



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2026 – 06:25 AM UTC

PDB ID : 3ZFG / pdb_00003zfg
Title : Human enterovirus 71 in complex with capsid binding inhibitor WIN51711
Authors : Plevka, P.; Perera, R.; Yap, M.L.; Cardoso, 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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

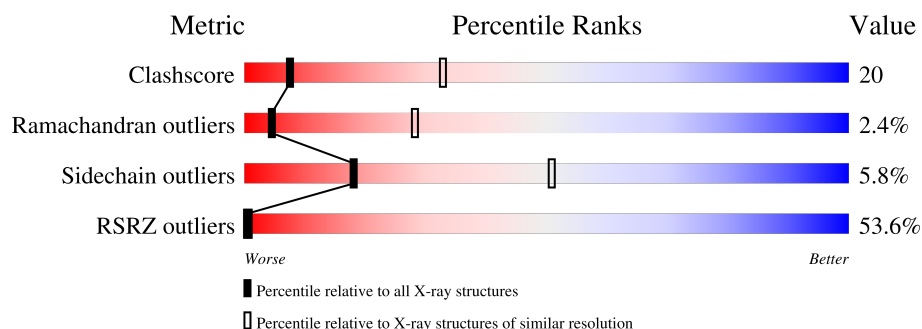
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (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 $\leq 5\%$. 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	298	54% 62% 31% 7%
2	B	254	51% 60% 30% 6% • •
3	C	242	48% 57% 33% 8% •
4	D	69	62% 52% 26% • 17%

2 Entry composition

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
1	A	297	Total	C	N	O	S	0	0	1
			2299	1447	395	444	13			

- Molecule 2 is a protein called VP2.

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

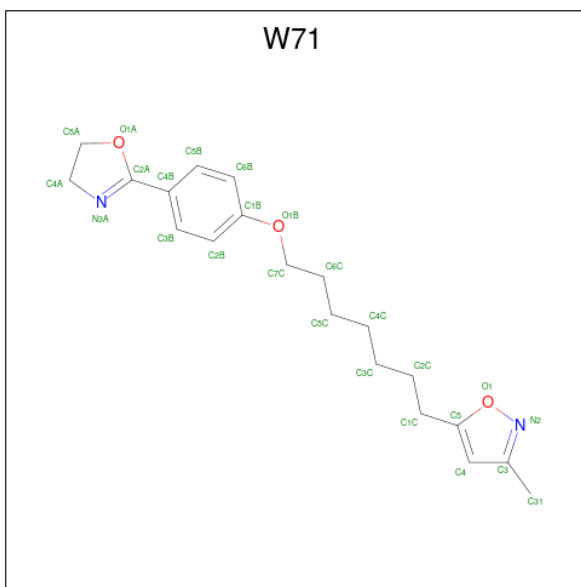
- Molecule 3 is a protein called VP3.

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

- Molecule 4 is a protein called VP4.

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

- Molecule 5 is 5-(7-(4-(4,5-DIHYDRO-2-OXAZOLYL)PHENOXY)HEPTYL)-3-METHYL ISOXAZOLE (CCD ID: W71) (formula: C₂₀H₂₆N₂O₃).

