



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 12:02 PM UTC

PDB ID : 4PJ7 / pdb_00004pj7
Title : Structure of human MR1-5-OP-RU in complex with human MAIT TRBV6-4 TCR
Authors : Birkinshaw, R.W.; Rossjohn, J.
Deposited on : 2014-05-12
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

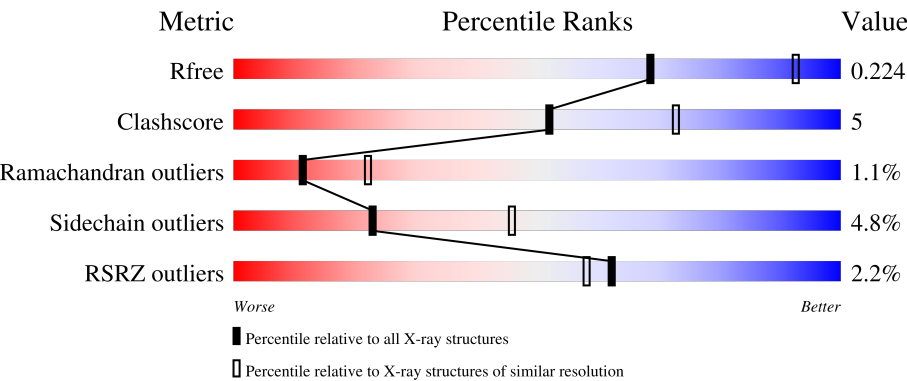
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

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

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	271	2% 80% 15% ...
1	C	271	3% 77% 17% ..
2	B	99	% 84% 13% .
2	D	99	4% 81% 9% .. 7%
3	E	203	% 85% 13% .

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Mol	Chain	Length	Quality of chain
3	G	203	4% 81% 13%
4	F	243	% 81% 15%
4	H	243	2% 81% 14%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12989 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 Major histocompatibility complex class I-related gene protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	0	0
			2150	1378	373	388	11			
1	C	264	Total	C	N	O	S	0	0	0
			2131	1363	371	387	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP Q95460
A	261	SER	CYS	engineered mutation	UNP Q95460
C	0	MET	-	initiating methionine	UNP Q95460
C	261	SER	CYS	engineered mutation	UNP Q95460

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	96	Total	C	N	O	S	0	0	0
			769	494	131	142	2			
2	D	92	Total	C	N	O	S	0	0	0
			704	455	119	128	2			

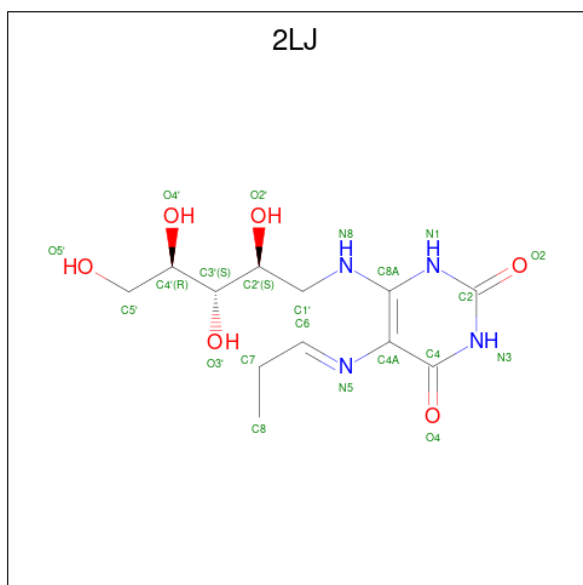
- Molecule 3 is a protein called TCR-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	199	Total	C	N	O	S	0	0	0
			1519	957	244	308	10			
3	G	199	Total	C	N	O	S	0	0	0
			1507	955	242	300	10			

- Molecule 4 is a protein called TCR-beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	238	Total	C	N	O	S	0	0	0
			1811	1141	315	347	8			
4	H	238	Total	C	N	O	S	0	0	0
			1826	1148	322	348	8			

- Molecule 5 is 1-deoxy-1-({2,6-dioxo-5-[(E)-propylideneamino]-1,2,3,6-tetrahydropyrimidin-4-yl}amino)-D-ribose (CCD ID: 2LJ) (formula: C₁₂H₂₀N₄O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			22	12	4	6		
5	C	1	Total	C	N	O	0	0
			22	12	4	6		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	121	Total	O	0	0
			121	121		
6	B	39	Total	O	0	0
			39	39		
6	C	80	Total	O	0	0
			80	80		
6	D	27	Total	O	0	0
			27	27		
6	E	63	Total	O	0	0
			63	63		

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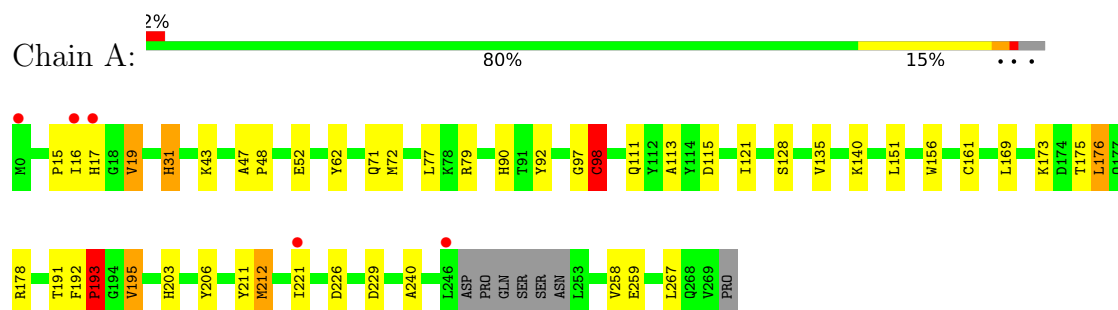
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	57	Total 57	O 57	0	0
6	G	54	Total 54	O 54	0	0
6	H	87	Total 87	O 87	0	0

