Full wwPDB X-ray Structure Validation Report (i)

Nov 16, 2023 – 06:00 AM JST

PDB ID	:	6L20
Title	:	Crystal structure of CK2a2 with hematein
Authors	:	Tsuyuguchi, M.; Kinoshita, T.
Deposited on	:	2019-10-02
Resolution	:	3.09 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

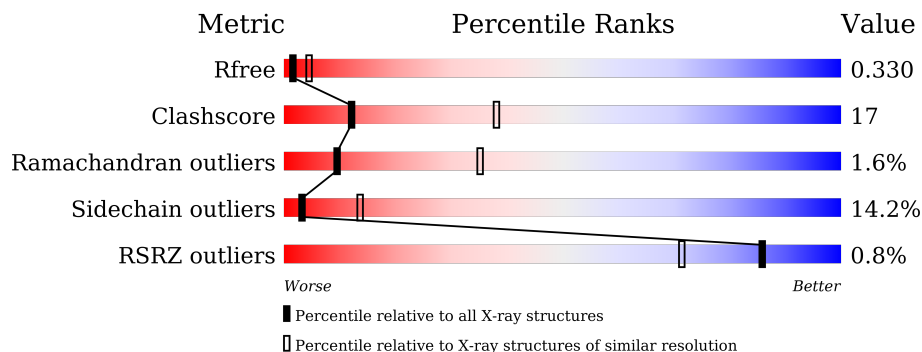|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.09 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	Percentile Ranks	Value
Rfree		0.330
Clashscore		17
Ramachandran outliers		1.6%
Sidechain outliers		14.2%
RSRZ outliers		0.8%

Worse　　　　　　　　　　　　　　　Better

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1447 (3.10-3.06)
Clashscore	141614	1546 (3.10-3.06)
Ramachandran outliers	138981	1487 (3.10-3.06)
Sidechain outliers	138945	1486 (3.10-3.06)
RSRZ outliers	127900	1416 (3.10-3.06)

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	338	% 49% 39% 5% 7%
1	D	338	% 46% 40% 7% 7%
1	G	338	% 47% 39% 8% 6%
1	J	338	57% 31% 5% 7%

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 10746 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 Casein kinase II subunit alpha'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	313	Total	C	N	O	S	0	0	0
			2655	1715	461	469	10			
1	D	313	Total	C	N	O	S	0	0	0
			2645	1710	458	467	10			
1	G	319	Total	C	N	O	S	0	0	0
			2699	1736	472	481	10			
1	J	314	Total	C	N	O	S	0	0	0
			2657	1712	463	472	10			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP P19784
A	-3	PRO	-	expression tag	UNP P19784
A	-2	LEU	-	expression tag	UNP P19784
A	-1	GLY	-	expression tag	UNP P19784
A	0	SER	-	expression tag	UNP P19784
D	-4	GLY	-	expression tag	UNP P19784
D	-3	PRO	-	expression tag	UNP P19784
D	-2	LEU	-	expression tag	UNP P19784
D	-1	GLY	-	expression tag	UNP P19784
D	0	SER	-	expression tag	UNP P19784
G	-4	GLY	-	expression tag	UNP P19784
G	-3	PRO	-	expression tag	UNP P19784
G	-2	LEU	-	expression tag	UNP P19784
G	-1	GLY	-	expression tag	UNP P19784
G	0	SER	-	expression tag	UNP P19784
J	-4	GLY	-	expression tag	UNP P19784
J	-3	PRO	-	expression tag	UNP P19784
J	-2	LEU	-	expression tag	UNP P19784
J	-1	GLY	-	expression tag	UNP P19784
J	0	SER	-	expression tag	UNP P19784

- Molecule 2 is (6aR)-3,4,6a,10-tetrakis(oxidanyl)-6,7-dihydroindeno[2,1-c]chromen-9-one (three-letter code: E3U) (formula: $C_{16}H_{12}O_6$) (labeled as "Ligand of Interest" by depositor).
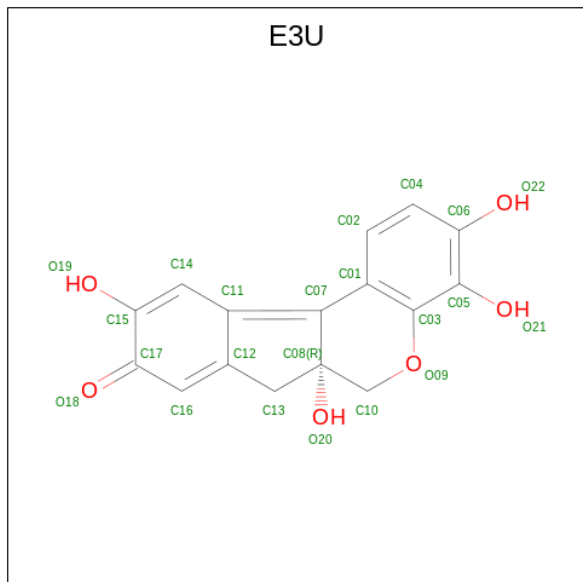
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 22	C 16	O 6	0	0
2	D	1	Total 22	C 16	O 6	0	0
2	G	1	Total 22	C 16	O 6	0	0
2	J	1	Total 22	C 16	O 6	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

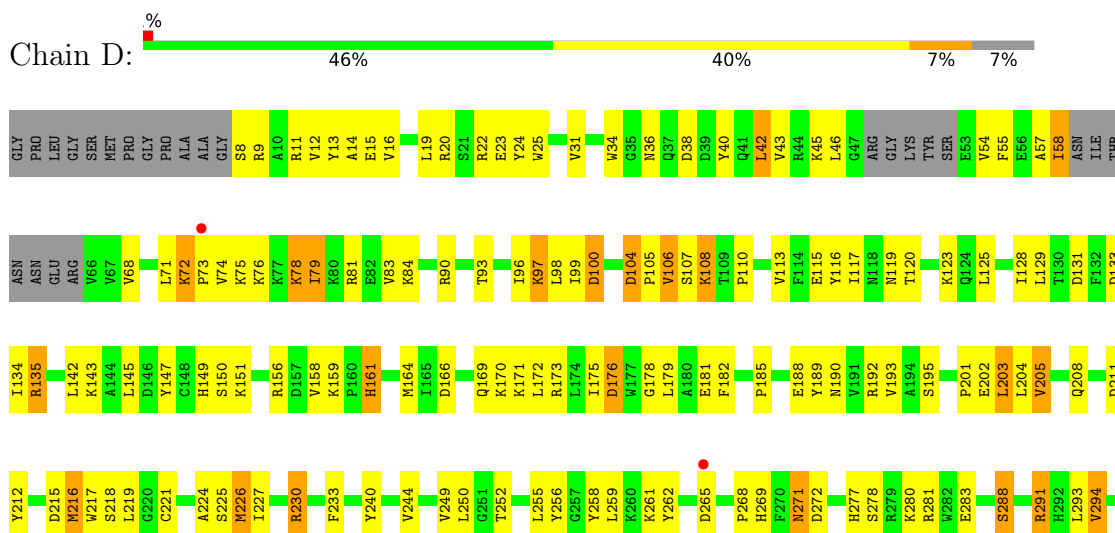| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Cl 1	0	0
3	D	1	Total 1	Cl 1	0	0

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Casein kinase II subunit alpha'

Chain A:

• Molecule 1: Casein kinase II subunit alpha'

Chain D:

D300 L301 L302 D303 K304 L305 L306 R307 Y308 D309 R313 L314 T315 E318 A319 M320 Y324 F325 V328 V329 Q332 SER

• Molecule 1: Casein kinase II subunit alpha'

Chain G:

%

| 47% | 39% | 8% | 6% |

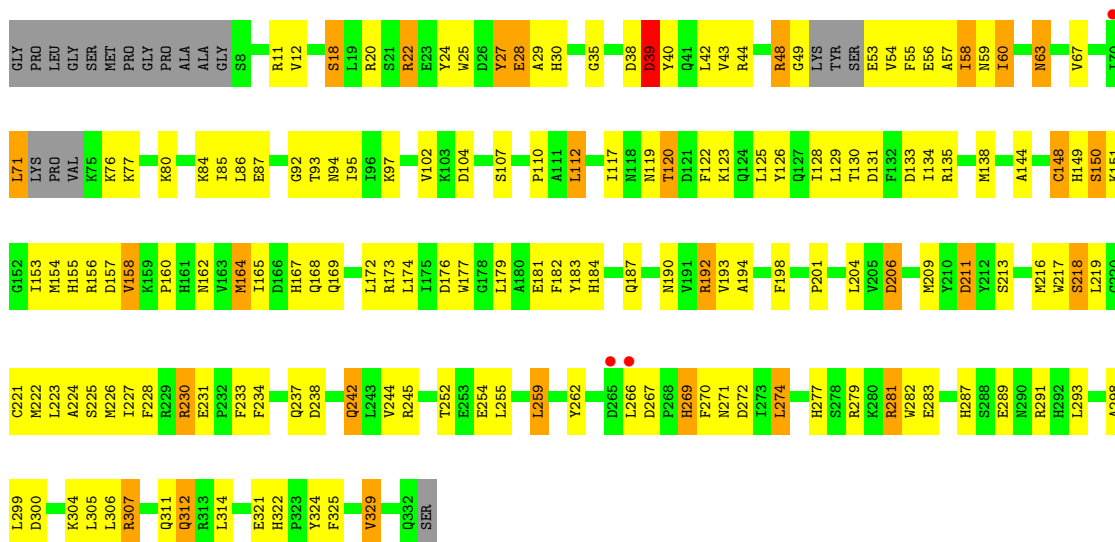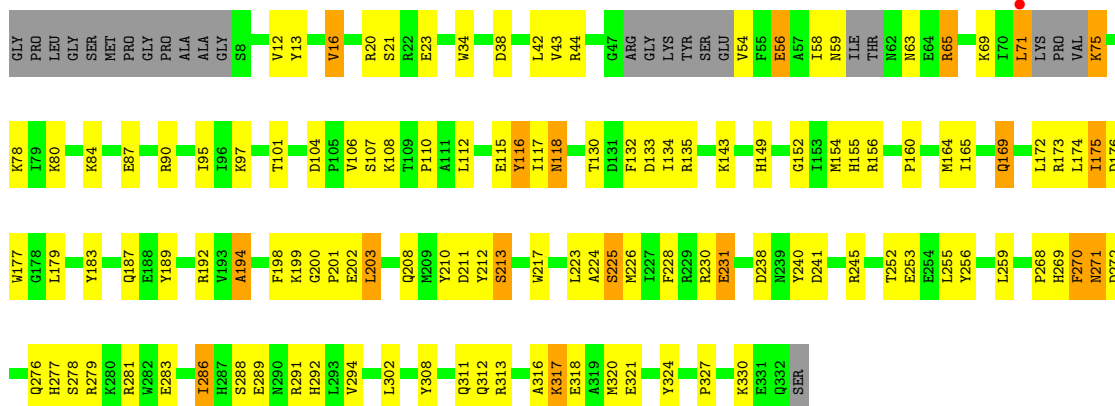GLY PRO LEU GLY SER MET PRO GLY PRO ALA ALA GLY S8 R11 V12 S18 L19 R20 S21 R22 E23 Y24 W25 D26 Y27 E28 A29 H30 G35 D38 D39 Y40 Q41 L42 V43 R44 R48 G49 LYS TYR SER E53 V54 F55 E56 A57 I58 N59 I60 N63 V67 I70

