Full wwPDB X-ray Structure Validation Report (i)

May 23, 2024 – 10:50 AM EDT

PDB ID	:	3ZFG
Title	:	Human enterovirus 71 in complex with capsid binding inhibitor WIN51711
Authors	:	Plevka, P.; Perera, R.; Yap, M.L.; Cardosa, J.; Kuhn, R.J.; Rossmann, M.G.
Deposited on	:	2012-12-11
Resolution	:	3.20 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 (1)) were used in the production of this report:

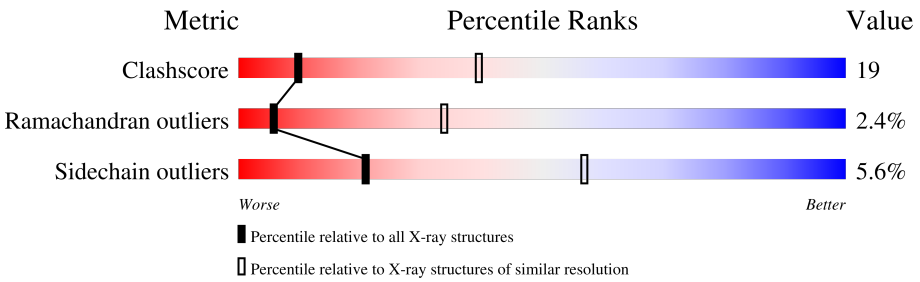
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)

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%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	298	66% 30% •
2	B	254	64% 30% • •
3	C	242	60% 36% • •
4	D	69	61% 20% • 17%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6532 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 VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	297	2299	1447	395	444	13	0	0	1

- Molecule 2 is a protein called VP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	245	1899	1215	314	361	9	0	0	0

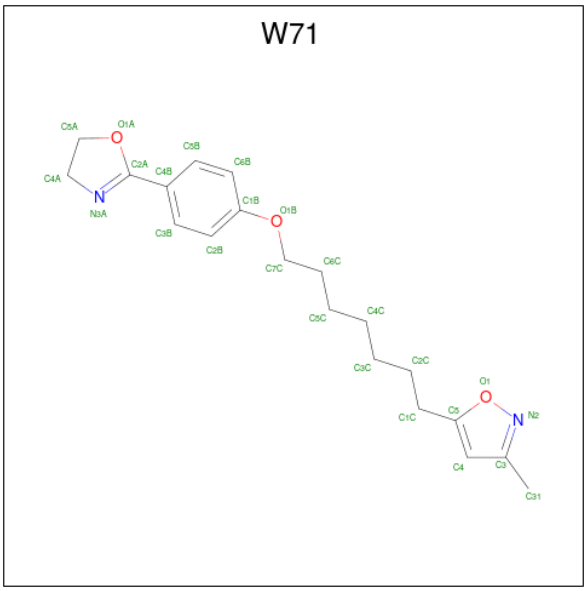
- Molecule 3 is a protein called VP3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	242	1866	1198	311	345	12	0	0	0

- Molecule 4 is a protein called VP4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	57	443	276	72	94	1	0	0	0

- Molecule 5 is 5-(7-(4-(4,5-DIHYDRO-2-OXAZOLYL)PHENOXY)HEPTYL)-3-METHYL ISOXAZOLE (three-letter code: W71) (formula: $C_{20}H_{26}N_2O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	25	20	2	3	0	0

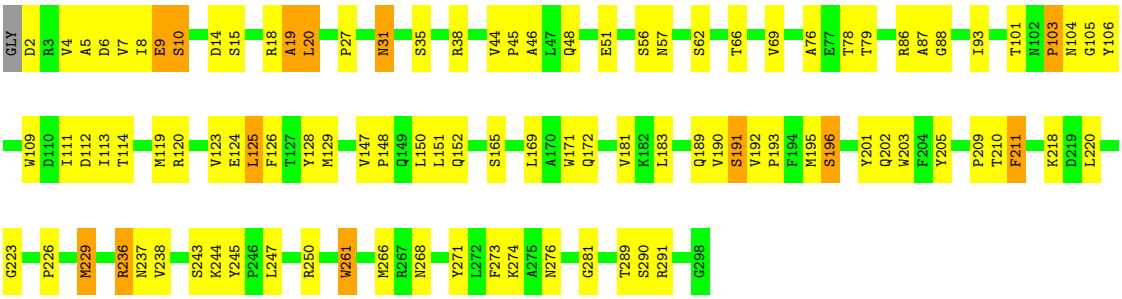
3 Residue-property plots (i)

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. 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 failed to run properly.

