



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 08:08 PM UTC

PDB ID : 3IAD / pdb_00003iad
Title : Crystal structure of human phosphodiesterase 4D with bound allosteric modulator
Authors : Staker, B.L.; Burgin Jr., A.B.
Deposited on : 2009-07-13
Resolution : 2.65 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

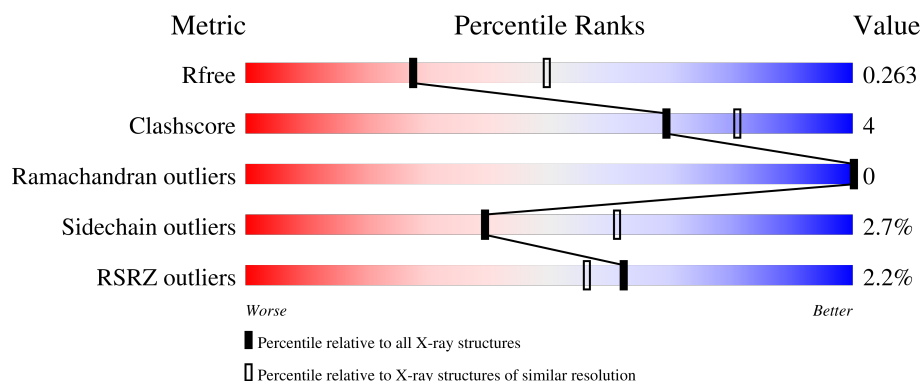
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	377	
1	B	377	
1	C	377	
1	D	377	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11397 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 cAMP-specific 3',5'-cyclic phosphodiesterase 4D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	0	0	0
			2743	1734	465	530	14			
1	B	338	Total	C	N	O	S	0	0	0
			2727	1726	462	525	14			
1	C	339	Total	C	N	O	S	0	0	0
			2740	1732	466	528	14			
1	D	339	Total	C	N	O	S	0	0	0
			2741	1733	467	527	14			

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	243	MET	-	initiating methionine	UNP Q08499
A	579	ALA	-	linker	UNP Q08499
A	580	PRO	-	linker	UNP Q08499
A	581	ALA	-	linker	UNP Q08499
A	582	PRO	-	linker	UNP Q08499
A	583	PRO	-	linker	UNP Q08499
A	584	LEU	-	linker	UNP Q08499
A	585	ASP	-	linker	UNP Q08499
A	586	GLU	-	linker	UNP Q08499
A	587	GLN	-	linker	UNP Q08499
A	588	ASN	-	linker	UNP Q08499
A	589	ARG	-	linker	UNP Q08499
A	590	ASP	-	linker	UNP Q08499
A	591	SER	-	linker	UNP Q08499
A	592	GLN	-	linker	UNP Q08499
A	607	GLU	-	expression tag	UNP Q08499
A	608	ASN	-	expression tag	UNP Q08499
A	609	LEU	-	expression tag	UNP Q08499
A	610	TYR	-	expression tag	UNP Q08499
A	611	PHE	-	expression tag	UNP Q08499
A	612	GLN	-	expression tag	UNP Q08499

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Chain	Residue	Modelled	Actual	Comment	Reference
A	613	GLY	-	expression tag	UNP Q08499
A	614	HIS	-	expression tag	UNP Q08499
A	615	HIS	-	expression tag	UNP Q08499
A	616	HIS	-	expression tag	UNP Q08499
A	617	HIS	-	expression tag	UNP Q08499
A	618	HIS	-	expression tag	UNP Q08499
A	619	HIS	-	expression tag	UNP Q08499
B	243	MET	-	initiating methionine	UNP Q08499
B	579	ALA	-	linker	UNP Q08499
B	580	PRO	-	linker	UNP Q08499
B	581	ALA	-	linker	UNP Q08499
B	582	PRO	-	linker	UNP Q08499
B	583	PRO	-	linker	UNP Q08499
B	584	LEU	-	linker	UNP Q08499
B	585	ASP	-	linker	UNP Q08499
B	586	GLU	-	linker	UNP Q08499
B	587	GLN	-	linker	UNP Q08499
B	588	ASN	-	linker	UNP Q08499
B	589	ARG	-	linker	UNP Q08499
B	590	ASP	-	linker	UNP Q08499
B	591	SER	-	linker	UNP Q08499
B	592	GLN	-	linker	UNP Q08499
B	607	GLU	-	expression tag	UNP Q08499
B	608	ASN	-	expression tag	UNP Q08499
B	609	LEU	-	expression tag	UNP Q08499
B	610	TYR	-	expression tag	UNP Q08499
B	611	PHE	-	expression tag	UNP Q08499
B	612	GLN	-	expression tag	UNP Q08499
B	613	GLY	-	expression tag	UNP Q08499
B	614	HIS	-	expression tag	UNP Q08499
B	615	HIS	-	expression tag	UNP Q08499
B	616	HIS	-	expression tag	UNP Q08499
B	617	HIS	-	expression tag	UNP Q08499
B	618	HIS	-	expression tag	UNP Q08499
B	619	HIS	-	expression tag	UNP Q08499
C	243	MET	-	initiating methionine	UNP Q08499
C	579	ALA	-	linker	UNP Q08499
C	580	PRO	-	linker	UNP Q08499
C	581	ALA	-	linker	UNP Q08499
C	582	PRO	-	linker	UNP Q08499
C	583	PRO	-	linker	UNP Q08499
C	584	LEU	-	linker	UNP Q08499

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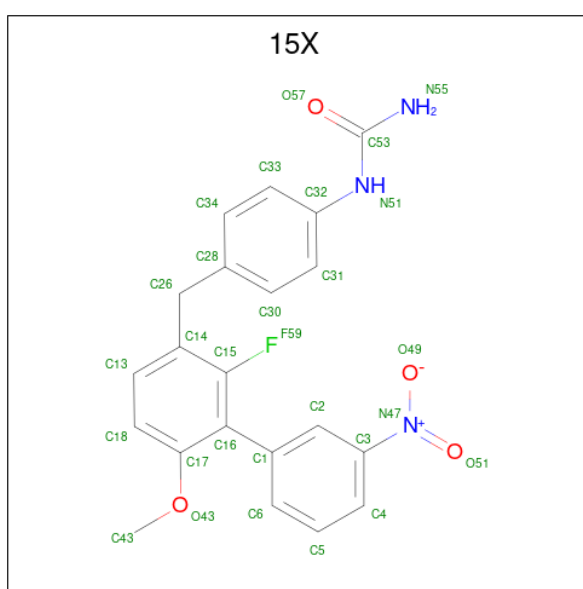
Chain	Residue	Modelled	Actual	Comment	Reference
C	585	ASP	-	linker	UNP Q08499
C	586	GLU	-	linker	UNP Q08499
C	587	GLN	-	linker	UNP Q08499
C	588	ASN	-	linker	UNP Q08499
C	589	ARG	-	linker	UNP Q08499
C	590	ASP	-	linker	UNP Q08499
C	591	SER	-	linker	UNP Q08499
C	592	GLN	-	linker	UNP Q08499
C	607	GLU	-	expression tag	UNP Q08499
C	608	ASN	-	expression tag	UNP Q08499
C	609	LEU	-	expression tag	UNP Q08499
C	610	TYR	-	expression tag	UNP Q08499
C	611	PHE	-	expression tag	UNP Q08499
C	612	GLN	-	expression tag	UNP Q08499
C	613	GLY	-	expression tag	UNP Q08499
C	614	HIS	-	expression tag	UNP Q08499
C	615	HIS	-	expression tag	UNP Q08499
C	616	HIS	-	expression tag	UNP Q08499
C	617	HIS	-	expression tag	UNP Q08499
C	618	HIS	-	expression tag	UNP Q08499
C	619	HIS	-	expression tag	UNP Q08499
D	243	MET	-	initiating methionine	UNP Q08499
D	579	ALA	-	linker	UNP Q08499
D	580	PRO	-	linker	UNP Q08499
D	581	ALA	-	linker	UNP Q08499
D	582	PRO	-	linker	UNP Q08499
D	583	PRO	-	linker	UNP Q08499
D	584	LEU	-	linker	UNP Q08499
D	585	ASP	-	linker	UNP Q08499
D	586	GLU	-	linker	UNP Q08499
D	587	GLN	-	linker	UNP Q08499
D	588	ASN	-	linker	UNP Q08499
D	589	ARG	-	linker	UNP Q08499
D	590	ASP	-	linker	UNP Q08499
D	591	SER	-	linker	UNP Q08499
D	592	GLN	-	linker	UNP Q08499
D	607	GLU	-	expression tag	UNP Q08499
D	608	ASN	-	expression tag	UNP Q08499
D	609	LEU	-	expression tag	UNP Q08499
D	610	TYR	-	expression tag	UNP Q08499
D	611	PHE	-	expression tag	UNP Q08499
D	612	GLN	-	expression tag	UNP Q08499