L71 LYS PRO VAL K75 K76 K77 K80 K84 I85 L86 E87 G92 T93 N94 I95 I96 K97 V102 K103 D104 S107 P110 A111 L112 I117 N118 N119 T120 D121 F122 K123 Q124 L125 Y126 Q127 I128 L129 T130 D131 F132 D133 I134 R135 M138 A144 C148 H149 S150 K151

G152 I153 M154 H155 R156 D157 V158 K159 P160 H161 N162 V163 M164 I165 D166 H167 Q168 Q169 L172 R173 L174 I175 D176 W177 G178 L179 A180 E181 F182 Y183 H184 Q187 N190 V191 R192 V193 A194 F198 P201 L204 V205 D206 M209 Y210 D211 Y212 S213 M216 W217 S218 L219 G220

C221 M222 L223 A224 S225 M226 I227 F228 R229 R230 E231 P232 F233 F234 Q237 D238 Q242 L243 V244 R245 T252 E253 E254 L255 L259 Y262 D265 L266 D267 P268 H269 F270 N271 D272 I273 L274 H277 S278 R279 K280 R281 W282 E283 H287 S288 E289 N290 R291 H292 L293 A298

L299 D300 K304 L305 L306 R307 Q311 Q312 R313 L314 E321 H322 P323 Y324 F325 V329 Q332 SER

• Molecule 1: Casein kinase II subunit alpha'

Chain J:

| 57% | 31% | 5% | 7% |

GLY PRO LEU GLY SER MET PRO GLY PRO ALA ALA GLY S8 V12 Y13 V16 R20 S21 R22 E23 W34 D38 L42 V43 R44 G47 ARG GLY LYS TYR SER GLU V54 F55 E56 A57 I58 N59 ILE THR N62 N63 E64 R65 K69 I70 L71 LYS PRO VAL K75

K78 I79 K80 K84 E87 R90 I95 I96 K97 T101 D104 P105 V106 S107 K108 T109 P110 A111 L112 E115 Y116 I117 N118 T130 D131 F132 D133 I134 R135 K143 H149 G152 I153 M154 H155 R156 P160 M164 I165 Q169 L172 R173 L174 I175 D176

W177 G178 L179 Y183 Q187 E188 Y189 R192 V193 A194 F198 K199 G200 P201 E202 L203 Q208 M209 Y210 D211 Y212 S213 W217 L223 A224 S225 M226 I227 F228 R229 R230 E231 D238 N239 Y240 D241 R245 T252 E253 E254 L255 Y256 L259 P268 H269 F270 N271 D272

Q276 H277 S278 R279 K280 R281 W282 E283 I286 H287 S288 E289 N290 R291 H292 L293 V294 L302 Y308 Q311 Q312 R313 A316 K317 E318 A319 M320 E321 Y324 P327 K330 E331 Q332 SER

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	46.70Å 89.14Å 95.99Å 81.15° 86.05° 90.06°	Depositor
Resolution (Å)	35.04 – 3.09 46.59 – 3.09	Depositor EDS
% Data completeness (in resolution range)	96.9 (35.04-3.09) 98.1 (46.59-3.09)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.07 (at 3.06Å)	Xtriage
Refinement program	REFMAC 5, PHENIX 1.9_1692+SVN	Depositor
R, R_{free}	0.241 , 0.326 0.246 , 0.330	Depositor DCC
R_{free} test set	2748 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å^2)	48.2	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 42.0	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10746	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 87.41 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.9114e-08. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CL, E3U

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	0.55	0/2723	0.67	0/3674
1	D	0.54	0/2713	0.66	0/3661
1	G	0.54	0/2766	0.66	0/3731
1	J	0.55	0/2723	0.66	0/3672
All	All	0.55	0/10925	0.66	0/14738

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2655	0	2635	91	0
1	D	2645	0	2623	104	0
1	G	2699	0	2667	102	0
1	J	2657	0	2622	71	0
2	A	22	0	0	4	0
2	D	22	0	0	6	0
2	G	22	0	0	5	0
2	J	22	0	0	2	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	1	0	0	0	0
All	All	10746	0	10547	365	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

