



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 05:52 AM UTC

PDB ID : 8W38 / pdb_00008w38
Title : TAS-120 covalent structure with FGFR2 molecular brake mutant
Authors : Hoffman, I.D.; Nelson, K.J.; Bensen, D.C.; Bailey, J.B.
Deposited on : 2024-02-22
Resolution : 2.60 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

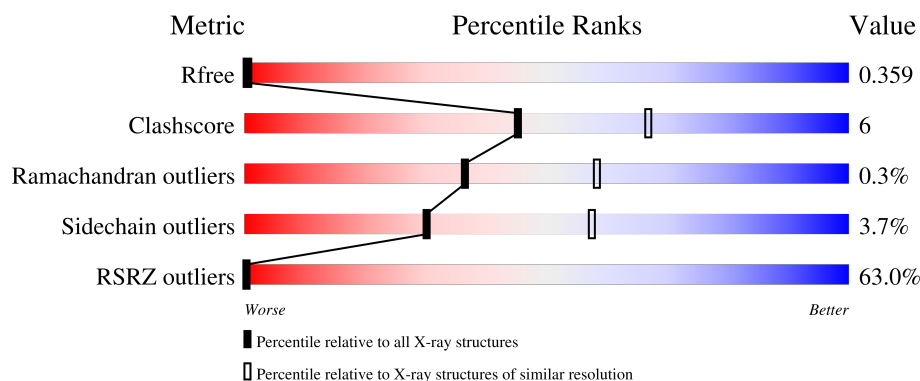
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	324	20% 80% 11% 8%
1	B	324	82% 74% 13% 11%
1	C	324	40% 75% 13% 11%
1	D	324	81% 69% 14% 16%

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
3	SO4	A	802	-	-	-	X
3	SO4	B	802	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9383 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 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	298	Total	C	N	O	S	0	3	0
			2392	1524	403	442	23			
1	B	288	Total	C	N	O	S	0	3	0
			2297	1462	389	424	22			
1	C	289	Total	C	N	O	S	0	3	0
			2314	1476	389	427	22			
1	D	271	Total	C	N	O	S	0	3	0
			2163	1380	368	394	21			

There are 60 discrepancies between the modelled and reference sequences:

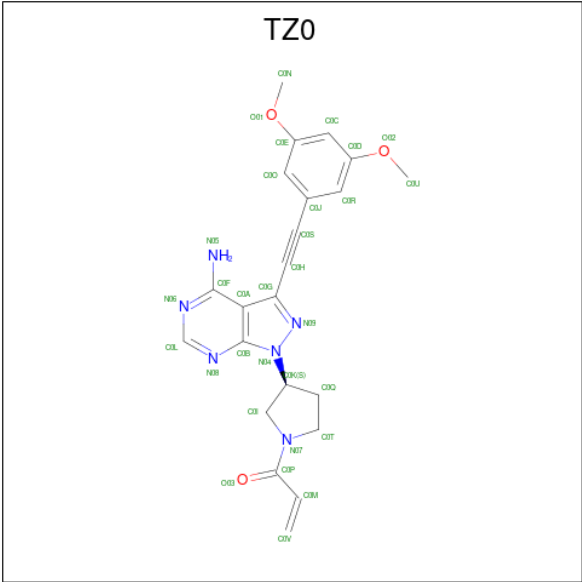
Chain	Residue	Modelled	Actual	Comment	Reference
A	445	MET	-	initiating methionine	UNP P21802
A	446	GLY	-	expression tag	UNP P21802
A	447	SER	-	expression tag	UNP P21802
A	448	SER	-	expression tag	UNP P21802
A	449	HIS	-	expression tag	UNP P21802
A	450	HIS	-	expression tag	UNP P21802
A	451	HIS	-	expression tag	UNP P21802
A	452	HIS	-	expression tag	UNP P21802
A	453	HIS	-	expression tag	UNP P21802
A	454	HIS	-	expression tag	UNP P21802
A	455	SER	-	expression tag	UNP P21802
A	456	GLN	-	expression tag	UNP P21802
A	457	ASP	-	expression tag	UNP P21802
A	549	ASP	ASN	engineered mutation	UNP P21802
A	650	VAL	ASP	engineered mutation	UNP P21802
B	445	MET	-	initiating methionine	UNP P21802
B	446	GLY	-	expression tag	UNP P21802
B	447	SER	-	expression tag	UNP P21802
B	448	SER	-	expression tag	UNP P21802
B	449	HIS	-	expression tag	UNP P21802
B	450	HIS	-	expression tag	UNP P21802

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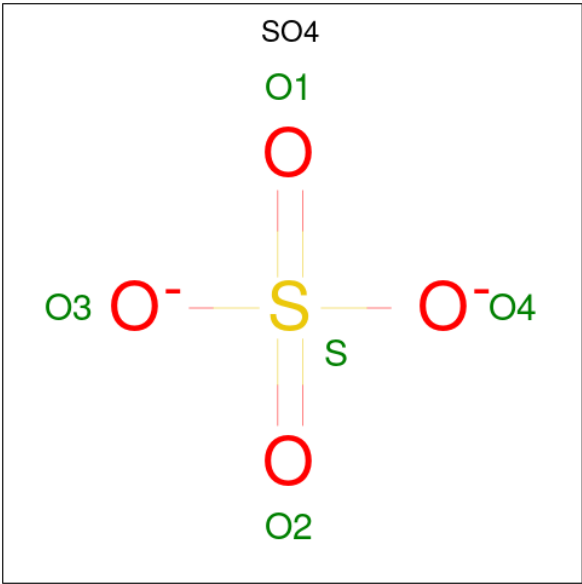
Chain	Residue	Modelled	Actual	Comment	Reference
B	451	HIS	-	expression tag	UNP P21802
B	452	HIS	-	expression tag	UNP P21802
B	453	HIS	-	expression tag	UNP P21802
B	454	HIS	-	expression tag	UNP P21802
B	455	SER	-	expression tag	UNP P21802
B	456	GLN	-	expression tag	UNP P21802
B	457	ASP	-	expression tag	UNP P21802
B	549	ASP	ASN	engineered mutation	UNP P21802
B	650	VAL	ASP	engineered mutation	UNP P21802
C	445	MET	-	initiating methionine	UNP P21802
C	446	GLY	-	expression tag	UNP P21802
C	447	SER	-	expression tag	UNP P21802
C	448	SER	-	expression tag	UNP P21802
C	449	HIS	-	expression tag	UNP P21802
C	450	HIS	-	expression tag	UNP P21802
C	451	HIS	-	expression tag	UNP P21802
C	452	HIS	-	expression tag	UNP P21802
C	453	HIS	-	expression tag	UNP P21802
C	454	HIS	-	expression tag	UNP P21802
C	455	SER	-	expression tag	UNP P21802
C	456	GLN	-	expression tag	UNP P21802
C	457	ASP	-	expression tag	UNP P21802
C	549	ASP	ASN	engineered mutation	UNP P21802
C	650	VAL	ASP	engineered mutation	UNP P21802
D	445	MET	-	initiating methionine	UNP P21802
D	446	GLY	-	expression tag	UNP P21802
D	447	SER	-	expression tag	UNP P21802
D	448	SER	-	expression tag	UNP P21802
D	449	HIS	-	expression tag	UNP P21802
D	450	HIS	-	expression tag	UNP P21802
D	451	HIS	-	expression tag	UNP P21802
D	452	HIS	-	expression tag	UNP P21802
D	453	HIS	-	expression tag	UNP P21802
D	454	HIS	-	expression tag	UNP P21802
D	455	SER	-	expression tag	UNP P21802
D	456	GLN	-	expression tag	UNP P21802
D	457	ASP	-	expression tag	UNP P21802
D	549	ASP	ASN	engineered mutation	UNP P21802
D	650	VAL	ASP	engineered mutation	UNP P21802