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Chain	Residue	Modelled	Actual	Comment	Reference
D	613	GLY	-	expression tag	UNP Q08499
D	614	HIS	-	expression tag	UNP Q08499
D	615	HIS	-	expression tag	UNP Q08499
D	616	HIS	-	expression tag	UNP Q08499
D	617	HIS	-	expression tag	UNP Q08499
D	618	HIS	-	expression tag	UNP Q08499
D	619	HIS	-	expression tag	UNP Q08499

- Molecule 2 is 1-{4-[(2-fluoro-6-methoxy-3'-nitrophenyl-3-yl)methyl]phenyl}urea (CCD ID: 15X) (formula: C₂₁H₁₈FN₃O₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 29	C 21	F 1	N 3	O 4	0	0
2	B	1	Total 58	C 42	F 2	N 6	O 8	0	1
2	C	1	Total 29	C 21	F 1	N 3	O 4	0	0
2	D	1	Total 29	C 21	F 1	N 3	O 4	0	0

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

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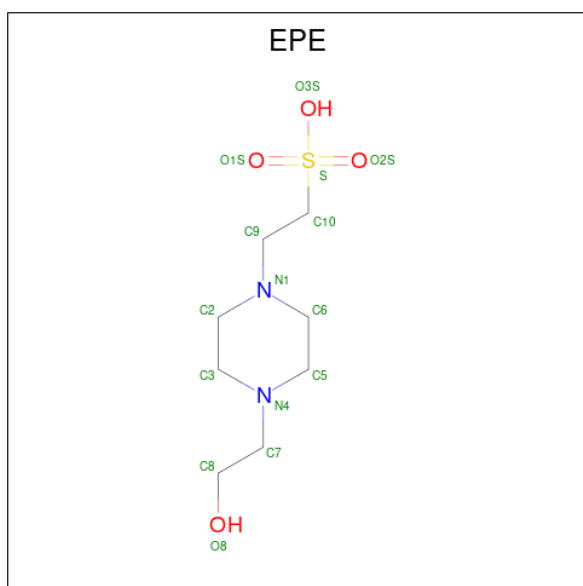
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
5	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

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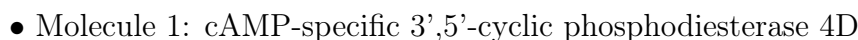
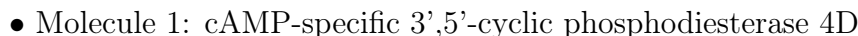
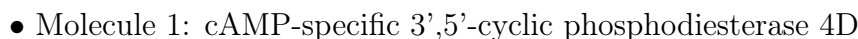
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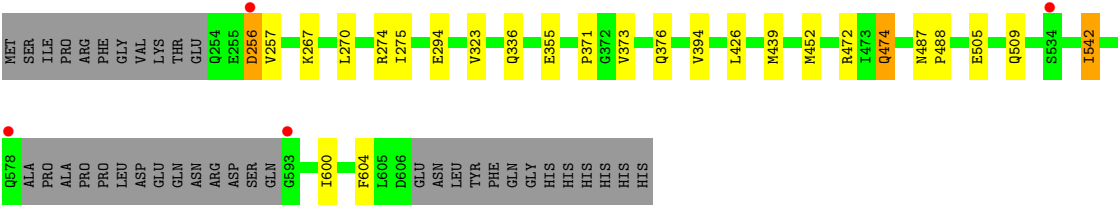
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
5	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
5	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
5	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	53	Total	O	0	0
			53	53		
6	B	46	Total	O	0	0
			46	46		
6	C	44	Total	O	0	0
			44	44		
6	D	60	Total	O	0	0
			60	60		

- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	97.55Å 112.00Å 162.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.65 50.00 – 2.65	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.65) 93.2 (50.00-2.65)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.214 , 0.267 0.214 , 0.263	Depositor DCC
R_{free} test set	2479 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å ²)	27.3	Xtriage
Anisotropy	0.151	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 30.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	11397	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% 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: EPE, ZN, MG, 15X

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	0.49	0/2797	0.73	0/3798
1	B	0.48	0/2782	0.73	0/3780
1	C	0.49	0/2794	0.73	0/3794
1	D	0.50	0/2796	0.73	0/3797
All	All	0.49	0/11169	0.73	0/15169

