



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:17 AM UTC

PDB ID : 8SL7 / pdb_00008sl7
Title : Butyricicoccus sp. BIOML-A1 tryptophanase complex with (3S) ALG-05
Authors : Graboski, A.L.; Redinbo, M.R.
Deposited on : 2023-04-21
Resolution : 2.07 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

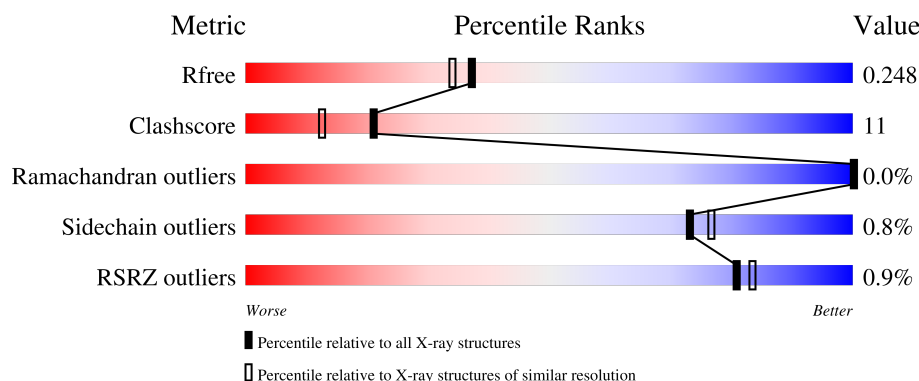
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.07 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	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

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	569	75% 20% 5%
1	B	569	% 78% 17% 5%
1	C	569	% 70% 25% 5%
1	D	569	% 72% 23% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17370 atoms, of which 64 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 Tryptophanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	541	Total	C	N	O	S	0	0	0
			4159	2639	718	772	30			
1	B	543	Total	C	N	O	S	0	0	0
			4147	2627	712	777	31			
1	C	543	Total	C	N	O	S	0	0	0
			4158	2637	722	769	30			
1	D	544	Total	C	N	O	S	0	0	0
			4211	2670	723	788	30			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	HIS	-	expression tag	UNP A0A845MXR5
A	-19	HIS	-	expression tag	UNP A0A845MXR5
A	-18	HIS	-	expression tag	UNP A0A845MXR5
A	-17	HIS	-	expression tag	UNP A0A845MXR5
A	-16	HIS	-	expression tag	UNP A0A845MXR5
A	-15	HIS	-	expression tag	UNP A0A845MXR5
A	-14	SER	-	expression tag	UNP A0A845MXR5
A	-13	SER	-	expression tag	UNP A0A845MXR5
A	-12	GLY	-	expression tag	UNP A0A845MXR5
A	-11	VAL	-	expression tag	UNP A0A845MXR5
A	-10	ASP	-	expression tag	UNP A0A845MXR5
A	-9	LEU	-	expression tag	UNP A0A845MXR5
A	-8	GLY	-	expression tag	UNP A0A845MXR5
A	-7	THR	-	expression tag	UNP A0A845MXR5
A	-6	GLU	-	expression tag	UNP A0A845MXR5
A	-5	ASN	-	expression tag	UNP A0A845MXR5
A	-4	LEU	-	expression tag	UNP A0A845MXR5
A	-3	TYR	-	expression tag	UNP A0A845MXR5
A	-2	PHE	-	expression tag	UNP A0A845MXR5
A	-1	GLN	-	expression tag	UNP A0A845MXR5
A	0	SER	-	expression tag	UNP A0A845MXR5

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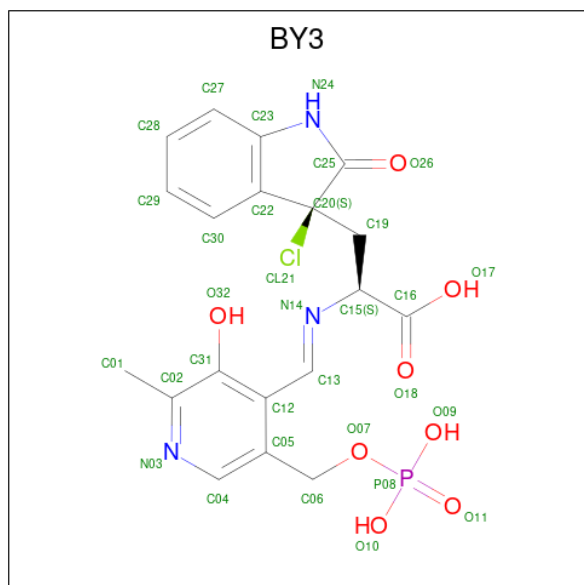
Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	HIS	-	expression tag	UNP A0A845MXR5
B	-19	HIS	-	expression tag	UNP A0A845MXR5
B	-18	HIS	-	expression tag	UNP A0A845MXR5
B	-17	HIS	-	expression tag	UNP A0A845MXR5
B	-16	HIS	-	expression tag	UNP A0A845MXR5
B	-15	HIS	-	expression tag	UNP A0A845MXR5
B	-14	SER	-	expression tag	UNP A0A845MXR5
B	-13	SER	-	expression tag	UNP A0A845MXR5
B	-12	GLY	-	expression tag	UNP A0A845MXR5
B	-11	VAL	-	expression tag	UNP A0A845MXR5
B	-10	ASP	-	expression tag	UNP A0A845MXR5
B	-9	LEU	-	expression tag	UNP A0A845MXR5
B	-8	GLY	-	expression tag	UNP A0A845MXR5
B	-7	THR	-	expression tag	UNP A0A845MXR5
B	-6	GLU	-	expression tag	UNP A0A845MXR5
B	-5	ASN	-	expression tag	UNP A0A845MXR5
B	-4	LEU	-	expression tag	UNP A0A845MXR5
B	-3	TYR	-	expression tag	UNP A0A845MXR5
B	-2	PHE	-	expression tag	UNP A0A845MXR5
B	-1	GLN	-	expression tag	UNP A0A845MXR5
B	0	SER	-	expression tag	UNP A0A845MXR5
C	-20	HIS	-	expression tag	UNP A0A845MXR5
C	-19	HIS	-	expression tag	UNP A0A845MXR5
C	-18	HIS	-	expression tag	UNP A0A845MXR5
C	-17	HIS	-	expression tag	UNP A0A845MXR5
C	-16	HIS	-	expression tag	UNP A0A845MXR5
C	-15	HIS	-	expression tag	UNP A0A845MXR5
C	-14	SER	-	expression tag	UNP A0A845MXR5
C	-13	SER	-	expression tag	UNP A0A845MXR5
C	-12	GLY	-	expression tag	UNP A0A845MXR5
C	-11	VAL	-	expression tag	UNP A0A845MXR5
C	-10	ASP	-	expression tag	UNP A0A845MXR5
C	-9	LEU	-	expression tag	UNP A0A845MXR5
C	-8	GLY	-	expression tag	UNP A0A845MXR5
C	-7	THR	-	expression tag	UNP A0A845MXR5
C	-6	GLU	-	expression tag	UNP A0A845MXR5
C	-5	ASN	-	expression tag	UNP A0A845MXR5
C	-4	LEU	-	expression tag	UNP A0A845MXR5
C	-3	TYR	-	expression tag	UNP A0A845MXR5
C	-2	PHE	-	expression tag	UNP A0A845MXR5
C	-1	GLN	-	expression tag	UNP A0A845MXR5
C	0	SER	-	expression tag	UNP A0A845MXR5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-20	HIS	-	expression tag	UNP A0A845MXR5
D	-19	HIS	-	expression tag	UNP A0A845MXR5
D	-18	HIS	-	expression tag	UNP A0A845MXR5
D	-17	HIS	-	expression tag	UNP A0A845MXR5
D	-16	HIS	-	expression tag	UNP A0A845MXR5
D	-15	HIS	-	expression tag	UNP A0A845MXR5
D	-14	SER	-	expression tag	UNP A0A845MXR5
D	-13	SER	-	expression tag	UNP A0A845MXR5
D	-12	GLY	-	expression tag	UNP A0A845MXR5
D	-11	VAL	-	expression tag	UNP A0A845MXR5
D	-10	ASP	-	expression tag	UNP A0A845MXR5
D	-9	LEU	-	expression tag	UNP A0A845MXR5
D	-8	GLY	-	expression tag	UNP A0A845MXR5
D	-7	THR	-	expression tag	UNP A0A845MXR5
D	-6	GLU	-	expression tag	UNP A0A845MXR5
D	-5	ASN	-	expression tag	UNP A0A845MXR5
D	-4	LEU	-	expression tag	UNP A0A845MXR5
D	-3	TYR	-	expression tag	UNP A0A845MXR5
D	-2	PHE	-	expression tag	UNP A0A845MXR5
D	-1	GLN	-	expression tag	UNP A0A845MXR5
D	0	SER	-	expression tag	UNP A0A845MXR5

- Molecule 2 is (E)-3-[(3S)-3-chloro-2-oxo-2,3-dihydro-1H-indol-3-yl]-N-({3-hydroxy-2-methyl-5-[(phosphonooxy)methyl]pyridin-4-yl}methylidene)-L-alanine (CCD ID: BY3) (formula: C₁₉H₁₉ClN₃O₈P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	A	1	Total 48	C 19	Cl 1	H 16	N 3	O 8	P 1	0	0
2	B	1	Total 48	C 19	Cl 1	H 16	N 3	O 8	P 1	0	0
2	C	1	Total 48	C 19	Cl 1	H 16	N 3	O 8	P 1	0	0
2	D	1	Total 48	C 19	Cl 1	H 16	N 3	O 8	P 1	0	0

