



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:57 AM UTC

PDB ID : 7LNP / pdb_00007lnp
Title : Structure of the exo-alpha-L-galactosidase BpGH29 (D264N mutant) from *Bacteroides plebeius* in complex with paranitrophenyl-alpha-L-galactopyranoside
Authors : Boraston, A.B.; Robb, C.S.
Deposited on : 2021-02-08
Resolution : 2.70 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

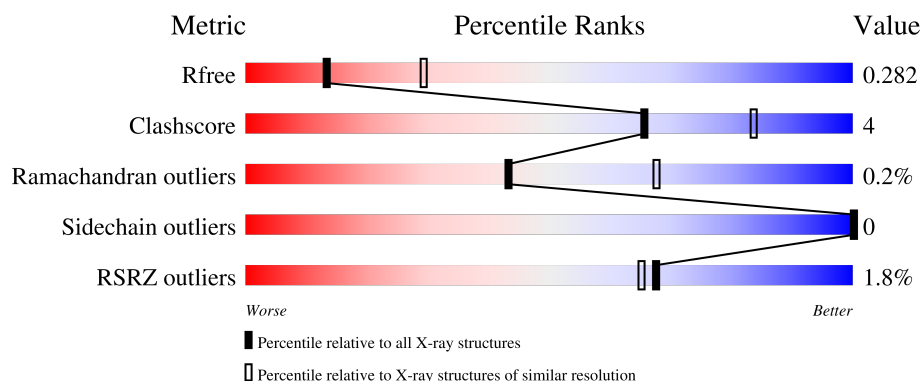
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

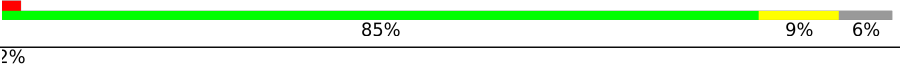
The reported resolution of this entry is 2.70 Å.

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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	599	 2% 85% 10% 6%
1	C	599	 2% 85% 9% 6%
1	D	599	 2% 83% 7% 9%
1	E	599	 2% 82% 9% 9%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 18496 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 Exo-alpha-L-galactosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	565	Total	C	N	O	S	0	0	0
			4488	2873	732	863	20			
1	C	565	Total	C	N	O	S	0	0	0
			4499	2881	732	866	20			
1	D	543	Total	C	N	O	S	0	0	0
			4341	2788	705	829	19			
1	E	548	Total	C	N	O	S	0	0	0
			4381	2812	713	837	19			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP B5CYA5
A	0	GLY	-	expression tag	UNP B5CYA5
A	1	SER	-	expression tag	UNP B5CYA5
A	2	SER	-	expression tag	UNP B5CYA5
A	3	HIS	-	expression tag	UNP B5CYA5
A	4	HIS	-	expression tag	UNP B5CYA5
A	5	HIS	-	expression tag	UNP B5CYA5
A	6	HIS	-	expression tag	UNP B5CYA5
A	7	HIS	-	expression tag	UNP B5CYA5
A	8	HIS	-	expression tag	UNP B5CYA5
A	9	SER	-	expression tag	UNP B5CYA5
A	10	SER	-	expression tag	UNP B5CYA5
A	11	GLY	-	expression tag	UNP B5CYA5
A	12	LEU	-	expression tag	UNP B5CYA5
A	13	VAL	-	expression tag	UNP B5CYA5
A	14	PRO	-	expression tag	UNP B5CYA5
A	15	ARG	-	expression tag	UNP B5CYA5
A	16	GLY	-	expression tag	UNP B5CYA5
A	17	SER	-	expression tag	UNP B5CYA5
A	18	HIS	-	expression tag	UNP B5CYA5
A	19	MET	-	expression tag	UNP B5CYA5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	20	ALA	-	expression tag	UNP B5CYA5
A	21	SER	-	expression tag	UNP B5CYA5
A	264	ASN	ASP	engineered mutation	UNP B5CYA5
C	-1	MET	-	initiating methionine	UNP B5CYA5
C	0	GLY	-	expression tag	UNP B5CYA5
C	1	SER	-	expression tag	UNP B5CYA5
C	2	SER	-	expression tag	UNP B5CYA5
C	3	HIS	-	expression tag	UNP B5CYA5
C	4	HIS	-	expression tag	UNP B5CYA5
C	5	HIS	-	expression tag	UNP B5CYA5
C	6	HIS	-	expression tag	UNP B5CYA5
C	7	HIS	-	expression tag	UNP B5CYA5
C	8	HIS	-	expression tag	UNP B5CYA5
C	9	SER	-	expression tag	UNP B5CYA5
C	10	SER	-	expression tag	UNP B5CYA5
C	11	GLY	-	expression tag	UNP B5CYA5
C	12	LEU	-	expression tag	UNP B5CYA5
C	13	VAL	-	expression tag	UNP B5CYA5
C	14	PRO	-	expression tag	UNP B5CYA5
C	15	ARG	-	expression tag	UNP B5CYA5
C	16	GLY	-	expression tag	UNP B5CYA5
C	17	SER	-	expression tag	UNP B5CYA5
C	18	HIS	-	expression tag	UNP B5CYA5
C	19	MET	-	expression tag	UNP B5CYA5
C	20	ALA	-	expression tag	UNP B5CYA5
C	21	SER	-	expression tag	UNP B5CYA5
C	264	ASN	ASP	engineered mutation	UNP B5CYA5
D	-1	MET	-	initiating methionine	UNP B5CYA5
D	0	GLY	-	expression tag	UNP B5CYA5
D	1	SER	-	expression tag	UNP B5CYA5
D	2	SER	-	expression tag	UNP B5CYA5
D	3	HIS	-	expression tag	UNP B5CYA5
D	4	HIS	-	expression tag	UNP B5CYA5
D	5	HIS	-	expression tag	UNP B5CYA5
D	6	HIS	-	expression tag	UNP B5CYA5
D	7	HIS	-	expression tag	UNP B5CYA5
D	8	HIS	-	expression tag	UNP B5CYA5
D	9	SER	-	expression tag	UNP B5CYA5
D	10	SER	-	expression tag	UNP B5CYA5
D	11	GLY	-	expression tag	UNP B5CYA5
D	12	LEU	-	expression tag	UNP B5CYA5
D	13	VAL	-	expression tag	UNP B5CYA5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	14	PRO	-	expression tag	UNP B5CYA5
D	15	ARG	-	expression tag	UNP B5CYA5
D	16	GLY	-	expression tag	UNP B5CYA5
D	17	SER	-	expression tag	UNP B5CYA5
D	18	HIS	-	expression tag	UNP B5CYA5
D	19	MET	-	expression tag	UNP B5CYA5
D	20	ALA	-	expression tag	UNP B5CYA5
D	21	SER	-	expression tag	UNP B5CYA5
D	264	ASN	ASP	engineered mutation	UNP B5CYA5
E	-1	MET	-	initiating methionine	UNP B5CYA5
E	0	GLY	-	expression tag	UNP B5CYA5
E	1	SER	-	expression tag	UNP B5CYA5
E	2	SER	-	expression tag	UNP B5CYA5
E	3	HIS	-	expression tag	UNP B5CYA5
E	4	HIS	-	expression tag	UNP B5CYA5
E	5	HIS	-	expression tag	UNP B5CYA5
E	6	HIS	-	expression tag	UNP B5CYA5
E	7	HIS	-	expression tag	UNP B5CYA5
E	8	HIS	-	expression tag	UNP B5CYA5
E	9	SER	-	expression tag	UNP B5CYA5
E	10	SER	-	expression tag	UNP B5CYA5
E	11	GLY	-	expression tag	UNP B5CYA5
E	12	LEU	-	expression tag	UNP B5CYA5
E	13	VAL	-	expression tag	UNP B5CYA5
E	14	PRO	-	expression tag	UNP B5CYA5
E	15	ARG	-	expression tag	UNP B5CYA5
E	16	GLY	-	expression tag	UNP B5CYA5
E	17	SER	-	expression tag	UNP B5CYA5
E	18	HIS	-	expression tag	UNP B5CYA5
E	19	MET	-	expression tag	UNP B5CYA5
E	20	ALA	-	expression tag	UNP B5CYA5
E	21	SER	-	expression tag	UNP B5CYA5
E	264	ASN	ASP	engineered mutation	UNP B5CYA5

