Full wwPDB X-ray Structure Validation Report (i)

Sep 26, 2023 – 02:02 AM EDT

PDB ID	:	6AM0
Title	:	Crystal structure of K. lactis Edc1-Dcp1-Dcp2-Edc3 decapping complex with synthetic cap substrate analog
Authors	:	Mugridge, J.S.; Gross, J.D.
Deposited on	:	2017-08-08
Resolution	:	2.84 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 (i) 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 (i)) were used in the production of this report:

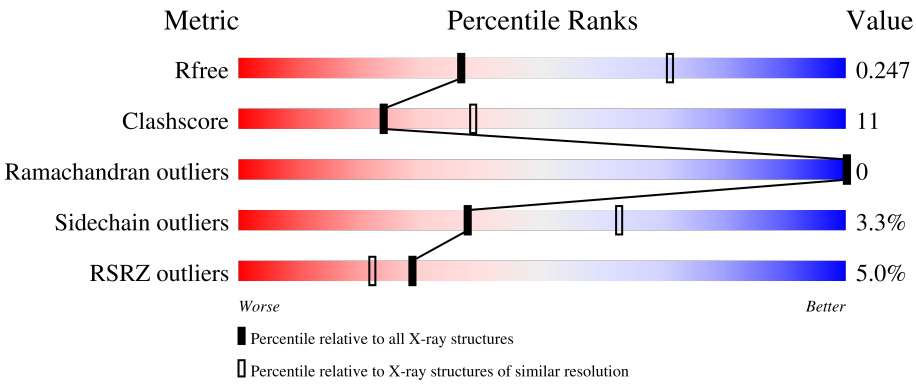
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.84 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1031 (2.86-2.82)
Clashscore	141614	1078 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)
RSRZ outliers	127900	1019 (2.86-2.82)

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	275	% 66% 27% • 5%
1	E	275	4% 70% 22% • 7%
2	B	190	5% 68% 23% • 8%
2	F	190	2% 71% 22% • 6%
3	C	26	62% 27% 12%

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Mol	Chain	Length	Quality of chain
3	G	26	4% 65% 35%
4	D	66	5% 65% 33%
4	H	66	30% 48% 36% 12%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 8599 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 KLLA0F23980p.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	260	2129	1386	352	385	6	0	0	0
1	E	257	2106	1372	348	380	6	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	152	GLN	GLU	engineered mutation	UNP Q6CIU1
E	152	GLN	GLU	engineered mutation	UNP Q6CIU1

- Molecule 2 is a protein called KLLA0E01827p.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	175	1443	928	242	269	4	0	0	0
2	F	178	1472	944	245	279	4	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	expression tag	UNP Q6CPV9
B	0	SER	-	expression tag	UNP Q6CPV9
F	-1	GLY	-	expression tag	UNP Q6CPV9
F	0	SER	-	expression tag	UNP Q6CPV9

- Molecule 3 is a protein called KLLA0A01474p.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	23	170	111	26	32	1	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	G	26	193	125	31	36	1	0	0	0

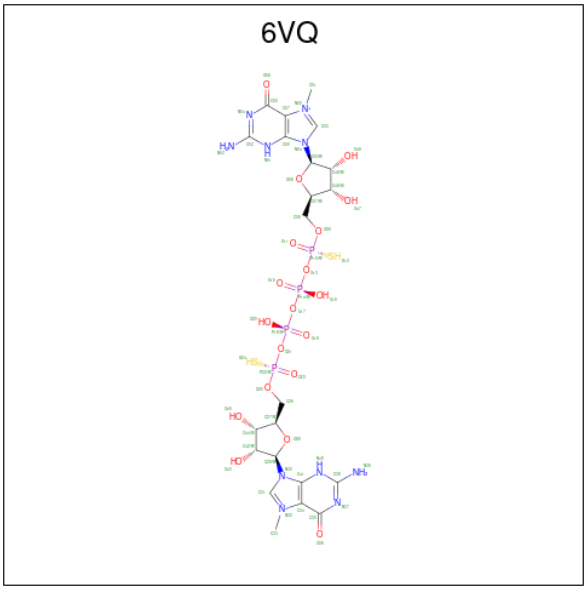
- Molecule 4 is a protein called KLLA0A11308p.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	65	510	333	83	93	1	0	0	0
			Total	C	N	O				
4	H	58	461	306	74	81		0	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
5	A	1	1	1	0	0

- Molecule 6 is [[(2 {R},3 {S},4 {R},5 {R})-5-(2-azanyl-7-methyl-6-oxidanylidene-3 {H}-purin-7-ium-9-yl)-3,4-bis(oxidanyl)oxolan-2-yl]methoxy-sulfanyl-phosphoryl] [[[(2 {R},3 {S},4 {R},5 {R})-5-(2-azanyl-7-methyl-6-oxidanylidene-3 {H}-purin-7-ium-9-yl)-3,4-bis(oxidanyl)oxolan-2-yl]methoxy-sulfanyl-phosphoryl]oxy-oxidanyl-phosphoryl] hydrogen phosphate (three-letter code: 6VQ) (formula: $C_{22}H_{34}N_{10}O_{19}P_4S_2$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
6	A	1	57	22	10	19	4	2	0	0

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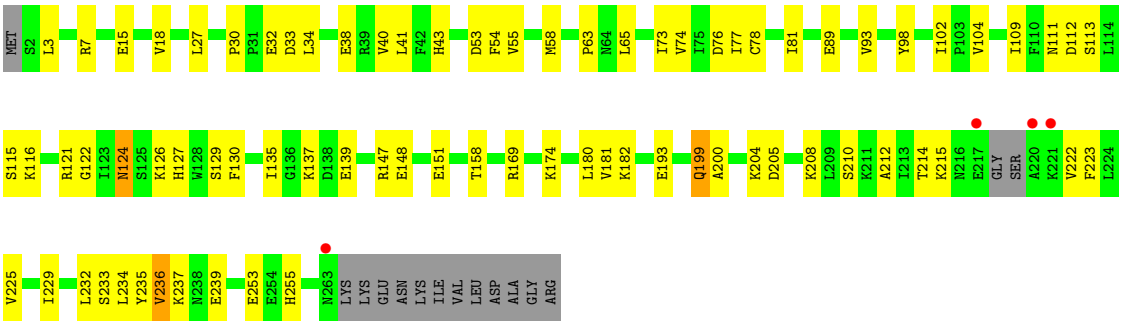
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
6	E	1	57	22	10	19	4	2	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

