



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:43 AM UTC

PDB ID : 8X7H / pdb_00008x7h
Title : Crystal structure of the ternary complex of GID4-PROTAC(NEP162)-BRD4 (BD1).
Authors : Dong, C.; Yan, X.; Li, Y.
Deposited on : 2023-11-24
Resolution : 2.90 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

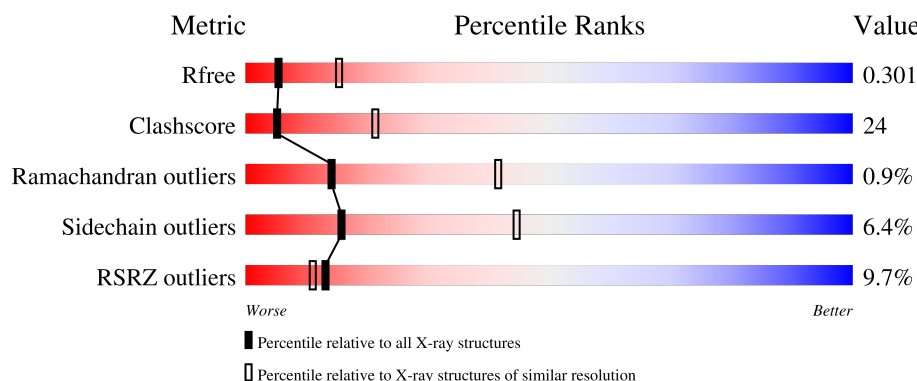
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	167	
1	C	167	
1	E	167	
1	G	167	
2	B	126	

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Mol	Chain	Length	Quality of chain
2	D	126	10% 54% 29% 17%
2	F	126	9% 60% 22% •• 16%
2	H	126	9% 56% 24% • 17%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8411 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 Glucose-induced degradation protein 4 homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	162	Total	C	N	O	S	0	0	0
			1211	788	192	228	3			
1	C	163	Total	C	N	O	S	0	0	0
			1196	775	192	226	3			
1	E	164	Total	C	N	O	S	0	0	0
			1260	821	204	232	3			
1	G	160	Total	C	N	O	S	0	0	0
			1240	805	203	229	3			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	123	GLY	-	expression tag	UNP Q8IVV7
C	123	GLY	-	expression tag	UNP Q8IVV7
E	123	GLY	-	expression tag	UNP Q8IVV7
G	123	GLY	-	expression tag	UNP Q8IVV7

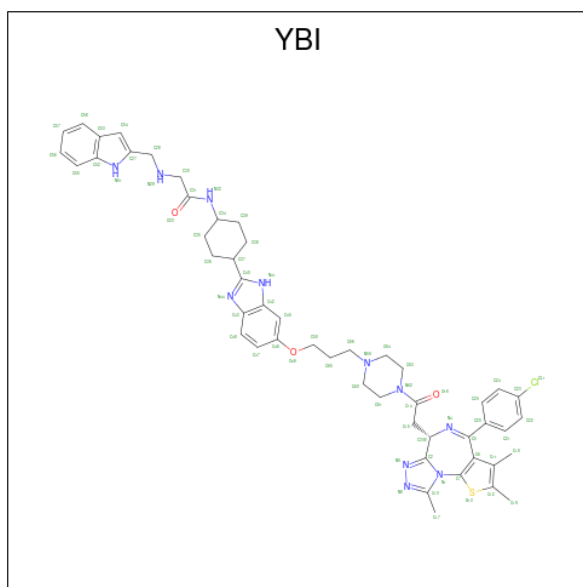
- Molecule 2 is a protein called Bromodomain-containing protein 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	105	Total	C	N	O	S	0	0	0
			800	519	126	149	6			
2	D	105	Total	C	N	O	S	0	0	0
			792	517	122	147	6			
2	F	106	Total	C	N	O	S	0	0	0
			760	487	124	143	6			
2	H	105	Total	C	N	O	S	0	0	0
			776	502	123	145	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	43	GLY	-	expression tag	UNP O60885
D	43	GLY	-	expression tag	UNP O60885
F	43	GLY	-	expression tag	UNP O60885
H	43	GLY	-	expression tag	UNP O60885

- Molecule 3 is {N}-[4-[6-[3-[4-[2-[(9 {S})-7-(4-chlorophenyl)-4,5,13-trimethyl-3-thia-1,8,11,12-tetrazatricyclo[8.3.0.0[^]{2,6}]trideca-2(6),4,7,10,12-pentaen-9-yl]ethanoyl]piperazin-1-yl]propoxy]-1 {H}-benzimidazol-2-yl]cyclohexyl]-2-(1 {H}-indol-2-ylmethylamino)ethanamide (CCD ID: YBI) (formula: C₅₀H₅₆ClN₁₁O₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	S	0	0
			66	50	1	11	3	1		
3	C	1	Total	C	Cl	N	O	S	0	0
			66	50	1	11	3	1		
3	E	1	Total	C	Cl	N	O	S	0	0
			66	50	1	11	3	1		
3	G	1	Total	C	Cl	N	O	S	0	0
			66	50	1	11	3	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	11	Total	O	0	0
			11	11		
5	B	11	Total	O	0	0
			11	11		
5	C	10	Total	O	0	0
			10	10		
5	D	12	Total	O	0	0
			12	12		

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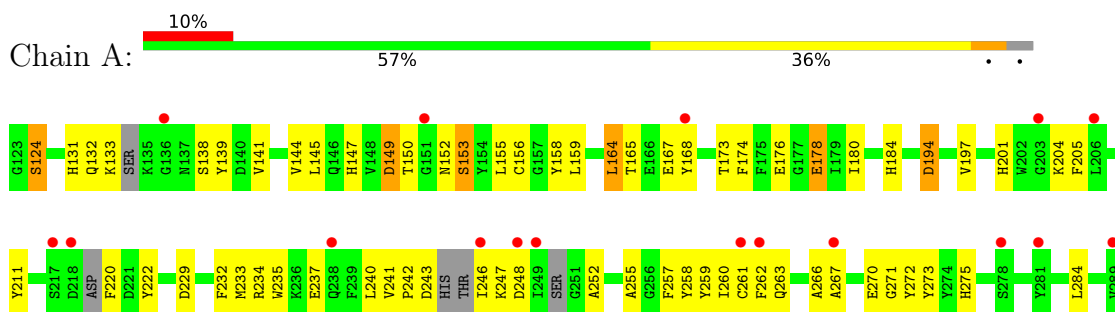
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	7	Total	O	0	0
			7	7		
5	F	4	Total	O	0	0
			4	4		
5	G	6	Total	O	0	0
			6	6		
5	H	3	Total	O	0	0
			3	3		

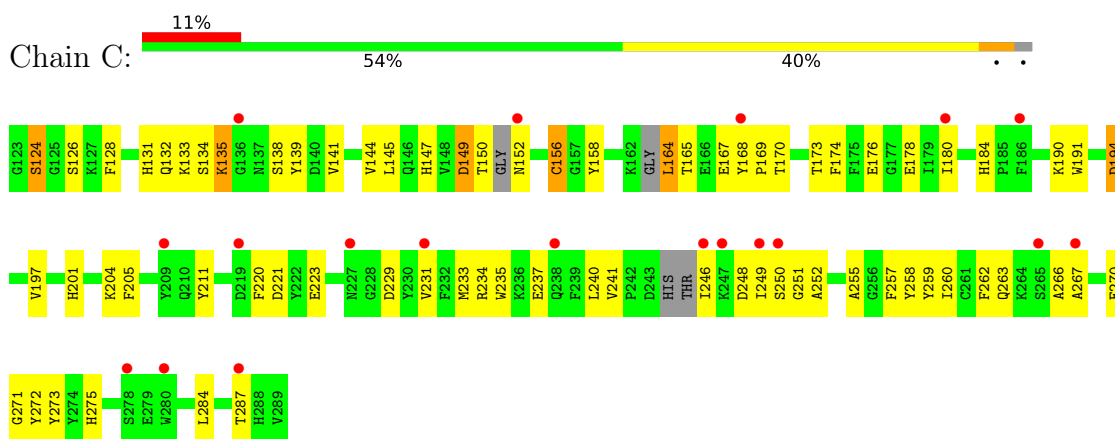
3 Residue-property plots [i](#)

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.

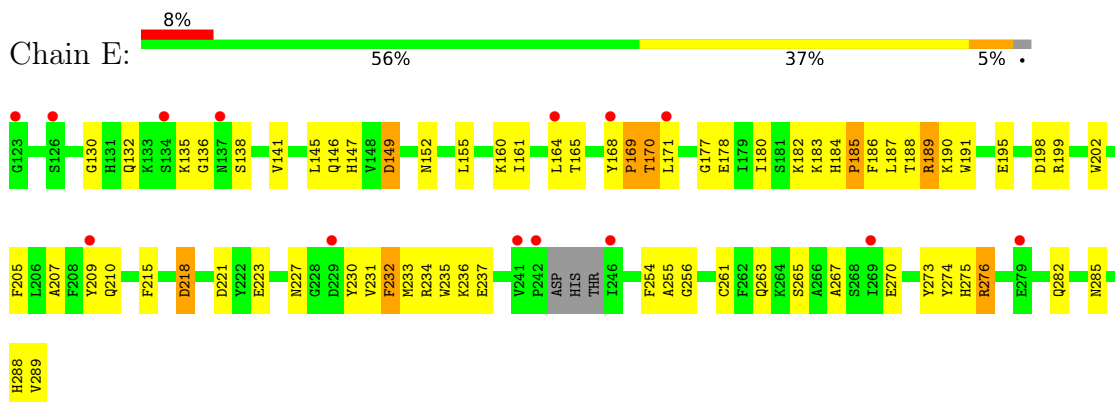
- Molecule 1: Glucose-induced degradation protein 4 homolog



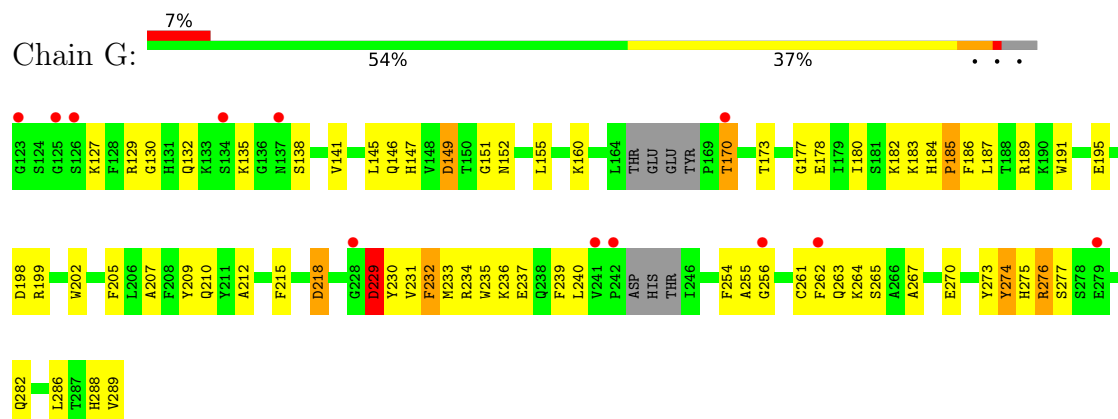
- Molecule 1: Glucose-induced degradation protein 4 homolog



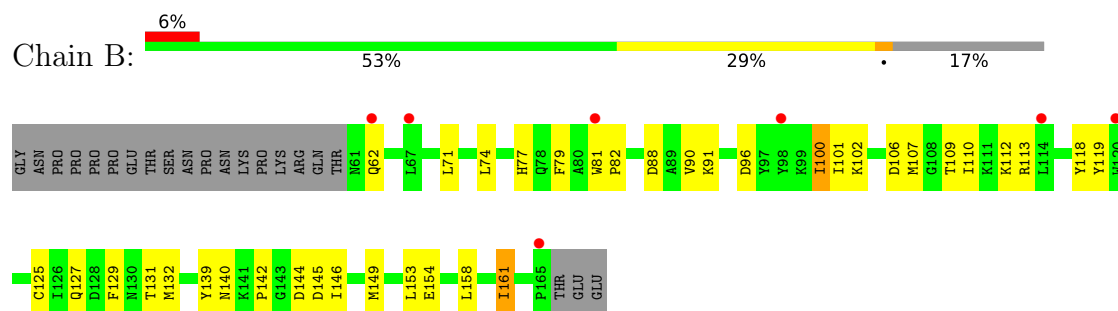
- Molecule 1: Glucose-induced degradation protein 4 homolog