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

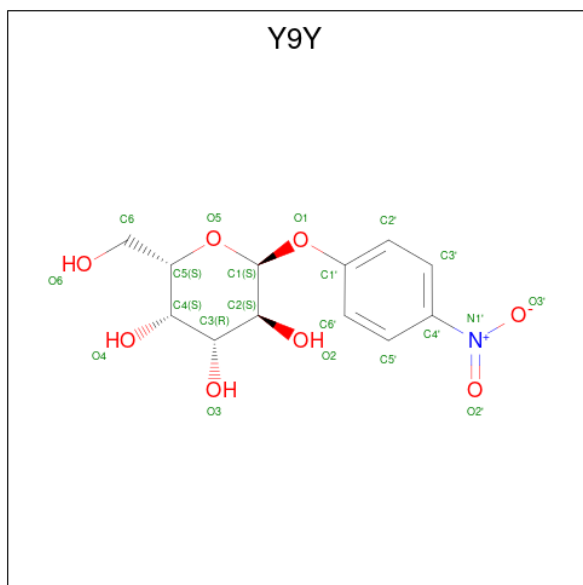
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Ca 1 1	0	0
2	C	1	Total Ca 1 1	0	0
2	D	1	Total Ca 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	1	Total	Ca	0	0
			1	1		

- Molecule 3 is paranitrophenyl-alpha-L-galactopyranoside (CCD ID: Y9Y) (formula: $C_{12}H_{15}NO_8$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			21	12	1	8		
3	C	1	Total	C	N	O	0	0
			21	12	1	8		
3	D	1	Total	C	N	O	0	0
			21	12	1	8		
3	E	1	Total	C	N	O	0	0
			21	12	1	8		

- Molecule 4 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Ni	0	0
			2	2		
4	C	3	Total	Ni	0	0
			3	3		
4	D	2	Total	Ni	0	0
			2	2		
4	E	2	Total	Ni	0	0
			2	2		

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total 3	Na 3	0	0
5	C	2	Total 2	Na 2	0	0
5	D	2	Total 2	Na 2	0	0
5	E	3	Total 3	Na 3	0	0

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total 1	Cl 1	0	0
6	E	1	Total 1	Cl 1	0	0

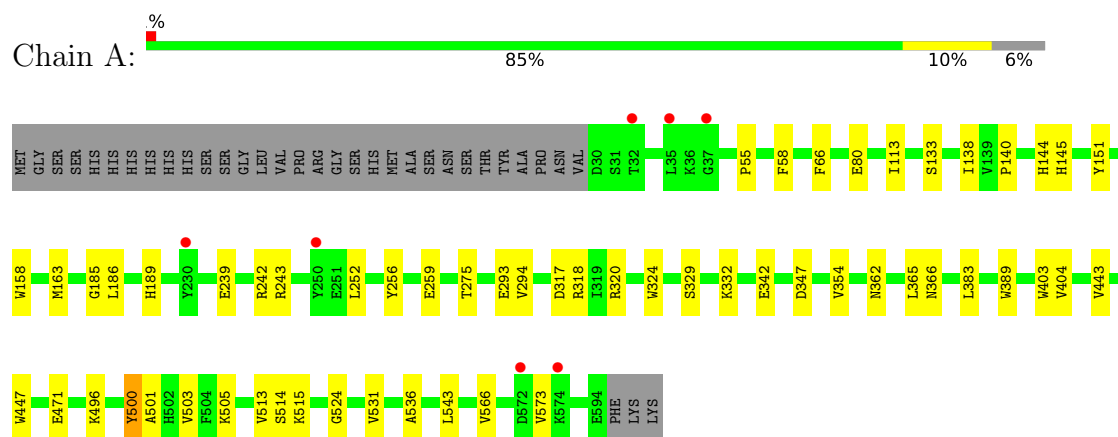
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	176	Total 176	O 176	0	0
7	C	183	Total 183	O 183	0	0
7	D	151	Total 151	O 151	0	0
7	E	168	Total 168	O 168	0	0

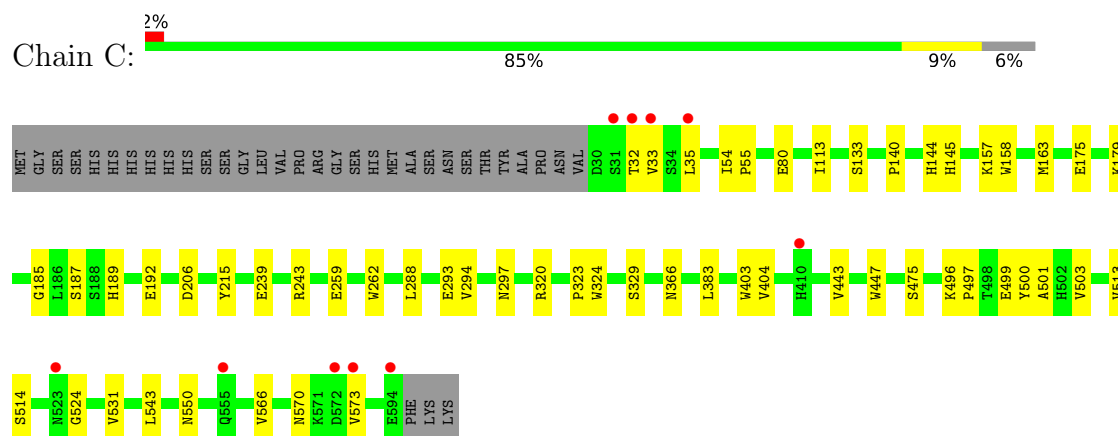
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