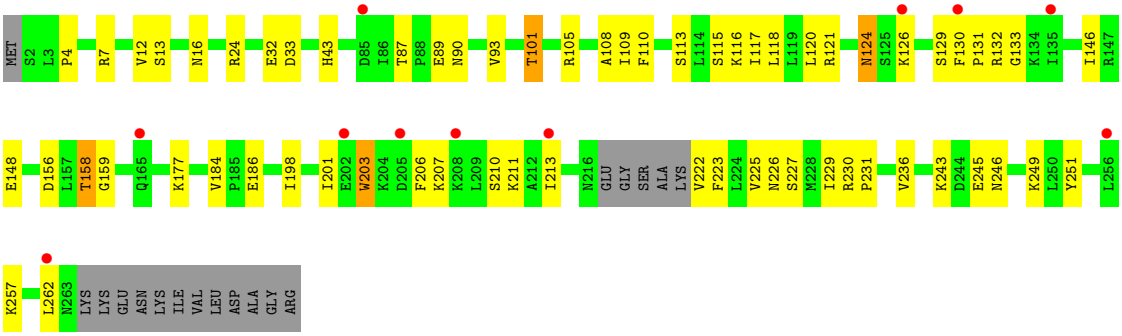
• Molecule 1: KLLA0F23980p

Chain A:



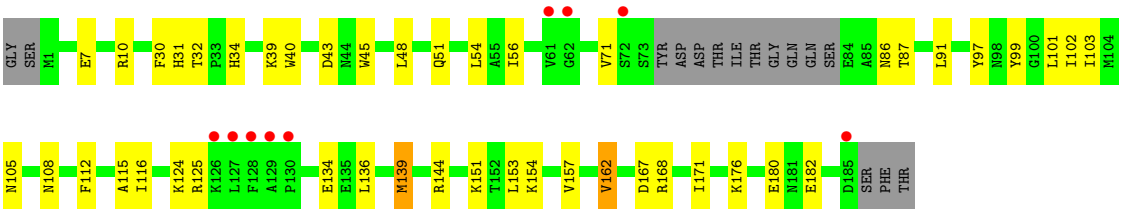
• Molecule 1: KLLA0F23980p

Chain E:



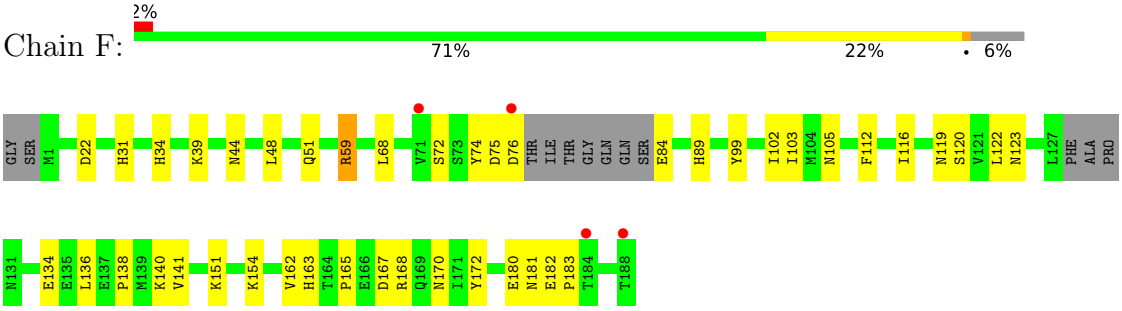
• Molecule 2: KLLA0E01827p

Chain B:



• Molecule 2: KLLA0E01827p

Chain F:

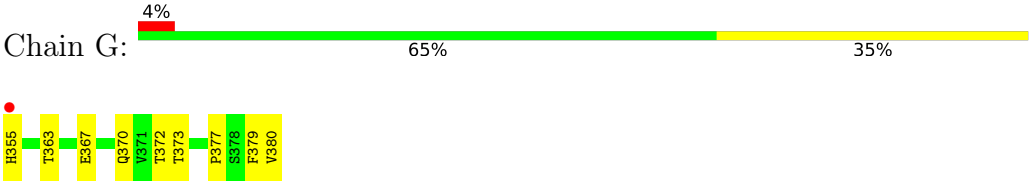


• Molecule 3: KLLA0A01474p

Chain C:

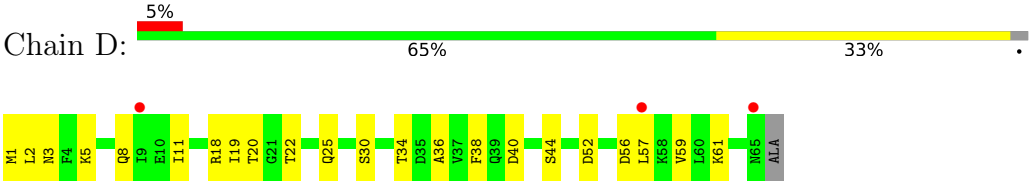
• Molecule 3: KLLA0A01474p

Chain G:



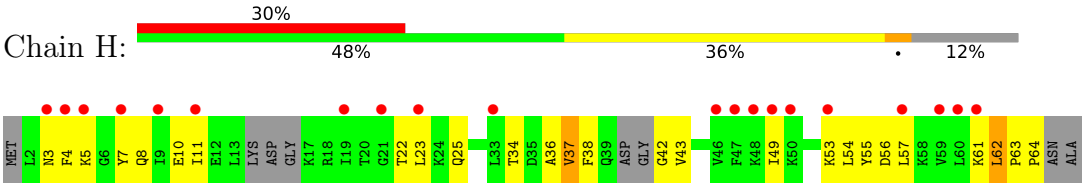
• Molecule 4: KLLA0A11308p

Chain D:



• Molecule 4: KLLA0A11308p

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	174.26Å 83.25Å 104.30Å 90.00° 93.62° 90.00°	Depositor
Resolution (Å)	45.96 – 2.84 45.95 – 2.84	Depositor EDS
% Data completeness (in resolution range)	99.7 (45.96-2.84) 99.7 (45.95-2.84)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.61 (at 2.86Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.225 , 0.248 0.225 , 0.247	Depositor DCC
R_{free} test set	1998 reflections (5.66%)	wwPDB-VP
Wilson B-factor (Å^2)	95.1	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 58.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8599	wwPDB-VP
Average B, all atoms (Å^2)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% of the height of the origin peak. No significant pseudotranslation is detected.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 6VQ

