



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 04:28 AM UTC

PDB ID : 5DF8 / pdb_00005df8
Title : CRYSTAL STRUCTURE OF PENICILLIN-BINDING PROTEIN 3 FROM PSEUDOMONAS AERUGINOSA IN COMPLEX WITH CEFOPERAZONE
Authors : Ren, J.; Nettleship, J.E.; Males, A.; Stuart, D.I.; Owens, R.J.
Deposited on : 2015-08-26
Resolution : 2.00 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

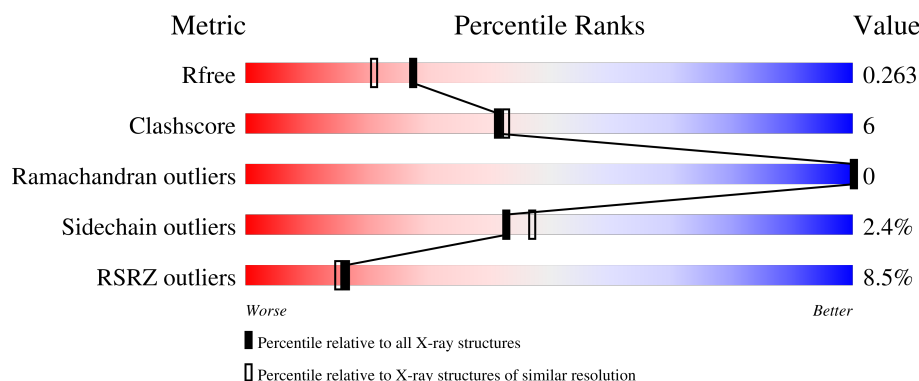
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	564	6% 78% 12% • 9%
1	B	564	9% 76% 10% • 13%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	59F	A	601	X	-	-	-
2	59F	B	601	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8353 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 Cell division protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	514	Total	C	N	O	S	0	0	0
			3922	2474	712	724	12			
1	B	489	Total	C	N	O	S	0	0	0
			3717	2349	666	690	12			

There are 38 discrepancies between the modelled and reference sequences:

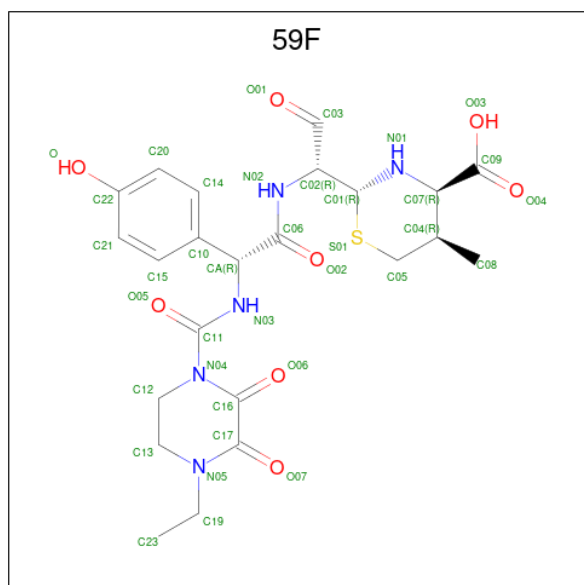
Chain	Residue	Modelled	Actual	Comment	Reference
A	16	MET	-	initiating methionine	UNP Q51504
A	17	ALA	-	expression tag	UNP Q51504
A	18	HIS	-	expression tag	UNP Q51504
A	19	HIS	-	expression tag	UNP Q51504
A	20	HIS	-	expression tag	UNP Q51504
A	21	HIS	-	expression tag	UNP Q51504
A	22	HIS	-	expression tag	UNP Q51504
A	23	HIS	-	expression tag	UNP Q51504
A	24	SER	-	expression tag	UNP Q51504
A	25	SER	-	expression tag	UNP Q51504
A	26	GLY	-	expression tag	UNP Q51504
A	27	LEU	-	expression tag	UNP Q51504
A	28	GLU	-	expression tag	UNP Q51504
A	29	VAL	-	expression tag	UNP Q51504
A	30	LEU	-	expression tag	UNP Q51504
A	31	PHE	-	expression tag	UNP Q51504
A	32	GLN	-	expression tag	UNP Q51504
A	33	GLY	-	expression tag	UNP Q51504
A	34	PRO	-	expression tag	UNP Q51504
B	16	MET	-	initiating methionine	UNP Q51504
B	17	ALA	-	expression tag	UNP Q51504
B	18	HIS	-	expression tag	UNP Q51504
B	19	HIS	-	expression tag	UNP Q51504
B	20	HIS	-	expression tag	UNP Q51504
B	21	HIS	-	expression tag	UNP Q51504

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Chain	Residue	Modelled	Actual	Comment	Reference
B	22	HIS	-	expression tag	UNP Q51504
B	23	HIS	-	expression tag	UNP Q51504
B	24	SER	-	expression tag	UNP Q51504
B	25	SER	-	expression tag	UNP Q51504
B	26	GLY	-	expression tag	UNP Q51504
B	27	LEU	-	expression tag	UNP Q51504
B	28	GLU	-	expression tag	UNP Q51504
B	29	VAL	-	expression tag	UNP Q51504
B	30	LEU	-	expression tag	UNP Q51504
B	31	PHE	-	expression tag	UNP Q51504
B	32	GLN	-	expression tag	UNP Q51504
B	33	GLY	-	expression tag	UNP Q51504
B	34	PRO	-	expression tag	UNP Q51504