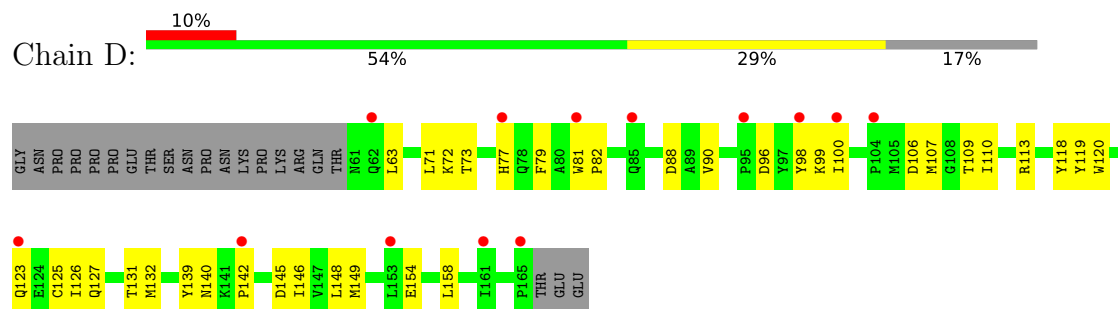
- Molecule 1: Glucose-induced degradation protein 4 homolog



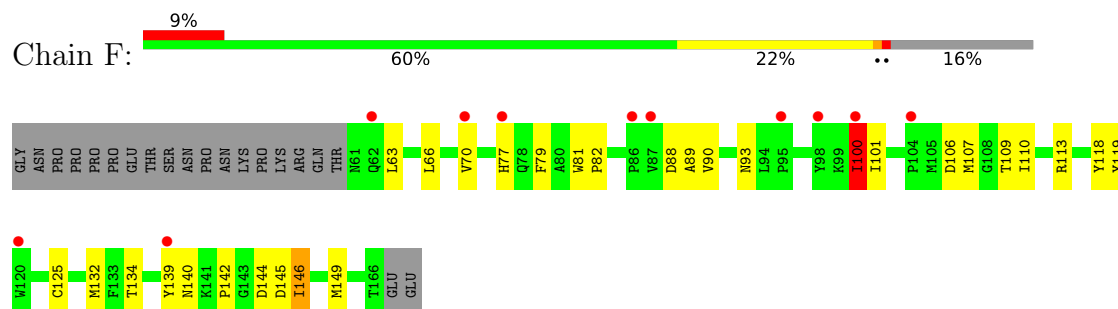
- Molecule 2: Bromodomain-containing protein 4



- Molecule 2: Bromodomain-containing protein 4

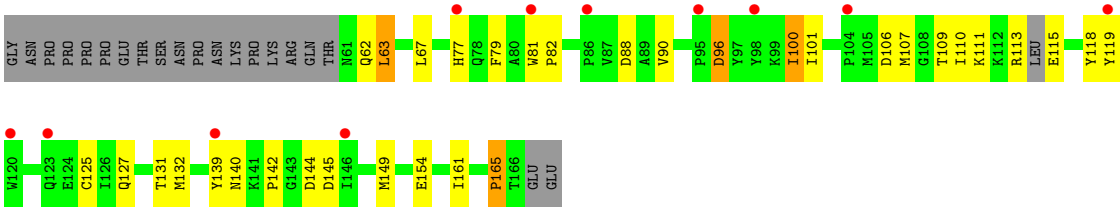


- Molecule 2: Bromodomain-containing protein 4



- Molecule 2: Bromodomain-containing protein 4





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	56.85Å 87.61Å 88.44Å 103.09° 90.90° 106.23°	Depositor
Resolution (Å)	38.46 – 2.90 38.46 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.1 (38.46-2.90) 97.1 (38.46-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 2.90Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.235 , 0.301 0.244 , 0.301	Depositor DCC
R_{free} test set	1718 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	59.9	Xtriage
Anisotropy	0.456	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 117.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8411	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.27% 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: GOL, YBI

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	0.64	0/1248	0.94	0/1700
1	C	0.66	0/1232	0.99	0/1685
1	E	0.77	0/1301	1.12	7/1771 (0.4%)
1	G	0.77	0/1278	1.17	7/1734 (0.4%)
2	B	0.64	0/824	1.00	1/1132 (0.1%)
2	D	0.61	0/816	1.02	3/1124 (0.3%)
2	F	0.60	0/780	0.98	2/1072 (0.2%)
2	H	0.60	0/796	1.04	2/1092 (0.2%)
All	All	0.68	0/8275	1.04	22/11310 (0.2%)

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	G	0	2

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	135	LYS	N-CA-C	-9.87	99.63	114.64
1	G	135	LYS	N-CA-C	-7.92	102.68	113.30
2	F	63	LEU	N-CA-C	-7.53	103.06	111.71
2	H	63	LEU	N-CA-C	-7.27	103.35	111.71
1	G	232	PHE	CA-C-N	-6.39	111.60	123.03
1	G	232	PHE	C-N-CA	-6.39	111.60	123.03
1	E	232	PHE	CA-C-N	-6.37	111.63	123.03
1	E	232	PHE	C-N-CA	-6.37	111.63	123.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	161	ILE	N-CA-C	-6.20	103.89	112.50
1	G	274	TYR	CB-CA-C	-6.14	100.85	110.74
1	G	229	ASP	N-CA-C	-5.98	105.64	113.17
2	D	63	LEU	N-CA-C	-5.76	105.14	111.82
2	H	165	PRO	N-CA-CB	-5.71	97.25	103.25
1	E	185	PRO	N-CA-C	5.66	119.42	111.33
1	G	185	PRO	N-CA-C	5.65	119.41	111.33
2	D	99	LYS	N-CA-C	-5.41	106.69	113.72
2	F	100	ILE	CA-C-O	-5.28	116.21	120.70
1	E	276	ARG	N-CA-CB	5.24	119.35	110.49
2	D	98	TYR	N-CA-C	-5.14	106.85	113.02
1	G	276	ARG	N-CA-CB	5.03	118.98	110.49
1	E	136	GLY	CA-C-N	-5.01	113.64	121.87
1	E	136	GLY	C-N-CA	-5.01	113.64	121.87

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	129	ARG	Sidechain
1	G	189	ARG	Sidechain

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	1211	0	958	61	0
1	C	1196	0	909	58	0
1	E	1260	0	1040	74	0
1	G	1240	0	1039	64	0
2	B	800	0	671	36	0
2	D	792	0	659	38	0
2	F	760	0	608	23	0
2	H	776	0	648	27	0
3	A	66	0	0	4	0
3	C	66	0	0	2	0
3	E	66	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	66	0	0	0	0
4	B	6	0	8	1	0
4	D	24	0	31	1	0
4	G	12	0	16	0	0
4	H	6	0	8	0	0
5	A	11	0	0	0	0
5	B	11	0	0	1	0
5	C	10	0	0	1	0
5	D	12	0	0	1	0
5	E	7	0	0	2	0
5	F	4	0	0	0	0
5	G	6	0	0	1	0
5	H	3	0	0	1	0
All	All	8411	0	6595	366	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 24.