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	0.27	0/2178	0.44	0/2941
1	E	0.27	0/2155	0.46	0/2911
2	B	0.27	0/1476	0.46	0/2004
2	F	0.26	0/1504	0.46	0/2040
3	C	0.27	0/175	0.48	0/239
3	G	0.26	0/199	0.46	0/272
4	D	0.26	0/518	0.56	0/696
4	H	0.34	0/467	0.64	0/626
All	All	0.27	0/8672	0.47	0/11729

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 (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	2129	0	2165	52	0
1	E	2106	0	2141	49	0
2	B	1443	0	1441	33	0
2	F	1472	0	1457	29	0
3	C	170	0	168	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	193	0	189	8	0
4	D	510	0	551	19	1
4	H	461	0	504	20	0
5	A	1	0	0	0	0
6	A	57	0	0	4	0
6	E	57	0	0	0	0
All	All	8599	0	8616	191	1

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 11.

All (191) 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:E:109:ILE:HG22	1:E:184:VAL:HG11	1.70	0.72
1:E:101:THR:HG21	3:G:355:HIS:HB2	1.72	0.71
4:H:56:ASP:OD1	4:H:57:LEU:N	2.24	0.70
1:E:133:GLY:HA3	1:E:148:GLU:HG2	1.73	0.70
2:F:99:TYR:HB2	2:F:116:ILE:HB	1.72	0.70
1:A:65:LEU:HD21	1:A:73:ILE:HD12	1.73	0.69
4:H:62:LEU:HB2	4:H:64:PRO:HD2	1.74	0.69
4:D:3:ASN:HD22	4:D:5:LYS:HD2	1.59	0.67
1:E:120:LEU:HB3	1:E:201:ILE:HG22	1.76	0.67
4:H:22:THR:HG1	4:H:34:THR:HG1	1.44	0.66
2:B:162:VAL:HG13	2:B:168:ARG:HG2	1.77	0.66
2:F:119:ASN:O	2:F:123:ASN:ND2	2.26	0.66
1:E:146:ILE:HG21	1:E:158:THR:HG23	1.78	0.65
2:F:120:SER:HA	2:F:123:ASN:HD21	1.61	0.65
1:A:33:ASP:HB3	1:A:43:HIS:HE2	1.61	0.65
2:B:151:LYS:HD2	2:B:157:VAL:HG12	1.78	0.65
2:B:151:LYS:HB2	3:C:379:PHE:HE1	1.62	0.65
1:A:255:HIS:ND1	1:E:159:GLY:O	2.29	0.65
4:D:8:GLN:HB3	4:D:61:LYS:H	1.62	0.64
1:E:118:LEU:HA	1:E:203:TRP:HB3	1.79	0.64
1:E:115:SER:O	1:E:206:PHE:N	2.21	0.64
4:D:25:GLN:HG3	3:G:372:THR:HG22	1.80	0.63
1:A:233:SER:O	1:A:237:LYS:HG3	1.99	0.62
4:D:22:THR:OG1	4:D:34:THR:OG1	2.17	0.62
4:D:19:ILE:HD12	4:D:38:PHE:CD1	2.34	0.61
2:B:56:ILE:HD11	2:B:101:LEU:HD12	1.82	0.61
2:B:105:ASN:ND2	2:B:108:ASN:OD1	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:GLU:HB3	4:D:59:VAL:HG12	1.83	0.60
3:G:377:PRO:HB2	3:G:380:VAL:HG22	1.82	0.60
2:B:40:TRP:HB3	2:B:157:VAL:HG23	1.83	0.60
1:A:127:HIS:ND1	6:A:302:6VQ:O56	2.35	0.60
1:E:105:ARG:HA	1:E:177:LYS:O	2.01	0.60
1:A:63:PRO:HG2	1:A:65:LEU:HD11	1.83	0.60
4:D:56:ASP:OD1	4:D:57:LEU:N	2.35	0.60
4:H:5:LYS:HE2	4:H:25:GLN:HA	1.85	0.59
2:B:176:LYS:O	2:B:180:GLU:HG2	2.03	0.58
1:A:27:LEU:HD21	2:B:10:ARG:HA	1.84	0.58
2:B:32:THR:HG22	2:B:54:LEU:HB3	1.86	0.58
1:A:15:GLU:HA	1:A:77:ILE:HD13	1.86	0.57
1:E:121:ARG:HH11	1:E:126:LYS:HG2	1.70	0.57
1:E:7:ARG:NH2	2:F:72:SER:O	2.30	0.57
1:A:234:LEU:HA	1:A:237:LYS:HD2	1.86	0.57
4:H:38:PHE:N	4:H:42:GLY:O	2.37	0.57
1:E:245:GLU:HB3	1:E:249:LYS:HE3	1.87	0.57
4:H:49:ILE:HD11	4:H:53:LYS:HB2	1.87	0.55
1:A:32:GLU:HG2	3:C:363:THR:HG21	1.87	0.55
2:F:134:GLU:HB2	2:F:136:LEU:HG	1.87	0.55
2:B:40:TRP:CZ2	2:B:43:ASP:HA	2.42	0.55
2:B:102:ILE:HA	2:B:112:PHE:O	2.07	0.54
2:F:89:HIS:CE1	2:F:154:LYS:HZ3	2.24	0.54
4:D:1:MET:HG2	4:D:2:LEU:H	1.73	0.54
1:A:104:VAL:HG23	1:A:174:LYS:HD2	1.90	0.54
4:H:7:TYR:CD1	4:H:63:PRO:HD2	2.43	0.53
4:H:61:LYS:HG2	4:H:62:LEU:N	2.24	0.53
1:A:130:PHE:CZ	1:A:225:VAL:HG22	2.44	0.53
4:H:3:ASN:HD21	4:H:5:LYS:HD2	1.74	0.53
1:A:151:GLU:HA	1:A:193:GLU:HG3	1.90	0.53
2:B:139:MET:HG2	2:B:153:LEU:HD23	1.91	0.53
2:F:165:PRO:HB3	2:F:168:ARG:NH1	2.24	0.53
1:A:3:LEU:HG	2:B:115:ALA:HB2	1.91	0.52
2:B:144:ARG:HD2	3:C:375:PRO:HB2	1.90	0.52
1:E:129:SER:HB3	1:E:223:PHE:HB3	1.90	0.52
1:A:124:ASN:N	1:A:124:ASN:OD1	2.39	0.52
1:E:32:GLU:HG3	3:G:363:THR:HG21	1.90	0.52
2:B:30:PHE:CE2	2:B:171:ILE:HG12	2.44	0.52
3:G:370:GLN:O	3:G:373:THR:HG22	2.10	0.52
1:E:12:VAL:HG13	1:E:16:ASN:HB2	1.92	0.51
1:E:116:LYS:NZ	1:E:186:GLU:OE1	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:ASN:OD1	1:A:112:ASP:N	2.44	0.51
2:B:40:TRP:HB3	2:B:157:VAL:CG2	2.40	0.51
2:B:34:HIS:CE1	2:B:51:GLN:HG2	2.45	0.50
4:D:18:ARG:NH2	4:H:55:TYR:CD1	2.79	0.50
2:F:182:GLU:HB3	2:F:183:PRO:HD2	1.93	0.50
1:A:121:ARG:HE	1:A:200:ALA:HB3	1.76	0.50
1:A:222:VAL:CG1	1:A:225:VAL:HB	2.42	0.50
1:A:53:ASP:OD2	6:A:302:6VQ:N37	2.45	0.49
1:A:222:VAL:HG11	1:A:225:VAL:HB	1.92	0.49
2:F:140:LYS:HD2	2:F:151:LYS:HD3	1.94	0.49
4:H:8:GLN:HB2	4:H:61:LYS:HD3	1.94	0.49
4:D:30:SER:HB3	3:G:372:THR:OG1	2.13	0.49
2:F:163:HIS:HD1	3:G:367:GLU:CD	2.16	0.49
2:B:144:ARG:O	3:C:375:PRO:HG3	2.12	0.49
1:E:4:PRO:HG3	2:F:68:LEU:HB3	1.93	0.49
2:F:103:ILE:HB	2:F:112:PHE:HB3	1.95	0.49
2:B:54:LEU:HD12	2:B:103:ILE:HD11	1.95	0.48
