



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 5, 2022 – 08:07 AM EST

PDB ID : 7UFJ
Title : Structure of human MR1-ethylvanillin in complex with human MAIT A-F7 TCR
Authors : Wang, C.J.; Rossjohn, J.; Le Nours, J.
Deposited on : 2022-03-22
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	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

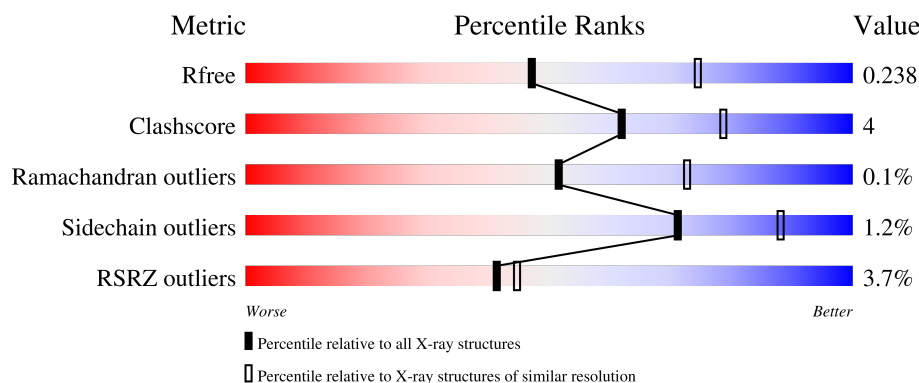
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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	<div> <div>86%</div> <div>12%</div> <div>•</div> </div>
1	C	271	<div> <div>83%</div> <div>14%</div> <div>•</div> </div>
2	B	100	<div> <div>3%</div> <div>91%</div> <div>9%</div> </div>
2	D	100	<div> <div>15%</div> <div>81%</div> <div>15%</div> <div>••</div> </div>
3	E	203	<div> <div>91%</div> <div>7%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
3	G	203	
4	F	245	
4	H	245	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	GOL	A	303	-	X	-	-
7	GOL	C	307	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 13149 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	266	Total	C	N	O	S	1	1	0
			2173	1392	377	393	11			
1	C	264	Total	C	N	O	S	0	1	0
			2146	1370	375	390	11			

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	conflict	UNP Q95460
C	0	MET	-	initiating methionine	UNP Q95460
C	261	SER	CYS	conflict	UNP Q95460

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	0	0
			813	518	137	154	4			
2	D	97	Total	C	N	O	S	0	0	0
			757	485	126	143	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769
D	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called MAIT T-cell receptor alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	194	Total	C	N	O	S	0	1	0
			1443	925	230	279	9			

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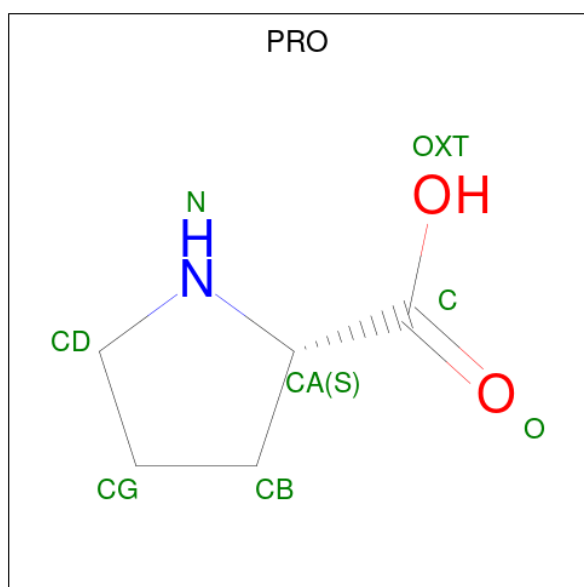
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	200	Total	C	N	O	S	0	0	0
			1543	975	247	312	9			

- Molecule 4 is a protein called MAIT T-cell receptor beta chain.

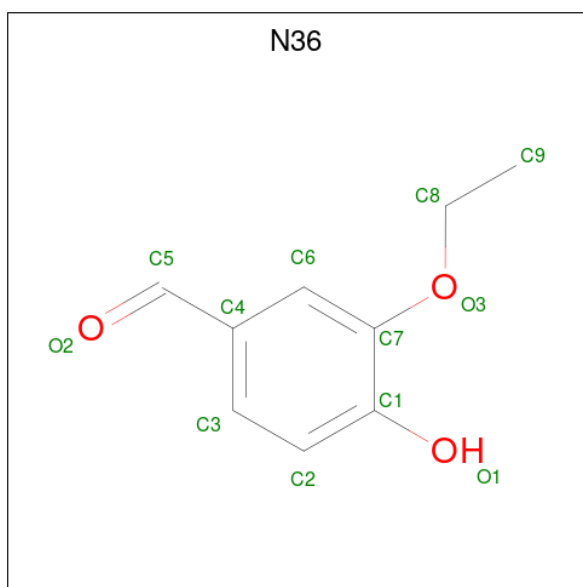
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	242	Total	C	N	O	S	0	2	0
			1874	1181	328	356	9			
4	F	244	Total	C	N	O	S	0	0	0
			1891	1192	330	360	9			

- Molecule 5 is PROLINE (three-letter code: PRO) (formula: C₅H₉NO₂).