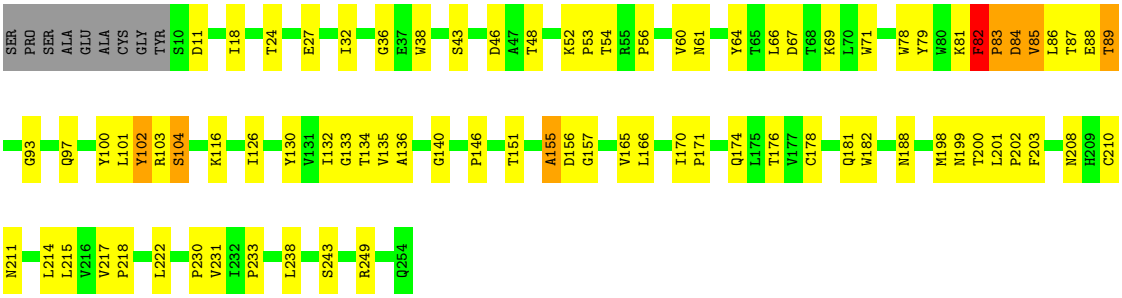
- Molecule 1: VP1

Chain A:



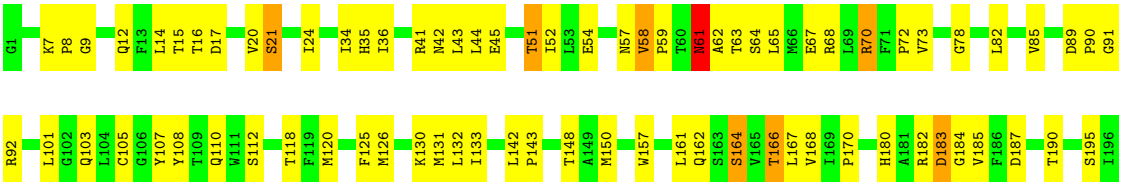
- Molecule 2: VP2

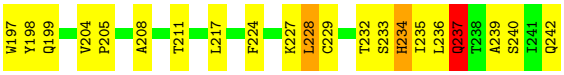
Chain B:



- Molecule 3: VP3

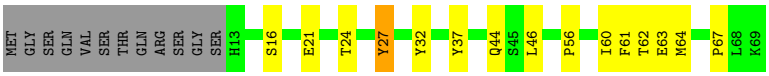
Chain C:





• Molecule 4: VP4

Chain D:



4 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α, β, γ	592.50Å 592.50Å 592.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.20 – 3.20	Depositor
% Data completeness (in resolution range)	66.8 (33.20-3.20)	Depositor
R_{merge}	0.33	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.28 (at 3.25Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.249 , (Not available)	Depositor
Wilson B-factor (Å^2)	50.1	Xtriage
Anisotropy	0.000	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.000 for -l,-k,-h	Xtriage
Total number of atoms	6532	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% 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: W71

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	0.57	1/2358 (0.0%)	0.71	0/3215
2	B	0.51	0/1954	0.72	1/2678 (0.0%)
3	C	0.52	0/1920	0.71	0/2626
4	D	0.62	0/452	0.73	0/611
All	All	0.54	1/6684 (0.0%)	0.71	1/9130 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	189	GLN	CD-OE1	5.59	1.36	1.24

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	82	PHE	N-CA-C	6.47	128.48	111.00

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	2299	0	2231	107	0
2	B	1899	0	1832	64	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1866	0	1837	97	0
4	D	443	0	420	20	0
5	A	25	0	26	5	0
All	All	6532	0	6346	247	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 19.