- Molecule 2 is (2R,4R,5R)-2-[(1R)-1-[(2R)-2-[(4-ethyl-2,3-dioxopiperazin-1-yl)carbonyl]amino]-2-(4-hydroxyphenyl)acetyl]amino}-2-oxoethyl]-5-methyl-1,3-thiazinane-4-carboxylic acid (CCD ID: 59F) (formula: C₂₃H₂₉N₅O₈S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			37	23	5	8	1		
2	B	1	Total	C	N	O	S	0	0
			37	23	5	8	1		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Cl	0	0
			3	3		
4	B	3	Total	Cl	0	0
			3	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	316	Total	O	0	0
			316	316		

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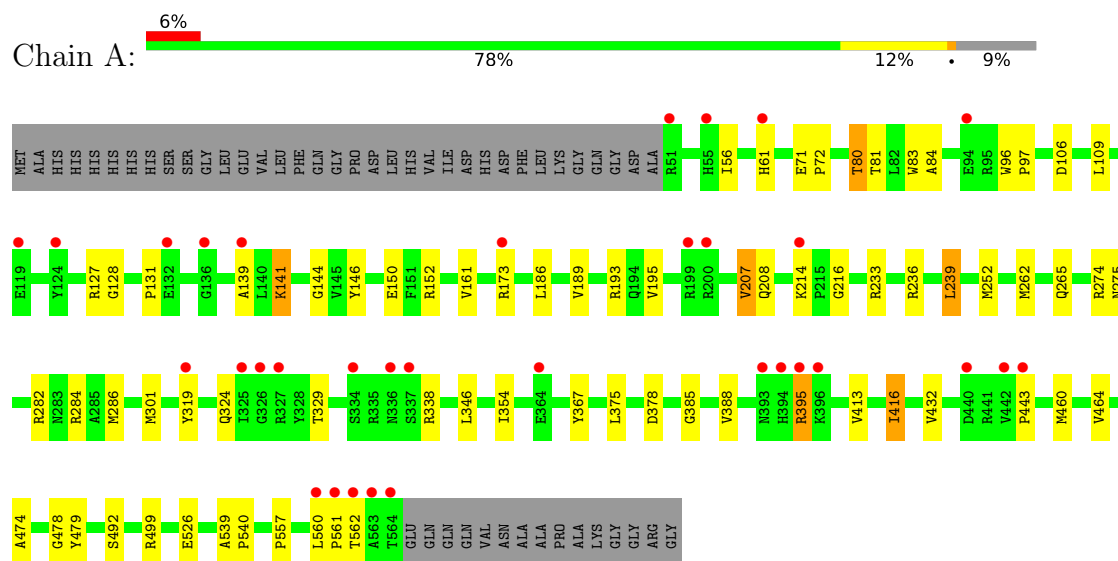
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	282	Total 282	O 282	0	0

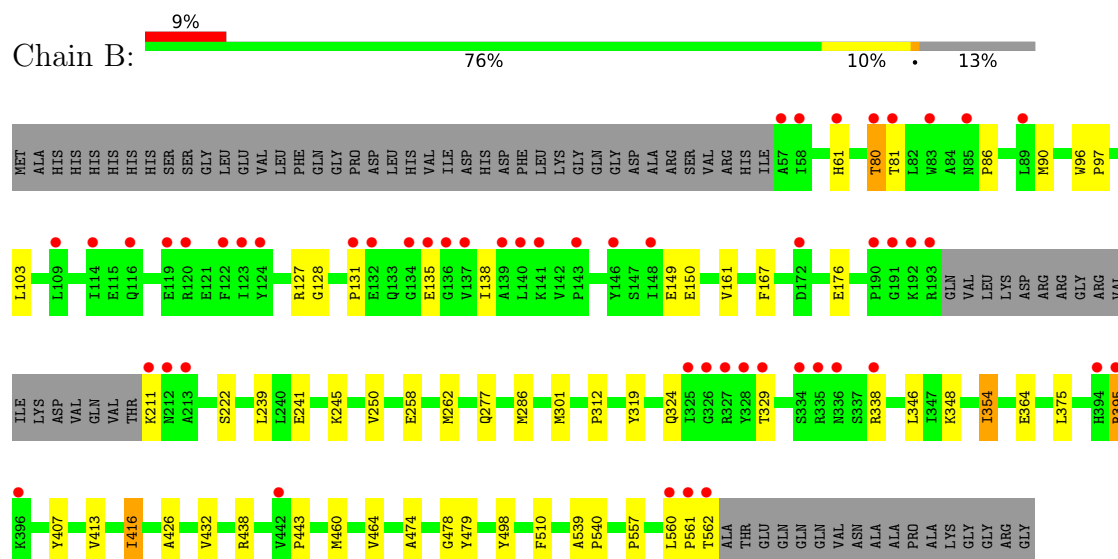
3 Residue-property plots [i](#)