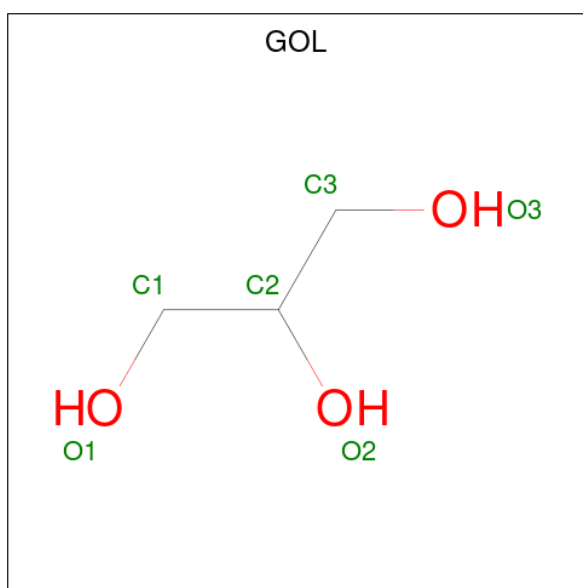
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			7	5	1	1		
5	C	1	Total	C	N	O	0	0
			7	5	1	1		

- Molecule 6 is 3-ethoxy-4-hydroxybenzaldehyde (three-letter code: N36) (formula: C₉H₁₀O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			11	9	2		
6	C	1	Total	C	O	0	0
			11	9	2		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



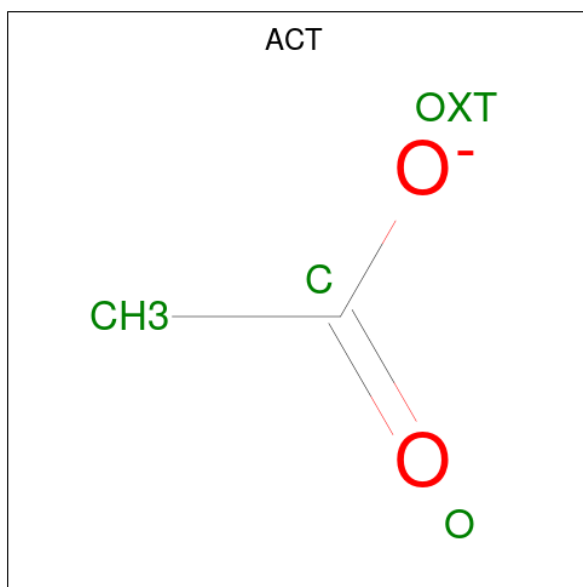
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	G	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		
7	E	1	Total	C	O	0	0
			6	3	3		
7	F	1	Total	C	O	0	0
			6	3	3		
7	F	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	1	Total C O 4 2 2	0	0
8	C	1	Total C O 4 2 2	0	0
8	E	1	Total C O 4 2 2	0	0
8	F	1	Total C O 4 2 2	0	0

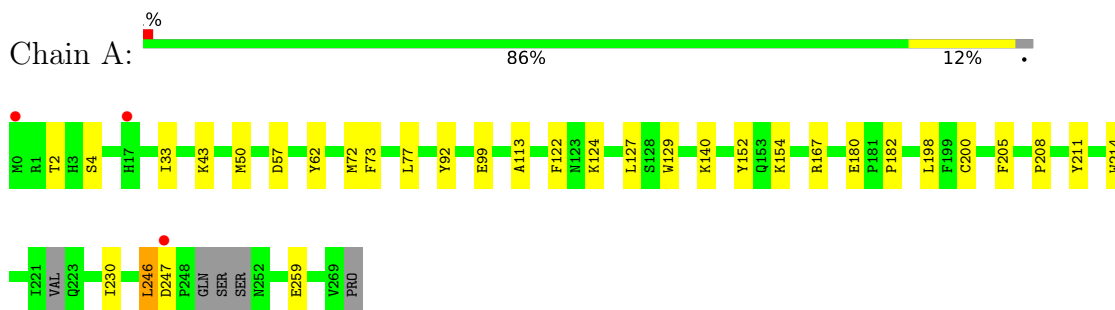
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	78	Total O 78 78	0	0
9	B	36	Total O 36 36	0	0
9	G	31	Total O 31 31	0	0
9	H	36	Total O 36 36	0	0
9	C	59	Total O 59 59	0	0
9	D	17	Total O 17 17	0	0
9	E	61	Total O 61 61	0	0
9	F	61	Total O 61 61	0	0

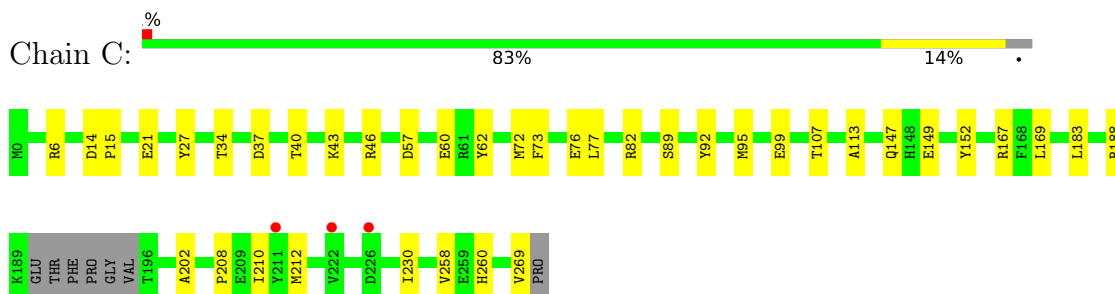
3 Residue-property plots [i](#)

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.

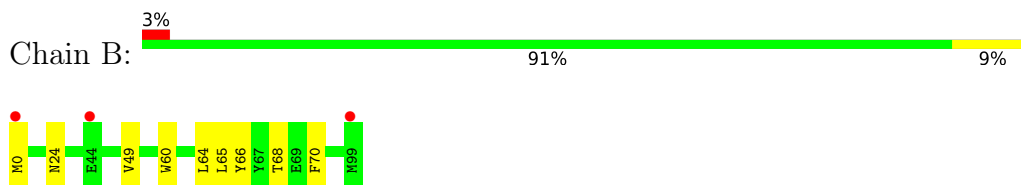
- Molecule 1: Major histocompatibility complex class I-related gene protein



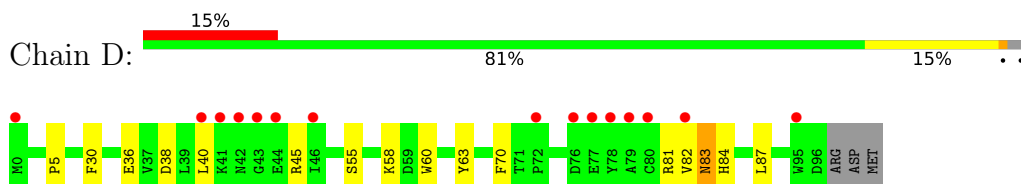
- Molecule 1: Major histocompatibility complex class I-related gene protein