All (247) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:ASP:OD1	1:A:114:THR:HG22	1.51	1.09
1:A:210:THR:O	1:A:211:PHE:HB2	1.71	0.90
1:A:114:THR:HG23	1:A:274:LYS:HB3	1.53	0.89
1:A:268:ASN:HB2	2:B:171:PRO:HD3	1.58	0.86
1:A:18:ARG:HB2	2:B:38:TRP:HB2	1.62	0.82
3:C:131:MET:HE2	3:C:198:TYR:HA	1.62	0.81
1:A:35:SER:HB3	1:A:66:THR:H	1.44	0.81
3:C:237:GLN:HE21	3:C:237:GLN:N	1.77	0.81
3:C:237:GLN:N	3:C:237:GLN:NE2	2.29	0.81
2:B:102:TYR:CE1	2:B:104:SER:HB3	2.18	0.79
3:C:235:ILE:HD11	3:C:237:GLN:OE1	1.82	0.79
1:A:27:PRO:HA	4:D:46:LEU:HD23	1.65	0.79
3:C:58:VAL:HB	3:C:59:PRO:HD3	1.64	0.78
2:B:82:PHE:O	2:B:83:PRO:C	2.22	0.78
1:A:19:ALA:O	1:A:20:LEU:HB2	1.84	0.77
2:B:249:ARG:HG3	2:B:249:ARG:HH11	1.50	0.77
1:A:192:VAL:HG22	3:C:24:ILE:HD13	1.69	0.75
3:C:89:ASP:OD2	3:C:190:THR:HA	1.88	0.73
2:B:66:LEU:HD13	2:B:85:VAL:HG22	1.73	0.71
2:B:86:LEU:HD13	2:B:238:LEU:HD11	1.73	0.70
2:B:43:SER:HB2	2:B:46:ASP:HB2	1.74	0.70
3:C:34:ILE:HG22	3:C:35:HIS:N	2.06	0.70
1:A:243:SER:O	1:A:244:LYS:HB3	1.91	0.69
1:A:114:THR:CG2	1:A:274:LYS:HB3	2.23	0.69
1:A:226:PRO:HA	1:A:229:MET:CG	2.22	0.69
1:A:150:LEU:HD23	1:A:238:VAL:HG21	1.75	0.68
2:B:54:THR:HG22	2:B:56:PRO:HD3	1.75	0.68
1:A:78:THR:HG21	3:C:44:LEU:HG	1.77	0.66
1:A:289:THR:HG22	1:A:290:SER:N	2.08	0.66
3:C:120:MET:HA	3:C:164:SER:HB3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:ASN:HB3	1:A:69:VAL:O	1.96	0.65
1:A:192:VAL:HG11	5:A:900:W71:H4C2	1.77	0.65
3:C:161:LEU:HD12	3:C:161:LEU:H	1.62	0.65
3:C:237:GLN:HE21	3:C:237:GLN:H	1.43	0.63
1:A:78:THR:HG22	3:C:43:LEU:HB2	1.79	0.63
2:B:32:ILE:HD12	4:D:56:PRO:HG2	1.80	0.63
3:C:126:MET:HE3	3:C:126:MET:HA	1.81	0.63
2:B:83:PRO:HG2	2:B:210:CYS:HA	1.79	0.63
1:A:78:THR:CG2	3:C:43:LEU:HB2	2.29	0.63
3:C:65:LEU:O	3:C:68:ARG:HG3	1.99	0.62
3:C:131:MET:HE1	3:C:198:TYR:CD2	2.34	0.62
1:A:171:TRP:CE2	1:A:236:ARG:HG2	2.35	0.62
2:B:64:TYR:CD2	2:B:86:LEU:HD21	2.35	0.62
3:C:108:TYR:CE2	3:C:229:CYS:HB3	2.35	0.61
4:D:62:THR:HG22	4:D:64:MET:H	1.65	0.61
2:B:83:PRO:HG2	2:B:211:ASN:H	1.64	0.61
3:C:142:LEU:HD12	3:C:143:PRO:HD2	1.83	0.61
1:A:88:GLY:HA3	1:A:119:MET:CE	2.31	0.60
3:C:204:VAL:HG22	3:C:208:ALA:HB3	1.83	0.60
1:A:191:SER:HB2	3:C:21:SER:O	2.02	0.60
4:D:62:THR:HG22	4:D:63:GLU:N	2.16	0.59
1:A:169:LEU:O	1:A:172:GLN:HG3	2.03	0.59
3:C:112:SER:O	3:C:224:PHE:HA	2.03	0.58
4:D:16:SER:HB3	4:D:21:GLU:OE2	2.03	0.58
3:C:61:ASN:C	3:C:63:THR:H	2.06	0.58
2:B:155:ALA:C	2:B:157:GLY:H	2.07	0.58
1:A:183:LEU:HD21	1:A:247:LEU:HD22	1.86	0.57
2:B:104:SER:HB2	2:B:243:SER:HA	1.87	0.57
1:A:9:GLU:O	1:A:10:SER:C	2.42	0.57
2:B:87:THR:HG22	2:B:88:GLU:N	2.20	0.57
1:A:123:VAL:HB	1:A:129:MET:HE3	1.85	0.57