- Molecule 2 is 1-[(3S)-3-{4-amino-3-[(3,5-dimethoxyphenyl)ethynyl]-1H-pyrazolo[3,4-d]pyrimidin-1-yl}pyrrolidin-1-yl]prop-2-en-1-one (CCD ID: TZ0) (formula: C₂₂H₂₂N₆O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			31	22	6	3		
2	B	1	Total	C	N	O	0	0
			31	22	6	3		
2	C	1	Total	C	N	O	0	0
			31	22	6	3		
2	D	1	Total	C	N	O	0	0
			31	22	6	3		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0

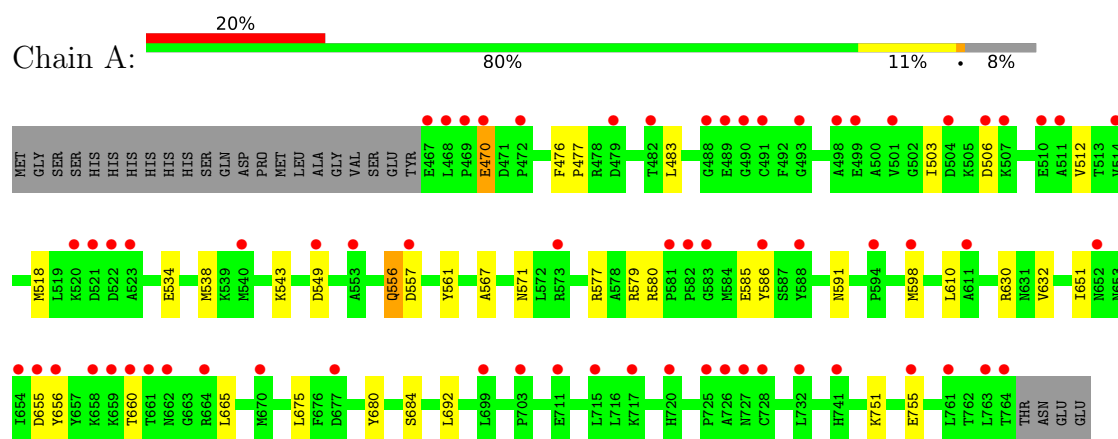
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	26	Total O 26 26	0	0
4	B	7	Total O 7 7	0	0
4	C	23	Total O 23 23	0	0
4	D	2	Total O 2 2	0	0

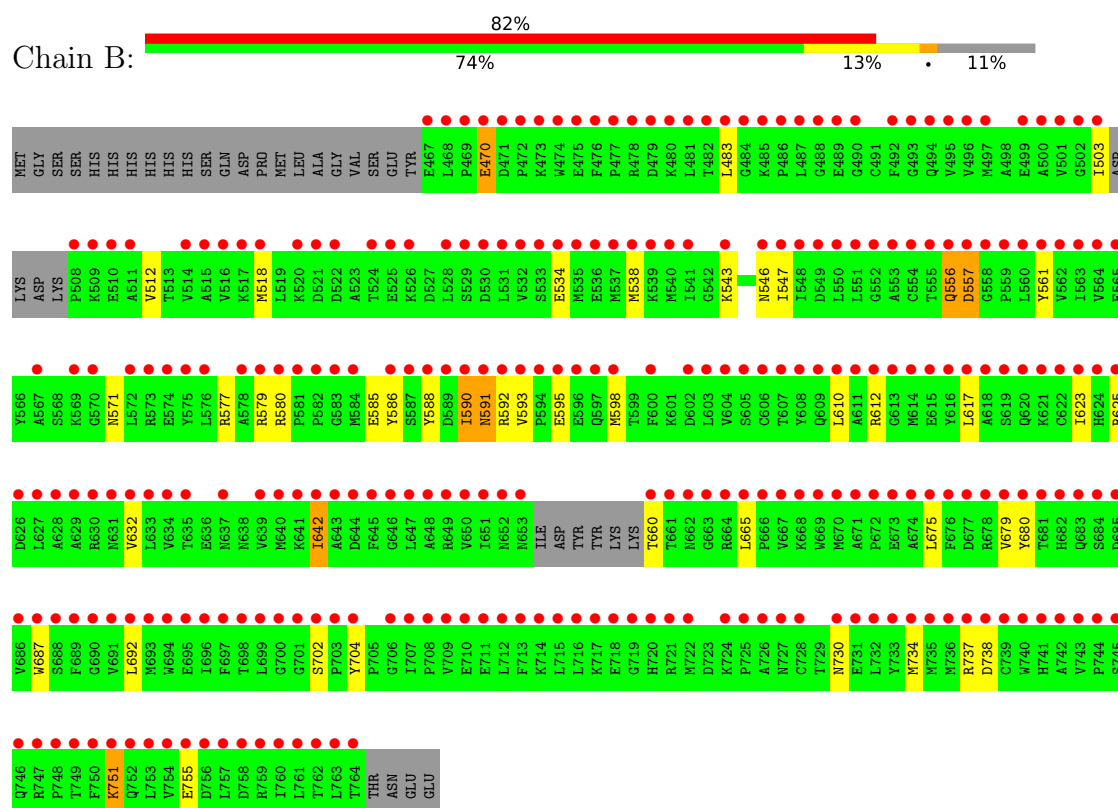
3 Residue-property plots [i](#)

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.

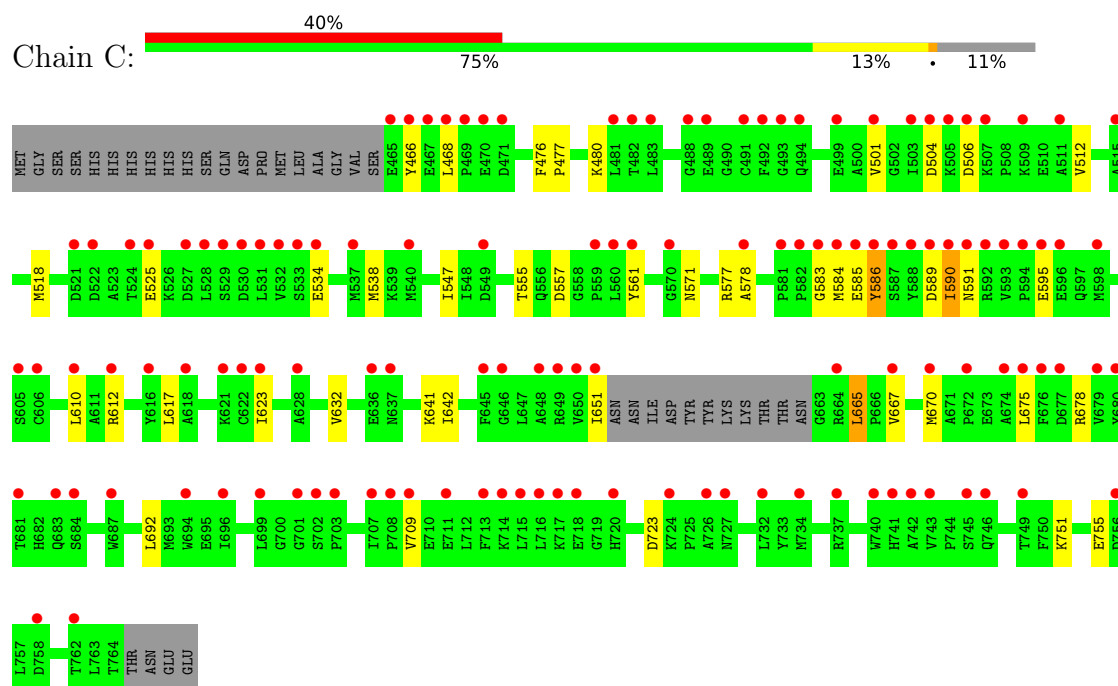
- Molecule 1: Fibroblast growth factor receptor 2