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	2743	0	2682	20	0
1	B	2727	0	2664	16	0
1	C	2740	0	2682	17	0
1	D	2741	0	2684	17	0
2	A	29	0	18	1	0
2	B	58	0	36	6	0
2	C	29	0	18	1	0
2	D	29	0	18	1	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	15	0	17	0	0
5	B	30	0	34	0	0
5	C	15	0	17	0	0
5	D	30	0	34	0	0
6	A	53	0	0	3	0
6	B	46	0	0	0	0
6	C	44	0	0	0	0
6	D	60	0	0	2	0
All	All	11397	0	10904	78	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 (78) 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:439:MET:HE2	1:D:604:PHE:HE2	1.39	0.86
1:A:542:ILE:HD11	1:A:600:ILE:HG23	1.54	0.86
1:C:542:ILE:HD11	1:C:600:ILE:HG23	1.59	0.84
1:D:542:ILE:HD11	1:D:600:ILE:HG23	1.58	0.83
2:B:901[A]:15X:O57	2:B:901[A]:15X:H31	1.80	0.80
1:B:542:ILE:HD11	1:B:600:ILE:HG23	1.66	0.77
2:B:901[B]:15X:O57	2:B:901[B]:15X:H33	1.90	0.70
1:D:439:MET:HE2	1:D:604:PHE:CE2	2.24	0.68
1:B:439:MET:HE2	1:B:604:PHE:HE2	1.58	0.68
1:B:358:ALA:HB2	1:B:426:LEU:HD12	1.78	0.65
1:B:439:MET:HE2	1:B:604:PHE:CE2	2.32	0.65
1:C:452:MET:HE1	1:C:474:GLN:HB3	1.82	0.62
1:A:270:LEU:HD11	1:A:275:ILE:HD11	1.86	0.58
1:C:270:LEU:HD11	1:C:275:ILE:HD11	1.85	0.57
1:A:459:THR:HG22	1:A:465:LEU:HD12	1.87	0.56
1:B:323:VAL:HG13	1:B:505:GLU:OE1	2.05	0.56
1:C:288:MET:HE3	1:C:312:LEU:HD21	1.87	0.55
1:C:323:VAL:HG13	1:C:505:GLU:OE1	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:267:LYS:NZ	6:D:30:HOH:O	2.40	0.54
1:B:400:LEU:HD21	1:B:434:VAL:HB	1.90	0.54
1:A:542:ILE:HD13	1:A:604:PHE:CE1	2.45	0.52
1:C:323:VAL:CG1	1:C:505:GLU:OE1	2.58	0.52
1:B:496:ARG:HD3	1:B:571:TRP:CH2	2.44	0.52
1:D:270:LEU:HD11	1:D:275:ILE:HD11	1.90	0.52
1:C:418:LEU:HD23	1:C:422:GLN:HB3	1.91	0.52
1:C:439:MET:HE2	1:C:604:PHE:HE2	1.75	0.51
1:C:439:MET:HE2	1:C:604:PHE:CE2	2.44	0.51
1:A:550:TRP:O	1:A:554:VAL:HG22	2.10	0.51
2:B:901[B]:15X:H30	2:B:901[B]:15X:F59	2.01	0.51
1:D:487:ASN:HB2	1:D:488:PRO:HD3	1.93	0.50
1:C:439:MET:HE3	1:C:439:MET:HA	1.93	0.49
1:A:474:GLN:HA	1:A:477:GLN:HE21	1.76	0.49
1:A:439:MET:HE2	1:A:604:PHE:CE2	2.48	0.48
1:B:449:LEU:HG	1:B:549:THR:HG22	1.96	0.48
1:A:523:MET:SD	1:A:534:SER:OG	2.71	0.48
1:D:371:PRO:HG2	1:D:373:VAL:HG22	1.96	0.47
1:D:439:MET:HE3	1:D:439:MET:HA	1.95	0.47
1:A:439:MET:HE1	1:A:485:LEU:HD21	1.96	0.47
2:A:901:15X:H31	2:A:901:15X:HN55	1.80	0.47
1:C:287:ILE:HD12	1:C:332:ALA:HB1	1.96	0.47
1:C:542:ILE:HD13	1:C:604:PHE:CD1	2.50	0.47
1:B:262:LEU:HD11	1:B:286:VAL:CG1	2.45	0.47
1:D:394:VAL:HG23	6:D:47:HOH:O	2.15	0.46
1:B:439:MET:HE3	1:B:439:MET:HA	1.97	0.46
1:D:323:VAL:HG13	1:D:505:GLU:OE1	2.15	0.46
1:A:249:GLY:N	6:A:93:HOH:O	2.48	0.46
1:A:426:LEU:O	1:A:430:VAL:HG23	2.15	0.46
1:D:256:ASP:OD2	1:D:257:VAL:HG23	2.15	0.46
2:B:901[A]:15X:O57	2:B:901[A]:15X:C31	2.48	0.46
2:D:901:15X:O57	2:D:901:15X:H33	2.16	0.45
1:A:439:MET:HE3	1:A:439:MET:HA	1.97	0.45
1:D:452:MET:HE1	1:D:474:GLN:HB3	1.98	0.45
1:A:250:VAL:HG22	6:A:93:HOH:O	2.17	0.45
2:C:901:15X:O57	2:C:901:15X:H33	2.17	0.45
1:D:373:VAL:HA	1:D:509:GLN:HE21	1.82	0.45
2:B:901[B]:15X:O57	2:B:901[B]:15X:C33	2.57	0.44
1:C:492:LEU:HD21	1:C:571:TRP:CE2	2.51	0.44
1:B:542:ILE:HD13	1:B:604:PHE:CE1	2.52	0.44
1:B:282:ARG:N	1:B:283:PRO:CD	2.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:ILE:HG22	1:A:313:MET:HE2	2.00	0.44
1:C:487:ASN:HB2	1:C:488:PRO:HD3	2.00	0.43
1:A:392:SER:O	1:A:393:SER:C	2.61	0.43
1:B:288:MET:HE3	1:B:312:LEU:HD21	1.99	0.43
1:A:253:GLU:O	1:A:257:VAL:HG23	2.19	0.43
1:D:373:VAL:HA	1:D:509:GLN:NE2	2.34	0.42
1:C:282:ARG:N	1:C:283:PRO:CD	2.83	0.42
1:A:439:MET:HE2	1:A:604:PHE:HE2	1.84	0.42
1:D:270:LEU:HD22	1:D:336:GLN:HG3	2.01	0.42
1:A:539:ILE:HA	1:A:543:VAL:HB	2.02	0.42
1:C:342:LEU:HD13	1:C:356:ILE:HG23	2.01	0.42
1:A:293:GLN:NE2	6:A:87:HOH:O	2.51	0.41
1:C:371:PRO:HG2	1:C:373:VAL:HG22	2.02	0.41
1:B:502:ILE:HG21	2:B:901[A]:15X:H43A	2.01	0.41
1:D:542:ILE:HD13	1:D:604:PHE:CE1	2.56	0.41
1:D:355:GLU:OE1	1:D:472:ARG:NH1	2.54	0.41
1:B:487:ASN:HB2	1:B:488:PRO:HD3	2.03	0.41
1:A:459:THR:HG23	1:A:465:LEU:HB2	2.04	0.40
1:B:562:LEU:HD23	1:B:562:LEU:HA	1.97	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	336/377 (89%)	326 (97%)	10 (3%)	0	100	100
1	B	334/377 (89%)	321 (96%)	13 (4%)	0	100	100
1	C	335/377 (89%)	325 (97%)	10 (3%)	0	100	100
1	D	335/377 (89%)	327 (98%)	8 (2%)	0	100	100
All	All	1340/1508 (89%)	1299 (97%)	41 (3%)	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	310/344 (90%)	305 (98%)	5 (2%)	55	74
1	B	308/344 (90%)	297 (96%)	11 (4%)	31	51
1	C	310/344 (90%)	299 (96%)	11 (4%)	32	52
1	D	310/344 (90%)	303 (98%)	7 (2%)	44	66
All	All	1238/1376 (90%)	1204 (97%)	34 (3%)	39	61

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	252	THR
1	A	323	VAL
1	A	445	LEU
1	A	452	MET
1	A	570	GLU
1	B	255	GLU
1	B	256	ASP
1	B	258	LEU
1	B	344	THR
1	B	421	LYS
1	B	445	LEU
1	B	452	MET
1	B	493	GLN
1	B	504	GLU
1	B	534	SER
1	B	567	ASP
1	C	253	GLU
1	C	254	GLN
1	C	344	THR
1	C	385	LEU
1	C	387	LEU
1	C	408	GLN