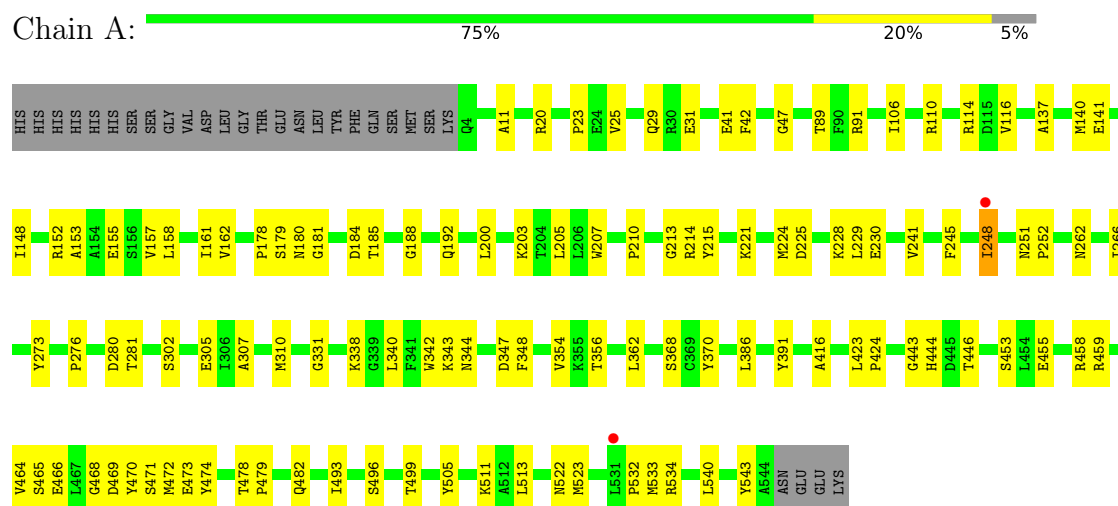
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	148	Total 148	O 148	0	0
3	B	139	Total 139	O 139	0	0
3	C	101	Total 101	O 101	0	0
3	D	115	Total 115	O 115	0	0

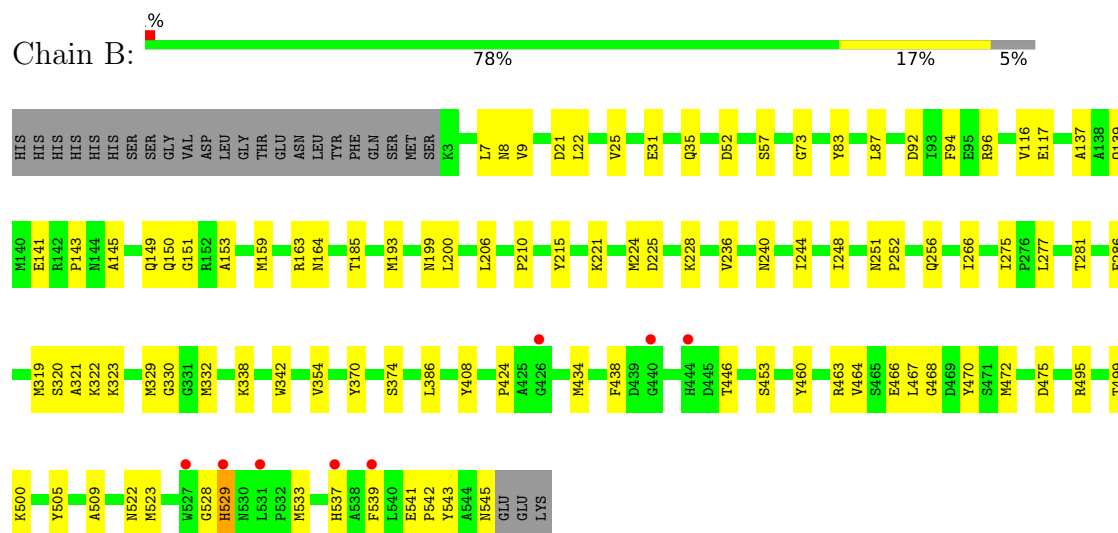
3 Residue-property plots

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: Tryptophanase

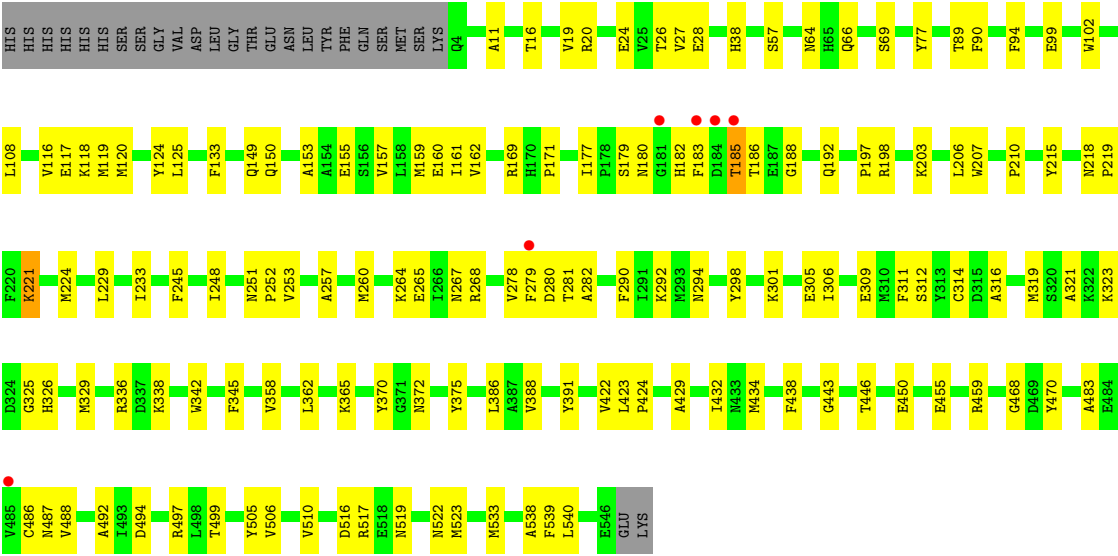


• Molecule 1: Tryptophanase

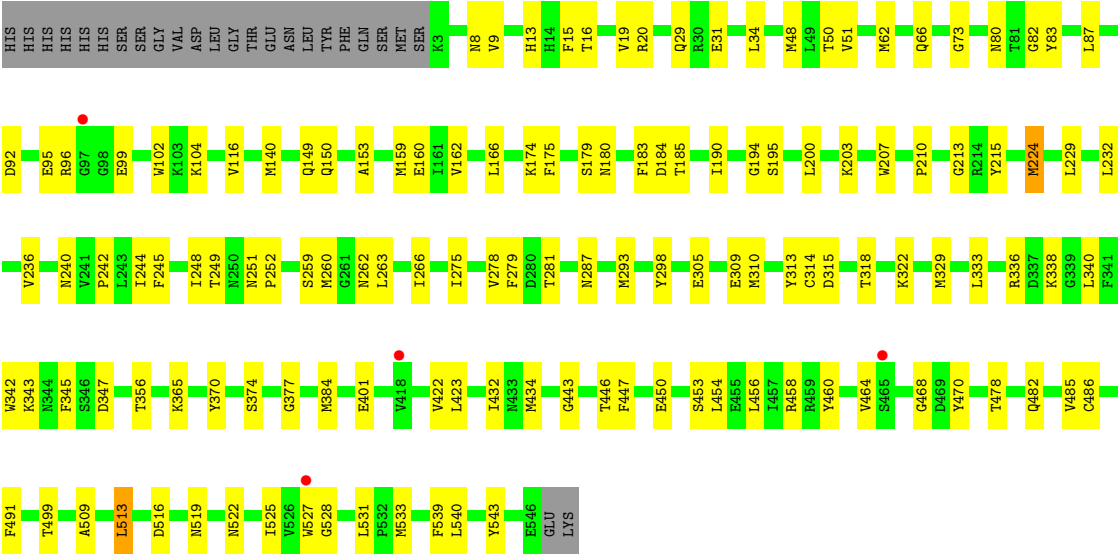


• Molecule 1: Tryptophanase





● Molecule 1: Tryptophanase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	62.64Å 93.95Å 105.60Å 65.24° 88.01° 74.30°	Depositor
Resolution (Å)	44.77 – 2.07 44.77 – 2.07	Depositor EDS
% Data completeness (in resolution range)	95.3 (44.77-2.07) 95.3 (44.77-2.07)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 2.07Å)	Xtriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
R, R_{free}	0.203 , 0.247 0.204 , 0.248	Depositor DCC
R_{free} test set	2000 reflections (1.56%)	wwPDB-VP
Wilson B-factor (Å ²)	45.7	Xtriage
Anisotropy	0.249	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 40.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	17370	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.36% 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: BY3

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	0.48	0/4256	0.67	0/5771
1	B	0.52	0/4242	0.73	0/5754
1	C	0.45	0/4257	0.66	0/5776
1	D	0.49	0/4311	0.67	0/5847
All	All	0.49	0/17066	0.68	0/23148

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	4159	0	3919	89	0
1	B	4147	0	3871	69	0
1	C	4158	0	3883	110	0
1	D	4211	0	3952	111	0
2	A	32	16	0	3	0
2	B	32	16	0	2	0
2	C	32	16	0	4	0
2	D	32	16	0	2	0
3	A	148	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	139	0	0	0	0
3	C	101	0	0	2	0
3	D	115	0	0	4	0
All	All	17306	64	15625	356	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 11.