All (365) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:156:ARG:HH11	1:G:181:GLU:HB2	1.13	1.08
1:G:156:ARG:NH1	1:G:181:GLU:HB2	1.69	1.05
1:G:156:ARG:HH21	1:G:193:VAL:HG11	1.28	0.96
1:G:156:ARG:HH11	1:G:181:GLU:CB	1.85	0.89
1:D:117:ILE:HG13	1:D:173:ARG:HG3	1.57	0.84
1:A:46:LEU:HB2	1:A:54:VAL:HG12	1.60	0.83
1:D:40:TYR:HA	1:D:58:ILE:HG23	1.65	0.78
1:J:199:LYS:HG2	1:J:203:LEU:HD23	1.66	0.76
1:J:291:ARG:O	1:J:291:ARG:NH1	2.18	0.76
1:D:205:VAL:HG21	1:D:259:LEU:HD21	1.67	0.75
1:A:68:VAL:HG22	1:A:113:VAL:HG22	1.68	0.74
1:D:68:VAL:HG22	1:D:113:VAL:HG22	1.70	0.74
1:A:141:LEU:HD23	1:A:219:LEU:HD12	1.70	0.72
1:G:134:ILE:HD13	1:G:226:MET:HB3	1.71	0.72
1:J:59:ASN:O	1:J:65:ARG:N	2.23	0.72
1:D:72:LYS:HB3	1:D:73:PRO:HD2	1.70	0.71
1:D:134:ILE:HD12	1:D:226:MET:HB2	1.72	0.71
1:J:87:GLU:HG2	1:J:90:ARG:HH12	1.54	0.70
1:D:90:ARG:NH1	1:D:98:LEU:O	2.23	0.70
1:J:58:ILE:HD11	1:J:63:ASN:HA	1.72	0.70
1:A:202:GLU:OE2	1:A:313:ARG:NH2	2.27	0.67
1:D:227:ILE:HD12	1:D:294:VAL:HG13	1.75	0.67
1:G:156:ARG:NH2	1:G:193:VAL:HG11	2.05	0.67
1:A:71:LEU:HD12	1:A:110:PRO:HB2	1.78	0.66
1:G:117:ILE:N	2:G:401:E3U:O22	2.26	0.65
1:G:156:ARG:NH1	1:G:181:GLU:CB	2.51	0.65
1:D:181:GLU:HG2	1:D:189:TYR:CE1	2.31	0.65
1:A:169:GLN:HB3	1:A:171:LYS:HG2	1.79	0.65
1:G:259:LEU:HD21	1:G:266:LEU:HB3	1.78	0.64
1:G:183:TYR:CE1	1:G:211:ASP:HB3	2.32	0.64
1:J:156:ARG:O	1:J:194:ALA:HB2	1.98	0.64
1:D:268:PRO:O	1:D:271:ASN:ND2	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:28:GLU:HG2	1:G:77:LYS:HG3	1.79	0.64
1:A:252:THR:HG23	1:A:277:HIS:HB2	1.80	0.63
1:D:79:ILE:O	1:D:83:VAL:HG23	1.98	0.63
1:D:71:LEU:HD23	1:D:79:ILE:HD13	1.79	0.63
1:J:327:PRO:HA	1:J:330:LYS:HE3	1.80	0.63
1:J:16:VAL:HB	1:J:20:ARG:HH12	1.65	0.62
1:A:272:ASP:OD1	1:A:272:ASP:N	2.32	0.62
1:G:157:ASP:OD2	1:G:162:ASN:ND2	2.32	0.61
1:A:43:VAL:HG23	1:A:57:ALA:HA	1.82	0.61
1:D:224:ALA:HB2	1:D:302:LEU:HD11	1.81	0.61
1:G:157:ASP:O	1:G:162:ASN:ND2	2.31	0.61
1:A:160:PRO:HD3	1:A:198:PHE:CZ	2.36	0.61
1:D:24:TYR:OH	1:D:151:LYS:HB3	2.00	0.61
1:A:40:TYR:HA	1:A:58:ILE:HG23	1.82	0.60
1:G:300:ASP:OD2	1:G:322:HIS:NE2	2.33	0.60
1:A:16:VAL:HG13	1:A:20:ARG:HH21	1.66	0.60
1:G:129:LEU:HD22	1:G:133:ASP:HB3	1.82	0.60
1:A:220:GLY:O	1:A:223:LEU:N	2.35	0.60
1:D:43:VAL:HG23	1:D:57:ALA:HA	1.84	0.60
1:J:44:ARG:H	1:J:56:GLU:HB2	1.67	0.60
1:G:135:ARG:NH1	1:G:324:TYR:O	2.35	0.59
1:G:154:MET:HB3	1:G:156:ARG:HG3	1.83	0.59
1:J:43:VAL:HB	1:J:56:GLU:HB3	1.84	0.59
1:A:122:PHE:HB2	1:A:126:TYR:CE1	2.37	0.59
1:D:147:TYR:O	1:D:151:LYS:HG2	2.02	0.59
1:A:97:LYS:N	1:A:115:GLU:OE2	2.36	0.59
1:D:216:MET:HG3	1:D:314:LEU:O	2.02	0.59
1:J:156:ARG:NH2	1:J:210:TYR:OH	2.29	0.59
1:D:252:THR:HG23	1:D:277:HIS:HB2	1.85	0.59
1:G:71:LEU:HD12	1:G:110:PRO:HB2	1.85	0.59
1:G:281:ARG:HB3	1:G:283:GLU:OE1	2.03	0.58
1:G:43:VAL:HG12	1:G:44:ARG:HG3	1.86	0.58
1:G:28:GLU:HA	1:G:80:LYS:HD2	1.84	0.58
1:A:57:ALA:HB3	1:A:66:VAL:HG23	1.85	0.58
1:G:158:VAL:HB	1:G:218:SER:HB2	1.84	0.58
1:A:162:ASN:ND2	1:A:176:ASP:HB3	2.19	0.58
1:A:309:ASP:HB3	1:A:312:GLN:HB2	1.86	0.57
1:G:184:HIS:HB2	1:G:187:GLN:HG3	1.85	0.57
1:J:54:VAL:HA	1:J:69:LYS:HA	1.86	0.57
1:J:256:TYR:HA	1:J:259:LEU:HD12	1.85	0.57
1:D:16:VAL:HG13	1:D:20:ARG:NH1	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:149:HIS:CD2	1:D:212:TYR:HB3	2.40	0.57
1:D:135:ARG:HB3	1:D:324:TYR:CE2	2.40	0.57
1:D:211:ASP:OD1	1:D:212:TYR:N	2.38	0.57
1:G:156:ARG:HH21	1:G:193:VAL:CG1	2.09	0.57
1:J:225:SER:OG	1:J:231:GLU:HG2	2.05	0.57
1:A:166:ASP:O	1:A:170:LYS:N	2.38	0.56
1:J:183:TYR:CE1	1:J:211:ASP:HB3	2.40	0.56
1:A:24:TYR:OH	1:A:151:LYS:HB3	2.05	0.56
1:A:135:ARG:HD3	1:A:324:TYR:O	2.05	0.56
1:G:85:ILE:HD13	1:G:153:ILE:HG12	1.86	0.56
1:A:117:ILE:HG13	1:A:173:ARG:HG3	1.87	0.56
1:J:13:TYR:O	1:J:16:VAL:HG22	2.06	0.56
1:D:314:LEU:HD22	1:D:318:GLU:HB3	1.88	0.56
1:A:232:PRO:HD2	1:A:235:HIS:ND1	2.21	0.55
1:J:154:MET:HG3	1:J:156:ARG:CG	2.37	0.55
1:A:152:GLY:O	1:A:183:TYR:N	2.26	0.55
1:G:244:VAL:HG22	1:G:274:LEU:HD23	1.88	0.55
1:D:307:ARG:HB2	1:D:313:ARG:HG3	1.88	0.55
1:J:132:PHE:HA	1:J:135:ARG:HD2	1.89	0.55
1:J:176:ASP:OD1	2:J:401:E3U:O21	2.25	0.54
1:J:116:TYR:OH	1:J:118:ASN:OD1	2.25	0.54
1:D:325:PHE:O	1:D:329:VAL:HG13	2.07	0.54
1:J:75:LYS:HE2	1:J:78:LYS:HE3	1.89	0.54
1:J:149:HIS:CE1	1:J:212:TYR:HB3	2.42	0.54
1:J:268:PRO:O	1:J:271:ASN:ND2	2.38	0.54
1:J:154:MET:HG3	1:J:156:ARG:HD2	1.88	0.54
1:D:288:SER:O	1:D:291:ARG:NH1	2.40	0.54
1:J:224:ALA:O	1:J:228:PHE:HB2	2.08	0.53
1:A:255:LEU:HB2	1:A:308:TYR:CZ	2.42	0.53
1:J:176:ASP:HA	2:J:401:E3U:O22	2.08	0.53
1:G:49:GLY:HA3	1:G:53:GLU:N	2.23	0.53
1:A:71:LEU:HD21	1:A:112:LEU:HG	1.91	0.53
1:D:97:LYS:HB3	1:D:115:GLU:HB2	1.91	0.53
1:A:192:ARG:HH21	1:G:206:ASP:HB3	1.74	0.52
1:J:316:ALA:O	1:J:320:MET:HG3	2.09	0.52
1:J:34:TRP:CH2	1:J:110:PRO:HB3	2.44	0.52
1:D:169:GLN:HB3	1:D:171:LYS:HG2	1.92	0.52
1:D:249:VAL:HG12	1:D:250:LEU:HD12	1.91	0.52
1:G:267:ASP:OD1	1:G:269:HIS:HB3	2.10	0.52
1:D:240:TYR:CE1	1:D:269:HIS:HB2	2.45	0.52
1:D:42:LEU:HD13	1:D:55:PHE:CG	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:134:ILE:HD12	1:G:293:LEU:HD22	1.92	0.52
1:J:164:MET:HG2	1:J:175:ILE:HD13	1.90	0.52
1:G:27:TYR:O	1:G:29:ALA:N	2.43	0.52
1:A:188:GLU:HB3	1:A:208:GLN:HB3	1.92	0.52
1:G:125:LEU:O	1:G:129:LEU:HG	2.10	0.52
1:J:134:ILE:HD13	1:J:226:MET:HB3	1.92	0.51
1:D:117:ILE:CG1	1:D:173:ARG:HG3	2.37	0.51
1:A:164:MET:HG3	1:A:175:ILE:HG21	1.92	0.51
1:G:254:GLU:OE1	1:G:254:GLU:N	2.44	0.51
1:D:181:GLU:HG2	1:D:189:TYR:HE1	1.71	0.51
1:D:281:ARG:HH22	1:G:312:GLN:HA	1.76	0.51
1:J:16:VAL:O	1:J:20:ARG:NH1	2.44	0.51
1:A:130:THR:C	1:A:132:PHE:H	2.13	0.51
1:D:156:ARG:NE	1:D:179:LEU:O	2.31	0.51
1:G:48:ARG:HG2	1:G:49:GLY:H	1.75	0.51
1:A:72:LYS:O	1:A:74:VAL:N	2.41	0.51
1:D:166:ASP:O	1:D:170:LYS:N	2.44	0.51
1:G:56:GLU:HG2	1:G:57:ALA:H	1.76	0.51
1:G:38:ASP:O	1:G:39:ASP:HB2	2.11	0.51
1:D:283:GLU:CD	1:G:11:ARG:HH22	2.14	0.50
1:G:282:TRP:CH2	1:G:306:LEU:HD12	2.47	0.50
1:A:292:HIS:NE2	1:A:293:LEU:HG	2.27	0.50
1:J:241:ASP:O	1:J:245:ARG:HG2	2.11	0.50
1:A:201:PRO:O	1:A:205:VAL:HG22	2.12	0.50
1:G:104:ASP:HB3	1:G:107:SER:OG	2.12	0.50
1:G:201:PRO:HA	1:G:204:LEU:HD12	1.94	0.50
1:J:143:LYS:HG3	1:J:320:MET:HE1	1.92	0.50
1:A:69:LYS:NZ	2:A:401:E3U:O18	2.36	0.50
1:G:160:PRO:HD3	1:G:198:PHE:CZ	2.47	0.50
1:A:160:PRO:HD3	1:A:198:PHE:CE2	2.47	0.50
1:G:24:TYR:OH	1:G:151:LYS:HB3	2.12	0.50
1:G:40:TYR:HA	1:G:58:ILE:O	2.12	0.50
1:J:211:ASP:OD2	1:J:213:SER:OG	2.30	0.50
1:G:190:ASN:OD1	1:G:192:ARG:HB2	2.12	0.49
1:D:104:ASP:OD1	1:D:106:VAL:HG13	2.12	0.49
1:D:188:GLU:HG2	1:D:208:GLN:HB2	1.93	0.49
1:A:34:TRP:CD2	1:A:103:LYS:HE3	2.47	0.49
1:D:164:MET:O	1:D:172:LEU:HA	2.12	0.49
1:G:234:PHE:HB2	1:G:242:GLN:HE22	1.77	0.49
1:J:71:LEU:HD21	1:J:112:LEU:HG	1.93	0.49
1:J:211:ASP:OD2	1:J:211:ASP:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:261:LYS:HE2	1:D:262:TYR:CZ	2.47	0.49
1:A:300:ASP:O	1:A:304:LYS:HG3	2.12	0.49
1:A:325:PHE:O	1:A:329:VAL:HG13	2.13	0.49
1:A:25:TRP:HA	1:A:182:PHE:CE1	2.47	0.49
1:A:142:LEU:HD21	1:A:216:MET:HE1	1.95	0.48
1:A:229:ARG:HE	1:A:293:LEU:HD12	1.78	0.48
1:D:176:ASP:HA	2:D:401:E3U:O18	2.14	0.48
1:A:310:HIS:HA	1:A:313:ARG:CZ	2.44	0.48
1:D:172:LEU:O	1:D:173:ARG:NH1	2.47	0.48
1:G:25:TRP:HA	1:G:182:PHE:CE1	2.49	0.48
1:A:103:LYS:HG2	1:A:110:PRO:HA	1.95	0.48
1:D:131:ASP:O	1:D:135:ARG:HG2	2.13	0.48
1:A:130:THR:O	1:A:132:PHE:N	2.47	0.48
1:D:300:ASP:OD2	1:D:304:LYS:NZ	2.44	0.48
1:G:59:ASN:O	1:G:63:ASN:N	2.46	0.48
1:G:218:SER:O	1:G:222:MET:HG3	2.13	0.48
1:J:255:LEU:HB2	1:J:308:TYR:CZ	2.48	0.48
1:A:16:VAL:O	1:A:20:ARG:HG3	2.14	0.48
1:A:289:GLU:OE2	1:A:289:GLU:HA	2.14	0.48
1:A:292:HIS:CD2	1:A:293:LEU:HG	2.48	0.47
1:D:12:VAL:HG22	1:D:13:TYR:CD2	2.49	0.47
1:J:283:GLU:O	1:J:286:ILE:HG13	2.14	0.47
1:A:183:TYR:CZ	1:A:185:PRO:HA	2.49	0.47
1:D:325:PHE:O	1:D:328:VAL:N	2.47	0.47
1:G:67:VAL:HG21	2:G:401:E3U:C06	2.44	0.47
1:D:22:ARG:HA	1:D:25:TRP:CE2	2.49	0.47
1:G:138:MET:HE2	1:G:223:LEU:HD13	1.96	0.47
1:D:22:ARG:HA	1:D:25:TRP:NE1	2.30	0.47
1:J:240:TYR:HD1	1:J:270:PHE:CZ	2.32	0.47
1:J:286:ILE:HD13	1:J:294:VAL:HG11	1.96	0.47
1:A:54:VAL:HG23	1:A:69:LYS:HG3	1.95	0.47