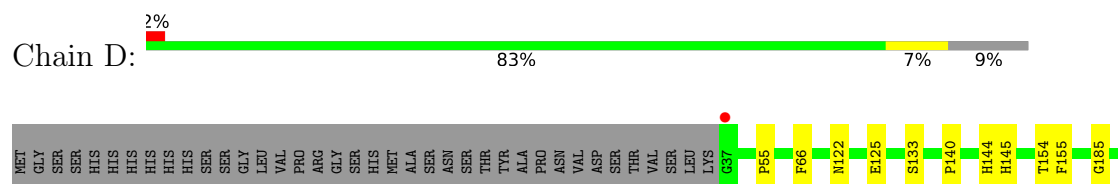
- Molecule 1: Exo-alpha-L-galactosidase

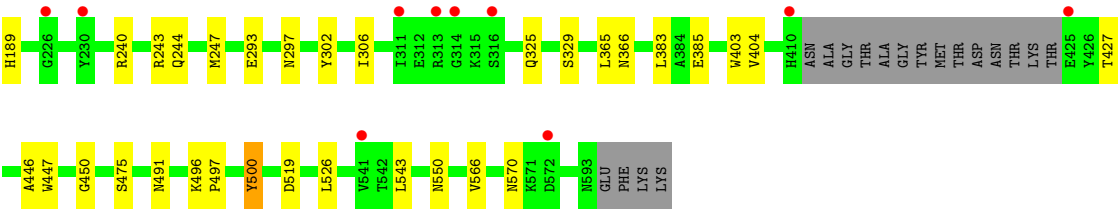


- Molecule 1: Exo-alpha-L-galactosidase

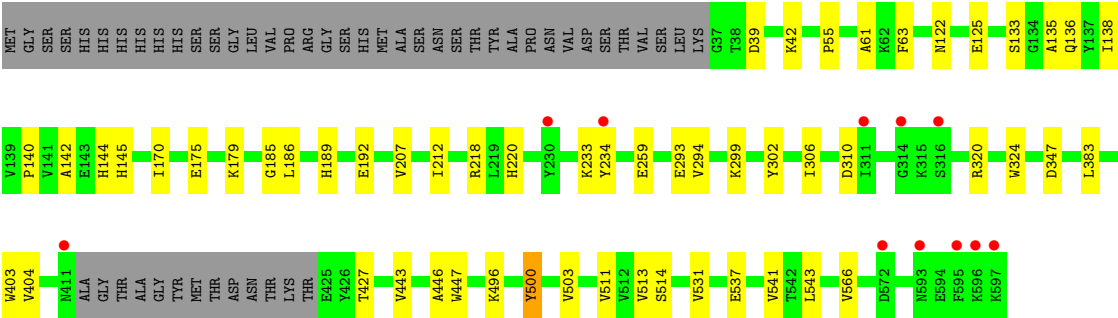
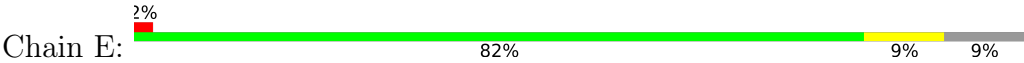


- Molecule 1: Exo-alpha-L-galactosidase





● Molecule 1: Exo-alpha-L-galactosidase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	157.32Å 106.64Å 155.90Å 90.00° 114.97° 90.00°	Depositor
Resolution (Å)	31.57 – 2.70 31.57 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.4 (31.57-2.70) 83.8 (31.57-2.70)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 2.68Å)	Xtrriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.230 , 0.284 0.230 , 0.282	Depositor DCC
R_{free} test set	3197 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	16.3	Xtrriage
Anisotropy	0.725	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 35.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	18496	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.90 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0711e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: CL, NA, NI, Y9Y, CA

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	0.08	0/4612	0.26	0/6267
1	C	0.08	0/4623	0.25	0/6282
1	D	0.08	0/4462	0.25	0/6060
1	E	0.09	0/4504	0.26	0/6118
All	All	0.08	0/18201	0.26	0/24727