All (356) 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:D:260:MET:HE3	1:D:313:TYR:HE2	1.15	1.10
1:B:145:ALA:HB1	1:B:332:MET:HE1	1.45	0.99
1:D:185:THR:HA	1:D:533:MET:HE3	1.49	0.95
1:D:260:MET:HE3	1:D:313:TYR:CE2	2.01	0.95
1:A:161:ILE:HG13	1:A:362:LEU:HD23	1.46	0.95
1:A:185:THR:HA	1:A:533:MET:HE2	1.51	0.92
1:A:499:THR:HG21	1:C:499:THR:HG21	1.50	0.90
1:D:185:THR:HA	1:D:533:MET:CE	2.01	0.89
1:D:13:HIS:HB2	1:D:401:GLU:OE1	1.71	0.88
1:C:282:ALA:HB1	1:C:323:LYS:HD3	1.59	0.84
1:D:104:LYS:HE2	3:D:717:HOH:O	1.76	0.84
1:D:174:LYS:HD2	1:D:194:GLY:O	1.78	0.82
1:A:137:ALA:O	1:A:141:GLU:HG3	1.80	0.82
1:A:342:TRP:CZ2	1:A:354:VAL:HG11	2.15	0.82
1:B:499:THR:HG21	1:D:499:THR:HG21	1.61	0.81
1:B:210:PRO:HG3	1:B:215:TYR:CE2	2.18	0.79
1:C:358:VAL:O	1:C:362:LEU:HD13	1.84	0.78
1:D:244:ILE:HG13	1:D:275:ILE:HG21	1.66	0.78
1:C:117:GLU:HA	1:C:120:MET:HE2	1.66	0.77
1:C:338:LYS:HA	1:C:342:TRP:CE3	2.21	0.76
1:D:34:LEU:HD22	1:D:454:LEU:HD12	1.70	0.74
1:C:117:GLU:HG2	1:D:29:GLN:HE21	1.51	0.73
1:C:116:VAL:O	1:C:120:MET:HG3	1.88	0.73
1:D:260:MET:HE1	1:D:309:GLU:C	2.12	0.73
1:A:210:PRO:HG3	1:A:215:TYR:CD1	2.24	0.73
1:C:28:GLU:CD	1:C:28:GLU:H	1.97	0.73
1:C:506:VAL:O	1:C:510:VAL:HG23	1.88	0.73
1:D:516:ASP:OD1	1:D:519:ASN:HB2	1.89	0.72
1:B:210:PRO:HG3	1:B:215:TYR:CD2	2.26	0.71
1:C:422:VAL:O	1:C:423:LEU:HD23	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:460:TYR:CD2	1:B:509:ALA:HB1	2.27	0.70
1:A:225:ASP:OD2	1:A:228:LYS:HE3	1.92	0.69
1:C:185:THR:HA	1:C:533:MET:HE3	1.75	0.69
1:A:106:ILE:HG12	1:A:110:ARG:HD2	1.73	0.69
1:B:541:GLU:HG2	1:B:542:PRO:HD2	1.76	0.68
1:A:444:HIS:ND1	1:A:469:ASP:OD2	2.22	0.68
1:D:149:GLN:HG2	1:D:150:GLN:HG2	1.76	0.68
1:A:251:ASN:ND2	3:A:702:HOH:O	2.27	0.67
1:A:473:GLU:HA	1:A:534:ARG:NH2	2.10	0.67
1:A:342:TRP:HZ2	1:A:354:VAL:HG11	1.60	0.66
1:A:302:SER:OG	1:A:305:GLU:HG3	1.96	0.66
1:D:450:GLU:O	1:D:454:LEU:HD23	1.95	0.65
1:B:145:ALA:HB1	1:B:332:MET:CE	2.24	0.65
1:A:158:LEU:O	1:A:162:VAL:HG23	1.96	0.64
1:B:523:MET:HE1	1:B:542:PRO:HB3	1.79	0.64
1:D:432:ILE:HG22	1:D:434:MET:CE	2.28	0.64
1:C:443:GLY:H	1:C:446:THR:HG21	1.61	0.63
1:C:278:VAL:HG22	1:C:316:ALA:HB3	1.80	0.63
1:B:466:GLU:OE1	1:B:470:TYR:HB3	1.99	0.63
1:C:161:ILE:HG21	1:C:362:LEU:CD1	2.29	0.63
1:C:161:ILE:HG13	1:C:362:LEU:HD12	1.81	0.62
1:A:161:ILE:HG13	1:A:362:LEU:CD2	2.25	0.62
1:A:205:LEU:HG	1:A:221:LYS:HG2	1.80	0.62
1:A:42:PHE:HE2	2:A:601:BY3:C29	2.12	0.62
1:B:137:ALA:O	1:B:141:GLU:HG3	2.00	0.62
1:D:210:PRO:HG3	1:D:215:TYR:CD2	2.35	0.61
1:C:27:VAL:HG23	3:C:774:HOH:O	1.99	0.61
1:C:292:LYS:HB2	1:C:306:ILE:CD1	2.31	0.61
1:C:161:ILE:HG21	1:C:362:LEU:HD11	1.83	0.60
1:D:50:THR:HG22	1:D:51:VAL:HG23	1.83	0.60
1:D:460:TYR:CD2	1:D:509:ALA:HB1	2.37	0.60
1:C:446:THR:HB	1:C:522:ASN:ND2	2.16	0.60
1:C:311:PHE:O	1:C:336:ARG:NH2	2.34	0.60
1:D:522:ASN:HB2	1:D:543:TYR:CE2	2.37	0.60
1:D:260:MET:HG2	1:D:298:TYR:OH	2.02	0.60
1:A:114:ARG:HH12	1:B:21:ASP:CB	2.15	0.59
1:D:347:ASP:HB2	1:D:356:THR:HB	1.84	0.59
1:C:251:ASN:HB3	1:C:252:PRO:HD3	1.84	0.59
1:A:453:SER:HB2	1:A:464:VAL:HG23	1.84	0.59
1:D:434:MET:HE2	1:D:434:MET:HA	1.85	0.59
1:C:160:GLU:CD	1:C:365:LYS:HE2	2.28	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:TYR:OH	1:A:540:LEU:HD21	2.04	0.58
1:D:446:THR:HB	1:D:522:ASN:OD1	2.03	0.58
1:A:348:PHE:CE1	1:A:354:VAL:HG12	2.38	0.58
1:B:31:GLU:O	1:B:35:GLN:HG2	2.03	0.58
1:D:92:ASP:HA	1:D:96:ARG:HG3	1.85	0.58
1:B:321:ALA:HB1	1:B:386:LEU:HD11	1.84	0.58
1:C:26:THR:HB	1:C:28:GLU:OE1	2.04	0.58
1:C:257:ALA:HB2	1:C:290:PHE:CD2	2.40	0.57
1:D:150:GLN:HB2	2:D:601:BY3:O10	2.05	0.57
1:B:468:GLY:O	1:B:472:MET:HB2	2.04	0.57
1:A:203:LYS:NZ	1:A:207:TRP:HE1	2.02	0.57
1:C:443:GLY:O	1:C:446:THR:HG23	2.05	0.56
1:C:455:GLU:OE1	1:C:459:ARG:NE	2.35	0.56
1:B:8:ASN:OD1	1:B:9:VAL:HG23	2.05	0.56
1:C:117:GLU:HG2	1:D:29:GLN:NE2	2.17	0.56
1:A:473:GLU:HA	1:A:534:ARG:HH21	1.71	0.56
1:A:496:SER:HB3	1:C:19:VAL:HG11	1.87	0.56
1:D:180:ASN:HB3	1:D:224:MET:HB2	1.88	0.56
1:C:523:MET:HE3	1:C:523:MET:HA	1.87	0.56
1:B:206:LEU:HA	1:B:221:LYS:HD3	1.88	0.56
1:C:470:TYR:OH	1:C:538:ALA:HB3	2.04	0.56
1:D:175:PHE:HB3	1:D:242:PRO:HD3	1.87	0.56
1:A:106:ILE:O	1:A:110:ARG:HG3	2.05	0.56
1:B:541:GLU:HG2	1:B:542:PRO:CD	2.36	0.56
1:A:25:VAL:HG22	1:B:116:VAL:HG21	1.88	0.55
1:A:205:LEU:O	1:A:221:LYS:HE2	2.05	0.55
1:A:188:GLY:O	1:A:192:GLN:HG3	2.07	0.55
1:C:372:ASN:HB3	1:C:375:TYR:CE1	2.40	0.55
1:C:38:HIS:HB2	1:D:140:MET:HE1	1.88	0.55
1:C:229:LEU:HD11	1:C:233:ILE:HD11	1.88	0.55
1:B:215:TYR:CD2	1:B:424:PRO:HD3	2.42	0.55
1:C:20:ARG:NH2	1:D:73:GLY:O	2.36	0.55
1:D:236:VAL:O	1:D:240:ASN:ND2	2.37	0.55
1:D:160:GLU:CD	1:D:365:LYS:HE2	2.32	0.55
1:D:185:THR:HA	1:D:533:MET:HE1	1.88	0.55
1:B:251:ASN:HB3	1:B:252:PRO:HD3	1.88	0.54
1:C:219:PRO:HG2	1:C:221:LYS:HE3	1.89	0.54
1:D:20:ARG:NE	3:D:703:HOH:O	2.40	0.54
1:B:225:ASP:CG	1:B:228:LYS:HD3	2.32	0.54
1:C:279:PHE:CD2	1:C:314:CYS:HB3	2.42	0.54
1:C:309:GLU:O	1:C:312:SER:OG	2.24	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:VAL:O	1:A:161:ILE:HG12	2.07	0.54
1:A:161:ILE:CG1	1:A:362:LEU:HD23	2.28	0.54
1:C:229:LEU:CD1	1:C:233:ILE:HD11	2.37	0.54
1:D:432:ILE:HG22	1:D:434:MET:HE2	1.89	0.54
1:A:42:PHE:CE2	2:A:601:BY3:C29	2.91	0.54
1:D:13:HIS:CB	1:D:401:GLU:OE1	2.51	0.54
1:D:516:ASP:OD1	1:D:516:ASP:O	2.26	0.54
1:D:340:LEU:HA	1:D:343:LYS:HE3	1.91	0.53
1:D:293:MET:HE2	1:D:293:MET:HA	1.89	0.53
1:D:249:THR:HG22	1:D:287:ASN:HB2	1.89	0.53
1:A:416:ALA:HB1	1:A:511:LYS:HD2	1.91	0.53
1:D:305:GLU:HG2	3:D:795:HOH:O	2.09	0.53
1:B:244:ILE:O	1:B:277:LEU:HD12	2.08	0.53
1:D:443:GLY:H	1:D:446:THR:CG2	2.22	0.53
1:A:200:LEU:HD23	1:A:229:LEU:N	2.24	0.53
1:A:455:GLU:OE2	1:A:459:ARG:NE	2.39	0.53
1:A:200:LEU:CD2	1:A:229:LEU:HA	2.39	0.52
1:B:523:MET:HE3	1:B:541:GLU:C	2.35	0.52
1:C:169:ARG:C	1:C:171:PRO:HD3	2.34	0.52
1:C:179:SER:HB2	1:C:245:PHE:HB2	1.92	0.52
1:A:203:LYS:HZ1	1:A:207:TRP:HE1	1.57	0.52
1:C:90:PHE:HB3	1:C:133:PHE:CZ	2.45	0.52
1:B:94:PHE:CZ	1:B:319:MET:HE1	2.45	0.51
1:B:522:ASN:HB2	1:B:543:TYR:CE1	2.45	0.51
1:C:77:TYR:OH	2:D:601:BY3:CL21	2.59	0.51
1:C:183:PHE:HA	1:C:252:PRO:HG3	1.92	0.51
1:A:152:ARG:HA	1:A:155:GLU:HG2	1.92	0.51
1:B:244:ILE:HG13	1:B:275:ILE:HG21	1.93	0.51
1:C:108:LEU:HD21	1:C:118:LYS:HE2	1.93	0.51
1:C:149:GLN:HG2	1:C:150:GLN:HG2	1.91	0.51
1:A:338:LYS:HA	1:A:342:TRP:CE3	2.46	0.51
1:B:225:ASP:OD2	1:B:228:LYS:HD3	2.11	0.51
1:C:443:GLY:H	1:C:446:THR:CG2	2.24	0.51
1:B:150:GLN:HB2	2:B:601:BY3:O10	2.11	0.51
1:A:210:PRO:HD3	1:A:215:TYR:CE1	2.45	0.51
1:A:470:TYR:CZ	1:A:540:LEU:HD21	2.45	0.51
1:C:290:PHE:O	1:C:294:ASN:ND2	2.42	0.51
1:C:188:GLY:O	1:C:192:GLN:HG3	2.11	0.50
1:C:321:ALA:HB1	1:C:386:LEU:HD11	1.92	0.50
1:A:474:TYR:CD1	1:A:482:GLN:HG2	2.46	0.50
1:B:248:ILE:HD11	1:B:281:THR:HG22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:153:ALA:HB1	1:C:370:TYR:CE1	2.46	0.50
1:D:244:ILE:HG13	1:D:275:ILE:CG2	2.39	0.50
1:D:248:ILE:HG23	1:D:287:ASN:CB	2.41	0.50
1:D:80:ASN:OD1	1:D:80:ASN:C	2.54	0.50
1:A:213:GLY:C	1:A:214:ARG:HG3	2.36	0.50
1:B:153:ALA:HB1	1:B:370:TYR:CE2	2.46	0.50
1:D:251:ASN:HB3	1:D:252:PRO:HD3	1.93	0.50
1:A:153:ALA:HB1	1:A:370:TYR:CE2	2.47	0.50
1:C:264:LYS:HE3	3:C:738:HOH:O	2.12	0.50
1:D:190:ILE:HG23	1:D:195:SER:HB2	1.93	0.50
1:C:248:ILE:HG13	1:C:248:ILE:O	2.12	0.50
1:D:315:ASP:HA	1:D:336:ARG:HG3	1.93	0.50
1:D:453:SER:OG	1:D:464:VAL:HG23	2.12	0.50
1:B:92:ASP:OD1	1:B:96:ARG:NH1	2.42	0.50
1:B:466:GLU:OE2	1:B:468:GLY:N	2.43	0.49
1:C:207:TRP:HZ3	1:C:422:VAL:HG22	1.77	0.49
1:D:232:LEU:O	1:D:236:VAL:HG22	2.12	0.49
1:B:236:VAL:O	1:B:240:ASN:OD1	2.30	0.49
1:C:450:GLU:HG2	1:C:540:LEU:CD1	2.41	0.49
1:D:159:MET:HE3	1:D:190:ILE:HG12	1.95	0.49
1:A:20:ARG:NH2	1:B:73:GLY:O	2.33	0.49
1:B:522:ASN:ND2	1:B:545:ASN:HA	2.27	0.49
1:D:443:GLY:H	1:D:446:THR:HG23	1.77	0.49
1:A:91:ARG:NH2	3:A:707:HOH:O	2.42	0.49
1:D:82:GLY:CA	1:D:384:MET:HE2	2.42	0.49
1:B:523:MET:HE1	1:B:542:PRO:CB	2.42	0.49
1:A:31:GLU:OE2	1:A:458:ARG:NH1	2.46	0.48