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Mol	Chain	Res	Type
1	C	421	LYS
1	C	463	VAL
1	C	474	GLN
1	C	523	MET
1	C	597	SER
1	D	256	ASP
1	D	274	ARG
1	D	294	GLU
1	D	376	GLN
1	D	426	LEU
1	D	474	GLN
1	D	542	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	477	GLN
1	A	478	ASN
1	A	528	ASN
1	A	535	GLN
1	A	594	ASN
1	B	390	ASN
1	B	474	GLN
1	B	497	GLN
1	B	595	GLN
1	C	376	GLN
1	C	408	GLN
1	C	487	ASN
1	C	535	GLN
1	C	594	ASN
1	C	595	GLN
1	D	254	GLN
1	D	293	GLN
1	D	390	ASN
1	D	424	GLN
1	D	478	ASN
1	D	487	ASN
1	D	497	GLN
1	D	509	GLN
1	D	528	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 19 ligands modelled in this entry, 8 are monoatomic - leaving 11 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$
5	EPE	C	803	-	15,15,15	0.74	1 (6%)	19,20,20	1.24	2 (10%)
2	15X	B	901[A]	-	31,31,31	2.60	5 (16%)	40,43,43	1.56	8 (20%)
5	EPE	D	804	-	15,15,15	0.74	1 (6%)	19,20,20	1.08	1 (5%)
2	15X	A	901	-	31,31,31	2.65	5 (16%)	40,43,43	2.59	12 (30%)
2	15X	B	901[B]	-	31,31,31	2.60	5 (16%)	40,43,43	1.48	7 (17%)
5	EPE	B	801	-	15,15,15	0.83	1 (6%)	19,20,20	1.08	0
5	EPE	D	805	-	15,15,15	0.78	1 (6%)	19,20,20	1.29	2 (10%)
5	EPE	B	802	-	15,15,15	0.89	1 (6%)	19,20,20	1.05	2 (10%)
2	15X	C	901	-	31,31,31	2.60	5 (16%)	40,43,43	1.75	9 (22%)
2	15X	D	901	-	31,31,31	2.51	5 (16%)	40,43,43	1.48	7 (17%)
5	EPE	A	806	-	15,15,15	0.77	1 (6%)	19,20,20	1.16	2 (10%)

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
5	EPE	C	803	-	-	3/9/19/19	0/1/1/1
2	15X	B	901[A]	-	-	1/16/18/18	0/3/3/3
5	EPE	D	804	-	-	2/9/19/19	0/1/1/1
2	15X	A	901	-	-	3/16/18/18	0/3/3/3
2	15X	B	901[B]	-	-	0/16/18/18	0/3/3/3
5	EPE	B	801	-	-	4/9/19/19	0/1/1/1
5	EPE	D	805	-	-	3/9/19/19	0/1/1/1
5	EPE	B	802	-	-	1/9/19/19	0/1/1/1
2	15X	C	901	-	-	2/16/18/18	0/3/3/3
2	15X	D	901	-	-	0/16/18/18	0/3/3/3
5	EPE	A	806	-	-	1/9/19/19	0/1/1/1

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	15X	O51-N47	10.10	1.40	1.22
2	C	901	15X	O51-N47	9.93	1.39	1.22
2	B	901[B]	15X	O51-N47	9.75	1.39	1.22
2	B	901[A]	15X	O51-N47	9.74	1.39	1.22
2	D	901	15X	O51-N47	9.52	1.39	1.22
2	C	901	15X	C16-C17	6.15	1.49	1.40
2	A	901	15X	C16-C15	5.97	1.48	1.39
2	D	901	15X	C16-C15	5.85	1.48	1.39
2	B	901[B]	15X	C16-C17	5.82	1.48	1.40
2	B	901[A]	15X	C16-C17	5.82	1.48	1.40
2	C	901	15X	C16-C15	5.74	1.48	1.39
2	A	901	15X	C16-C17	5.72	1.48	1.40
2	B	901[B]	15X	C16-C15	5.71	1.48	1.39
2	B	901[A]	15X	C16-C15	5.68	1.47	1.39
2	D	901	15X	C16-C17	5.50	1.48	1.40
2	A	901	15X	C14-C15	5.41	1.49	1.38
2	B	901[B]	15X	C14-C15	4.97	1.48	1.38
2	B	901[A]	15X	C14-C15	4.88	1.47	1.38
2	D	901	15X	C14-C15	4.65	1.47	1.38
2	C	901	15X	C14-C15	4.57	1.47	1.38
5	B	802	EPE	C10-S	3.07	1.81	1.77
5	B	801	EPE	C10-S	2.88	1.81	1.77
2	B	901[A]	15X	C32-N51	-2.76	1.36	1.41
5	A	806	EPE	C10-S	2.66	1.81	1.77
5	D	805	EPE	C10-S	2.60	1.81	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901[B]	15X	C32-N51	-2.58	1.36	1.41
5	C	803	EPE	C10-S	2.54	1.81	1.77
5	D	804	EPE	C10-S	2.53	1.81	1.77
2	D	901	15X	C32-N51	-2.25	1.37	1.41
2	A	901	15X	C32-N51	-2.19	1.37	1.41
2	C	901	15X	C32-N51	-2.07	1.37	1.41