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	4488	0	4196	33	0
1	C	4499	0	4221	40	0
1	D	4341	0	4080	28	0
1	E	4381	0	4104	35	0
2	A	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
3	A	21	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	21	0	0	0	0
3	D	21	0	0	0	0
3	E	21	0	0	0	0
4	A	2	0	0	0	0
4	C	3	0	0	0	0
4	D	2	0	0	0	0
4	E	2	0	0	0	0
5	A	3	0	0	0	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
5	E	3	0	0	0	0
6	A	1	0	0	0	0
6	E	1	0	0	0	0
7	A	176	0	0	0	0
7	C	183	0	0	0	0
7	D	151	0	0	0	0
7	E	168	0	0	0	0
All	All	18496	0	16601	129	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (129) 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:C:33:VAL:HG21	1:D:155:PHE:HB2	1.70	0.74
1:E:142:ALA:HB2	1:E:186:LEU:HD22	1.71	0.72
1:C:33:VAL:HG13	1:D:244:GLN:HG2	1.75	0.69
1:D:302:TYR:HB3	1:D:306:ILE:HD11	1.76	0.66
1:E:212:ILE:O	1:E:218:ARG:NH2	2.31	0.63
1:C:32:THR:O	1:D:243:ARG:NH1	2.32	0.62
1:C:524:GLY:HA2	1:C:573:VAL:HB	1.81	0.62
1:E:133:SER:HB3	1:E:383:LEU:HB3	1.82	0.61
1:D:450:GLY:O	1:D:491:ASN:ND2	2.34	0.60
1:C:144:HIS:HA	1:C:189:HIS:HB2	1.84	0.60
1:E:39:ASP:O	1:E:42:LYS:NZ	2.35	0.59
1:C:404:VAL:HB	1:C:514:SER:HB3	1.84	0.59
1:A:329:SER:HA	1:A:366:ASN:HB3	1.84	0.59
1:E:404:VAL:HB	1:E:514:SER:HB3	1.86	0.58
1:E:347:ASP:HB2	1:E:500:TYR:HD1	1.69	0.57
1:C:329:SER:HA	1:C:366:ASN:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:VAL:HB	1:A:514:SER:HB3	1.86	0.57
1:C:543:LEU:HD12	1:C:566:VAL:HG11	1.87	0.56
1:D:133:SER:HB3	1:D:383:LEU:HB3	1.87	0.56
1:E:55:PRO:HB3	1:E:293:GLU:HB3	1.88	0.56
1:E:513:VAL:HG23	1:E:531:VAL:HG22	1.87	0.55
1:C:550:ASN:OD1	1:C:570:ASN:ND2	2.35	0.55
1:D:122:ASN:HB3	1:D:125:GLU:HB2	1.88	0.55
1:A:144:HIS:HA	1:A:189:HIS:HB2	1.89	0.54
1:C:133:SER:HB3	1:C:383:LEU:HB3	1.91	0.53
1:A:133:SER:HB3	1:A:383:LEU:HB3	1.90	0.53
1:A:524:GLY:HA2	1:A:573:VAL:HB	1.90	0.52
1:C:443:VAL:HG22	1:C:503:VAL:HG22	1.90	0.52
1:A:259:GLU:HA	1:A:294:VAL:HG12	1.92	0.51
1:A:55:PRO:HB3	1:A:293:GLU:HB3	1.92	0.51
1:D:385:GLU:OE1	1:D:500:TYR:OH	2.26	0.51
1:D:55:PRO:HB3	1:D:293:GLU:HB3	1.92	0.51
1:E:233:LYS:NZ	1:E:234:TYR:CE2	2.79	0.51
1:A:543:LEU:HD12	1:A:566:VAL:HG11	1.92	0.51
1:E:537:GLU:N	1:E:537:GLU:OE1	2.45	0.50
1:A:443:VAL:HG22	1:A:503:VAL:HG22	1.93	0.50
1:D:519:ASP:HB2	1:D:526:LEU:HD23	1.92	0.50
1:E:543:LEU:HD12	1:E:566:VAL:HG11	1.93	0.50
1:E:144:HIS:HA	1:E:189:HIS:HB2	1.94	0.50
1:C:55:PRO:HB3	1:C:293:GLU:HB3	1.93	0.50
1:C:113:ILE:HG21	1:C:163:MET:HE3	1.94	0.50
1:C:33:VAL:HG21	1:D:155:PHE:CB	2.40	0.49
1:A:113:ILE:HG21	1:A:163:MET:HE3	1.95	0.49
1:C:513:VAL:HG23	1:C:531:VAL:HG22	1.95	0.49
1:D:550:ASN:OD1	1:D:570:ASN:ND2	2.41	0.49
1:C:145:HIS:CE1	1:C:189:HIS:HB3	2.47	0.49
1:E:511:VAL:HG11	1:E:541:VAL:HG21	1.94	0.49
1:D:144:HIS:HA	1:D:189:HIS:HB2	1.94	0.48
1:A:145:HIS:CE1	1:A:189:HIS:HB3	2.48	0.48
1:C:243:ARG:HD2	1:D:154:THR:HB	1.95	0.48
1:C:447:TRP:CG	1:C:496:LYS:HE2	2.48	0.48
1:D:140:PRO:HD2	1:D:185:GLY:O	2.13	0.48
1:A:447:TRP:CG	1:A:496:LYS:HE2	2.48	0.47
1:A:58:PHE:O	1:A:362:ASN:ND2	2.47	0.47
1:A:317:ASP:OD1	1:A:318:ARG:HG2	2.15	0.47
1:E:175:GLU:O	1:E:179:LYS:HG3	2.15	0.47
1:C:187:SER:HB3	1:C:262:TRP:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:GLU:H	1:A:80:GLU:CD	2.22	0.46
1:E:175:GLU:HG2	1:E:179:LYS:HE2	1.97	0.46
1:A:347:ASP:HB2	1:A:500:TYR:HD1	1.79	0.46
1:E:403:TRP:CG	1:E:404:VAL:H	2.33	0.46
1:A:158:TRP:HE3	1:A:163:MET:HE1	1.81	0.46
1:A:239:GLU:O	1:A:243:ARG:HG3	2.15	0.46
1:D:297:ASN:OD1	1:D:325:GLN:NE2	2.49	0.46
1:E:138:ILE:HG12	1:E:140:PRO:HD3	1.98	0.46
1:C:140:PRO:HD2	1:C:185:GLY:O	2.16	0.46
1:C:499:GLU:O	1:C:501:ALA:N	2.49	0.46
1:E:140:PRO:HD2	1:E:185:GLY:O	2.15	0.46
1:E:207:VAL:O	1:E:218:ARG:NH1	2.50	0.45
1:C:475:SER:HB2	1:C:497:PRO:HG3	1.99	0.45
1:D:244:GLN:HA	1:D:247:MET:HE3	1.99	0.44
1:E:220:HIS:HB3	1:E:234:TYR:CE2	2.52	0.44
1:A:471:GLU:O	1:A:505:LYS:N	2.37	0.44
1:C:35:LEU:O	1:D:243:ARG:NH2	2.44	0.44
1:E:145:HIS:CE1	1:E:189:HIS:HB3	2.52	0.44
1:E:220:HIS:CB	1:E:234:TYR:CE2	3.01	0.44
1:C:158:TRP:HE3	1:C:163:MET:HE1	1.82	0.44
1:D:243:ARG:HG2	1:D:247:MET:HE2	1.99	0.44
1:C:80:GLU:H	1:C:80:GLU:CD	2.25	0.44
1:D:403:TRP:CG	1:D:404:VAL:H	2.35	0.44
1:E:63:PHE:HB3	1:E:135:ALA:HA	2.00	0.44
1:E:170:ILE:HD12	1:E:186:LEU:HD21	2.00	0.44
1:C:145:HIS:ND1	1:C:192:GLU:HB2	2.33	0.44
1:C:259:GLU:HA	1:C:294:VAL:HG12	1.99	0.44
1:A:403:TRP:CG	1:A:404:VAL:H	2.36	0.43
1:C:320:ARG:HD3	1:C:324:TRP:CG	2.54	0.43
1:A:513:VAL:HG23	1:A:531:VAL:HG22	2.00	0.43
1:C:262:TRP:HA	1:C:297:ASN:HB2	2.00	0.43
1:E:122:ASN:HB3	1:E:125:GLU:HB2	2.00	0.43
1:C:239:GLU:OE2	1:C:243:ARG:NE	2.47	0.43
1:D:447:TRP:CG	1:D:496:LYS:HE2	2.53	0.43
1:D:66:PHE:N	1:D:365:LEU:O	2.34	0.43
1:D:329:SER:HA	1:D:366:ASN:HB3	2.00	0.43
1:E:443:VAL:HG22	1:E:503:VAL:HG22	2.01	0.43
1:C:157:LYS:HA	1:C:157:LYS:HD3	1.85	0.43
1:E:320:ARG:HD3	1:E:324:TRP:CD1	2.54	0.43
1:E:299:LYS:HE2	1:E:310:ASP:HB3	2.01	0.43
1:D:475:SER:HB2	1:D:497:PRO:HG3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:LYS:HB3	1:A:515:LYS:HE3	1.77	0.42
1:D:543:LEU:HD12	1:D:566:VAL:HG11	2.01	0.42
1:C:54:ILE:HD12	1:C:323:PRO:HD2	2.01	0.42
1:D:427:THR:C	1:D:446:ALA:HB3	2.45	0.42
1:A:140:PRO:HD2	1:A:185:GLY:O	2.18	0.42
1:A:242:ARG:HB3	1:A:275:THR:HG21	2.01	0.42
1:C:320:ARG:HD3	1:C:324:TRP:CD1	2.55	0.42
1:A:320:ARG:HD3	1:A:324:TRP:CD1	2.54	0.42
1:C:206:ASP:OD2	1:C:215:TYR:OH	2.36	0.42
1:E:427:THR:C	1:E:446:ALA:HB3	2.45	0.42
1:A:138:ILE:HG12	1:A:140:PRO:HD3	2.01	0.42
1:A:389:TRP:CZ2	1:A:501:ALA:HB3	2.55	0.42
1:D:145:HIS:CE1	1:D:189:HIS:HB3	2.55	0.42
1:C:175:GLU:HG3	1:C:179:LYS:HE3	2.00	0.42
1:C:403:TRP:CG	1:C:404:VAL:H	2.37	0.42
1:E:61:ALA:HB1	1:E:136:GLN:HB2	2.02	0.42
1:E:233:LYS:NZ	1:E:234:TYR:CZ	2.88	0.42
1:E:302:TYR:HB3	1:E:306:ILE:HD11	2.00	0.42
1:A:354:VAL:HG11	1:A:443:VAL:HG11	2.02	0.42
1:D:240:ARG:O	1:D:244:GLN:HG3	2.20	0.42
1:A:66:PHE:N	1:A:365:LEU:O	2.44	0.41
1:A:151:TYR:HB2	1:A:256:TYR:OH	2.21	0.41
1:A:536:ALA:HB1	1:C:288:LEU:HD13	2.03	0.41
1:C:163:MET:HE3	1:C:163:MET:HB2	1.86	0.41
1:C:239:GLU:O	1:C:243:ARG:HG3	2.21	0.41
1:E:447:TRP:CG	1:E:496:LYS:HE2	2.56	0.41
1:E:145:HIS:ND1	1:E:192:GLU:HB2	2.37	0.40
1:A:332:LYS:HD2	1:A:342:GLU:HG2	2.03	0.40
1:A:186:LEU:CD1	1:A:252:LEU:HD13	2.50	0.40
1:E:259:GLU:HA	1:E:294:VAL:HG12	2.03	0.40
1:C:145:HIS:ND1	1:C:189:HIS:HB3	2.37	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	563/599 (94%)	547 (97%)	15 (3%)	1 (0%)	43	68
1	C	563/599 (94%)	544 (97%)	18 (3%)	1 (0%)	43	68
1	D	539/599 (90%)	524 (97%)	14 (3%)	1 (0%)	43	68
1	E	544/599 (91%)	528 (97%)	15 (3%)	1 (0%)	43	68
All	All	2209/2396 (92%)	2143 (97%)	62 (3%)	4 (0%)	43	68