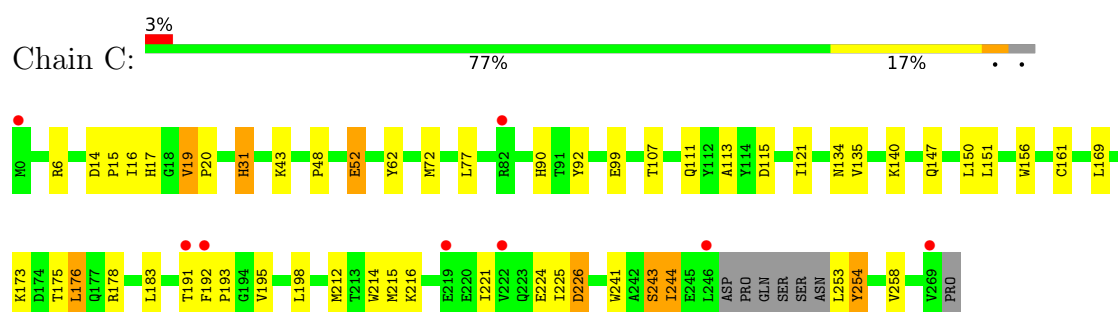
3 Residue-property plots [i](#)

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.

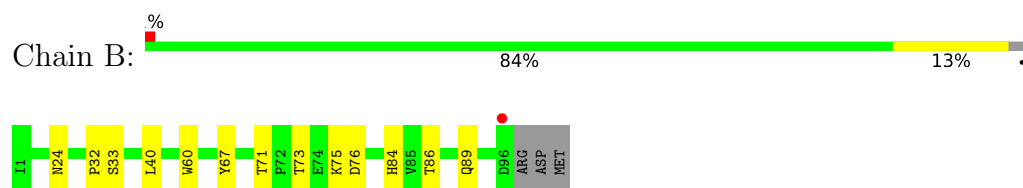
- Molecule 1: Major histocompatibility complex class I-related gene protein



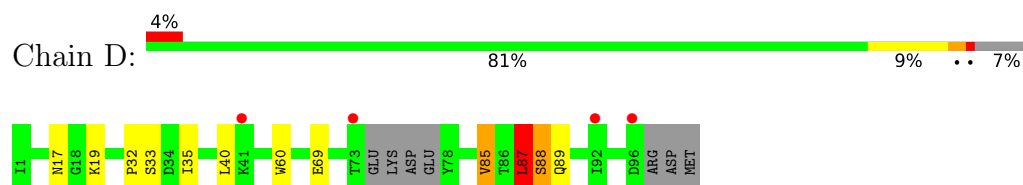
- Molecule 1: Major histocompatibility complex class I-related gene protein



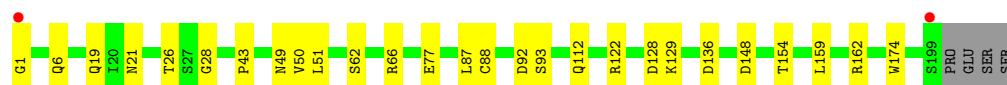
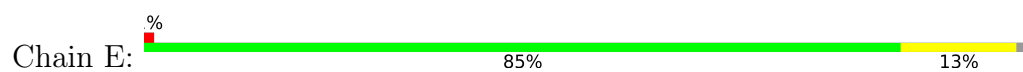
- Molecule 2: Beta-2-microglobulin



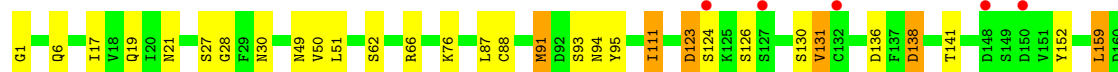
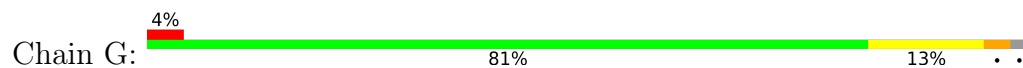
- Molecule 2: Beta-2-microglobulin



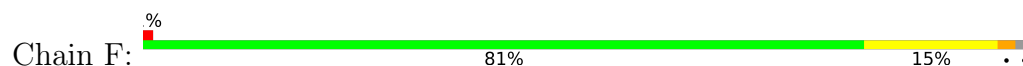
- Molecule 3: TCR-alpha



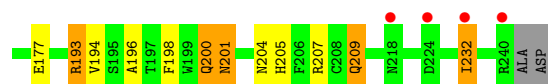
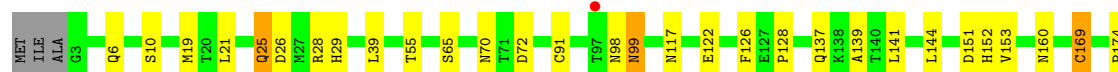
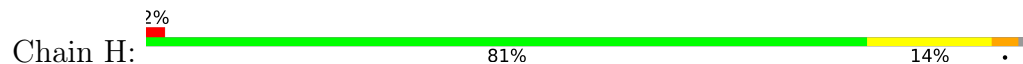
• Molecule 3: TCR-alpha



• Molecule 4: TCR-beta



• Molecule 4: TCR-beta



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	216.59Å 70.43Å 142.61Å 90.00° 104.00° 90.00°	Depositor
Resolution (Å)	36.60 – 2.50 36.60 – 2.50	Depositor EDS
% Data completeness (in resolution range)	88.3 (36.60-2.50) 88.3 (36.60-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 2.51Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.171 , 0.219 0.178 , 0.224	Depositor DCC
R_{free} test set	3223 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	39.8	Xtriage
Anisotropy	0.799	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 59.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12989	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 2LJ

