



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 28, 2026 – 02:11 PM JST

PDB ID : 9VM9 / pdb_00009vm9
Title : Crystal structure of FGFR3 in complex with 10s
Authors : Chen, X.J.; Liu, X.R.; Zhang, L.
Deposited on : 2025-06-27
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 : 1.8.5 (274361), CSD as541be (2020)
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

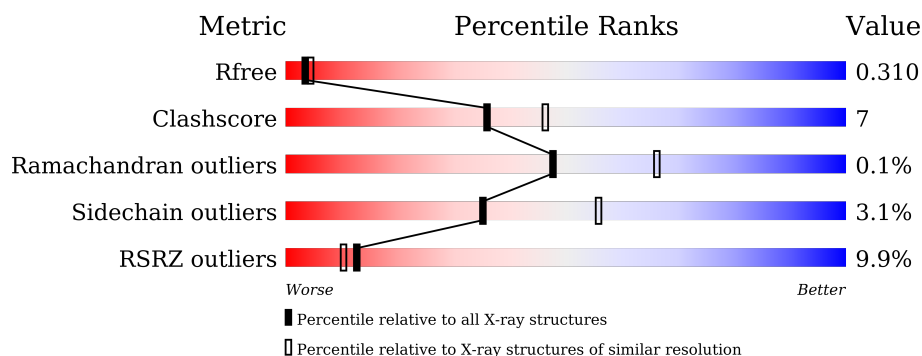
1 Overall quality at a glance

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	292	<div> <div>7%</div> <div>83%</div> <div>15%</div> <div>.</div> </div>
1	B	292	<div> <div>8%</div> <div>84%</div> <div>13%</div> <div>..</div> </div>
1	C	292	<div> <div>9%</div> <div>75%</div> <div>20%</div> <div>..</div> </div>
1	D	292	<div> <div>14%</div> <div>75%</div> <div>22%</div> <div>.</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9210 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 Fibroblast growth factor receptor 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	287	Total	C	N	O	S	0	1	0
			2269	1444	392	414	19			
1	B	285	Total	C	N	O	S	0	1	0
			2262	1441	391	411	19			
1	C	281	Total	C	N	O	S	0	1	0
			2223	1414	386	404	19			
1	D	284	Total	C	N	O	S	0	1	0
			2247	1431	390	407	19			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	453	GLY	-	expression tag	UNP P22607
A	454	PRO	-	expression tag	UNP P22607
A	584	SER	PRO	conflict	UNP P22607
A	585	GLY	PRO	conflict	UNP P22607
A	?	-	GLY	deletion	UNP P22607
A	?	-	LEU	deletion	UNP P22607
A	?	-	ASP	deletion	UNP P22607
A	?	-	TYR	deletion	UNP P22607
A	?	-	SER	deletion	UNP P22607
A	?	-	PHE	deletion	UNP P22607
A	?	-	ASP	deletion	UNP P22607
A	?	-	THR	deletion	UNP P22607
A	?	-	CYS	deletion	UNP P22607
A	?	-	LYS	deletion	UNP P22607
A	?	-	PRO	deletion	UNP P22607
A	?	-	PRO	deletion	UNP P22607
B	453	GLY	-	expression tag	UNP P22607
B	454	PRO	-	expression tag	UNP P22607
B	584	SER	PRO	conflict	UNP P22607
B	585	GLY	PRO	conflict	UNP P22607
B	?	-	GLY	deletion	UNP P22607

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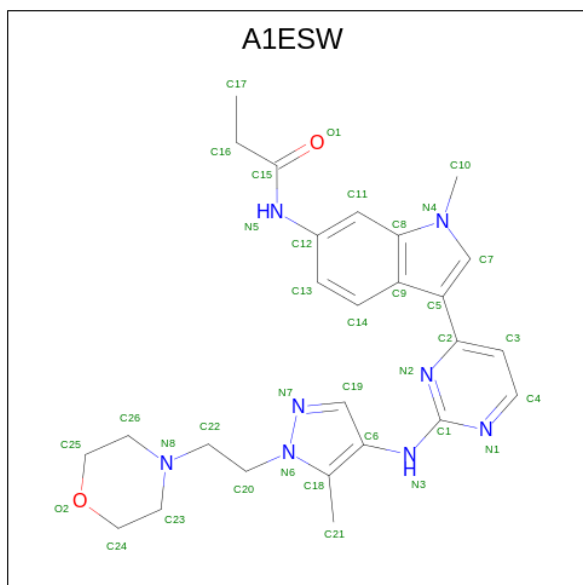
Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	LEU	deletion	UNP P22607
B	?	-	ASP	deletion	UNP P22607
B	?	-	TYR	deletion	UNP P22607
B	?	-	SER	deletion	UNP P22607
B	?	-	PHE	deletion	UNP P22607
B	?	-	ASP	deletion	UNP P22607
B	?	-	THR	deletion	UNP P22607
B	?	-	CYS	deletion	UNP P22607
B	?	-	LYS	deletion	UNP P22607
B	?	-	PRO	deletion	UNP P22607
B	?	-	PRO	deletion	UNP P22607
C	453	GLY	-	expression tag	UNP P22607
C	454	PRO	-	expression tag	UNP P22607
C	584	SER	PRO	conflict	UNP P22607
C	585	GLY	PRO	conflict	UNP P22607
C	?	-	GLY	deletion	UNP P22607
C	?	-	LEU	deletion	UNP P22607
C	?	-	ASP	deletion	UNP P22607
C	?	-	TYR	deletion	UNP P22607
C	?	-	SER	deletion	UNP P22607
C	?	-	PHE	deletion	UNP P22607
C	?	-	ASP	deletion	UNP P22607
C	?	-	THR	deletion	UNP P22607
C	?	-	CYS	deletion	UNP P22607
C	?	-	LYS	deletion	UNP P22607
C	?	-	PRO	deletion	UNP P22607
C	?	-	PRO	deletion	UNP P22607
D	453	GLY	-	expression tag	UNP P22607
D	454	PRO	-	expression tag	UNP P22607
D	584	SER	PRO	conflict	UNP P22607
D	585	GLY	PRO	conflict	UNP P22607
D	?	-	GLY	deletion	UNP P22607
D	?	-	LEU	deletion	UNP P22607
D	?	-	ASP	deletion	UNP P22607
D	?	-	TYR	deletion	UNP P22607
D	?	-	SER	deletion	UNP P22607
D	?	-	PHE	deletion	UNP P22607
D	?	-	ASP	deletion	UNP P22607
D	?	-	THR	deletion	UNP P22607
D	?	-	CYS	deletion	UNP P22607
D	?	-	LYS	deletion	UNP P22607
D	?	-	PRO	deletion	UNP P22607

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Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	PRO	deletion	UNP P22607

- Molecule 2 is {N}-[1-methyl-3-[2-[[5-methyl-1-(2-morpholin-4-ylethyl)pyrazol-4-yl]amino]pyrimidin-4-yl]indol-6-yl]propanamide (CCD ID: A1ESW) (formula: C₂₆H₃₂N₈O₂) (labeled as "Ligand of Interest" by depositor).

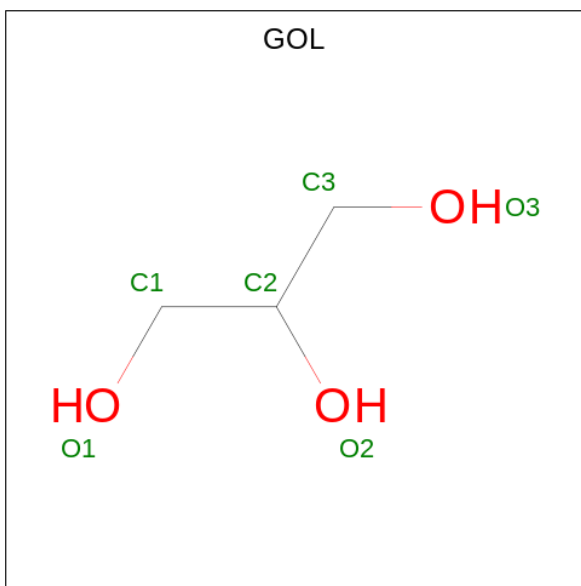


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			36	26	8	2		
2	B	1	Total	C	N	O	0	0
			36	26	8	2		
2	C	1	Total	C	N	O	0	0
			36	26	8	2		
2	D	1	Total	C	N	O	0	0
			36	26	8	2		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

