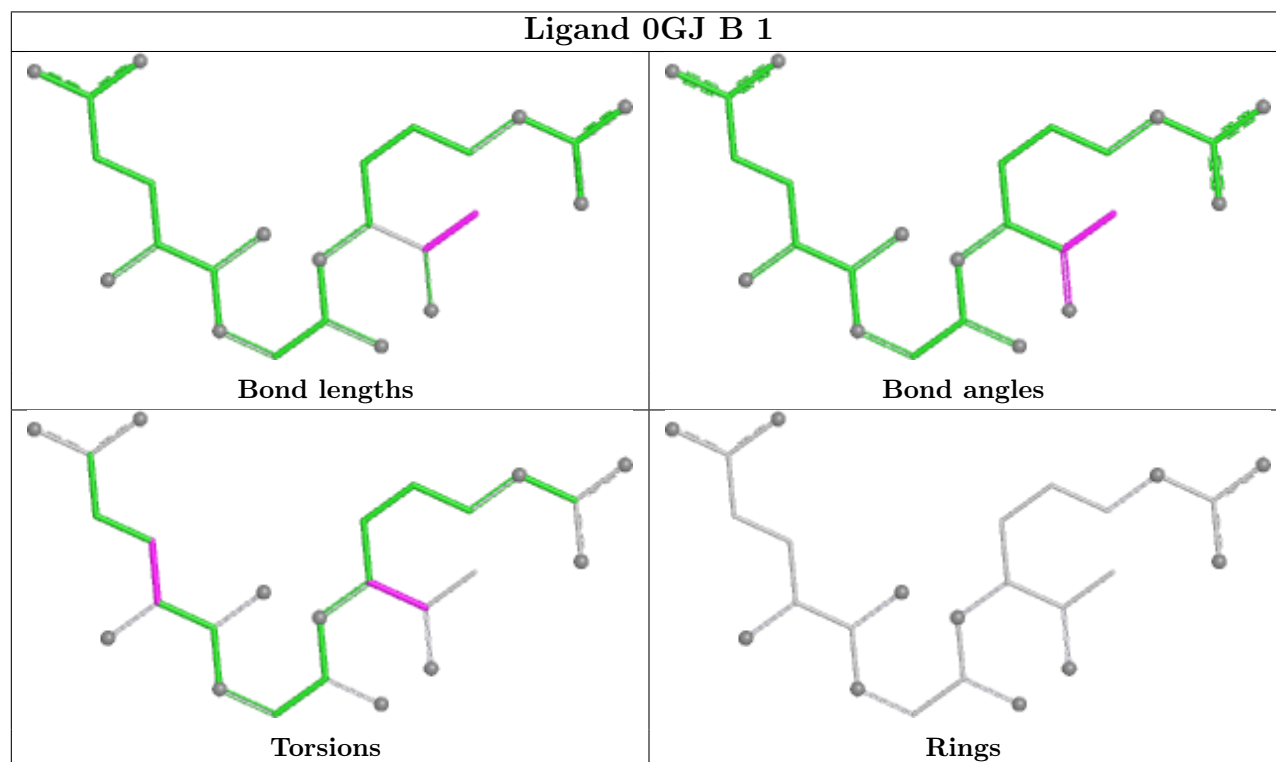
There are no ring outliers.

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 [i](#)

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.