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	15X	N55-C53-N51	11.04	127.80	115.47
2	A	901	15X	O57-C53-N51	-6.40	115.42	122.39
2	B	901[B]	15X	O43-C17-C16	4.17	120.86	115.45
2	C	901	15X	O43-C17-C16	4.16	120.86	115.45
2	B	901[A]	15X	O43-C17-C16	4.15	120.84	115.45
2	B	901[A]	15X	C13-C14-C15	3.84	119.28	116.46
2	B	901[B]	15X	C13-C14-C15	3.67	119.15	116.46
2	C	901	15X	C13-C14-C15	3.61	119.12	116.46
2	D	901	15X	C43-O43-C17	3.54	122.71	117.51
2	C	901	15X	C1-C16-C15	-3.49	116.22	122.12
2	C	901	15X	C1-C16-C17	3.46	125.53	120.73
2	A	901	15X	C43-O43-C17	3.28	122.32	117.51
2	D	901	15X	C13-C14-C15	3.27	118.86	116.46
2	A	901	15X	O57-C53-N55	-3.19	116.77	123.18
2	C	901	15X	C4-C3-N47	3.12	122.07	119.34
5	D	805	EPE	O2S-S-C10	3.08	111.38	106.73
5	D	804	EPE	O2S-S-C10	3.05	111.34	106.73
2	A	901	15X	F59-C15-C14	3.00	122.06	118.00
2	A	901	15X	C1-C16-C15	-2.93	117.17	122.12
2	A	901	15X	C13-C14-C15	2.85	118.55	116.46
2	B	901[A]	15X	C14-C26-C28	-2.80	108.04	114.21
5	C	803	EPE	O2S-S-C10	2.73	110.86	106.73
2	A	901	15X	O43-C17-C16	2.73	119.00	115.45
2	B	901[B]	15X	C16-C15-C14	-2.72	118.76	123.38
2	D	901	15X	O57-C53-N55	-2.71	117.72	123.18
2	C	901	15X	C43-O43-C17	2.63	121.37	117.51
2	B	901[A]	15X	O43-C17-C18	-2.63	119.86	124.30
2	B	901[A]	15X	C16-C15-C14	-2.63	118.92	123.38
5	C	803	EPE	O1S-S-C10	2.58	110.63	106.73
2	B	901[B]	15X	O43-C17-C18	-2.58	119.95	124.30
2	A	901	15X	C16-C15-C14	-2.58	119.00	123.38
2	C	901	15X	O57-C53-N55	-2.56	118.04	123.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901[A]	15X	C1-C16-C15	-2.50	117.90	122.12
5	B	802	EPE	O1S-S-C10	2.47	110.46	106.73
2	D	901	15X	O43-C17-C16	2.47	118.66	115.45
2	A	901	15X	C1-C16-C17	2.47	124.15	120.73
2	D	901	15X	C16-C15-C14	-2.47	119.18	123.38
2	D	901	15X	O57-C53-N51	2.46	125.07	122.39
2	C	901	15X	C16-C15-C14	-2.44	119.24	123.38
2	B	901[A]	15X	C1-C16-C17	2.40	124.05	120.73
2	B	901[B]	15X	C1-C16-C15	-2.38	118.10	122.12
2	D	901	15X	C1-C16-C15	-2.32	118.20	122.12
5	A	806	EPE	O1S-S-C10	2.28	110.17	106.73
5	B	802	EPE	O3S-S-C10	2.26	110.43	106.00
2	C	901	15X	O43-C17-C18	-2.20	120.59	124.30
2	B	901[B]	15X	F59-C15-C14	2.17	120.93	118.00
5	A	806	EPE	C6-N1-C2	2.16	113.50	108.84
2	A	901	15X	C4-C3-N47	2.13	121.19	119.34
2	A	901	15X	C31-C32-N51	2.12	127.53	120.41
5	D	805	EPE	O1S-S-C10	2.10	109.91	106.73
2	B	901[B]	15X	C1-C16-C17	2.10	123.64	120.73
2	B	901[A]	15X	F59-C15-C14	2.03	120.74	118.00

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	801	EPE	C9-C10-S-O1S
5	C	803	EPE	C9-C10-S-O2S
5	C	803	EPE	C9-C10-S-O3S
5	A	806	EPE	N4-C7-C8-O8
5	D	804	EPE	N4-C7-C8-O8
5	B	801	EPE	C9-C10-S-O3S
5	D	805	EPE	C9-C10-S-O3S
5	B	801	EPE	N4-C7-C8-O8
2	A	901	15X	N55-C53-N51-C32
2	A	901	15X	O57-C53-N51-C32
5	B	802	EPE	N4-C7-C8-O8
5	D	804	EPE	S-C10-C9-N1
2	C	901	15X	C18-C17-O43-C43
2	C	901	15X	C16-C17-O43-C43
2	B	901[A]	15X	C15-C14-C26-C28
5	B	801	EPE	C9-C10-S-O2S
5	C	803	EPE	C9-C10-S-O1S

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Mol	Chain	Res	Type	Atoms
5	D	805	EPE	C9-C10-S-O1S
5	D	805	EPE	C9-C10-S-O2S
2	A	901	15X	C15-C14-C26-C28

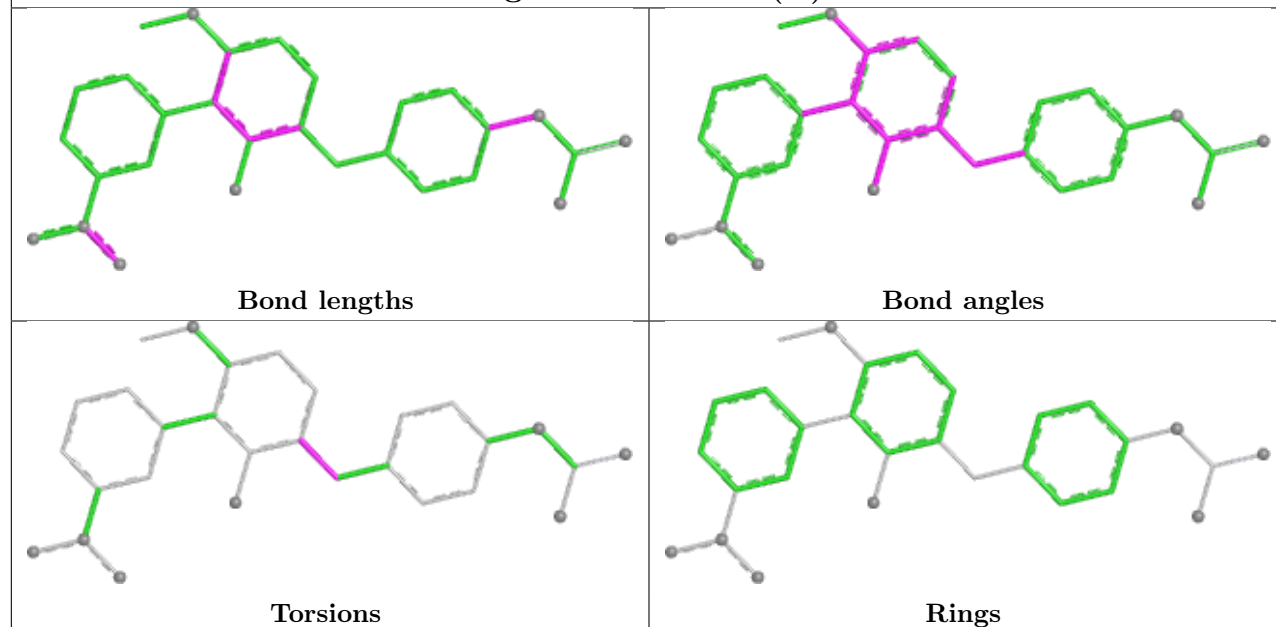
There are no ring outliers.

5 monomers are involved in 9 short contacts:

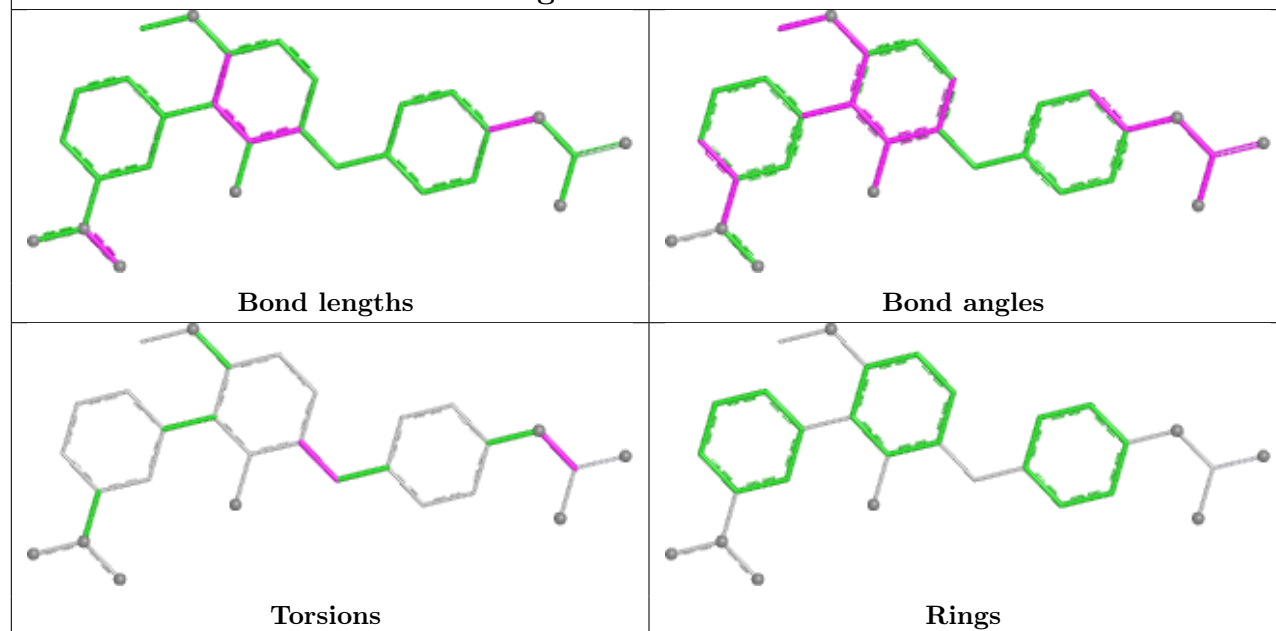
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	901[A]	15X	3	0
2	A	901	15X	1	0
2	B	901[B]	15X	3	0
2	C	901	15X	1	0
2	D	901	15X	1	0

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

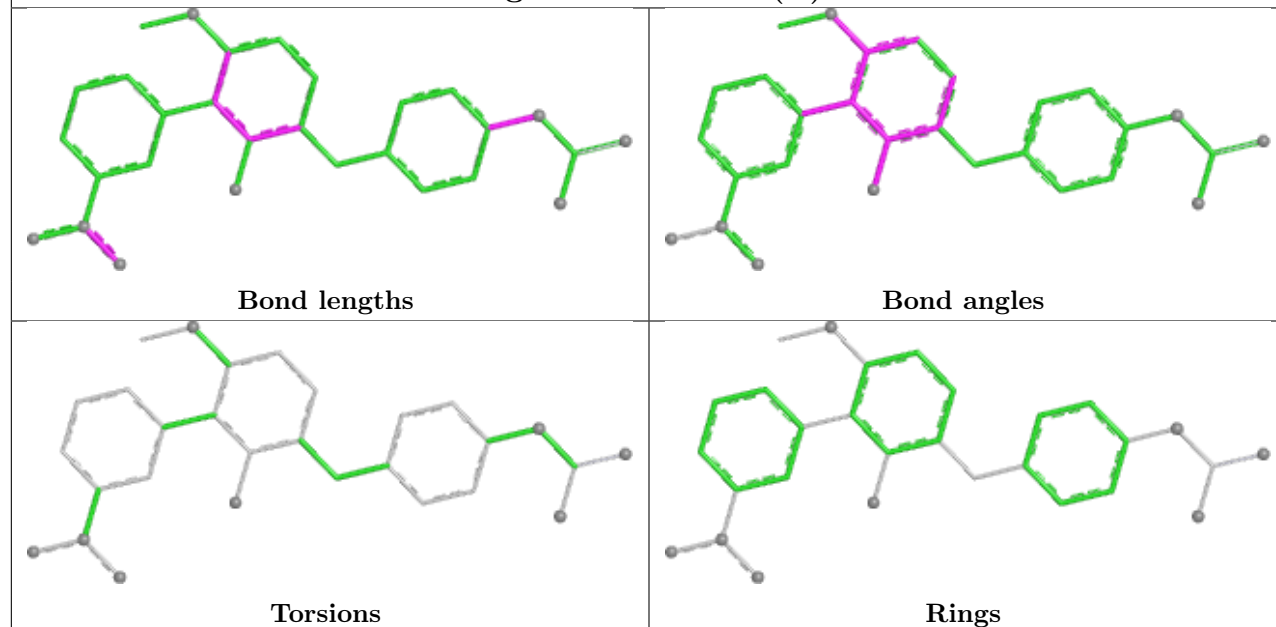
Ligand 15X B 901 (A)