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	500	TYR
1	C	500	TYR
1	D	500	TYR
1	E	500	TYR

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	468/521 (90%)	468 (100%)	0	100	100
1	C	472/521 (91%)	472 (100%)	0	100	100
1	D	455/521 (87%)	455 (100%)	0	100	100
1	E	459/521 (88%)	459 (100%)	0	100	100
All	All	1854/2084 (89%)	1854 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

Mol	Chain	Res	Type
1	A	193	ASN
1	A	393	ASN

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Mol	Chain	Res	Type
1	A	464	ASN
1	A	491	ASN
1	A	540	ASN
1	C	99	GLN
1	C	136	GLN
1	C	193	ASN
1	C	410	HIS
1	C	464	ASN
1	D	348	HIS
1	D	491	ASN
1	E	136	GLN
1	E	264	ASN
1	E	348	HIS
1	E	411	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](#)

Of 29 ligands modelled in this entry, 25 are monoatomic - leaving 4 for Mogul analysis.

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
3	Y9Y	E	602	-	22,22,22	0.47	0	29,31,31	0.50	0
3	Y9Y	C	602	-	22,22,22	0.46	0	29,31,31	0.47	0
3	Y9Y	D	602	-	22,22,22	0.46	0	29,31,31	0.48	0
3	Y9Y	A	602	-	22,22,22	0.46	0	29,31,31	0.47	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
3	Y9Y	E	602	-	-	3/8/30/30	0/2/2/2
3	Y9Y	C	602	-	-	2/8/30/30	0/2/2/2
3	Y9Y	D	602	-	-	4/8/30/30	0/2/2/2
3	Y9Y	A	602	-	-	2/8/30/30	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

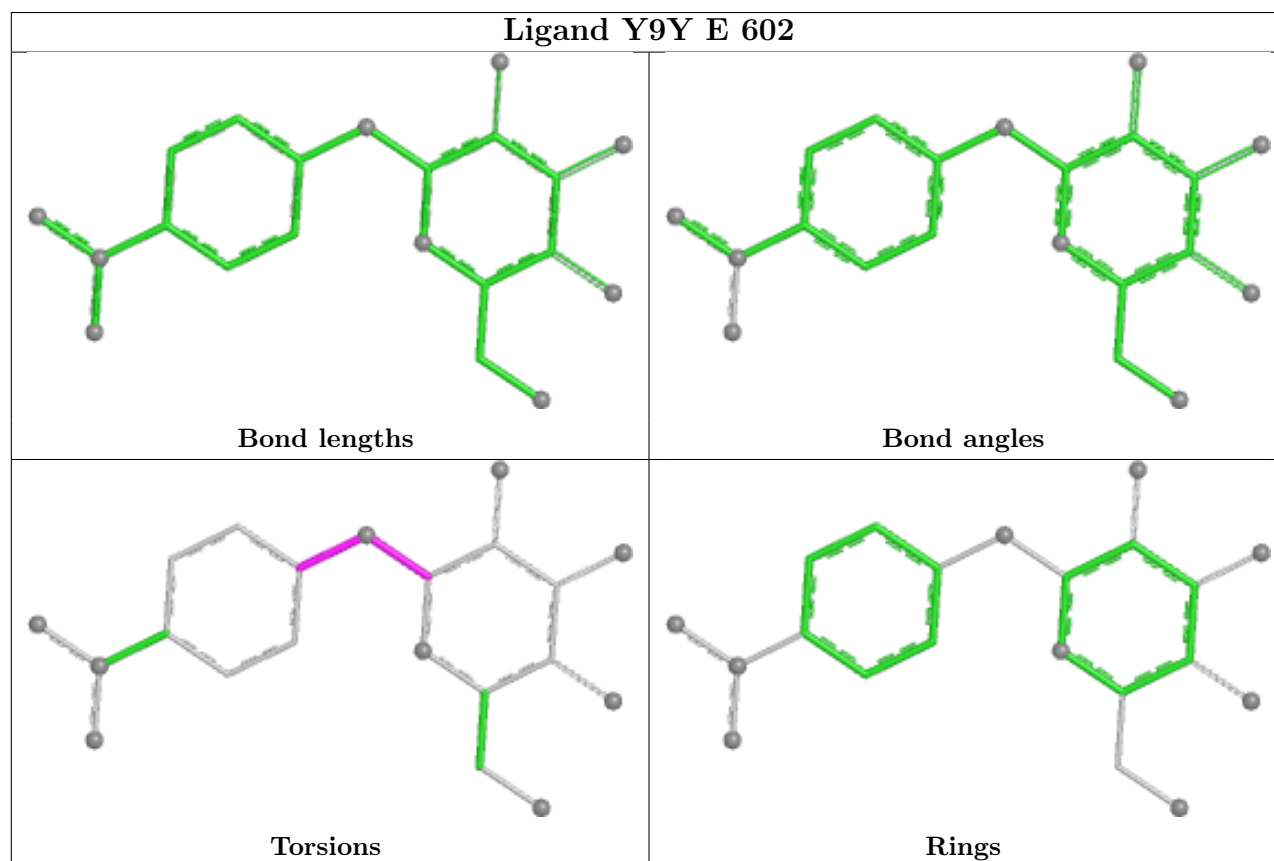
Mol	Chain	Res	Type	Atoms
3	A	602	Y9Y	O5-C1-O1-C1'
3	C	602	Y9Y	O5-C1-O1-C1'
3	A	602	Y9Y	C2-C1-O1-C1'
3	C	602	Y9Y	C2-C1-O1-C1'
3	E	602	Y9Y	C6'-C1'-O1-C1
3	E	602	Y9Y	C2'-C1'-O1-C1
3	D	602	Y9Y	O5-C1-O1-C1'
3	D	602	Y9Y	C2-C1-O1-C1'
3	E	602	Y9Y	C2-C1-O1-C1'
3	D	602	Y9Y	C6'-C1'-O1-C1
3	D	602	Y9Y	C2'-C1'-O1-C1

There are no ring outliers.