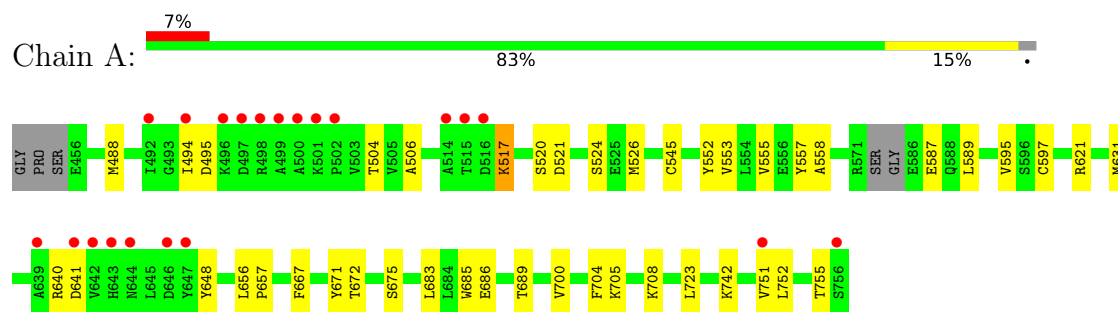
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	11	Total	O	0	0
			11	11		
5	B	17	Total	O	0	0
			17	17		
5	C	12	Total	O	0	0
			12	12		
5	D	15	Total	O	0	0
			15	15		

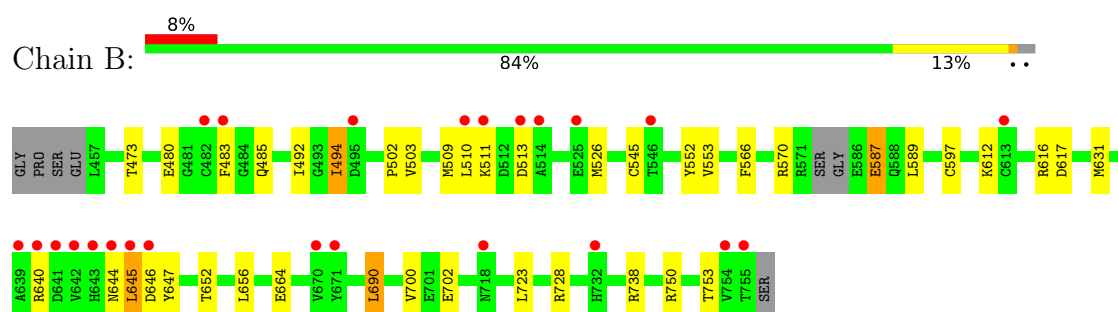
3 Residue-property plots [i](#)

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.

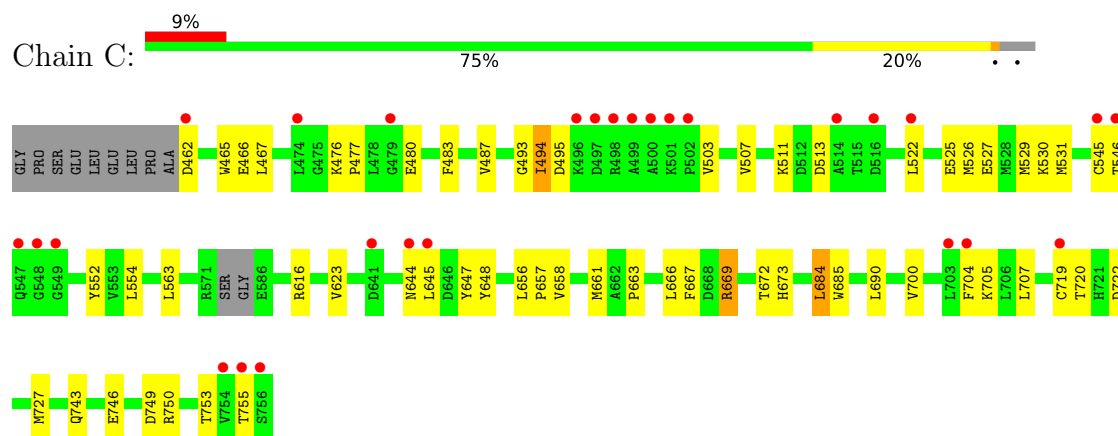
• Molecule 1: Fibroblast growth factor receptor 3



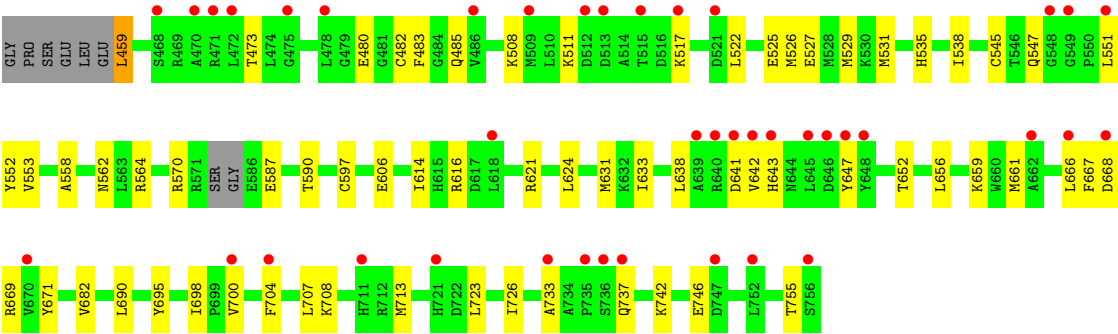
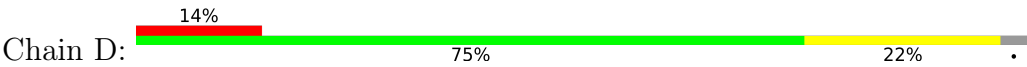
• Molecule 1: Fibroblast growth factor receptor 3



• Molecule 1: Fibroblast growth factor receptor 3



• Molecule 1: Fibroblast growth factor receptor 3



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.70Å 113.51Å 87.90Å 90.00° 94.97° 90.00°	Depositor
Resolution (Å)	17.93 – 2.65 17.93 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.2 (17.93-2.65) 98.8 (17.93-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 2.66Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.259 , 0.312 0.259 , 0.310	Depositor DCC
R_{free} test set	1697 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	48.0	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 45.4	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	0.88	EDS
Total number of atoms	9210	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.34% 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: MG, GOL, A1ESW

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	0.09	0/2318	0.26	0/3134
1	B	0.08	0/2311	0.26	0/3123
1	C	0.10	0/2271	0.32	0/3069
1	D	0.16	0/2296	0.34	0/3103
All	All	0.11	0/9196	0.30	0/12429

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	2269	0	2276	26	0
1	B	2262	0	2280	24	0
1	C	2223	0	2230	42	0
1	D	2247	0	2264	44	0
2	A	36	0	0	1	0
2	B	36	0	0	0	0
2	C	36	0	0	0	0
2	D	36	0	0	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	D	6	0	8	1	0
5	A	11	0	0	1	0
5	B	17	0	0	0	0
5	C	12	0	0	4	0
5	D	15	0	0	3	0
All	All	9210	0	9058	133	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 7.