3:C:34:ILE:HG22	3:C:35:HIS:H	1.69	0.56
1:A:281:GLY:HA3	2:B:135:VAL:HB	1.87	0.56
1:A:6:ASP:O	1:A:10:SER:HB2	2.05	0.56
1:A:112:ASP:CG	1:A:114:THR:HG22	2.24	0.56
1:A:147:VAL:HG11	1:A:245:TYR:CG	2.41	0.56
1:A:289:THR:CG2	1:A:290:SER:N	2.68	0.56
2:B:116:LYS:HD3	3:C:125:PHE:CD2	2.39	0.56
1:A:15:SER:HB2	2:B:43:SER:HA	1.88	0.56
1:A:51:GLU:HA	2:B:182:TRP:HB2	1.87	0.56
3:C:108:TYR:HA	3:C:229:CYS:HA	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:105:CYS:HB3	3:C:180:HIS:HE1	1.71	0.56
1:A:243:SER:O	1:A:244:LYS:CB	2.54	0.56
1:A:193:PRO:HG2	1:A:195:MET:HE3	1.87	0.55
1:A:226:PRO:HA	1:A:229:MET:HG3	1.87	0.55
1:A:18:ARG:O	1:A:19:ALA:HB3	2.07	0.55
2:B:130:TYR:CE2	2:B:215:LEU:HD11	2.43	0.54
3:C:14:LEU:HB3	3:C:17:ASP:HB2	1.90	0.54
1:A:291:ARG:HD2	3:C:57:ASN:OD1	2.08	0.54
3:C:64:SER:O	3:C:67:GLU:HB2	2.08	0.54
2:B:66:LEU:CD1	2:B:85:VAL:HG22	2.37	0.54
3:C:91:GLY:HA3	3:C:180:HIS:ND1	2.24	0.53
2:B:116:LYS:HD3	3:C:125:PHE:CE2	2.43	0.53
2:B:93:GLY:O	2:B:97:GLN:HG3	2.08	0.53
1:A:268:ASN:HB2	2:B:171:PRO:CD	2.35	0.53
1:A:48:GLN:HA	4:D:67:PRO:HG2	1.90	0.53
3:C:239:ALA:O	3:C:240:SER:C	2.47	0.53
1:A:120:ARG:O	1:A:124:GLU:HG3	2.08	0.53
1:A:87:ALA:O	3:C:15:THR:HG23	2.08	0.52
2:B:81:LYS:HG3	2:B:151:THR:O	2.09	0.52
1:A:171:TRP:CZ2	1:A:236:ARG:HG2	2.44	0.52
1:A:113:ILE:HD11	1:A:203:TRP:CH2	2.44	0.52
1:A:261:TRP:CD1	1:A:261:TRP:N	2.76	0.52
2:B:82:PHE:CZ	2:B:238:LEU:HD22	2.44	0.52
2:B:249:ARG:HG3	2:B:249:ARG:NH1	2.19	0.52
3:C:9:GLY:O	3:C:12:GLN:HG2	2.10	0.52
2:B:102:TYR:HE1	2:B:104:SER:HB3	1.69	0.52
1:A:193:PRO:HB3	4:D:37:TYR:CD2	2.45	0.52
1:A:78:THR:HB	3:C:42:ASN:OD1	2.10	0.52
2:B:155:ALA:O	2:B:156:ASP:HB2	2.10	0.51
1:A:201:TYR:CG	5:A:900:W71:H2B	2.46	0.51
2:B:66:LEU:O	2:B:67:ASP:HB2	2.11	0.51
1:A:19:ALA:O	1:A:20:LEU:CB	2.56	0.51
1:A:129:MET:CE	1:A:203:TRP:HE1	2.23	0.51
1:A:150:LEU:CD2	1:A:238:VAL:HG21	2.40	0.51
2:B:126:ILE:O	2:B:178:CYS:HB3	2.10	0.51
1:A:56:SER:OG	3:C:166:THR:HG21	2.11	0.51
1:A:261:TRP:CE3	3:C:36:ILE:HB	2.46	0.51
1:A:218:LYS:C	1:A:220:LEU:H	2.13	0.50
3:C:20:VAL:HG21	4:D:32:TYR:CD2	2.47	0.50
1:A:266:MET:HE1	3:C:107:TYR:HE2	1.75	0.50
1:A:151:LEU:HD23	1:A:237:ASN:HA	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:61:PHE:O	4:D:62:THR:HB	2.11	0.50
1:A:129:MET:HE3	1:A:203:TRP:HE1	1.77	0.50
4:D:60:ILE:HG22	4:D:61:PHE:N	2.26	0.50
1:A:4:VAL:O	1:A:5:ALA:HB3	2.11	0.50
1:A:51:GLU:O	2:B:181:GLN:HG3	2.12	0.50
1:A:76:ALA:O	1:A:79:THR:HG23	2.12	0.50
3:C:67:GLU:HG2	3:C:70:ARG:NH2	2.27	0.50
1:A:103:PRO:O	1:A:105:GLY:N	2.43	0.49
2:B:200:THR:O	2:B:201:LEU:HD23	2.12	0.49
2:B:174:GLN:HA	3:C:51:THR:HG22	1.93	0.49
3:C:70:ARG:HD3	3:C:70:ARG:N	2.27	0.49