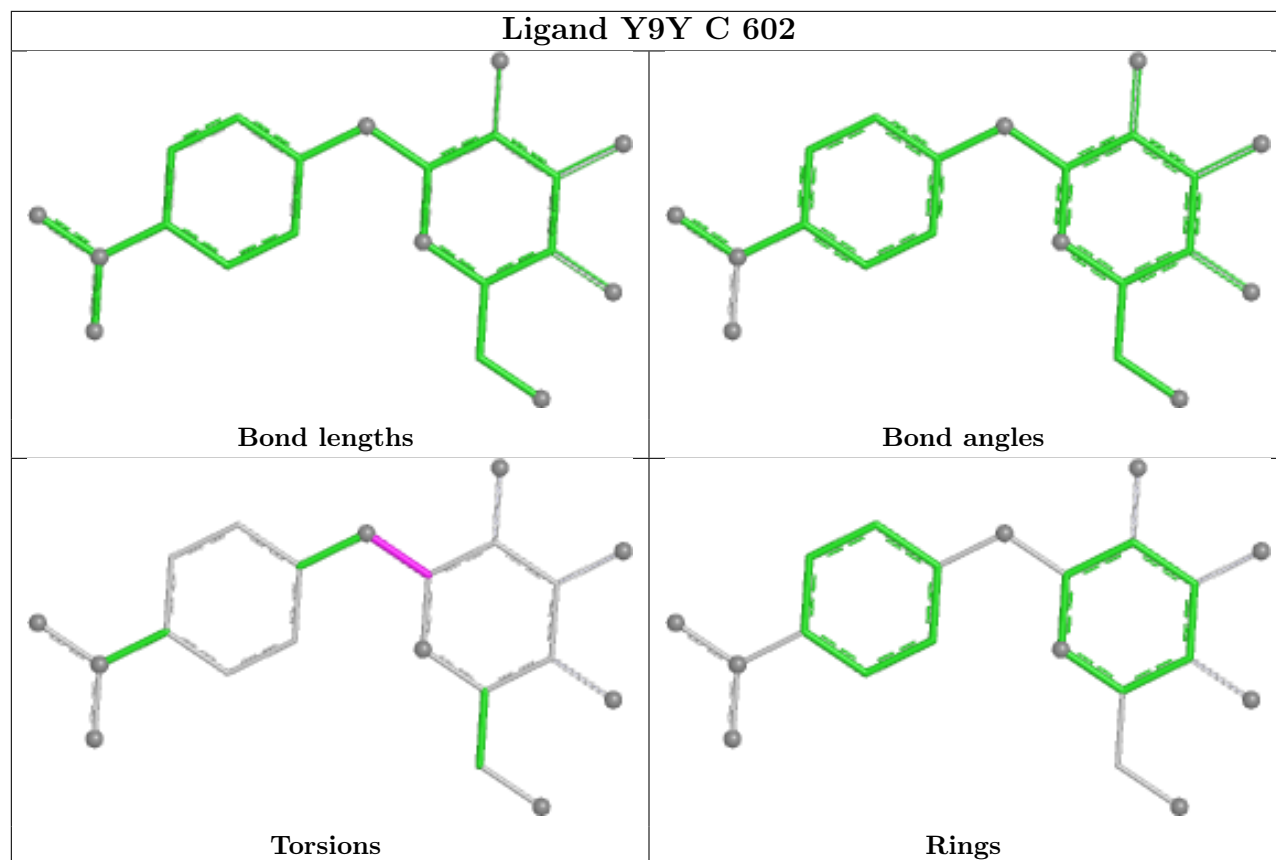
No monomer is involved in short contacts.

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

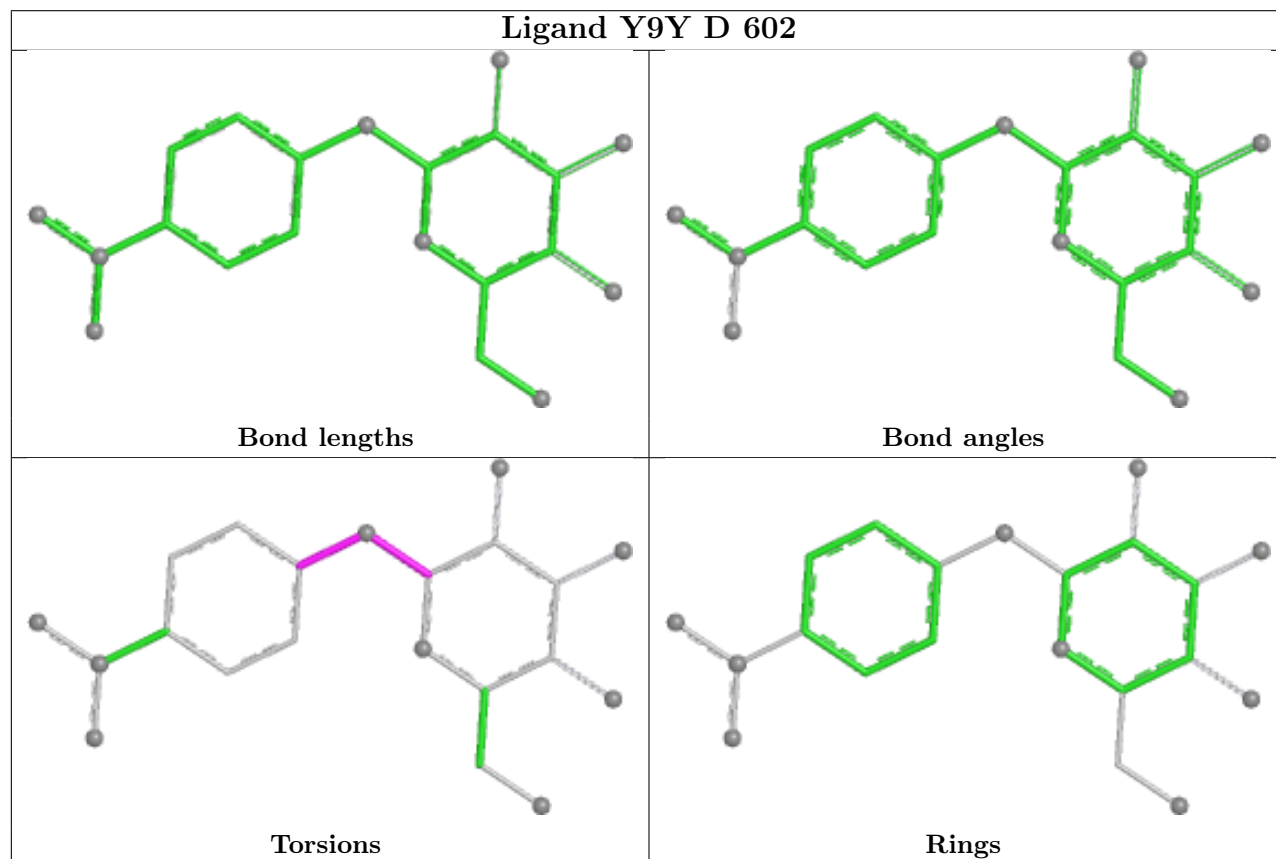
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.