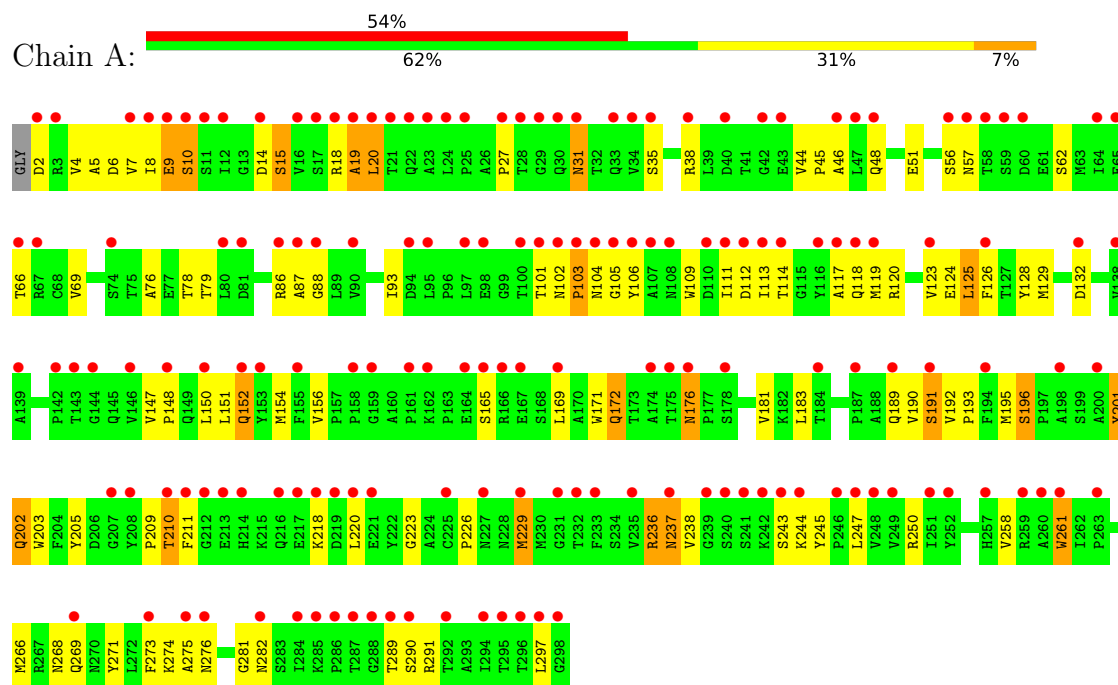


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	25	20	2	3	0	0

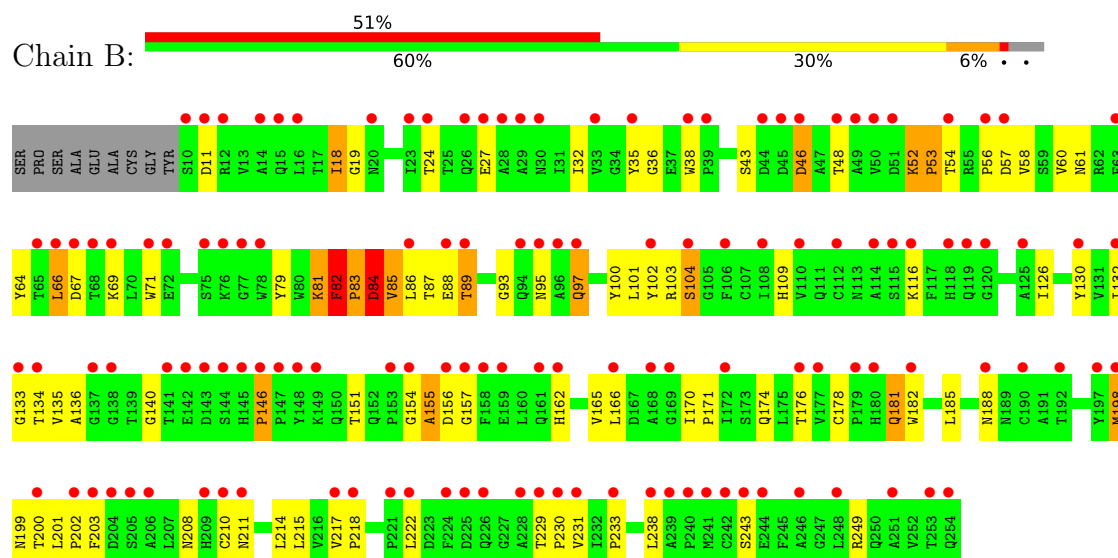
3 Residue-property plots [i](#)

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 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.

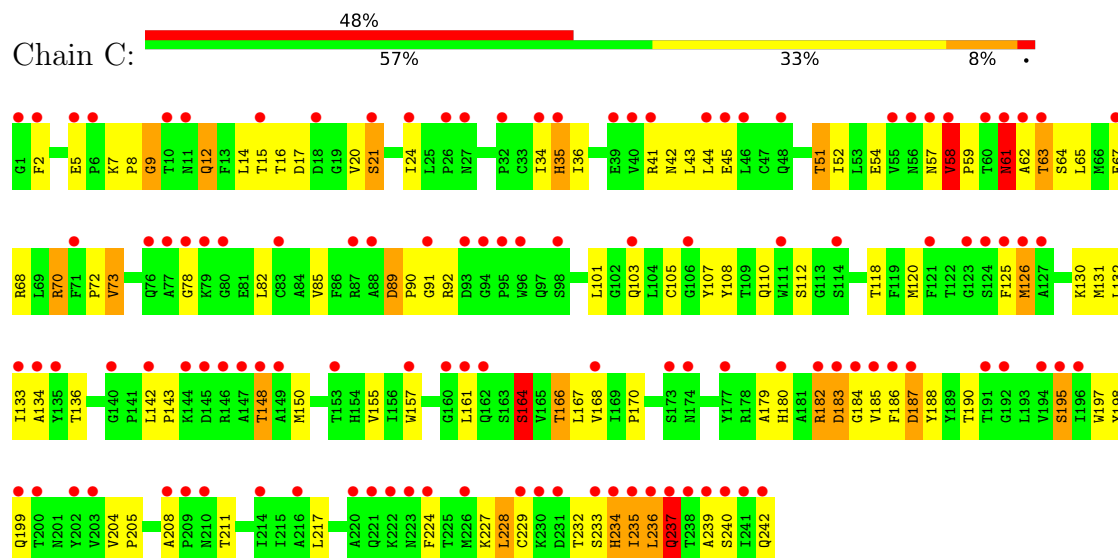
• Molecule 1: VP1



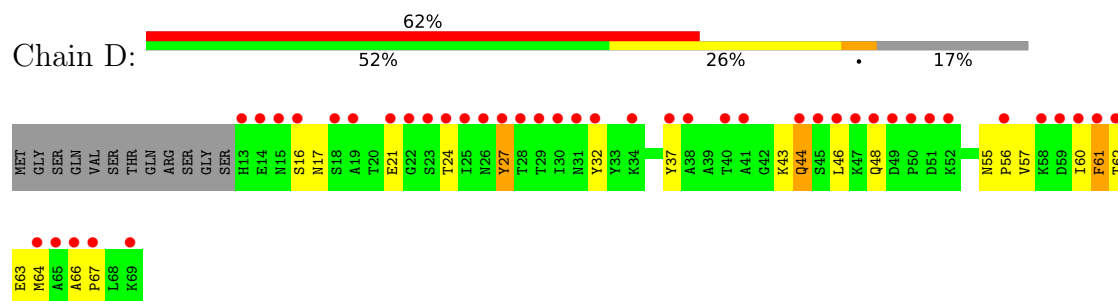
• Molecule 2: VP2



• Molecule 3: VP3



• Molecule 4: VP4



4 Data and refinement statistics

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 33.20 – 3.25	Depositor EDS
% Data completeness (in resolution range)	66.8 (33.20-3.20) 66.3 (33.20-3.25)	Depositor EDS
R_{merge}	0.33	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 3.25Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.249 , (Not available) (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	50.1	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 32.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.000 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.15	EDS
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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.70	11/2358 (0.5%)	1.04	8/3215 (0.2%)
2	B	0.63	5/1954 (0.3%)	1.14	19/2678 (0.7%)
3	C	0.62	3/1920 (0.2%)	1.09	21/2626 (0.8%)
4	D	0.73	3/452 (0.7%)	1.07	4/611 (0.7%)
All	All	0.66	22/6684 (0.3%)	1.09	52/9130 (0.6%)