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: Cell division protein



• Molecule 1: Cell division protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	57.22Å 74.37Å 82.45Å 71.69° 86.06° 85.88°	Depositor
Resolution (Å)	47.21 – 2.00 47.21 – 2.00	Depositor EDS
% Data completeness (in resolution range)	92.8 (47.21-2.00) 92.8 (47.21-2.00)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.7.0032, PHENIX	Depositor
R, R_{free}	0.226 , 0.263 0.226 , 0.263	Depositor DCC
R_{free} test set	4067 reflections (4.68%)	wwPDB-VP
Wilson B-factor (Å ²)	18.1	Xtriage
Anisotropy	0.330	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 53.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8353	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.80% 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: 59F, GOL, CL

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	0.50	0/3999	0.82	2/5426 (0.0%)
1	B	0.49	0/3792	0.80	0/5147
All	All	0.49	0/7791	0.81	2/10573 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	526	GLU	CA-C-N	-6.14	113.45	119.78
1	A	526	GLU	C-N-CA	-6.14	113.45	119.78

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	3922	0	3983	51	0
1	B	3717	0	3755	48	0
2	A	37	0	25	1	0
2	B	37	0	25	1	0
3	A	18	0	24	2	0
3	B	18	0	24	1	0
4	A	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	3	0	0	0	0
5	A	316	0	0	5	0
5	B	282	0	0	8	0
All	All	8353	0	7836	99	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 6.