1:A:172:LEU:O	1:A:173:ARG:NH1	2.45	0.47
1:D:81:ARG:NH2	1:D:178:GLY:O	2.47	0.47
1:D:129:LEU:HD22	1:D:133:ASP:HB3	1.97	0.47
1:G:155:HIS:HD2	1:G:174:LEU:HD21	1.80	0.47
1:D:175:ILE:HD12	2:D:401:E3U:C11	2.44	0.47
1:D:181:GLU:HG3	1:D:182:PHE:N	2.30	0.47
1:D:252:THR:O	1:D:256:TYR:HD2	1.97	0.47
1:G:221:CYS:N	1:G:306:LEU:HD21	2.29	0.47
1:D:72:LYS:HB3	1:D:73:PRO:CD	2.43	0.47
1:J:149:HIS:ND1	1:J:212:TYR:HB3	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:GLU:O	1:A:18:SER:N	2.48	0.47
1:A:67:VAL:HG21	2:A:401:E3U:C04	2.44	0.47
1:G:262:TYR:OH	1:G:311:GLN:HB2	2.15	0.47
1:J:154:MET:HG3	1:J:156:ARG:CD	2.45	0.47
1:J:179:LEU:HD12	1:J:179:LEU:HA	1.78	0.47
1:D:145:LEU:O	1:D:149:HIS:ND1	2.48	0.46
1:G:27:TYR:O	1:G:30:HIS:N	2.49	0.46
1:A:155:HIS:HD2	1:A:177:TRP:CZ3	2.34	0.46
1:D:14:ALA:O	1:D:185:PRO:HG3	2.14	0.46
1:J:117:ILE:HG13	1:J:173:ARG:HG3	1.97	0.46
1:A:248:LYS:O	1:A:280:LYS:NZ	2.46	0.46
1:D:203:LEU:O	1:D:204:LEU:HB2	2.15	0.46
1:J:200:GLY:HA2	1:J:217:TRP:CD1	2.50	0.46
1:A:40:TYR:CD1	1:A:66:VAL:HG21	2.51	0.46
1:D:22:ARG:HG3	1:D:25:TRP:CZ2	2.51	0.46
1:D:179:LEU:HD23	1:D:193:VAL:HB	1.97	0.46
1:D:159:LYS:NZ	1:D:195:SER:HB2	2.31	0.46
1:D:240:TYR:O	1:D:244:VAL:HG23	2.16	0.46
1:D:302:LEU:HG	1:D:306:LEU:HD12	1.98	0.46
1:G:216:MET:HG3	1:G:314:LEU:O	2.16	0.46
1:J:252:THR:O	1:J:255:LEU:HB3	2.16	0.46
1:J:291:ARG:NH1	1:J:294:VAL:O	2.43	0.46
1:D:42:LEU:HD22	1:D:55:PHE:HB2	1.98	0.46
1:D:117:ILE:O	2:D:401:E3U:O22	2.34	0.46
1:G:86:LEU:HD21	1:G:177:TRP:CD1	2.51	0.46
1:G:149:HIS:HE1	1:G:216:MET:CE	2.28	0.46
1:A:155:HIS:CD2	1:A:174:LEU:HD21	2.51	0.45
1:D:15:GLU:O	1:D:19:LEU:HG	2.16	0.45
1:D:79:ILE:HD12	1:D:110:PRO:HG2	1.99	0.45
1:D:307:ARG:O	1:D:313:ARG:NE	2.39	0.45
1:G:122:PHE:HB2	1:G:126:TYR:CE2	2.51	0.45
1:G:238:ASP:OD1	1:G:238:ASP:N	2.50	0.45
1:G:305:LEU:HD23	1:G:314:LEU:HB2	1.97	0.45
1:A:93:THR:HG21	1:A:143:LYS:HD2	1.98	0.45
1:A:159:LYS:O	1:A:163:VAL:HG23	2.16	0.45
1:A:304:LYS:HG2	1:A:307:ARG:NH2	2.31	0.45
1:A:322:HIS:CG	1:A:323:PRO:HD2	2.51	0.45
1:A:96:ILE:HD12	1:A:175:ILE:HG22	1.99	0.45
1:A:254:GLU:H	1:A:254:GLU:CD	2.18	0.45
1:G:71:LEU:HD11	1:G:112:LEU:HD22	1.99	0.45
1:G:86:LEU:HA	1:G:86:LEU:HD23	1.72	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:172:LEU:O	1:G:173:ARG:NH1	2.35	0.45
1:J:160:PRO:HD3	1:J:198:PHE:CZ	2.51	0.45
1:G:42:LEU:HD12	1:G:55:PHE:HB2	1.98	0.45
1:G:252:THR:HG23	1:G:277:HIS:HB2	1.98	0.45
1:G:119:ASN:HD22	1:G:165:ILE:H	1.64	0.45
1:G:289:GLU:OE1	1:G:289:GLU:HA	2.17	0.45
1:G:230:ARG:HD2	1:G:233:PHE:CD1	2.52	0.45
1:J:289:GLU:O	1:J:292:HIS:HE1	2.00	0.45
1:G:131:ASP:HA	1:G:293:LEU:HD23	1.99	0.45
1:A:286:ILE:HG21	1:A:291:ARG:HD3	1.99	0.44
1:J:201:PRO:HD2	1:J:313:ARG:NH2	2.32	0.44
1:D:34:TRP:CH2	1:D:110:PRO:HB3	2.52	0.44
1:D:320:MET:HE2	1:D:320:MET:HB3	1.80	0.44
1:G:20:ARG:NH2	1:G:151:LYS:HD2	2.33	0.44
1:G:22:ARG:HG2	1:G:25:TRP:CZ2	2.52	0.44
1:G:35:GLY:H	1:G:102:VAL:HA	1.83	0.44
1:G:54:VAL:HG11	2:G:401:E3U:O20	2.17	0.44
1:J:187:GLN:HB3	1:J:189:TYR:CE2	2.52	0.44
1:G:282:TRP:HB3	1:G:299:LEU:HD22	1.99	0.44
1:D:218:SER:O	1:D:221:CYS:HB2	2.18	0.44
1:G:176:ASP:HA	2:G:401:E3U:C17	2.46	0.44
1:D:75:LYS:HG3	1:D:78:LYS:HB2	2.00	0.44
1:D:175:ILE:HD12	2:D:401:E3U:C07	2.48	0.44
1:A:158:VAL:HB	1:A:218:SER:HB3	1.98	0.44
1:D:226:MET:O	1:D:293:LEU:HD13	2.17	0.44
1:G:224:ALA:O	1:G:228:PHE:HB2	2.17	0.44
1:G:225:SER:HB2	1:G:231:GLU:HB2	2.00	0.44
1:G:304:LYS:HB3	1:G:314:LEU:HG	2.00	0.44
1:A:15:GLU:O	1:A:17:ASN:N	2.51	0.44
1:A:304:LYS:HA	1:A:307:ARG:CZ	2.47	0.44
1:J:201:PRO:HD3	1:J:217:TRP:CD2	2.53	0.44
1:J:202:GLU:HG2	1:J:203:LEU:N	2.33	0.44
1:J:211:ASP:HB2	1:J:212:TYR:H	1.63	0.44
1:D:99:ILE:O	1:D:100:ASP:HB2	2.17	0.44
1:D:307:ARG:HB2	1:D:313:ARG:CG	2.47	0.44
1:J:223:LEU:HD23	1:J:302:LEU:HD13	2.00	0.44
1:A:234:PHE:CE1	1:A:246:ILE:HA	2.52	0.44
1:G:42:LEU:HD22	1:G:42:LEU:H	1.82	0.44
1:A:117:ILE:O	2:A:401:E3U:O22	2.36	0.43
1:A:141:LEU:CD2	1:A:219:LEU:HD12	2.45	0.43
1:G:56:GLU:HG2	1:G:57:ALA:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:ILE:N	2:A:401:E3U:O22	2.39	0.43
1:G:128:ILE:HD11	1:G:167:HIS:HD2	1.82	0.43
1:A:102:VAL:O	1:A:111:ALA:N	2.52	0.43
1:G:179:LEU:HD13	1:G:193:VAL:HB	2.00	0.43
1:J:97:LYS:N	1:J:115:GLU:OE2	2.52	0.43
1:J:252:THR:HG23	1:J:277:HIS:HB2	2.00	0.43
1:A:22:ARG:HG3	1:A:25:TRP:CH2	2.54	0.43
1:D:159:LYS:HG3	1:D:161:HIS:ND1	2.34	0.43
1:D:278:SER:O	1:D:280:LYS:NZ	2.45	0.43
1:G:298:ALA:HB2	1:G:324:TYR:CE1	2.54	0.43
1:A:199:LYS:HG2	1:A:203:LEU:HD12	2.01	0.43
1:D:271:ASN:HD22	1:D:272:ASP:N	2.16	0.43
1:G:311:GLN:HB3	1:G:312:GLN:NE2	2.33	0.43
1:D:315:THR:HG23	1:D:318:GLU:OE1	2.18	0.43
1:G:149:HIS:HE1	1:G:216:MET:HE2	1.84	0.43
1:G:227:ILE:HG13	1:G:228:PHE:N	2.34	0.43
1:D:125:LEU:O	1:D:129:LEU:HG	2.19	0.43
1:D:202:GLU:HG2	1:D:203:LEU:H	1.83	0.43
1:G:201:PRO:HD3	1:G:217:TRP:CE2	2.54	0.43
1:A:164:MET:O	1:A:172:LEU:HA	2.19	0.42
1:A:295:SER:HB2	1:A:297:GLU:OE1	2.18	0.42
1:D:143:LYS:HG3	1:D:320:MET:HE3	2.00	0.42
1:D:240:TYR:HE1	1:D:269:HIS:HB2	1.82	0.42
1:G:60:ILE:H	1:G:60:ILE:HG13	1.43	0.42
1:G:92:GLY:HA3	1:G:95:ILE:HG13	2.00	0.42
1:J:130:THR:O	1:J:133:ASP:HB2	2.19	0.42
1:J:169:GLN:H	1:J:169:GLN:HG3	1.66	0.42
1:J:311:GLN:O	1:J:311:GLN:HG2	2.18	0.42
1:A:35:GLY:H	1:A:102:VAL:HA	1.85	0.42
1:G:119:ASN:HB2	1:G:164:MET:HG3	2.01	0.42
1:G:307:ARG:HE	1:G:307:ARG:HB3	1.41	0.42
1:D:158:VAL:HB	1:D:218:SER:HB3	2.00	0.42
1:J:143:LYS:CG	1:J:320:MET:HE1	2.49	0.42
1:J:155:HIS:HD2	1:J:174:LEU:HD21	1.84	0.42
1:A:159:LYS:HB3	1:A:198:PHE:CD2	2.55	0.42
1:D:105:PRO:O	1:D:108:LYS:HE2	2.20	0.42
1:A:298:ALA:HB2	1:A:324:TYR:CE1	2.55	0.42
1:D:215:ASP:O	1:D:218:SER:HB2	2.19	0.42
1:J:202:GLU:HG2	1:J:203:LEU:H	1.85	0.42
1:G:20:ARG:HH22	1:G:151:LYS:HD2	1.83	0.42
1:J:135:ARG:NH1	1:J:324:TYR:O	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:22:ARG:HG3	1:D:25:TRP:CH2	2.55	0.42
1:D:201:PRO:HD3	1:D:217:TRP:CD2	2.55	0.42
1:G:325:PHE:O	1:G:329:VAL:HG13	2.20	0.42
1:A:72:LYS:HB3	1:A:73:PRO:HD2	2.01	0.42
1:A:260:LYS:HB3	1:A:260:LYS:HE2	1.85	0.42
1:D:230:ARG:HG2	1:D:230:ARG:HH11	1.84	0.42
1:A:310:HIS:HA	1:A:313:ARG:NH1	2.34	0.41
1:G:176:ASP:HA	2:G:401:E3U:O18	2.19	0.41
1:J:104:ASP:HB3	1:J:107:SER:OG	2.20	0.41
1:J:130:THR:HG22	1:J:133:ASP:CG	2.40	0.41
1:A:280:LYS:HB3	1:A:284:ASN:ND2	2.34	0.41
1:A:230:ARG:HH21	1:A:285:PHE:HE1	1.66	0.41
1:D:255:LEU:HD13	1:D:308:TYR:CE1	2.55	0.41
1:A:130:THR:C	1:A:132:PHE:N	2.73	0.41
1:D:36:ASN:OD1	1:D:105:PRO:HG3	2.20	0.41
1:J:95:ILE:HD13	1:J:177:TRP:CZ2	2.56	0.41
1:D:54:VAL:HG11	2:D:401:E3U:O20	2.21	0.41
1:D:201:PRO:HD2	1:D:313:ARG:NH2	2.36	0.41
1:G:156:ARG:HB3	1:G:193:VAL:HG21	2.02	0.41
1:D:135:ARG:HD3	1:D:324:TYR:O	2.20	0.41
1:A:267:ASP:HA	1:A:268:PRO:HD2	1.73	0.41
1:D:131:ASP:CG	1:D:135:ARG:HH21	2.24	0.41
1:D:135:ARG:HB3	1:D:324:TYR:CZ	2.56	0.41
1:D:258:TYR:CE1	1:D:309:ASP:HA	2.56	0.41
1:A:72:LYS:HB3	1:A:73:PRO:CD	2.51	0.41
1:A:104:ASP:OD1	1:A:106:VAL:HG13	2.21	0.41
1:A:241:ASP:O	1:A:245:ARG:HG2	2.20	0.41
1:D:45:LYS:HG3	1:D:46:LEU:N	2.35	0.41
1:G:120:THR:HB	1:G:125:LEU:HB2	2.02	0.41
1:J:130:THR:HG23	1:J:133:ASP:H	1.86	0.41
1:G:144:ALA:O	1:G:148:CYS:HB3	2.21	0.41
1:G:156:ARG:O	1:G:194:ALA:HB2	2.20	0.41
1:A:159:LYS:HE2	1:A:195:SER:HB2	2.02	0.40
1:G:252:THR:O	1:G:255:LEU:HB3	2.21	0.40
1:J:152:GLY:HA2	1:J:212:TYR:OH	2.22	0.40
1:J:317:LYS:O	1:J:317:LYS:HD2	2.21	0.40
1:D:175:ILE:HB	2:D:401:E3U:C14	2.52	0.40
1:A:55:PHE:O	1:A:67:VAL:HA	2.21	0.40
1:D:142:LEU:HD22	1:D:319:ALA:HB3	2.04	0.40
1:A:291:ARG:HD3	1:A:291:ARG:HA	1.88	0.40
1:D:203:LEU:H	1:D:203:LEU:HG	1.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:93:THR:O	1:G:94:ASN:HB2	2.22	0.40
1:D:96:ILE:HA	1:D:173:ARG:HD2	2.04	0.40
1:D:230:ARG:NH1	1:D:233:PHE:O	2.55	0.40
1:G:305:LEU:CD2	1:G:314:LEU:HB2	2.51	0.40
1:J:34:TRP:CZ3	1:J:101:THR:HB	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	307/338 (91%)	276 (90%)	26 (8%)	5 (2%)	9	35
1	D	307/338 (91%)	276 (90%)	25 (8%)	6 (2%)	7	29
1	G	313/338 (93%)	282 (90%)	24 (8%)	7 (2%)	6	27
1	J	306/338 (90%)	287 (94%)	17 (6%)	2 (1%)	22	54
All	All	1233/1352 (91%)	1121 (91%)	92 (8%)	20 (2%)	9	35