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	0.91	4/2216 (0.2%)	1.30	16/3014 (0.5%)
1	C	0.82	0/2195	1.30	14/2987 (0.5%)
2	B	0.78	0/792	1.24	5/1080 (0.5%)
2	D	0.77	0/726	1.25	6/996 (0.6%)
3	E	0.83	0/1553	1.21	3/2113 (0.1%)
3	G	0.88	1/1541 (0.1%)	1.24	7/2096 (0.3%)
4	F	0.82	0/1860	1.25	7/2545 (0.3%)
4	H	0.83	1/1875 (0.1%)	1.24	5/2563 (0.2%)
All	All	0.84	6/12758 (0.0%)	1.26	63/17394 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	98	CYS	CA-C	-9.34	1.41	1.52
4	H	232	ILE	CG1-CD1	8.78	1.85	1.51
1	A	212	MET	SD-CE	-8.42	1.58	1.79
3	G	111	ILE	CG1-CD1	-7.92	1.20	1.51
1	A	72	MET	SD-CE	6.60	1.96	1.79
1	A	47	ALA	CA-C	5.05	1.57	1.52

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	96	GLY	CA-C-N	8.20	131.10	120.44
4	F	96	GLY	C-N-CA	8.20	131.10	120.44
1	C	215	MET	CA-C-N	7.85	131.01	120.65
1	C	215	MET	C-N-CA	7.85	131.01	120.65
1	A	97	GLY	CA-C-N	7.60	134.83	122.29
1	A	97	GLY	C-N-CA	7.60	134.83	122.29
2	B	33	SER	N-CA-C	6.88	118.78	111.28
1	C	254	TYR	N-CA-C	6.77	121.06	110.17
2	D	19	LYS	N-CA-C	6.56	120.21	109.72
1	C	226	ASP	CA-CB-CG	6.49	119.08	112.60
1	A	98	CYS	CA-C-O	-6.47	113.55	121.06
4	F	72	ASP	N-CA-C	6.37	119.21	111.82
4	H	72	ASP	N-CA-C	6.35	119.19	111.82
1	A	229	ASP	CA-CB-CG	6.15	118.75	112.60
3	E	92	ASP	CA-CB-CG	6.10	118.70	112.60
1	A	193	PRO	N-CA-C	6.09	125.01	112.47
3	G	179	ASP	CA-C-N	6.01	130.94	121.56
3	G	179	ASP	C-N-CA	6.01	130.94	121.56
1	C	134	ASN	CA-CB-CG	-6.00	106.60	112.60
3	G	178	SER	CA-C-N	5.91	132.33	121.70
3	G	178	SER	C-N-CA	5.91	132.33	121.70
1	C	175	THR	CA-C-N	5.90	128.19	120.28
1	C	175	THR	C-N-CA	5.90	128.19	120.28
4	F	12	ILE	N-CA-C	-5.90	99.92	108.71
4	H	201	ASN	CA-CB-CG	5.88	118.48	112.60
1	C	52	GLU	CB-CG-CD	5.86	122.56	112.60
2	B	76	ASP	N-CA-C	5.80	118.13	109.25
1	C	176	LEU	N-CA-C	5.71	117.50	111.28
1	A	175	THR	CA-C-N	5.70	127.91	120.28
1	A	175	THR	C-N-CA	5.70	127.91	120.28
4	H	26	ASP	CA-CB-CG	5.66	118.26	112.60
3	G	123	ASP	CA-C-N	5.65	132.33	121.54
3	G	123	ASP	C-N-CA	5.65	132.33	121.54
1	A	31	HIS	N-CA-C	5.62	117.05	109.24
1	A	17	HIS	N-CA-C	5.59	117.84	111.02
1	A	176	LEU	N-CA-C	5.58	117.37	111.28
4	F	26	ASP	CA-CB-CG	5.53	118.13	112.60
2	B	71	THR	CB-CA-C	5.53	117.87	110.13
3	G	130	SER	N-CA-C	5.52	117.57	109.24
2	D	87	LEU	CA-C-N	5.50	132.04	121.54
2	D	87	LEU	C-N-CA	5.50	132.04	121.54
1	A	135	VAL	N-CA-C	-5.46	105.18	110.42
4	H	99	ASN	N-CA-C	5.43	118.46	110.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	148	ASP	CA-CB-CG	5.42	118.02	112.60
2	D	33	SER	N-CA-C	5.38	117.89	111.71
1	C	31	HIS	N-CA-C	5.34	116.67	109.24
1	A	195	VAL	N-CA-C	5.26	117.42	109.12
4	F	200	GLN	N-CA-C	5.20	119.25	113.01
2	B	32	PRO	CA-C-N	5.17	127.21	120.28
2	B	32	PRO	C-N-CA	5.17	127.21	120.28
1	C	135	VAL	N-CA-C	-5.14	105.69	110.53
4	H	126	PHE	CA-CB-CG	-5.12	108.68	113.80
1	C	191	THR	CA-C-N	5.11	134.27	121.80
1	C	191	THR	C-N-CA	5.11	134.27	121.80
4	F	122	GLU	N-CA-C	-5.09	100.44	108.73
1	A	19	VAL	N-CA-C	5.08	119.84	108.88
1	A	173	LYS	N-CA-C	5.07	117.47	111.33
2	D	32	PRO	CA-C-N	5.06	127.57	120.28
2	D	32	PRO	C-N-CA	5.06	127.57	120.28
3	E	128	ASP	CA-CB-CG	5.06	117.66	112.60
1	C	17	HIS	N-CA-C	5.05	117.19	111.02
1	A	267	LEU	CA-C-N	5.03	128.02	120.87
1	A	267	LEU	C-N-CA	5.03	128.02	120.87

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	98	CYS	Mainchain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2150	0	2021	23	0
1	C	2131	0	1988	27	0
2	B	769	0	715	4	0
2	D	704	0	619	2	0
3	E	1519	0	1395	14	0
3	G	1507	0	1391	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	1811	0	1685	19	0
4	H	1826	0	1711	28	0
5	A	22	0	18	2	0
5	C	22	0	18	0	0
6	A	121	0	0	0	0
6	B	39	0	0	1	0
6	C	80	0	0	0	0
6	D	27	0	0	0	0
6	E	63	0	0	1	0
6	F	57	0	0	0	0
6	G	54	0	0	0	0
6	H	87	0	0	2	0
All	All	12989	0	11561	123	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 5.