All (133) 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:666:LEU:HD21	1:D:704:PHE:CE1	2.20	0.76
1:D:621:ARG:HH12	4:D:801:GOL:H2	1.52	0.75
1:B:617:ASP:OD2	1:B:647:TYR:OH	2.05	0.74
1:B:616:ARG:NH2	1:D:737:GLN:OE1	2.21	0.73
1:D:526:MET:HE1	1:D:551:LEU:HD11	1.71	0.72
1:C:704:PHE:CE1	1:C:707:LEU:HD12	2.26	0.70
1:D:517:LYS:NZ	1:D:641:ASP:O	2.27	0.68
1:A:708:LYS:NZ	5:A:903:HOH:O	2.27	0.67
1:D:638:LEU:HD22	1:D:642:VAL:HG11	1.76	0.66
1:C:720:THR:HG22	1:C:722:ASP:H	1.61	0.66
1:D:667:PHE:HE2	1:D:708:LYS:HD3	1.61	0.66
1:D:659:LYS:HG2	1:D:695:TYR:HD1	1.62	0.65
1:C:647:TYR:O	5:C:901:HOH:O	2.15	0.65
1:C:648:TYR:HD1	1:C:657:PRO:HB2	1.62	0.65
1:C:476:LYS:NZ	5:C:902:HOH:O	2.32	0.62
1:C:483:PHE:CD2	1:C:522:LEU:HB2	2.35	0.62
1:D:723:LEU:HA	1:D:726:ILE:HD12	1.80	0.62
1:D:508:LYS:HB2	1:D:553:VAL:HB	1.81	0.62
1:D:535:HIS:HB3	1:D:538:ILE:HG12	1.83	0.60
1:D:666:LEU:HA	1:D:669:ARG:HD3	1.84	0.59
1:B:545:CYS:HB2	1:B:552:TYR:HB2	1.84	0.59
1:A:517:LYS:NZ	1:A:641:ASP:O	2.35	0.59
1:B:570:ARG:HD3	1:B:589:LEU:HD21	1.85	0.59
1:C:648:TYR:CD1	1:C:657:PRO:HB2	2.38	0.58
1:D:527:GLU:O	1:D:531:MET:HG3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:493:GLY:O	1:C:495:ASP:N	2.37	0.57
1:C:750:ARG:NH1	5:C:904:HOH:O	2.38	0.57
1:C:616:ARG:NH1	5:C:903:HOH:O	2.38	0.56
1:D:511:LYS:NZ	5:D:903:HOH:O	2.39	0.56
1:D:666:LEU:HD21	1:D:704:PHE:CZ	2.40	0.56
1:C:661:MET:HE2	1:C:666:LEU:HG	1.87	0.56
1:B:656:LEU:HD22	1:B:700:VAL:HG11	1.87	0.56
1:D:659:LYS:NZ	5:D:901:HOH:O	2.39	0.56
1:A:742:LYS:NZ	1:B:753:THR:O	2.27	0.55
1:D:545:CYS:HB2	1:D:552:TYR:HB2	1.89	0.55
1:A:672:THR:HG23	1:A:675:SER:H	1.72	0.54
1:A:520:SER:O	1:A:524:SER:OG	2.25	0.54
1:D:614:ILE:HG22	1:D:616:ARG:HG3	1.90	0.54
1:D:459:LEU:O	1:D:547:GLN:NE2	2.40	0.54
1:D:570:ARG:NH2	1:D:587:GLU:OE2	2.41	0.54
1:A:723:LEU:HD21	1:A:751:VAL:HG11	1.89	0.53
1:C:645:LEU:HD23	1:C:645:LEU:H	1.73	0.53
1:A:545:CYS:HB2	1:A:552:TYR:HB2	1.91	0.52
1:B:664:GLU:OE2	1:B:738:ARG:NH1	2.38	0.52
1:D:522:LEU:HD11	1:D:553:VAL:HG21	1.92	0.51
1:A:621:ARG:O	1:A:621:ARG:HD3	2.11	0.51
1:B:483:PHE:HB3	1:B:510:LEU:HD23	1.93	0.51
1:B:612:LYS:HG3	1:D:733:ALA:HB3	1.93	0.50
1:C:666:LEU:HB2	1:C:704:PHE:HE2	1.77	0.50
1:C:526:MET:HA	1:C:529:MET:HE3	1.94	0.50
1:B:644:ASN:O	1:B:647:TYR:HB3	2.11	0.50
1:D:682:VAL:HG13	1:D:713:MET:HE1	1.94	0.50
1:C:684:LEU:HB3	1:C:727:MET:HG2	1.93	0.50
1:C:467:LEU:HD13	1:C:494:ILE:HD12	1.94	0.49
1:C:666:LEU:HB2	1:C:704:PHE:CE2	2.47	0.49
1:D:661:MET:HE2	1:D:666:LEU:HD23	1.94	0.49
1:C:616:ARG:O	1:C:648:TYR:OH	2.24	0.49
1:C:645:LEU:HD13	1:C:669:ARG:NH1	2.28	0.49
1:A:705:LYS:O	1:A:708:LYS:HG2	2.13	0.49
1:D:558:ALA:O	2:D:802:A1ESW:N3	2.46	0.49
1:C:466:GLU:OE2	1:C:546:THR:N	2.46	0.48
1:B:494:ILE:HG22	1:B:503:VAL:HG21	1.94	0.48
1:A:640:ARG:HH21	1:A:671:TYR:HD2	1.60	0.48
1:A:526:MET:HE2	1:A:553:VAL:HG22	1.94	0.48
1:D:656:LEU:HD13	1:D:700:VAL:HG11	1.94	0.48
1:D:606:GLU:OE2	1:D:742:LYS:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:667:PHE:CZ	1:A:704:PHE:HB3	2.49	0.47
1:B:702:GLU:O	1:B:702:GLU:HG3	2.15	0.47
1:D:667:PHE:CE2	1:D:708:LYS:HD3	2.46	0.47
1:B:480:GLU:HA	1:B:485:GLN:HA	1.97	0.46
1:C:656:LEU:HD13	1:C:700:VAL:HG11	1.96	0.46
1:C:648:TYR:O	1:C:658:VAL:HB	2.16	0.46
1:C:685:TRP:HD1	1:C:727:MET:HE1	1.81	0.46
1:C:477:PRO:HA	1:C:487:VAL:HA	1.97	0.46
1:D:597[B]:CYS:SG	1:D:631:MET:HE3	2.55	0.46
1:A:488:MET:HE3	1:A:557:TYR:CZ	2.51	0.46
1:B:509:MET:HE2	1:B:552:TYR:CE1	2.51	0.46
1:A:495:ASP:OD1	1:A:495:ASP:N	2.44	0.45
1:A:667:PHE:HZ	1:A:704:PHE:HB3	1.80	0.45
1:D:525:GLU:O	1:D:529:MET:HG3	2.16	0.45
1:C:705:LYS:HB3	1:C:705:LYS:HE3	1.67	0.45
1:D:562:ASN:HA	1:D:624:LEU:HD23	1.97	0.45
1:A:488:MET:HE2	1:A:504:THR:HG21	1.99	0.45
1:C:743:GLN:HA	1:C:746:GLU:OE1	2.16	0.45
1:B:566:PHE:O	1:B:570:ARG:HD2	2.16	0.45
1:B:587:GLU:H	1:B:587:GLU:HG2	1.47	0.45
1:A:595:VAL:HG12	1:A:752:LEU:HD13	1.98	0.45
1:A:506:ALA:HB3	1:A:555:VAL:HG23	1.97	0.44
1:A:597[B]:CYS:SG	1:A:631:MET:HE3	2.57	0.44
1:D:659:LYS:HG2	1:D:695:TYR:CD1	2.48	0.44
1:C:531:MET:H	1:C:531:MET:HG2	1.44	0.44
1:C:545:CYS:HB2	1:C:552:TYR:HB2	1.99	0.44
1:B:492:ILE:HA	1:B:502:PRO:HA	2.00	0.44
1:A:648:TYR:HD1	1:A:657:PRO:HB2	1.83	0.44
1:D:666:LEU:HD21	1:D:704:PHE:CD1	2.52	0.44
1:A:685:TRP:O	1:A:689:THR:OG1	2.34	0.44
1:A:558:ALA:O	2:A:801:A1ESW:N3	2.51	0.44
1:B:616:ARG:NE	1:B:640:ARG:HG2	2.32	0.43
1:C:527:GLU:O	1:C:531:MET:HG2	2.18	0.43
1:B:597[B]:CYS:SG	1:B:631:MET:HE3	2.58	0.43
1:A:521:ASP:N	1:A:521:ASP:OD1	2.51	0.43
1:C:667:PHE:HZ	1:C:704:PHE:HB3	1.84	0.43
1:B:526:MET:HE2	1:B:553:VAL:HG22	2.01	0.43
1:A:683:LEU:HA	1:A:686:GLU:OE1	2.19	0.42
1:D:746:GLU:HA	1:D:746:GLU:OE1	2.19	0.42
1:B:728:ARG:HD2	1:B:728:ARG:HA	1.83	0.42
1:D:526:MET:HE2	1:D:553:VAL:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:645:LEU:H	1:B:645:LEU:HD22	1.83	0.42
1:D:690:LEU:HD13	1:D:690:LEU:HA	1.93	0.42
1:B:690:LEU:HD13	1:B:690:LEU:HA	1.81	0.41
1:C:644:ASN:OD1	1:C:645:LEU:HD23	2.19	0.41
1:D:564:ARG:CZ	1:D:621:ARG:HD3	2.50	0.41
1:D:704:PHE:CE2	1:D:707:LEU:HD12	2.55	0.41
1:A:656:LEU:HD13	1:A:700:VAL:HG11	2.01	0.41
1:D:643:HIS:HB3	1:D:647:TYR:CD1	2.55	0.41
1:B:511:LYS:HE3	1:B:513:ASP:HB3	2.02	0.41
1:C:663:PRO:HA	1:C:704:PHE:CE2	2.55	0.41
1:A:648:TYR:CD1	1:A:657:PRO:HB2	2.55	0.41
1:D:698:ILE:O	5:D:901:HOH:O	2.21	0.41
1:D:704:PHE:CD2	1:D:707:LEU:HD12	2.56	0.41
1:C:672:THR:OG1	1:C:673:HIS:N	2.54	0.41
1:C:719:CYS:SG	1:C:720:THR:N	2.93	0.41
1:C:465:TRP:NE1	1:C:530:LYS:HD3	2.36	0.41
1:C:563:LEU:N	1:C:623:VAL:O	2.52	0.41
1:D:708:LYS:HD2	1:D:708:LYS:HA	1.78	0.41
1:C:525:GLU:HG2	1:C:529:MET:HE2	2.02	0.40
1:C:511:LYS:HE3	1:C:513:ASP:HB3	2.03	0.40
1:D:616:ARG:HG2	1:D:671:TYR:CD1	2.56	0.40
1:C:507:VAL:HG22	1:C:554:LEU:HD22	2.04	0.40
1:D:538:ILE:HA	1:D:633:ILE:H	1.85	0.40
1:C:667:PHE:CZ	1:C:704:PHE:HB3	2.56	0.40
1:C:690:LEU:HD13	1:C:690:LEU:HA	1.91	0.40
1:C:749:ASP:O	1:C:753:THR:HG23	2.21	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	284/292 (97%)	280 (99%)	4 (1%)	0	100	100
1	B	282/292 (97%)	277 (98%)	5 (2%)	0	100	100
1	C	278/292 (95%)	271 (98%)	6 (2%)	1 (0%)	30	45
1	D	281/292 (96%)	275 (98%)	6 (2%)	0	100	100
All	All	1125/1168 (96%)	1103 (98%)	21 (2%)	1 (0%)	48	66