All (366) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:155:LEU:HD22	1:E:233:MET:HE2	1.45	0.98
1:G:180:ILE:HG12	1:G:232:PHE:O	1.64	0.97
1:E:180:ILE:HG12	1:E:232:PHE:O	1.64	0.96
1:G:155:LEU:HD22	1:G:233:MET:HE2	1.45	0.95
1:A:205:PHE:HE1	1:A:270:GLU:HG2	1.36	0.90
1:C:205:PHE:HE1	1:C:270:GLU:HG2	1.36	0.89
1:C:233:MET:HE3	1:C:235:TRP:HE1	1.40	0.87
1:G:155:LEU:CD2	1:G:233:MET:HE2	2.06	0.85
1:A:233:MET:HE3	1:A:235:TRP:HE1	1.40	0.84
1:E:155:LEU:CD2	1:E:233:MET:HE2	2.06	0.84
2:H:67:LEU:HD11	5:H:301:HOH:O	1.78	0.83
1:C:124:SER:HB3	1:C:147:HIS:HA	1.59	0.83
1:C:252:ALA:HA	1:C:255:ALA:HB2	1.61	0.82
2:F:109:THR:O	2:F:113:ARG:HG3	1.79	0.82
2:D:109:THR:O	2:D:113:ARG:HG3	1.79	0.82
2:B:109:THR:O	2:B:113:ARG:HG3	1.79	0.81
2:H:109:THR:O	2:H:113:ARG:HG3	1.79	0.81
1:A:124:SER:HB3	1:A:147:HIS:HA	1.64	0.78
1:G:230:TYR:HB2	5:G:403:HOH:O	1.84	0.77
1:E:188:THR:HG22	1:E:190:LYS:HG3	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:LYS:HB3	1:A:272:TYR:HE2	1.53	0.74
1:E:218:ASP:N	1:E:218:ASP:OD1	2.20	0.73
1:A:252:ALA:HA	1:A:255:ALA:HB2	1.70	0.72
1:E:188:THR:HG22	1:E:190:LYS:CG	2.19	0.72
2:B:106:ASP:OD2	2:B:109:THR:N	2.21	0.72
2:D:149:MET:HE3	1:E:169:PRO:HG3	1.72	0.71
1:C:271:GLY:O	1:C:272:TYR:HD1	1.74	0.71
2:D:154:GLU:CD	1:G:147:HIS:HD1	1.99	0.71
1:A:271:GLY:O	1:A:272:TYR:HD1	1.74	0.70
2:D:79:PHE:HZ	1:E:165:THR:HA	1.57	0.70
2:F:106:ASP:OD2	2:F:109:THR:N	2.21	0.70
1:G:191:TRP:CZ2	1:G:236:LYS:HG3	2.27	0.69
1:E:191:TRP:CZ2	1:E:236:LYS:HG3	2.27	0.69
1:G:202:TRP:O	1:G:205:PHE:HB2	1.93	0.68
2:B:71:LEU:C	2:B:71:LEU:HD23	2.17	0.68
1:A:211:TYR:HB3	1:A:220:PHE:HE2	1.59	0.68
1:E:202:TRP:O	1:E:205:PHE:HB2	1.93	0.67
1:C:126:SER:HB3	1:C:128:PHE:CE1	2.30	0.67
1:G:149:ASP:OD2	1:G:152:ASN:HB2	1.95	0.67
1:A:204:LYS:HB3	1:A:272:TYR:CE2	2.29	0.66
2:H:106:ASP:OD2	2:H:109:THR:N	2.21	0.66
2:F:66:LEU:HA	2:F:70:VAL:HB	1.76	0.66
1:C:211:TYR:HB3	1:C:220:PHE:HE2	1.60	0.66
2:D:123:GLN:NE2	2:D:126:ILE:HD11	2.11	0.66
1:A:233:MET:HE3	1:A:235:TRP:NE1	2.11	0.65
2:D:154:GLU:OE2	1:G:147:HIS:ND1	2.23	0.65
1:E:149:ASP:OD2	1:E:152:ASN:HB2	1.95	0.65
1:A:178:GLU:HB3	1:A:184:HIS:ND1	2.12	0.64
1:E:230:TYR:CE1	1:E:263:GLN:HG3	2.33	0.64
1:G:230:TYR:CE1	1:G:263:GLN:HG3	2.33	0.64
1:G:273:TYR:CE1	1:G:275:HIS:HB2	2.33	0.64
1:G:218:ASP:OD1	1:G:218:ASP:N	2.20	0.64
1:A:194:ASP:OD1	1:A:194:ASP:N	2.30	0.64
1:G:160:LYS:HE3	1:G:170:THR:HG21	1.77	0.64
2:D:106:ASP:OD2	2:D:109:THR:N	2.21	0.64
1:C:233:MET:HE3	1:C:235:TRP:NE1	2.11	0.63
1:E:256:GLY:HA3	1:E:273:TYR:CE1	2.33	0.63
1:G:256:GLY:HA3	1:G:273:TYR:CE1	2.33	0.63
1:E:267:ALA:HB1	1:E:288:HIS:HB2	1.80	0.63
1:A:153:SER:O	1:A:153:SER:OG	2.09	0.63
1:C:178:GLU:HB3	1:C:184:HIS:ND1	2.12	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:227:ASN:HA	5:E:405:HOH:O	1.98	0.63
1:C:165:THR:HG23	1:C:168:TYR:H	1.64	0.62
1:E:230:TYR:HB2	5:E:403:HOH:O	1.98	0.62
2:B:113:ARG:HB3	2:B:118:TYR:CD2	2.35	0.62
2:D:113:ARG:HB3	2:D:118:TYR:CD2	2.35	0.62
2:H:113:ARG:HB3	2:H:118:TYR:CD2	2.35	0.62
2:B:154:GLU:CD	1:E:147:HIS:HD1	2.08	0.62
1:C:190:LYS:HG2	1:C:191:TRP:N	2.15	0.61
1:C:194:ASP:OD1	1:C:194:ASP:N	2.30	0.61
2:F:113:ARG:HB3	2:F:118:TYR:CD2	2.35	0.61
1:E:273:TYR:HD1	1:E:274:TYR:N	1.99	0.61
1:E:155:LEU:HD22	1:E:233:MET:CE	2.26	0.61
1:C:275:HIS:ND1	1:C:275:HIS:O	2.33	0.61
1:G:229:ASP:HA	1:G:264:LYS:HD3	1.82	0.60
2:H:88:ASP:OD2	2:H:90:VAL:HG22	2.02	0.60
1:A:263:GLN:HG2	1:A:266:ALA:HB3	1.84	0.60
1:C:178:GLU:HB3	1:C:184:HIS:CE1	2.36	0.60
2:F:88:ASP:OD2	2:F:90:VAL:HG22	2.02	0.60
1:A:178:GLU:HB3	1:A:184:HIS:CE1	2.36	0.60
1:A:275:HIS:O	1:A:275:HIS:ND1	2.33	0.60
1:A:273:TYR:HE2	1:A:275:HIS:HB2	1.67	0.60
1:C:204:LYS:CB	5:C:405:HOH:O	2.50	0.60
1:C:273:TYR:HE2	1:C:275:HIS:HB2	1.67	0.60
2:D:88:ASP:OD2	2:D:90:VAL:HG22	2.02	0.60
1:C:263:GLN:HG2	1:C:266:ALA:HB3	1.84	0.60
1:C:134:SER:O	1:C:135:LYS:C	2.44	0.59
2:D:123:GLN:CD	2:D:126:ILE:HD11	2.27	0.59
1:A:242:PRO:O	1:A:243:ASP:HB2	2.02	0.59
1:E:190:LYS:HD2	1:E:191:TRP:CE3	2.38	0.59
2:B:88:ASP:OD2	2:B:90:VAL:HG22	2.02	0.59
5:B:304:HOH:O	1:E:146:GLN:HG2	2.02	0.59
2:D:107:MET:HG3	2:D:132:MET:SD	2.43	0.59
1:G:155:LEU:HD22	1:G:233:MET:CE	2.26	0.59
1:A:174:PHE:HE1	1:A:176:GLU:HG2	1.68	0.58
2:H:107:MET:HG3	2:H:132:MET:SD	2.43	0.58
1:C:174:PHE:HE1	1:C:176:GLU:HG2	1.68	0.58
2:H:100:ILE:HD11	2:H:139:TYR:HD1	1.68	0.58
1:E:152:ASN:O	1:E:183:LYS:NZ	2.36	0.58
2:B:74:LEU:HD23	2:B:153:LEU:HD22	1.85	0.58
2:B:107:MET:HG3	2:B:132:MET:SD	2.43	0.58
1:C:246:ILE:O	1:C:246:ILE:HD12	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:107:MET:HG3	2:F:132:MET:SD	2.43	0.57
1:G:230:TYR:HE1	1:G:263:GLN:HE21	1.52	0.57
1:E:230:TYR:HE1	1:E:263:GLN:HE21	1.52	0.57
1:A:220:PHE:HE1	1:A:222:TYR:HA	1.68	0.57
1:A:246:ILE:HD12	1:A:246:ILE:O	2.04	0.57
2:D:127:GLN:HE21	1:G:151:GLY:HA3	1.70	0.57
2:H:142:PRO:C	2:H:144:ASP:H	2.13	0.57
2:F:113:ARG:HB3	2:F:118:TYR:HD2	1.70	0.56
2:D:113:ARG:HB3	2:D:118:TYR:HD2	1.70	0.56
2:B:113:ARG:HB3	2:B:118:TYR:HD2	1.70	0.56
2:B:145:ASP:O	2:B:149:MET:HG3	2.06	0.56
1:G:152:ASN:O	1:G:183:LYS:NZ	2.36	0.56
1:C:211:TYR:HB3	1:C:220:PHE:CE2	2.40	0.56
1:C:240:LEU:HD23	1:C:241:VAL:O	2.05	0.56
2:D:145:ASP:O	2:D:149:MET:HG3	2.06	0.56
2:B:100:ILE:HG13	2:B:101:ILE:H	1.71	0.56
2:B:140:ASN:OD1	2:B:146:ILE:HG21	2.06	0.55
1:G:155:LEU:HD21	1:G:177:GLY:HA3	1.89	0.55
3:A:301:YBI:C25	2:B:146:ILE:HD13	2.36	0.55
2:D:145:ASP:HB3	1:E:169:PRO:HG2	1.87	0.55
1:E:188:THR:OG1	1:E:234:ARG:NH1	2.40	0.55
2:H:113:ARG:HB3	2:H:118:TYR:HD2	1.70	0.55
1:A:240:LEU:HD23	1:A:241:VAL:O	2.05	0.55
1:E:178:GLU:O	1:E:233:MET:HB3	2.07	0.55
1:E:155:LEU:CD2	1:E:177:GLY:HA3	2.37	0.55
1:G:191:TRP:CE2	1:G:236:LYS:HG3	2.41	0.55
1:C:149:ASP:OD1	1:C:152:ASN:N	2.40	0.55
1:C:221:ASP:C	1:C:223:GLU:N	2.64	0.55
1:G:267:ALA:HB1	1:G:288:HIS:HB2	1.89	0.55
1:G:273:TYR:HD1	1:G:274:TYR:N	2.05	0.55
1:G:155:LEU:CD2	1:G:177:GLY:HA3	2.37	0.54
1:G:178:GLU:O	1:G:233:MET:HB3	2.07	0.54
1:A:149:ASP:OD1	1:A:152:ASN:N	2.40	0.54
2:B:74:LEU:HD12	2:B:129:PHE:HE2	1.72	0.54
1:C:263:GLN:HG2	1:C:266:ALA:CB	2.37	0.54
1:A:204:LYS:HD2	1:A:272:TYR:CE2	2.42	0.54
1:A:263:GLN:HG2	1:A:266:ALA:CB	2.37	0.54
1:A:173:THR:OG1	1:A:237:GLU:HG2	2.07	0.54
1:E:155:LEU:HD21	1:E:177:GLY:HA3	1.89	0.54
1:E:191:TRP:CE2	1:E:236:LYS:HG3	2.42	0.54
1:G:254:PHE:O	1:G:254:PHE:CD1	2.61	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:SER:HB3	1:C:128:PHE:HE1	1.70	0.54
1:C:173:THR:OG1	1:C:237:GLU:HG2	2.07	0.54
2:F:142:PRO:C	2:F:144:ASP:H	2.16	0.54
2:B:139:TYR:C	2:B:140:ASN:HD22	2.17	0.53
1:E:207:ALA:O	1:E:210:GLN:HG3	2.08	0.53
1:E:254:PHE:O	1:E:254:PHE:CD1	2.61	0.53
1:C:174:PHE:CE1	1:C:176:GLU:HG2	2.44	0.53
2:D:127:GLN:NE2	1:G:151:GLY:HA3	2.24	0.53
1:G:207:ALA:O	1:G:210:GLN:HG3	2.08	0.53
2:H:139:TYR:C	2:H:140:ASN:HD22	2.17	0.53
1:A:133:LYS:HA	1:A:138:SER:HA	1.91	0.52
1:E:188:THR:HG22	1:E:190:LYS:HG2	1.92	0.52
1:C:205:PHE:CE1	1:C:270:GLU:HG2	2.28	0.52
1:G:255:ALA:HB3	1:G:275:HIS:NE2	2.24	0.52
1:A:174:PHE:CE1	1:A:176:GLU:HG2	2.44	0.52
1:C:158:TYR:CE1	1:C:174:PHE:HD2	2.27	0.52
2:F:139:TYR:C	2:F:140:ASN:HD22	2.17	0.52
1:G:130:GLY:HA3	1:G:286:LEU:HD23	1.91	0.52
1:A:158:TYR:CE1	1:A:174:PHE:HD2	2.28	0.52
1:E:205:PHE:HE2	1:E:270:GLU:HG2	1.75	0.52
2:D:139:TYR:C	2:D:140:ASN:HD22	2.17	0.51
1:A:220:PHE:CE1	1:A:222:TYR:HA	2.44	0.51
1:G:205:PHE:HE2	1:G:270:GLU:HG2	1.75	0.51
1:G:149:ASP:OD1	1:G:149:ASP:C	2.54	0.51
1:E:149:ASP:OD1	1:E:149:ASP:C	2.54	0.51
2:H:67:LEU:HD21	2:H:115:GLU:N	2.25	0.51
1:A:141:VAL:HG21	1:A:284:LEU:HD11	1.93	0.50
1:A:167:GLU:OE1	3:A:301:YBI:N59	2.44	0.50
1:C:141:VAL:HG21	1:C:284:LEU:HD11	1.93	0.50
2:F:145:ASP:O	2:F:149:MET:HG3	2.12	0.50
2:H:81:TRP:CG	2:H:82:PRO:HD3	2.47	0.50
3:C:301:YBI:C25	2:D:146:ILE:HD13	2.40	0.50
1:C:221:ASP:C	1:C:223:GLU:H	2.17	0.50
1:A:205:PHE:CE1	1:A:270:GLU:HG2	2.28	0.50
1:A:259:TYR:O	1:A:260:ILE:HD13	2.12	0.50
2:D:81:TRP:CG	2:D:82:PRO:HD3	2.47	0.50
1:C:259:TYR:O	1:C:260:ILE:HD13	2.12	0.50
1:E:182:LYS:O	1:E:185:PRO:HD3	2.12	0.50
1:C:131:HIS:HA	1:C:139:TYR:O	2.12	0.49
2:F:81:TRP:CG	2:F:82:PRO:HD3	2.47	0.49
2:F:140:ASN:OD1	2:F:146:ILE:HG21	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:81:TRP:CG	2:B:82:PRO:HD3	2.47	0.49
2:D:140:ASN:OD1	2:D:146:ILE:HG21	2.11	0.49