1:C:301:LYS:HA	1:C:305:GLU:OE2	2.14	0.48
1:D:179:SER:HA	1:D:245:PHE:O	2.13	0.48
1:A:368:SER:HB3	1:B:533:MET:CE	2.43	0.48
1:C:57:SER:HB2	1:C:323:LYS:HE3	1.95	0.48
1:D:62:MET:HB3	1:D:66:GLN:HB2	1.95	0.48
1:C:177:ILE:O	1:C:182:HIS:HE1	1.97	0.48
1:C:218:ASN:ND2	1:C:424:PRO:HG2	2.29	0.48
1:C:338:LYS:HA	1:C:342:TRP:CD2	2.49	0.48
1:A:41:GLU:OE1	1:A:465:SER:HA	2.14	0.48
1:A:180:ASN:HB3	1:A:224:MET:HG3	1.96	0.47
1:B:22:LEU:HD21	1:D:15:PHE:CD1	2.48	0.47
1:C:24:GLU:O	1:D:116:VAL:HG21	2.14	0.47
1:B:22:LEU:HD21	1:D:15:PHE:HD1	1.79	0.47
1:B:52:ASP:OD1	1:B:463:ARG:NH2	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:408:TYR:CE2	1:B:500:LYS:HE2	2.49	0.47
1:D:153:ALA:HB1	1:D:370:TYR:CE2	2.48	0.47
1:D:432:ILE:CG2	1:D:434:MET:CE	2.92	0.47
1:A:347:ASP:HB2	1:A:356:THR:HB	1.97	0.47
1:B:528:GLY:O	1:B:529:HIS:CB	2.62	0.47
1:C:253:VAL:HG12	1:C:253:VAL:O	2.14	0.47
1:B:163:ARG:NH2	1:B:164:ASN:OD1	2.47	0.47
1:D:207:TRP:HZ3	1:D:422:VAL:HG22	1.79	0.47
1:D:338:LYS:HA	1:D:342:TRP:CE3	2.49	0.47
1:B:342:TRP:HZ2	1:B:354:VAL:HG21	1.80	0.47
1:B:7:LEU:HD11	1:D:509:ALA:HB2	1.96	0.46
1:B:224:MET:HE3	1:B:266:ILE:HD13	1.96	0.46
1:D:322:LYS:HG2	1:D:329:MET:HA	1.96	0.46
1:C:280:ASP:C	1:C:280:ASP:OD1	2.59	0.46
1:A:468:GLY:O	1:A:472:MET:HB2	2.16	0.46
1:D:200:LEU:CD1	1:D:229:LEU:HA	2.46	0.46
1:D:527:TRP:CE3	1:D:528:GLY:N	2.84	0.46
1:A:221:LYS:NZ	1:A:423:LEU:O	2.44	0.46
1:B:163:ARG:HB2	1:B:193:MET:HE3	1.97	0.46
1:A:23:PRO:HG3	1:A:47:GLY:O	2.16	0.46
1:A:533:MET:HB2	3:A:741:HOH:O	2.15	0.46
1:D:525:ILE:HA	1:D:540:LEU:HD23	1.98	0.46
1:C:89:THR:HG23	1:C:391:TYR:CZ	2.51	0.46
1:C:265:GLU:OE2	1:C:268:ARG:NH2	2.47	0.46
1:A:532:PRO:O	1:A:533:MET:HB2	2.16	0.46
1:C:539:PHE:O	1:C:540:LEU:HD23	2.17	0.46
1:D:279:PHE:CD2	1:D:314:CYS:HB3	2.50	0.46
1:C:99:GLU:HG3	1:C:102:TRP:CH2	2.51	0.45
1:C:149:GLN:HG2	1:C:150:GLN:N	2.29	0.45
1:C:494:ASP:OD1	1:C:497:ARG:NE	2.35	0.45
1:D:279:PHE:HB3	1:D:281:THR:HG23	1.98	0.45
1:C:438:PHE:CE1	1:C:517:ARG:HB2	2.52	0.45
1:A:474:TYR:CE1	1:A:482:GLN:HG2	2.51	0.45
1:B:522:ASN:O	1:B:542:PRO:HA	2.17	0.45
1:D:83:TYR:CD1	1:D:374:SER:HA	2.51	0.45
1:A:11:ALA:HB2	1:C:505:TYR:CE2	2.51	0.45
1:A:20:ARG:HG3	1:C:64:ASN:OD1	2.17	0.45
1:B:221:LYS:HB2	1:B:256:GLN:HG3	1.99	0.45
1:B:329:MET:HG3	1:B:330:GLY:N	2.32	0.45
1:C:248:ILE:HD11	1:C:281:THR:HG22	1.98	0.45
1:D:82:GLY:HA2	1:D:384:MET:HE2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:207:TRP:HZ3	1:D:422:VAL:CG2	2.30	0.45
1:D:468:GLY:HA2	1:D:486:CYS:O	2.17	0.45
1:A:522:ASN:HB2	1:A:543:TYR:CZ	2.52	0.45
1:C:203:LYS:NZ	1:C:483:ALA:O	2.29	0.45
1:D:80:ASN:HB3	3:D:744:HOH:O	2.16	0.45
1:B:149:GLN:HG2	1:B:150:GLN:HG2	1.98	0.44
1:C:26:THR:CB	1:C:28:GLU:OE1	2.65	0.44
1:C:89:THR:HG23	1:C:391:TYR:CE2	2.52	0.44
1:C:265:GLU:CD	1:C:268:ARG:HH21	2.25	0.44
1:C:362:LEU:CD1	1:C:362:LEU:N	2.80	0.44
1:D:432:ILE:HD12	1:D:491:PHE:CE1	2.52	0.44
1:A:89:THR:HG23	1:A:391:TYR:CZ	2.52	0.44
1:A:307:ALA:HA	1:A:310:MET:HE2	2.00	0.44
1:C:28:GLU:CD	1:C:28:GLU:N	2.73	0.44
1:D:259:SER:O	1:D:263:LEU:HG	2.18	0.44
1:D:450:GLU:OE1	1:D:450:GLU:HA	2.17	0.44
1:A:423:LEU:HA	1:A:424:PRO:C	2.42	0.44
1:A:443:GLY:H	1:A:446:THR:HG21	1.81	0.44
1:C:210:PRO:HD3	1:C:215:TYR:CE1	2.53	0.44
1:C:362:LEU:HD12	1:C:362:LEU:N	2.32	0.44
1:D:99:GLU:HG3	1:D:102:TRP:CH2	2.53	0.44
1:D:318:THR:HG22	1:D:333:LEU:HD13	1.99	0.44
1:A:276:PRO:HD3	1:A:344:ASN:ND2	2.32	0.44
1:D:478:THR:O	1:D:482:GLN:HG3	2.18	0.44
1:A:148:ILE:O	1:A:331:GLY:N	2.51	0.44
1:A:340:LEU:HA	1:A:343:LYS:HE2	1.99	0.44
1:D:432:ILE:HD12	1:D:491:PHE:HE1	1.83	0.44
1:C:179:SER:HA	1:C:245:PHE:O	2.17	0.44
1:C:206:LEU:HD22	1:C:253:VAL:HG13	1.99	0.44
1:C:119:MET:HB3	1:C:124:TYR:CE2	2.52	0.43
1:A:184:ASP:N	1:A:184:ASP:OD1	2.52	0.43
1:D:525:ILE:HA	1:D:540:LEU:CD2	2.49	0.43
1:B:446:THR:HB	1:B:522:ASN:OD1	2.18	0.43
1:A:29:GLN:HE21	1:B:117:GLU:HG2	1.84	0.43
1:D:539:PHE:O	1:D:540:LEU:HD23	2.18	0.43
1:B:453:SER:HB2	1:B:464:VAL:HG23	1.99	0.43
1:C:260:MET:HG2	1:C:298:TYR:OH	2.18	0.43
1:D:16:THR:HG21	1:D:19:VAL:CG1	2.48	0.43
1:D:183:PHE:CD2	1:D:184:ASP:OD2	2.72	0.43
1:B:83:TYR:CD1	1:B:374:SER:HA	2.53	0.43
1:C:323:LYS:NZ	2:C:601:BY3:C13	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:429:ALA:HB2	1:C:492:ALA:HA	2.00	0.43
1:D:347:ASP:HB2	1:D:356:THR:CB	2.47	0.43
1:B:286:GLU:OE1	1:B:495:ARG:NH2	2.52	0.43
1:C:124:TYR:C	1:C:125:LEU:HD23	2.43	0.43
1:C:468:GLY:HA2	1:C:486:CYS:O	2.19	0.43
1:D:262:ASN:O	1:D:266:ILE:HD12	2.19	0.43
1:D:513:LEU:HD13	1:D:513:LEU:HA	1.79	0.43
1:A:140:MET:HE2	1:A:140:MET:HB3	1.85	0.43
1:B:434:MET:HE3	1:B:438:PHE:CE1	2.54	0.43
1:A:342:TRP:CZ2	1:A:354:VAL:CG1	2.95	0.43
1:B:322:LYS:HG2	1:B:329:MET:HA	2.00	0.43
1:C:280:ASP:OD2	2:C:601:BY3:N03	2.52	0.42
1:A:141:GLU:HG2	1:B:539:PHE:CZ	2.54	0.42
1:B:453:SER:HB2	1:B:464:VAL:CG2	2.50	0.42
1:B:505:TYR:HA	1:D:9:VAL:HG21	2.01	0.42
1:C:155:GLU:O	1:C:159:MET:HG2	2.19	0.42
1:D:456:LEU:HD23	1:D:513:LEU:HD23	2.01	0.42
1:A:89:THR:HG23	1:A:391:TYR:CE2	2.54	0.42
1:B:151:GLY:HA3	1:B:320:SER:HB2	2.00	0.42
1:D:531:LEU:HD23	1:D:531:LEU:HA	1.89	0.42
1:B:57:SER:HA	1:B:323:LYS:HD2	2.02	0.42
1:D:87:LEU:HA	1:D:87:LEU:HD23	1.77	0.42
1:A:443:GLY:H	1:A:446:THR:CG2	2.32	0.42
1:C:157:VAL:O	1:C:161:ILE:HG12	2.20	0.42
1:C:66:GLN:HA	1:C:69:SER:OG	2.20	0.42
1:D:213:GLY:O	1:D:423:LEU:HD13	2.20	0.42
1:D:539:PHE:N	1:D:539:PHE:CD1	2.86	0.42
1:A:523:MET:HE3	1:A:540:LEU:HB3	2.01	0.42
1:D:447:PHE:CD1	1:D:470:TYR:HB2	2.55	0.42
1:C:329:MET:HE3	1:D:377:GLY:C	2.45	0.42
1:B:467:LEU:HD21	2:B:601:BY3:C28	2.50	0.42
1:C:16:THR:HG21	1:C:19:VAL:HG12	2.02	0.42
1:D:540:LEU:HD23	1:D:540:LEU:HA	1.80	0.42
1:A:478:THR:HB	1:A:479:PRO:CD	2.50	0.41
1:B:338:LYS:HA	1:B:342:TRP:CE3	2.54	0.41
1:B:87:LEU:HD23	1:B:87:LEU:HA	1.89	0.41
1:C:69:SER:OG	1:C:388:VAL:HG21	2.19	0.41
1:D:340:LEU:HA	1:D:340:LEU:HD12	1.84	0.41
1:B:139:GLN:OE1	1:B:143:PRO:HA	2.20	0.41
1:D:260:MET:HE1	1:D:309:GLU:O	2.20	0.41
1:D:525:ILE:HG12	1:D:540:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:GLY:C	1:A:252:PRO:HG2	2.45	0.41
1:A:280:ASP:OD1	2:A:601:BY3:N03	2.53	0.41
1:A:466:GLU:O	1:A:471:SER:OG	2.21	0.41
1:C:323:LYS:HE2	2:C:601:BY3:C13	2.51	0.41
1:C:434:MET:HB2	1:C:487:ASN:ND2	2.35	0.41
1:D:245:PHE:HA	1:D:278:VAL:O	2.21	0.41
1:A:251:ASN:HB3	1:A:252:PRO:HD3	2.02	0.41
1:C:94:PHE:CZ	1:C:319:MET:HE1	2.56	0.41
1:C:150:GLN:HB2	2:C:601:BY3:O10	2.20	0.41
1:A:116:VAL:HG21	1:B:25:VAL:HG22	2.03	0.41
1:A:262:ASN:O	1:A:266:ILE:HG13	2.21	0.41
1:C:323:LYS:C	1:C:325:GLY:H	2.29	0.41
1:D:249:THR:HG22	1:D:287:ASN:CB	2.51	0.41
1:A:248:ILE:HD11	1:A:281:THR:HG22	2.02	0.41
1:B:199:ASN:C	1:B:200:LEU:HD23	2.46	0.41
1:C:161:ILE:HG13	1:C:362:LEU:CD1	2.50	0.41
1:C:162:VAL:HG13	1:C:345:PHE:CE1	2.55	0.41
1:A:148:ILE:HD11	1:A:370:TYR:CG	2.55	0.41
1:D:8:ASN:OD1	1:D:9:VAL:HG13	2.21	0.41
1:D:31:GLU:HG2	1:D:458:ARG:HD2	2.03	0.41
1:D:48:MET:HE2	1:D:48:MET:HB3	1.82	0.41
1:D:162:VAL:HG13	1:D:345:PHE:HE2	1.86	0.41
1:A:178:PRO:HD3	1:A:241:VAL:HG13	2.03	0.41
1:C:264:LYS:O	1:C:267:ASN:HB3	2.21	0.41
1:C:432:ILE:O	1:C:488:VAL:HA	2.21	0.41
1:C:197:PRO:O	1:C:198:ARG:HG2	2.21	0.40
1:D:166:LEU:HD22	1:D:175:PHE:CZ	2.56	0.40
1:D:203:LYS:NZ	1:D:485:VAL:O	2.42	0.40
1:A:179:SER:HB2	1:A:245:PHE:HB2	2.03	0.40
1:C:281:THR:O	1:C:282:ALA:C	2.64	0.40
1:C:516:ASP:OD1	1:C:519:ASN:HB2	2.21	0.40
1:A:230:GLU:OE2	1:A:273:TYR:OH	2.23	0.40
1:A:386:LEU:HD12	1:A:386:LEU:O	2.21	0.40
1:C:180:ASN:N	1:C:224:MET:HE2	2.36	0.40
1:C:207:TRP:CZ3	1:C:422:VAL:HG22	2.55	0.40
1:A:505:TYR:CD2	1:C:11:ALA:HA	2.57	0.40
1:D:260:MET:HE1	1:D:310:MET:N	2.36	0.40
1:A:31:GLU:HG2	1:A:458:ARG:HG3	2.03	0.40
1:D:456:LEU:HD23	1:D:456:LEU:HA	1.71	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	539/569 (95%)	519 (96%)	20 (4%)	0	100	100
1	B	541/569 (95%)	516 (95%)	24 (4%)	1 (0%)	43	38
1	C	541/569 (95%)	514 (95%)	27 (5%)	0	100	100
1	D	542/569 (95%)	521 (96%)	21 (4%)	0	100	100
All	All	2163/2276 (95%)	2070 (96%)	92 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	529	HIS