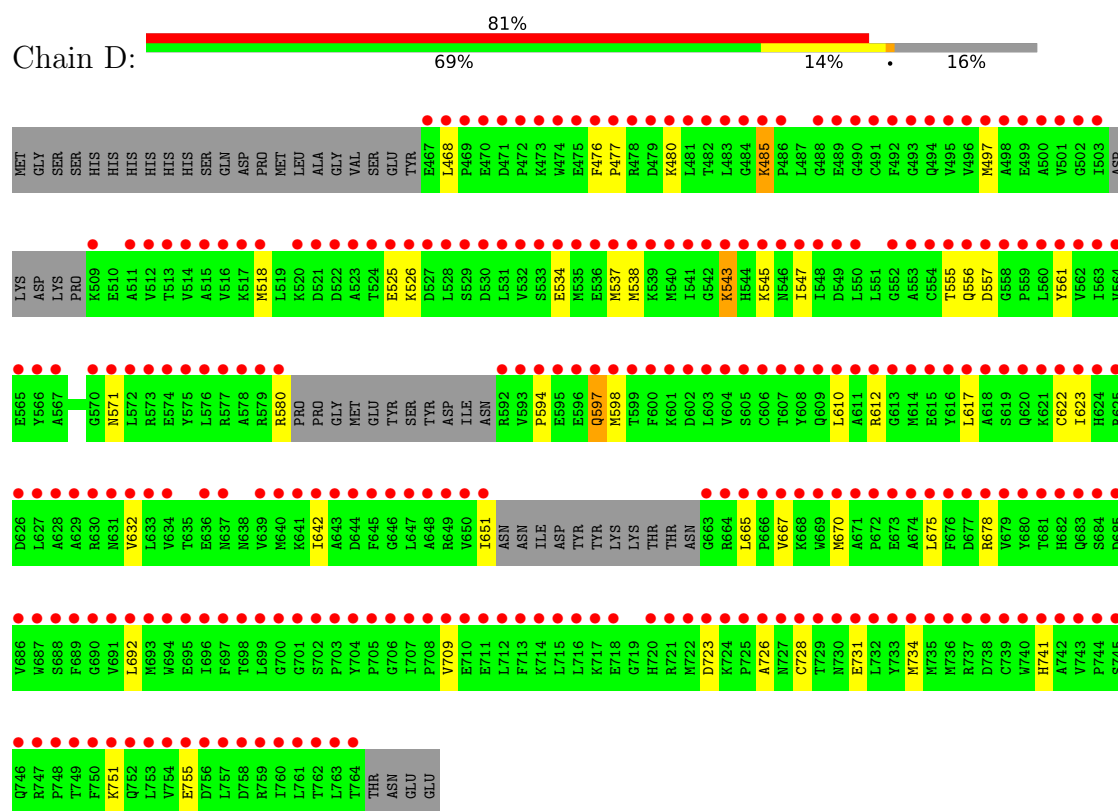
- Molecule 1: Fibroblast growth factor receptor 2



• Molecule 1: Fibroblast growth factor receptor 2



• Molecule 1: Fibroblast growth factor receptor 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	80.25Å 129.87Å 131.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.00 – 2.60 35.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (35.00-2.60) 99.7 (35.00-2.60)	Depositor EDS
R_{merge}	0.31	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.72 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.336 , 0.359 0.335 , 0.359	Depositor DCC
R_{free} test set	2002 reflections (4.65%)	wwPDB-VP
Wilson B-factor (Å ²)	30.8	Xtriage
Anisotropy	0.529	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 68.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	9383	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.00 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.9360e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, TZ0

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	0.45	0/2447	0.96	0/3307
1	B	0.44	0/2345	0.96	0/3168
1	C	0.45	0/2364	0.96	0/3193
1	D	0.43	0/2205	0.96	0/2973
All	All	0.44	0/9361	0.96	0/12641

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	2392	0	2399	24	0
1	B	2297	0	2300	38	1
1	C	2314	0	2317	26	0
1	D	2163	0	2183	26	4
2	A	31	0	0	1	0
2	B	31	0	0	0	0
2	C	31	0	0	0	0
2	D	31	0	0	0	0
3	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	15	0	0	1	0
3	C	15	0	0	0	0
4	A	26	0	0	2	0
4	B	7	0	0	4	0
4	C	23	0	0	1	0
4	D	2	0	0	0	0
All	All	9383	0	9199	109	4