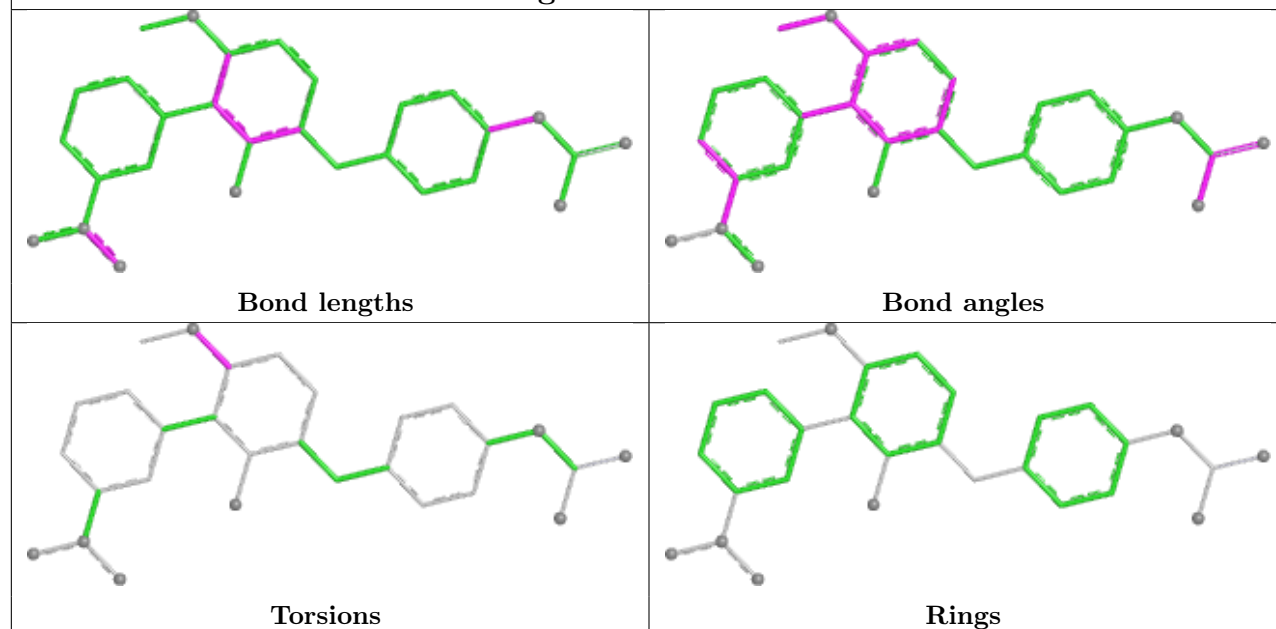
Ligand 15X A 901

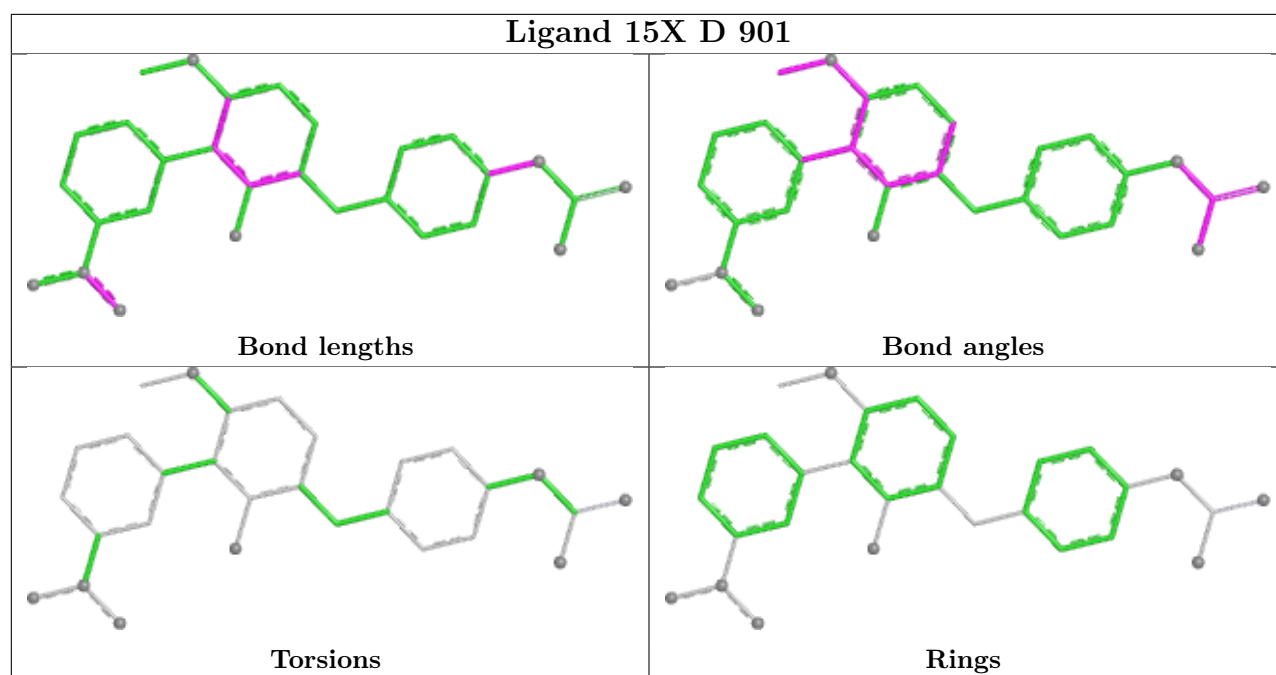


Ligand 15X B 901 (B)



Ligand 15X C 901





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	340/377 (90%)	0.08	12 (3%) 47 38	7, 19, 40, 51	0
1	B	338/377 (89%)	0.11	3 (0%) 81 78	8, 24, 38, 53	0
1	C	339/377 (89%)	0.21	11 (3%) 50 42	10, 23, 43, 56	0
1	D	339/377 (89%)	-0.15	4 (1%) 76 72	6, 14, 32, 41	0
All	All	1356/1508 (89%)	0.06	30 (2%) 62 56	6, 20, 39, 56	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	593	GLY	4.5
1	A	461	SER	4.1
1	C	254	GLN	4.0
1	B	254	GLN	3.7
1	C	467	ASP	3.6
1	A	458	VAL	3.4
1	D	256	ASP	3.2
1	C	593	GLY	3.1
1	A	460	SER	3.1
1	C	576	ILE	2.9
1	A	464	LEU	2.7
1	A	575	THR	2.7
1	C	253	GLU	2.6
1	A	249	GLY	2.4
1	C	575	THR	2.4
1	C	597	SER	2.4
1	A	606	ASP	2.4
1	D	578	GLN	2.4
1	B	255	GLU	2.3
1	C	252	THR	2.3
1	A	462	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	594	ASN	2.2
1	A	250	VAL	2.2
1	C	460	SER	2.2
1	A	515	GLU	2.2
1	C	517	GLY	2.1
1	C	606	ASP	2.1
1	D	534	SER	2.1
1	A	528	ASN	2.0
1	A	463	VAL	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
2	15X	B	901[A]	29/29	0.84	0.13	19,20,21,21	29
2	15X	B	901[B]	29/29	0.84	0.13	13,14,16,16	29
5	EPE	D	804	15/15	0.86	0.15	41,43,43,44	0
5	EPE	A	806	15/15	0.87	0.18	52,57,58,59	0
5	EPE	B	801	15/15	0.88	0.15	48,51,51,51	0
2	15X	A	901	29/29	0.88	0.12	22,27,35,37	0
5	EPE	D	805	15/15	0.89	0.17	34,41,44,45	0
2	15X	C	901	29/29	0.90	0.12	26,29,34,35	0
5	EPE	B	802	15/15	0.90	0.15	44,47,49,49	0
4	MG	A	621	1/1	0.91	0.10	17,17,17,17	0
2	15X	D	901	29/29	0.92	0.12	16,19,26,27	0
4	MG	B	621	1/1	0.96	0.07	17,17,17,17	0
5	EPE	C	803	15/15	0.96	0.10	31,33,37,37	0
4	MG	C	621	1/1	0.98	0.05	10,10,10,10	0

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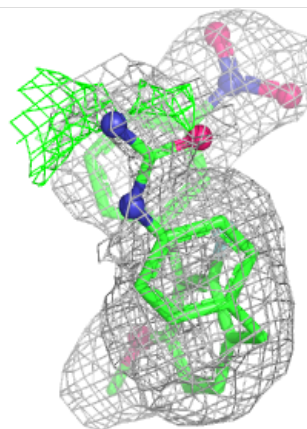
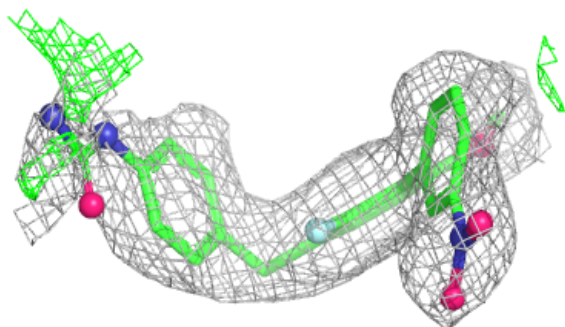
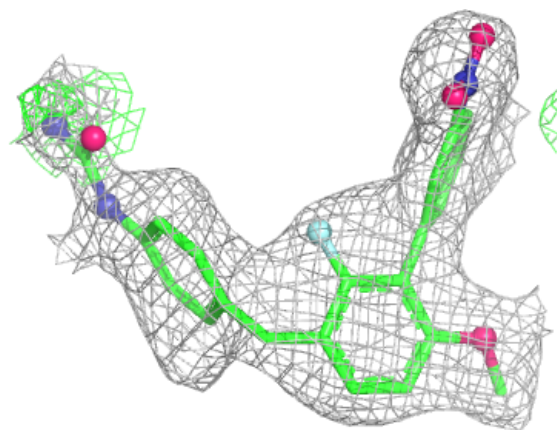
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ZN	C	620	1/1	0.99	0.02	16,16,16,16	0
4	MG	D	621	1/1	0.99	0.06	3,3,3,3	0
3	ZN	A	620	1/1	1.00	0.01	14,14,14,14	0
3	ZN	D	620	1/1	1.00	0.01	10,10,10,10	0
3	ZN	B	620	1/1	1.00	0.01	13,13,13,13	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.