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	494	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	243/248 (98%)	238 (98%)	5 (2%)	47	69
1	B	243/248 (98%)	234 (96%)	9 (4%)	30	50
1	C	238/248 (96%)	232 (98%)	6 (2%)	42	64
1	D	241/248 (97%)	231 (96%)	10 (4%)	27	46
All	All	965/992 (97%)	935 (97%)	30 (3%)	35	56

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	494	ILE
1	A	517	LYS
1	A	587	GLU
1	A	589	LEU
1	A	755	THR
1	B	473	THR
1	B	494	ILE
1	B	587	GLU
1	B	645	LEU
1	B	646	ASP

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Mol	Chain	Res	Type
1	B	652	THR
1	B	690	LEU
1	B	723	LEU
1	B	750	ARG
1	C	462	ASP
1	C	480	GLU
1	C	503	VAL
1	C	669	ARG
1	C	684	LEU
1	C	755	THR
1	D	459	LEU
1	D	473	THR
1	D	480	GLU
1	D	482	CYS
1	D	483	PHE
1	D	485	GLN
1	D	590	THR
1	D	652	THR
1	D	668	ASP
1	D	755	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	537	ASN
1	B	537	ASN
1	B	547	GLN
1	C	673	HIS
1	C	718	ASN
1	D	718	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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
2	A1ESW	A	801	1	37,40,40	3.41	16 (43%)	51,56,56	5.21	21 (41%)
2	A1ESW	C	801	1	37,40,40	3.38	15 (40%)	51,56,56	5.24	20 (39%)
2	A1ESW	D	802	1	37,40,40	3.45	18 (48%)	51,56,56	5.20	20 (39%)
4	GOL	D	801	-	5,5,5	0.94	0	5,5,5	0.99	0
2	A1ESW	B	801	1	37,40,40	3.38	15 (40%)	51,56,56	5.20	19 (37%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A1ESW	A	801	1	-	4/19/27/27	0/5/5/5
2	A1ESW	C	801	1	-	9/19/27/27	0/5/5/5
2	A1ESW	D	802	1	-	6/19/27/27	0/5/5/5
4	GOL	D	801	-	-	0/4/4/4	-
2	A1ESW	B	801	1	-	5/19/27/27	0/5/5/5

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	A1ESW	C18-N6	7.71	1.44	1.35
2	D	802	A1ESW	C6-N3	7.59	1.52	1.36
2	A	801	A1ESW	C6-N3	7.59	1.52	1.36
2	C	801	A1ESW	C6-N3	7.45	1.51	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	A1ESW	C6-N3	7.44	1.51	1.36
2	D	802	A1ESW	C18-N6	7.42	1.43	1.35
2	B	801	A1ESW	C18-N6	7.41	1.43	1.35
2	A	801	A1ESW	C1-N3	7.41	1.48	1.38
2	B	801	A1ESW	C22-N8	-7.40	1.30	1.47
2	C	801	A1ESW	C22-N8	-7.37	1.30	1.47
2	D	802	A1ESW	C1-N3	7.36	1.48	1.38
2	C	801	A1ESW	C18-N6	7.36	1.43	1.35
2	C	801	A1ESW	C1-N3	7.22	1.48	1.38
2	B	801	A1ESW	C1-N3	7.05	1.48	1.38
2	A	801	A1ESW	C22-N8	-6.95	1.31	1.47
2	D	802	A1ESW	C22-N8	-6.95	1.31	1.47
2	D	802	A1ESW	C7-N4	-6.34	1.27	1.37
2	B	801	A1ESW	C26-N8	-6.15	1.29	1.46
2	A	801	A1ESW	C26-N8	-6.11	1.30	1.46
2	C	801	A1ESW	C26-N8	-6.11	1.30	1.46
2	D	802	A1ESW	C26-N8	-6.01	1.30	1.46
2	A	801	A1ESW	C7-N4	-5.87	1.27	1.37
2	B	801	A1ESW	C7-N4	-5.79	1.28	1.37
2	C	801	A1ESW	C7-N4	-5.73	1.28	1.37
2	A	801	A1ESW	C9-C8	5.32	1.48	1.41
2	D	802	A1ESW	C9-C8	5.31	1.48	1.41
2	B	801	A1ESW	C9-C8	5.26	1.48	1.41
2	C	801	A1ESW	C9-C8	5.25	1.48	1.41
2	B	801	A1ESW	C23-N8	-4.42	1.34	1.46
2	A	801	A1ESW	C15-N5	4.37	1.45	1.35
2	C	801	A1ESW	C23-N8	-4.32	1.35	1.46
2	D	802	A1ESW	C23-N8	-4.29	1.35	1.46
2	C	801	A1ESW	C15-N5	4.21	1.44	1.35
2	B	801	A1ESW	C15-N5	4.17	1.44	1.35
2	A	801	A1ESW	C23-N8	-4.15	1.35	1.46
2	D	802	A1ESW	C15-N5	4.06	1.44	1.35
2	C	801	A1ESW	C21-C18	3.89	1.55	1.49
2	B	801	A1ESW	C21-C18	3.85	1.55	1.49
2	A	801	A1ESW	C21-C18	3.85	1.55	1.49
2	D	802	A1ESW	C21-C18	3.80	1.55	1.49
2	D	802	A1ESW	C19-N7	2.94	1.37	1.32
2	D	802	A1ESW	C9-C5	2.86	1.53	1.47
2	D	802	A1ESW	C22-C20	2.78	1.61	1.51
2	A	801	A1ESW	C22-C20	2.77	1.61	1.51
2	A	801	A1ESW	C19-N7	2.72	1.37	1.32
2	C	801	A1ESW	C19-N7	2.71	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	A1ESW	C19-N7	2.69	1.37	1.32
2	B	801	A1ESW	C22-C20	2.61	1.61	1.51
2	C	801	A1ESW	C22-C20	2.60	1.61	1.51
2	D	802	A1ESW	C13-C12	2.50	1.43	1.39
2	A	801	A1ESW	C12-N5	2.38	1.46	1.41
2	C	801	A1ESW	C9-C5	2.37	1.52	1.47
2	A	801	A1ESW	C9-C5	2.35	1.52	1.47
2	D	802	A1ESW	C11-C8	-2.33	1.35	1.39
2	B	801	A1ESW	C9-C5	2.28	1.52	1.47
2	D	802	A1ESW	C12-N5	2.28	1.46	1.41
2	C	801	A1ESW	C13-C12	2.19	1.42	1.39
2	B	801	A1ESW	C13-C12	2.18	1.42	1.39
2	D	802	A1ESW	C20-N6	2.18	1.50	1.46
2	A	801	A1ESW	C13-C12	2.17	1.42	1.39
2	C	801	A1ESW	C12-N5	2.13	1.46	1.41
2	B	801	A1ESW	C12-N5	2.13	1.46	1.41
2	A	801	A1ESW	C20-N6	2.05	1.49	1.46
2	D	802	A1ESW	C14-C13	2.03	1.42	1.38