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 (109) 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:597:GLN:NE2	1:D:597:GLN:HA	1.83	0.93
1:B:546:ASN:O	1:B:642:ILE:HG22	1.72	0.89
1:A:549:ASP:HB2	4:A:912:HOH:O	1.78	0.83
1:A:577:ARG:HD3	1:A:586:TYR:HB3	1.64	0.79
1:B:577:ARG:HD3	1:B:586:TYR:HB3	1.65	0.79
1:B:704:TYR:OH	4:B:901:HOH:O	2.06	0.72
1:B:617:LEU:HD11	1:B:642:ILE:CD1	2.20	0.71
1:B:617:LEU:HD11	1:B:642:ILE:HD11	1.72	0.70
1:D:597:GLN:HA	1:D:597:GLN:HE21	1.56	0.69
1:B:579:ARG:HD3	1:B:598:MET:HE3	1.75	0.68
1:A:503:ILE:HG22	1:A:512:VAL:CG1	2.24	0.67
1:B:503:ILE:HG22	1:B:512:VAL:CG1	2.23	0.67
1:C:589:ASP:O	1:C:590:ILE:HB	1.95	0.66
1:D:597:GLN:NE2	1:D:597:GLN:CA	2.58	0.66
1:A:579:ARG:HD3	1:A:598:MET:HE3	1.77	0.66
1:C:610:LEU:HD13	1:C:692:LEU:HD21	1.78	0.64
1:C:534:GLU:O	1:C:538:MET:HG3	1.99	0.63
1:A:534:GLU:O	1:A:538:MET:HG3	1.99	0.62
1:B:534:GLU:O	1:B:538:MET:HG3	1.99	0.62
1:A:610:LEU:HD13	1:A:692:LEU:HD21	1.80	0.62
1:A:577:ARG:HD3	1:A:586:TYR:CB	2.29	0.61
1:D:534:GLU:O	1:D:538:MET:HG3	2.00	0.61
1:D:610:LEU:HD13	1:D:692:LEU:HD21	1.82	0.61
1:B:610:LEU:HD13	1:B:692:LEU:HD21	1.82	0.60
1:C:667:VAL:HG21	1:C:709:VAL:HG13	1.83	0.60
1:D:667:VAL:HG21	1:D:709:VAL:HG13	1.83	0.60
1:A:518:MET:HE2	1:A:561:TYR:CE1	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:546:ASN:O	1:B:642:ILE:CG2	2.48	0.59
1:B:577:ARG:HD3	1:B:586:TYR:CB	2.31	0.59
1:B:518:MET:HE2	1:B:561:TYR:CE1	2.38	0.59
1:A:506:ASP:HA	1:D:612:ARG:HH12	1.66	0.59
1:D:543:LYS:N	1:D:543:LYS:HD3	2.20	0.57
1:B:617:LEU:CD1	1:B:642:ILE:CD1	2.83	0.56
1:C:585:GLU:O	1:C:586:TYR:HD1	1.88	0.56
1:A:580:ARG:NH1	1:A:585:GLU:O	2.35	0.56
1:D:731:GLU:HA	1:D:734:MET:HE2	1.89	0.55
1:B:580:ARG:NH1	1:B:585:GLU:O	2.37	0.55
1:B:543:LYS:HD2	1:B:543:LYS:N	2.23	0.54
1:C:480:LYS:HD3	1:C:501:VAL:HG23	1.90	0.54
1:B:612:ARG:HH12	1:C:506:ASP:HA	1.72	0.54
1:B:687:TRP:HZ2	4:B:901:HOH:O	1.92	0.53
1:C:667:VAL:HA	1:C:670:MET:HE3	1.90	0.53
1:B:734[A]:MET:HE3	1:B:738:ASP:OD1	2.08	0.53
1:D:518:MET:HE2	1:D:561:TYR:CE1	2.44	0.52
1:D:667:VAL:HA	1:D:670:MET:HE3	1.91	0.52
1:C:468:LEU:HD23	1:C:555:THR:HB	1.90	0.52
1:A:503:ILE:HG22	1:A:512:VAL:HG11	1.93	0.51
1:A:503:ILE:CG2	1:A:512:VAL:HG11	2.41	0.51
1:D:468:LEU:HD23	1:D:555:THR:HB	1.93	0.51
1:C:583:GLY:O	1:C:584:MET:HB2	2.10	0.51
1:B:503:ILE:HG22	1:B:512:VAL:HG11	1.93	0.50
1:B:503:ILE:CG2	1:B:512:VAL:HG11	2.42	0.50
1:B:590:ILE:O	1:B:591:ASN:C	2.54	0.50
1:B:503:ILE:CG2	1:B:512:VAL:CG1	2.90	0.50
1:C:518:MET:HE2	1:C:561:TYR:CE1	2.47	0.50
1:A:503:ILE:CG2	1:A:512:VAL:CG1	2.91	0.49
1:C:480:LYS:HD3	1:C:501:VAL:CG2	2.42	0.49
1:B:625:ARG:HH21	1:B:680:TYR:HB3	1.78	0.48
1:B:737:ARG:HB3	3:B:802:SO4:S	2.54	0.48
1:C:623:ILE:HG23	1:C:651:ILE:HD11	1.94	0.48
1:D:547:ILE:HD13	1:D:642:ILE:HB	1.95	0.47
1:C:547:ILE:HD13	1:C:642:ILE:HB	1.96	0.47
1:D:623:ILE:HG23	1:D:651:ILE:HD11	1.95	0.47
1:A:651:ILE:HG21	1:A:656:TYR:HB2	1.97	0.47
1:D:537:MET:HE3	1:D:622[A]:CYS:SG	2.55	0.47
1:A:470:GLU:HB2	1:A:556:GLN:OE1	2.15	0.46
1:B:751:LYS:O	1:B:755:GLU:HG2	2.16	0.46
1:C:504:ASP:HB3	1:C:512:VAL:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:597:GLN:CD	1:D:598:MET:H	2.25	0.45
1:B:588:TYR:CE2	1:B:590:ILE:HG13	2.52	0.45
1:A:630:ARG:HD3	4:A:923:HOH:O	2.16	0.45
1:A:751:LYS:O	1:A:755:GLU:HG3	2.15	0.45
1:B:470:GLU:HB2	1:B:556:GLN:OE1	2.17	0.45
1:C:751:LYS:O	1:C:755:GLU:HG3	2.16	0.45
1:A:506:ASP:CG	1:D:545:LYS:HD3	2.42	0.45
1:D:751:LYS:O	1:D:755:GLU:HG3	2.16	0.45
1:B:617:LEU:CD1	1:B:642:ILE:HD11	2.44	0.44
1:C:665:LEU:HD23	1:C:665:LEU:N	2.32	0.44
1:A:571:ASN:HA	1:A:632:VAL:O	2.19	0.43
1:B:571:ASN:HA	1:B:632:VAL:O	2.18	0.43
1:D:571:ASN:HA	1:D:632:VAL:O	2.19	0.43
1:B:556:GLN:HB3	1:B:557:ASP:OD1	2.19	0.43
1:B:687:TRP:CZ2	4:B:901:HOH:O	2.57	0.42
1:B:612:ARG:HG3	1:B:612:ARG:HH11	1.84	0.42
1:A:591:ASN:O	1:C:466:TYR:HA	2.20	0.42
1:C:571:ASN:HA	1:C:632:VAL:O	2.19	0.42
1:B:679:VAL:HG12	1:D:485:LYS:HD2	2.02	0.42
1:B:625:ARG:HE	1:B:680:TYR:CB	2.32	0.42
1:D:665:LEU:N	1:D:665:LEU:HD23	2.34	0.42
1:A:556:GLN:HB3	1:A:557:ASP:OD1	2.19	0.42
1:C:578:ALA:HB1	1:C:591:ASN:O	2.20	0.42
1:B:702:SER:HB2	4:B:903:HOH:O	2.19	0.41
1:B:623:ILE:HD12	1:B:625:ARG:NE	2.35	0.41
1:C:595:GLU:CD	1:C:595:GLU:H	2.28	0.41
1:D:476:PHE:HA	1:D:477:PRO:HD3	1.92	0.41
1:A:567:ALA:H	2:A:801:TZ0:C0L	2.33	0.41
1:A:680:TYR:CE1	1:A:684:SER:HB2	2.55	0.41
1:B:593:VAL:O	1:B:595:GLU:OE2	2.39	0.41
1:C:476:PHE:HA	1:C:477:PRO:HD3	1.92	0.41
1:C:585:GLU:O	1:C:586:TYR:CD1	2.71	0.41
1:C:617:LEU:HD23	1:C:617:LEU:HA	1.88	0.41
1:D:485:LYS:HG2	1:D:497:MET:HE2	2.03	0.41
1:D:612:ARG:HG3	1:D:612:ARG:HH11	1.86	0.41
1:D:617:LEU:HD23	1:D:617:LEU:HA	1.88	0.41
1:A:476:PHE:HA	1:A:477:PRO:HD3	1.93	0.41
1:B:547:ILE:HA	1:B:642:ILE:HG23	2.03	0.41
1:C:612:ARG:HG3	1:C:612:ARG:HH11	1.86	0.40
1:D:597:GLN:CD	1:D:598:MET:N	2.79	0.40
1:C:525:GLU:OE2	4:C:901:HOH:O	2.22	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:597:GLN:NE2	1:D:726:ALA:O[2_455]	1.93	0.27
1:D:580:ARG:O	1:D:726:ALA:CB[2_455]	2.16	0.04
1:B:730:ASN:ND2	1:D:741:HIS:CD2[2_455]	2.17	0.03
1:D:594:PRO:O	1:D:728:CYS:O[2_455]	2.17	0.03

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	297/324 (92%)	289 (97%)	8 (3%)	0	100	100
1	B	282/324 (87%)	272 (96%)	8 (3%)	2 (1%)	18	38
1	C	285/324 (88%)	275 (96%)	9 (3%)	1 (0%)	30	51
1	D	263/324 (81%)	257 (98%)	6 (2%)	0	100	100
All	All	1127/1296 (87%)	1093 (97%)	31 (3%)	3 (0%)	36	58

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	591	ASN
1	C	590	ILE
1	B	592	ARG

5.3.2 Protein sidechains [i](#)

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	263/285 (92%)	255 (97%)	8 (3%)	36	64
1	B	252/285 (88%)	242 (96%)	10 (4%)	28	55
1	C	253/285 (89%)	245 (97%)	8 (3%)	34	62
1	D	236/285 (83%)	225 (95%)	11 (5%)	23	48
All	All	1004/1140 (88%)	967 (96%)	37 (4%)	30	57

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	470	GLU
1	A	483	LEU
1	A	543	LYS
1	A	556	GLN
1	A	655	ASP
1	A	660	THR
1	A	665	LEU
1	A	675	LEU
1	B	470	GLU
1	B	483	LEU
1	B	556	GLN
1	B	557	ASP
1	B	590	ILE
1	B	642	ILE
1	B	660	THR
1	B	665	LEU
1	B	675	LEU
1	B	751	LYS
1	C	557	ASP
1	C	577	ARG
1	C	586	TYR
1	C	641	LYS
1	C	665	LEU
1	C	675	LEU
1	C	678	ARG
1	C	723	ASP
1	D	480	LYS
1	D	485	LYS
1	D	525	GLU
1	D	526	LYS
1	D	543	LYS
1	D	556	GLN
1	D	557	ASP

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Mol	Chain	Res	Type
1	D	597	GLN
1	D	675	LEU
1	D	678	ARG
1	D	723	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	597	GLN
1	A	720	HIS
1	B	720	HIS
1	C	494	GLN
1	C	597	GLN
1	C	682	HIS
1	C	720	HIS
1	C	727	ASN
1	D	597	GLN
1	D	682	HIS
1	D	727	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