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	189	GLN	CD-OE1	6.68	1.36	1.23
2	B	181	GLN	CD-OE1	5.75	1.34	1.23
2	B	95	ASN	CG-OD1	5.70	1.34	1.23
1	A	202	GLN	CD-OE1	5.67	1.34	1.23
1	A	297	LEU	C-N	-5.51	1.25	1.33
1	A	172	GLN	CD-OE1	5.48	1.33	1.23
4	D	44	GLN	CD-OE1	5.45	1.33	1.23
1	A	102	ASN	CG-OD1	5.43	1.33	1.23
4	D	48	GLN	CD-OE1	5.40	1.33	1.23
3	C	35	HIS	ND1-CE1	5.34	1.37	1.32
2	B	162	HIS	ND1-CE1	5.33	1.37	1.32
2	B	109	HIS	ND1-CE1	5.26	1.37	1.32
1	A	282	ASN	CG-OD1	5.25	1.33	1.23
1	A	269	GLN	CD-OE1	5.22	1.33	1.23
2	B	97	GLN	CD-OE1	5.22	1.33	1.23
1	A	118	GLN	CD-OE1	5.21	1.33	1.23
4	D	17	ASN	CG-OD1	5.20	1.33	1.23
1	A	176	ASN	CG-ND2	-5.12	1.22	1.33
3	C	61	ASN	CG-OD1	5.10	1.33	1.23
1	A	176	ASN	CG-OD1	5.05	1.33	1.23
1	A	152	GLN	CD-OE1	5.01	1.33	1.23
3	C	12	GLN	CD-OE1	5.01	1.33	1.23

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	66	LEU	N-CA-C	10.79	124.34	111.82
1	A	117	ALA	N-CA-C	8.68	121.84	111.33
2	B	82	PHE	N-CA-C	8.45	128.48	109.81
1	A	210	THR	N-CA-C	8.44	124.26	113.88
3	C	187	ASP	N-CA-C	-8.26	103.21	113.20
2	B	229	THR	CA-C-N	8.11	129.45	120.45
2	B	229	THR	C-N-CA	8.11	129.45	120.45
1	A	237	ASN	N-CA-C	-6.88	98.05	109.46
3	C	164	SER	N-CA-C	6.85	120.76	110.14
3	C	35	HIS	CB-CG-CD2	-6.77	122.40	131.20
3	C	63	THR	N-CA-C	-6.73	105.36	113.97
2	B	109	HIS	CB-CG-CD2	-6.56	122.67	131.20
2	B	162	HIS	CB-CG-CD2	-6.56	122.68	131.20
2	B	52	LYS	CA-C-N	6.55	126.50	120.21
2	B	52	LYS	C-N-CA	6.55	126.50	120.21
1	A	258	VAL	N-CA-C	6.44	117.97	109.21
3	C	73	VAL	N-CA-C	-6.44	99.45	108.27
1	A	172	GLN	N-CA-C	-6.43	104.70	112.54
4	D	61	PHE	N-CA-C	6.42	124.05	114.09
2	B	146	PRO	CA-C-N	6.31	126.28	120.03
2	B	146	PRO	C-N-CA	6.31	126.28	120.03
3	C	179	ALA	N-CA-C	-6.22	101.31	110.52
2	B	81	LYS	N-CA-C	-6.01	100.76	110.32
3	C	235	ILE	N-CA-C	5.98	118.06	108.85
2	B	84	ASP	N-CA-C	5.93	118.26	111.02
4	D	66	ALA	N-CA-C	-5.88	101.07	109.24
1	A	132	ASP	N-CA-C	-5.87	101.77	110.46
2	B	109	HIS	CB-CG-ND1	5.68	131.22	122.70
2	B	46	ASP	N-CA-C	-5.63	106.57	113.50
3	C	58	VAL	CA-C-N	5.59	125.53	119.78
3	C	58	VAL	C-N-CA	5.59	125.53	119.78
2	B	57	ASP	CB-CA-C	-5.55	110.19	116.63
2	B	162	HIS	CB-CG-ND1	5.55	131.02	122.70
3	C	35	HIS	CB-CG-ND1	5.54	131.00	122.70
3	C	182	ARG	N-CA-C	5.49	116.88	107.28
4	D	17	ASN	N-CA-C	5.40	119.01	111.56
2	B	58	VAL	N-CA-C	5.37	118.59	111.17
3	C	5	GLU	CA-C-N	5.36	125.28	119.76
3	C	5	GLU	C-N-CA	5.36	125.28	119.76
3	C	136	THR	CA-C-N	5.33	125.87	120.38
3	C	136	THR	C-N-CA	5.33	125.87	120.38
2	B	53	PRO	N-CA-C	5.33	118.68	111.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	43	LYS	N-CA-C	-5.31	103.38	110.55
1	A	201	TYR	N-CA-C	-5.26	103.09	110.50
3	C	9	GLY	N-CA-C	-5.21	107.35	114.64
1	A	15	SER	N-CA-C	5.16	117.80	111.82
3	C	134	ALA	N-CA-C	5.13	117.43	108.76
3	C	2	PHE	CA-C-N	5.09	126.20	119.84
3	C	2	PHE	C-N-CA	5.09	126.20	119.84
2	B	185	LEU	N-CA-C	5.06	117.46	111.33
3	C	89	ASP	CA-C-N	5.01	126.10	119.84
3	C	89	ASP	C-N-CA	5.01	126.10	119.84

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	111	0
2	B	1899	0	1832	72	0
3	C	1866	0	1837	99	0
4	D	443	0	420	21	0
5	A	25	0	26	5	0
All	All	6532	0	6346	261	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 20.