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	801	A1ESW	C5-C7-N4	-23.99	103.60	111.05
2	B	801	A1ESW	C5-C7-N4	-23.89	103.64	111.05
2	A	801	A1ESW	C5-C7-N4	-23.53	103.75	111.05
2	D	802	A1ESW	C5-C7-N4	-23.05	103.90	111.05
2	A	801	A1ESW	C8-N4-C7	17.56	121.28	108.54
2	C	801	A1ESW	C8-N4-C7	17.35	121.13	108.54
2	B	801	A1ESW	C8-N4-C7	17.19	121.01	108.54
2	D	802	A1ESW	C8-N4-C7	17.17	121.00	108.54
2	D	802	A1ESW	C8-C9-C5	-12.48	99.97	106.92
2	B	801	A1ESW	C8-C9-C5	-10.57	101.04	106.92
2	B	801	A1ESW	C9-C5-C7	10.44	112.11	106.00
2	C	801	A1ESW	C8-C9-C5	-10.42	101.12	106.92
2	D	802	A1ESW	C9-C5-C7	10.39	112.08	106.00
2	C	801	A1ESW	C9-C5-C7	10.25	112.00	106.00
2	A	801	A1ESW	C9-C5-C7	10.01	111.86	106.00
2	A	801	A1ESW	C8-C9-C5	-9.93	101.39	106.92
2	A	801	A1ESW	C9-C8-N4	-9.79	101.72	107.89
2	C	801	A1ESW	C9-C8-N4	-9.11	102.15	107.89
2	B	801	A1ESW	C9-C8-N4	-9.02	102.20	107.89
2	D	802	A1ESW	C9-C8-N4	-7.68	103.05	107.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	A1ESW	C10-N4-C7	-6.78	118.37	125.71
2	D	802	A1ESW	C10-N4-C8	-6.58	119.20	125.69
2	C	801	A1ESW	C10-N4-C8	-6.41	119.37	125.69
2	B	801	A1ESW	C10-N4-C8	-6.10	119.68	125.69
2	B	801	A1ESW	C10-N4-C7	-5.91	119.31	125.71
2	C	801	A1ESW	C10-N4-C7	-5.73	119.50	125.71
2	D	802	A1ESW	C10-N4-C7	-5.46	119.80	125.71
2	A	801	A1ESW	C10-N4-C8	-5.42	120.34	125.69
2	D	802	A1ESW	C14-C9-C5	4.66	143.13	132.39
2	C	801	A1ESW	C20-N6-C18	-4.30	124.21	128.60
2	D	802	A1ESW	C20-N6-C18	-4.30	124.21	128.60
2	B	801	A1ESW	C20-N6-C18	-4.15	124.36	128.60
2	C	801	A1ESW	C12-N5-C15	-3.98	120.53	127.50
2	D	802	A1ESW	N1-C1-N2	-3.96	122.80	126.55
2	D	802	A1ESW	C20-N6-N7	3.81	125.26	119.88
2	B	801	A1ESW	C1-N3-C6	-3.74	120.80	128.09
2	A	801	A1ESW	C21-C18-N6	3.71	127.24	123.07
2	C	801	A1ESW	C14-C9-C5	3.56	140.61	132.39
2	B	801	A1ESW	C14-C9-C5	3.50	140.46	132.39
2	A	801	A1ESW	C14-C9-C5	3.50	140.46	132.39
2	A	801	A1ESW	C24-C23-N8	3.45	115.33	110.10
2	A	801	A1ESW	N1-C1-N2	-3.44	123.29	126.55
2	C	801	A1ESW	C20-N6-N7	3.39	124.66	119.88
2	B	801	A1ESW	C21-C18-N6	3.35	126.84	123.07
2	B	801	A1ESW	N1-C1-N2	-3.34	123.38	126.55
2	A	801	A1ESW	C26-N8-C23	3.34	116.36	108.83
2	D	802	A1ESW	C2-N2-C1	3.33	119.49	116.80
2	C	801	A1ESW	N1-C1-N2	-3.25	123.47	126.55
2	B	801	A1ESW	C20-N6-N7	3.24	124.46	119.88
2	A	801	A1ESW	C20-N6-C18	-3.19	125.34	128.60
2	B	801	A1ESW	C2-N2-C1	3.14	119.34	116.80
2	A	801	A1ESW	C2-N2-C1	3.13	119.33	116.80
2	C	801	A1ESW	C21-C18-N6	3.08	126.54	123.07
2	C	801	A1ESW	C2-N2-C1	3.04	119.26	116.80
2	D	802	A1ESW	C21-C18-N6	3.03	126.48	123.07
2	C	801	A1ESW	C1-N3-C6	-2.97	122.30	128.09
2	A	801	A1ESW	C11-C8-N4	2.90	136.11	131.25
2	A	801	A1ESW	C20-N6-N7	2.81	123.84	119.88
2	D	802	A1ESW	C4-N1-C1	2.77	117.91	115.45
2	D	802	A1ESW	C26-N8-C23	2.67	114.84	108.83
2	B	801	A1ESW	C11-C8-N4	2.64	135.67	131.25
2	C	801	A1ESW	C11-C8-N4	2.60	135.60	131.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	801	A1ESW	C3-C2-N2	-2.56	119.92	122.92
2	D	802	A1ESW	C18-N6-N7	-2.54	110.53	112.75
2	A	801	A1ESW	C3-C2-N2	-2.46	120.04	122.92
2	B	801	A1ESW	C12-N5-C15	-2.41	123.28	127.50
2	B	801	A1ESW	C3-C2-N2	-2.40	120.11	122.92
2	A	801	A1ESW	C1-N3-C6	-2.39	123.44	128.09
2	B	801	A1ESW	C22-C20-N6	-2.28	107.41	111.70
2	A	801	A1ESW	C18-N6-N7	-2.21	110.82	112.75
2	B	801	A1ESW	C4-N1-C1	2.21	117.41	115.45
2	A	801	A1ESW	C4-N1-C1	2.16	117.37	115.45
2	D	802	A1ESW	C3-C2-N2	-2.15	120.40	122.92
2	C	801	A1ESW	C26-N8-C23	2.13	113.62	108.83
2	D	802	A1ESW	C1-N3-C6	-2.09	124.03	128.09
2	A	801	A1ESW	C22-N8-C23	2.07	116.52	111.23
2	C	801	A1ESW	C5-C2-N2	2.06	119.65	116.60
2	D	802	A1ESW	C14-C9-C8	-2.05	116.89	119.24
2	D	802	A1ESW	C22-C20-N6	-2.03	107.86	111.70
2	C	801	A1ESW	C4-N1-C1	2.01	117.23	115.45

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	A1ESW	C20-C22-N8-C23
2	C	801	A1ESW	C22-C20-N6-C18
2	C	801	A1ESW	C22-C20-N6-N7
2	D	802	A1ESW	C20-C22-N8-C26
2	C	801	A1ESW	C13-C12-N5-C15
2	C	801	A1ESW	C11-C12-N5-C15
2	C	801	A1ESW	N6-C20-C22-N8
2	A	801	A1ESW	C20-C22-N8-C26
2	D	802	A1ESW	C20-C22-N8-C23
2	A	801	A1ESW	N2-C2-C5-C9
2	B	801	A1ESW	N2-C2-C5-C9
2	C	801	A1ESW	N2-C2-C5-C9
2	D	802	A1ESW	N2-C2-C5-C9
2	B	801	A1ESW	C13-C12-N5-C15
2	D	802	A1ESW	C11-C12-N5-C15
2	A	801	A1ESW	C3-C2-C5-C7
2	B	801	A1ESW	N2-C2-C5-C7
2	C	801	A1ESW	C3-C2-C5-C7
2	D	802	A1ESW	C13-C12-N5-C15

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Mol	Chain	Res	Type	Atoms
2	B	801	A1ESW	C11-C12-N5-C15
2	C	801	A1ESW	N5-C15-C16-C17
2	C	801	A1ESW	O1-C15-C16-C17
2	B	801	A1ESW	C3-C2-C5-C7
2	D	802	A1ESW	N6-C20-C22-N8