1:E:231:VAL:O	1:E:231:VAL:HG13	2.13	0.49
1:A:156:CYS:HA	1:A:176:GLU:HA	1.93	0.49
2:B:100:ILE:HG13	2:B:101:ILE:N	2.28	0.49
1:C:133:LYS:HA	1:C:138:SER:HA	1.93	0.49
1:C:263:GLN:O	1:C:267:ALA:N	2.46	0.49
1:A:131:HIS:HA	1:A:139:TYR:O	2.12	0.49
1:A:263:GLN:O	1:A:267:ALA:N	2.46	0.49
1:E:209:TYR:O	1:E:210:GLN:C	2.56	0.49
1:G:132:GLN:O	1:G:138:SER:HA	2.13	0.49
5:D:305:HOH:O	1:G:146:GLN:HG2	2.11	0.48
1:G:209:TYR:O	1:G:210:GLN:C	2.56	0.48
1:G:182:LYS:O	1:G:185:PRO:HD3	2.12	0.48
1:G:231:VAL:HG13	1:G:231:VAL:O	2.12	0.48
1:C:229:ASP:OD1	1:C:263:GLN:NE2	2.46	0.48
1:E:191:TRP:CZ2	1:E:236:LYS:CG	2.96	0.48
1:A:229:ASP:OD1	1:A:263:GLN:NE2	2.46	0.48
2:B:154:GLU:OE2	1:E:147:HIS:ND1	2.32	0.48
1:G:186:PHE:O	1:G:187:LEU:C	2.57	0.48
2:H:132:MET:HE2	2:H:132:MET:HB3	1.75	0.48
1:G:173:THR:HG22	1:G:240:LEU:HD12	1.95	0.48
1:G:185:PRO:O	1:G:234:ARG:NH2	2.47	0.48
2:H:100:ILE:HG13	2:H:101:ILE:H	1.79	0.48
2:B:88:ASP:OD1	2:B:91:LYS:HB2	2.13	0.48
2:D:77:HIS:CD2	2:D:79:PHE:H	2.32	0.48
1:A:164:LEU:HD11	3:A:301:YBI:N41	2.29	0.48
1:C:271:GLY:O	1:C:272:TYR:CD1	2.62	0.48
2:D:142:PRO:HD2	1:G:239:PHE:HZ	1.79	0.47
2:H:77:HIS:CD2	2:H:79:PHE:H	2.32	0.47
2:B:109:THR:HG23	2:B:112:LYS:HE2	1.96	0.47
1:E:132:GLN:O	1:E:138:SER:HA	2.14	0.47
1:A:165:THR:HG23	1:A:168:TYR:H	1.80	0.47
1:C:156:CYS:HA	1:C:176:GLU:HA	1.95	0.47
1:E:232:PHE:HD1	1:E:261:CYS:HB2	1.80	0.47
1:G:236:LYS:HD3	1:G:237:GLU:N	2.29	0.47
1:G:191:TRP:CZ2	1:G:236:LYS:CG	2.96	0.47
2:B:112:LYS:HG3	2:B:113:ARG:N	2.29	0.47
1:E:236:LYS:HD3	1:E:237:GLU:N	2.29	0.47
1:G:178:GLU:HB3	1:G:184:HIS:CD2	2.50	0.47
1:E:130:GLY:HA3	1:E:285:ASN:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:77:HIS:CD2	2:F:79:PHE:H	2.32	0.47
1:G:262:PHE:HE2	1:G:264:LYS:HG2	1.78	0.47
1:G:232:PHE:HD1	1:G:261:CYS:HB2	1.79	0.47
1:A:271:GLY:C	1:A:272:TYR:CD1	2.93	0.47
2:F:100:ILE:HD11	2:F:139:TYR:HD1	1.80	0.47
2:F:106:ASP:O	2:F:110:ILE:HG13	2.15	0.47
2:B:77:HIS:CD2	2:B:79:PHE:H	2.32	0.46
1:C:164:LEU:HD11	3:C:301:YBI:N41	2.29	0.46
1:C:271:GLY:C	1:C:272:TYR:CD1	2.93	0.46
2:D:106:ASP:O	2:D:110:ILE:HG13	2.15	0.46
1:E:186:PHE:O	1:E:187:LEU:C	2.56	0.46
1:E:188:THR:O	1:E:190:LYS:N	2.48	0.46
1:A:271:GLY:C	1:A:272:TYR:HD1	2.23	0.46
1:E:178:GLU:HB3	1:E:184:HIS:CD2	2.50	0.46
2:B:74:LEU:CD2	2:B:153:LEU:HD22	2.44	0.46
1:E:188:THR:O	1:E:189:ARG:C	2.59	0.46
1:E:254:PHE:O	1:E:254:PHE:HD1	1.97	0.46
1:G:127:LYS:HB3	1:G:127:LYS:NZ	2.31	0.46
2:B:106:ASP:O	2:B:110:ILE:HG13	2.15	0.46
1:E:185:PRO:O	1:E:234:ARG:NH2	2.47	0.46
1:C:271:GLY:C	1:C:272:TYR:HD1	2.23	0.46
2:D:142:PRO:HD2	1:G:239:PHE:CZ	2.51	0.46
1:E:145:LEU:HD23	1:E:145:LEU:HA	1.60	0.46
1:E:187:LEU:HD23	1:E:187:LEU:HA	1.71	0.45
1:E:221:ASP:C	1:E:223:GLU:H	2.24	0.45
1:E:190:LYS:HD2	1:E:191:TRP:CD2	2.51	0.45
2:D:127:GLN:OE1	2:D:127:GLN:O	2.34	0.45
2:H:106:ASP:O	2:H:110:ILE:HG13	2.15	0.45
1:G:254:PHE:O	1:G:254:PHE:HD1	1.98	0.45
2:H:96:ASP:OD2	2:H:96:ASP:N	2.41	0.45
1:G:199:ARG:NH1	1:G:215:PHE:CE1	2.85	0.45
1:E:199:ARG:NH1	1:E:215:PHE:CE1	2.85	0.45
1:E:255:ALA:HB3	1:E:275:HIS:NE2	2.32	0.45
1:G:141:VAL:HA	1:G:160:LYS:O	2.17	0.45
1:G:230:TYR:HE1	1:G:263:GLN:HG3	1.82	0.45
2:F:100:ILE:HG13	2:F:101:ILE:N	2.32	0.45
1:A:201:HIS:O	1:A:204:LYS:HB2	2.16	0.44
1:E:161:ILE:O	1:E:170:THR:HA	2.17	0.44
1:E:168:TYR:HA	1:E:169:PRO:HD3	1.78	0.44
1:E:199:ARG:NH1	1:E:215:PHE:HE1	2.16	0.44
1:G:234:ARG:C	1:G:235:TRP:HD1	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:276:ARG:O	1:G:277:SER:C	2.60	0.44
1:E:234:ARG:C	1:E:235:TRP:HD1	2.25	0.44
1:A:271:GLY:O	1:A:272:TYR:CD1	2.62	0.44
1:C:197:VAL:O	1:C:201:HIS:ND1	2.51	0.44
1:E:141:VAL:HA	1:E:160:LYS:O	2.17	0.44
2:H:111:LYS:O	2:H:115:GLU:N	2.50	0.44
1:G:199:ARG:NH1	1:G:215:PHE:HE1	2.16	0.44
1:E:171:LEU:HD23	1:E:171:LEU:HA	1.88	0.44
2:F:81:TRP:CH2	2:F:149:MET:HE1	2.53	0.44
2:H:145:ASP:O	2:H:149:MET:HG3	2.18	0.44
2:B:100:ILE:HD11	2:B:139:TYR:HD1	1.83	0.43
1:C:248:ASP:O	1:C:249:ILE:C	2.61	0.43
1:C:271:GLY:O	1:C:284:LEU:N	2.51	0.43
2:H:81:TRP:CH2	2:H:149:MET:HE1	2.53	0.43
2:D:71:LEU:O	2:D:73:THR:N	2.51	0.43
2:D:81:TRP:CH2	2:D:149:MET:HE1	2.53	0.43
1:E:187:LEU:HA	1:E:198:ASP:OD2	2.18	0.43
2:F:119:TYR:CD2	2:F:125:CYS:HB2	2.53	0.43
2:H:100:ILE:HD11	2:H:139:TYR:CD1	2.50	0.43
2:H:119:TYR:CD2	2:H:125:CYS:HB2	2.53	0.43
1:C:145:LEU:HA	1:C:145:LEU:HD23	1.65	0.43
1:C:259:TYR:C	1:C:260:ILE:HD13	2.43	0.43
2:D:79:PHE:CZ	1:E:165:THR:HA	2.46	0.43
1:G:230:TYR:CD1	1:G:263:GLN:HG3	2.53	0.43
2:B:132:MET:HE2	2:B:132:MET:HB3	1.75	0.43
2:D:119:TYR:CD2	2:D:125:CYS:HB2	2.53	0.43
1:G:187:LEU:HA	1:G:198:ASP:OD2	2.18	0.43
2:B:81:TRP:CH2	2:B:149:MET:HE1	2.53	0.43
2:B:119:TYR:CD2	2:B:125:CYS:HB2	2.53	0.43
1:A:259:TYR:C	1:A:260:ILE:HD13	2.43	0.43
2:D:71:LEU:O	2:D:72:LYS:C	2.61	0.43
2:D:71:LEU:C	2:D:73:THR:N	2.75	0.43
1:E:164:LEU:HD12	1:E:171:LEU:HB2	2.01	0.43
1:G:195:GLU:HG2	1:G:199:ARG:NH2	2.34	0.43
1:E:230:TYR:CD1	1:E:263:GLN:HG3	2.53	0.42
1:A:165:THR:CG2	1:A:168:TYR:HB2	2.49	0.42
1:E:195:GLU:HG2	1:E:199:ARG:NH2	2.33	0.42
2:F:100:ILE:HG13	2:F:101:ILE:H	1.84	0.42
1:C:132:GLN:O	1:C:139:TYR:N	2.41	0.42
2:D:131:THR:OG1	1:G:152:ASN:OD1	2.36	0.42
2:F:132:MET:HE2	2:F:132:MET:HB3	1.75	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:GLN:O	1:A:139:TYR:N	2.41	0.42
2:B:79:PHE:N	2:B:79:PHE:CD1	2.87	0.42
1:A:262:PHE:CZ	1:A:267:ALA:HA	2.55	0.42
1:C:132:GLN:O	1:C:138:SER:HA	2.19	0.42
1:C:262:PHE:CZ	1:C:267:ALA:HA	2.55	0.42
2:D:158:LEU:HA	2:D:158:LEU:HD23	1.84	0.42
1:A:132:GLN:O	1:A:138:SER:HA	2.19	0.42
1:A:247:LYS:HB3	1:A:248:ASP:H	1.55	0.42
1:A:257:PHE:CE1	1:A:259:TYR:CE1	3.08	0.42
2:B:74:LEU:CD2	2:B:153:LEU:HB3	2.50	0.42
1:G:199:ARG:HH11	1:G:215:PHE:HE1	1.68	0.42
1:C:257:PHE:CE1	1:C:259:TYR:CE1	3.08	0.42
1:A:197:VAL:O	1:A:201:HIS:ND1	2.51	0.42
1:E:233:MET:HB2	1:E:235:TRP:HE1	1.85	0.42
2:B:71:LEU:C	2:B:71:LEU:CD2	2.92	0.41
1:C:250:SER:C	1:C:252:ALA:H	2.28	0.41
2:F:100:ILE:O	2:F:101:ILE:C	2.63	0.41
1:G:233:MET:HB2	1:G:235:TRP:HE1	1.85	0.41
2:D:96:ASP:O	2:D:100:ILE:HG23	2.20	0.41
2:D:120:TRP:HA	4:D:204:GOL:H31	2.01	0.41
2:H:79:PHE:CG	2:H:149:MET:HE2	2.54	0.41
2:H:142:PRO:C	2:H:144:ASP:N	2.78	0.41
1:G:275:HIS:O	1:G:275:HIS:ND1	2.53	0.41
2:H:100:ILE:HG13	2:H:101:ILE:N	2.34	0.41
1:A:220:PHE:CD1	1:A:220:PHE:C	2.99	0.41
1:C:144:VAL:O	1:C:145:LEU:HD23	2.21	0.41
1:E:188:THR:O	1:E:190:LYS:HG2	2.21	0.41
1:A:132:GLN:N	1:A:139:TYR:O	2.47	0.41
1:A:234:ARG:HA	1:A:258:TYR:O	2.21	0.41
2:B:109:THR:O	2:B:112:LYS:HG2	2.21	0.41
1:E:145:LEU:HD22	1:E:155:LEU:HD12	2.02	0.41
1:A:147:HIS:NE2	2:F:134:THR:OG1	2.44	0.41
2:B:127:GLN:OE1	2:B:131:THR:OG1	2.38	0.41
2:D:96:ASP:OD2	2:D:96:ASP:N	2.45	0.41
1:E:188:THR:C	1:E:190:LYS:N	2.78	0.41
1:G:145:LEU:HD22	1:G:155:LEU:HD12	2.02	0.41
2:D:77:HIS:HD2	2:D:79:PHE:H	1.69	0.41
1:E:186:PHE:HB3	1:E:215:PHE:HD2	1.86	0.41
2:F:89:ALA:O	2:F:93:ASN:N	2.55	0.40
2:H:127:GLN:O	2:H:131:THR:N	2.45	0.40
2:B:102:LYS:H	4:B:201:GOL:H2	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:HIS:ND1	2:H:154:GLU:OE2	2.47	0.40
2:D:120:TRP:HA	2:D:120:TRP:CE3	2.56	0.40
1:E:230:TYR:HE1	1:E:263:GLN:HG3	1.82	0.40
1:A:273:TYR:CD2	1:A:273:TYR:C	3.00	0.40
1:A:273:TYR:CE1	3:A:301:YBI:C31	3.04	0.40
2:B:142:PRO:C	2:B:144:ASP:H	2.29	0.40
1:C:132:GLN:N	1:C:139:TYR:O	2.47	0.40
1:E:256:GLY:HA3	1:E:273:TYR:HE1	1.83	0.40
1:A:141:VAL:HG21	1:A:284:LEU:CD1	2.51	0.40
1:A:232:PHE:C	1:A:233:MET:HG3	2.47	0.40
1:C:141:VAL:HG21	1:C:284:LEU:CD1	2.51	0.40
1:C:273:TYR:CD2	1:C:273:TYR:C	3.00	0.40
1:A:144:VAL:O	1:A:145:LEU:HD23	2.21	0.40
1:A:260:ILE:HG22	1:A:261:CYS:N	2.37	0.40
2:B:158:LEU:HD23	2:B:158:LEU:HA	1.91	0.40
1:C:234:ARG:HA	1:C:258:TYR:O	2.21	0.40
1:E:199:ARG:HH11	1:E:215:PHE:HE1	1.68	0.40
1:G:212:ALA:O	1:G:215:PHE:HD1	2.05	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	152/167 (91%)	131 (86%)	20 (13%)	1 (1%)	18	48
1	C	155/167 (93%)	132 (85%)	19 (12%)	4 (3%)	4	17
1	E	160/167 (96%)	138 (86%)	19 (12%)	3 (2%)	6	23
1	G	154/167 (92%)	138 (90%)	16 (10%)	0	100	100
2	B	103/126 (82%)	82 (80%)	21 (20%)	0	100	100
2	D	103/126 (82%)	84 (82%)	19 (18%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	104/126 (82%)	84 (81%)	20 (19%)	0	100	100
2	H	101/126 (80%)	81 (80%)	19 (19%)	1 (1%)	12	39
All	All	1032/1172 (88%)	870 (84%)	153 (15%)	9 (1%)	14	41