1:E:105:ARG:HD2	1:E:177:LYS:HB3	1.95	0.48
4:D:20:THR:O	4:D:36:ALA:HA	2.14	0.48
1:A:129:SER:OG	1:A:223:PHE:O	2.27	0.48
4:D:25:GLN:OE1	2:F:44:ASN:ND2	2.36	0.48
1:E:207:LYS:HA	1:E:210:SER:HB2	1.96	0.48
4:H:62:LEU:HD23	4:H:62:LEU:H	1.77	0.48
1:A:182:LYS:NZ	1:A:239:GLU:OE1	2.40	0.47
1:A:53:ASP:OD1	6:A:302:6VQ:N39	2.46	0.47
1:A:113:SER:O	1:A:115:SER:N	2.41	0.47
3:C:357:LYS:HB2	3:C:357:LYS:NZ	2.29	0.47
1:E:226:ASN:O	1:E:229:ILE:HG22	2.14	0.47
1:A:18:VAL:HG13	1:A:74:VAL:HG22	1.96	0.47
2:B:91:LEU:HD13	2:B:97:TYR:CZ	2.49	0.47
1:A:34:LEU:HD23	1:A:40:VAL:HG12	1.97	0.47
2:B:39:LYS:HB2	2:B:48:LEU:HD11	1.97	0.47
1:E:109:ILE:O	1:E:117:ILE:HA	2.15	0.47
1:E:226:ASN:OD1	1:E:227:SER:N	2.48	0.47
1:E:257:LYS:HB3	1:E:262:LEU:HD12	1.97	0.47
1:A:102:ILE:HD13	3:C:360:ALA:HB2	1.96	0.46
2:B:154:LYS:HA	2:B:154:LYS:HE2	1.98	0.46
2:F:102:ILE:HA	2:F:112:PHE:O	2.16	0.46
1:A:122:GLY:O	1:A:199:GLN:HB2	2.15	0.46
4:D:2:LEU:HD11	1:E:158:THR:OG1	2.16	0.46
1:E:206:PHE:O	1:E:210:SER:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:109:ILE:HD11	1:E:131:PRO:HG3	1.96	0.46
2:F:123:ASN:H	2:F:123:ASN:HD22	1.62	0.46
1:E:213:ILE:HD11	1:E:229:ILE:HD13	1.97	0.46
1:E:230:ARG:HH11	1:E:231:PRO:HD3	1.81	0.46
2:B:167:ASP:O	2:B:171:ILE:HG13	2.16	0.46
4:D:1:MET:HB3	4:D:3:ASN:OD1	2.15	0.46
4:H:7:TYR:HD1	4:H:63:PRO:HD2	1.81	0.46
2:B:86:ASN:OD1	2:B:86:ASN:N	2.49	0.46
2:B:139:MET:HA	2:B:151:LYS:O	2.16	0.45
1:E:113:SER:C	1:E:115:SER:H	2.20	0.45
2:F:180:GLU:N	2:F:180:GLU:OE2	2.50	0.45
4:H:37:VAL:HG23	4:H:43:VAL:HG12	1.98	0.45
1:E:108:ALA:HB2	1:E:130:PHE:HE2	1.82	0.45
1:A:38:GLU:OE2	1:A:38:GLU:N	2.44	0.45
2:F:162:VAL:HB	2:F:168:ARG:HG2	1.99	0.45
4:D:1:MET:HG2	4:D:2:LEU:N	2.30	0.45
1:A:212:ALA:O	1:A:215:LYS:HB2	2.16	0.45
2:F:39:LYS:HB2	2:F:48:LEU:HD11	1.99	0.45
2:F:151:LYS:HB2	3:G:379:PHE:CE1	2.51	0.45
2:B:151:LYS:HB2	3:C:379:PHE:CE1	2.47	0.45
1:E:101:THR:O	1:E:101:THR:OG1	2.34	0.45
1:E:186:GLU:HA	1:E:203:TRP:CZ2	2.52	0.44
1:A:109:ILE:HA	1:A:181:VAL:HG23	1.98	0.44
4:H:36:ALA:O	4:H:43:VAL:HA	2.18	0.44
4:H:62:LEU:HD12	4:H:64:PRO:HG2	2.00	0.44
1:E:13:SER:OG	1:E:16:ASN:OD1	2.36	0.44
1:E:24:ARG:NH1	2:F:105:ASN:O	2.46	0.44
2:F:22:ASP:OD2	2:F:59:ARG:NH1	2.49	0.44
4:D:52:ASP:N	4:D:52:ASP:OD1	2.51	0.44
1:E:222:VAL:HG13	1:E:225:VAL:HG13	2.00	0.44
1:E:262:LEU:HD23	4:H:56:ASP:HA	2.00	0.44
1:A:139:GLU:OE2	1:A:147:ARG:NH2	2.51	0.44
2:F:34:HIS:NE2	2:F:51:GLN:HG2	2.32	0.44
1:A:232:LEU:O	1:A:236:VAL:HG13	2.18	0.43
2:F:167:ASP:HA	2:F:170:ASN:HB2	2.00	0.43
1:A:30:PRO:HG2	1:A:33:ASP:OD1	2.18	0.43
1:A:33:ASP:HB3	1:A:43:HIS:NE2	2.32	0.43
1:A:137:LYS:HD3	3:C:359:TYR:CZ	2.53	0.43
2:B:124:LYS:HB2	2:B:124:LYS:HE3	1.75	0.43
1:E:90:ASN:O	1:E:93:VAL:HG22	2.19	0.43
1:A:122:GLY:C	1:A:199:GLN:HB2	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:7:GLU:OE2	2:B:10:ARG:NH1	2.51	0.43
1:E:110:PHE:CE1	1:E:117:ILE:HB	2.53	0.43
2:B:99:TYR:HB2	2:B:116:ILE:HB	1.99	0.43
4:D:2:LEU:HD22	1:E:156:ASP:OD2	2.18	0.43
4:D:18:ARG:NH2	4:H:55:TYR:CG	2.86	0.43
1:A:127:HIS:HD1	6:A:302:6VQ:C55	2.27	0.43
1:A:147:ARG:NH1	1:A:148:GLU:OE2	2.36	0.43
1:E:33:ASP:HB3	1:E:43:HIS:HE2	1.84	0.43
1:E:87:THR:HG22	1:E:89:GLU:H	1.84	0.43
1:A:7:ARG:HH11	2:B:71:VAL:HG23	1.84	0.42
2:F:89:HIS:CE1	2:F:154:LYS:NZ	2.87	0.42
2:B:136:LEU:HD13	2:B:153:LEU:HD13	1.99	0.42
2:B:40:TRP:HB2	2:B:45:TRP:CZ3	2.54	0.42
2:F:122:LEU:HD11	2:F:138:PRO:HG3	2.02	0.42
1:A:78:CYS:O	1:A:81:ILE:HG12	2.19	0.42
1:A:205:ASP:HB3	1:A:208:LYS:HB2	2.00	0.42
1:A:63:PRO:HG2	1:A:65:LEU:CD1	2.50	0.42
1:E:120:LEU:HD22	1:E:198:ILE:HD13	2.00	0.42
1:E:211:LYS:HA	1:E:211:LYS:HD3	1.67	0.42
1:A:233:SER:O	1:A:236:VAL:HG22	2.20	0.42
1:E:124:ASN:N	1:E:124:ASN:OD1	2.53	0.42
1:E:243:LYS:O	1:E:246:ASN:HB3	2.20	0.42
4:D:11:ILE:O	4:D:18:ARG:HA	2.19	0.41
1:E:118:LEU:HB2	1:E:203:TRP:CE3	2.55	0.41
4:H:11:ILE:HB	4:H:54:LEU:HD22	2.02	0.41
1:A:116:LYS:HA	1:A:204:LYS:O	2.21	0.41
1:A:169:ARG:HA	1:A:169:ARG:HD3	1.97	0.41
1:A:38:GLU:HG2	1:A:98:TYR:HB2	2.03	0.41
1:A:54:PHE:O	1:A:58:MET:HG3	2.21	0.41
1:A:210:SER:HA	1:A:229:ILE:HD11	2.01	0.41
1:E:110:PHE:O	1:E:184:VAL:HG12	2.21	0.41
2:F:75:ASP:OD1	2:F:84:GLU:N	2.54	0.41
2:F:141:VAL:HG22	2:F:172:TYR:HD1	1.86	0.41
2:F:165:PRO:HB3	2:F:168:ARG:HH12	1.86	0.41
1:A:124:ASN:O	1:A:126:LYS:HB2	2.21	0.40
1:A:180:LEU:HD22	1:A:235:TYR:CG	2.56	0.40
2:B:125:ARG:NH2	2:B:134:GLU:O	2.54	0.40
1:E:146:ILE:HD13	1:E:158:THR:HA	2.03	0.40
4:H:4:PHE:O	4:H:23:LEU:HD23	2.20	0.40
1:E:213:ILE:HD11	1:E:229:ILE:HG21	2.04	0.40
2:F:74:TYR:CE2	2:F:76:ASP:HB3	2.57	0.40