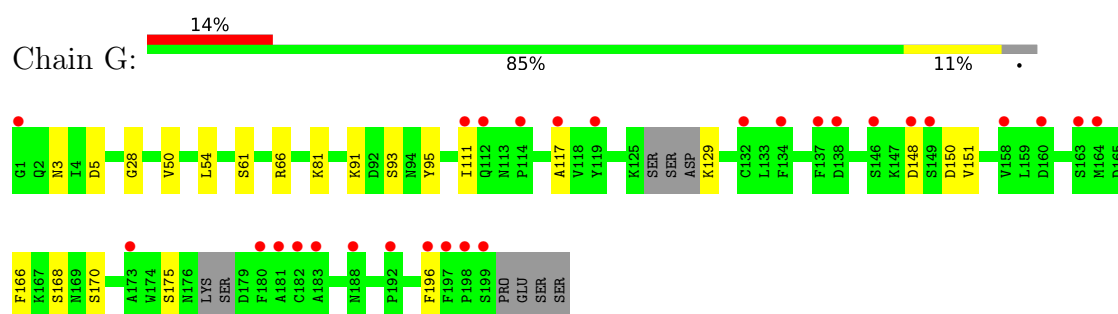
- Molecule 2: Beta-2-microglobulin



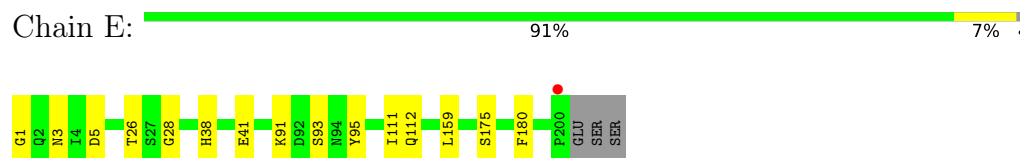
- Molecule 2: Beta-2-microglobulin



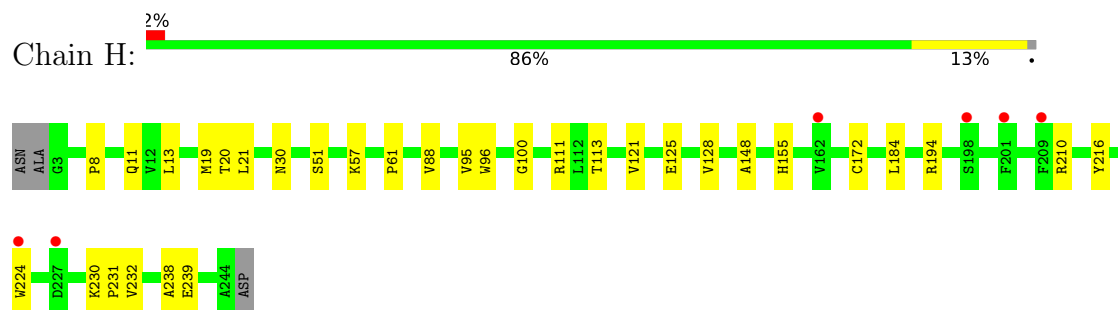
- Molecule 3: MAIT T-cell receptor alpha chain



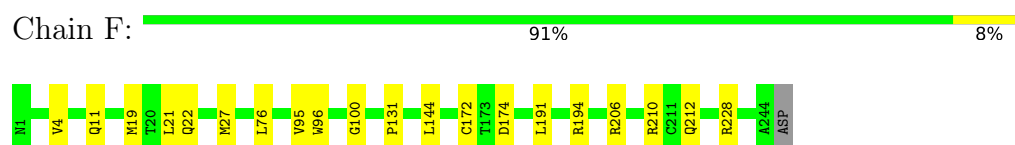
- Molecule 3: MAIT T-cell receptor alpha chain



- Molecule 4: MAIT T-cell receptor beta chain



- Molecule 4: MAIT T-cell receptor beta chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	217.94Å 70.89Å 144.39Å 90.00° 104.86° 90.00°	Depositor
Resolution (Å)	48.43 – 2.50 48.43 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.8 (48.43-2.50) 98.8 (48.43-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.180 , 0.238 0.180 , 0.238	Depositor DCC
R_{free} test set	3728 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	41.9	Xtriage
Anisotropy	0.468	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13149	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.86% 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: GOL, N36, ACT

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	0.45	0/2238	0.65	0/3042
1	C	0.43	0/2211	0.62	0/3006
2	B	0.43	0/836	0.61	0/1137
2	D	0.37	0/780	0.57	0/1067
3	E	0.42	0/1578	0.65	0/2143
3	G	0.41	0/1475	0.61	0/2006
4	F	0.46	0/1942	0.63	0/2647
4	H	0.42	0/1925	0.63	0/2627
All	All	0.43	0/12985	0.63	0/17675

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2173	0	2042	23	0
1	C	2146	0	1991	24	0
2	B	813	0	753	4	0
2	D	757	0	667	12	0
3	E	1543	0	1439	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	1443	0	1297	11	0
4	F	1891	0	1773	15	0
4	H	1874	0	1717	20	0
5	A	7	0	7	0	0
5	C	7	0	7	1	0
6	A	11	0	0	0	0
6	C	11	0	0	0	0
7	A	18	0	24	1	0
7	B	12	0	15	0	0
7	C	18	0	24	1	0
7	D	6	0	8	1	0
7	E	6	0	8	2	0
7	F	12	0	16	2	0
7	G	6	0	8	0	0
8	C	8	0	6	0	0
8	E	4	0	3	0	0
8	F	4	0	3	1	0
9	A	78	0	0	0	0
9	B	36	0	0	0	0
9	C	59	0	0	0	0
9	D	17	0	0	1	0
9	E	61	0	0	1	0
9	F	61	0	0	1	0
9	G	31	0	0	1	0
9	H	36	0	0	0	0
All	All	13149	0	11808	108	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 4.