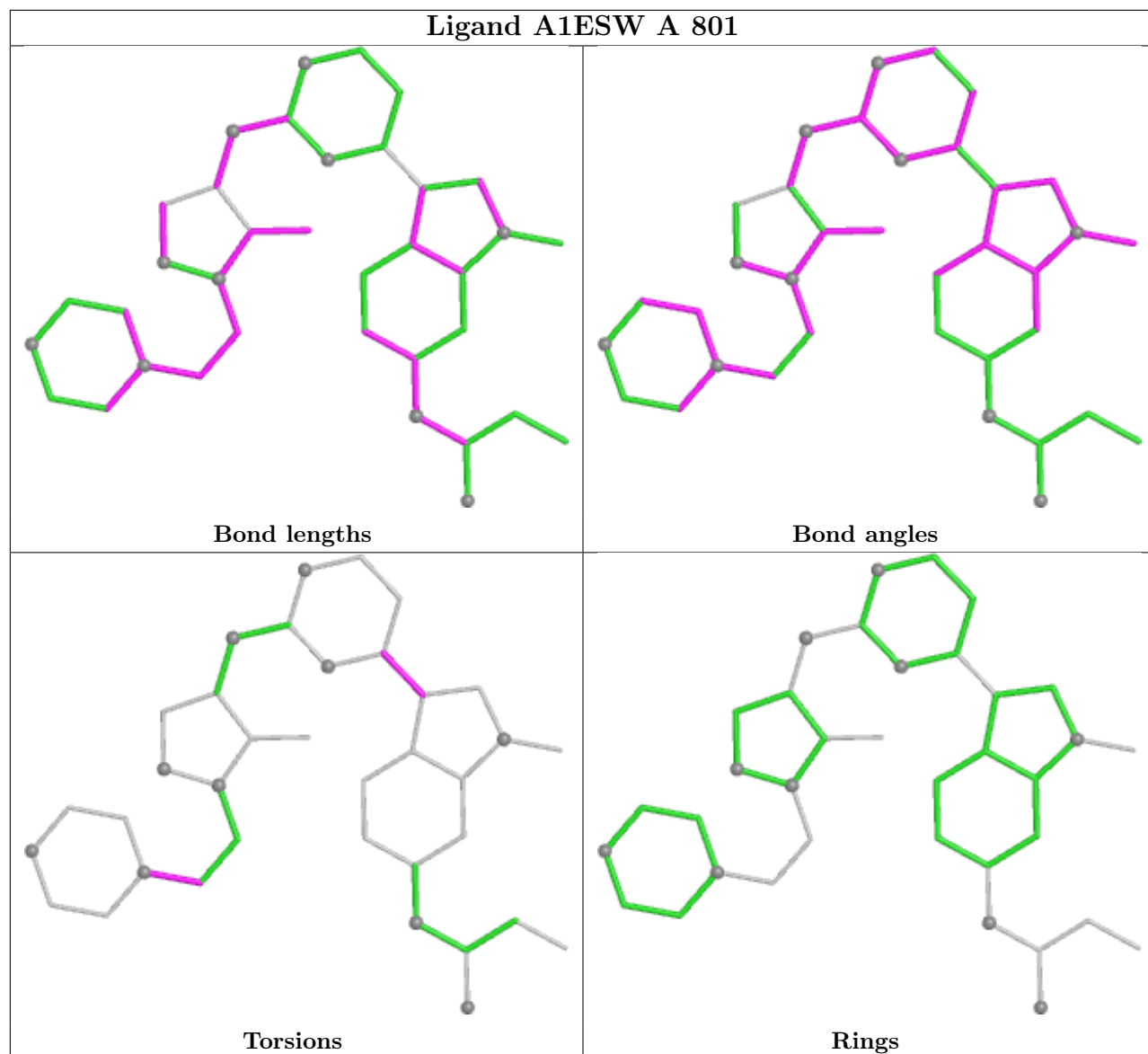
There are no ring outliers.

3 monomers are involved in 3 short contacts:

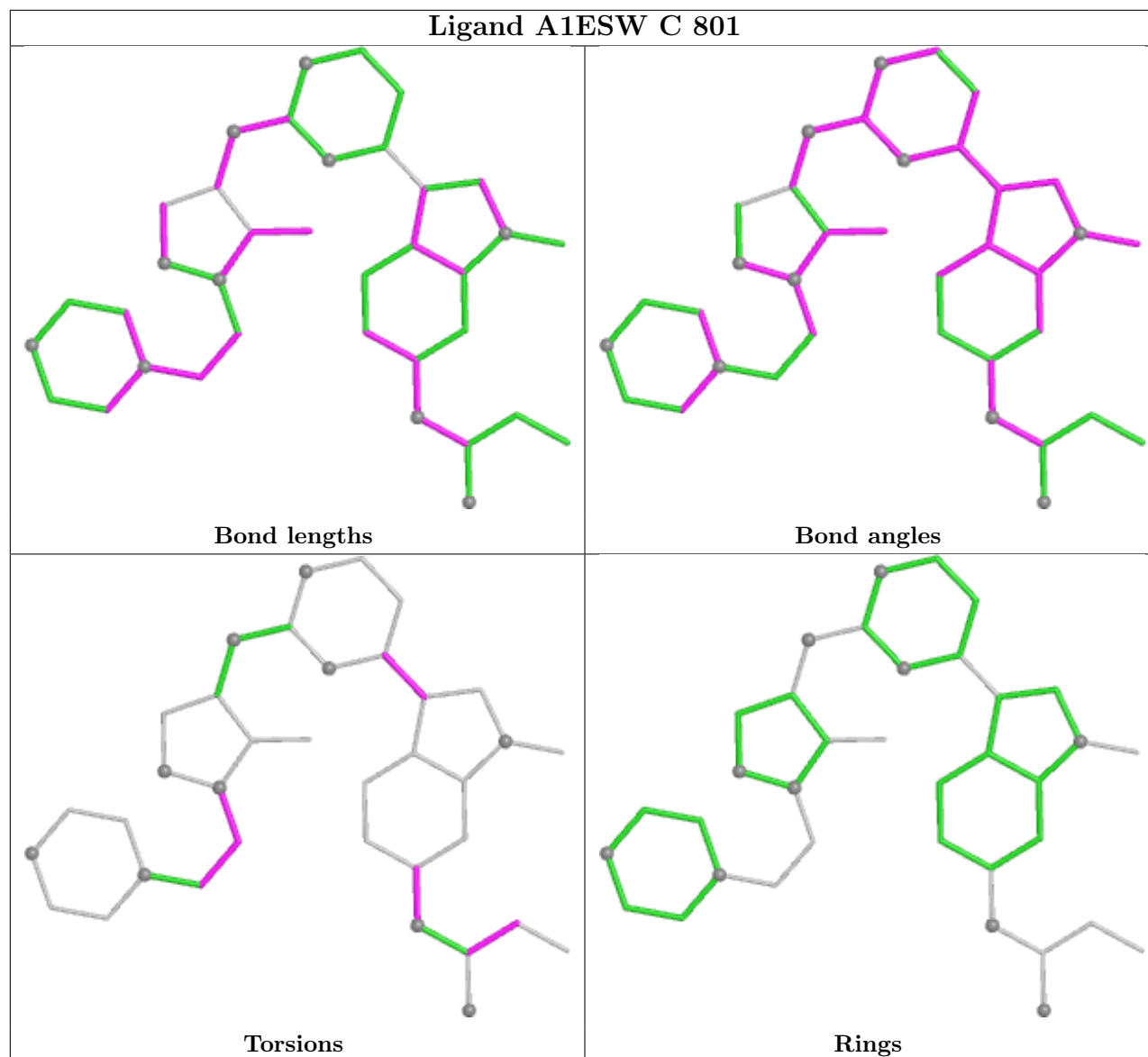
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	A1ESW	1	0
2	D	802	A1ESW	1	0
4	D	801	GOL	1	0