All (99) 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:A:478:GLY:H	1:A:562:THR:HG23	1.31	0.95
1:B:478:GLY:H	1:B:562:THR:HG23	1.32	0.90
1:B:395:ARG:HG3	1:B:395:ARG:HH11	1.37	0.87
1:B:319:TYR:HB2	1:B:338:ARG:HG3	1.61	0.82
1:A:319:TYR:HB2	1:A:338:ARG:HG3	1.64	0.79
1:A:286:MET:HG2	1:A:416:ILE:HD13	1.68	0.74
1:A:81:THR:HG22	1:A:127:ARG:HA	1.71	0.72
1:B:81:THR:HG22	1:B:128:GLY:H	1.54	0.72
1:B:432:VAL:HG13	1:B:443:PRO:HG2	1.71	0.72
1:A:395:ARG:HG2	1:A:395:ARG:HH11	1.56	0.70
1:A:432:VAL:HG13	1:A:443:PRO:HG2	1.74	0.70
1:B:81:THR:HG22	1:B:127:ARG:HA	1.75	0.69
1:A:189:VAL:HG12	1:A:214:LYS:HB2	1.75	0.69
1:A:173:ARG:NH1	5:A:702:HOH:O	2.26	0.68
1:B:81:THR:HG21	1:B:150:GLU:OE2	1.94	0.67
1:B:364:GLU:HG2	5:B:723:HOH:O	1.96	0.66
1:A:346:LEU:HD12	1:A:460:MET:HE2	1.78	0.64
1:A:152:ARG:HH11	1:A:152:ARG:HG2	1.61	0.64
1:B:211:LYS:N	5:B:702:HOH:O	2.31	0.64
1:A:186:LEU:O	1:A:216:GLY:HA3	1.99	0.63
1:B:324:GLN:HG2	1:B:329:THR:HG22	1.81	0.61
1:B:562:THR:HG21	5:B:813:HOH:O	2.00	0.60
1:B:286:MET:HE2	1:B:416:ILE:HG12	1.85	0.59
1:A:81:THR:HG21	1:A:150:GLU:OE2	2.06	0.55
1:B:286:MET:HG2	1:B:416:ILE:HD13	1.89	0.55
1:B:262:MET:SD	1:B:286:MET:HE3	2.47	0.54
1:A:81:THR:CG2	1:A:150:GLU:OE2	2.56	0.54
1:B:81:THR:HG22	1:B:128:GLY:N	2.23	0.53
1:A:346:LEU:CD1	1:A:460:MET:HE2	2.38	0.53
1:B:395:ARG:HH11	1:B:395:ARG:CG	2.17	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:560:LEU:N	1:A:561:PRO:HD2	2.24	0.52
1:B:222:SER:HB2	1:B:258:GLU:HB3	1.91	0.52
1:B:250:VAL:HG21	1:B:416:ILE:HD12	1.91	0.52
1:B:395:ARG:HG3	1:B:395:ARG:NH1	2.15	0.52
1:B:540:PRO:HB2	3:B:603:GOL:H31	1.92	0.52
1:B:81:THR:CG2	1:B:150:GLU:OE2	2.58	0.51
1:A:474:ALA:HB2	1:A:539:ALA:HB1	1.92	0.51
1:B:460:MET:O	1:B:464:VAL:HG23	2.10	0.51
1:B:86:PRO:O	1:B:90:MET:HG2	2.11	0.51
1:B:354:ILE:HG21	1:B:407:TYR:HB3	1.93	0.51
1:A:81:THR:HG22	1:A:128:GLY:H	1.77	0.50
1:A:80:THR:OG1	1:A:131:PRO:HA	2.11	0.50
1:B:498:TYR:CE1	2:B:601:59F:H2	2.46	0.50
1:A:284:ARG:HD2	5:A:750:HOH:O	2.11	0.49
1:A:499:ARG:HD2	5:A:730:HOH:O	2.12	0.49
1:A:96:TRP:HB2	1:A:97:PRO:HD3	1.94	0.49
1:A:395:ARG:HG2	1:A:395:ARG:NH1	2.25	0.48
1:A:282:ARG:HG2	3:A:603:GOL:H12	1.95	0.48
1:B:135:GLU:HA	1:B:138:ILE:HB	1.95	0.48
1:B:560:LEU:N	1:B:561:PRO:HD2	2.28	0.48
1:B:81:THR:HG22	1:B:127:ARG:CA	2.42	0.48
1:A:239:LEU:HD13	1:A:265:GLN:HB2	1.96	0.47
1:B:80:THR:OG1	1:B:131:PRO:HA	2.14	0.47
1:A:385:GLY:HA2	1:B:241:GLU:O	2.15	0.47
1:A:301:MET:HG2	1:A:460:MET:HE1	1.96	0.47
1:B:312:PRO:HB3	5:B:785:HOH:O	2.14	0.47
1:B:167:PHE:CE2	1:B:176:GLU:HG3	2.50	0.47
1:A:207:VAL:HG23	1:A:208:GLN:HG2	1.97	0.47
1:B:438:ARG:NH1	5:B:701:HOH:O	2.31	0.46
1:B:474:ALA:HB2	1:B:539:ALA:HB1	1.96	0.46
1:A:84:ALA:HA	1:A:144:GLY:O	2.16	0.46
1:A:56:ILE:HD11	1:A:193:ARG:CZ	2.45	0.45
1:A:56:ILE:HD11	1:A:193:ARG:NH1	2.31	0.45
1:A:262:MET:SD	1:A:286:MET:HE3	2.56	0.45
1:A:106:ASP:OD2	1:A:109:LEU:HG	2.16	0.45
1:A:81:THR:HG21	1:A:127:ARG:HE	1.81	0.44
1:B:375:LEU:HD22	1:B:413:VAL:HG11	1.99	0.44
1:B:277:GLN:NE2	5:B:710:HOH:O	2.47	0.44
1:A:539:ALA:N	1:A:540:PRO:HD2	2.31	0.44
1:B:161:VAL:O	1:B:161:VAL:HG22	2.18	0.44
1:A:460:MET:O	1:A:464:VAL:HG23	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:ALA:O	1:A:141:LYS:HG2	2.18	0.43
1:B:324:GLN:CG	1:B:329:THR:HG22	2.48	0.43
1:A:274:ARG:HG2	1:A:275:ASN:OD1	2.18	0.43
1:A:83:TRP:CE2	1:A:146:TYR:HB2	2.52	0.43
1:A:252:MET:HE2	1:A:252:MET:HB3	1.73	0.43
1:A:265:GLN:HB3	5:A:732:HOH:O	2.18	0.43
1:A:432:VAL:CG1	1:A:443:PRO:HG2	2.45	0.43
1:A:479:TYR:CE1	1:A:557:PRO:HA	2.53	0.43
1:A:81:THR:HG22	1:A:127:ARG:CA	2.43	0.42
1:B:426:ALA:HB2	1:B:510:PHE:CG	2.54	0.42
1:A:233:ARG:HG2	5:A:950:HOH:O	2.19	0.42
1:A:375:LEU:HD22	1:A:413:VAL:HG11	2.00	0.42
1:A:282:ARG:CG	3:A:603:GOL:H12	2.49	0.42
1:B:96:TRP:HB2	1:B:97:PRO:HD3	2.02	0.41
1:B:539:ALA:N	1:B:540:PRO:HD2	2.34	0.41
1:A:378:ASP:HA	1:A:388:VAL:HG22	2.01	0.41
1:B:245:LYS:HE3	5:B:859:HOH:O	2.19	0.41
1:B:432:VAL:CG1	1:B:443:PRO:HG2	2.45	0.41
2:A:601:59F:O06	2:A:601:59F:N03	2.44	0.41
1:B:478:GLY:N	1:B:562:THR:HG23	2.16	0.41
1:B:346:LEU:HD12	1:B:460:MET:HE2	2.03	0.41
1:A:324:GLN:HG2	1:A:329:THR:HG22	2.03	0.41
1:A:492:SER:HA	1:A:499:ARG:HG2	2.02	0.41
1:B:301:MET:HG2	1:B:460:MET:HE1	2.03	0.41
1:B:348:LYS:HD3	5:B:808:HOH:O	2.21	0.41
1:B:479:TYR:CE1	1:B:557:PRO:HA	2.55	0.41
1:A:71:GLU:HA	1:A:72:PRO:HD3	1.94	0.41
1:A:367:TYR:CD2	1:A:367:TYR:C	2.99	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	512/564 (91%)	500 (98%)	12 (2%)	0	100	100
1	B	485/564 (86%)	475 (98%)	10 (2%)	0	100	100
All	All	997/1128 (88%)	975 (98%)	22 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	410/448 (92%)	399 (97%)	11 (3%)	39	42
1	B	387/448 (86%)	379 (98%)	8 (2%)	47	52
All	All	797/896 (89%)	778 (98%)	19 (2%)	43	47

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	HIS
1	A	80	THR
1	A	141	LYS
1	A	161	VAL
1	A	195	VAL
1	A	207	VAL
1	A	236	ARG
1	A	239	LEU
1	A	354	ILE
1	A	395	ARG
1	A	416	ILE
1	B	61	HIS
1	B	80	THR
1	B	103	LEU
1	B	149	GLU
1	B	239	LEU
1	B	354	ILE
1	B	395	ARG