3:C:108:TYR:CD2	3:C:229:CYS:HB3	2.46	0.49
1:A:192:VAL:HG21	5:A:900:W71:H2C2	1.94	0.49
2:B:18:ILE:HG22	2:B:61:ASN:O	2.12	0.49
2:B:134:THR:HG23	2:B:146:PRO:HD3	1.94	0.49
3:C:199:GLN:OE1	3:C:199:GLN:HA	2.13	0.49
1:A:238:VAL:HG23	1:A:238:VAL:O	2.12	0.49
2:B:87:THR:C	2:B:89:THR:H	2.16	0.49
1:A:86:ARG:HG2	3:C:16:THR:HG22	1.95	0.49
1:A:103:PRO:C	1:A:105:GLY:H	2.16	0.49
1:A:106:TYR:CE2	1:A:165:SER:HA	2.48	0.49
1:A:266:MET:CE	3:C:107:TYR:HE2	2.26	0.49
3:C:228:LEU:C	3:C:228:LEU:HD12	2.33	0.49
3:C:182:ARG:O	3:C:182:ARG:HG3	2.12	0.49
3:C:236:LEU:N	3:C:236:LEU:HD23	2.28	0.48
1:A:193:PRO:HG2	1:A:195:MET:CE	2.43	0.48
3:C:143:PRO:HB3	3:C:148:THR:HG22	1.96	0.48
1:A:271:TYR:H	3:C:237:GLN:HG3	1.78	0.48
1:A:38:ARG:HG3	1:A:38:ARG:HH11	1.79	0.48
1:A:123:VAL:HA	1:A:129:MET:CE	2.44	0.48
1:A:125:LEU:HD13	1:A:126:PHE:CZ	2.49	0.48
1:A:203:TRP:HA	1:A:203:TRP:CE3	2.49	0.48
1:A:250:ARG:HG3	1:A:250:ARG:HH11	1.78	0.48
3:C:131:MET:CE	3:C:198:TYR:HA	2.41	0.48
1:A:147:VAL:HG13	1:A:148:PRO:HD2	1.96	0.47
3:C:132:LEU:HD23	3:C:132:LEU:C	2.34	0.47
2:B:27:GLU:O	2:B:188:ASN:HB2	2.14	0.47
4:D:60:ILE:HG22	4:D:61:PHE:H	1.80	0.47
1:A:195:MET:O	1:A:196:SER:CB	2.63	0.47
1:A:88:GLY:HA3	1:A:119:MET:HE2	1.96	0.47
2:B:176:THR:C	2:B:178:CYS:H	2.19	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:62:THR:HG22	4:D:63:GLU:H	1.80	0.47
3:C:20:VAL:HG21	4:D:32:TYR:HD2	1.80	0.47
3:C:62:ALA:HA	3:C:65:LEU:HG	1.97	0.46
1:A:123:VAL:C	1:A:125:LEU:H	2.17	0.46
3:C:52:ILE:HA	3:C:217:LEU:HD23	1.98	0.46
2:B:166:LEU:HD12	2:B:170:ILE:HG13	1.97	0.46
3:C:130:LYS:HA	3:C:157:TRP:O	2.16	0.46
2:B:66:LEU:HD12	2:B:238:LEU:HD21	1.98	0.46
2:B:83:PRO:CG	2:B:210:CYS:HA	2.46	0.46
2:B:231:VAL:O	2:B:233:PRO:HD3	2.15	0.46
2:B:79:TYR:HA	2:B:214:LEU:O	2.17	0.45
3:C:34:ILE:CG2	3:C:35:HIS:N	2.75	0.45
1:A:150:LEU:HD23	1:A:238:VAL:CG2	2.43	0.45
2:B:101:LEU:HB3	2:B:203:PHE:HB3	1.97	0.45
1:A:192:VAL:HG22	3:C:24:ILE:CD1	2.42	0.45
2:B:100:TYR:HA	2:B:249:ARG:HH21	1.82	0.45
3:C:110:GLN:OE1	3:C:227:LYS:HE3	2.16	0.45
2:B:82:PHE:O	2:B:84:ASP:N	2.49	0.45
3:C:233:SER:O	3:C:234:HIS:C	2.54	0.45
1:A:266:MET:HG3	3:C:103:GLN:HB3	1.99	0.45
3:C:133:ILE:HG22	3:C:167:LEU:HD22	1.99	0.45
3:C:161:LEU:HD12	3:C:161:LEU:N	2.30	0.45
1:A:201:TYR:CD1	5:A:900:W71:H2B	2.52	0.45
1:A:218:LYS:C	1:A:220:LEU:N	2.70	0.44
1:A:123:VAL:CB	1:A:129:MET:HE3	2.48	0.44
2:B:71:TRP:CE2	2:B:222:LEU:HB2	2.52	0.44
3:C:54:GLU:HG2	3:C:68:ARG:HB2	1.98	0.44
3:C:126:MET:HA	3:C:126:MET:CE	2.48	0.44
1:A:171:TRP:CD2	1:A:236:ARG:HG2	2.52	0.44
3:C:133:ILE:CG2	3:C:167:LEU:HD22	2.47	0.44
1:A:93:ILE:HD11	1:A:109:TRP:HB2	2.00	0.44
3:C:7:LYS:HB3	3:C:8:PRO:HD2	1.99	0.44