All (108) 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)
3:E:28:GLY:HA3	3:E:93:SER:HB3	1.72	0.71
1:A:211:TYR:HB3	1:A:259:GLU:HB3	1.73	0.71
4:H:88:VAL:HG22	4:H:111[B]:ARG:HG2	1.73	0.71
4:H:11:GLN:HG2	4:H:19:MET:SD	2.32	0.69
4:F:11:GLN:HG2	4:F:19:MET:SD	2.34	0.67
4:H:224:TRP:HB2	4:H:230:LYS:HD2	1.75	0.67
3:G:28:GLY:HA3	3:G:93:SER:HB3	1.77	0.67
3:G:151:VAL:HG12	3:G:175:SER:HB2	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:SER:HB3	1:A:99:GLU:HG2	1.78	0.65
1:C:167:ARG:HH11	7:C:305:GOL:H32	1.62	0.64
3:G:54:LEU:HD11	3:G:61:SER:HB3	1.81	0.63
3:E:112:GLN:N	7:E:302:GOL:O2	2.25	0.61
1:C:43:LYS:HD2	1:C:62:TYR:HB3	1.83	0.60
1:A:152:TYR:CD1	4:H:100:GLY:HA3	2.37	0.60
4:H:128:VAL:HG23	4:H:238:ALA:HB3	1.85	0.59
3:E:1:GLY:HA3	3:E:26:THR:HA	1.84	0.59
3:E:159:LEU:HB3	4:F:172:CYS:HB2	1.86	0.58
3:G:3:ASN:ND2	3:G:5:ASP:OD2	2.37	0.57
4:H:155:HIS:HB3	4:H:216:TYR:HB2	1.89	0.54
4:F:21:LEU:HD12	4:F:76:LEU:HD23	1.87	0.54
1:A:129:TRP:O	1:A:140:LYS:HE2	2.08	0.54
1:A:77:LEU:HD13	1:A:92:TYR:HB2	1.91	0.53
4:H:13:LEU:HD11	4:H:19:MET:HE2	1.91	0.53
2:B:24:ASN:HB3	2:B:65:LEU:HD11	1.90	0.53
1:C:77:LEU:HD13	1:C:92:TYR:HB2	1.90	0.52
4:F:11:GLN:NE2	9:F:501:HOH:O	2.26	0.52
1:C:57:ASP:HA	1:C:60:GLU:HB2	1.91	0.52
3:E:111:ILE:HA	7:E:302:GOL:H2	1.91	0.52
4:H:57:LYS:HB2	4:H:61:PRO:HG3	1.92	0.51
3:E:38:HIS:HB2	3:E:41:GLU:HG3	1.90	0.51
1:C:269:VAL:HA	5:C:301:PRO:HD2	1.91	0.51
4:H:19:MET:HG2	4:H:20:THR:N	2.25	0.51
1:C:72:MET:HG3	4:F:96:TRP:CE2	2.46	0.51
4:F:131:PRO:HD3	4:F:144:LEU:HG	1.93	0.51
2:B:49:VAL:HG22	2:B:68:THR:HB	1.93	0.50
1:A:127:LEU:HD11	1:A:154:LYS:HD2	1.94	0.50
3:E:91:LYS:HG2	3:E:95:TYR:HA	1.94	0.49
1:A:113:ALA:HB2	2:B:60:TRP:CE2	2.48	0.49
4:H:30:ASN:O	4:H:51:SER:HA	2.13	0.49
1:C:208:PRO:O	1:C:230:ILE:HD13	2.12	0.49
1:A:2:THR:OG1	8:F:401:ACT:H2	2.13	0.48
1:A:43:LYS:HD2	1:A:62:TYR:HB3	1.95	0.48
3:E:175:SER:HB3	3:E:180:PHE:CG	2.49	0.48
1:C:113:ALA:HB2	2:D:60:TRP:CE2	2.48	0.48
1:C:99:GLU:HB2	1:C:107:THR:OG1	2.14	0.48
3:E:3:ASN:ND2	3:E:5:ASP:OD2	2.45	0.47
1:A:152:TYR:CE1	4:H:100:GLY:HA3	2.49	0.47
3:G:148:ASP:C	3:G:150:ASP:H	2.17	0.47
4:H:111[A]:ARG:NH1	4:H:113:THR:OG1	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:PHE:HB2	1:A:129:TRP:CZ3	2.50	0.47
1:C:14:ASP:HB3	1:C:89:SER:HB2	1.95	0.47
4:H:8:PRO:HD2	4:H:21:LEU:HD22	1.97	0.47
2:D:40:LEU:HD11	2:D:81:ARG:HD3	1.96	0.47
4:F:4:VAL:HG23	4:F:27:MET:HE1	1.96	0.46
1:C:15:PRO:HG3	1:C:21:GLU:HB3	1.97	0.46
4:F:95:VAL:HG12	4:F:96:TRP:CD1	2.50	0.46
2:D:55:SER:HB3	2:D:63:TYR:CE1	2.52	0.45
2:D:55:SER:HB3	2:D:63:TYR:CZ	2.51	0.45
1:A:180:GLU:O	1:A:205:PHE:HA	2.17	0.45
1:C:152:TYR:CE1	4:F:100:GLY:HA2	2.51	0.44
1:A:167:ARG:HH11	7:A:305:GOL:H11	1.83	0.44
3:G:166:PHE:CE2	3:G:168:SER:HB3	2.53	0.44
1:A:198:LEU:HG	1:A:246:LEU:HD21	1.99	0.44
2:D:83:ASN:ND2	2:D:87:LEU:HB2	2.32	0.44
1:A:72:MET:HG3	4:H:96:TRP:CZ2	2.53	0.44
1:A:208:PRO:O	1:A:230:ILE:HD13	2.18	0.44
4:H:230:LYS:HZ2	4:H:232:VAL:HG12	1.83	0.44
1:C:34:THR:HB	1:C:43:LYS:HE3	2.00	0.44
4:F:210:ARG:NH1	4:F:212:GLN:HB2	2.33	0.44
1:A:43:LYS:CD	1:A:62:TYR:HB3	2.48	0.43
2:D:83:ASN:HD22	2:D:83:ASN:HA	1.64	0.43
3:G:91:LYS:HG2	3:G:95:TYR:HA	2.01	0.43
1:C:72:MET:O	1:C:76:GLU:HG3	2.18	0.43
2:D:83:ASN:ND2	2:D:84:HIS:H	2.17	0.43
4:H:121:VAL:HG12	4:H:231:PRO:HB2	2.01	0.43
4:H:210:ARG:HG3	4:H:239:GLU:HG2	2.01	0.43
1:A:230:ILE:HD11	4:F:206:ARG:HD3	1.99	0.43
3:G:129:LYS:N	9:G:404:HOH:O	2.52	0.43
3:E:5:ASP:OD1	9:E:401:HOH:O	2.21	0.42
1:C:183:LEU:O	1:C:202:ALA:HA	2.18	0.42
2:D:40:LEU:HD23	2:D:45:ARG:HA	2.00	0.42
1:A:124:LYS:O	1:A:154:LYS:NZ	2.43	0.42
1:A:198:LEU:HG	1:A:246:LEU:CD2	2.50	0.42
3:G:111:ILE:HD13	3:G:111:ILE:HA	1.87	0.42
4:F:206:ARG:NE	7:F:403:GOL:O2	2.53	0.42
2:D:36:GLU:O	2:D:82:VAL:HA	2.19	0.42
4:H:125:GLU:O	4:H:148:ALA:HA	2.20	0.42
1:C:95:MET:CE	2:D:58:LYS:HA	2.50	0.41
2:D:5:PRO:HB3	2:D:30:PHE:HB3	2.02	0.41
3:G:50:VAL:O	3:G:66:ARG:HD3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:184:LEU:HD23	4:H:184:LEU:HA	1.92	0.41
1:C:46[B]:ARG:HD3	1:C:46[B]:ARG:HA	1.84	0.41
1:C:212:MET:HG2	1:C:258:VAL:HG22	2.02	0.41
2:D:38:ASP:OD2	2:D:81:ARG:NH2	2.54	0.41
3:G:117:ALA:HB2	3:G:196:PHE:HB3	2.03	0.41
4:H:95:VAL:HG12	4:H:96:TRP:CD1	2.55	0.41
1:A:33:ILE:HB	1:A:50:MET:HG3	2.03	0.41
1:C:6:ARG:HD2	9:D:205:HOH:O	2.21	0.41
1:C:27:TYR:CG	7:D:101:GOL:H12	2.56	0.41
1:C:149:GLU:OE2	4:F:100:GLY:HA3	2.21	0.41
1:C:210:ILE:HG13	1:C:260:HIS:HB2	2.03	0.41
4:F:174:ASP:HB2	4:F:191:LEU:HD12	2.02	0.41
2:B:64:LEU:HD13	2:B:66:TYR:HE1	1.86	0.41
1:C:37:ASP:OD1	1:C:40:THR:HG23	2.21	0.40
1:A:200:CYS:HB2	1:A:214:TRP:CZ2	2.56	0.40
1:C:169:LEU:HA	1:C:169:LEU:HD23	1.87	0.40
1:A:182:PRO:HB3	1:A:205:PHE:HB3	2.03	0.40
4:F:228:ARG:O	7:F:402:GOL:H12	2.22	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	261/271 (96%)	252 (97%)	8 (3%)	1 (0%)	34	54
1	C	261/271 (96%)	254 (97%)	7 (3%)	0	100	100
2	B	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
2	D	95/100 (95%)	95 (100%)	0	0	100	100
3	E	198/203 (98%)	193 (98%)	5 (2%)	0	100	100
3	G	189/203 (93%)	182 (96%)	6 (3%)	1 (0%)	29	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	F	242/245 (99%)	233 (96%)	9 (4%)	0	100	100
4	H	242/245 (99%)	235 (97%)	7 (3%)	0	100	100
All	All	1586/1638 (97%)	1541 (97%)	43 (3%)	2 (0%)	51	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	247	ASP
3	G	81	LYS