11 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	B	803	-	4,4,4	0.34	0	6,6,6	0.08	0
2	TZ0	B	801	1	32,34,34	2.19	7 (21%)	44,48,48	2.67	17 (38%)
2	TZ0	D	800	1	32,34,34	2.97	10 (31%)	44,48,48	2.67	16 (36%)
2	TZ0	A	801	1	32,34,34	2.59	9 (28%)	44,48,48	2.61	18 (40%)
3	SO4	B	802	-	4,4,4	0.35	0	6,6,6	0.07	0
2	TZ0	C	801	1	32,34,34	2.80	10 (31%)	44,48,48	2.80	19 (43%)
3	SO4	B	804	-	4,4,4	0.34	0	6,6,6	0.07	0
3	SO4	C	804	-	4,4,4	0.35	0	6,6,6	0.07	0
3	SO4	C	803	-	4,4,4	0.35	0	6,6,6	0.09	0
3	SO4	A	802	-	4,4,4	0.36	0	6,6,6	0.07	0
3	SO4	C	802	-	4,4,4	0.33	0	6,6,6	0.07	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
2	TZ0	C	801	1	-	5/17/28/28	0/4/4/4
2	TZ0	D	800	1	-	6/17/28/28	0/4/4/4
2	TZ0	A	801	1	-	3/17/28/28	0/4/4/4
2	TZ0	B	801	1	-	3/17/28/28	0/4/4/4

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	800	TZ0	C0H-C0S	-11.07	1.03	1.20
2	C	801	TZ0	C0A-C0F	-8.42	1.33	1.42
2	C	801	TZ0	C0H-C0S	-8.29	1.07	1.20
2	A	801	TZ0	C0H-C0S	-7.78	1.08	1.20
2	A	801	TZ0	C0A-C0F	-7.13	1.34	1.42
2	D	800	TZ0	C0A-C0F	-6.80	1.34	1.42
2	B	801	TZ0	C0A-C0F	-6.21	1.35	1.42
2	C	801	TZ0	C0A-C0B	-5.46	1.33	1.40
2	A	801	TZ0	C0A-C0B	-5.40	1.33	1.40
2	D	800	TZ0	C0A-C0B	-4.94	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	801	TZ0	C0V-C0M	4.86	1.53	1.30
2	A	801	TZ0	C0V-C0M	4.84	1.53	1.30
2	B	801	TZ0	C0A-C0B	-4.83	1.34	1.40
2	D	800	TZ0	C0V-C0M	4.83	1.53	1.30
2	B	801	TZ0	C0V-C0M	4.80	1.53	1.30
2	B	801	TZ0	C0H-C0S	-4.78	1.12	1.20
2	D	800	TZ0	C0J-C0S	-3.53	1.35	1.44
2	D	800	TZ0	C0L-N06	3.49	1.40	1.33
2	B	801	TZ0	C0L-N08	3.43	1.40	1.33
2	D	800	TZ0	C0L-N08	3.28	1.39	1.33
2	A	801	TZ0	C0M-C0P	3.28	1.58	1.49
2	B	801	TZ0	C0L-N06	3.27	1.39	1.33
2	C	801	TZ0	C0L-N08	3.14	1.39	1.33
2	C	801	TZ0	C0I-N07	3.00	1.52	1.46
2	A	801	TZ0	C0L-N06	2.86	1.39	1.33
2	C	801	TZ0	C0L-N06	2.84	1.39	1.33
2	A	801	TZ0	C0B-N04	-2.77	1.33	1.36
2	D	800	TZ0	C0K-N04	2.62	1.51	1.46
2	A	801	TZ0	C0L-N08	2.55	1.38	1.33
2	D	800	TZ0	C0B-N04	-2.51	1.33	1.36
2	C	801	TZ0	N04-N09	-2.49	1.33	1.38
2	D	800	TZ0	C0I-N07	2.34	1.51	1.46
2	A	801	TZ0	N04-N09	-2.27	1.34	1.38
2	C	801	TZ0	C0K-N04	2.24	1.50	1.46
2	B	801	TZ0	C0M-C0P	2.15	1.55	1.49
2	C	801	TZ0	C0B-N04	-2.15	1.34	1.36

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	800	TZ0	N08-C0L-N06	-7.29	117.54	128.58
2	C	801	TZ0	N08-C0L-N06	-7.28	117.56	128.58
2	B	801	TZ0	N08-C0L-N06	-6.98	118.01	128.58
2	A	801	TZ0	N08-C0L-N06	-6.53	118.70	128.58
2	B	801	TZ0	C0A-C0B-N08	-6.04	120.56	126.97
2	C	801	TZ0	C0A-C0B-N08	-5.94	120.67	126.97
2	B	801	TZ0	C0F-C0A-C0B	5.61	119.94	115.74
2	D	800	TZ0	C0A-C0B-N08	-5.58	121.05	126.97
2	D	800	TZ0	C0V-C0M-C0P	-5.47	110.17	121.27
2	A	801	TZ0	C0F-C0A-C0B	5.42	119.80	115.74
2	D	800	TZ0	C0F-C0A-C0B	5.40	119.78	115.74
2	C	801	TZ0	C0V-C0M-C0P	-5.38	110.34	121.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	TZ0	C0A-C0B-N08	-5.35	121.30	126.97
2	C	801	TZ0	C0B-N04-N09	-5.31	107.50	110.90
2	C	801	TZ0	C0F-C0A-C0B	5.30	119.71	115.74
2	B	801	TZ0	C0V-C0M-C0P	-5.14	110.83	121.27
2	D	800	TZ0	C0F-C0A-C0G	-5.02	133.91	139.12
2	C	801	TZ0	C0F-C0A-C0G	-4.91	134.03	139.12
2	B	801	TZ0	C0F-C0A-C0G	-4.70	134.25	139.12
2	C	801	TZ0	C0A-C0F-N05	-4.70	117.20	123.40
2	C	801	TZ0	C0A-C0F-N06	4.68	122.84	118.64
2	A	801	TZ0	C0F-C0A-C0G	-4.62	134.33	139.12
2	B	801	TZ0	C0T-N07-C0I	-4.42	107.22	112.38
2	D	800	TZ0	C0B-N04-N09	-4.38	108.10	110.90
2	A	801	TZ0	C0M-C0P-N07	-4.29	112.93	117.66
2	A	801	TZ0	C0A-C0F-N05	-4.02	118.09	123.40
2	D	800	TZ0	C0K-N04-N09	3.91	129.06	119.89
2	D	800	TZ0	C0A-C0F-N05	-3.90	118.26	123.40
2	B	801	TZ0	C0A-C0F-N05	-3.84	118.33	123.40
2	B	801	TZ0	C0A-C0F-N06	3.84	122.08	118.64
2	B	801	TZ0	C0B-N04-N09	-3.74	108.50	110.90
2	C	801	TZ0	C0G-N09-N04	3.69	107.33	103.81
2	D	800	TZ0	C0A-C0F-N06	3.67	121.93	118.64
2	A	801	TZ0	C0T-N07-C0I	-3.65	108.12	112.38
2	B	801	TZ0	N08-C0B-N04	3.57	130.70	126.05
2	B	801	TZ0	C0L-N08-C0B	3.53	120.46	111.83
2	C	801	TZ0	C0L-N08-C0B	3.50	120.39	111.83
2	A	801	TZ0	C0A-C0F-N06	3.47	121.76	118.64
2	D	800	TZ0	C0L-N08-C0B	3.47	120.31	111.83
2	A	801	TZ0	C0B-N04-N09	-3.42	108.71	110.90
2	C	801	TZ0	N08-C0B-N04	3.37	130.44	126.05
2	A	801	TZ0	C0L-N08-C0B	3.22	119.70	111.83
2	D	800	TZ0	N08-C0B-N04	3.18	130.19	126.05
2	A	801	TZ0	C0V-C0M-C0P	-3.17	114.84	121.27
2	A	801	TZ0	C0K-N04-N09	3.16	127.30	119.89
2	A	801	TZ0	C0Q-C0K-C0I	3.12	107.48	102.22
2	D	800	TZ0	C0G-N09-N04	3.09	106.76	103.81
2	A	801	TZ0	N08-C0B-N04	3.06	130.04	126.05
2	D	800	TZ0	C0T-N07-C0I	-2.79	109.12	112.38
2	C	801	TZ0	C0A-C0B-N04	2.68	108.89	107.19
2	B	801	TZ0	C0K-N04-N09	2.63	126.06	119.89
2	B	801	TZ0	C0G-N09-N04	2.61	106.30	103.81
2	A	801	TZ0	C0N-O01-C0E	-2.51	112.12	117.50
2	D	800	TZ0	C0B-N04-C0K	-2.47	122.83	128.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	800	TZ0	C0A-C0B-N04	2.47	108.76	107.19
2	A	801	TZ0	C0G-N09-N04	2.44	106.14	103.81
2	B	801	TZ0	C0A-C0B-N04	2.43	108.74	107.19
2	C	801	TZ0	C0A-C0G-C0H	2.39	129.34	123.49
2	C	801	TZ0	C0K-N04-N09	2.37	125.46	119.89
2	C	801	TZ0	C0R-C0J-C0S	-2.36	115.95	120.22
2	A	801	TZ0	C0A-C0B-N04	2.32	108.66	107.19
2	C	801	TZ0	C0O-C0J-C0S	2.30	124.37	120.22
2	D	800	TZ0	C0B-C0A-C0G	2.24	106.30	104.74
2	C	801	TZ0	C0Q-C0T-N07	2.19	105.75	102.93
2	C	801	TZ0	C0B-C0A-C0G	2.19	106.26	104.74
2	B	801	TZ0	C0U-O02-C0D	-2.14	112.90	117.50
2	B	801	TZ0	C0I-C0K-N04	-2.08	110.53	112.48
2	B	801	TZ0	C0Q-C0K-C0I	2.06	105.70	102.22
2	A	801	TZ0	C0B-N04-C0K	-2.00	123.99	128.97
2	C	801	TZ0	C0T-N07-C0I	-2.00	110.04	112.38