All (123) 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)
4:H:232:ILE:CD1	4:H:232:ILE:CG1	1.86	1.54
3:G:91:MET:HE1	4:H:98:ASN:HA	1.38	1.00
1:A:191:THR:HG23	1:A:192:PHE:H	1.36	0.86
1:A:193:PRO:HG3	1:C:14:ASP:HB2	1.64	0.78
4:H:201:ASN:HB3	4:H:204:ASN:ND2	2.00	0.74
3:G:159:LEU:HB2	4:H:169:CYS:HB3	1.72	0.71
3:G:111:ILE:HD13	3:G:138:ASP:HA	1.75	0.67
4:H:196:ALA:O	4:H:200:GLN:HG2	1.95	0.67
1:A:31:HIS:HE1	1:A:206:TYR:OH	1.79	0.65
3:G:136:ASP:OD1	4:H:193:ARG:NH2	2.29	0.64
1:C:99:GLU:HB2	1:C:107:THR:OG1	1.98	0.64
1:C:48:PRO:O	1:C:52:GLU:HG2	1.99	0.62
3:E:19:GLN:HE21	3:E:21:ASN:HD21	1.48	0.61
1:A:203:HIS:HE1	6:B:136:HOH:O	1.83	0.60
4:F:12:ILE:HD12	4:F:214:GLY:HA2	1.83	0.60
3:G:19:GLN:HE21	3:G:21:ASN:HD21	1.49	0.59
4:F:25:GLN:HE22	4:F:29:HIS:H	1.50	0.59
4:H:25:GLN:HE22	4:H:29:HIS:H	1.50	0.58
1:C:43:LYS:HD2	1:C:62:TYR:HB3	1.86	0.58
1:C:111:GLN:HG2	1:C:121:ILE:HG12	1.86	0.57
1:C:151:LEU:HD22	3:E:51:LEU:HD12	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:84:HIS:HD2	2:B:86:THR:OG1	1.86	0.57
3:E:129:LYS:HD3	3:E:174:TRP:CD1	2.39	0.57
3:G:159:LEU:HD11	4:H:193:ARG:HB2	1.86	0.57
4:H:151:ASP:HB2	4:H:174:PRO:HG3	1.87	0.56
1:A:211:TYR:HB2	1:A:259:GLU:HB3	1.87	0.56
1:A:111:GLN:HG2	1:A:121:ILE:HG12	1.86	0.56
1:C:241:TRP:HZ3	1:C:243:SER:HB2	1.71	0.56
3:G:1:GLY:HA2	3:G:27:SER:H	1.70	0.56
4:H:160:ASN:HD21	4:H:204:ASN:HA	1.71	0.56
4:F:13:LEU:HD21	4:F:19:MET:HB2	1.89	0.55
4:H:194:VAL:HG21	4:H:198:PHE:CD2	2.41	0.55
4:F:125:VAL:HG13	4:F:235:ALA:HB3	1.89	0.55
1:A:43:LYS:HD2	1:A:62:TYR:HB3	1.88	0.54
3:G:91:MET:HE1	4:H:98:ASN:CA	2.26	0.54
1:C:77:LEU:HD13	1:C:92:TYR:HB2	1.90	0.54
4:H:160:ASN:ND2	4:H:205:HIS:H	2.06	0.53
2:B:73:THR:HG22	2:B:75:LYS:H	1.73	0.53
4:F:128:PRO:HD3	4:F:141:LEU:HG	1.91	0.53
4:H:117:ASN:HB3	6:H:306:HOH:O	2.08	0.52
1:A:77:LEU:HD13	1:A:92:TYR:HB2	1.92	0.52
1:A:62:TYR:HE2	3:G:94:ASN:HD22	1.57	0.52
1:A:90:HIS:HD2	1:A:115:ASP:OD2	1.94	0.51
1:C:113:ALA:HB2	2:D:60:TRP:CE2	2.45	0.51
1:C:198:LEU:HB2	1:C:244:ILE:HG22	1.93	0.50
1:A:212:MET:HE1	1:A:240:ALA:HB3	1.91	0.50
1:C:90:HIS:HD2	1:C:115:ASP:OD2	1.94	0.50
4:H:207:ARG:HH12	4:H:209:GLN:CG	2.24	0.50
1:A:48:PRO:O	1:A:52:GLU:HG3	2.11	0.49
3:G:178:SER:HA	3:G:180:PHE:N	2.27	0.49
4:H:19:MET:HE2	4:H:21:LEU:HD23	1.94	0.49
3:G:6:GLN:HE22	3:G:88:CYS:H	1.59	0.49
3:E:6:GLN:HE22	3:E:88:CYS:H	1.60	0.49
1:A:191:THR:CG2	1:A:192:PHE:H	2.16	0.49
1:C:221:ILE:HD11	1:C:254:TYR:CD1	2.48	0.48
4:H:201:ASN:HB3	4:H:204:ASN:HD22	1.76	0.48
3:G:30:ASN:HB2	3:G:91:MET:HG2	1.95	0.48
4:H:10:SER:OG	4:H:152:HIS:CE1	2.67	0.48
4:H:128:PRO:HD3	4:H:141:LEU:HG	1.94	0.48
3:G:17:ILE:HG12	3:G:76:LYS:HG2	1.95	0.48
4:F:19:MET:HE2	4:F:21:LEU:HD23	1.95	0.47
4:F:201:ASN:OD1	4:F:203:ARG:HG3	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:PRO:HB2	1:A:19:VAL:HG23	1.97	0.47
2:B:24:ASN:HD22	2:B:67:TYR:HB3	1.80	0.47
1:C:214:TRP:HB3	1:C:221:ILE:HD12	1.97	0.47
1:C:221:ILE:HD11	1:C:254:TYR:HD1	1.78	0.47
1:A:151:LEU:HD22	3:G:51:LEU:HD12	1.97	0.47