1:A:125:LEU:O	1:A:125:LEU:HD22	2.17	0.44
1:A:5:ALA:O	1:A:8:ILE:N	2.50	0.44
1:A:147:VAL:HG11	1:A:245:TYR:CD2	2.53	0.44
2:B:56:PRO:HG2	2:B:60:VAL:HG21	1.99	0.44
3:C:42:ASN:O	3:C:45:GLU:HB2	2.18	0.44
1:A:57:ASN:HD21	4:D:61:PHE:HE1	1.65	0.44
3:C:195:SER:HB2	3:C:197:TRP:NE1	2.33	0.43
4:D:27:TYR:N	4:D:27:TYR:CD1	2.86	0.43
3:C:82:LEU:HB2	3:C:197:TRP:CZ3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:168:VAL:O	3:C:170:PRO:HD3	2.18	0.43
3:C:61:ASN:C	3:C:63:THR:N	2.72	0.43
1:A:5:ALA:C	1:A:7:VAL:N	2.71	0.43
1:A:45:PRO:HA	4:D:63:GLU:O	2.18	0.43
3:C:120:MET:CA	3:C:164:SER:HB3	2.45	0.43
1:A:195:MET:O	1:A:196:SER:HB2	2.18	0.43
2:B:136:ALA:HB3	2:B:140:GLY:HA2	1.99	0.43
1:A:226:PRO:HA	1:A:229:MET:HG2	1.97	0.43
1:A:273:PHE:CD2	3:C:242:GLN:HB3	2.53	0.43
1:A:46:ALA:O	3:C:166:THR:HG22	2.19	0.43
2:B:52:LYS:HA	2:B:53:PRO:HD2	1.90	0.43
3:C:233:SER:OG	3:C:234:HIS:N	2.51	0.43
2:B:67:ASP:OD2	2:B:69:LYS:HE2	2.19	0.43
2:B:217:VAL:HA	2:B:218:PRO:HD3	1.77	0.43
3:C:233:SER:O	3:C:235:ILE:N	2.52	0.43
3:C:142:LEU:HA	3:C:143:PRO:HD2	1.88	0.43
1:A:27:PRO:HA	4:D:46:LEU:CD2	2.43	0.42
3:C:89:ASP:HA	3:C:90:PRO:HD3	1.78	0.42
3:C:41:ARG:HH22	4:D:24:THR:HG21	1.84	0.42
3:C:204:VAL:HG22	3:C:205:PRO:HD2	2.01	0.42
1:A:210:THR:O	1:A:211:PHE:CB	2.50	0.42
2:B:155:ALA:O	2:B:157:GLY:N	2.52	0.42
3:C:185:VAL:C	3:C:187:ASP:H	2.22	0.42
2:B:136:ALA:CB	2:B:140:GLY:HA2	2.49	0.42
1:A:291:ARG:NH2	3:C:85:VAL:O	2.49	0.42
2:B:202:PRO:HD3	3:C:34:ILE:HD11	2.00	0.42
1:A:111:ILE:HG21	5:A:900:W71:H5C2	2.01	0.42
3:C:161:LEU:H	3:C:161:LEU:CD1	2.30	0.42
1:A:152:GLN:OE1	1:A:236:ARG:NH1	2.53	0.41
3:C:7:LYS:HB3	3:C:8:PRO:CD	2.50	0.41
1:A:205:TYR:O	1:A:223:GLY:HA2	2.20	0.41
3:C:73:VAL:O	3:C:73:VAL:HG13	2.19	0.41
4:D:61:PHE:HD1	4:D:62:THR:O	2.04	0.41
2:B:155:ALA:C	2:B:157:GLY:N	2.72	0.41
3:C:118:THR:HA	3:C:166:THR:HA	2.01	0.41
4:D:61:PHE:O	4:D:62:THR:CB	2.68	0.41
2:B:102:TYR:CG	2:B:103:ARG:N	2.86	0.41
1:A:128:TYR:CE1	1:A:202:GLN:HG3	2.56	0.41
2:B:100:TYR:HA	2:B:249:ARG:NH2	2.35	0.41
2:B:199:ASN:OD1	2:B:200:THR:N	2.51	0.41
3:C:235:ILE:HG12	3:C:237:GLN:HE22	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:ALA:O	2:B:36:GLY:O	2.38	0.41
2:B:165:VAL:HA	2:B:170:ILE:O	2.20	0.41
3:C:183:ASP:O	3:C:187:ASP:HB2	2.20	0.41
3:C:204:VAL:HG22	3:C:205:PRO:CD	2.51	0.41
1:A:203:TRP:HA	1:A:203:TRP:HE3	1.85	0.41
3:C:92:ARG:NH2	3:C:183:ASP:H	2.19	0.41
3:C:184:GLY:O	3:C:185:VAL:HB	2.21	0.41
1:A:195:MET:H	1:A:195:MET:HG2	1.57	0.40
3:C:118:THR:OG1	3:C:166:THR:HB	2.22	0.40
3:C:195:SER:HB2	3:C:197:TRP:HE1	1.86	0.40
1:A:44:VAL:HG23	1:A:44:VAL:O	2.21	0.40
2:B:132:ILE:HG22	2:B:133:GLY:N	2.36	0.40