There are no chirality outliers.

All (17) torsion outliers are listed below:

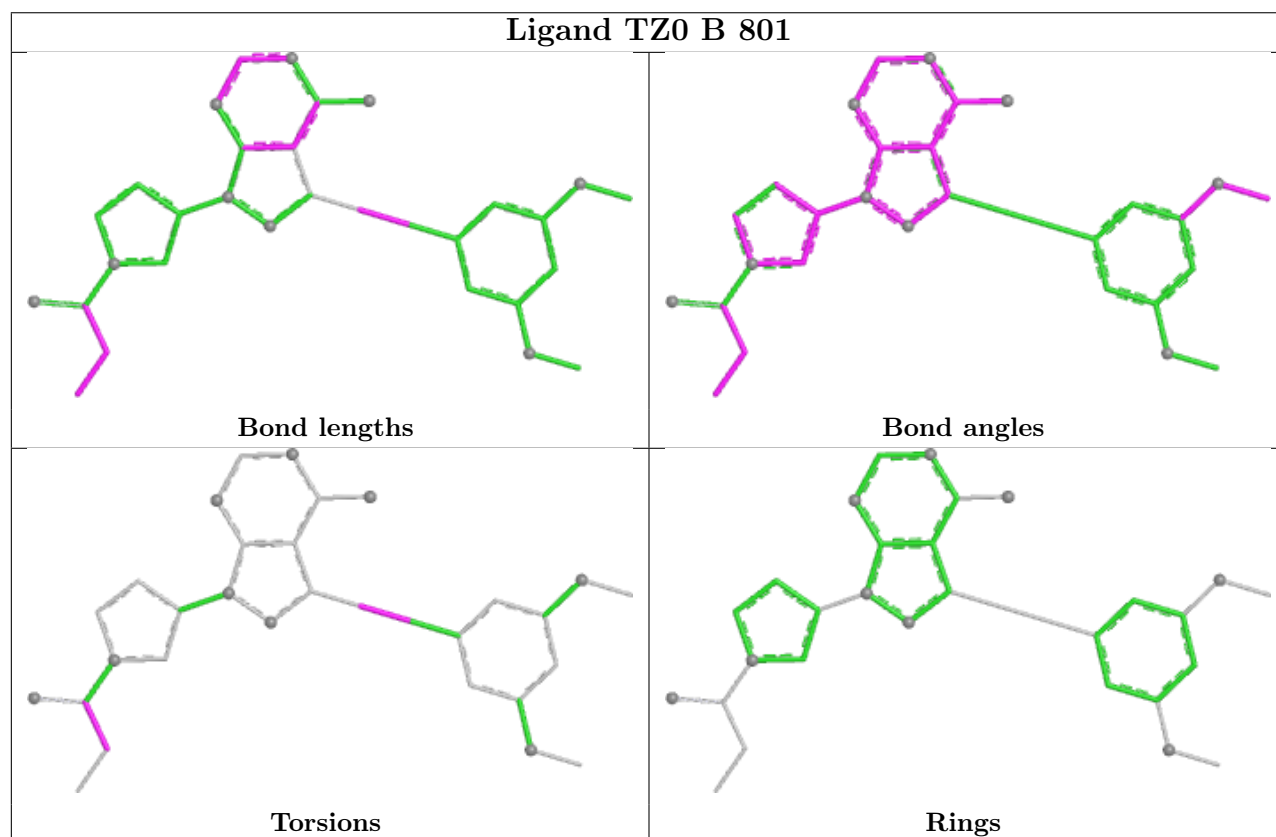
Mol	Chain	Res	Type	Atoms
2	B	801	TZ0	C0V-C0M-C0P-O03
2	C	801	TZ0	C0G-C0H-C0S-C0J
2	C	801	TZ0	C0I-C0K-N04-N09
2	C	801	TZ0	C0Q-C0K-N04-C0B
2	B	801	TZ0	C0V-C0M-C0P-N07
2	D	800	TZ0	C0I-C0K-N04-N09
2	A	801	TZ0	C0G-C0H-C0S-C0J
2	B	801	TZ0	C0G-C0H-C0S-C0J
2	D	800	TZ0	C0G-C0H-C0S-C0J
2	A	801	TZ0	C0Q-C0K-N04-C0B
2	C	801	TZ0	C0I-C0K-N04-C0B
2	D	800	TZ0	C0Q-C0K-N04-C0B
2	C	801	TZ0	C0Q-C0K-N04-N09
2	D	800	TZ0	C0Q-C0K-N04-N09
2	D	800	TZ0	C0C-C0D-O02-C0U
2	D	800	TZ0	C0R-C0D-O02-C0U
2	A	801	TZ0	C0I-C0K-N04-N09

There are no ring outliers.