1:C:31:HIS:HD2	1:C:176:LEU:CD2	2.28	0.47
3:E:1:GLY:HA3	3:E:26:THR:HA	1.96	0.47
4:F:207:ARG:NH1	4:F:209:GLN:HG3	2.30	0.47
4:F:110:THR:OG1	4:F:152:HIS:HE1	1.97	0.46
4:H:207:ARG:NH1	4:H:209:GLN:CG	2.79	0.46
5:A:301:2LJ:H10	5:A:301:2LJ:H17	1.77	0.46
3:E:28:GLY:HA3	3:E:93:SER:HB3	1.97	0.46
3:E:136:ASP:OD1	4:F:193:ARG:NH2	2.48	0.46
1:C:31:HIS:CD2	1:C:176:LEU:HD23	2.51	0.46
1:A:169:LEU:HD23	1:A:176:LEU:HD13	1.97	0.45
3:G:28:GLY:HA3	3:G:93:SER:HB3	1.97	0.45
3:G:50:VAL:O	3:G:66:ARG:HD3	2.16	0.45
1:C:212:MET:HG2	1:C:258:VAL:HG22	1.98	0.45
1:A:191:THR:HG23	1:A:192:PHE:N	2.18	0.45
4:F:207:ARG:HH12	4:F:209:GLN:HG3	1.82	0.45
1:C:15:PRO:HB2	1:C:19:VAL:HG23	1.99	0.45
3:E:154:THR:HG21	4:F:189:SER:OG	2.17	0.45
3:E:49:ASN:HD21	3:E:62:SER:CB	2.30	0.45
4:F:3:GLY:O	4:F:27:MET:HE2	2.16	0.45
4:F:110:THR:OG1	4:F:152:HIS:CE1	2.70	0.45
1:A:113:ALA:HB2	2:B:60:TRP:CE2	2.53	0.44
1:C:221:ILE:HG21	1:C:244:ILE:HD11	1.98	0.44
3:G:141:THR:HG21	3:G:192:PRO:HD3	2.00	0.44
1:A:212:MET:HG2	1:A:258:VAL:HG22	2.00	0.44
1:A:156:TRP:CZ3	1:A:161:CYS:HB2	2.53	0.44
3:G:91:MET:HE3	3:G:95:TYR:HD1	1.83	0.44
4:H:128:PRO:HG3	4:H:139:ALA:HB1	2.00	0.44
1:C:216:LYS:O	1:C:253:LEU:O	2.36	0.43
3:E:50:VAL:O	3:E:66:ARG:HD3	2.18	0.43
1:C:19:VAL:HA	1:C:20:PRO:HD3	1.97	0.43
1:C:169:LEU:HD23	1:C:176:LEU:HD13	2.00	0.43
1:A:212:MET:HE1	1:A:240:ALA:CB	2.49	0.43
1:C:225:ILE:HG12	1:C:244:ILE:HD11	1.99	0.43
3:E:122:ARG:HB2	4:F:127:GLU:HB2	2.00	0.43
4:H:10:SER:HG	4:H:152:HIS:CE1	2.37	0.43
1:C:156:TRP:CZ3	1:C:161:CYS:HB2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:112:GLN:HA	6:E:333:HOH:O	2.18	0.42
1:C:147:GLN:HA	1:C:150:LEU:HD12	2.01	0.42
2:D:87:LEU:HB2	2:D:88:SER:H	1.68	0.42
4:H:207:ARG:NH1	4:H:209:GLN:HG2	2.33	0.42
1:A:71:GLN:HG3	6:H:328:HOH:O	2.18	0.42
4:H:194:VAL:HG22	4:H:198:PHE:HB3	2.02	0.42
1:A:212:MET:CE	1:A:240:ALA:HB3	2.50	0.42
1:C:225:ILE:HG12	1:C:244:ILE:CD1	2.50	0.41
4:F:128:PRO:HG3	4:F:139:ALA:HB1	2.01	0.41
3:G:49:ASN:HD21	3:G:62:SER:CB	2.33	0.41
4:F:152:HIS:HB3	4:F:213:TYR:HB2	2.03	0.41
3:G:131:VAL:CG2	4:H:144:LEU:HD11	2.51	0.41
3:E:43:PRO:HD2	4:F:103:PHE:CG	2.56	0.41
1:C:31:HIS:CD2	1:C:176:LEU:CD2	3.04	0.41
5:A:301:2LJ:H1	5:A:301:2LJ:O4	2.21	0.40
4:F:6:GLN:NE2	4:F:91:CYS:H	2.19	0.40
3:G:152:TYR:CE1	4:H:177:GLU:HA	2.55	0.40
4:H:6:GLN:NE2	4:H:91:CYS:H	2.19	0.40
3:E:49:ASN:HD21	3:E:62:SER:HB2	1.85	0.40
4:H:207:ARG:NH1	4:H:209:GLN:HG3	2.37	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	260/271 (96%)	249 (96%)	9 (4%)	2 (1%)	16	31
1	C	260/271 (96%)	245 (94%)	10 (4%)	5 (2%)	6	11
2	B	94/99 (95%)	93 (99%)	1 (1%)	0	100	100
2	D	88/99 (89%)	79 (90%)	4 (4%)	5 (6%)	1	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	E	197/203 (97%)	192 (98%)	5 (2%)	0	100	100
3	G	197/203 (97%)	185 (94%)	7 (4%)	5 (2%)	4	7
4	F	236/243 (97%)	226 (96%)	10 (4%)	0	100	100
4	H	236/243 (97%)	228 (97%)	8 (3%)	0	100	100
All	All	1568/1632 (96%)	1497 (96%)	54 (3%)	17 (1%)	11	22