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Mol	Chain	Res	Type
1	B	416	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	394	HIS
1	A	475	GLN
1	A	501	ASN
1	B	277	GLN
1	B	393	ASN
1	B	468	GLN
1	B	475	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 6 are monoatomic - leaving 8 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	GOL	B	602	-	5,5,5	0.28	0	5,5,5	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	A	604	-	5,5,5	0.30	0	5,5,5	0.31	0
2	59F	B	601	1	35,39,39	2.02	6 (17%)	40,55,55	2.07	10 (25%)
2	59F	A	601	1	35,39,39	1.98	8 (22%)	40,55,55	2.26	14 (35%)
3	GOL	B	604	-	5,5,5	0.26	0	5,5,5	0.66	0
3	GOL	B	603	-	5,5,5	0.27	0	5,5,5	0.48	0
3	GOL	A	603	-	5,5,5	0.37	0	5,5,5	0.47	0
3	GOL	A	602	-	5,5,5	0.26	0	5,5,5	0.69	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	GOL	B	602	-	-	2/4/4/4	-
3	GOL	A	604	-	-	0/4/4/4	-
2	59F	B	601	1	1/1/12/16	3/25/62/62	0/2/3/3
2	59F	A	601	1	1/1/12/16	3/25/62/62	0/2/3/3
3	GOL	B	604	-	-	2/4/4/4	-
3	GOL	B	603	-	-	0/4/4/4	-
3	GOL	A	603	-	-	2/4/4/4	-
3	GOL	A	602	-	-	2/4/4/4	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	59F	C06-N02	5.57	1.46	1.34
2	A	601	59F	C06-N02	4.93	1.44	1.34
2	B	601	59F	C17-N05	4.85	1.40	1.35
2	A	601	59F	C17-N05	4.65	1.40	1.35
2	A	601	59F	C16-C17	-4.64	1.45	1.53
2	B	601	59F	C11-N03	4.54	1.45	1.35
2	B	601	59F	C16-C17	-4.22	1.46	1.53
2	A	601	59F	C11-N03	4.15	1.44	1.35
2	B	601	59F	C11-N04	3.58	1.48	1.41
2	A	601	59F	C11-N04	3.20	1.47	1.41
2	A	601	59F	CA-C06	-2.43	1.48	1.54
2	A	601	59F	C02-N02	-2.38	1.43	1.46
2	A	601	59F	O04-C09	2.27	1.28	1.22
2	B	601	59F	O04-C09	2.22	1.28	1.22

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	59F	C08-C04-C07	7.02	122.39	112.24
2	A	601	59F	C08-C04-C07	6.74	121.98	112.24
2	B	601	59F	C08-C04-C05	5.28	118.96	108.99
2	A	601	59F	C08-C04-C05	4.90	118.25	108.99
2	A	601	59F	C02-N02-C06	-4.60	117.81	123.08
2	A	601	59F	C13-C12-N04	4.08	115.39	109.06
2	B	601	59F	C19-N05-C17	4.04	124.43	119.59
2	B	601	59F	C02-N02-C06	-3.57	119.00	123.08
2	A	601	59F	C01-C02-N02	3.35	117.03	109.93
2	B	601	59F	C10-CA-C06	3.18	115.91	108.42
2	A	601	59F	C03-C02-N02	-3.11	104.89	109.80
2	A	601	59F	O05-C11-N04	2.73	122.75	119.59
2	B	601	59F	C01-C02-N02	2.73	115.71	109.93
2	A	601	59F	O07-C17-N05	-2.70	120.48	123.55
2	A	601	59F	C19-N05-C17	2.64	122.75	119.59
2	A	601	59F	C12-C13-N05	2.52	115.43	110.42
2	B	601	59F	C09-C07-N01	2.40	114.39	108.68
2	A	601	59F	C15-C10-CA	-2.36	116.99	120.78
2	B	601	59F	O07-C17-N05	-2.31	120.93	123.55
2	A	601	59F	C10-CA-C06	2.30	113.83	108.42
2	A	601	59F	O01-C03-C02	-2.20	119.05	124.86
2	A	601	59F	C13-N05-C19	-2.07	112.94	116.63
2	B	601	59F	C04-C05-S01	-2.06	111.86	114.48
2	B	601	59F	O03-C09-O04	-2.02	119.50	124.08

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	601	59F	C04
2	B	601	59F	C04

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	59F	C23-C19-N05-C13
2	B	601	59F	N01-C07-C09-O04
3	A	602	GOL	O1-C1-C2-C3
3	A	603	GOL	C1-C2-C3-O3
3	B	602	GOL	O1-C1-C2-C3
3	B	604	GOL	C1-C2-C3-O3
3	B	602	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	B	604	GOL	O2-C2-C3-O3
3	A	602	GOL	O1-C1-C2-O2
3	A	603	GOL	O2-C2-C3-O3
2	A	601	59F	C23-C19-N05-C17
2	B	601	59F	C04-C07-C09-O03
2	A	601	59F	N01-C07-C09-O04
2	B	601	59F	C04-C07-C09-O04

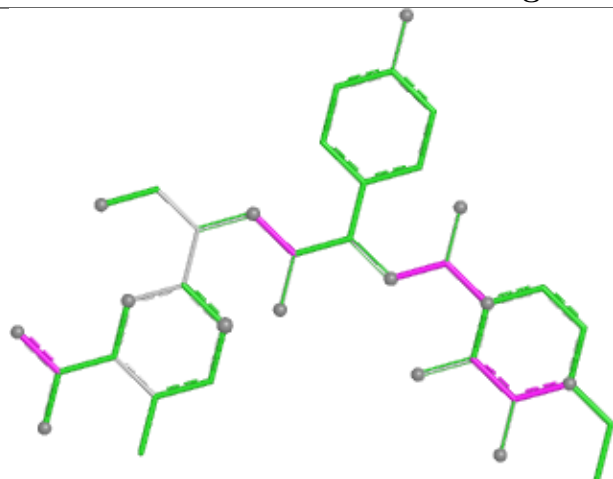
There are no ring outliers.