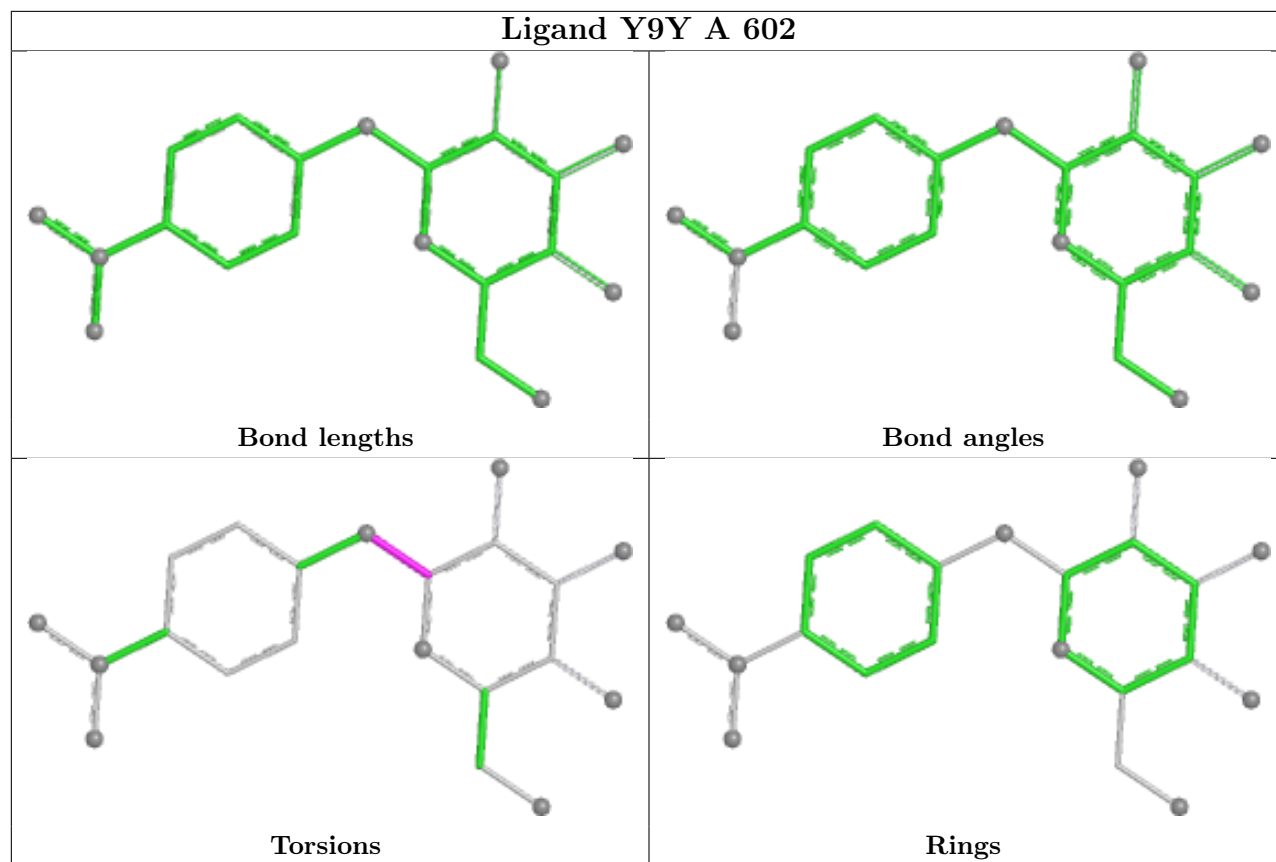


Ligand Y9Y C 602



Ligand Y9Y D 602





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	565/599 (94%)	0.02	7 (1%) 76 75	11, 19, 33, 49	0
1	C	565/599 (94%)	0.06	10 (1%) 67 65	11, 18, 37, 61	0
1	D	543/599 (90%)	0.06	11 (2%) 65 62	11, 20, 34, 52	0
1	E	548/599 (91%)	0.07	11 (2%) 65 62	11, 19, 38, 62	0
All	All	2221/2396 (92%)	0.05	39 (1%) 67 65	11, 19, 36, 62	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	572	ASP	4.9
1	E	597	LYS	3.6
1	E	316	SER	3.4
1	D	37	GLY	3.4
1	E	311	ILE	3.4
1	E	230	TYR	3.4
1	A	572	ASP	3.3
1	C	32	THR	3.2
1	C	594	GLU	3.2
1	A	230	TYR	3.0
1	E	314	GLY	3.0
1	E	595	PHE	3.0
1	E	234	TYR	2.9
1	D	311	ILE	2.9
1	C	523	ASN	2.8
1	D	316	SER	2.8
1	A	250	TYR	2.7
1	D	230	TYR	2.6
1	A	32	THR	2.6
1	E	593	ASN	2.4
1	C	35	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	574	LYS	2.3
1	C	33	VAL	2.3
1	C	410	HIS	2.2
1	E	596	LYS	2.2
1	D	425	GLU	2.2
1	D	541	VAL	2.2
1	D	313	ARG	2.2
1	E	411	ASN	2.2
1	C	573	VAL	2.2
1	C	555	GLN	2.2
1	D	410	HIS	2.2
1	A	35	LEU	2.1
1	D	226	GLY	2.1
1	D	314	GLY	2.1
1	D	572	ASP	2.1
1	E	572	ASP	2.1
1	C	31	SER	2.1
1	A	37	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NA	E	607	1/1	0.73	0.25	20,20,20,20	0
3	Y9Y	E	602	21/21	0.74	0.14	27,35,43,53	0
3	Y9Y	C	602	21/21	0.78	0.15	20,26,42,49	0
3	Y9Y	D	602	21/21	0.81	0.13	23,35,46,56	0
5	NA	A	605	1/1	0.84	0.13	26,26,26,26	0