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	193	PRO
1	C	192	PHE
2	D	88	SER
3	G	123	ASP
3	G	124	SER
2	D	87	LEU
3	G	178	SER
3	G	126	SER
1	C	224	GLU
2	D	17	ASN
3	G	179	ASP
2	D	85	VAL
2	D	89	GLN
1	C	19	VAL
1	C	16	ILE
1	A	16	ILE
1	C	193	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	224/241 (93%)	216 (96%)	8 (4%)	31	58
1	C	219/241 (91%)	209 (95%)	10 (5%)	24	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	83/94 (88%)	81 (98%)	2 (2%)	43	70
2	D	71/94 (76%)	66 (93%)	5 (7%)	14	29
3	E	165/180 (92%)	161 (98%)	4 (2%)	43	70
3	G	161/180 (89%)	156 (97%)	5 (3%)	35	62
4	F	189/205 (92%)	175 (93%)	14 (7%)	13	27
4	H	192/205 (94%)	178 (93%)	14 (7%)	13	27
All	All	1304/1440 (91%)	1242 (95%)	62 (5%)	23	46

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	ARG
1	A	98	CYS
1	A	128	SER
1	A	140	LYS
1	A	178	ARG
1	A	195	VAL
1	A	221	ILE
1	A	226	ASP
2	B	40	LEU
2	B	89	GLN
1	C	6	ARG
1	C	72	MET
1	C	140	LYS
1	C	173	LYS
1	C	178	ARG
1	C	183	LEU
1	C	195	VAL
1	C	226	ASP
1	C	243	SER
1	C	244	ILE
2	D	35	ILE
2	D	40	LEU
2	D	69	GLU
2	D	85	VAL
2	D	87	LEU
3	E	77	GLU
3	E	87	LEU
3	E	159	LEU
3	E	162	ARG

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Mol	Chain	Res	Type
4	F	13	LEU
4	F	18	ARG
4	F	25	GLN
4	F	39	LEU
4	F	55	THR
4	F	65	SER
4	F	70	ASN
4	F	80	SER
4	F	82	VAL
4	F	94	SER
4	F	151	ASP
4	F	169	CYS
4	F	193	ARG
4	F	203	ARG
3	G	87	LEU
3	G	91	MET
3	G	131	VAL
3	G	138	ASP
3	G	159	LEU
4	H	25	GLN
4	H	28	ARG
4	H	39	LEU
4	H	55	THR
4	H	65	SER
4	H	70	ASN
4	H	99	ASN
4	H	122	GLU
4	H	137	GLN
4	H	153	VAL
4	H	169	CYS
4	H	193	ARG
4	H	200	GLN
4	H	209	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	HIS
1	A	58	HIS
1	A	81	GLN
1	A	90	HIS
1	A	93	GLN

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Mol	Chain	Res	Type
1	A	111	GLN
1	A	146	ASN
1	A	147	GLN
1	A	177	GLN
1	A	203	HIS
1	A	239	GLN
1	A	257	HIS
2	B	8	GLN
2	B	24	ASN
2	B	42	ASN
2	B	84	HIS
1	C	58	HIS
1	C	64	GLN
1	C	81	GLN
1	C	90	HIS
1	C	134	ASN
1	C	137	HIS
1	C	147	GLN
1	C	203	HIS
1	C	239	GLN
1	C	257	HIS
2	D	8	GLN
2	D	13	HIS
3	E	6	GLN
3	E	19	GLN
3	E	37	GLN
3	E	49	ASN
3	E	169	ASN
3	E	187	ASN
4	F	6	GLN
4	F	25	GLN
4	F	37	GLN
4	F	152	HIS
4	F	178	GLN
4	F	211	GLN
4	F	231	GLN
3	G	2	GLN
3	G	6	GLN
3	G	19	GLN
3	G	37	GLN
3	G	38	HIS
3	G	49	ASN

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Mol	Chain	Res	Type
3	G	94	ASN
3	G	145	GLN
3	G	187	ASN
4	H	6	GLN
4	H	25	GLN
4	H	37	GLN
4	H	98	ASN
4	H	117	ASN
4	H	135	HIS
4	H	160	ASN
4	H	201	ASN
4	H	209	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	2LJ	A	301	1	22,22,22	1.29	3 (13%)	24,29,29	1.26	3 (12%)
5	2LJ	C	301	1	22,22,22	1.90	3 (13%)	24,29,29	1.52	2 (8%)

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	2LJ	A	301	1	-	2/18/19/19	0/1/1/1
5	2LJ	C	301	1	-	1/18/19/19	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	301	2LJ	C7-C6	6.05	1.55	1.49
5	C	301	2LJ	C8A-N8	5.69	1.41	1.32
5	A	301	2LJ	C8A-N8	4.22	1.39	1.32
5	A	301	2LJ	C7-C6	3.09	1.52	1.49
5	C	301	2LJ	C1'-C2'	2.74	1.56	1.52
5	A	301	2LJ	C4A-C8A	-2.19	1.39	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	301	2LJ	C6-N5-C4A	5.97	129.65	121.17
5	A	301	2LJ	C6-N5-C4A	3.69	126.42	121.17
5	A	301	2LJ	N1-C8A-N8	2.55	122.37	118.66
5	A	301	2LJ	C8-C7-C6	2.43	118.04	113.75
5	C	301	2LJ	C8-C7-C6	2.40	117.99	113.75

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	301	2LJ	N8-C1'-C2'-C3'
5	C	301	2LJ	N8-C1'-C2'-C3'
5	A	301	2LJ	C2'-C3'-C4'-C5'