4 monomers are involved in 5 short contacts:

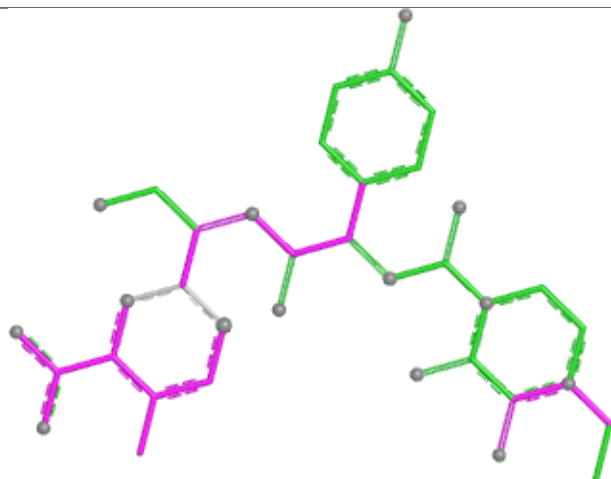
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	59F	1	0
2	A	601	59F	1	0
3	B	603	GOL	1	0
3	A	603	GOL	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

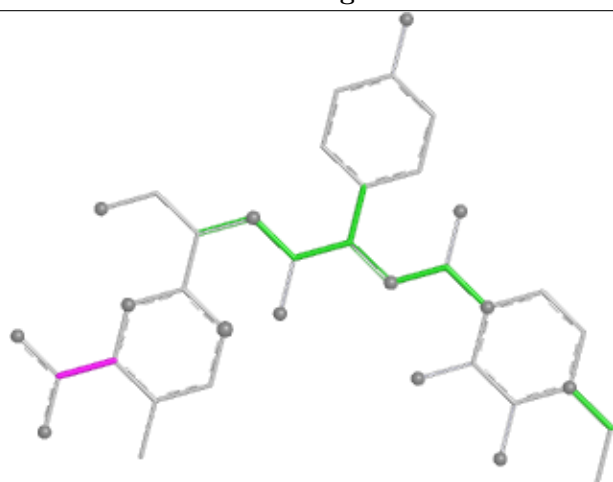
Ligand 59F B 601



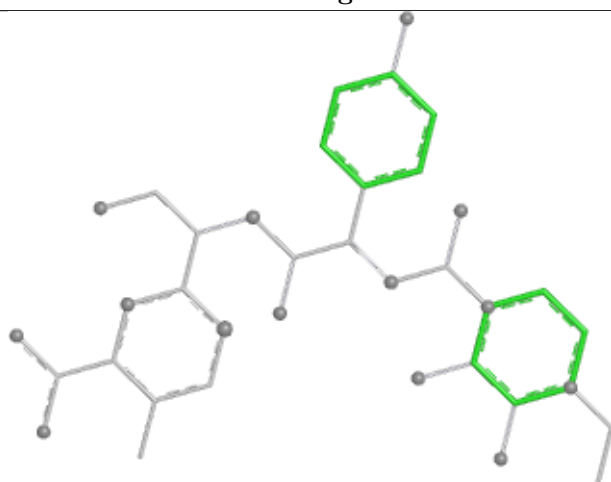
Bond lengths



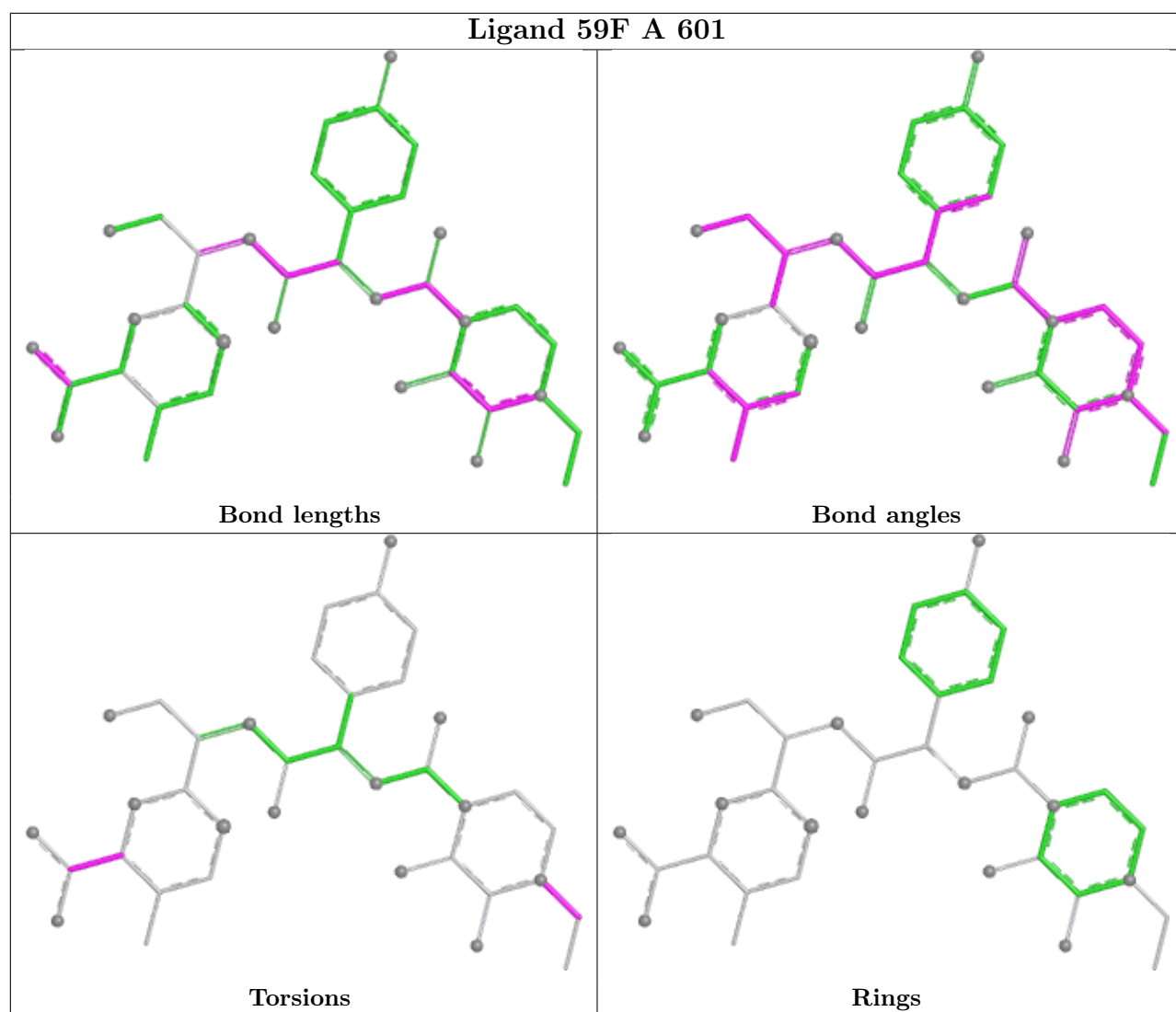
Bond angles



Torsions



Rings



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	514/564 (91%)	0.33	33 (6%) 25 24	8, 24, 60, 92	0
1	B	489/564 (86%)	0.48	52 (10%) 11 10	10, 26, 68, 102	0
All	All	1003/1128 (88%)	0.40	85 (8%) 16 15	8, 25, 65, 102	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	442	VAL	4.9
1	A	564	THR	4.7
1	A	560	LEU	4.5
1	B	193	ARG	4.3
1	A	563	ALA	4.2
1	A	561	PRO	3.9
1	B	146	TYR	3.8
1	B	136	GLY	3.7
1	B	139	ALA	3.7
1	B	58	ILE	3.7
1	B	560	LEU	3.6
1	A	396	LYS	3.6
1	B	212	ASN	3.5
1	A	334	SER	3.5
1	B	213	ALA	3.4
1	B	561	PRO	3.4
1	A	395	ARG	3.4
1	B	338	ARG	3.3
1	B	132	GLU	3.3
1	B	334	SER	3.2
1	B	141	LYS	3.2
1	B	134	GLY	3.2
1	B	140	LEU	3.1
1	B	192	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	124	TYR	3.1
1	A	364	GLU	3.0
1	B	119	GLU	3.0