All (261) 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:129:MET:HE3	1:A:203:TRP:HE1	1.31	0.95
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:82:PHE:O	2:B:83:PRO:C	2.22	0.82
1:A:18:ARG:HB2	2:B:38:TRP:HB2	1.62	0.82
1:A:35:SER:HB3	1:A:66:THR:H	1.44	0.81
3:C:237:GLN:NE2	3:C:237:GLN:N	2.29	0.81
3:C:237:GLN:N	3:C:237:GLN:HE21	1.77	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
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:123:VAL:HA	1:A:129:MET:HE1	1.66	0.77
1:A:192:VAL:HG22	3:C:24:ILE:HD13	1.69	0.75
3:C:126:MET:HE3	3:C:126:MET:HA	1.67	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
2:B:35:TYR:CD2	2:B:198:MET:HE1	2.27	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
3:C:131:MET:HE1	3:C:198:TYR:CD2	2.30	0.67
1:A:78:THR:HG21	3:C:44:LEU:HG	1.77	0.66
1:A:129:MET:HE3	1:A:203:TRP:NE1	2.09	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
1:A:266:MET:HE1	3:C:107:TYR:HE2	1.62	0.65
2:B:35:TYR:HD2	2:B:198:MET:HE1	1.61	0.65
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:61:ASN:C	3:C:63:THR:H	2.06	0.63
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:155:ALA:C	2:B:157:GLY:H	2.07	0.62
3:C:65:LEU:O	3:C:68:ARG:HG3	1.99	0.62
1:A:171:TRP:CE2	1:A:236:ARG:HG2	2.35	0.62
1:A:9:GLU:O	1:A:10:SER:C	2.42	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
1:A:112:ASP:CG	1:A:114:THR:HG22	2.24	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
1:A:183:LEU:HD21	1:A:247:LEU:HD22	1.86	0.57
3:C:239:ALA:O	3:C:240:SER:C	2.47	0.57
2:B:104:SER:HB2	2:B:243:SER:HA	1.87	0.57
2:B:87:THR:HG22	2:B:88:GLU:N	2.20	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: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
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: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
2:B:87:THR:C	2:B:89:THR:H	2.16	0.54
1:A:103:PRO:C	1:A:105:GLY:H	2.16	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
1:A:218:LYS:C	1:A:220:LEU:H	2.13	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:C:228:LEU:C	3:C:228:LEU:HD12	2.33	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:132:LEU:HD23	3:C:132:LEU:C	2.34	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: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:154:MET:HE2	1:A:156:VAL:HG22	1.92	0.51
1:A:261:TRP:CE3	3:C:36:ILE:HB	2.46	0.51
1:A:123:VAL:C	1:A:125:LEU:H	2.17	0.51
3:C:20:VAL:HG21	4:D:32:TYR:CD2	2.47	0.50
3:C:131:MET:CE	3:C:198:TYR:HA	2.41	0.50
1:A:151:LEU:HD23	1:A:237:ASN:HA	1.94	0.50
2:B:176:THR:C	2:B:178:CYS:H	2.19	0.50
4:D:61:PHE:O	4:D:62:THR:HB	2.11	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
3:C:233:SER:O	3:C:234:HIS:C	2.54	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:86:ARG:HG2	3:C:16:THR:HG22	1.95	0.49
1:A:106:TYR:CE2	1:A:165:SER:HA	2.48	0.49
1:A:218:LYS:C	1:A:220:LEU:N	2.70	0.49
3:C:130:LYS:O	3:C:131:MET:HE2	2.13	0.49
1:A:88:GLY:HA3	1:A:119:MET:HE2	1.95	0.49
3:C:182:ARG:O	3:C:182:ARG:HG3	2.12	0.49
1:A:266:MET:CE	3:C:107:TYR:HE2	2.26	0.48
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:125:LEU:HD13	1:A:126:PHE:CZ	2.49	0.48
3:C:61:ASN:C	3:C:63:THR:N	2.72	0.48
1:A:5:ALA:C	1:A:7:VAL:N	2.71	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
1:A:147:VAL:HG13	1:A:148:PRO:HD2	1.96	0.47
3:C:185:VAL:C	3:C:187:ASP:H	2.22	0.47
2:B:27:GLU:O	2:B:188:ASN:HB2	2.14	0.47
3:C:131:MET:HE2	3:C:131:MET:HA	1.95	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
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:193:PRO:HG2	1:A:195:MET:HE3	1.98	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
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
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
2:B:155:ALA:C	2:B:157:GLY:N	2.72	0.44
2:B:238:LEU:HD12	2:B:238:LEU:C	2.43	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
3:C:168:VAL:O	3:C:170:PRO:HD3	2.18	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
2:B:154:GLY:C	2:B:155:ALA:O	2.59	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:154:MET:HE3	1:A:176:ASN:OD1	2.19	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
2:B:136:ALA:CB	2:B:140:GLY:HA2	2.49	0.42
1:A:123:VAL:C	1:A:125:LEU:N	2.78	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
1:A:266:MET:HE1	3:C:107:TYR:CE2	2.47	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
2:B:18:ILE:O	2:B:19:GLY:C	2.61	0.41
3:C:73:VAL:O	3:C:73:VAL:HG13	2.19	0.41
4:D:55:ASN:C	4:D:57:VAL:H	2.28	0.41
4:D:61:PHE:HD1	4:D:62:THR:O	2.04	0.41
3:C:118:THR:HA	3:C:166:THR:HA	2.01	0.41
3:C:186:PHE:C	3:C:188:TYR:N	2.78	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
1:A:19:ALA:O	2:B:36:GLY:O	2.38	0.41
1:A:274:LYS:O	1:A:275:ALA:C	2.63	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:5:ALA:C	1:A:7:VAL:H	2.28	0.41
1:A:203:TRP:HA	1:A:203:TRP:HE3	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:79:TYR:CD1	2:B:79:TYR:C	2.99	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
2:B:176:THR:C	2:B:178:CYS:N	2.79	0.40
2:B:198:MET:HE2	2:B:198:MET:HB3	1.91	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%)	3	22
2	B	235/254 (92%)	203 (86%)	27 (12%)	5 (2%)	5	31
3	C	210/242 (87%)	185 (88%)	20 (10%)	5 (2%)	4	28
4	D	55/69 (80%)	47 (86%)	8 (14%)	0	100	100
All	All	795/863 (92%)	696 (88%)	80 (10%)	19 (2%)	4	28

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	196	SER
3	C	234	HIS
1	A	10	SER
1	A	101	THR
2	B	11	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	85	VAL
3	C	78	GLY
3	C	183	ASP
1	A	20	LEU
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 ⓘ

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%)	241 (95%)	12 (5%)	23	57
2	B	209/215 (97%)	200 (96%)	9 (4%)	26	59
3	C	203/203 (100%)	185 (91%)	18 (9%)	9	34
4	D	48/58 (83%)	46 (96%)	2 (4%)	26	60
All	All	713/729 (98%)	672 (94%)	41 (6%)	18	51

All (41) 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
1	A	62	SER
1	A	125	LEU
1	A	181	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	190	VAL
1	A	191	SER
1	A	229	MET
1	A	236	ARG
1	A	261	TRP
2	B	18	ILE
2	B	24	THR
2	B	48	THR
2	B	84	ASP
2	B	89	THR
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	126	MET
3	C	148	THR
3	C	150	MET
3	C	155	VAL
3	C	164	SER
3	C	166	THR
3	C	195	SER
3	C	211	THR
3	C	228	LEU
3	C	232	THR
3	C	236	LEU
3	C	237	GLN
4	D	27	TYR
4	D	44	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	31	ASN
1	A	118	GLN
2	B	111	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	145	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	-	27,27,27	3.18	13 (48%)	33,34,34	3.32	13 (39%)