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	226/241 (94%)	223 (99%)	3 (1%)	69	87
1	C	221/241 (92%)	217 (98%)	4 (2%)	59	81
2	B	89/95 (94%)	87 (98%)	2 (2%)	52	77
2	D	77/95 (81%)	75 (97%)	2 (3%)	46	72
3	E	169/180 (94%)	169 (100%)	0	100	100
3	G	141/180 (78%)	139 (99%)	2 (1%)	67	86
4	F	200/211 (95%)	198 (99%)	2 (1%)	76	90
4	H	192/211 (91%)	190 (99%)	2 (1%)	76	90
All	All	1315/1454 (90%)	1298 (99%)	17 (1%)	71	87

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	ASP
1	A	73	PHE
1	A	246	LEU
2	B	0	MET
2	B	70	PHE

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Mol	Chain	Res	Type
3	G	170[A]	SER
3	G	170[B]	SER
4	H	172	CYS
4	H	194	ARG
1	C	73	PHE
1	C	82	ARG
1	C	147	GLN
1	C	188	ARG
2	D	70	PHE
2	D	83	ASN
4	F	22	GLN
4	F	194	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	13	HIS
3	G	96	GLN
4	H	120	ASN
1	C	147	GLN
1	C	264	HIS
2	D	83	ASN
3	E	188	ASN
4	F	208	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry

21 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	$\# Z > 2$
7	GOL	D	101	-	5,5,5	0.84	0	5,5,5	0.96	0
6	N36	C	302	1	11,11,12	0.58	0	14,14,15	0.51	0
7	GOL	A	305	-	5,5,5	0.84	0	5,5,5	1.05	0
5	PRO	A	301	-	5,7,8	0.62	0	7,8,10	1.41	1 (14%)
7	GOL	E	302	-	5,5,5	1.08	0	5,5,5	1.04	0
8	ACT	C	304	-	3,3,3	0.96	0	3,3,3	0.48	0
7	GOL	G	301	-	5,5,5	1.16	0	5,5,5	0.81	0
8	ACT	C	303	-	3,3,3	1.30	1 (33%)	3,3,3	0.41	0
7	GOL	A	304	-	5,5,5	1.28	1 (20%)	5,5,5	0.73	0
7	GOL	A	303	-	5,5,5	1.38	2 (40%)	5,5,5	0.87	0
7	GOL	B	102	-	5,5,5	0.93	0	5,5,5	0.98	0
7	GOL	C	307	-	5,5,5	0.93	0	5,5,5	0.99	0
7	GOL	F	403	-	5,5,5	0.10	0	5,5,5	0.28	0
8	ACT	F	401	-	3,3,3	0.99	0	3,3,3	0.54	0
5	PRO	C	301	-	5,7,8	0.59	0	7,8,10	1.51	1 (14%)
7	GOL	C	305	-	5,5,5	0.77	0	5,5,5	1.18	0
7	GOL	B	101	-	5,5,5	0.75	0	5,5,5	1.20	0
6	N36	A	302	1	11,11,12	0.53	0	14,14,15	0.50	0
8	ACT	E	301	-	3,3,3	1.01	0	3,3,3	0.57	0
7	GOL	C	306	-	5,5,5	1.34	1 (20%)	5,5,5	0.96	0
7	GOL	F	402	-	5,5,5	0.74	0	5,5,5	1.14	1 (20%)