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	417/479 (87%)	414 (99%)	3 (1%)	76	79
1	B	412/479 (86%)	408 (99%)	4 (1%)	68	71
1	C	411/479 (86%)	407 (99%)	4 (1%)	68	71
1	D	425/479 (89%)	422 (99%)	3 (1%)	76	79
All	All	1665/1916 (87%)	1651 (99%)	14 (1%)	73	77

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	248	ILE
1	A	493	ILE
1	A	513	LEU
1	B	159	MET
1	B	185	THR
1	B	475	ASP
1	B	537	HIS
1	C	185	THR
1	C	186	THR
1	C	221	LYS
1	C	326	HIS
1	D	95	GLU
1	D	224	MET
1	D	513	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	182	HIS
1	A	192	GLN
1	A	240	ASN
1	A	251	ASN
1	B	192	GLN
1	B	240	ASN
1	B	349	ASN
1	C	4	GLN
1	C	101	ASN
1	C	182	HIS
1	C	192	GLN
1	C	231	GLN
1	C	271	HIS
1	C	522	ASN
1	C	545	ASN
1	D	234	GLN
1	D	372	ASN
1	D	405	GLN

5.3.3 RNA ⓘ

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](#)

4 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
2	BY3	B	601	-	32,34,34	3.22	12 (37%)	39,51,51	4.15	13 (33%)
2	BY3	C	601	-	32,34,34	3.09	11 (34%)	39,51,51	3.41	15 (38%)
2	BY3	D	601	-	32,34,34	3.23	14 (43%)	39,51,51	3.43	15 (38%)
2	BY3	A	601	-	32,34,34	3.11	10 (31%)	39,51,51	3.16	10 (25%)

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
2	BY3	B	601	-	-	3/19/36/36	0/3/3/3
2	BY3	C	601	-	-	2/19/36/36	0/3/3/3
2	BY3	D	601	-	-	2/19/36/36	0/3/3/3
2	BY3	A	601	-	-	4/19/36/36	0/3/3/3