1	A	139	ALA	3.0
1	B	137	VAL	3.0
1	B	562	THR	3.0
1	A	51	ARG	2.9
1	B	327	ARG	2.9
1	B	395	ARG	2.9
1	B	148	ILE	2.9
1	B	57	ALA	2.9
1	B	396	LYS	2.9
1	B	80	THR	2.8
1	B	114	ILE	2.8
1	B	131	PRO	2.8
1	B	120	ARG	2.8
1	A	325	ILE	2.8
1	A	200	ARG	2.8
1	A	393	ASN	2.7
1	A	336	ASN	2.6
1	A	394	HIS	2.6
1	A	440	ASP	2.6
1	B	325	ILE	2.6
1	B	335	ARG	2.6
1	B	394	HIS	2.5
1	B	329	THR	2.5
1	A	119	GLU	2.5
1	A	443	PRO	2.5
1	A	442	VAL	2.4
1	A	124	TYR	2.4
1	A	327	ARG	2.4
1	B	85	ASN	2.4
1	B	81	THR	2.4
1	B	326	GLY	2.3
1	A	319	TYR	2.3
1	B	172	ASP	2.3
1	B	135	GLU	2.3
1	A	214	LYS	2.3
1	B	109	LEU	2.3
1	B	122	PHE	2.2
1	B	328	TYR	2.2
1	A	173	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	89	LEU	2.2
1	A	337	SER	2.2
1	A	199	ARG	2.2
1	B	83	TRP	2.1
1	A	55	HIS	2.1
1	A	326	GLY	2.1
1	B	191	GLY	2.1
1	B	336	ASN	2.1
1	A	61	HIS	2.1
1	B	61	HIS	2.1
1	B	123	ILE	2.1
1	A	94	GLU	2.1
1	A	132	GLU	2.1
1	B	116	GLN	2.1
1	A	562	THR	2.1
1	A	136	GLY	2.1
1	B	211	LYS	2.1
1	B	143	PRO	2.0
1	B	190	PRO	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
3	GOL	A	603	6/6	0.80	0.22	39,55,61,62	0
3	GOL	B	603	6/6	0.82	0.18	40,46,52,58	0
3	GOL	A	604	6/6	0.88	0.13	28,50,52,53	0
3	GOL	B	604	6/6	0.88	0.14	23,30,35,39	0