There are no symmetry-related clashes.

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	295/298 (99%)	261 (88%)	25 (8%)	9 (3%)	4 26
2	B	243/254 (96%)	209 (86%)	29 (12%)	5 (2%)	7 37
3	C	240/242 (99%)	212 (88%)	22 (9%)	6 (2%)	5 32
4	D	55/69 (80%)	47 (86%)	8 (14%)	0	100 100
All	All	833/863 (96%)	729 (88%)	84 (10%)	20 (2%)	6 34

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	196	SER
3	C	234	HIS
1	A	10	SER

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Mol	Chain	Res	Type
1	A	101	THR
2	B	11	ASP
2	B	85	VAL
3	C	78	GLY
3	C	183	ASP
1	A	20	LEU
3	C	61	ASN
1	A	19	ALA
1	A	103	PRO
1	A	104	ASN
1	A	209	PRO
2	B	155	ALA
2	B	82	PHE
3	C	58	VAL
3	C	237	GLN
1	A	276	ASN
2	B	83	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	253/253 (100%)	240 (95%)	13 (5%)	24	60
2	B	209/215 (97%)	198 (95%)	11 (5%)	22	58
3	C	203/203 (100%)	189 (93%)	14 (7%)	15	49
4	D	48/58 (83%)	46 (96%)	2 (4%)	30	65
All	All	713/729 (98%)	673 (94%)	40 (6%)	21	57

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASP
1	A	9	GLU
1	A	14	ASP
1	A	31	ASN

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Mol	Chain	Res	Type
1	A	62	SER
1	A	125	LEU
1	A	181	VAL
1	A	190	VAL
1	A	191	SER
1	A	211	PHE
1	A	229	MET
1	A	236	ARG
1	A	261	TRP
2	B	24	THR
2	B	48	THR
2	B	78	TRP
2	B	82	PHE
2	B	84	ASP
2	B	89	THR
2	B	102	TYR
2	B	104	SER
2	B	198	MET
2	B	208	ASN
2	B	230	PRO
3	C	21	SER
3	C	51	THR
3	C	61	ASN
3	C	70	ARG
3	C	72	PRO
3	C	101	LEU
3	C	150	MET
3	C	162	GLN
3	C	164	SER
3	C	166	THR
3	C	211	THR
3	C	228	LEU
3	C	232	THR
3	C	237	GLN
4	D	27	TYR
4	D	44	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

1 ligand is 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	$\#\|Z\| > 2$
5	W71	A	900	-	24,27,27	2.37	11 (45%)	29,34,34	2.40	9 (31%)