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	BY3	C23-N24	10.57	1.57	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	BY3	C23-C22	10.26	1.50	1.39
2	C	601	BY3	C23-N24	10.25	1.57	1.38
2	B	601	BY3	C23-N24	10.12	1.57	1.38
2	A	601	BY3	C23-N24	10.01	1.56	1.38
2	A	601	BY3	C23-C22	9.80	1.50	1.39
2	C	601	BY3	C23-C22	9.75	1.50	1.39
2	D	601	BY3	C23-C22	9.67	1.50	1.39
2	B	601	BY3	C19-C15	5.29	1.59	1.53
2	D	601	BY3	O26-C25	-4.32	1.15	1.22
2	A	601	BY3	O26-C25	-3.98	1.16	1.22
2	D	601	BY3	C19-C15	3.76	1.57	1.53
2	B	601	BY3	O26-C25	-3.69	1.16	1.22
2	C	601	BY3	C30-C22	-3.66	1.34	1.39
2	A	601	BY3	C13-N14	3.62	1.34	1.27
2	C	601	BY3	O26-C25	-3.57	1.16	1.22
2	C	601	BY3	O32-C31	3.18	1.44	1.36
2	A	601	BY3	O32-C31	3.18	1.44	1.36
2	A	601	BY3	C30-C22	-3.13	1.35	1.39
2	D	601	BY3	C13-N14	3.13	1.33	1.27
2	D	601	BY3	O32-C31	2.97	1.43	1.36
2	D	601	BY3	C12-C13	2.96	1.52	1.46
2	B	601	BY3	O32-C31	2.87	1.43	1.36
2	B	601	BY3	C29-C28	2.84	1.44	1.38
2	A	601	BY3	C01-C02	2.79	1.54	1.50
2	C	601	BY3	C12-C05	-2.78	1.38	1.42
2	D	601	BY3	C25-N24	-2.77	1.32	1.35
2	D	601	BY3	C29-C28	2.76	1.44	1.38
2	D	601	BY3	C27-C23	-2.70	1.35	1.39
2	A	601	BY3	C29-C28	2.69	1.44	1.38
2	C	601	BY3	C15-C16	-2.68	1.49	1.52
2	D	601	BY3	C01-C02	2.56	1.54	1.50
2	C	601	BY3	C01-C02	2.56	1.54	1.50
2	B	601	BY3	C27-C23	-2.54	1.35	1.39
2	A	601	BY3	C12-C13	2.52	1.52	1.46
2	C	601	BY3	C29-C28	2.51	1.43	1.38
2	D	601	BY3	C30-C22	-2.47	1.35	1.39
2	B	601	BY3	C12-C13	2.38	1.51	1.46
2	C	601	BY3	P08-O09	-2.37	1.46	1.54
2	C	601	BY3	P08-O10	-2.16	1.46	1.54
2	A	601	BY3	P08-O09	-2.10	1.47	1.54
2	B	601	BY3	C01-C02	2.09	1.53	1.50
2	B	601	BY3	C13-N14	2.08	1.31	1.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	BY3	P08-O07	2.07	1.66	1.60
2	D	601	BY3	P08-O07	2.06	1.66	1.60
2	D	601	BY3	C15-C16	-2.04	1.50	1.52
2	B	601	BY3	P08-O09	-2.03	1.47	1.54

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	BY3	C15-N14-C13	17.01	142.04	116.77
2	D	601	BY3	C23-N24-C25	-11.69	104.12	111.85
2	B	601	BY3	C23-N24-C25	-11.39	104.31	111.85
2	C	601	BY3	C23-N24-C25	-10.56	104.86	111.85
2	A	601	BY3	C23-N24-C25	-10.25	105.07	111.85
2	C	601	BY3	C15-N14-C13	8.74	129.75	116.77
2	D	601	BY3	C19-C15-C16	8.47	123.56	109.48
2	B	601	BY3	C19-C15-N14	8.08	123.72	110.57
2	B	601	BY3	C19-C15-C16	8.01	122.80	109.48
2	A	601	BY3	C15-N14-C13	8.00	128.65	116.77
2	C	601	BY3	C19-C15-C16	7.64	122.18	109.48
2	D	601	BY3	C15-N14-C13	7.56	128.00	116.77
2	D	601	BY3	C19-C15-N14	7.53	122.83	110.57
2	A	601	BY3	O26-C25-N24	-7.21	118.63	126.28
2	A	601	BY3	C22-C23-N24	-6.17	105.46	109.60
2	C	601	BY3	C22-C23-N24	-6.14	105.48	109.60
2	C	601	BY3	C12-C13-N14	6.10	134.70	122.73
2	A	601	BY3	C19-C15-N14	5.72	119.88	110.57
2	B	601	BY3	O26-C25-N24	-5.62	120.31	126.28
2	A	601	BY3	C19-C15-C16	5.27	118.25	109.48
2	D	601	BY3	C22-C20-CL21	-5.14	102.36	110.50
2	C	601	BY3	C12-C31-C02	-5.10	117.27	120.14
2	D	601	BY3	C22-C23-N24	-4.50	106.58	109.60
2	C	601	BY3	O26-C25-N24	-4.50	121.51	126.28
2	D	601	BY3	C27-C23-C22	-3.80	118.37	121.92
2	B	601	BY3	C22-C23-N24	-3.80	107.05	109.60
2	C	601	BY3	C31-C12-C05	3.72	121.27	118.28
2	D	601	BY3	C30-C22-C23	3.69	123.02	119.81
2	B	601	BY3	C12-C31-C02	-3.45	118.20	120.14
2	A	601	BY3	C12-C31-C02	-3.28	118.30	120.14
2	A	601	BY3	C04-N03-C02	3.14	124.90	119.20
2	B	601	BY3	C12-C13-N14	2.98	128.59	122.73
2	C	601	BY3	C22-C20-CL21	-2.92	105.88	110.50
2	A	601	BY3	C05-C04-N03	-2.84	119.22	123.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	BY3	C05-C04-N03	-2.79	119.28	123.83
2	D	601	BY3	C29-C28-C27	2.77	123.65	120.24
2	B	601	BY3	O07-P08-O11	2.64	113.58	106.44
2	C	601	BY3	C27-C23-C22	-2.58	119.51	121.92
2	C	601	BY3	C04-N03-C02	2.54	123.81	119.20
2	B	601	BY3	O17-C16-O18	-2.52	118.36	124.08
2	A	601	BY3	C31-C12-C13	-2.49	115.91	120.40
2	B	601	BY3	C05-C04-N03	-2.47	119.81	123.83
2	D	601	BY3	O09-P08-O07	2.35	112.81	106.67
2	B	601	BY3	C27-C23-C22	-2.30	119.77	121.92
2	B	601	BY3	C04-N03-C02	2.22	123.22	119.20
2	D	601	BY3	O26-C25-N24	-2.20	123.94	126.28
2	C	601	BY3	C31-C12-C13	-2.18	116.46	120.40
2	D	601	BY3	O17-C16-O18	-2.15	119.20	124.08
2	D	601	BY3	C27-C23-N24	2.09	135.05	130.83
2	C	601	BY3	C27-C23-N24	2.06	135.00	130.83
2	C	601	BY3	C01-C02-C31	-2.06	118.39	120.80
2	D	601	BY3	C05-C04-N03	-2.05	120.49	123.83
2	D	601	BY3	C12-C13-N14	2.01	126.69	122.73

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	BY3	C19-C15-N14-C13
2	A	601	BY3	C15-C19-C20-C22
2	A	601	BY3	C15-C19-C20-C25
2	B	601	BY3	C16-C15-N14-C13
2	B	601	BY3	C19-C15-N14-C13
2	C	601	BY3	C05-C12-C13-N14
2	D	601	BY3	C19-C15-N14-C13
2	C	601	BY3	C31-C12-C13-N14
2	B	601	BY3	C06-O07-P08-O11
2	D	601	BY3	N14-C15-C16-O18
2	A	601	BY3	C31-C12-C13-N14

There are no ring outliers.

4 monomers are involved in 11 short contacts:

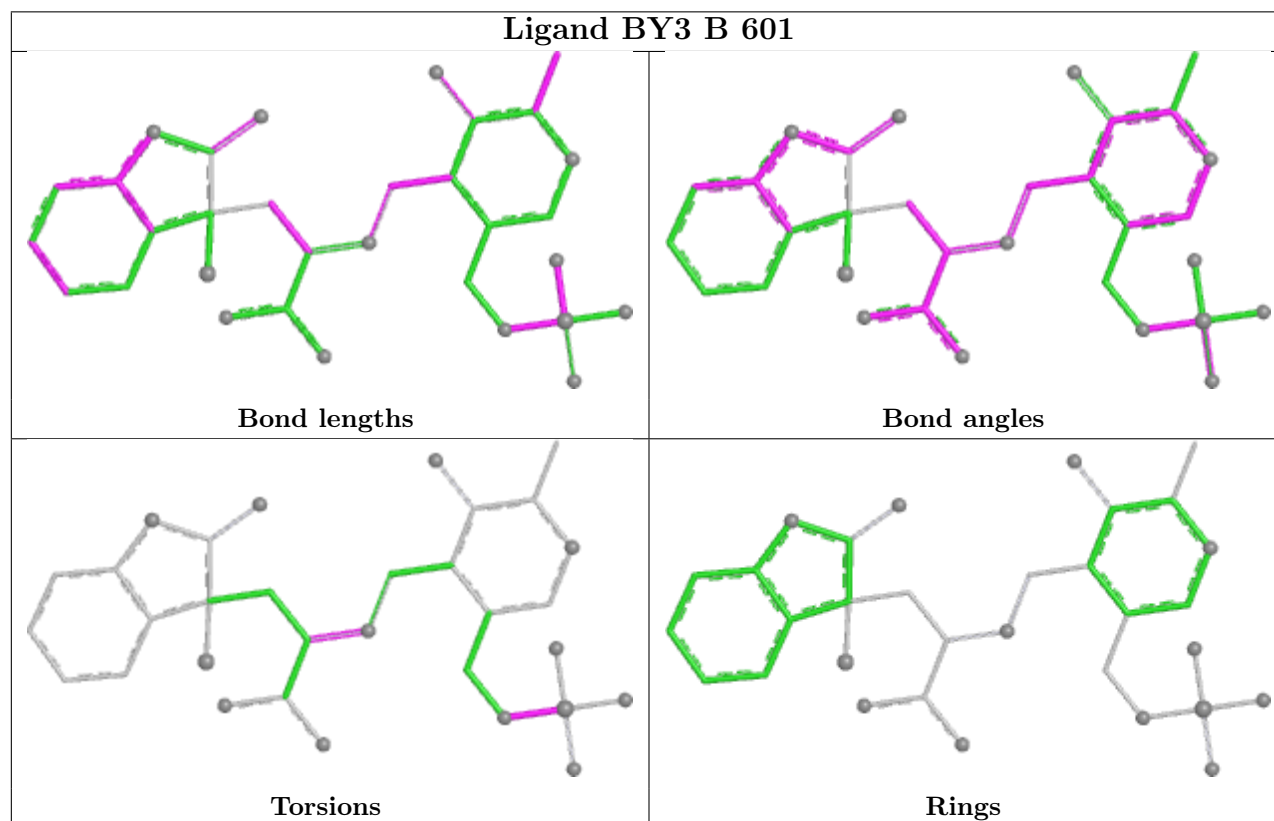
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	BY3	2	0