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	169	PRO
1	E	276	ARG
1	C	169	PRO
1	E	189	ARG
1	C	135	LYS
2	H	165	PRO
1	C	251	GLY
1	A	180	ILE
1	C	180	ILE

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	100/147 (68%)	91 (91%)	9 (9%)	9	28
1	C	92/147 (63%)	82 (89%)	10 (11%)	6	20
1	E	109/147 (74%)	103 (94%)	6 (6%)	19	50
1	G	110/147 (75%)	103 (94%)	7 (6%)	16	44
2	B	72/118 (61%)	68 (94%)	4 (6%)	19	50
2	D	70/118 (59%)	69 (99%)	1 (1%)	59	85
2	F	62/118 (52%)	60 (97%)	2 (3%)	34	68
2	H	68/118 (58%)	63 (93%)	5 (7%)	13	38
All	All	683/1060 (64%)	639 (94%)	44 (6%)	16	44

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	124	SER
1	A	149	ASP
1	A	150	THR
1	A	153	SER
1	A	155	LEU
1	A	159	LEU
1	A	164	LEU
1	A	178	GLU
1	A	194	ASP
2	B	62	GLN
2	B	96	ASP
2	B	100	ILE
2	B	161	ILE
1	C	124	SER
1	C	149	ASP
1	C	150	THR
1	C	156	CYS
1	C	164	LEU
1	C	167	GLU
1	C	170	THR
1	C	194	ASP
1	C	231	VAL
1	C	287	THR
2	D	148	LEU
1	E	149	ASP
1	E	170	THR
1	E	218	ASP
1	E	265	SER
1	E	282	GLN
1	E	289	VAL
2	F	100	ILE
2	F	146	ILE
1	G	149	ASP
1	G	170	THR
1	G	218	ASP
1	G	229	ASP
1	G	265	SER
1	G	282	GLN
1	G	289	VAL
2	H	62	GLN
2	H	63	LEU
2	H	96	ASP
2	H	100	ILE

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Mol	Chain	Res	Type
2	H	161	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	77	HIS
2	B	127	GLN
2	B	140	ASN
1	C	184	HIS
2	D	77	HIS
2	D	123	GLN
2	D	140	ASN
1	E	216	ASN
1	E	238	GLN
1	E	263	GLN
2	F	77	HIS
2	F	140	ASN
1	G	238	GLN
1	G	263	GLN
2	H	77	HIS
2	H	140	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 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	$\# Z > 2$
4	GOL	D	203	-	5,5,5	1.68	1 (20%)	5,5,5	0.91	0
4	GOL	D	204	-	5,5,5	0.89	0	5,5,5	1.21	0
3	YBI	G	301	-	69,75,75	2.89	32 (46%)	87,108,108	2.83	30 (34%)
4	GOL	H	201	-	5,5,5	0.82	0	5,5,5	1.33	0
4	GOL	G	302	-	5,5,5	1.12	0	5,5,5	0.99	0
3	YBI	E	301	-	69,75,75	2.90	32 (46%)	87,108,108	2.84	31 (35%)
4	GOL	D	201	-	5,5,5	1.21	1 (20%)	5,5,5	1.39	0
4	GOL	D	202	-	5,5,5	1.34	1 (20%)	5,5,5	0.91	0
4	GOL	G	303	-	5,5,5	0.98	0	5,5,5	1.00	0
3	YBI	A	301	-	69,75,75	2.95	33 (47%)	87,108,108	3.31	43 (49%)
3	YBI	C	301	-	69,75,75	2.95	33 (47%)	87,108,108	3.31	43 (49%)
4	GOL	B	201	-	5,5,5	0.09	0	5,5,5	0.29	0

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
4	GOL	D	203	-	-	4/4/4/4	-
4	GOL	D	204	-	-	1/4/4/4	-
3	YBI	G	301	-	-	6/33/69/69	0/9/10/10
4	GOL	H	201	-	-	3/4/4/4	-
4	GOL	G	302	-	-	0/4/4/4	-
3	YBI	E	301	-	-	5/33/69/69	0/9/10/10
4	GOL	D	201	-	-	4/4/4/4	-
4	GOL	D	202	-	-	2/4/4/4	-
4	GOL	G	303	-	-	2/4/4/4	-
3	YBI	A	301	-	-	5/33/69/69	0/9/10/10
3	YBI	C	301	-	-	5/33/69/69	0/9/10/10
4	GOL	B	201	-	-	0/4/4/4	-

All (133) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	301	YBI	C43-N44	7.25	1.54	1.39
3	A	301	YBI	C43-N44	7.22	1.54	1.39
3	G	301	YBI	C66-N59	-7.19	1.31	1.47
3	E	301	YBI	C66-N59	-7.14	1.31	1.47
3	E	301	YBI	C14-N62	7.08	1.48	1.35
3	C	301	YBI	C66-N59	-7.00	1.31	1.47
3	A	301	YBI	C66-N59	-6.98	1.31	1.47
3	G	301	YBI	C14-N62	6.96	1.48	1.35
3	G	301	YBI	C43-N44	6.88	1.53	1.39
3	E	301	YBI	C43-N44	6.78	1.53	1.39
3	G	301	YBI	C7-S13	6.73	1.87	1.74
3	A	301	YBI	C31-N32	6.62	1.48	1.34
3	C	301	YBI	C31-N32	6.61	1.48	1.34
3	E	301	YBI	C7-S13	6.53	1.87	1.74
3	A	301	YBI	C7-S13	6.53	1.87	1.74
3	C	301	YBI	C7-S13	6.49	1.86	1.74
3	C	301	YBI	C14-N62	6.47	1.47	1.35
3	A	301	YBI	C14-N62	6.47	1.47	1.35
3	E	301	YBI	C31-N32	6.05	1.46	1.34
3	A	301	YBI	C3-N4	6.02	1.52	1.47
3	C	301	YBI	C3-N4	5.88	1.52	1.47
3	G	301	YBI	C31-N32	5.87	1.46	1.34
3	G	301	YBI	C42-N41	-5.81	1.28	1.38
3	E	301	YBI	C42-N41	-5.65	1.28	1.38
3	A	301	YBI	C42-N41	-5.62	1.28	1.38
3	C	301	YBI	C42-N41	-5.59	1.28	1.38
3	E	301	YBI	C60-N59	-5.03	1.33	1.46
3	G	301	YBI	C60-N59	-5.00	1.33	1.46
3	C	301	YBI	C61-N62	-4.83	1.38	1.47
3	A	301	YBI	C61-N62	-4.80	1.38	1.47
3	C	301	YBI	C60-N59	-4.79	1.34	1.46
3	A	301	YBI	C60-N59	-4.76	1.34	1.46
3	C	301	YBI	C20-C5	4.62	1.55	1.48
3	A	301	YBI	C20-C5	4.60	1.55	1.48
3	E	301	YBI	C6-C7	4.52	1.47	1.38
3	G	301	YBI	C40-N44	4.44	1.38	1.32
3	G	301	YBI	C64-N59	-4.33	1.35	1.46
3	G	301	YBI	C6-C7	4.31	1.47	1.38
3	E	301	YBI	C40-N44	4.29	1.38	1.32
3	E	301	YBI	C64-N59	-4.22	1.35	1.46
3	E	301	YBI	C20-C5	4.18	1.54	1.48
3	E	301	YBI	C61-N62	-3.96	1.39	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	301	YBI	C6-C7	3.95	1.46	1.38
3	G	301	YBI	C61-N62	-3.94	1.40	1.47
3	C	301	YBI	C40-N44	3.94	1.37	1.32
3	A	301	YBI	C40-N44	3.93	1.37	1.32
3	C	301	YBI	C6-C7	3.93	1.46	1.38
3	C	301	YBI	C64-N59	-3.81	1.36	1.46
3	A	301	YBI	C64-N59	-3.80	1.36	1.46
3	A	301	YBI	C63-N62	-3.78	1.40	1.47
3	G	301	YBI	C12-C11	-3.77	1.22	1.37
3	C	301	YBI	C12-C11	-3.76	1.22	1.37
3	G	301	YBI	C63-N62	-3.76	1.40	1.47
3	A	301	YBI	C12-C11	-3.75	1.22	1.37
3	E	301	YBI	C12-S13	-3.72	1.58	1.73
3	C	301	YBI	C63-N62	-3.72	1.40	1.47
3	E	301	YBI	C12-C11	-3.71	1.22	1.37
3	E	301	YBI	C63-N62	-3.67	1.40	1.47
3	G	301	YBI	C20-C5	3.65	1.53	1.48
3	E	301	YBI	C28-C27	3.60	1.54	1.49
3	G	301	YBI	C12-S13	-3.60	1.58	1.73
3	G	301	YBI	C40-N41	-3.57	1.30	1.36
3	G	301	YBI	C28-C27	3.47	1.54	1.49
3	A	301	YBI	C12-S13	-3.46	1.59	1.73
3	C	301	YBI	C12-S13	-3.44	1.59	1.73
3	E	301	YBI	C40-N41	-3.42	1.30	1.36
3	C	301	YBI	C10-N8	3.25	1.35	1.31
3	C	301	YBI	C58-C53	-3.25	1.35	1.41
3	C	301	YBI	C28-C27	3.24	1.54	1.49
3	E	301	YBI	C3-N4	3.24	1.50	1.47
3	A	301	YBI	C10-N8	3.24	1.35	1.31
3	E	301	YBI	C58-C53	-3.23	1.35	1.41
3	A	301	YBI	C28-C27	3.23	1.54	1.49
3	A	301	YBI	C40-N41	-3.22	1.30	1.36
3	A	301	YBI	C58-C53	-3.22	1.35	1.41
3	E	301	YBI	C52-N51	3.19	1.44	1.38
3	C	301	YBI	C40-N41	-3.19	1.30	1.36
3	G	301	YBI	C52-N51	3.17	1.44	1.38
3	C	301	YBI	C52-N51	3.10	1.44	1.38
3	A	301	YBI	C52-N51	3.05	1.44	1.38
3	G	301	YBI	C58-C53	-3.05	1.35	1.41
3	E	301	YBI	C10-N8	3.03	1.35	1.31
3	G	301	YBI	C10-N8	2.97	1.35	1.31
3	G	301	YBI	C3-N4	2.93	1.50	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	301	YBI	O33-C31	-2.83	1.17	1.23
4	D	203	GOL	C3-C2	2.74	1.62	1.51
3	E	301	YBI	C15-C14	2.74	1.56	1.51
3	G	301	YBI	C2-N1	2.73	1.42	1.38
3	G	301	YBI	C15-C14	2.71	1.56	1.51
3	E	301	YBI	O33-C31	-2.71	1.17	1.23
3	C	301	YBI	C48-C47	2.71	1.43	1.38
3	G	301	YBI	C53-C52	2.70	1.45	1.41
3	A	301	YBI	C48-C47	2.70	1.43	1.38
3	E	301	YBI	C53-C52	2.67	1.45	1.41
3	E	301	YBI	C2-N1	2.67	1.42	1.38
3	G	301	YBI	C57-C56	2.58	1.43	1.38
3	E	301	YBI	C57-C56	2.55	1.43	1.38
3	A	301	YBI	C53-C52	2.55	1.45	1.41
3	C	301	YBI	C53-C52	2.52	1.44	1.41
3	A	301	YBI	C55-C52	-2.46	1.35	1.39
3	C	301	YBI	C55-C52	-2.44	1.35	1.39
3	E	301	YBI	C17-C10	2.44	1.53	1.49
3	G	301	YBI	C17-C10	2.44	1.53	1.49
3	C	301	YBI	O33-C31	-2.42	1.18	1.23
3	A	301	YBI	O33-C31	-2.40	1.18	1.23
3	C	301	YBI	C17-C10	2.39	1.52	1.49
3	E	301	YBI	C55-C52	-2.38	1.35	1.39
3	A	301	YBI	C37-C40	2.38	1.53	1.49
3	A	301	YBI	C17-C10	2.38	1.52	1.49
3	C	301	YBI	C37-C40	2.34	1.53	1.49
3	G	301	YBI	C55-C52	-2.33	1.35	1.39
4	D	201	GOL	O2-C2	-2.32	1.36	1.43
3	A	301	YBI	N9-N8	2.29	1.44	1.39
3	C	301	YBI	C57-C56	2.26	1.43	1.38
3	E	301	YBI	C37-C40	2.26	1.53	1.49
3	C	301	YBI	N9-N8	2.26	1.44	1.39
3	A	301	YBI	C57-C56	2.26	1.43	1.38
3	E	301	YBI	N9-N8	2.25	1.44	1.39
3	C	301	YBI	O49-C46	2.22	1.42	1.37
4	D	202	GOL	O2-C2	-2.21	1.36	1.43
3	A	301	YBI	O49-C46	2.19	1.42	1.37
3	G	301	YBI	N9-N8	2.18	1.44	1.39
3	A	301	YBI	C21-C20	-2.18	1.36	1.39
3	E	301	YBI	O49-C46	2.17	1.42	1.37
3	E	301	YBI	O16-C14	-2.17	1.18	1.23
3	G	301	YBI	C37-C40	2.15	1.53	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	301	YBI	O49-C46	2.13	1.42	1.37
3	G	301	YBI	O16-C14	-2.13	1.18	1.23
3	C	301	YBI	C21-C20	-2.12	1.36	1.39
3	A	301	YBI	C65-C50	2.07	1.59	1.51
3	A	301	YBI	C47-C46	2.06	1.42	1.38
3	C	301	YBI	C47-C46	2.06	1.42	1.38
3	C	301	YBI	C65-C50	2.05	1.59	1.51