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	-	-	2/15/22/22	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	900	W71	O1-N2	-9.94	1.24	1.42
5	A	900	W71	C2A-N3A	5.55	1.34	1.27
5	A	900	W71	C4-C5	4.54	1.41	1.34
5	A	900	W71	C4A-N3A	4.47	1.55	1.47
5	A	900	W71	C4-C3	4.47	1.47	1.40
5	A	900	W71	C5B-C4B	4.29	1.45	1.39
5	A	900	W71	C6B-C1B	4.00	1.46	1.38
5	A	900	W71	C2B-C1B	3.18	1.44	1.38
5	A	900	W71	C6B-C5B	2.69	1.43	1.38
5	A	900	W71	C3B-C2B	2.41	1.42	1.38
5	A	900	W71	O1A-C2A	2.38	1.40	1.36
5	A	900	W71	C5A-C4A	2.37	1.57	1.52
5	A	900	W71	O1B-C1B	2.31	1.42	1.37

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	900	W71	O1A-C2A-C4B	7.17	124.91	115.85
5	A	900	W71	O1A-C2A-N3A	-7.11	112.10	118.25
5	A	900	W71	C4-C3-N2	-7.07	106.40	111.54
5	A	900	W71	C5-O1-N2	6.78	113.40	108.30
5	A	900	W71	C31-C3-N2	5.61	124.56	119.97
5	A	900	W71	O1-C5-C1C	5.16	123.73	115.87
5	A	900	W71	O1-C5-C4	-5.07	105.02	109.73
5	A	900	W71	O1-N2-C3	4.15	112.07	105.18
5	A	900	W71	C7C-O1B-C1B	-3.77	108.13	117.93
5	A	900	W71	C5A-O1A-C2A	2.96	108.64	105.90
5	A	900	W71	C5C-C4C-C3C	-2.63	101.08	114.37
5	A	900	W71	O1A-C5A-C4A	-2.42	99.73	104.24
5	A	900	W71	C5C-C6C-C7C	-2.24	103.75	113.47

There are no chirality outliers.

All (2) torsion outliers are listed below:

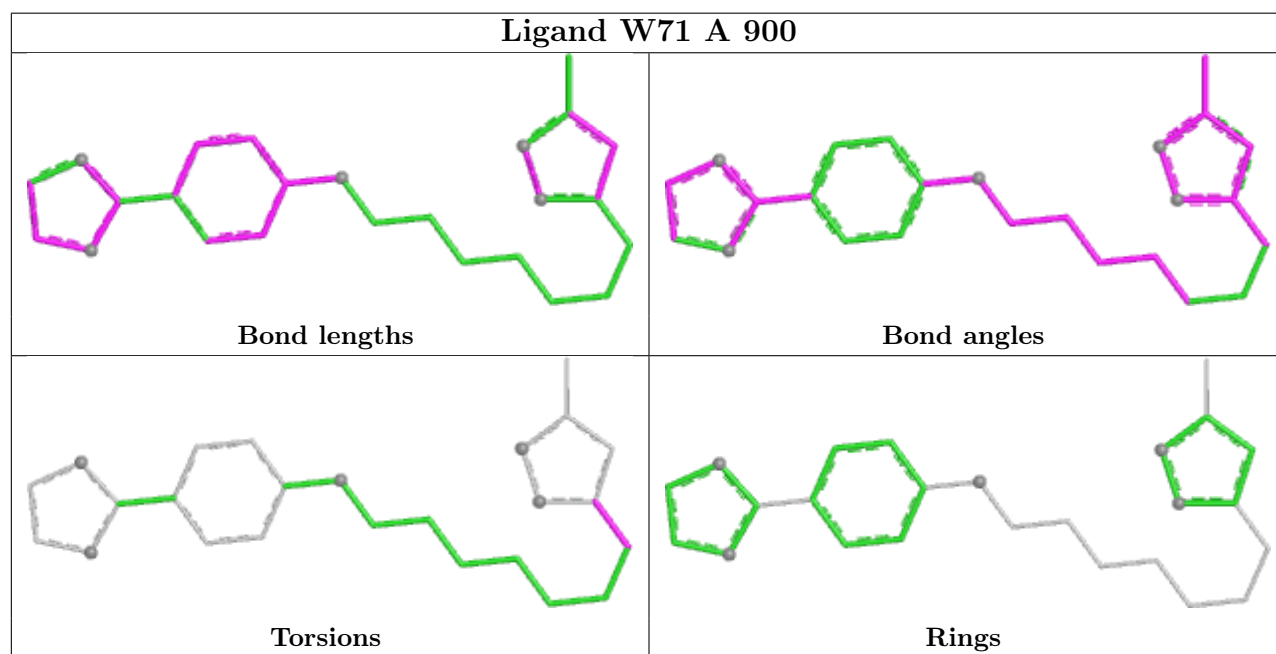
Mol	Chain	Res	Type	Atoms
5	A	900	W71	C2C-C1C-C5-O1
5	A	900	W71	C2C-C1C-C5-C4

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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	297/298 (99%)	2.48	162 (54%) 0 0	14, 33, 83, 145	0
2	B	245/254 (96%)	2.22	130 (53%) 0 1	11, 29, 60, 96	0
3	C	242/242 (100%)	2.16	116 (47%) 0 1	13, 30, 66, 130	0
4	D	57/69 (82%)	2.92	43 (75%) 0 0	21, 51, 115, 163	0
All	All	841/863 (97%)	2.34	451 (53%) 0 1	11, 31, 76, 163	0