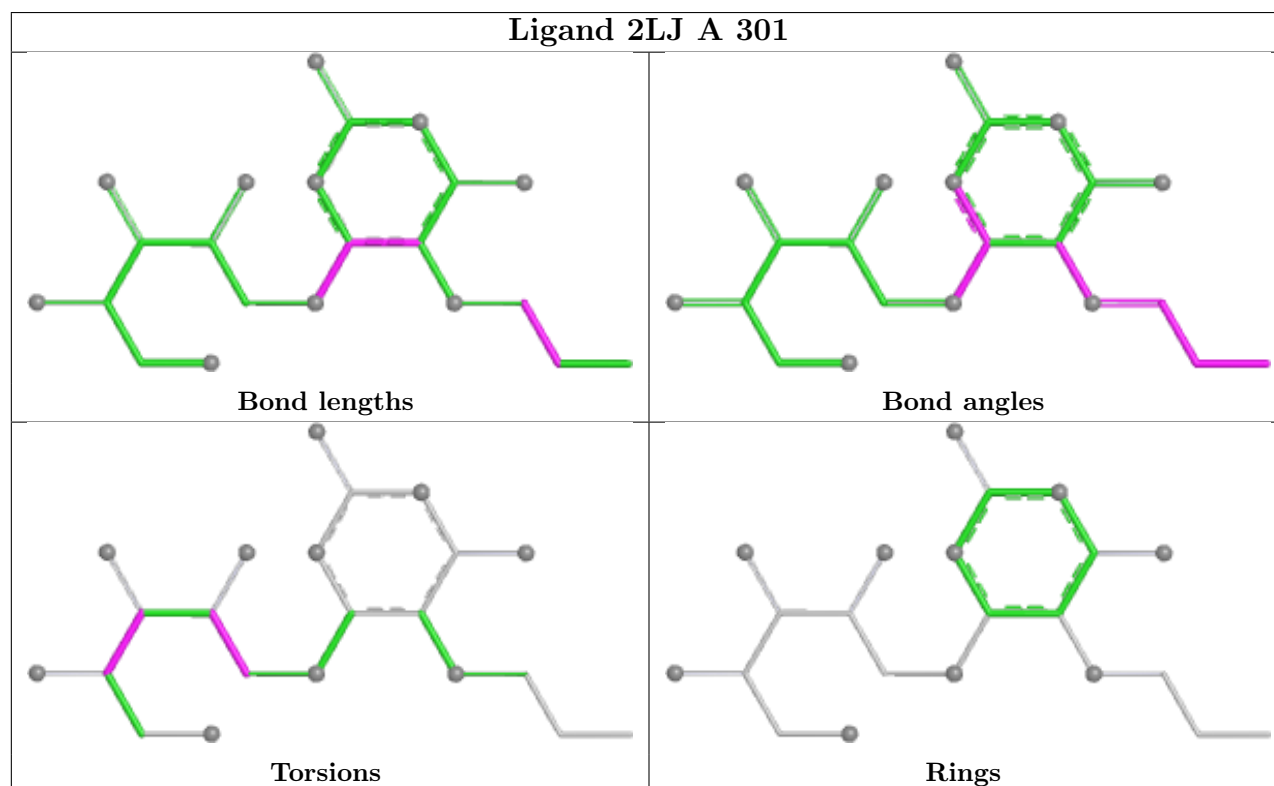
There are no ring outliers.

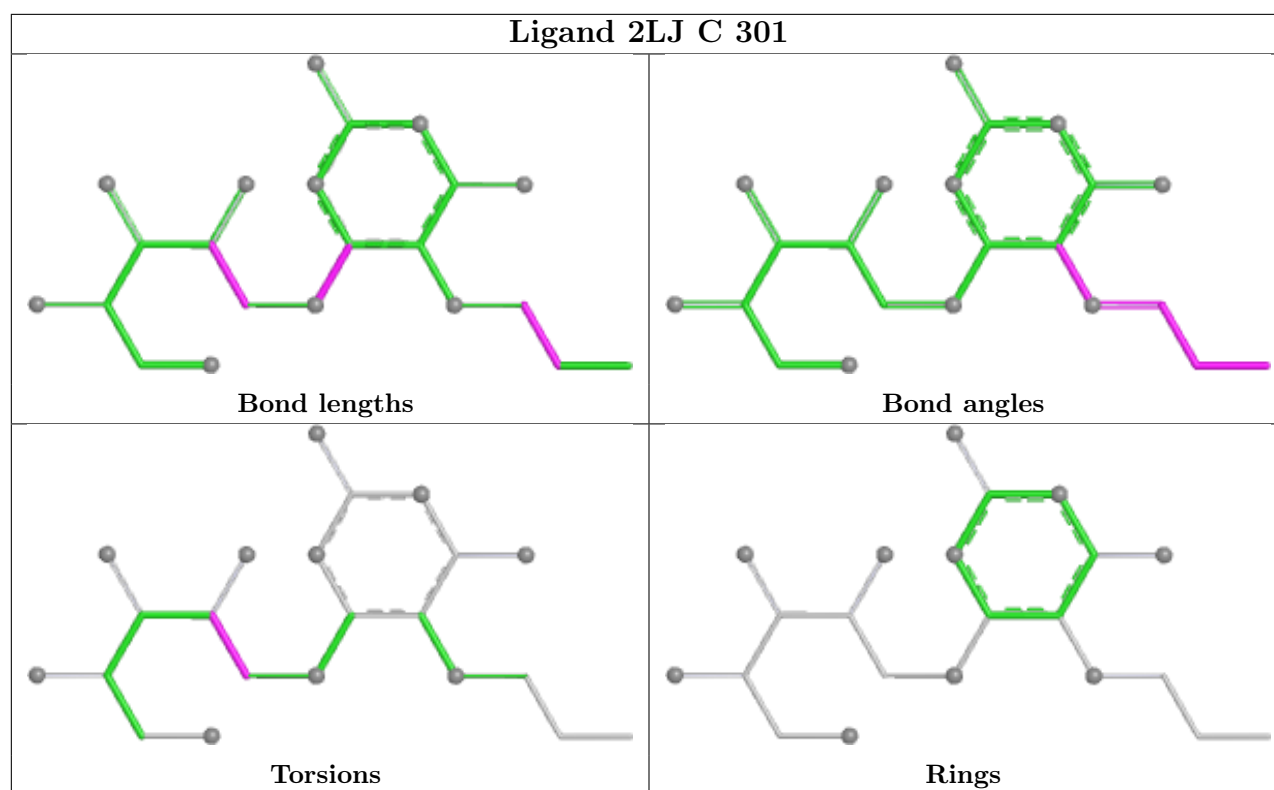
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	301	2LJ	2	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	264/271 (97%)	-0.28	5 (1%) 66 62	20, 38, 72, 95	0
1	C	264/271 (97%)	0.04	8 (3%) 52 48	30, 52, 88, 103	0
2	B	96/99 (96%)	-0.17	1 (1%) 79 76	26, 50, 77, 86	0
2	D	92/99 (92%)	0.51	4 (4%) 40 35	40, 77, 104, 118	0
3	E	199/203 (98%)	-0.19	2 (1%) 79 76	25, 43, 76, 99	0
3	G	199/203 (98%)	0.20	8 (4%) 42 38	23, 54, 99, 114	0
4	F	238/243 (97%)	-0.07	2 (0%) 82 80	30, 50, 74, 88	0
4	H	238/243 (97%)	-0.11	5 (2%) 63 59	23, 48, 88, 103	0
All	All	1590/1632 (97%)	-0.05	35 (2%) 62 58	20, 48, 89, 118	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	240	ARG	5.2
2	D	73	THR	4.6
2	D	96	ASP	4.5
3	E	199	SER	4.3
3	G	150	ASP	3.6
1	C	191	THR	3.5
3	G	199	SER	3.5
1	C	246	LEU	3.4
1	C	222	VAL	2.9
1	C	219	GLU	2.8
3	G	148	ASP	2.7
1	A	246	LEU	2.7
3	G	124	SER	2.6
4	H	224	ASP	2.6
4	H	218	ASN	2.6
3	G	178	SER	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	41	LYS	2.5
4	F	240	ARG	2.4
4	F	182	ASN	2.3
1	A	221	ILE	2.2
2	B	96	ASP	2.2
1	C	192	PHE	2.2
1	C	269	VAL	2.2
2	D	92	ILE	2.2
1	A	16	ILE	2.2
3	G	132	CYS	2.1
3	G	127	SER	2.1
3	G	161	MET	2.1
4	H	97	THR	2.1
1	A	17	HIS	2.1
4	H	232	ILE	2.1
1	C	0	MET	2.1
3	E	1	GLY	2.1
1	C	82	ARG	2.0
1	A	0	MET	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.