All (1) 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)
4:D:44:SER:OG	4:D:44:SER:OG[2_556]	2.08	0.12

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	256/275 (93%)	242 (94%)	14 (6%)	0	100	100
1	E	253/275 (92%)	242 (96%)	11 (4%)	0	100	100
2	B	171/190 (90%)	161 (94%)	10 (6%)	0	100	100
2	F	172/190 (90%)	163 (95%)	9 (5%)	0	100	100
3	C	21/26 (81%)	21 (100%)	0	0	100	100
3	G	24/26 (92%)	24 (100%)	0	0	100	100
4	D	63/66 (96%)	62 (98%)	1 (2%)	0	100	100
4	H	52/66 (79%)	52 (100%)	0	0	100	100
All	All	1012/1114 (91%)	967 (96%)	45 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	239/251 (95%)	228 (95%)	11 (5%)	27	51
1	E	237/251 (94%)	230 (97%)	7 (3%)	41	65
2	B	160/173 (92%)	155 (97%)	5 (3%)	40	64
2	F	164/173 (95%)	161 (98%)	3 (2%)	59	78
3	C	18/21 (86%)	17 (94%)	1 (6%)	21	40
3	G	21/21 (100%)	21 (100%)	0	100	100
4	D	58/58 (100%)	57 (98%)	1 (2%)	60	80
4	H	53/58 (91%)	50 (94%)	3 (6%)	20	39
All	All	950/1006 (94%)	919 (97%)	31 (3%)	38	63