All (147) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	301	YBI	C10-N8-N9	-11.96	95.76	107.95
3	A	301	YBI	C10-N8-N9	-11.90	95.82	107.95
3	G	301	YBI	C10-N8-N9	-11.24	96.49	107.95
3	E	301	YBI	C10-N8-N9	-11.15	96.58	107.95
3	C	301	YBI	N1-C10-N8	8.53	118.21	109.57
3	A	301	YBI	N1-C10-N8	8.51	118.19	109.57
3	G	301	YBI	N1-C10-N8	8.49	118.17	109.57
3	E	301	YBI	N1-C10-N8	8.28	117.95	109.57
3	G	301	YBI	C2-N9-N8	8.24	117.19	107.82
3	E	301	YBI	C2-N9-N8	8.21	117.15	107.82
3	A	301	YBI	C3-N4-C5	8.17	125.66	117.67
3	C	301	YBI	C3-N4-C5	8.11	125.60	117.67
3	C	301	YBI	C2-N9-N8	7.64	116.51	107.82
3	A	301	YBI	C2-N9-N8	7.60	116.46	107.82
3	A	301	YBI	C42-N41-C40	7.48	121.48	107.57
3	C	301	YBI	C42-N41-C40	7.46	121.45	107.57
3	G	301	YBI	C42-N41-C40	7.23	121.01	107.57
3	E	301	YBI	C42-N41-C40	7.18	120.92	107.57
3	C	301	YBI	C21-C22-C23	6.90	126.18	119.24
3	A	301	YBI	C21-C22-C23	6.84	126.12	119.24
3	C	301	YBI	C38-C39-C34	6.54	118.67	111.49
3	A	301	YBI	C38-C39-C34	6.52	118.65	111.49
3	C	301	YBI	C28-C27-N51	6.49	127.92	121.10
3	A	301	YBI	C28-C27-N51	6.48	127.91	121.10
3	E	301	YBI	C28-C27-N51	6.36	127.78	121.10
3	G	301	YBI	C6-C7-S13	-6.16	106.60	112.53
3	G	301	YBI	C28-C27-N51	5.96	127.37	121.10
3	C	301	YBI	C53-C52-N51	-5.83	101.58	107.65
3	A	301	YBI	C53-C52-N51	-5.81	101.60	107.65
3	E	301	YBI	C6-C7-S13	-5.78	106.97	112.53
3	A	301	YBI	C6-C7-S13	-5.55	107.19	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	301	YBI	C6-C7-S13	-5.49	107.25	112.53
3	C	301	YBI	C22-C21-C20	-5.49	114.94	120.80
3	A	301	YBI	C22-C21-C20	-5.46	114.97	120.80
3	G	301	YBI	C53-C52-N51	-5.43	102.00	107.65
3	E	301	YBI	C3-N4-C5	5.38	122.93	117.67
3	E	301	YBI	C53-C52-N51	-5.23	102.20	107.65
3	E	301	YBI	C52-C53-C54	-5.12	102.61	106.80
3	G	301	YBI	C3-N4-C5	4.93	122.49	117.67
3	G	301	YBI	C52-C53-C54	-4.90	102.79	106.80
3	A	301	YBI	C63-C64-N59	4.42	119.57	110.65
3	C	301	YBI	C63-C64-N59	4.42	119.56	110.65
3	A	301	YBI	C11-C12-S13	4.41	120.06	111.56
3	C	301	YBI	C11-C12-S13	4.40	120.03	111.56
3	A	301	YBI	C52-C53-C54	-4.36	103.23	106.80
3	C	301	YBI	C52-C53-C54	-4.32	103.26	106.80
3	A	301	YBI	C36-C35-C34	4.31	116.22	111.49
3	C	301	YBI	C36-C35-C34	4.29	116.20	111.49
3	E	301	YBI	N1-C2-N9	-4.27	104.41	109.44
3	E	301	YBI	C17-C10-N8	-4.19	119.42	125.96
3	G	301	YBI	C17-C10-N8	-4.13	119.52	125.96
3	G	301	YBI	N1-C2-N9	-4.12	104.59	109.44
3	G	301	YBI	C11-C12-S13	4.00	119.27	111.56
3	E	301	YBI	C11-C12-S13	3.99	119.25	111.56
3	C	301	YBI	C17-C10-N8	-3.87	119.93	125.96
3	A	301	YBI	C17-C10-N8	-3.86	119.93	125.96
3	G	301	YBI	C19-C12-C11	-3.82	119.81	128.63
3	A	301	YBI	C19-C12-C11	-3.76	119.97	128.63
3	C	301	YBI	C19-C12-C11	-3.75	119.98	128.63
3	E	301	YBI	C19-C12-C11	-3.58	120.37	128.63
3	A	301	YBI	C2-C3-N4	-3.53	100.97	106.80
3	C	301	YBI	C39-C34-N32	-3.52	103.54	110.57
3	C	301	YBI	C2-C3-N4	-3.52	100.99	106.80
3	A	301	YBI	C38-C37-C40	-3.51	106.88	111.94
3	A	301	YBI	C39-C34-N32	-3.50	103.58	110.57
3	C	301	YBI	C38-C37-C40	-3.50	106.90	111.94
3	E	301	YBI	C63-C64-N59	3.45	117.61	110.65
3	G	301	YBI	C61-C60-N59	3.28	117.27	110.65
3	A	301	YBI	C47-C46-C45	-3.23	116.16	120.50
3	E	301	YBI	C6-C11-C12	3.23	118.27	111.91
3	C	301	YBI	C47-C46-C45	-3.22	116.17	120.50
3	A	301	YBI	N1-C2-N9	-3.16	105.71	109.44
3	C	301	YBI	N1-C2-N9	-3.13	105.75	109.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	301	YBI	C6-C11-C12	3.12	118.06	111.91
3	C	301	YBI	C35-C36-C37	3.00	116.47	111.18
3	A	301	YBI	C35-C36-C37	3.00	116.47	111.18
3	G	301	YBI	C20-C5-C6	-2.95	114.86	118.75
3	E	301	YBI	C61-C60-N59	2.95	116.60	110.65
3	G	301	YBI	C63-C64-N59	2.90	116.50	110.65
3	E	301	YBI	C55-C52-N51	2.84	136.57	130.83
3	A	301	YBI	C30-C31-N32	2.83	122.89	116.16
3	C	301	YBI	C30-C31-N32	2.83	122.88	116.16
3	G	301	YBI	C55-C52-N51	2.82	136.53	130.83
3	E	301	YBI	C18-C11-C12	-2.74	118.38	124.21
3	C	301	YBI	C24-C25-C20	2.70	123.68	120.80
3	A	301	YBI	C24-C25-C20	2.68	123.67	120.80
3	A	301	YBI	N41-C40-N44	-2.62	105.22	112.51
3	C	301	YBI	N41-C40-N44	-2.61	105.25	112.51
3	C	301	YBI	C20-C5-N4	2.59	120.27	117.30
3	A	301	YBI	C20-C5-N4	2.59	120.27	117.30
3	C	301	YBI	C55-C52-N51	2.59	136.06	130.83
3	A	301	YBI	C55-C52-N51	2.58	136.03	130.83
3	A	301	YBI	C18-C11-C12	-2.54	118.79	124.21
3	C	301	YBI	C18-C11-C12	-2.53	118.82	124.21
3	C	301	YBI	C6-C11-C12	2.53	116.89	111.91
3	A	301	YBI	C6-C11-C12	2.53	116.89	111.91
3	A	301	YBI	C28-C27-C54	-2.51	128.59	131.55
3	C	301	YBI	C28-C27-C54	-2.51	128.59	131.55
3	G	301	YBI	C64-N59-C60	2.48	114.18	108.84
3	G	301	YBI	C18-C11-C12	-2.47	118.95	124.21
3	G	301	YBI	N41-C40-N44	-2.47	105.64	112.51
3	E	301	YBI	C38-C39-C34	2.47	114.20	111.49
3	E	301	YBI	N41-C40-N44	-2.46	105.67	112.51
3	E	301	YBI	C34-N32-C31	-2.43	119.29	122.88
3	G	301	YBI	C38-C39-C34	2.43	114.16	111.49
3	E	301	YBI	C66-N59-C60	-2.42	104.79	111.24
3	G	301	YBI	C34-N32-C31	-2.41	119.31	122.88
3	A	301	YBI	C25-C24-C23	-2.39	116.84	119.24
3	A	301	YBI	C66-N59-C60	-2.38	104.89	111.24
3	E	301	YBI	C47-C46-C45	-2.38	117.31	120.50
3	C	301	YBI	C66-N59-C60	-2.37	104.92	111.24
3	C	301	YBI	C25-C24-C23	-2.36	116.86	119.24
3	C	301	YBI	C24-C23-C22	-2.34	118.34	121.24
3	E	301	YBI	C45-C42-N41	2.34	135.44	130.65
3	E	301	YBI	C28-C27-C54	-2.33	128.80	131.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	301	YBI	C47-C46-C45	-2.31	117.40	120.50
3	E	301	YBI	C64-N59-C60	2.31	113.82	108.84
3	G	301	YBI	O33-C31-N32	-2.30	119.06	122.95
3	A	301	YBI	C24-C23-C22	-2.27	118.42	121.24
3	E	301	YBI	O33-C31-N32	-2.27	119.12	122.95
3	C	301	YBI	C42-C43-N44	-2.26	106.32	109.42
3	A	301	YBI	C42-C43-N44	-2.25	106.34	109.42
3	A	301	YBI	C66-N59-C64	-2.23	105.29	111.24
3	C	301	YBI	C66-N59-C64	-2.23	105.30	111.24
3	G	301	YBI	C36-C35-C34	2.22	113.93	111.49
3	G	301	YBI	C45-C42-N41	2.16	135.09	130.65
3	A	301	YBI	C35-C34-N32	2.16	114.89	110.57
3	A	301	YBI	C45-C42-N41	2.16	135.07	130.65
3	C	301	YBI	C35-C34-N32	2.16	114.88	110.57
3	C	301	YBI	C45-C42-N41	2.15	135.05	130.65
3	G	301	YBI	C42-C43-N44	-2.14	106.49	109.42
3	C	301	YBI	C48-C43-N44	2.12	134.23	128.21
3	C	301	YBI	O33-C31-N32	-2.12	119.36	122.95
3	A	301	YBI	O33-C31-N32	-2.12	119.37	122.95
3	A	301	YBI	C48-C43-N44	2.12	134.21	128.21
3	G	301	YBI	C28-C27-C54	-2.09	129.09	131.55
3	E	301	YBI	C20-C5-C6	-2.08	116.01	118.75
3	A	301	YBI	C48-C47-C46	2.08	122.11	119.73
3	G	301	YBI	C66-N59-C60	-2.06	105.74	111.24
3	A	301	YBI	C63-N62-C61	2.06	116.88	112.68
3	C	301	YBI	C63-N62-C61	2.05	116.86	112.68
3	C	301	YBI	C48-C47-C46	2.04	122.06	119.73
3	E	301	YBI	O16-C14-N62	-2.04	118.49	122.12
3	E	301	YBI	C42-C43-N44	-2.02	106.65	109.42
3	E	301	YBI	C36-C35-C34	2.02	113.71	111.49
3	A	301	YBI	C43-C42-N41	-2.02	103.28	105.71
3	C	301	YBI	C43-C42-N41	-2.00	103.30	105.71