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	72	LYS
1	J	65	ARG
1	A	324	TYR
1	D	324	TYR
1	G	18	SER
1	G	28	GLU
1	G	39	ASP
1	J	194	ALA
1	A	16	VAL
1	A	131	ASP

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Mol	Chain	Res	Type
1	D	176	ASP
1	D	288	SER
1	G	242	GLN
1	A	282	TRP
1	D	42	LEU
1	G	274	LEU
1	A	108	LYS
1	D	116	TYR
1	G	150	SER
1	G	168	GLN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	288/305 (94%)	252 (88%)	36 (12%)	4	17
1	D	286/305 (94%)	246 (86%)	40 (14%)	3	14
1	G	292/305 (96%)	246 (84%)	46 (16%)	2	10
1	J	287/305 (94%)	245 (85%)	42 (15%)	3	13
All	All	1153/1220 (94%)	989 (86%)	164 (14%)	3	14

All (164) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	VAL
1	A	19	LEU
1	A	21	SER
1	A	28	GLU
1	A	34	TRP
1	A	38	ASP
1	A	44	ARG
1	A	45	LYS
1	A	54	VAL
1	A	58	ILE
1	A	65	ARG

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Mol	Chain	Res	Type
1	A	76	LYS
1	A	84	LYS
1	A	97	LYS
1	A	100	ASP
1	A	106	VAL
1	A	107	SER
1	A	115	GLU
1	A	118	ASN
1	A	120	THR
1	A	125	LEU
1	A	135	ARG
1	A	159	LYS
1	A	179	LEU
1	A	213	SER
1	A	214	LEU
1	A	219	LEU
1	A	225	SER
1	A	260	LYS
1	A	265	ASP
1	A	272	ASP
1	A	283	GLU
1	A	291	ARG
1	A	295	SER
1	A	297	GLU
1	A	332	GLN
1	D	8	SER
1	D	9	ARG
1	D	11	ARG
1	D	23	GLU
1	D	31	VAL
1	D	38	ASP
1	D	58	ILE
1	D	74	VAL
1	D	76	LYS
1	D	78	LYS
1	D	79	ILE
1	D	84	LYS
1	D	93	THR
1	D	97	LYS
1	D	100	ASP
1	D	104	ASP
1	D	106	VAL

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Mol	Chain	Res	Type
1	D	107	SER
1	D	108	LYS
1	D	119	ASN
1	D	120	THR
1	D	123	LYS
1	D	128	ILE
1	D	135	ARG
1	D	150	SER
1	D	161	HIS
1	D	190	ASN
1	D	192	ARG
1	D	203	LEU
1	D	205	VAL
1	D	216	MET
1	D	219	LEU
1	D	225	SER
1	D	226	MET
1	D	230	ARG
1	D	265	ASP
1	D	271	ASN
1	D	291	ARG
1	D	294	VAL
1	D	320	MET
1	G	12	VAL
1	G	18	SER
1	G	22	ARG
1	G	27	TYR
1	G	39	ASP
1	G	48	ARG
1	G	58	ILE
1	G	60	ILE
1	G	63	ASN
1	G	71	LEU
1	G	76	LYS
1	G	84	LYS
1	G	87	GLU
1	G	97	LYS
1	G	112	LEU
1	G	120	THR
1	G	123	LYS
1	G	130	THR
1	G	148	CYS