All (451) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	161	GLN	9.6
1	A	18	ARG	9.3
4	D	13	HIS	8.5
1	A	213	GLU	8.4
1	A	298	GLY	7.5
1	A	98	GLU	7.4
4	D	22	GLY	7.3
3	C	234	HIS	7.2
1	A	3	ARG	7.2
2	B	66	LEU	6.9
1	A	2	ASP	6.9
1	A	38	ARG	6.7
1	A	242	LYS	6.6
1	A	11	SER	6.6
1	A	100	THR	6.3
2	B	226	GLN	6.3
1	A	243	SER	6.2
1	A	101	THR	6.2
2	B	10	SER	5.9
4	D	45	SER	5.9
3	C	63	THR	5.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	216	GLN	5.7
4	D	14	GLU	5.7
2	B	44	ASP	5.6
1	A	97	LEU	5.6
1	A	217	GLU	5.5
2	B	156	ASP	5.5
3	C	24	ILE	5.4
3	C	221	GLN	5.3
3	C	71	PHE	5.1
1	A	220	LEU	5.0
2	B	149	LYS	5.0
4	D	21	GLU	5.0
1	A	104	ASN	4.9
3	C	61	ASN	4.9
1	A	164	GLU	4.8
1	A	9	GLU	4.7
2	B	45	ASP	4.7
2	B	76	LYS	4.6
1	A	43	GLU	4.6
1	A	19	ALA	4.5
4	D	26	ASN	4.5
2	B	133	GLY	4.5
2	B	142	GLU	4.5
1	A	94	ASP	4.5
1	A	118	GLN	4.5
1	A	285	LYS	4.5
1	A	218	LYS	4.4
1	A	246	PRO	4.4
2	B	134	THR	4.4
1	A	169	LEU	4.3
1	A	102	ASN	4.3
1	A	107	ALA	4.3
3	C	58	VAL	4.3
1	A	103	PRO	4.3
2	B	30	ASN	4.3
2	B	29	ALA	4.2
1	A	227	ASN	4.2
2	B	46	ASP	4.2
1	A	167	GLU	4.2
1	A	297	LEU	4.2
1	A	294	ILE	4.2
3	C	239	ALA	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	231	GLY	4.2
1	A	287	THR	4.2
1	A	30	GLN	4.2
1	A	288	GLY	4.2
2	B	125	ALA	4.1
2	B	116	LYS	4.1
1	A	25	PRO	4.1
2	B	78	TRP	4.1
1	A	269	GLN	4.1
3	C	144	LYS	4.1
3	C	77	ALA	4.1
2	B	11	ASP	4.0
1	A	225	CYS	4.0
1	A	57	ASN	4.0
3	C	41	ARG	4.0
2	B	14	ALA	4.0
3	C	114	SER	4.0
2	B	38	TRP	3.9
4	D	61	PHE	3.9
1	A	56	SER	3.9
3	C	226	MET	3.9
3	C	121	PHE	3.9
4	D	69	LYS	3.9
3	C	195	SER	3.9
3	C	11	ASN	3.8
1	A	40	ASP	3.8
3	C	231	ASP	3.8
3	C	185	VAL	3.8
4	D	50	PRO	3.8
3	C	56	ASN	3.8
3	C	210	ASN	3.8
3	C	220	ALA	3.8
4	D	23	SER	3.8
3	C	1	GLY	3.7
4	D	24	THR	3.7
3	C	62	ALA	3.7
3	C	79	LYS	3.7
2	B	231	VAL	3.7
1	A	275	ALA	3.7
2	B	115	SER	3.7
1	A	187	PRO	3.7
1	A	111	ILE	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	D	29	THR	3.7
1	A	178	SER	3.6
1	A	237	ASN	3.6
2	B	146	PRO	3.6
3	C	87	ARG	3.6
2	B	198	MET	3.6
2	B	238	LEU	3.6
1	A	210	THR	3.6
3	C	48	GLN	3.6
2	B	180	HIS	3.5
3	C	60	THR	3.5
3	C	182	ARG	3.5
3	C	191	THR	3.5
2	B	203	PHE	3.5
3	C	233	SER	3.5
2	B	143	ASP	3.5
3	C	106	GLY	3.5
3	C	242	GLN	3.5
4	D	48	GLN	3.5
2	B	224	PHE	3.5
1	A	24	LEU	3.5
4	D	34	LYS	3.5
1	A	150	LEU	3.5
3	C	187	ASP	3.4
1	A	211	PHE	3.4
4	D	65	ALA	3.4
1	A	284	ILE	3.4
1	A	158	PRO	3.4
4	D	18	SER	3.4
2	B	110	VAL	3.4
3	C	147	ALA	3.4
2	B	211	ASN	3.4
3	C	199	GLN	3.4
2	B	120	GLY	3.4
3	C	26	PRO	3.4
2	B	182	TRP	3.3
1	A	33	GLN	3.3
1	A	10	SER	3.3
3	C	83	CYS	3.3
2	B	154	GLY	3.3
4	D	62	THR	3.3
4	D	47	LYS	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	137	GLY	3.3
3	C	235	ILE	3.3
1	A	295	THR	3.3
2	B	148	TYR	3.2
1	A	165	SER	3.2
4	D	16	SER	3.2
4	D	32	TYR	3.2
2	B	54	THR	3.2
2	B	88	GLU	3.2
1	A	22	GLN	3.2
3	C	160	GLY	3.2
1	A	276	ASN	3.2
4	D	59	ASP	3.2
1	A	198	ALA	3.2
1	A	144	GLY	3.2
3	C	236	LEU	3.2
1	A	233	PHE	3.2
1	A	189	GLN	3.2
4	D	51	ASP	3.1
3	C	161	LEU	3.1
2	B	39	PRO	3.1
3	C	222	LYS	3.1
3	C	238	THR	3.1
3	C	95	PRO	3.1
4	D	60	ILE	3.1
3	C	88	ALA	3.1
3	C	123	GLY	3.1
2	B	50	VAL	3.1
2	B	210	CYS	3.1
3	C	135	TYR	3.1
2	B	28	ALA	3.1
2	B	49	ALA	3.1
2	B	86	LEU	3.1
2	B	24	THR	3.1
4	D	15	ASN	3.1
3	C	127	ALA	3.1
3	C	93	ASP	3.1
1	A	66	THR	3.0
1	A	244	LYS	3.0
1	A	81	ASP	3.0
4	D	38	ALA	3.0
1	A	257	HIS	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	80	LEU	3.0
2	B	145	HIS	3.0
4	D	64	MET	3.0
1	A	286	PRO	3.0
1	A	87	ALA	3.0
3	C	180	HIS	3.0
2	B	200	THR	3.0
4	D	28	THR	3.0
2	B	159	GLU	3.0
1	A	282	ASN	3.0
3	C	45	GLU	2.9
1	A	90	VAL	2.9
2	B	77	GLY	2.9
3	C	174	ASN	2.9
1	A	273	PHE	2.9
3	C	183	ASP	2.9
2	B	69	LYS	2.9
2	B	240	PRO	2.9
1	A	208	TYR	2.9
3	C	184	GLY	2.9
2	B	158	PHE	2.9
1	A	232	THR	2.9
1	A	46	ALA	2.9
2	B	97	GLN	2.9
2	B	57	ASP	2.9
4	D	49	ASP	2.9
3	C	111	TRP	2.9
3	C	78	GLY	2.9
2	B	209	HIS	2.8
2	B	26	GLN	2.8
3	C	237	GLN	2.8
1	A	112	ASP	2.8
2	B	27	GLU	2.8
2	B	16	LEU	2.8
3	C	192	GLY	2.8
2	B	15	GLN	2.8
1	A	142	PRO	2.8
1	A	175	THR	2.8