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	LEU
1	A	55	VAL
1	A	76	ASP
1	A	89	GLU
1	A	93	VAL
1	A	124	ASN
1	A	135	ILE
1	A	158	THR
1	A	199	GLN
1	A	214	THR
1	A	236	VAL
2	B	31	HIS
2	B	87	THR
2	B	139	MET
2	B	162	VAL
2	B	182	GLU
3	C	371	VAL
4	D	40	ASP
1	E	101	THR
1	E	124	ASN
1	E	132	ARG
1	E	158	THR
1	E	203	TRP
1	E	236	VAL
1	E	251	TYR
2	F	31	HIS
2	F	59	ARG

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Mol	Chain	Res	Type
2	F	181	ASN
4	H	10	GLU
4	H	37	VAL
4	H	62	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	F	123	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	$\#\|Z\| > 2$
6	6VQ	A	302	-	42,62,62	3.86	14 (33%)	45,99,99	1.33	5 (11%)
6	6VQ	E	301	-	42,62,62	3.90	14 (33%)	45,99,99	1.54	7 (15%)

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
6	6VQ	A	302	-	-	7/22/70/70	0/6/6/6
6	6VQ	E	301	-	-	4/22/70/70	0/6/6/6

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	301	6VQ	P22-O25	16.95	1.85	1.57
6	A	302	6VQ	P22-O25	16.81	1.84	1.57
6	E	301	6VQ	P10-O09	13.90	1.80	1.57
6	A	302	6VQ	P10-O09	13.53	1.79	1.57
6	A	302	6VQ	C03-N04	5.02	1.42	1.33
6	E	301	6VQ	C03-N04	5.00	1.42	1.33
6	E	301	6VQ	C38-N39	3.83	1.43	1.34
6	A	302	6VQ	C38-N39	3.77	1.43	1.34
6	A	302	6VQ	C31-N30	3.69	1.39	1.33
6	A	302	6VQ	C03-N02	3.47	1.39	1.33
6	A	302	6VQ	C52-N53	3.44	1.42	1.34
6	E	301	6VQ	C03-N02	3.43	1.39	1.33
6	A	302	6VQ	C31-N32	3.42	1.39	1.33
6	E	301	6VQ	C26-C27	3.39	1.62	1.51
6	E	301	6VQ	C52-N53	3.38	1.42	1.34
6	E	301	6VQ	C31-N30	3.36	1.39	1.33
6	A	302	6VQ	C26-C27	3.30	1.61	1.51
6	E	301	6VQ	C31-N32	3.20	1.39	1.33
6	E	301	6VQ	C08-C07	2.78	1.60	1.51
6	A	302	6VQ	O09-C08	-2.64	1.34	1.44
6	E	301	6VQ	O09-C08	-2.60	1.34	1.44
6	A	302	6VQ	C08-C07	2.60	1.59	1.51
6	A	302	6VQ	O25-C26	-2.26	1.36	1.44
6	A	302	6VQ	C44-C27	2.22	1.58	1.53
6	A	302	6VQ	C52-N54	2.21	1.38	1.33
6	E	301	6VQ	C44-C27	2.21	1.58	1.53
6	E	301	6VQ	C52-N54	2.20	1.38	1.33
6	E	301	6VQ	O25-C26	-2.20	1.36	1.44

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	E	301	6VQ	O25-P22-O23	-4.88	96.42	114.42
6	E	301	6VQ	O09-P10-O11	-4.43	98.08	114.42
6	A	302	6VQ	O25-P22-O23	-3.95	99.86	114.42
6	A	302	6VQ	O09-P10-O11	-3.54	101.38	114.42
6	E	301	6VQ	O21-P22-O25	2.74	111.18	101.37
6	E	301	6VQ	C46-C48-C05	2.49	104.73	100.98
6	E	301	6VQ	O45-C44-C42	-2.49	103.77	111.82
6	A	302	6VQ	C42-C44-C27	2.13	106.78	102.64
6	E	301	6VQ	O06-C07-C08	2.10	116.30	109.37
6	E	301	6VQ	P10-O09-C08	2.09	126.78	120.16
6	A	302	6VQ	O45-C44-C42	-2.08	105.10	111.82
6	A	302	6VQ	C34-C35-N37	-2.01	115.05	117.85

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	302	6VQ	O25-C26-C27-C44
6	A	302	6VQ	O25-C26-C27-O28
6	E	301	6VQ	C26-O25-P22-O23
6	A	302	6VQ	O06-C07-C08-O09
6	A	302	6VQ	C27-C26-O25-P22
6	E	301	6VQ	C08-O09-P10-O11
6	E	301	6VQ	C27-C26-O25-P22
6	A	302	6VQ	P22-O21-P18-O20
6	A	302	6VQ	C26-O25-P22-O23
6	A	302	6VQ	C08-O09-P10-O11
6	E	301	6VQ	P18-O21-P22-O23

There are no ring outliers.