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Mol	Chain	Res	Type
1	G	150	SER
1	G	158	VAL
1	G	164	MET
1	G	169	GLN
1	G	192	ARG
1	G	206	ASP
1	G	209	MET
1	G	211	ASP
1	G	213	SER
1	G	218	SER
1	G	219	LEU
1	G	230	ARG
1	G	237	GLN
1	G	245	ARG
1	G	259	LEU
1	G	269	HIS
1	G	270	PHE
1	G	271	ASN
1	G	272	ASP
1	G	279	ARG
1	G	281	ARG
1	G	287	HIS
1	G	291	ARG
1	G	307	ARG
1	G	312	GLN
1	G	321	GLU
1	G	329	VAL
1	J	12	VAL
1	J	16	VAL
1	J	21	SER
1	J	23	GLU
1	J	38	ASP
1	J	42	LEU
1	J	56	GLU
1	J	71	LEU
1	J	75	LYS
1	J	80	LYS
1	J	84	LYS
1	J	106	VAL
1	J	108	LYS
1	J	116	TYR
1	J	118	ASN

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Mol	Chain	Res	Type
1	J	165	ILE
1	J	169	GLN
1	J	172	LEU
1	J	175	ILE
1	J	192	ARG
1	J	203	LEU
1	J	208	GLN
1	J	213	SER
1	J	225	SER
1	J	230	ARG
1	J	231	GLU
1	J	238	ASP
1	J	253	GLU
1	J	269	HIS
1	J	270	PHE
1	J	271	ASN
1	J	272	ASP
1	J	276	GLN
1	J	278	SER
1	J	279	ARG
1	J	281	ARG
1	J	286	ILE
1	J	288	SER
1	J	312	GLN
1	J	317	LYS
1	J	318	GLU
1	J	321	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	271	ASN
1	G	119	ASN
1	G	149	HIS
1	J	184	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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	$\#|Z| > 2$
2	E3U	J	401	-	23,25,25	4.27	10 (43%)	25,40,40	1.65	5 (20%)
2	E3U	G	401	-	23,25,25	4.19	13 (56%)	25,40,40	2.06	13 (52%)
2	E3U	D	401	-	23,25,25	4.33	13 (56%)	25,40,40	1.65	7 (28%)
2	E3U	A	401	-	23,25,25	4.33	14 (60%)	25,40,40	2.15	10 (40%)

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
2	E3U	J	401	-	-	-	0/4/4/4
2	E3U	G	401	-	-	-	0/4/4/4
2	E3U	D	401	-	-	-	0/4/4/4
2	E3U	A	401	-	-	-	0/4/4/4

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	E3U	O09-C03	13.60	1.58	1.37
2	J	401	E3U	O09-C03	13.01	1.58	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	E3U	O09-C03	12.94	1.57	1.37
2	G	401	E3U	O09-C03	12.75	1.57	1.37
2	D	401	E3U	C11-C07	7.56	1.62	1.37
2	G	401	E3U	C11-C07	7.35	1.61	1.37
2	A	401	E3U	C11-C07	7.23	1.61	1.37
2	J	401	E3U	C11-C07	7.10	1.60	1.37
2	J	401	E3U	C11-C12	-6.85	1.28	1.43
2	D	401	E3U	C11-C12	-6.80	1.29	1.43
2	A	401	E3U	C11-C12	-6.32	1.30	1.43
2	G	401	E3U	C11-C12	-6.18	1.30	1.43
2	D	401	E3U	O18-C17	5.94	1.40	1.24
2	A	401	E3U	O18-C17	5.89	1.40	1.24
2	G	401	E3U	O18-C17	5.80	1.40	1.24
2	G	401	E3U	O09-C10	5.67	1.49	1.43
2	J	401	E3U	O18-C17	5.52	1.39	1.24
2	D	401	E3U	C13-C12	-4.96	1.43	1.51
2	J	401	E3U	O09-C10	4.94	1.48	1.43
2	J	401	E3U	C13-C12	-4.86	1.43	1.51
2	D	401	E3U	O09-C10	4.63	1.48	1.43
2	A	401	E3U	O09-C10	4.49	1.48	1.43
2	A	401	E3U	C13-C12	-4.43	1.43	1.51
2	G	401	E3U	C13-C12	-4.15	1.44	1.51
2	D	401	E3U	C15-C17	-4.12	1.34	1.47
2	J	401	E3U	C15-C17	-4.08	1.34	1.47
2	G	401	E3U	C16-C12	3.65	1.44	1.34
2	A	401	E3U	C16-C12	3.53	1.43	1.34
2	D	401	E3U	C16-C12	3.48	1.43	1.34
2	J	401	E3U	C16-C12	3.46	1.43	1.34
2	G	401	E3U	C15-C17	-3.35	1.37	1.47
2	A	401	E3U	C15-C17	-3.25	1.37	1.47
2	J	401	E3U	C16-C17	-3.20	1.36	1.44
2	A	401	E3U	C16-C17	-2.95	1.36	1.44
2	D	401	E3U	C16-C17	-2.91	1.36	1.44
2	A	401	E3U	O19-C15	2.91	1.41	1.34
2	A	401	E3U	O20-C08	-2.76	1.38	1.43
2	G	401	E3U	C16-C17	-2.73	1.37	1.44
2	J	401	E3U	O19-C15	2.67	1.40	1.34
2	G	401	E3U	O19-C15	2.60	1.40	1.34
2	D	401	E3U	O19-C15	2.50	1.40	1.34
2	D	401	E3U	C08-C07	-2.47	1.48	1.52
2	G	401	E3U	O20-C08	-2.34	1.38	1.43
2	A	401	E3U	C01-C07	-2.33	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	E3U	C04-C06	2.31	1.43	1.39
2	A	401	E3U	C04-C06	2.27	1.43	1.39
2	G	401	E3U	C01-C07	-2.22	1.43	1.47
2	A	401	E3U	O21-C05	2.18	1.42	1.37
2	G	401	E3U	C04-C06	2.16	1.43	1.39
2	D	401	E3U	O21-C05	2.10	1.41	1.37

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	E3U	C12-C11-C07	-4.18	101.42	109.74
2	A	401	E3U	C01-C03-C05	-4.17	117.50	121.66
2	J	401	E3U	C12-C11-C07	-4.07	101.63	109.74
2	A	401	E3U	C02-C01-C03	3.63	124.04	118.37
2	D	401	E3U	C01-C03-C05	-3.59	118.08	121.66
2	G	401	E3U	C12-C11-C07	-3.44	102.89	109.74
2	G	401	E3U	O19-C15-C17	3.43	125.53	117.75
2	D	401	E3U	C12-C11-C07	-3.37	103.04	109.74
2	G	401	E3U	C16-C17-C15	3.14	122.35	117.03
2	A	401	E3U	O09-C03-C05	2.98	122.18	116.57
2	J	401	E3U	C01-C03-C05	-2.98	118.68	121.66
2	D	401	E3U	C02-C01-C03	2.98	123.02	118.37
2	A	401	E3U	C16-C17-C15	2.97	122.07	117.03
2	A	401	E3U	C14-C11-C12	2.88	123.12	120.11
2	J	401	E3U	C16-C17-C15	2.85	121.87	117.03
2	G	401	E3U	O09-C03-C01	-2.78	119.18	122.50
2	G	401	E3U	O09-C03-C05	2.78	121.79	116.57
2	G	401	E3U	C14-C15-C17	-2.65	118.52	121.26
2	A	401	E3U	O20-C08-C10	-2.65	102.97	110.01
2	G	401	E3U	C01-C03-C05	-2.63	119.03	121.66
2	G	401	E3U	C02-C01-C03	2.49	122.26	118.37
2	G	401	E3U	C14-C11-C12	2.49	122.71	120.11
2	J	401	E3U	C02-C01-C03	2.41	122.13	118.37
2	G	401	E3U	C02-C01-C07	-2.40	120.33	123.90
2	D	401	E3U	C04-C06-C05	2.33	122.44	120.06
2	D	401	E3U	C16-C17-C15	2.29	120.91	117.03
2	A	401	E3U	C02-C01-C07	-2.25	120.56	123.90
2	D	401	E3U	C02-C04-C06	-2.19	118.25	120.50
2	G	401	E3U	C06-C05-C03	2.15	120.57	118.43
2	J	401	E3U	C14-C11-C12	2.15	122.35	120.11
2	A	401	E3U	C12-C16-C17	-2.13	118.51	122.52
2	G	401	E3U	C12-C16-C17	-2.11	118.55	122.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401	E3U	O18-C17-C16	-2.08	117.00	121.78
2	G	401	E3U	O18-C17-C16	-2.04	117.11	121.78
2	D	401	E3U	C12-C16-C17	-2.00	118.75	122.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	401	E3U	2	0
2	G	401	E3U	5	0
2	D	401	E3U	6	0
2	A	401	E3U	4	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 then 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.