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

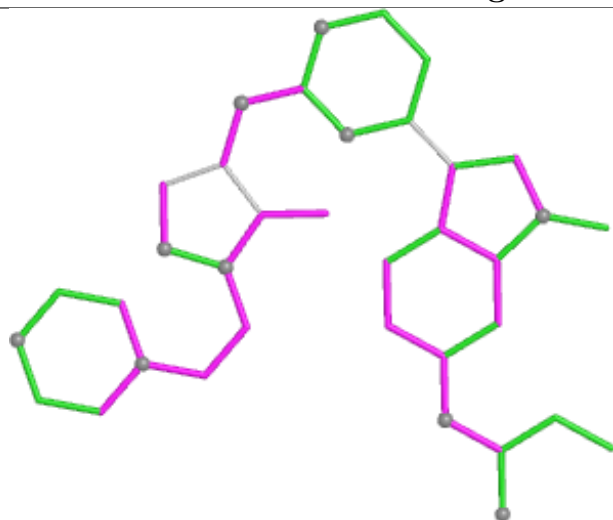
Ligand A1ESW A 801



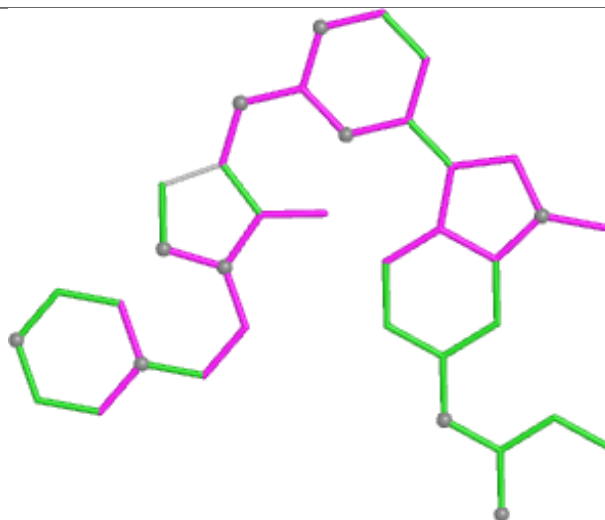
Ligand A1ESW C 801



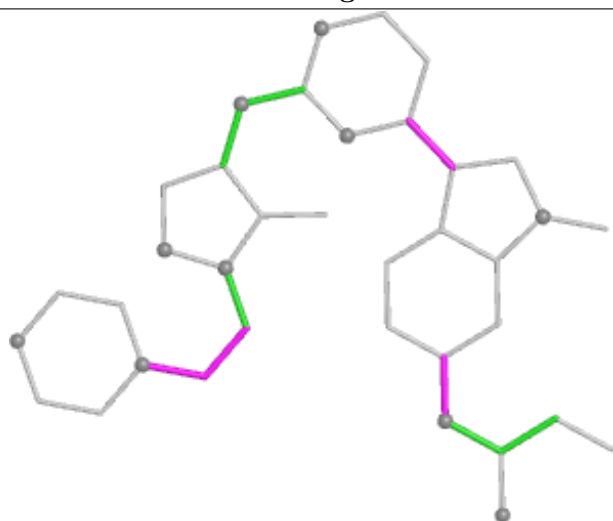
Ligand A1ESW D 802



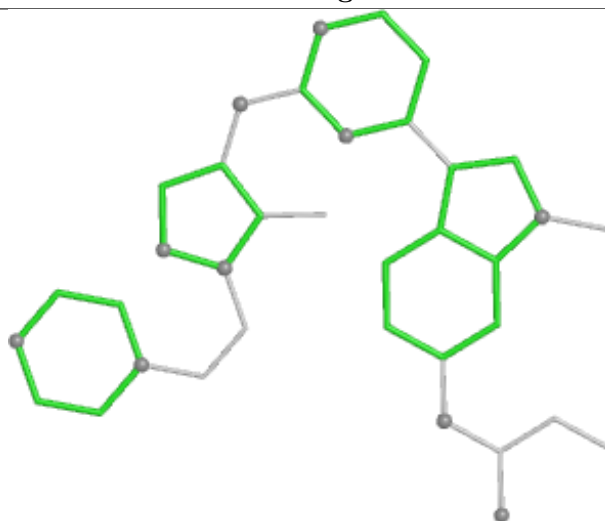
Bond lengths



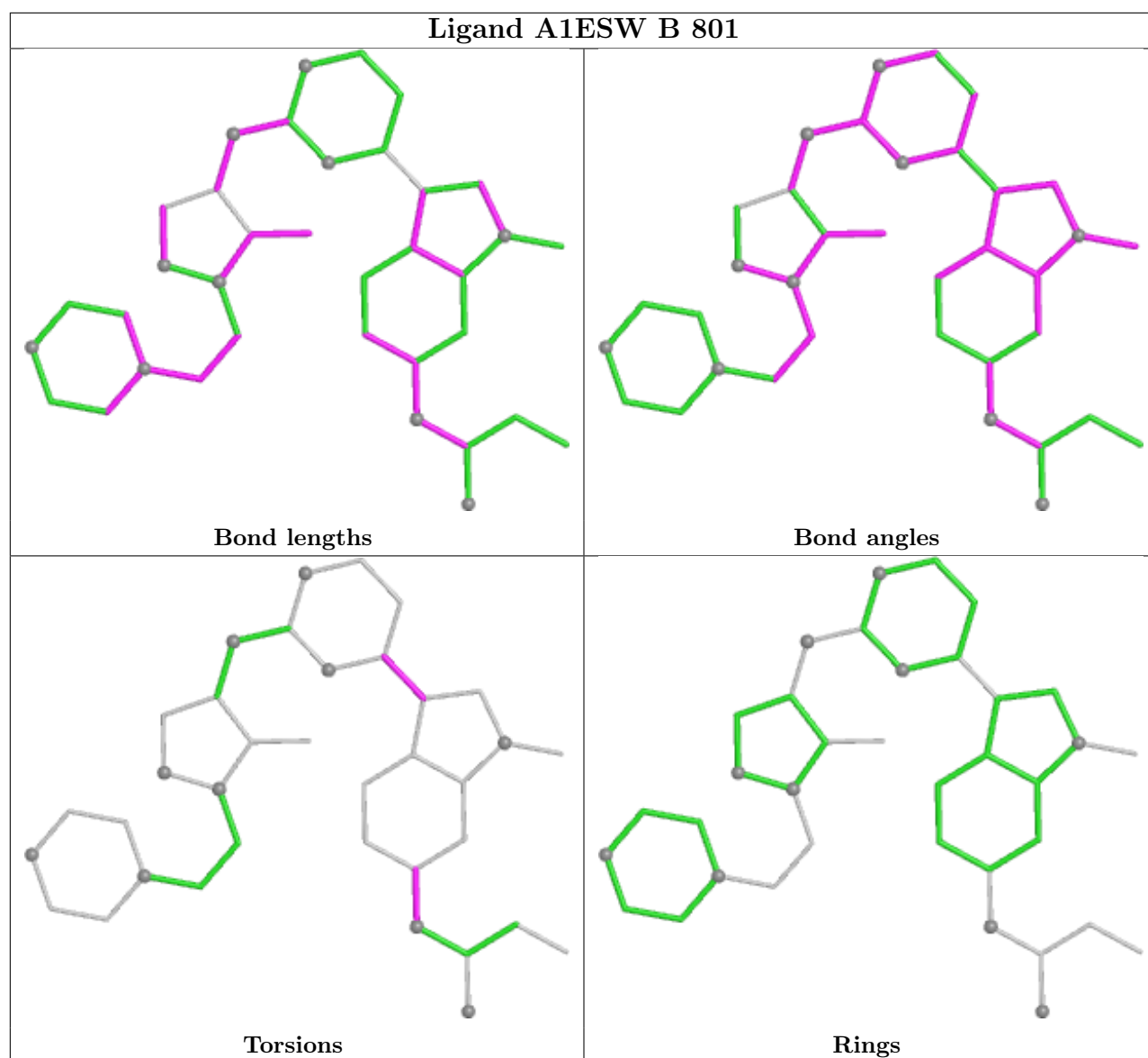
Bond angles



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	287/292 (98%)	0.78	21 (7%)	21	15	29, 45, 83, 101	1 (0%)
1	B	285/292 (97%)	0.75	24 (8%)	17	12	27, 45, 73, 86	1 (0%)
1	C	281/292 (96%)	0.86	27 (9%)	13	11	33, 50, 83, 113	1 (0%)
1	D	284/292 (97%)	1.02	41 (14%)	6	4	32, 51, 79, 96	1 (0%)
All	All	1137/1168 (97%)	0.85	113 (9%)	13	10	27, 48, 80, 113	4 (0%)