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
5	W71	A	900	-	-	0/14/22/22	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	900	W71	C2A-N3A	5.13	1.34	1.27
5	A	900	W71	C4A-N3A	4.17	1.55	1.47
5	A	900	W71	C4-C3	3.90	1.47	1.39
5	A	900	W71	C5B-C4B	3.86	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	900	W71	C6B-C1B	3.79	1.46	1.38
5	A	900	W71	C2B-C1B	3.02	1.44	1.38
5	A	900	W71	C6B-C5B	2.42	1.43	1.38
5	A	900	W71	O1A-C2A	2.30	1.40	1.36
5	A	900	W71	O1B-C1B	2.27	1.42	1.37
5	A	900	W71	C5A-C4A	2.23	1.57	1.52
5	A	900	W71	C3B-C2B	2.17	1.42	1.38

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	900	W71	O1A-C2A-N3A	-7.13	112.10	118.23
5	A	900	W71	O1A-C2A-C4B	6.84	124.91	115.85
5	A	900	W71	C7C-O1B-C1B	-3.75	108.13	117.93
5	A	900	W71	C5A-O1A-C2A	2.73	108.64	105.90
5	A	900	W71	C5C-C4C-C3C	-2.63	101.08	114.42
5	A	900	W71	C4-C3-N2	-2.39	106.40	110.85
5	A	900	W71	C31-C3-N2	2.27	124.56	120.06
5	A	900	W71	O1A-C5A-C4A	-2.23	99.73	104.28
5	A	900	W71	C5C-C6C-C7C	-2.20	103.75	113.49

There are no chirality outliers.

There are no torsion outliers.

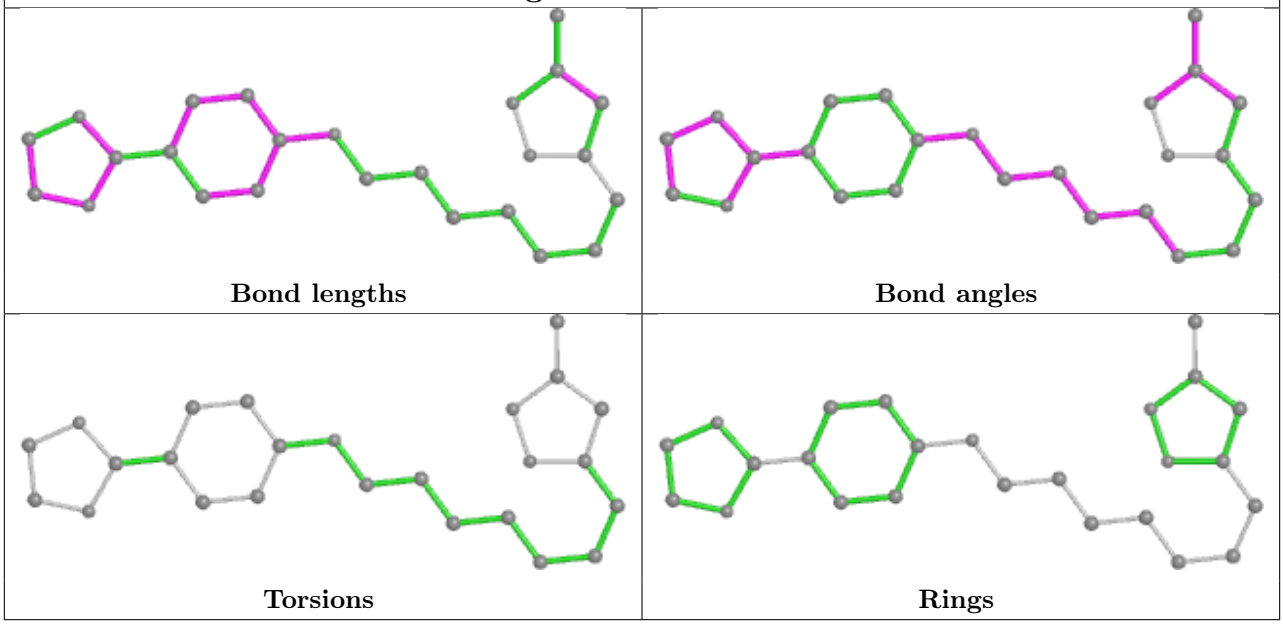
There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	900	W71	5	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 W71 A 900



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)

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates (i)

EDS failed to run properly - this section is therefore empty.

6.4 Ligands (i)

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers (i)

EDS failed to run properly - this section is therefore empty.