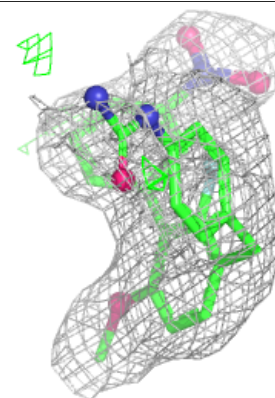
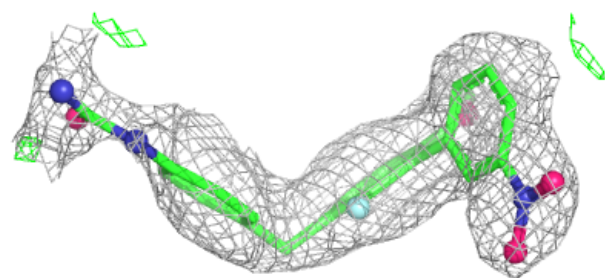
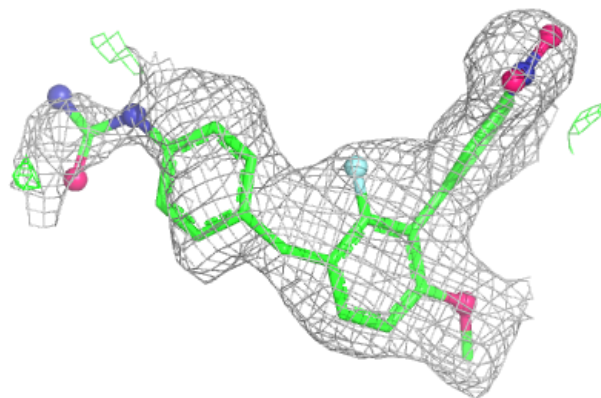
Electron density around 15X B 901 (A):

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

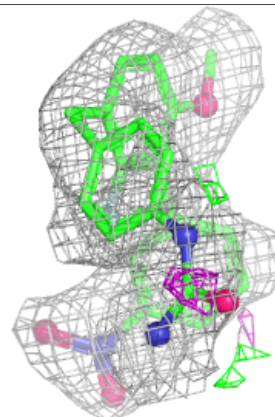
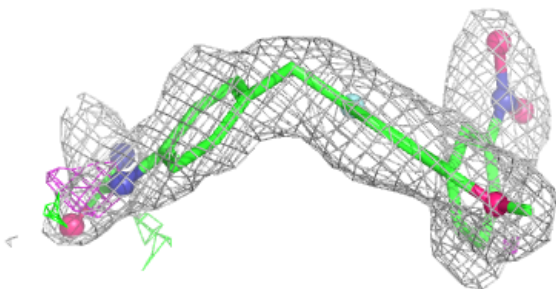
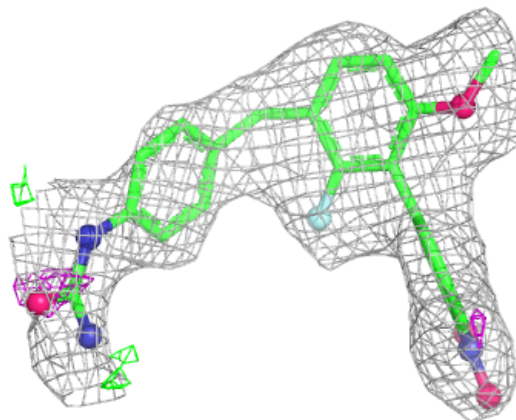


Electron density around 15X B 901 (B):

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

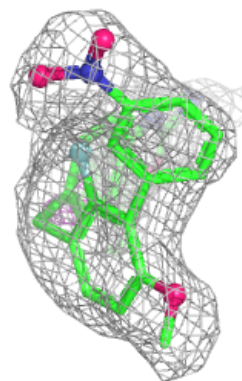
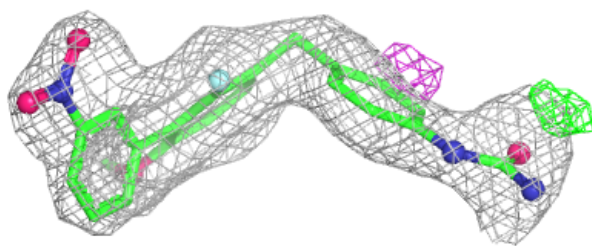
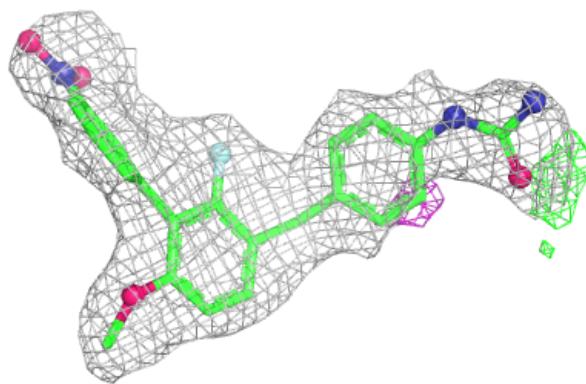
**Electron density around 15X A 901:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

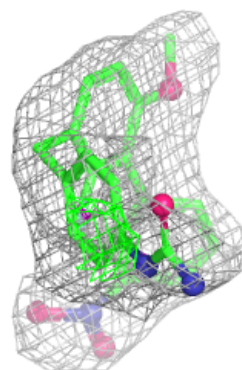
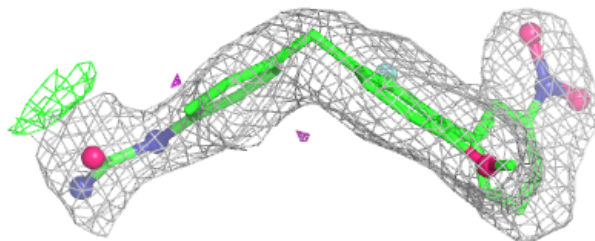
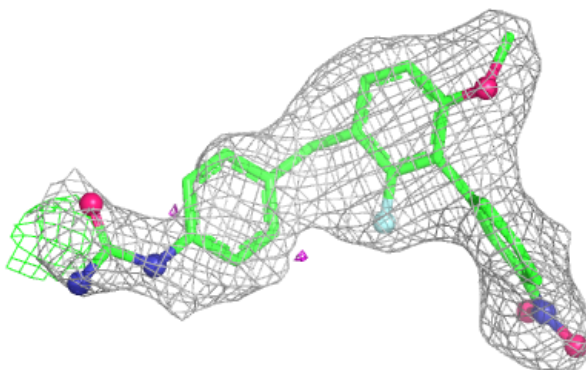


Electron density around 15X C 901:

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

**Electron density around 15X D 901:**

$2mF_o-DF_c$ (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.