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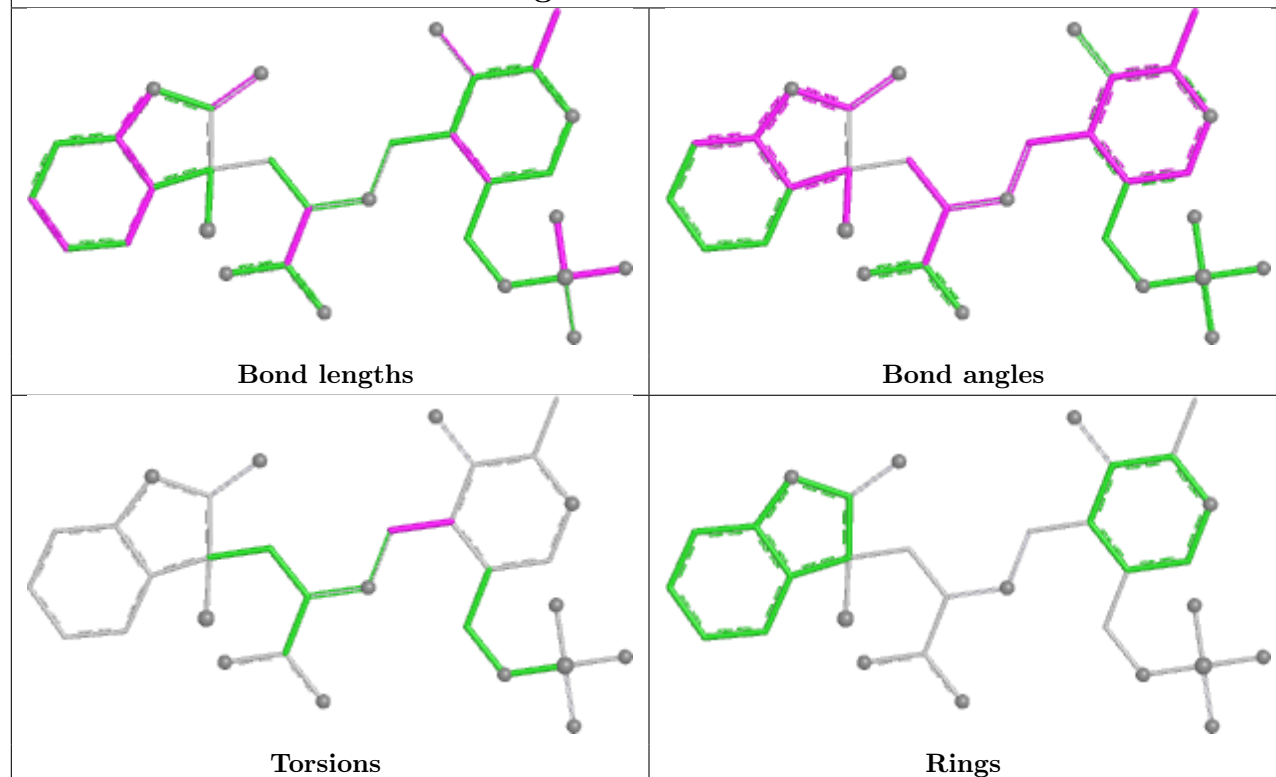
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	601	BY3	4	0
2	D	601	BY3	2	0
2	A	601	BY3	3	0

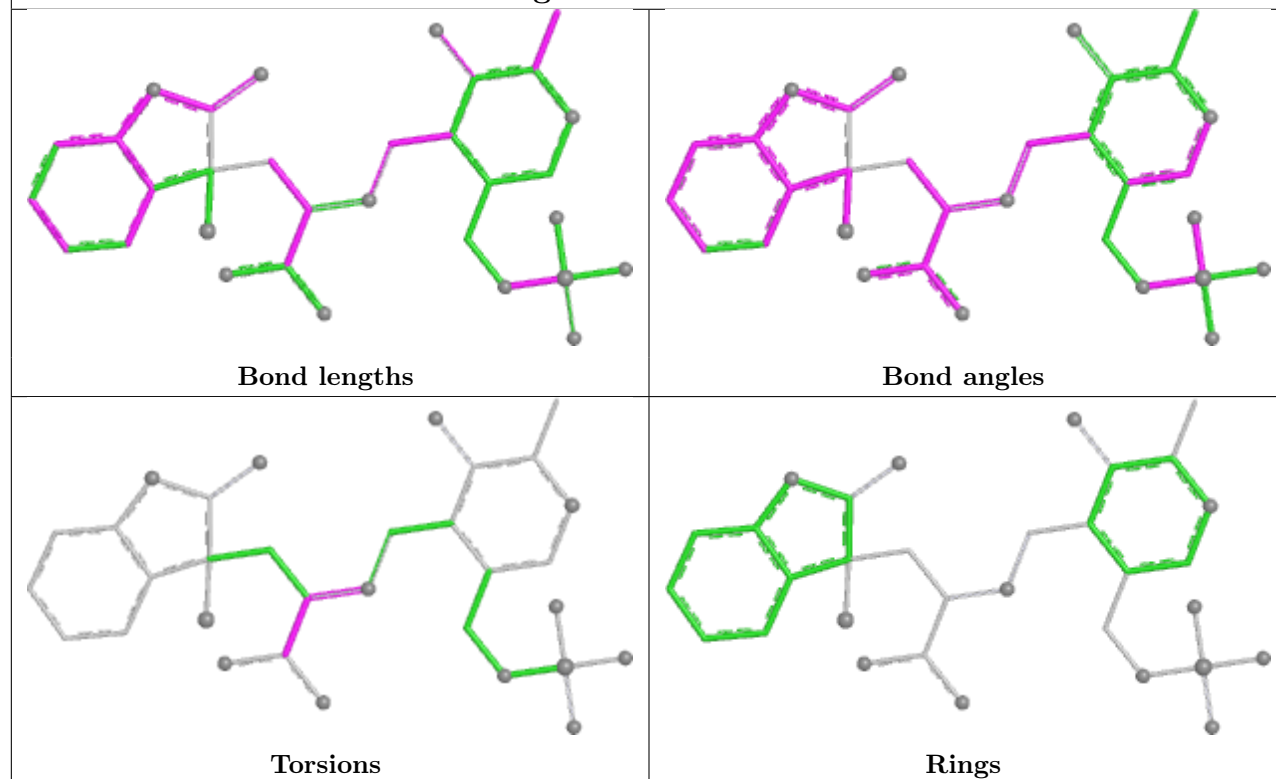
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

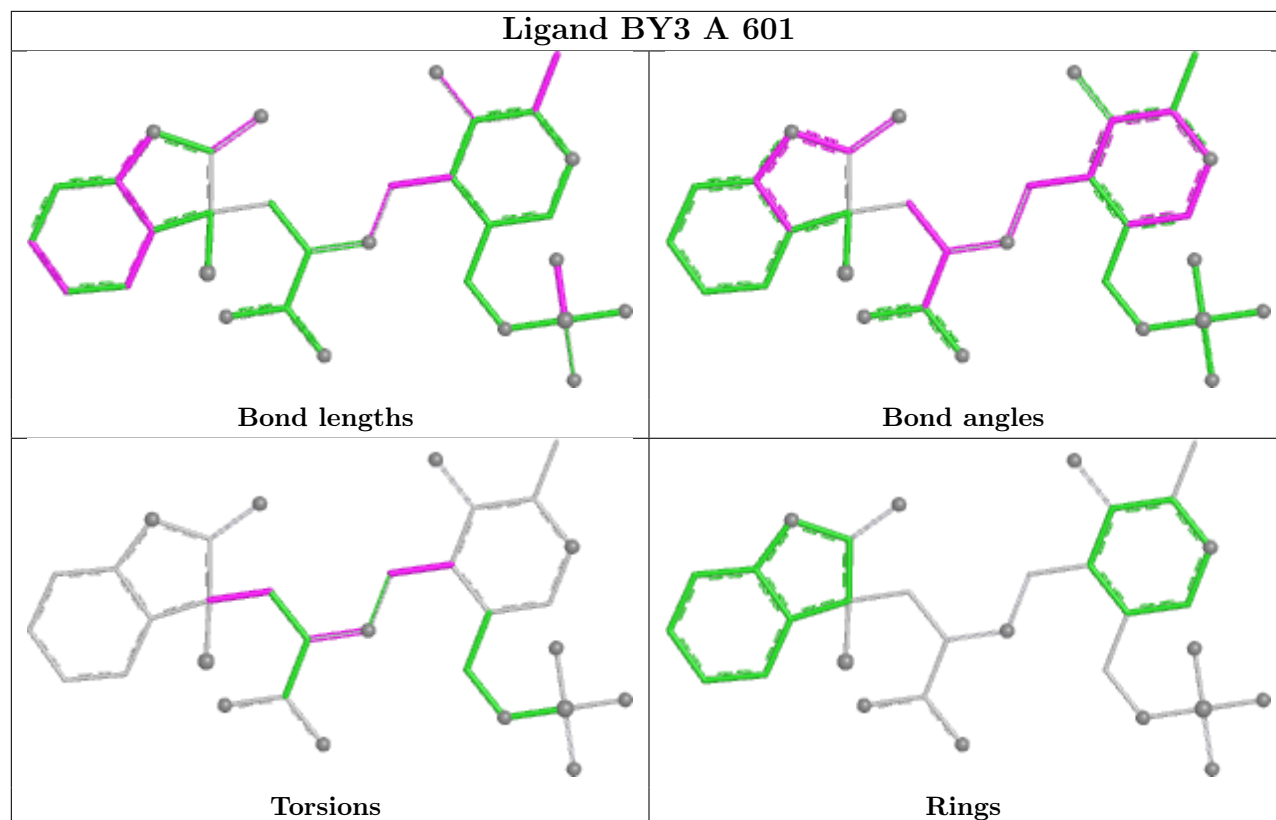


Ligand BY3 C 601



Ligand BY3 D 601





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	541/569 (95%)	0.08	2 (0%) 88 90	29, 48, 70, 83	0
1	B	543/569 (95%)	0.16	8 (1%) 72 74	29, 47, 70, 77	0
1	C	543/569 (95%)	0.31	6 (1%) 78 80	33, 53, 72, 82	1 (0%)
1	D	544/569 (95%)	0.13	4 (0%) 84 86	28, 48, 69, 83	0
All	All	2171/2276 (95%)	0.17	20 (0%) 81 83	28, 49, 71, 83	1 (0%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	248	ILE	2.8
1	B	529	HIS	2.7
1	D	527	TRP	2.7
1	D	97	GLY	2.6
1	B	539	PHE	2.5
1	D	418	VAL	2.5
1	B	444	HIS	2.5
1	B	537	HIS	2.4
1	B	440	GLY	2.3
1	C	183	PHE	2.3
1	D	465	SER	2.2
1	C	185	THR	2.2
1	C	184	ASP	2.2
1	C	181	GLY	2.1
1	B	527	TRP	2.1
1	C	485	VAL	2.1
1	C	279	PHE	2.1
1	A	531	LEU	2.0
1	B	426	GLY	2.0
1	B	531	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