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	644	ASN	4.7
1	C	755	THR	4.6
1	D	646	ASP	4.5
1	A	500	ALA	4.5
1	A	502	PRO	4.5
1	A	643	HIS	4.2
1	A	497	ASP	4.2
1	D	513	ASP	4.0
1	C	499	ALA	4.0
1	A	642	VAL	3.9
1	C	704	PHE	3.9
1	D	551	LEU	3.8
1	D	647	TYR	3.7
1	A	639	ALA	3.7
1	D	470	ALA	3.6
1	D	704	PHE	3.6
1	B	645	LEU	3.6
1	C	641	ASP	3.6
1	A	496	LYS	3.6
1	B	482	CYS	3.6
1	B	755	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	756	SER	3.5
1	D	670	VAL	3.5
1	D	549	GLY	3.5
1	C	501	LYS	3.4
1	B	513	ASP	3.4
1	D	643	HIS	3.4
1	D	711	HIS	3.4
1	D	475	GLY	3.3
1	A	494	ILE	3.3
1	C	516	ASP	3.3
1	A	514	ALA	3.3
1	B	646	ASP	3.3
1	D	512	ASP	3.3
1	A	756	SER	3.2
1	A	644	ASN	3.2
1	A	498	ARG	3.2
1	A	647	TYR	3.2
1	A	501	LYS	3.1
1	A	646	ASP	3.0
1	D	517	LYS	3.0
1	D	642	VAL	3.0
1	C	497	ASP	3.0
1	C	498	ARG	3.0
1	D	548	GLY	2.9
1	D	641	ASP	2.9
1	B	546	THR	2.9
1	C	462	ASP	2.9
1	D	521	ASP	2.9
1	B	671	TYR	2.9
1	A	499	ALA	2.9
1	C	754	VAL	2.9
1	D	700	VAL	2.8
1	C	547	GLN	2.8
1	B	643	HIS	2.8
1	B	639	ALA	2.8
1	C	514	ALA	2.8
1	B	642	VAL	2.8
1	D	645	LEU	2.7
1	B	670	VAL	2.7
1	D	733	ALA	2.7
1	D	648	TYR	2.6
1	C	522	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	472	LEU	2.6
1	B	511	LYS	2.6
1	C	500	ALA	2.6
1	B	495	ASP	2.6
1	A	492	ILE	2.6
1	B	613	CYS	2.6
1	B	514	ALA	2.6
1	B	510	LEU	2.5
1	D	618	LEU	2.5
1	B	732	HIS	2.5
1	B	641	ASP	2.5
1	B	640	ARG	2.4
1	D	721	HIS	2.4
1	D	747	ASP	2.4
1	D	756	SER	2.4
1	C	719	CYS	2.4
1	C	502	PRO	2.4
1	A	515	THR	2.4
1	A	516	ASP	2.4
1	B	483	PHE	2.4
1	C	644	ASN	2.3
1	B	525	GLU	2.3
1	D	639	ALA	2.3
1	D	662	ALA	2.3
1	A	641	ASP	2.3
1	C	703	LEU	2.3
1	C	545	CYS	2.2
1	D	668	ASP	2.2
1	D	640	ARG	2.2
1	C	496	LYS	2.2
1	C	479	GLY	2.2
1	D	471	ARG	2.2
1	B	718	ASN	2.2
1	D	737	GLN	2.2
1	D	515	THR	2.1
1	C	549	GLY	2.1
1	C	474	LEU	2.1
1	C	645	LEU	2.1
1	D	666	LEU	2.1
1	D	468	SER	2.1
1	D	478	LEU	2.1
1	D	486	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	736	SER	2.1
1	C	546	THR	2.1
1	B	754	VAL	2.1
1	D	735	PRO	2.0
1	D	752	LEU	2.0
1	D	509	MET	2.0
1	C	548	GLY	2.0
1	A	751	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](#)

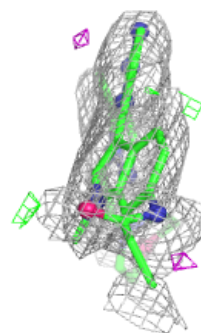
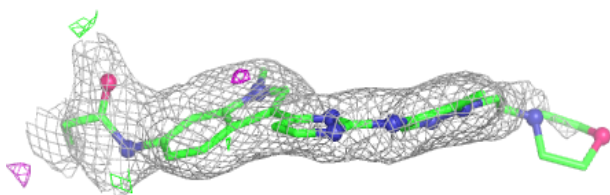
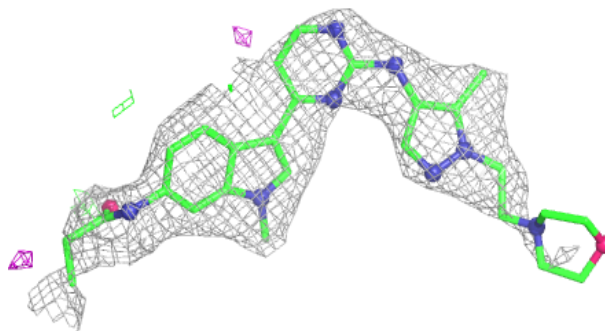
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GOL	D	801	6/6	0.77	0.14	52,53,54,56	0
2	A1ESW	C	801	36/36	0.79	0.14	44,52,74,80	0
2	A1ESW	D	802	36/36	0.81	0.14	38,49,61,63	0
2	A1ESW	A	801	36/36	0.83	0.13	34,47,66,70	0
2	A1ESW	B	801	36/36	0.84	0.12	34,40,54,56	0
3	MG	B	802	1/1	0.93	0.07	34,34,34,34	0
3	MG	D	803	1/1	0.95	0.17	40,40,40,40	0
3	MG	A	802	1/1	0.96	0.05	34,34,34,34	0
3	MG	C	802	1/1	0.96	0.08	42,42,42,42	0

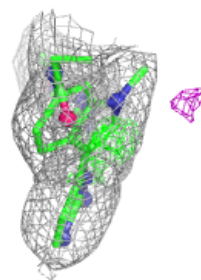
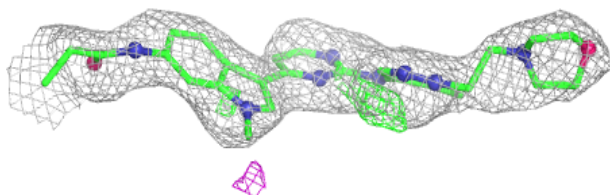
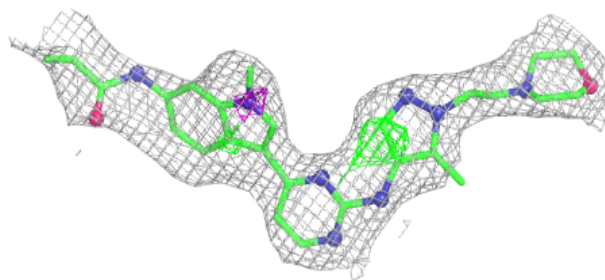
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1ESW C 801:

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

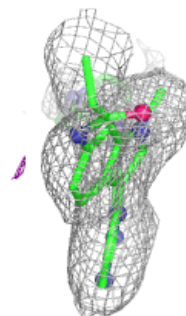
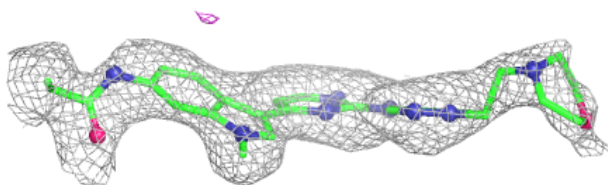
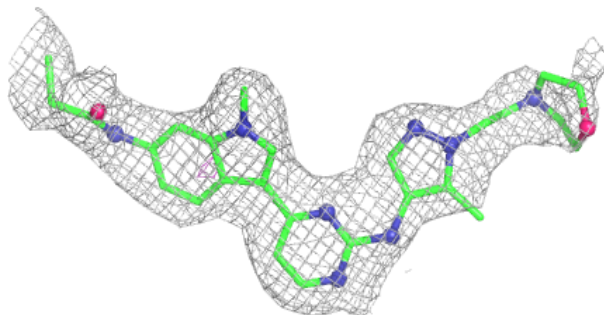
**Electron density around A1ESW D 802:**

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

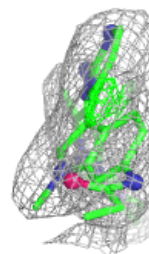
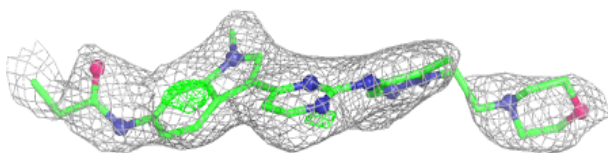
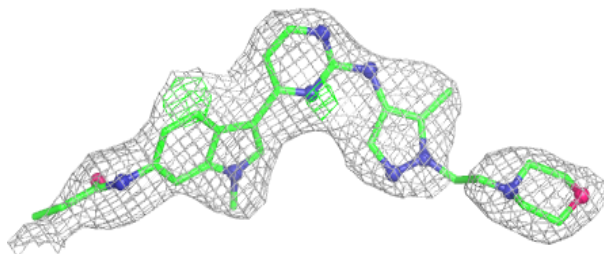


Electron density around A1ESW A 801:

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

**Electron density around A1ESW B 801:**

$2mF_o-DF_c$ (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.