Ligand E3U J 401

Bond lengths

Bond angles

Torsions

Rings

Ligand E3U G 401

Bond lengths

Bond angles

Torsions

Rings

Ligand E3U D 401 — Bond lengths, Bond angles, Torsions, Rings

Ligand E3U A 401 — Bond lengths, Bond angles, Torsions, Rings
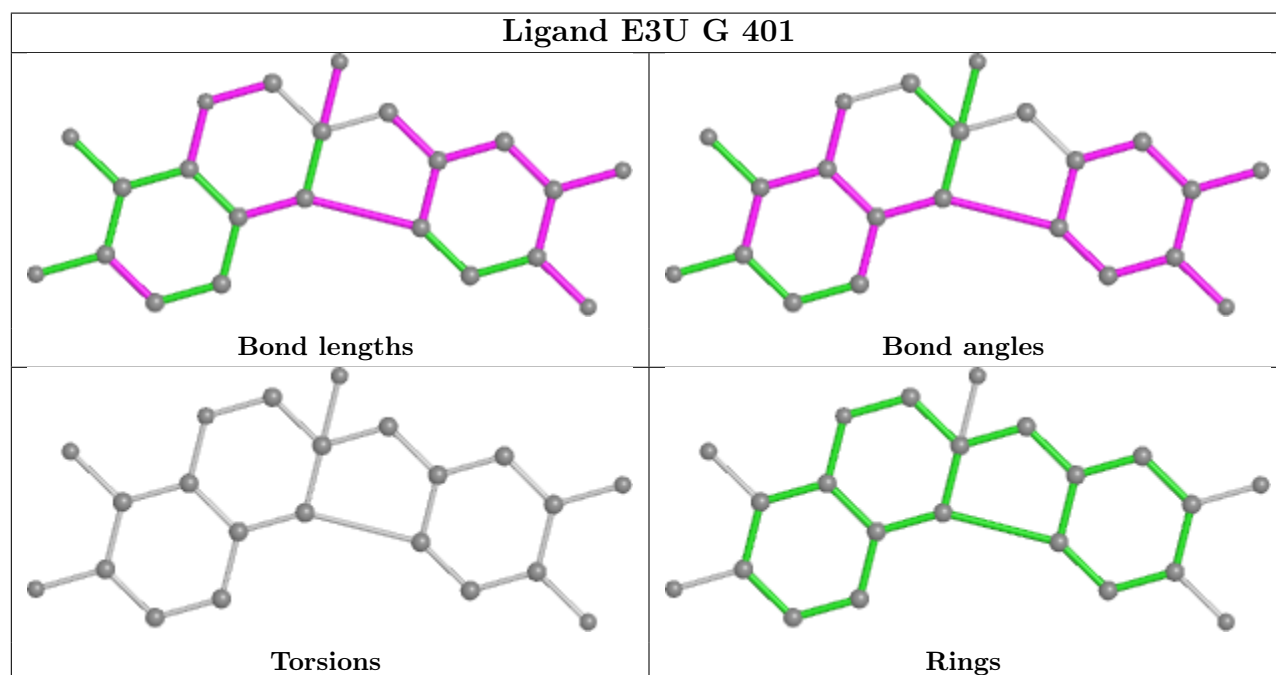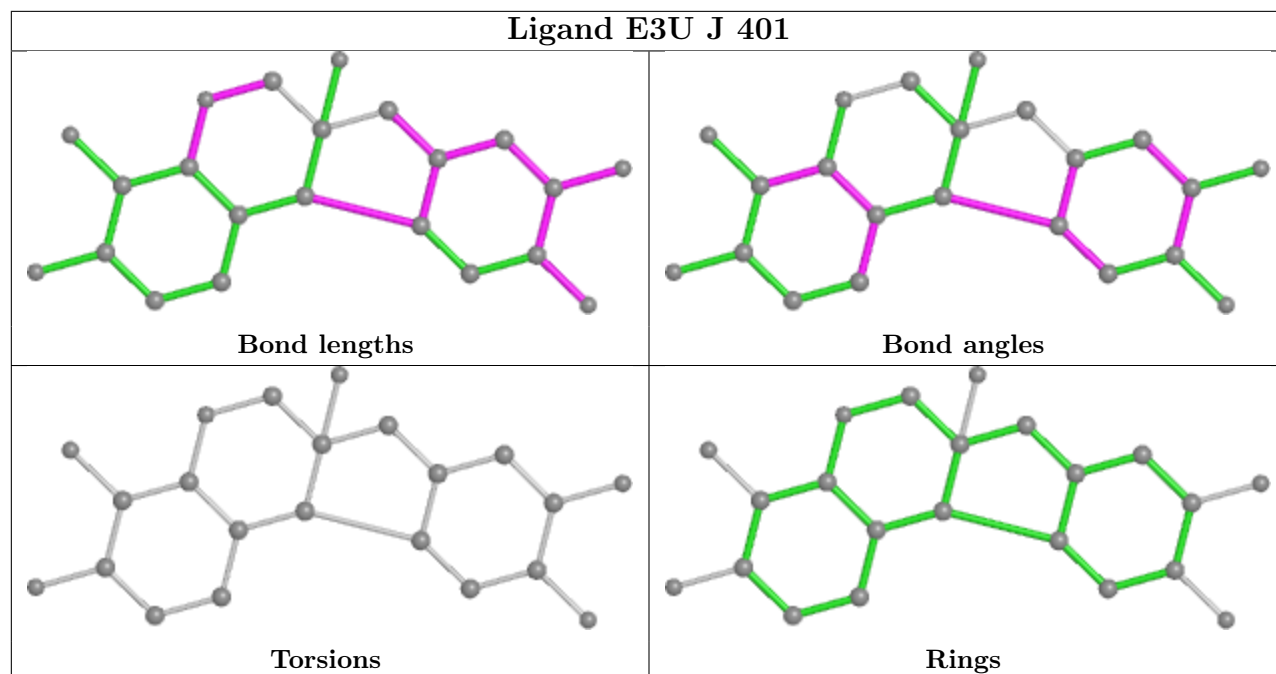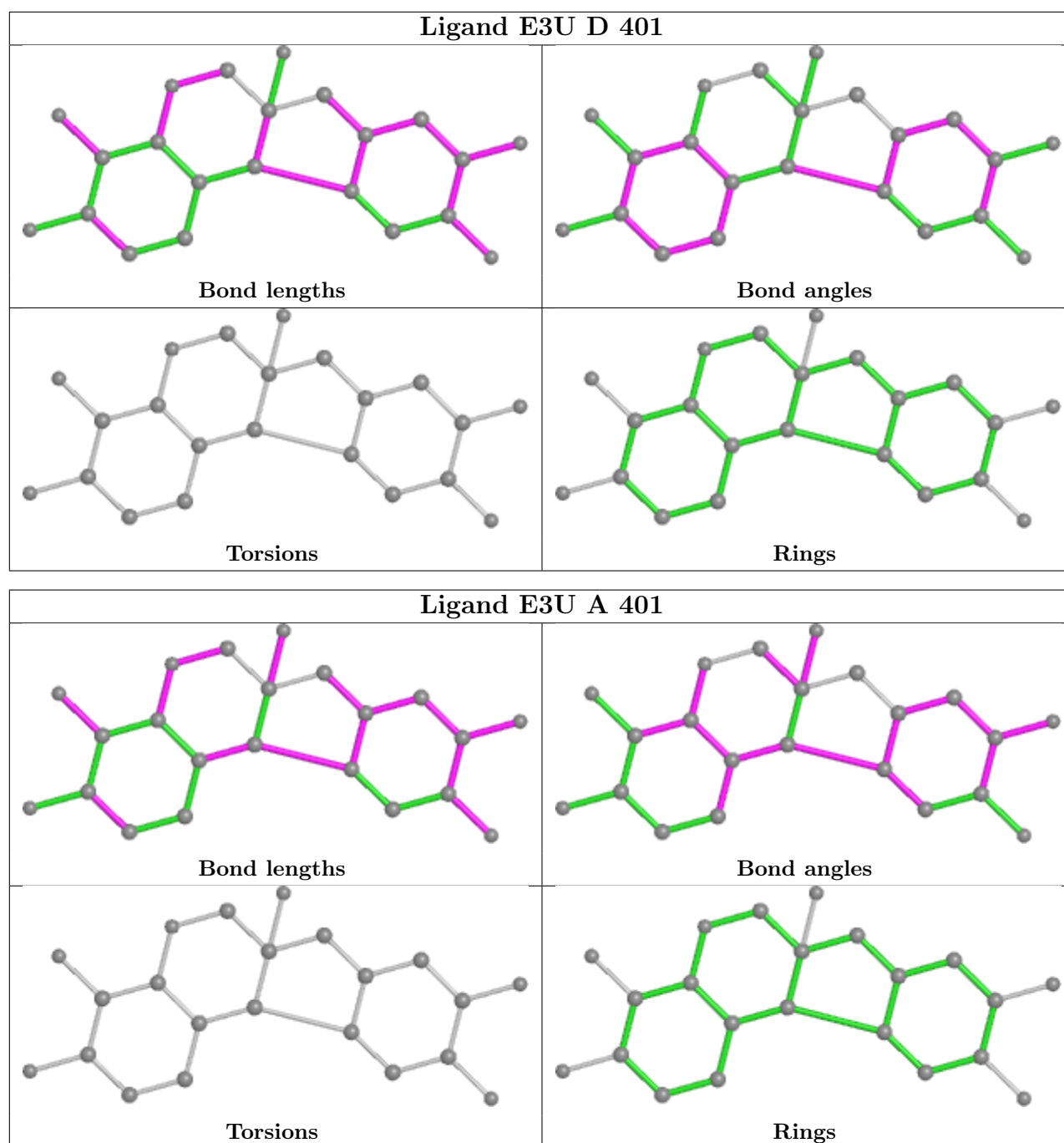
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	313/338 (92%)	-0.30	3 (0%)	82	66	14, 32, 63, 87	2 (0%)
1	D	313/338 (92%)	-0.30	3 (0%)	82	66	15, 31, 66, 86	1 (0%)
1	G	319/338 (94%)	-0.31	3 (0%)	84	68	14, 33, 70, 90	1 (0%)
1	J	314/338 (92%)	-0.32	1 (0%)	94	87	14, 33, 66, 79	1 (0%)
All	All	1259/1352 (93%)	-0.31	10 (0%)	86	71	14, 32, 66, 90	5 (0%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	73	PRO	4.3
1	A	73	PRO	3.3
1	G	265	ASP	3.3
1	A	269	HIS	2.9
1	G	266	LEU	2.2
1	D	332	GLN	2.2
1	G	70	ILE	2.1
1	D	265	ASP	2.1
1	A	332	GLN	2.1
1	J	71	LEU	2.0