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	201	GOL	O1-C1-C2-O2
4	D	201	GOL	O1-C1-C2-C3
4	D	202	GOL	C1-C2-C3-O3
4	D	203	GOL	O1-C1-C2-C3
4	D	203	GOL	C1-C2-C3-O3

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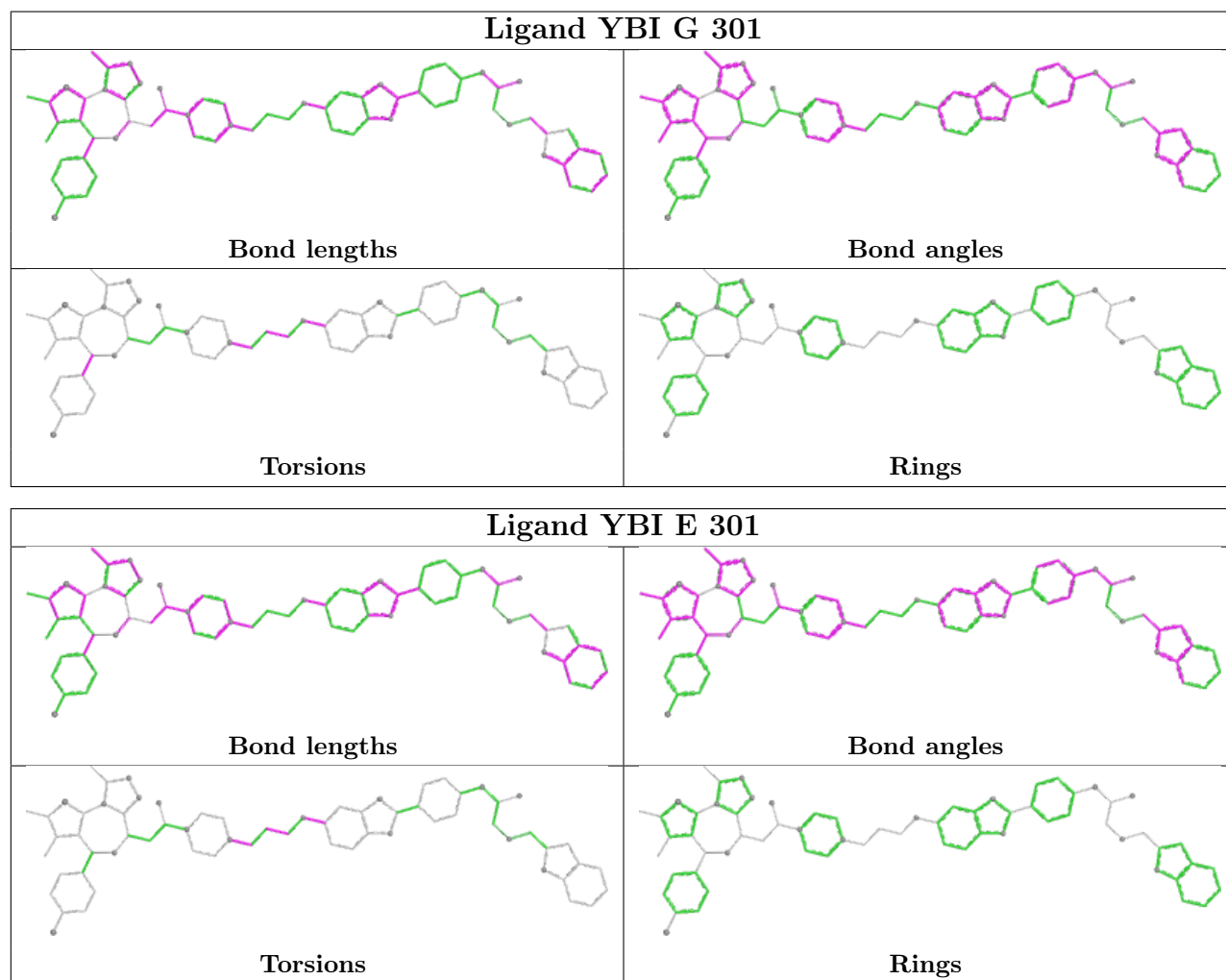
Mol	Chain	Res	Type	Atoms
4	G	303	GOL	C1-C2-C3-O3
4	H	201	GOL	O1-C1-C2-C3
3	E	301	YBI	O49-C50-C65-C66
3	G	301	YBI	O49-C50-C65-C66
3	G	301	YBI	C47-C46-O49-C50
3	G	301	YBI	C45-C46-O49-C50
3	A	301	YBI	C47-C46-O49-C50
3	C	301	YBI	C47-C46-O49-C50
3	A	301	YBI	C45-C46-O49-C50
3	C	301	YBI	C45-C46-O49-C50
4	G	303	GOL	O2-C2-C3-O3
3	E	301	YBI	C47-C46-O49-C50
3	E	301	YBI	C45-C46-O49-C50
4	D	201	GOL	C1-C2-C3-O3
3	G	301	YBI	C65-C66-N59-C60
3	G	301	YBI	C65-C66-N59-C64
4	D	202	GOL	O2-C2-C3-O3
4	H	201	GOL	O1-C1-C2-O2
3	E	301	YBI	C65-C66-N59-C64
4	D	201	GOL	O2-C2-C3-O3
4	D	203	GOL	O1-C1-C2-O2
3	E	301	YBI	C65-C66-N59-C60
4	D	203	GOL	O2-C2-C3-O3
4	D	204	GOL	O2-C2-C3-O3
4	H	201	GOL	O2-C2-C3-O3
3	A	301	YBI	C50-C65-C66-N59
3	C	301	YBI	C50-C65-C66-N59
3	A	301	YBI	C65-C66-N59-C64
3	C	301	YBI	C65-C66-N59-C64
3	G	301	YBI	C25-C20-C5-N4
3	A	301	YBI	C65-C66-N59-C60
3	C	301	YBI	C65-C66-N59-C60