1	A	292	THR	2.8
1	A	138	VAL	2.8
1	A	108	ASN	2.8
3	C	126	MET	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	D	67	PRO	2.8
1	A	132	ASP	2.8
3	C	15	THR	2.8
3	C	91	GLY	2.8
2	B	242	CYS	2.8
1	A	248	VAL	2.8
3	C	40	VAL	2.8
3	C	98	SER	2.8
3	C	148	THR	2.8
1	A	176	ASN	2.8
2	B	94	GLN	2.8
1	A	240	SER	2.8
3	C	153	THR	2.8
3	C	186	PHE	2.7
4	D	27	TYR	2.7
1	A	200	ALA	2.7
2	B	112	CYS	2.7
2	B	104	SER	2.7
1	A	21	THR	2.7
3	C	146	ARG	2.7
2	B	20	ASN	2.7
2	B	102	TYR	2.7
3	C	224	PHE	2.7
1	A	58	THR	2.7
1	A	191	SER	2.7
1	A	23	ALA	2.7
2	B	217	VAL	2.7
1	A	247	LEU	2.7
2	B	68	THR	2.7
1	A	110	ASP	2.7
2	B	225	ASP	2.7
1	A	47	LEU	2.7
2	B	71	TRP	2.7
3	C	21	SER	2.7
3	C	168	VAL	2.7
1	A	219	ASP	2.7
2	B	51	ASP	2.7
1	A	251	ILE	2.6
2	B	119	GLN	2.6
2	B	147	PRO	2.6
2	B	218	PRO	2.6
2	B	241	MET	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	289	THR	2.6
3	C	214	ILE	2.6
2	B	56	PRO	2.6
2	B	188	ASN	2.6
1	A	42	GLY	2.6
2	B	72	GLU	2.6
2	B	65	THR	2.6
3	C	35	HIS	2.6
1	A	194	PHE	2.6
2	B	138	GLY	2.6
2	B	48	THR	2.6
3	C	133	ILE	2.6
4	D	58	LYS	2.6
2	B	67	ASP	2.6
1	A	249	VAL	2.6
1	A	28	THR	2.6
2	B	228	ALA	2.6
2	B	12	ARG	2.6
4	D	40	THR	2.6
1	A	106	TYR	2.6
3	C	177	TYR	2.6
1	A	27	PRO	2.6
2	B	230	PRO	2.6
1	A	146	VAL	2.6
2	B	190	CYS	2.5
1	A	241	SER	2.5
1	A	60	ASP	2.5
3	C	18	ASP	2.5
1	A	8	ILE	2.5
2	B	153	PRO	2.5
2	B	206	ALA	2.5
3	C	196	ILE	2.5
2	B	162	HIS	2.5
1	A	17	SER	2.5
3	C	124	SER	2.5
1	A	117	ALA	2.5
4	D	66	ALA	2.5
1	A	48	GLN	2.5
2	B	132	ILE	2.5
3	C	5	GLU	2.5
3	C	34	ILE	2.5
2	B	253	THR	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	64	ILE	2.4
2	B	144	SER	2.4
4	D	25	ILE	2.4
1	A	229	MET	2.4
2	B	166	LEU	2.4
1	A	263	PRO	2.4
2	B	197	TYR	2.4
1	A	239	GLY	2.4
2	B	108	ILE	2.4
2	B	254	GLN	2.4
1	A	35	SER	2.4
1	A	143	THR	2.4
2	B	176	THR	2.4
3	C	6	PRO	2.4
3	C	57	ASN	2.4
1	A	14	ASP	2.4
1	A	16	VAL	2.4
3	C	55	VAL	2.4
1	A	290	SER	2.4
1	A	261	TRP	2.4
3	C	200	THR	2.4
2	B	204	ASP	2.4
3	C	80	GLY	2.4
1	A	113	ILE	2.4
3	C	230	LYS	2.4
3	C	125	PHE	2.4
1	A	235	VAL	2.4
2	B	177	VAL	2.4
1	A	86	ARG	2.3
3	C	149	ALA	2.3
1	A	20	LEU	2.3
1	A	95	LEU	2.3
2	B	222	LEU	2.3
2	B	141	THR	2.3
2	B	169	GLY	2.3
1	A	214	HIS	2.3
1	A	31	ASN	2.3
4	D	31	ASN	2.3
4	D	46	LEU	2.3
3	C	103	GLN	2.3
1	A	159	GLY	2.3
2	B	229	THR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	208	ALA	2.3
3	C	229	CYS	2.3
4	D	37	TYR	2.3
3	C	76	GLN	2.3
2	B	114	ALA	2.3
2	B	168	ALA	2.3
1	A	166	ARG	2.3
1	A	139	ALA	2.3
1	A	212	GLY	2.3
2	B	118	HIS	2.3
2	B	192	THR	2.3
1	A	74	SER	2.3
1	A	155	PHE	2.3
2	B	130	TYR	2.3
2	B	202	PRO	2.2
1	A	119	MET	2.2
2	B	251	ALA	2.2
1	A	116	TYR	2.2
3	C	240	SER	2.2
1	A	259	ARG	2.2
3	C	162	GLN	2.2
3	C	96	TRP	2.2
1	A	126	PHE	2.2
1	A	162	LYS	2.2
2	B	35	TYR	2.2
3	C	27	ASN	2.2
3	C	223	ASN	2.2
3	C	145	ASP	2.2
3	C	134	ALA	2.2
2	B	75	SER	2.2
2	B	205	SER	2.2
2	B	23	ILE	2.2
3	C	46	LEU	2.2
1	A	67	ARG	2.2
4	D	30	ILE	2.2
1	A	65	GLU	2.2
2	B	157	GLY	2.2
2	B	221	PRO	2.2
1	A	296	THR	2.1
3	C	202	TYR	2.1
2	B	244	GLU	2.1
2	B	246	ALA	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	D	56	PRO	2.1
1	A	152	GLN	2.1
2	B	96	ALA	2.1
1	A	148	PRO	2.1
2	B	179	PRO	2.1
2	B	233	PRO	2.1
3	C	2	PHE	2.1
1	A	114	THR	2.1
2	B	89	THR	2.1
3	C	44	LEU	2.1
1	A	174	ALA	2.1
2	B	239	ALA	2.1
1	A	221	GLU	2.1
3	C	67	GLU	2.1
2	B	106	PHE	2.1
2	B	243	SER	2.1
3	C	142	LEU	2.1
3	C	241	ILE	2.1
1	A	184	THR	2.1
1	A	252	TYR	2.1
1	A	260	ALA	2.1
4	D	19	ALA	2.1
4	D	44	GLN	2.1
3	C	32	PRO	2.1
3	C	173	SER	2.1
1	A	7	VAL	2.1
1	A	34	VAL	2.1
3	C	203	VAL	2.1
4	D	52	LYS	2.1
3	C	157	TRP	2.1
1	A	153	TYR	2.1
1	A	88	GLY	2.1
1	A	105	GLY	2.1
1	A	207	GLY	2.1
3	C	39	GLU	2.1
3	C	209	PRO	2.1
2	B	172	ILE	2.0
3	C	10	THR	2.0
2	B	63	PHE	2.0
3	C	94	GLY	2.0
3	C	140	GLY	2.0
1	A	123	VAL	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	194	VAL	2.0
1	A	12	ILE	2.0
1	A	59	SER	2.0
2	B	95	ASN	2.0
3	C	216	ALA	2.0
4	D	41	ALA	2.0
1	A	29	GLY	2.0
1	A	161	PRO	2.0
2	B	33	VAL	2.0
2	B	248	LEU	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](#)