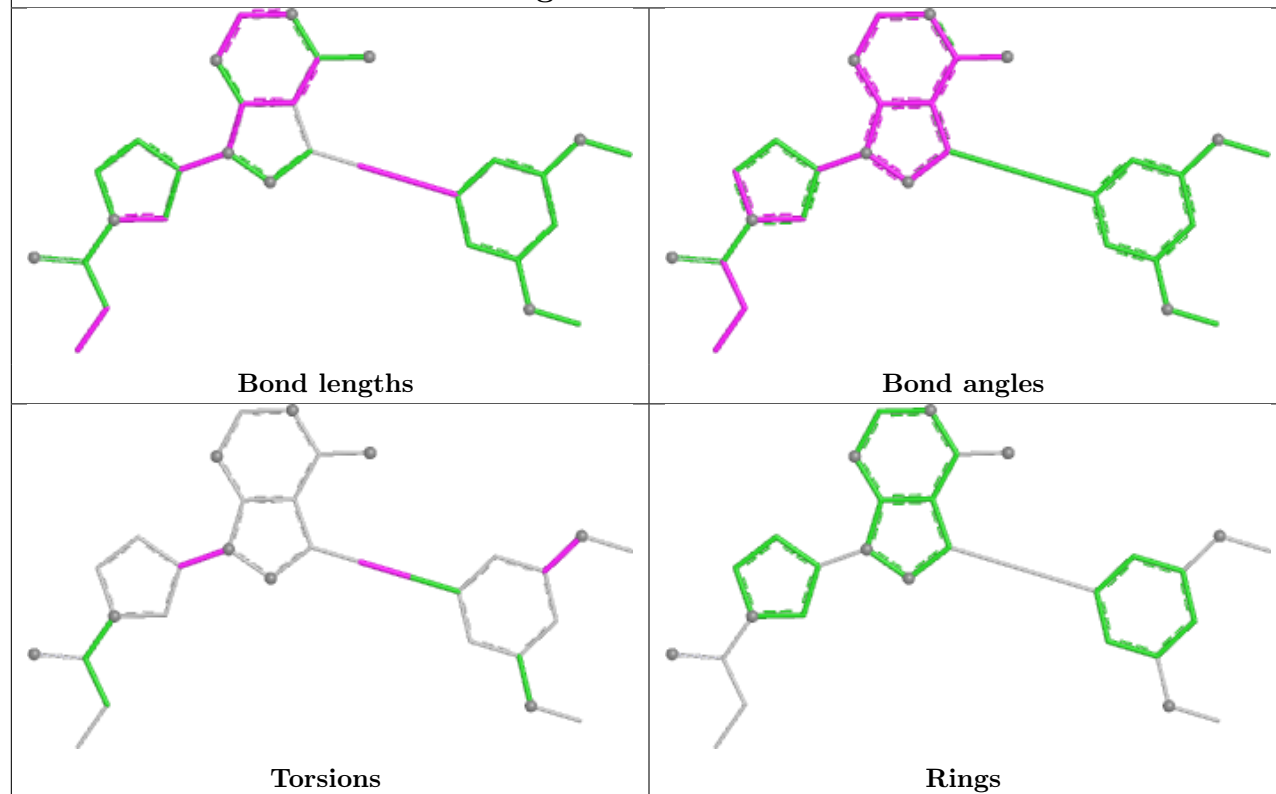
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	TZ0	1	0
3	B	802	SO4	1	0

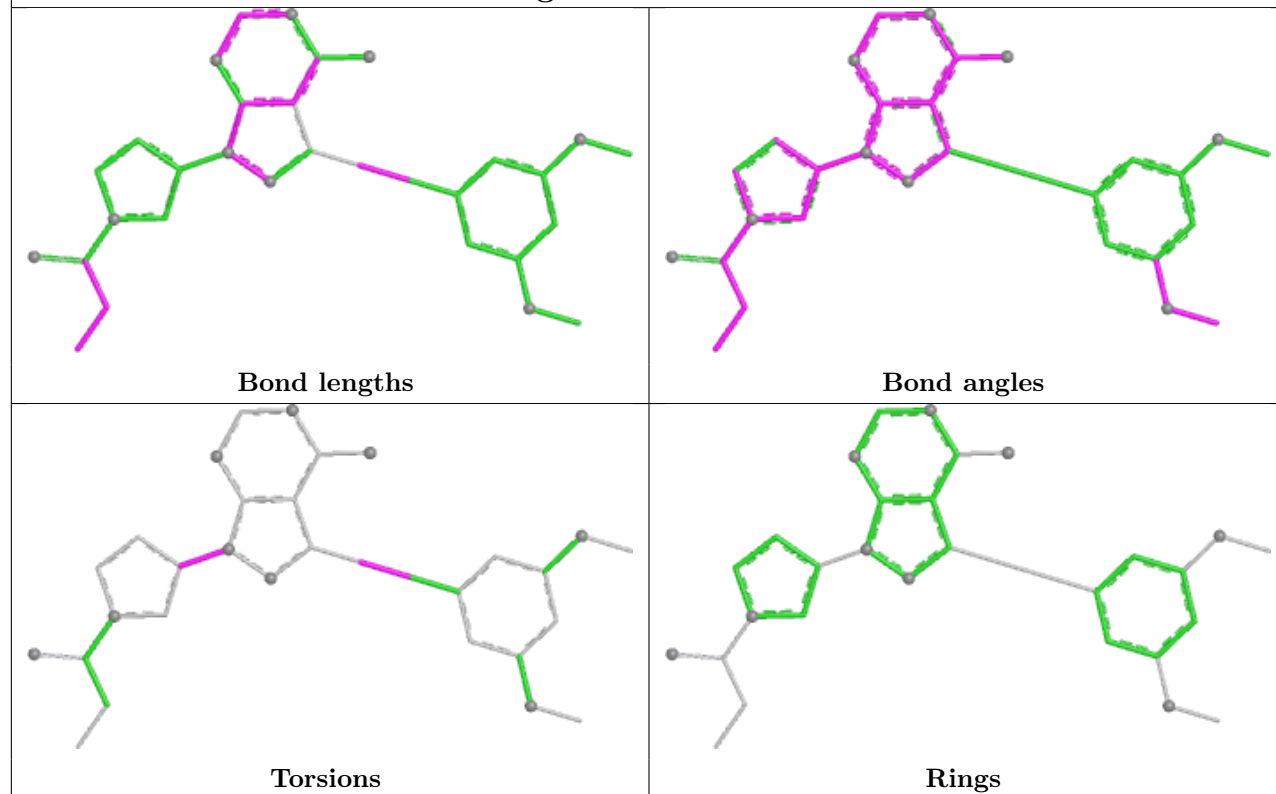
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