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
7	GOL	B	102	-	-	2/4/4/4	-
7	GOL	D	101	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	N36	C	302	1	-	0/3/3/5	0/1/1/1
7	GOL	C	305	-	-	2/4/4/4	-
7	GOL	A	305	-	-	2/4/4/4	-
5	PRO	A	301	-	-	0/0/9/11	0/1/1/1
7	GOL	C	307	-	-	2/4/4/4	-
7	GOL	E	302	-	-	2/4/4/4	-
7	GOL	G	301	-	-	2/4/4/4	-
7	GOL	B	101	-	-	3/4/4/4	-
7	GOL	F	403	-	-	0/4/4/4	-
7	GOL	A	304	-	-	0/4/4/4	-
6	N36	A	302	1	-	0/3/3/5	0/1/1/1
5	PRO	C	301	-	-	0/0/9/11	0/1/1/1
7	GOL	A	303	-	-	4/4/4/4	-
7	GOL	C	306	-	-	3/4/4/4	-
7	GOL	F	402	-	-	0/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	304	GOL	C3-C2	2.32	1.61	1.51
7	A	303	GOL	C1-C2	2.24	1.60	1.51
8	C	303	ACT	CH3-C	2.23	1.58	1.49
7	C	306	GOL	C3-C2	2.12	1.60	1.51
7	A	303	GOL	C3-C2	2.01	1.60	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	301	PRO	O-C-CA	-2.71	117.67	124.78
5	A	301	PRO	O-C-CA	-2.54	118.12	124.78
7	F	402	GOL	C3-C2-C1	-2.11	103.50	111.70

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	303	GOL	O1-C1-C2-C3
7	A	303	GOL	C1-C2-C3-O3
7	B	101	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
7	B	101	GOL	O2-C2-C3-O3
7	B	102	GOL	C1-C2-C3-O3
7	G	301	GOL	C1-C2-C3-O3
7	G	301	GOL	O2-C2-C3-O3
7	C	305	GOL	C1-C2-C3-O3
7	C	305	GOL	O2-C2-C3-O3
7	C	307	GOL	O1-C1-C2-C3
7	E	302	GOL	O1-C1-C2-C3
7	E	302	GOL	O1-C1-C2-O2
7	A	305	GOL	O1-C1-C2-C3
7	A	303	GOL	O1-C1-C2-O2
7	A	303	GOL	O2-C2-C3-O3
7	C	307	GOL	O1-C1-C2-O2
7	A	305	GOL	O1-C1-C2-O2
7	C	306	GOL	O1-C1-C2-O2
7	C	306	GOL	O2-C2-C3-O3
7	B	102	GOL	O2-C2-C3-O3
7	C	306	GOL	O1-C1-C2-C3
7	B	101	GOL	O1-C1-C2-C3