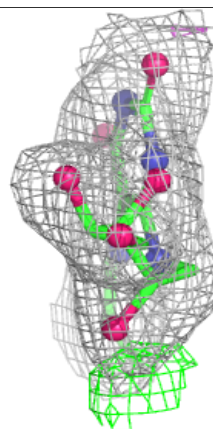
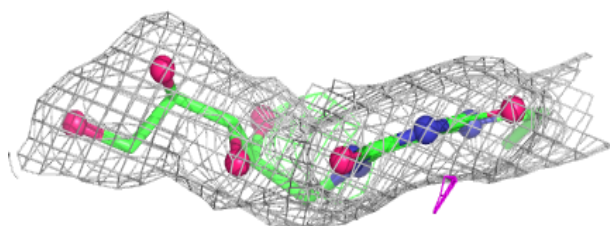
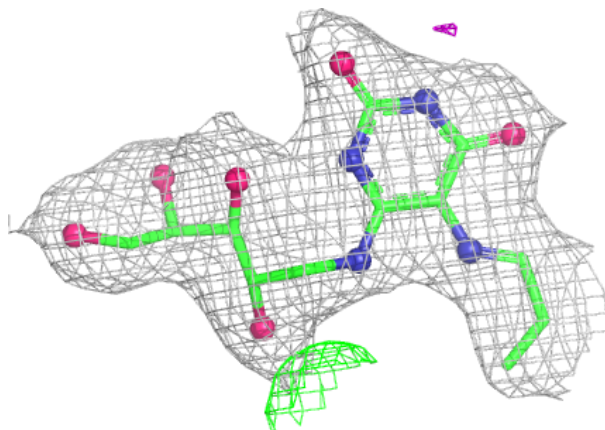
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	2LJ	C	301	22/22	0.96	0.06	22,28,32,34	0
5	2LJ	A	301	22/22	0.97	0.06	18,26,31,33	0

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.

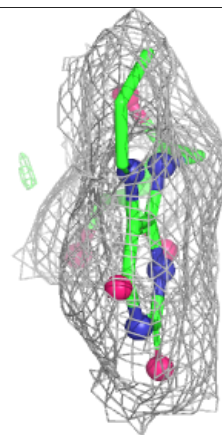
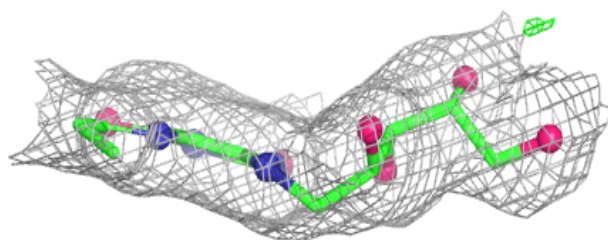
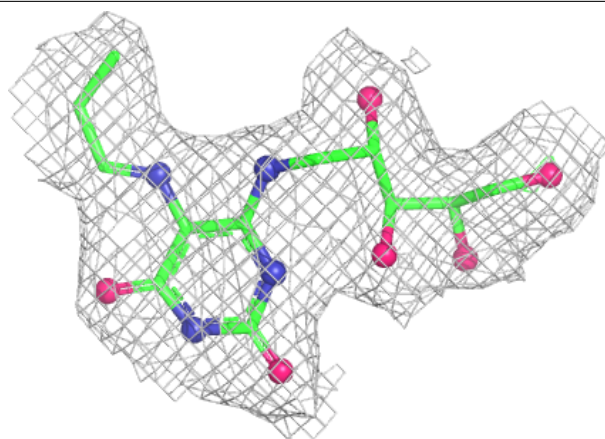
Electron density around 2LJ C 301:

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



Electron density around 2LJ A 301:

$2mF_o - DF_c$ (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.