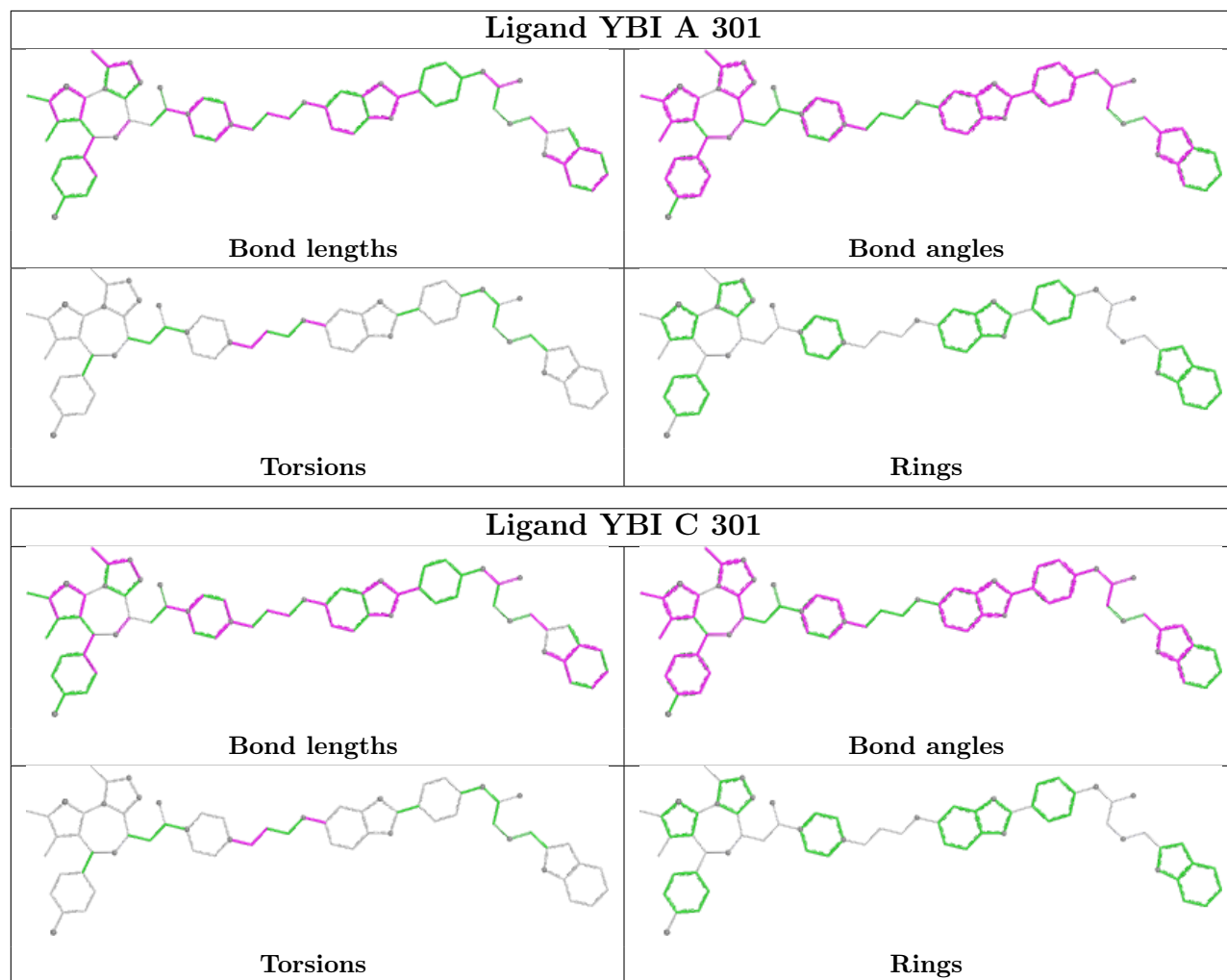
There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	204	GOL	1	0
3	A	301	YBI	4	0
3	C	301	YBI	2	0
4	B	201	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	162/167 (97%)	0.85	17 (10%)	11 10	37, 81, 125, 182	0
1	C	163/167 (97%)	0.82	19 (11%)	9 8	37, 81, 125, 167	0
1	E	164/167 (98%)	0.77	14 (8%)	16 14	27, 72, 120, 135	0
1	G	160/167 (95%)	0.70	12 (7%)	20 16	27, 71, 117, 135	0
2	B	105/126 (83%)	0.74	7 (6%)	24 19	42, 74, 112, 139	0
2	D	105/126 (83%)	0.83	13 (12%)	8 7	42, 73, 113, 157	0
2	F	106/126 (84%)	0.71	11 (10%)	11 10	42, 74, 107, 127	0
2	H	105/126 (83%)	0.83	11 (10%)	11 10	43, 74, 112, 135	0
All	All	1070/1172 (91%)	0.78	104 (9%)	13 11	27, 76, 121, 182	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	249	ILE	4.9
1	C	250	SER	4.3
2	D	123	GLN	4.0
2	F	98	TYR	3.7
1	G	242	PRO	3.6
2	D	62	GLN	3.6
1	A	278	SER	3.5
1	E	164	LEU	3.5
2	H	146	ILE	3.4
2	D	100	ILE	3.3
1	A	289	VAL	3.2
1	E	126	SER	3.2
1	A	206	LEU	3.2
2	D	98	TYR	3.1
1	E	279	GLU	3.1
1	C	280	TRP	3.0

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Mol	Chain	Res	Type	RSRZ
2	H	120	TRP	3.0
2	H	123	GLN	3.0
1	C	227	ASN	3.0
2	H	104	PRO	3.0
1	G	123	GLY	2.9
2	D	142	PRO	2.9
2	F	104	PRO	2.9
1	E	241	VAL	2.9
1	G	137	ASN	2.8
2	H	86	PRO	2.8
1	C	180	ILE	2.8
2	B	62	GLN	2.8
2	F	86	PRO	2.7
2	B	81	TRP	2.7
2	F	139	TYR	2.7
1	A	262	PHE	2.7
1	C	219	ASP	2.7
1	C	278	SER	2.7
2	D	85	GLN	2.7
1	G	134	SER	2.7
1	C	247	LYS	2.6
2	F	77	HIS	2.6
2	D	77	HIS	2.6
2	H	139	TYR	2.6
2	F	120	TRP	2.6
1	E	242	PRO	2.6
1	G	125	GLY	2.5
2	F	95	PRO	2.5
1	E	168	TYR	2.5
1	C	186	PHE	2.5
2	D	104	PRO	2.5
1	E	269	ILE	2.5
1	A	168	TYR	2.5
2	H	95	PRO	2.5
2	B	98	TYR	2.5
1	A	151	GLY	2.4
1	A	218	ASP	2.4
2	H	98	TYR	2.4
2	D	81	TRP	2.4
2	H	119	TYR	2.4
2	B	114	LEU	2.4
2	H	77	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	246	ILE	2.4
2	B	165	PRO	2.3
1	C	231	VAL	2.3
1	E	171	LEU	2.3
1	G	241	VAL	2.3
1	C	238	GLN	2.3
1	C	246	ILE	2.3
1	E	246	ILE	2.3
1	E	134	SER	2.3
1	G	170	THR	2.3
1	C	209	TYR	2.3
2	F	100	ILE	2.2
2	D	165	PRO	2.2
1	A	281	TYR	2.2
1	E	137	ASN	2.2
1	G	256	GLY	2.2
1	C	267	ALA	2.2
2	B	120	TRP	2.2
1	E	123	GLY	2.2
1	C	249	ILE	2.2
1	A	136	GLY	2.2
1	A	238	GLN	2.1
2	F	62	GLN	2.1
1	C	287	THR	2.1
1	C	265	SER	2.1
2	D	161	ILE	2.1
1	A	248	ASP	2.1
1	G	262	PHE	2.1
1	G	228	GLY	2.1
1	C	168	TYR	2.1
2	F	87	VAL	2.1
1	C	152	ASN	2.1
1	A	203	GLY	2.1
1	E	209	TYR	2.1
1	G	126	SER	2.0
2	F	70	VAL	2.0
2	D	95	PRO	2.0
2	B	67	LEU	2.0
2	D	153	LEU	2.0
1	C	136	GLY	2.0
1	A	267	ALA	2.0
1	E	229	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	G	279	GLU	2.0
1	A	217	SER	2.0
1	A	261	CYS	2.0
2	H	81	TRP	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](#)

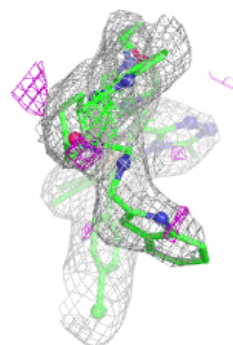
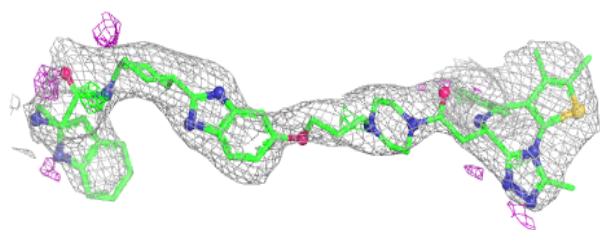
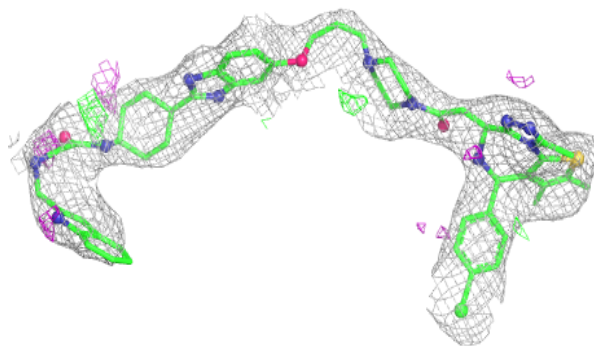
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
4	GOL	G	302	6/6	0.74	0.17	67,98,104,156	0
4	GOL	G	303	6/6	0.82	0.15	41,98,123,222	0
4	GOL	D	204	6/6	0.86	0.10	43,96,127,166	0
4	GOL	B	201	6/6	0.87	0.17	7,26,86,91	0
4	GOL	D	202	6/6	0.88	0.16	32,52,80,248	0
3	YBI	G	301	66/66	0.88	0.18	17,67,157,257	0
4	GOL	D	203	6/6	0.90	0.09	53,78,106,139	0
3	YBI	E	301	66/66	0.90	0.17	17,67,157,257	0
3	YBI	A	301	66/66	0.94	0.14	2,51,179,342	0
3	YBI	C	301	66/66	0.94	0.14	2,51,179,342	0
4	GOL	H	201	6/6	0.95	0.10	20,61,89,95	0
4	GOL	D	201	6/6	0.97	0.09	2,30,59,183	0

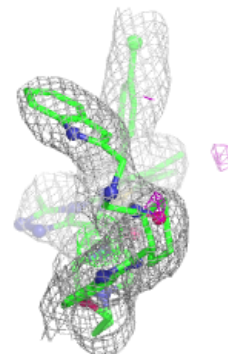
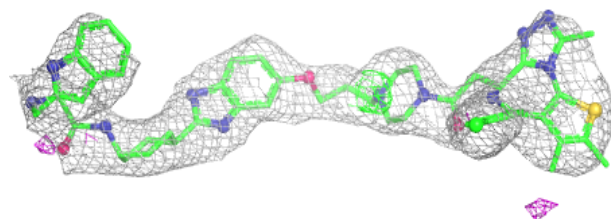
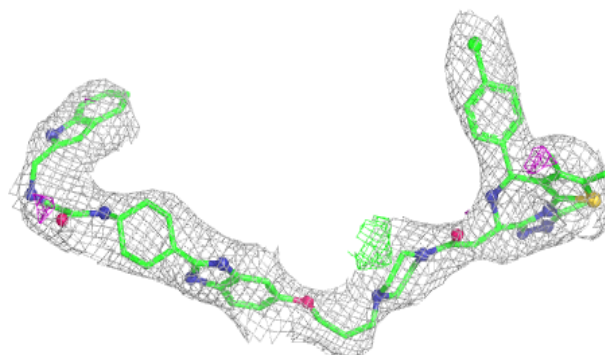
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around YBI G 301:

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

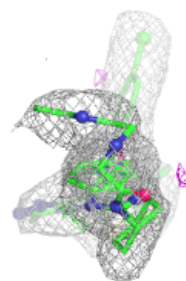
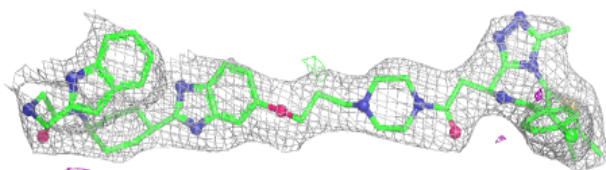
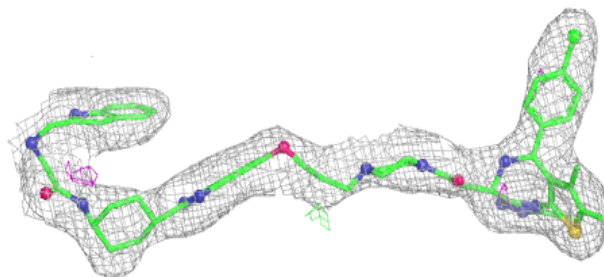
**Electron density around YBI E 301:**

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

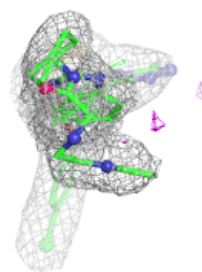
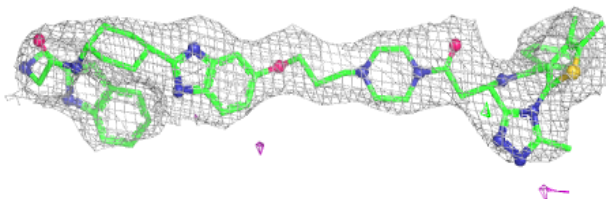
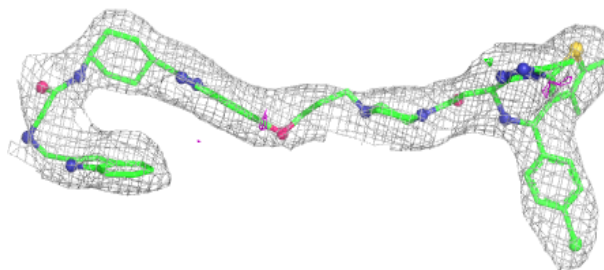


Electron density around YBI A 301:

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

**Electron density around YBI 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.