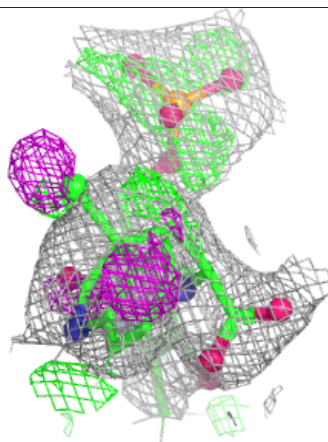
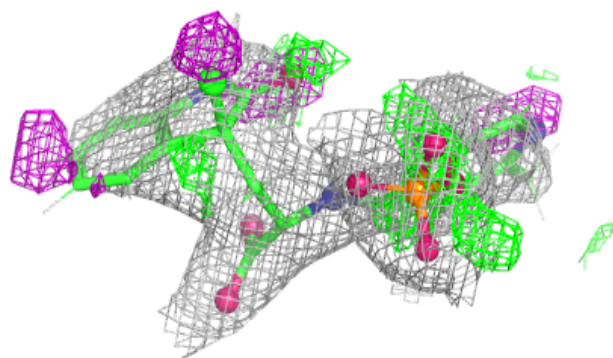
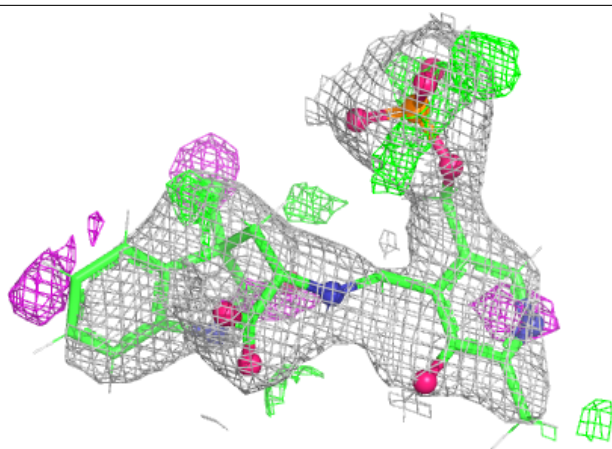
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BY3	C	601	32/32	0.84	0.15	34,45,60,72	48
2	BY3	B	601	32/32	0.85	0.14	31,42,51,86	48
2	BY3	A	601	32/32	0.85	0.18	29,43,52,72	48
2	BY3	D	601	32/32	0.86	0.13	35,43,53,80	48

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.

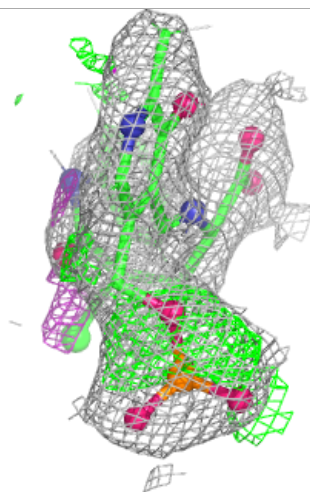
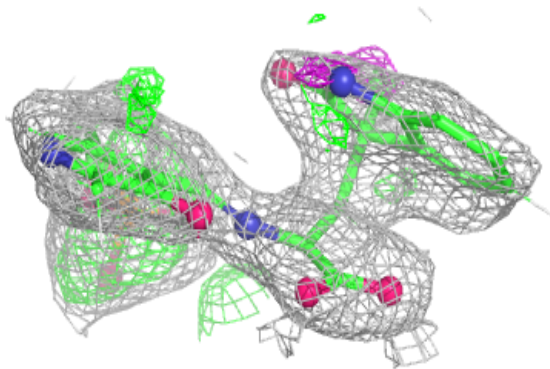
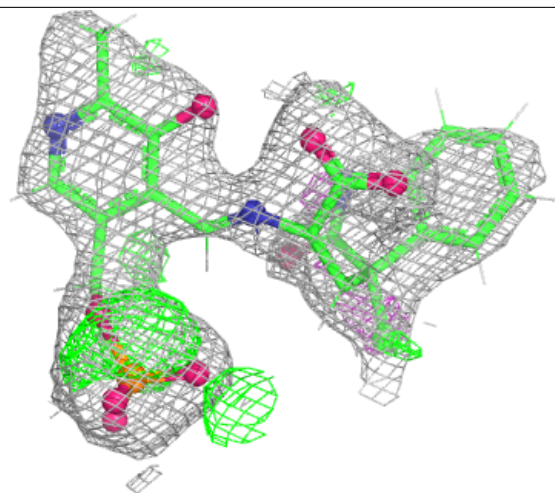
Electron density around BY3 C 601:

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



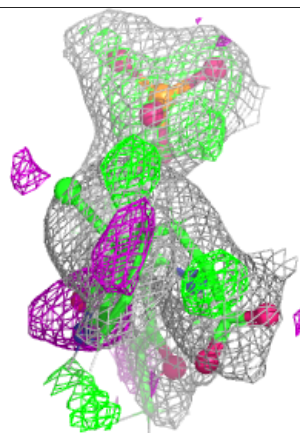
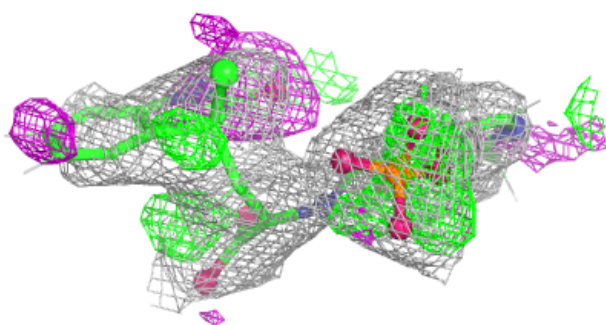
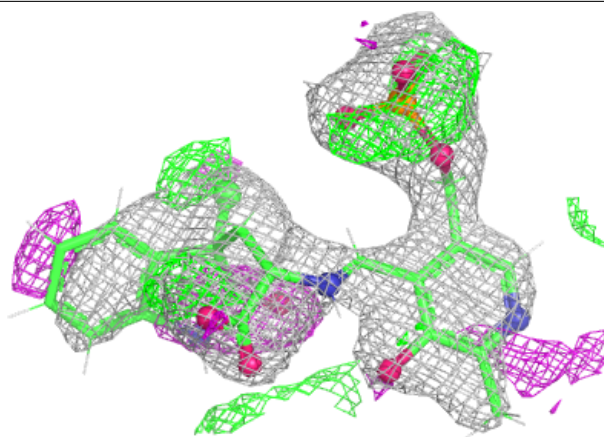
Electron density around BY3 B 601:

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



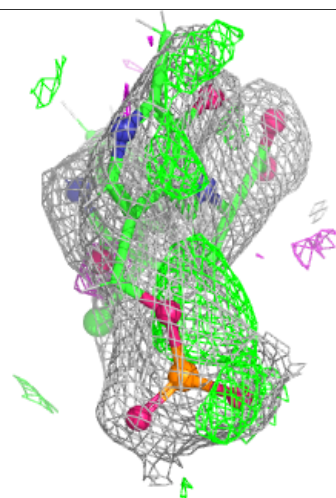
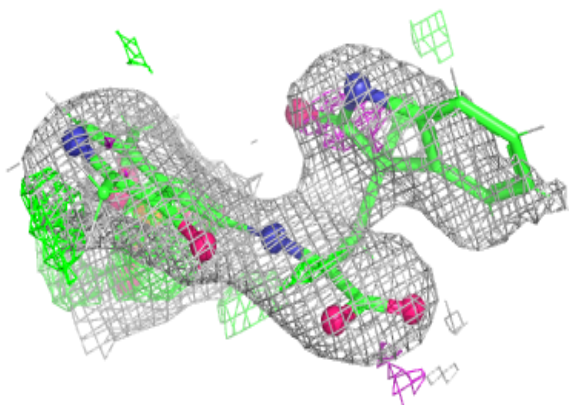
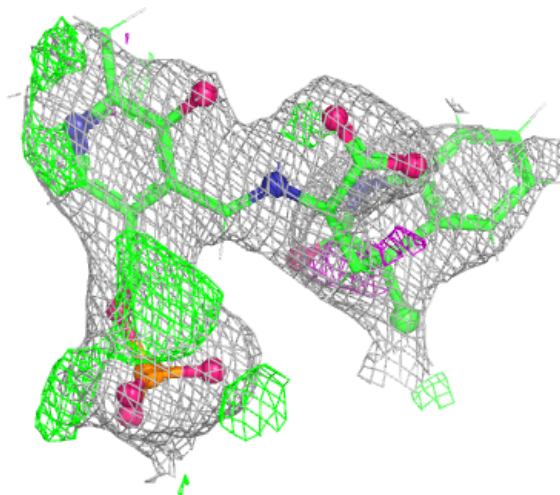
Electron density around BY3 A 601:

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



Electron density around BY3 D 601:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.