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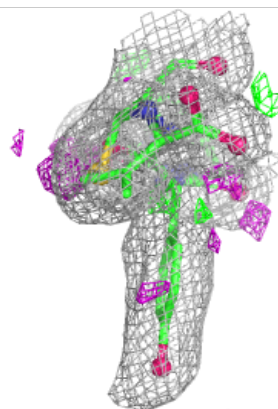
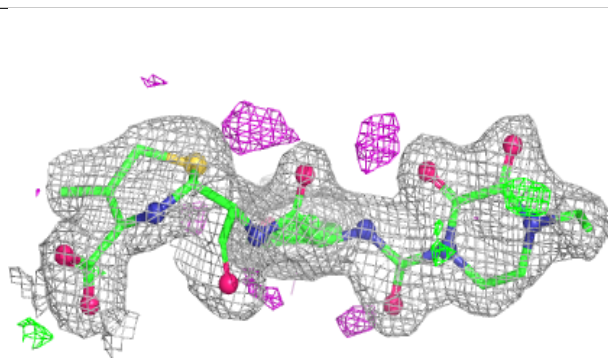
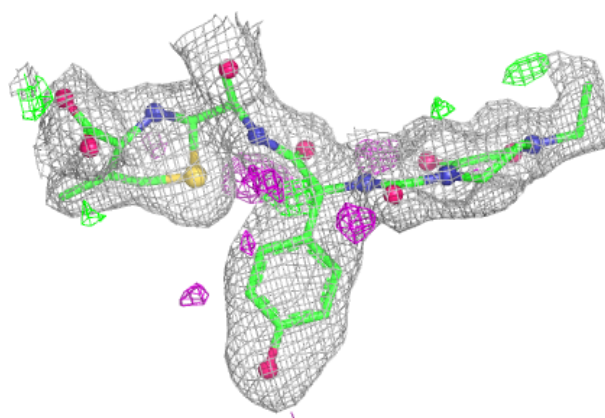
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	B	602	6/6	0.91	0.10	22,26,27,32	0
4	CL	A	605	1/1	0.93	0.11	34,34,34,34	0
4	CL	B	607	1/1	0.94	0.08	51,51,51,51	0
3	GOL	A	602	6/6	0.95	0.08	13,19,27,27	0
2	59F	B	601	37/37	0.95	0.08	12,23,33,38	0
2	59F	A	601	37/37	0.96	0.07	11,19,32,39	0
4	CL	B	605	1/1	0.97	0.09	38,38,38,38	0
4	CL	A	606	1/1	0.97	0.06	48,48,48,48	0
4	CL	B	606	1/1	0.98	0.04	31,31,31,31	0
4	CL	A	607	1/1	0.98	0.06	33,33,33,33	0

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

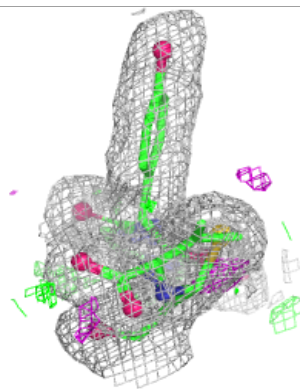
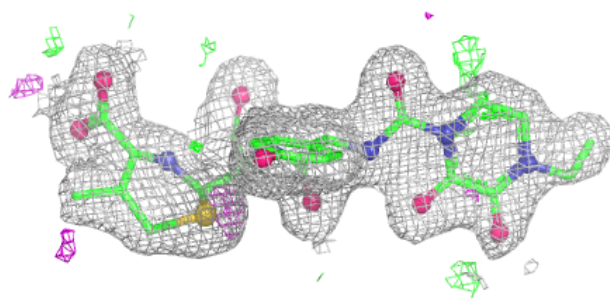
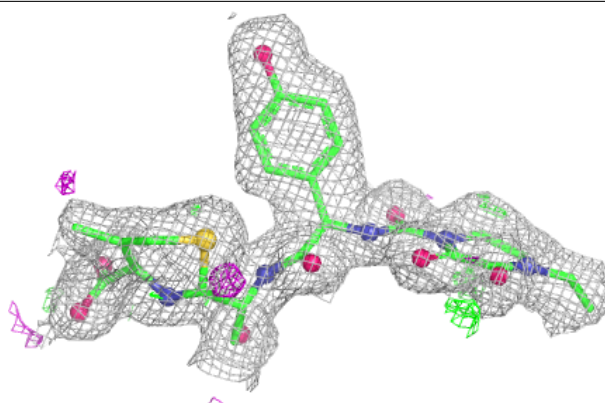
Electron density around 59F B 601:

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 59F 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.