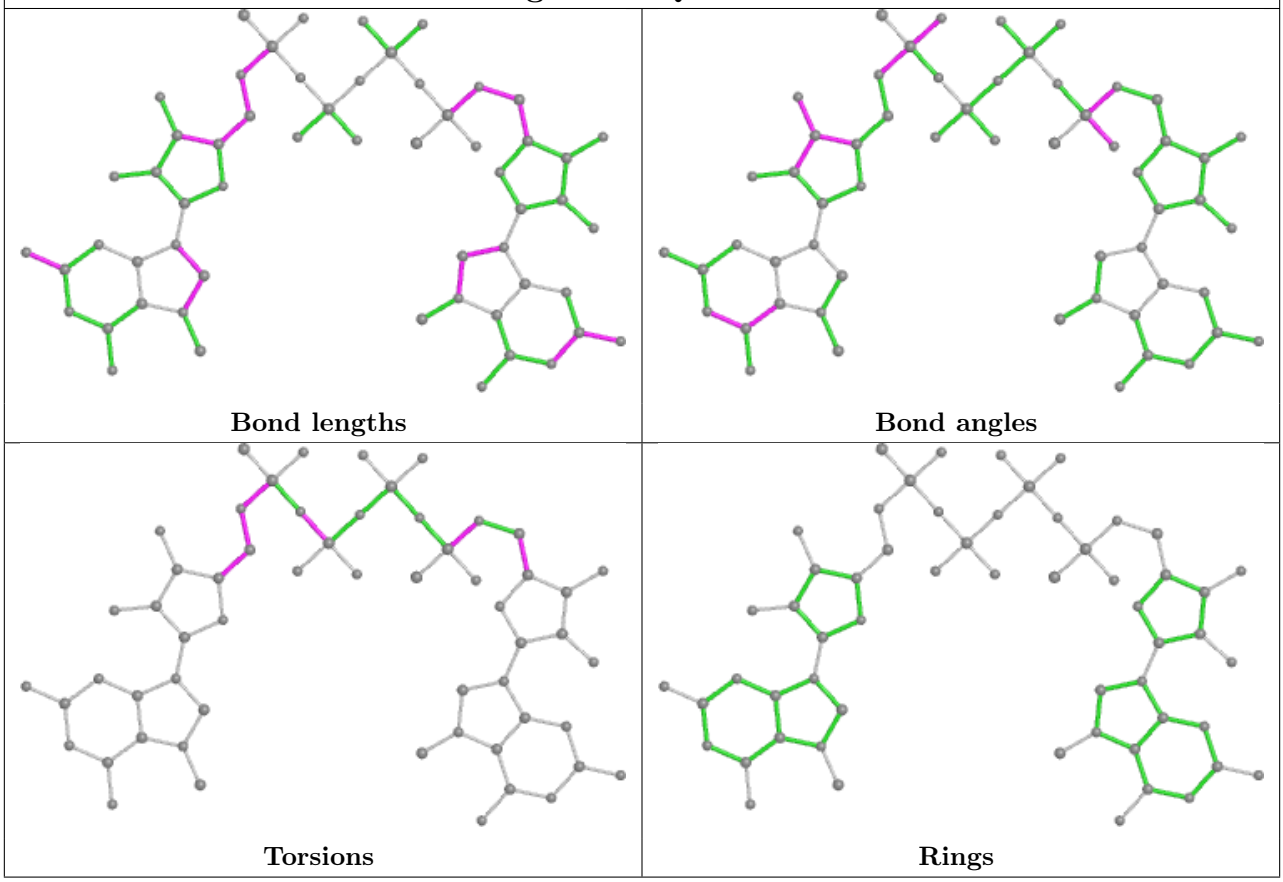
1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	302	6VQ	4	0

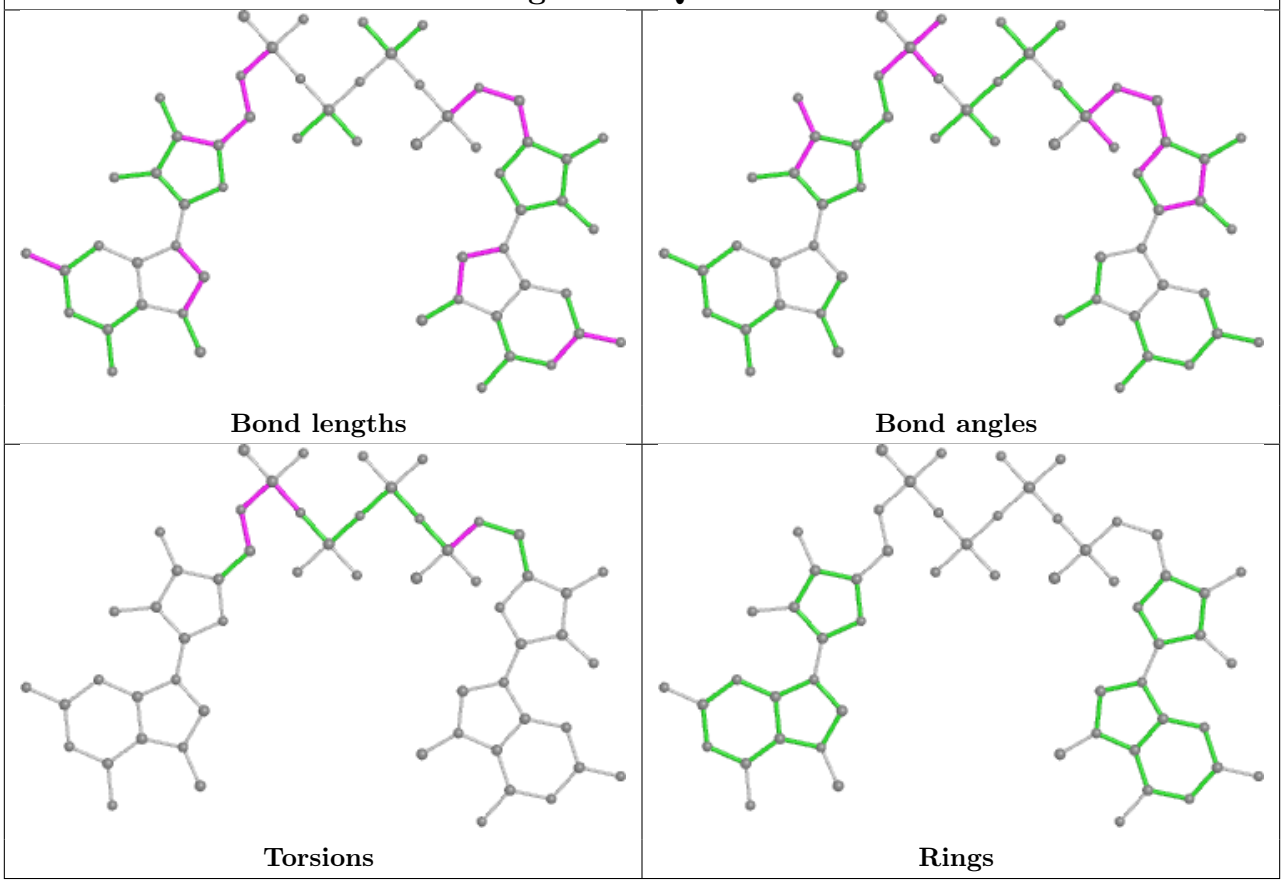
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 6VQ A 302