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

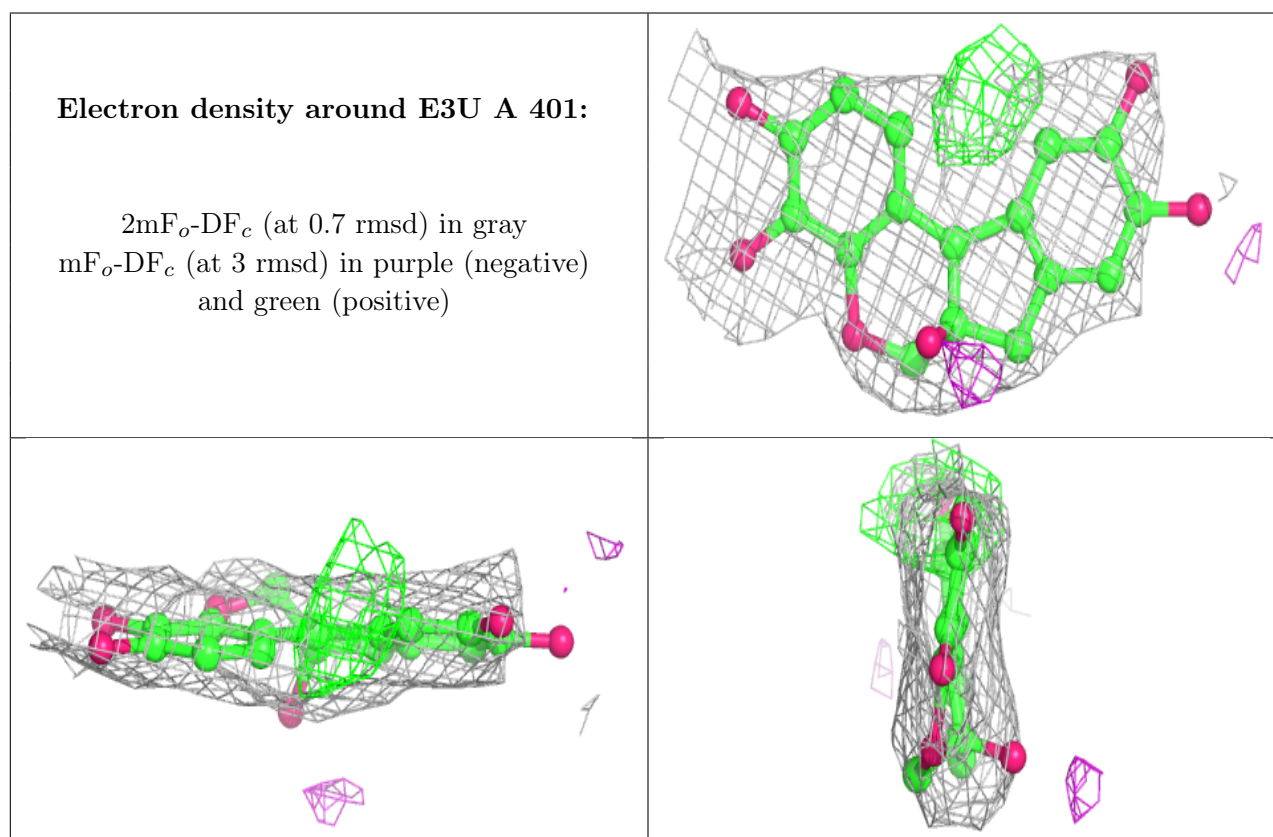There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
3	CL	A	402	1/1	0.83	0.60	44,44,44,44	0
2	E3U	A	401	22/22	0.84	0.31	30,35,42,48	22
2	E3U	D	401	22/22	0.85	0.36	28,35,50,62	22
2	E3U	G	401	22/22	0.86	0.33	28,33,40,44	22
2	E3U	J	401	22/22	0.88	0.33	29,39,45,55	22
3	CL	D	402	1/1	0.93	0.27	47,47,47,47	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.


Electron density around E3U A 401:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

Electron density around E3U D 401:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
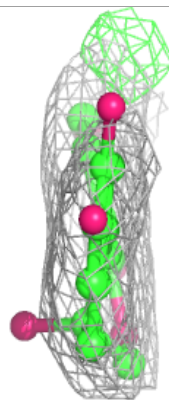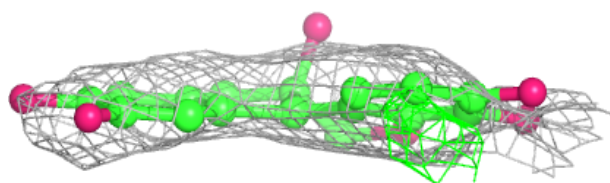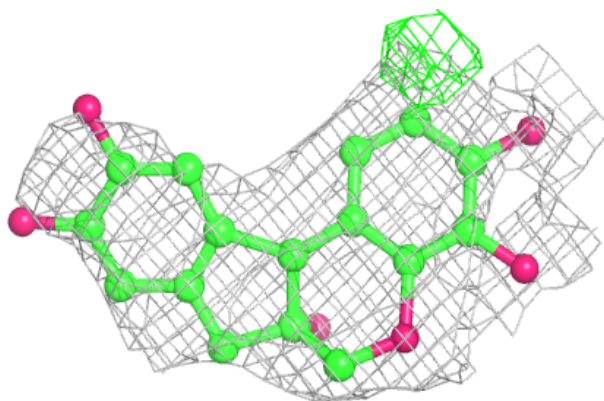
Electron density around E3U G 401:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around E3U J 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
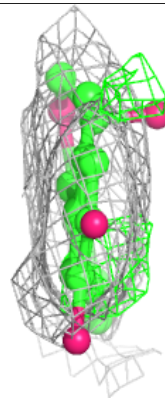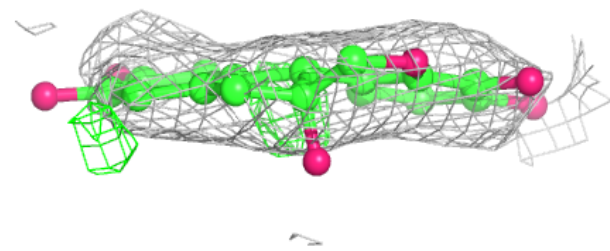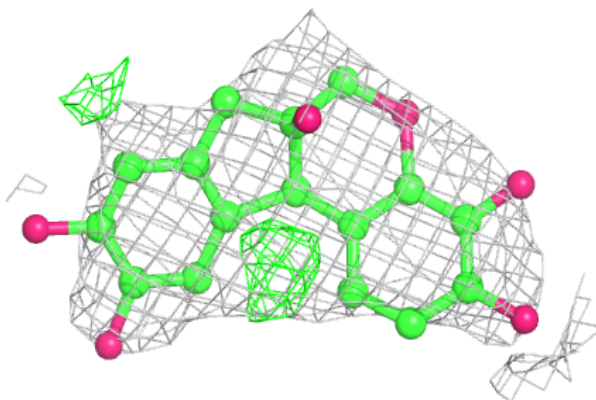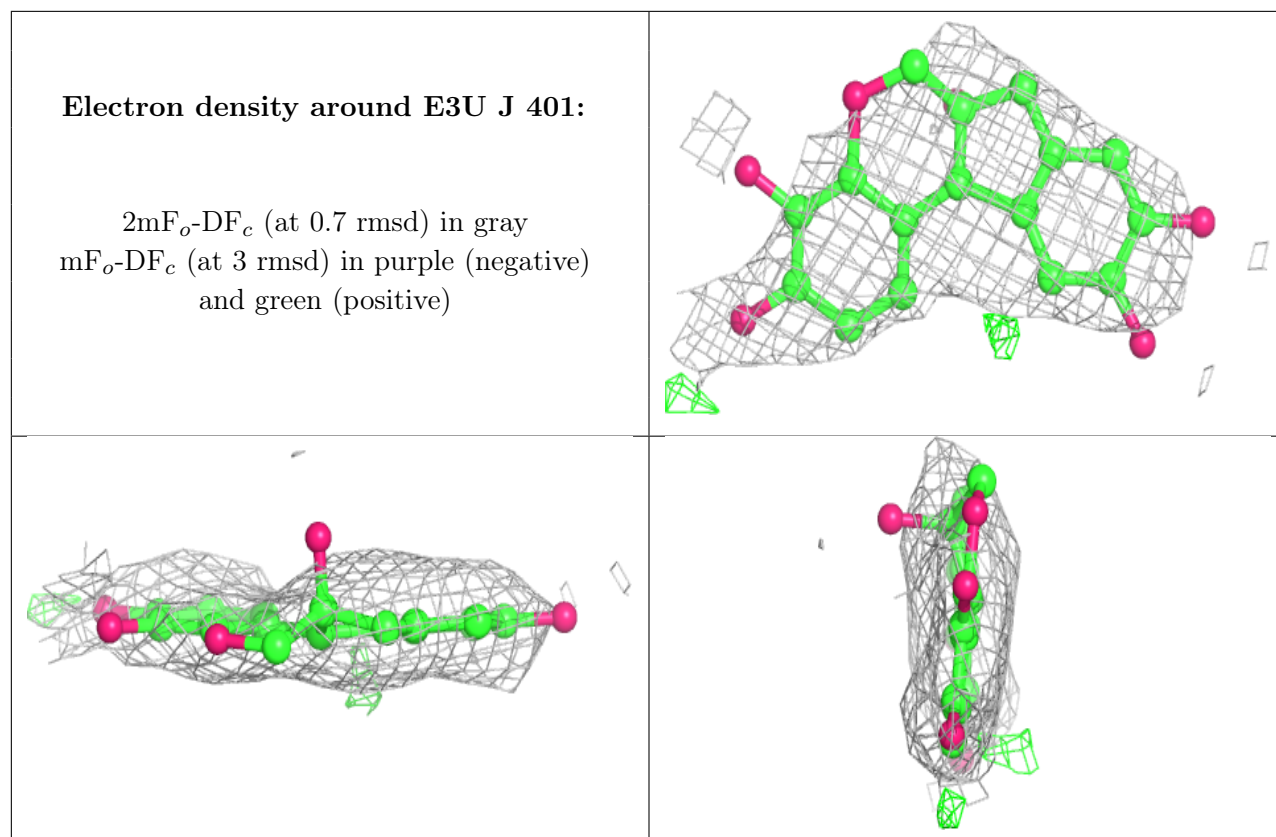
6.5 Other polymers (i)

There are no such residues in this entry.