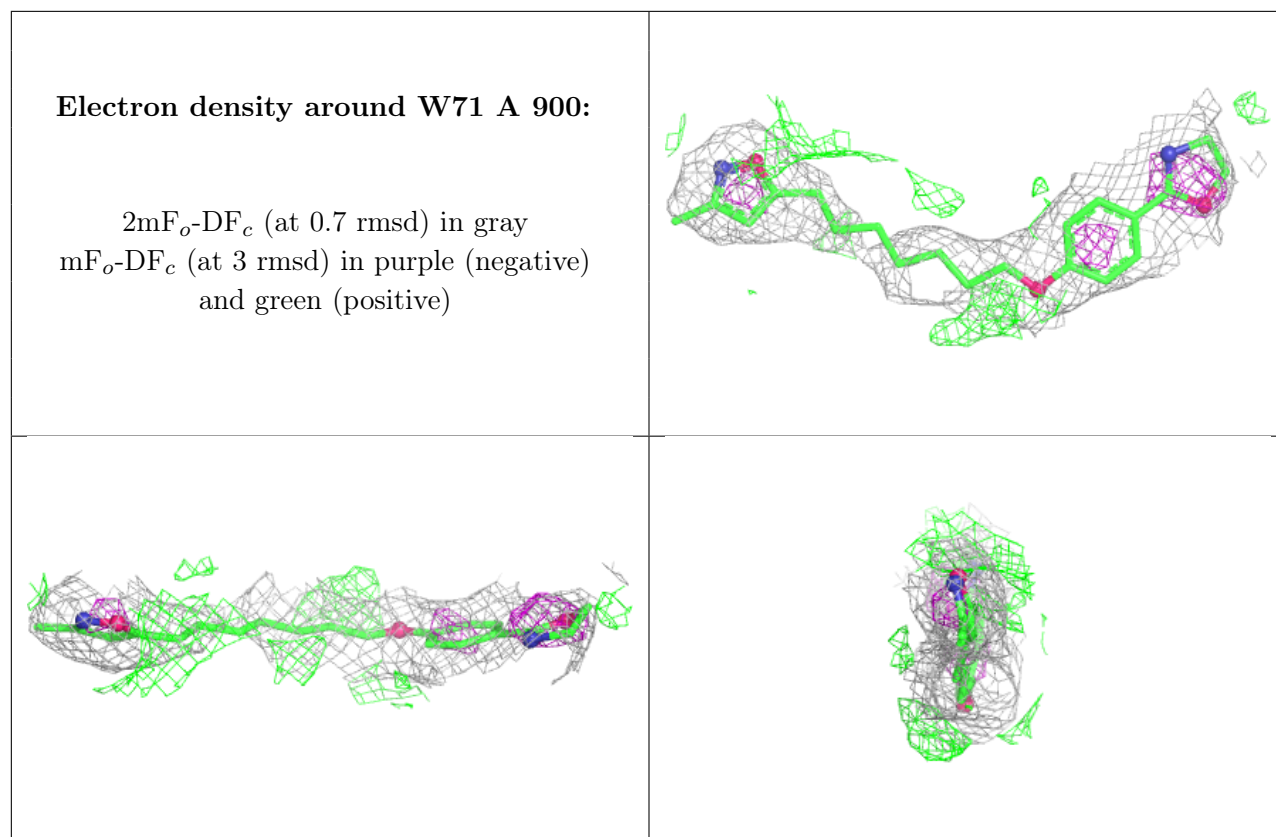
There are no oligosaccharides in this entry.

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	W71	A	900	25/25	0.89	0.24	11,11,11,11	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.