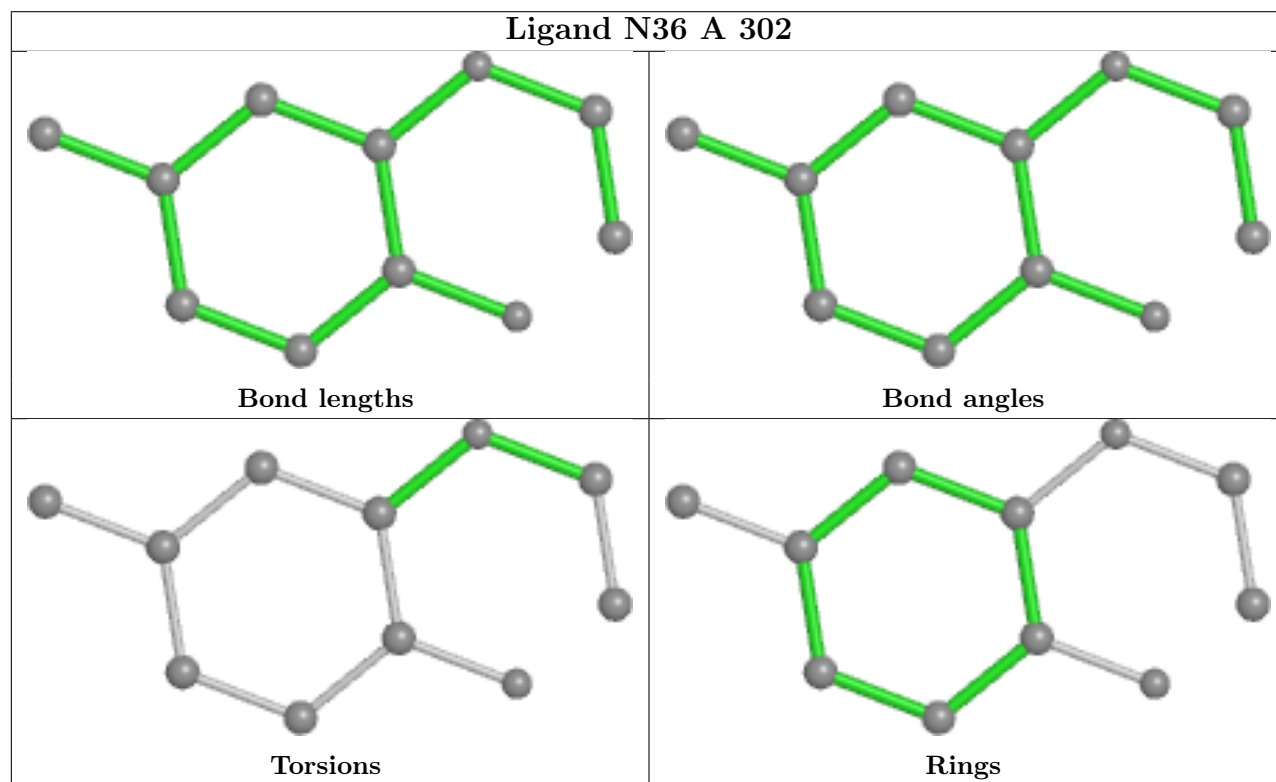
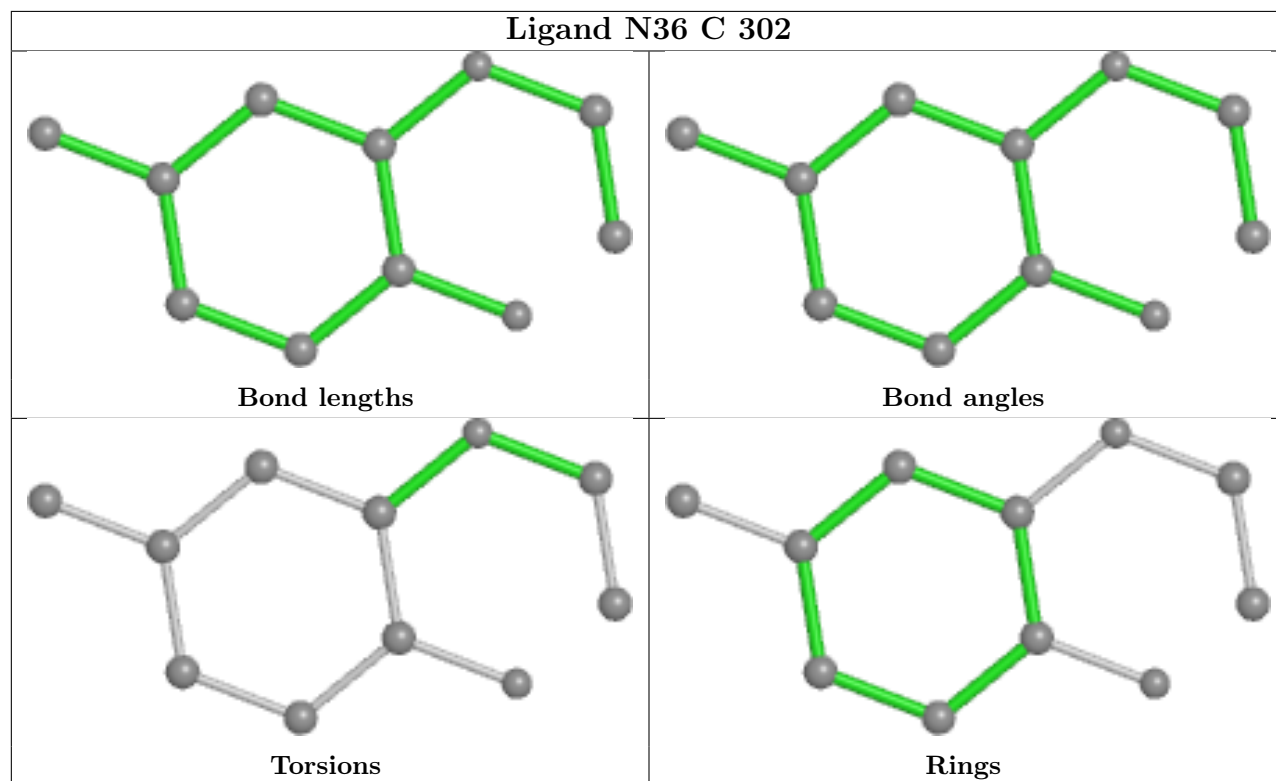
There are no ring outliers.

8 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	101	GOL	1	0
7	A	305	GOL	1	0
7	E	302	GOL	2	0
7	F	403	GOL	1	0
8	F	401	ACT	1	0
5	C	301	PRO	1	0
7	C	305	GOL	1	0
7	F	402	GOL	1	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	266/271 (98%)	-0.05	3 (1%) 80 82	27, 38, 62, 84	1 (0%)
1	C	264/271 (97%)	0.00	3 (1%) 80 82	28, 40, 72, 88	0
2	B	100/100 (100%)	0.07	3 (3%) 50 53	26, 41, 61, 70	0
2	D	97/100 (97%)	0.85	15 (15%) 2 1	33, 55, 74, 80	0
3	E	200/203 (98%)	0.04	1 (0%) 91 91	29, 40, 62, 76	0
3	G	194/203 (95%)	0.62	28 (14%) 2 2	30, 50, 82, 94	0
4	F	244/245 (99%)	-0.03	0 100 100	30, 39, 57, 81	0
4	H	242/245 (98%)	0.11	6 (2%) 57 61	28, 45, 74, 83	0
All	All	1607/1638 (98%)	0.14	59 (3%) 41 45	26, 41, 73, 94	1 (0%)

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	79	ALA	4.7
3	G	180	PHE	4.5
3	G	117	ALA	4.5
3	G	197	PHE	4.4
2	D	78	TYR	3.9
4	H	227	ASP	3.9
2	D	42	ASN	3.8
3	G	188	ASN	3.7
2	D	0	MET	3.5
2	D	46	ILE	3.4
2	D	76	ASP	3.4
3	G	132	CYS	3.4
3	G	181	ALA	3.3
3	E	200	PRO	3.3
1	A	247	ASP	3.3
3	G	119	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
3	G	196	PHE	3.1
3	G	164	MET	3.1
3	G	1	GLY	3.1
2	D	40	LEU	3.0
3	G	112	GLN	3.0
3	G	198	PRO	2.8
2	D	43	GLY	2.8
3	G	183	ALA	2.8
2	B	0	MET	2.8
1	A	17	HIS	2.7
3	G	134	PHE	2.7
1	A	0	MET	2.7
3	G	114	PRO	2.6
3	G	199	SER	2.6
3	G	148	ASP	2.5
2	D	80	CYS	2.5
4	H	224	TRP	2.4
3	G	192	PRO	2.4
2	D	44	GLU	2.4
2	D	72	PRO	2.4
3	G	158	VAL	2.3
3	G	111	ILE	2.3
1	C	222	VAL	2.3
2	D	82	VAL	2.3
2	D	41	LYS	2.3
3	G	173	ALA	2.3
3	G	137	PHE	2.2
4	H	201	PHE	2.2
4	H	209	PHE	2.2
3	G	146	SER	2.2
2	B	44	GLU	2.2
1	C	226	ASP	2.2
3	G	138	ASP	2.2
3	G	160	ASP	2.2
3	G	149	SER	2.2
3	G	163	SER	2.2
4	H	198	SER	2.1
2	D	77	GLU	2.1
4	H	162	VAL	2.1
2	D	95	TRP	2.0
2	B	99	MET	2.0
3	G	182	CYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	211	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