Ligand 6VQ E 301



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	260/275 (94%)	-0.08	4 (1%)	73	70	50, 84, 124, 165	0
1	E	257/275 (93%)	0.21	11 (4%)	35	27	59, 109, 157, 176	0
2	B	175/190 (92%)	0.18	9 (5%)	28	21	53, 88, 156, 178	0
2	F	178/190 (93%)	-0.00	4 (2%)	62	57	54, 82, 147, 179	0
3	C	23/26 (88%)	-0.32	0	100	100	59, 90, 111, 118	0
3	G	26/26 (100%)	0.03	1 (3%)	40	32	72, 87, 118, 149	0
4	D	65/66 (98%)	0.12	3 (4%)	32	25	65, 91, 123, 136	0
4	H	58/66 (87%)	1.55	20 (34%)	0	0	145, 186, 213, 223	0
All	All	1042/1114 (93%)	0.15	52 (4%)	28	22	50, 93, 169, 223	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	4	PHE	11.1
4	H	7	TYR	6.0
4	H	49	ILE	5.2
4	H	47	PHE	4.6
4	H	48	LYS	3.8
4	H	21	GLY	3.6
2	F	76	ASP	3.6
4	H	19	ILE	3.6
4	H	59	VAL	3.5
2	B	72	SER	3.3
1	A	221	LYS	3.2
1	A	217	GLU	3.1
4	D	65	ASN	3.1
4	H	9	ILE	3.0
4	H	5	LYS	3.0
4	H	11	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	128	PHE	3.0
4	H	46	VAL	3.0
1	E	202	GLU	2.8
4	H	53	LYS	2.7
1	E	213	ILE	2.7
1	A	263	ASN	2.7
4	H	33	LEU	2.7
4	H	57	LEU	2.6
2	B	129	ALA	2.6
4	H	60	LEU	2.6
2	B	62	GLY	2.6
2	F	71	VAL	2.6
1	E	85	ASP	2.5
4	H	61	LYS	2.4
2	B	127	LEU	2.4
4	H	23	LEU	2.4
2	B	61	VAL	2.4
2	B	126	LYS	2.3
4	H	50	LYS	2.3
2	F	184	THR	2.3
1	E	130	PHE	2.3
1	E	205	ASP	2.3
2	B	185	ASP	2.3
2	B	130	PRO	2.2
3	G	355	HIS	2.2
1	E	208	LYS	2.2
1	E	262	LEU	2.2
2	F	188	THR	2.2
1	E	256	LEU	2.1
4	D	9	ILE	2.1
4	H	3	ASN	2.1
1	E	165	GLN	2.1
1	E	126	LYS	2.1
4	D	57	LEU	2.1
1	A	220	ALA	2.0
1	E	135	ILE	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

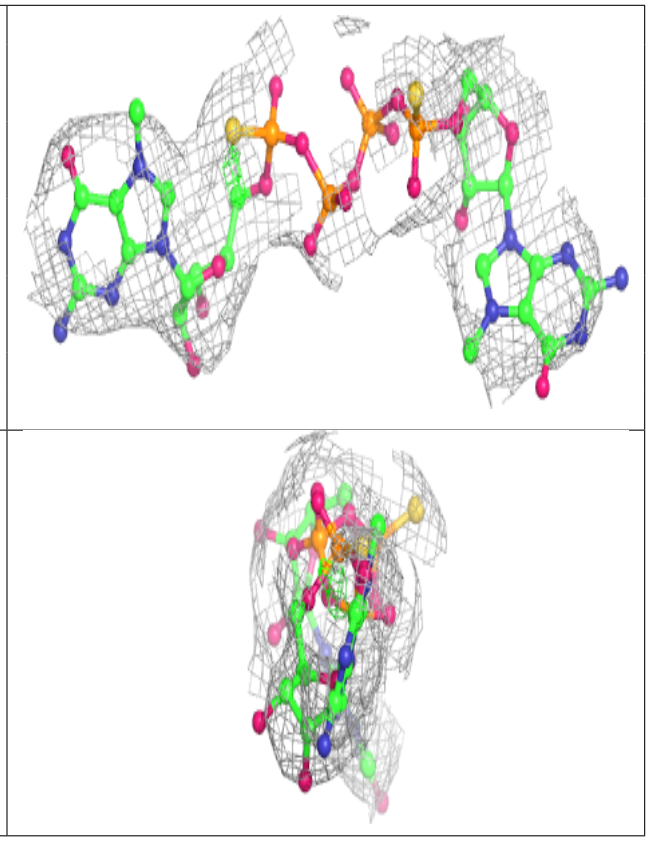
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	MG	A	301	1/1	0.87	0.33	94,94,94,94	0
6	6VQ	E	301	57/57	0.89	0.18	75,130,155,168	0
6	6VQ	A	302	57/57	0.95	0.16	68,96,122,130	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.

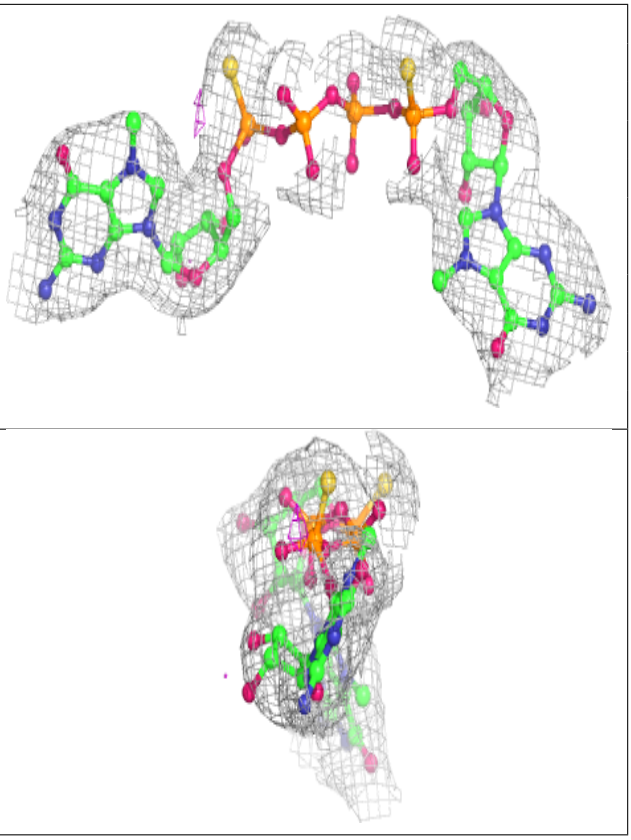
Electron density around 6VQ E 301:

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 6VQ A 302:

$2mF_o$-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.