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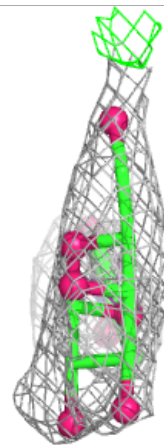
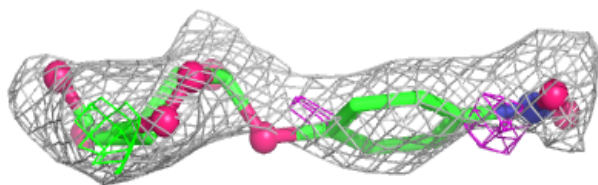
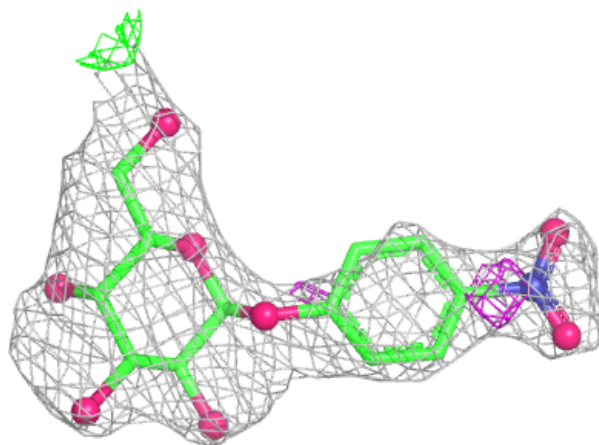
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	Y9Y	A	602	21/21	0.85	0.13	17,25,37,42	0
6	CL	E	608	1/1	0.87	0.18	41,41,41,41	0
5	NA	A	607	1/1	0.88	0.17	23,23,23,23	0
4	NI	C	605	1/1	0.90	0.10	51,51,51,51	0
5	NA	E	606	1/1	0.92	0.20	21,21,21,21	0
5	NA	D	605	1/1	0.93	0.07	24,24,24,24	0
5	NA	C	606	1/1	0.93	0.06	22,22,22,22	0
5	NA	D	606	1/1	0.94	0.23	25,25,25,25	0
5	NA	A	606	1/1	0.94	0.05	24,24,24,24	0
5	NA	C	607	1/1	0.94	0.07	15,15,15,15	0
2	CA	D	601	1/1	0.94	0.04	30,30,30,30	0
2	CA	E	601	1/1	0.95	0.04	25,25,25,25	0
6	CL	A	608	1/1	0.95	0.06	25,25,25,25	0
2	CA	A	601	1/1	0.95	0.04	22,22,22,22	0
4	NI	D	604	1/1	0.96	0.12	42,42,42,42	0
2	CA	C	601	1/1	0.96	0.06	16,16,16,16	0
4	NI	E	603	1/1	0.98	0.13	38,38,38,38	0
4	NI	E	604	1/1	0.98	0.11	28,28,28,28	0
4	NI	C	604	1/1	0.98	0.14	38,38,38,38	0
5	NA	E	605	1/1	0.98	0.04	16,16,16,16	0
4	NI	D	603	1/1	0.99	0.11	36,36,36,36	0
4	NI	C	603	1/1	0.99	0.19	39,39,39,39	0
4	NI	A	603	1/1	0.99	0.09	26,26,26,26	0
4	NI	A	604	1/1	0.99	0.13	35,35,35,35	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.

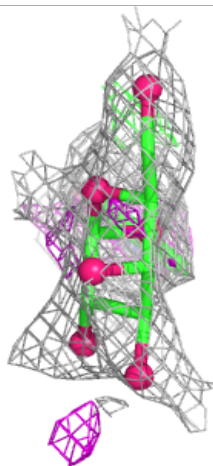
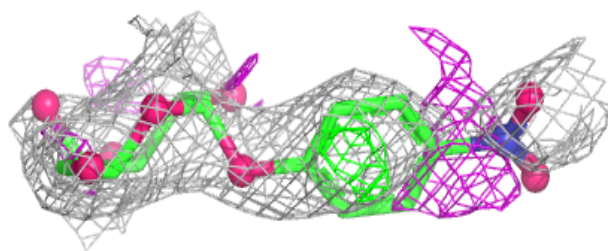
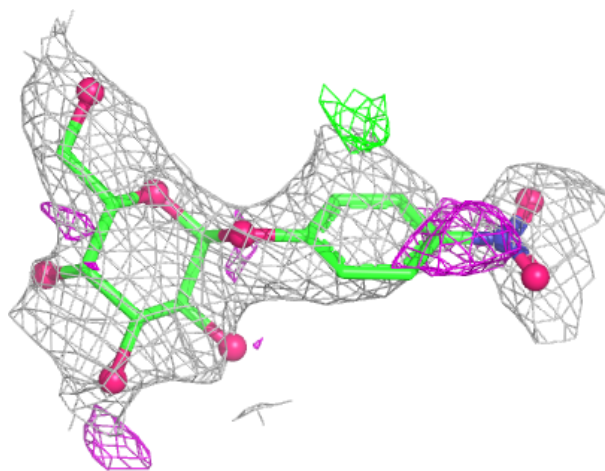
Electron density around Y9Y E 602:

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



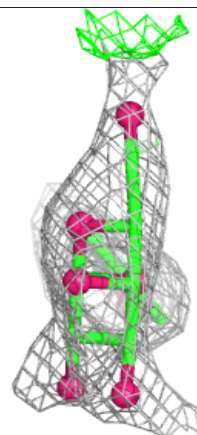
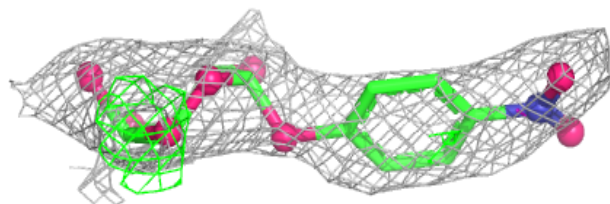
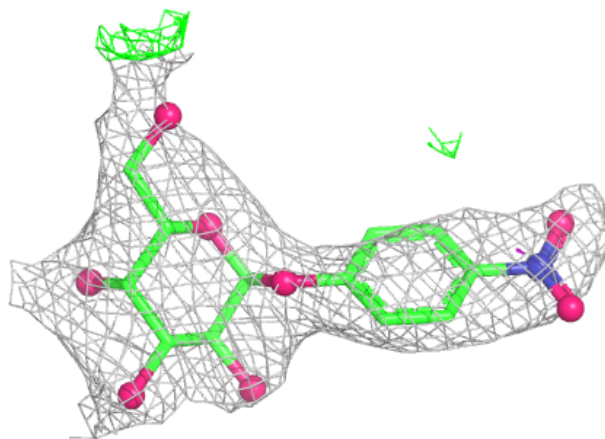
Electron density around Y9Y C 602:

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



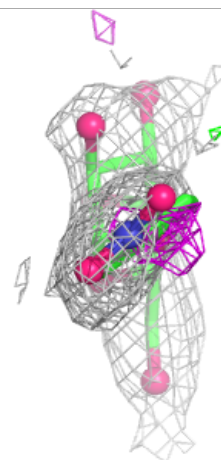
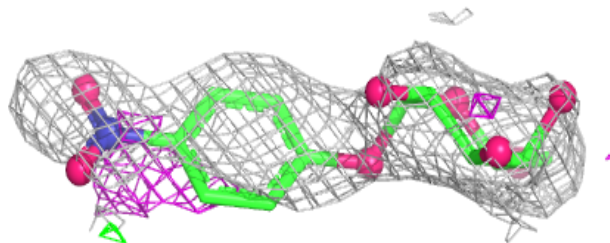
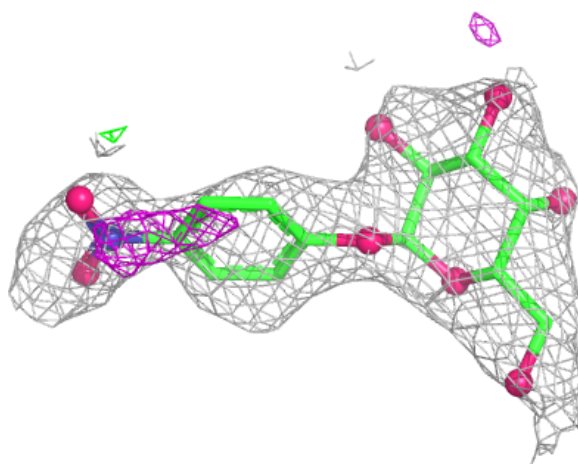
Electron density around Y9Y D 602:

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



Electron density around Y9Y A 602:

$2mF_o-DF_c$ (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.