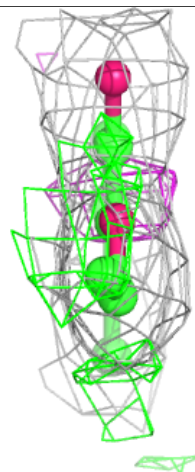
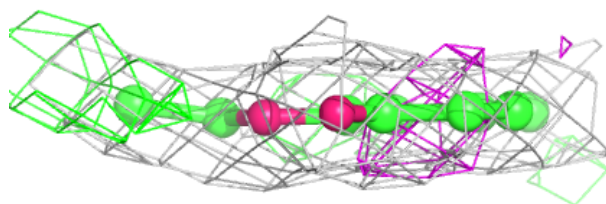
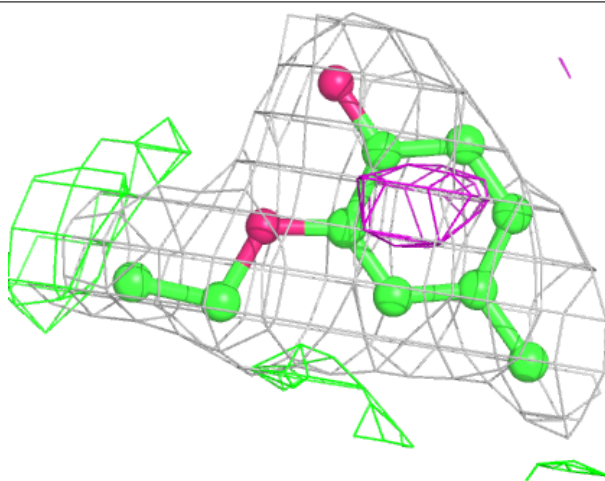
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	GOL	C	307	6/6	0.35	0.51	81,82,87,95	0
7	GOL	C	306	6/6	0.80	0.20	50,52,56,57	0
8	ACT	E	301	4/4	0.80	0.27	54,60,63,66	0
5	PRO	C	301	7/8	0.83	0.35	77,79,94,102	0
5	PRO	A	301	7/8	0.83	0.27	54,69,76,78	0
7	GOL	C	305	6/6	0.84	0.32	47,53,57,60	0
7	GOL	G	301	6/6	0.85	0.19	51,63,69,70	0
8	ACT	C	304	4/4	0.86	0.22	47,61,64,71	0
6	N36	C	302	11/12	0.88	0.21	34,40,50,55	0
7	GOL	A	303	6/6	0.88	0.18	51,54,56,57	0
7	GOL	A	304	6/6	0.88	0.22	40,47,50,52	0
7	GOL	A	305	6/6	0.89	0.30	49,53,59,59	0
8	ACT	C	303	4/4	0.89	0.18	32,47,53,55	0
6	N36	A	302	11/12	0.90	0.17	40,46,48,51	0
7	GOL	E	302	6/6	0.90	0.30	48,52,54,56	0
7	GOL	F	403	6/6	0.90	0.26	37,44,55,57	0
7	GOL	B	102	6/6	0.91	0.33	38,44,47,48	0
8	ACT	F	401	4/4	0.91	0.25	48,51,62,65	0
7	GOL	D	101	6/6	0.92	0.16	49,53,58,61	0
7	GOL	F	402	6/6	0.97	0.20	42,42,50,52	0
7	GOL	B	101	6/6	0.98	0.17	27,33,35,38	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.

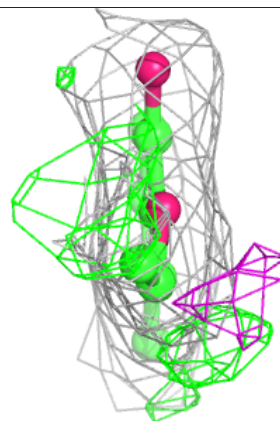
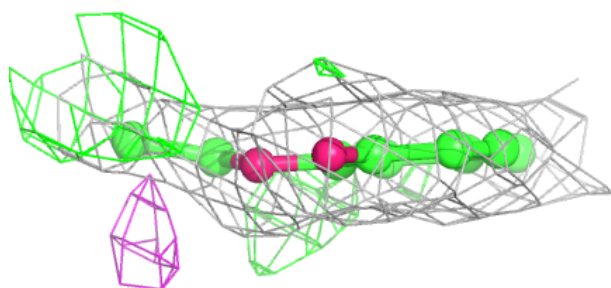
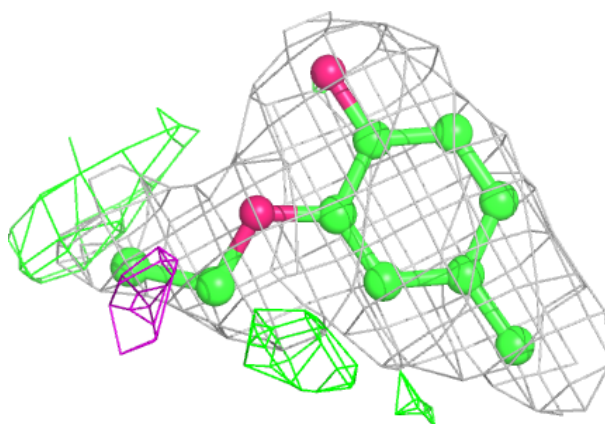
Electron density around N36 C 302:

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



Electron density around N36 A 302:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.