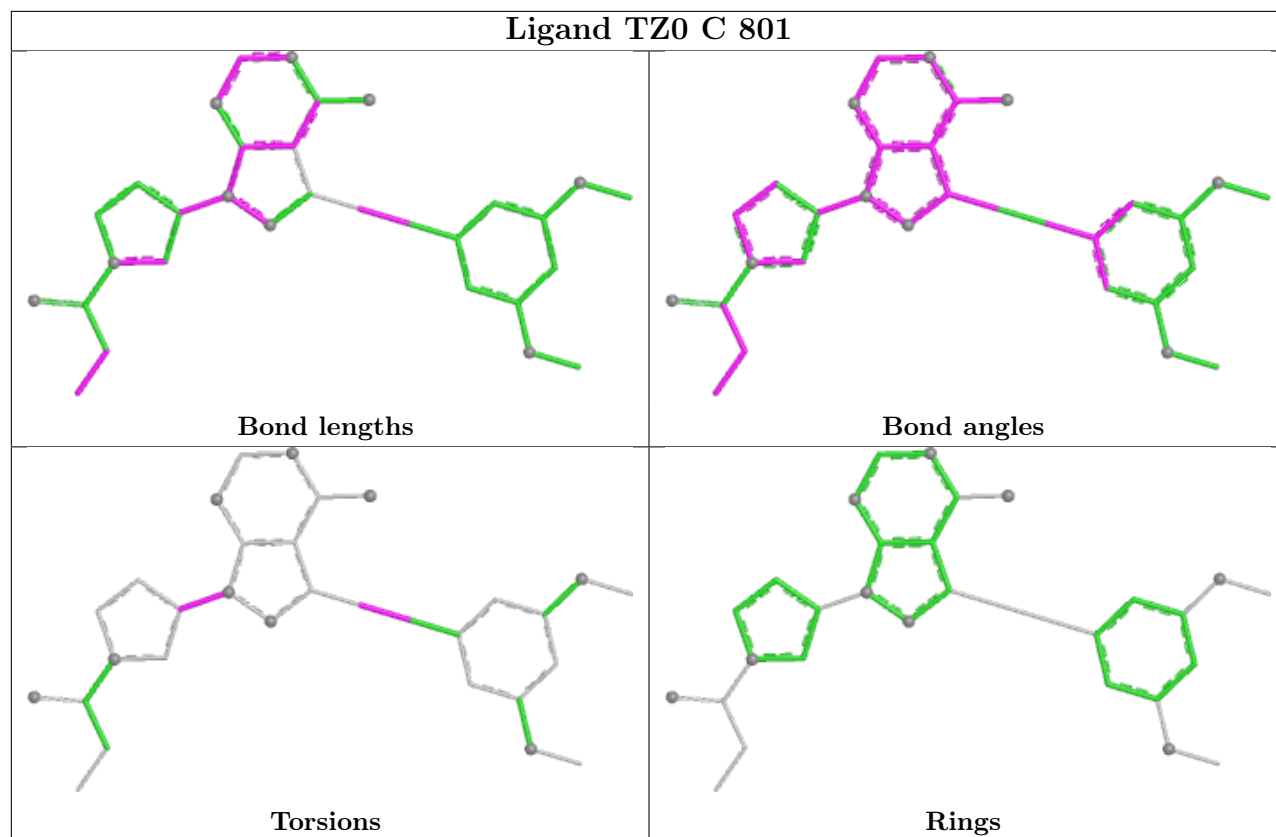


Ligand TZ0 D 800



Ligand TZ0 A 801





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	298/324 (91%)	1.40	66 (22%) 2 2	26, 47, 69, 82	1 (0%)
1	B	288/324 (88%)	3.58	266 (92%) 0 0	61, 72, 94, 107	0
1	C	289/324 (89%)	2.08	128 (44%) 0 0	37, 48, 63, 76	0
1	D	271/324 (83%)	3.98	262 (96%) 0 0	66, 75, 87, 96	0
All	All	1146/1296 (88%)	2.73	722 (63%) 0 0	26, 65, 87, 107	1 (0%)

All (722) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	593	VAL	10.6
1	D	553	ALA	9.4
1	B	553	ALA	9.3
1	D	597	GLN	9.3
1	B	594	PRO	8.9
1	D	593	VAL	8.8
1	C	583	GLY	8.4
1	C	713	PHE	8.0
1	C	586	TYR	7.7
1	D	622[A]	CYS	7.2
1	B	622[A]	CYS	7.1
1	D	533[A]	SER	7.1
1	B	652	ASN	6.8
1	D	532	VAL	6.7
1	B	745	SER	6.7
1	D	474	TRP	6.6
1	D	754	VAL	6.6
1	D	492	PHE	6.5
1	B	501	VAL	6.4
1	B	533	SER	6.4
1	B	508	PRO	6.4

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Mol	Chain	Res	Type	RSRZ
1	B	494	GLN	6.4
1	B	589	ASP	6.2
1	C	509	LYS	6.2
1	D	678	ARG	6.2
1	B	661	THR	6.2
1	D	735	MET	6.2
1	D	667	VAL	6.1
1	D	687	TRP	6.0
1	D	627	LEU	6.0
1	D	484	GLY	5.9
1	D	726	ALA	5.9
1	B	671	ALA	5.9
1	D	514	VAL	5.9
1	D	674	ALA	5.8
1	B	742	ALA	5.8
1	D	679	VAL	5.8
1	D	671	ALA	5.8
1	B	493	GLY	5.7
1	B	676	PHE	5.7
1	B	672	PRO	5.7
1	D	494	GLN	5.7
1	D	688	SER	5.7
1	C	584	MET	5.7
1	D	651	ILE	5.7
1	C	587	SER	5.7
1	D	634	VAL	5.7
1	D	561	TYR	5.7
1	B	525	GLU	5.6
1	B	653	ASN	5.6
1	D	740	TRP	5.6
1	D	643	ALA	5.5
1	C	582	PRO	5.5
1	D	704	TYR	5.5
1	D	742	ALA	5.5
1	D	664	ARG	5.5
1	D	604	VAL	5.5
1	B	555	THR	5.5
1	C	589	ASP	5.4
1	B	588	TYR	5.4
1	B	712	LEU	5.4
1	D	681	THR	5.4
1	B	754	VAL	5.4

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Mol	Chain	Res	Type	RSRZ
1	D	650	VAL	5.4
1	B	667	VAL	5.3
1	D	743	VAL	5.3
1	B	616	TYR	5.3
1	D	554	CYS	5.3
1	B	743	VAL	5.3
1	D	547	ILE	5.3
1	B	536	GLU	5.3
1	B	643	ALA	5.2
1	D	525	GLU	5.2
1	D	739	CYS	5.2
1	B	618	ALA	5.2
1	B	592	ARG	5.2
1	D	646	GLY	5.2
1	D	528	LEU	5.2
1	D	665	LEU	5.2
1	B	687	TRP	5.2
1	B	468	LEU	5.1
1	D	692	LEU	5.1
1	D	536	GLU	5.1
1	D	560	LEU	5.1
1	D	563	ILE	5.1
1	D	745	SER	5.1
1	D	686	VAL	5.1
1	D	498	ALA	5.1
1	D	555	THR	5.1
1	D	675	LEU	5.1
1	D	613	GLY	5.1
1	D	642	ILE	5.1
1	D	579	ARG	5.0
1	D	526	LYS	5.0
1	D	516	VAL	5.0
1	B	681	THR	5.0
1	D	596	GLU	5.0
1	D	647	LEU	5.0
1	D	599	THR	5.0
1	B	547	ILE	5.0
1	D	715	LEU	4.9
1	D	749	THR	4.9
1	B	591	ASN	4.9
1	D	747	ARG	4.9
1	D	716	LEU	4.9

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Mol	Chain	Res	Type	RSRZ
1	B	686	VAL	4.9
1	D	757	LEU	4.9
1	C	506	ASP	4.9
1	D	623	ILE	4.9
1	D	485	LYS	4.9
1	D	610	LEU	4.9
1	B	590	ILE	4.9
1	D	503	ILE	4.9
1	B	717	LYS	4.9
1	D	725	PRO	4.9
1	D	475	GLU	4.8
1	B	474	TRP	4.8
1	D	697	PHE	4.8
1	D	592	ARG	4.8
1	B	749	THR	4.8
1	B	675	LEU	4.8
1	D	732	LEU	4.8
1	C	606[A]	CYS	4.7
1	B	625	ARG	4.7
1	B	481	LEU	4.7
1	B	634	VAL	4.7
1	C	507	LYS	4.7
1	D	531	LEU	4.6
1	D	713	PHE	4.6
1	D	470	GLU	4.6
1	D	670	MET	4.6
1	D	611	ALA	4.6
1	D	629	ALA	4.6
1	B	517	LYS	4.6
1	D	748	PRO	4.6
1	D	562	VAL	4.6
1	D	734	MET	4.6
1	B	522	ASP	4.6
1	B	557	ASP	4.6
1	C	727	ASN	4.6
1	D	717	LYS	4.6
1	B	753	LEU	4.6
1	D	472	PRO	4.6
1	D	549	ASP	4.6
1	D	625	ARG	4.5
1	D	541	ILE	4.5
1	D	718	GLU	4.5

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Mol	Chain	Res	Type	RSRZ
1	D	617	LEU	4.5
1	D	607	THR	4.5
1	B	561	TYR	4.5
1	B	509	LYS	4.5
1	B	663	GLY	4.5
1	D	683	GLN	4.5
1	D	689	PHE	4.5
1	D	501	VAL	4.5
1	D	639	VAL	4.5
1	B	586	TYR	4.5
1	D	676	PHE	4.5
1	B	479	ASP	4.5
1	B	688	SER	4.4
1	D	714	LYS	4.4
1	D	575	TYR	4.4
1	B	747	ARG	4.4
1	B	528	LEU	4.4
1	D	550	LEU	4.4
1	D	600	PHE	4.4
1	D	755	GLU	4.4
1	D	685	ASP	4.4
1	B	692	LEU	4.4
1	B	720	HIS	4.4
1	B	763	LEU	4.4
1	C	718	GLU	4.4
1	B	562	VAL	4.4
1	B	651	ILE	4.4
1	D	633	LEU	4.4
1	B	722	MET	4.4
1	B	607	THR	4.4
1	D	606[A]	CYS	4.4
1	D	760	ILE	4.4
1	B	757	LEU	4.3
1	D	481	LEU	4.3
1	B	511	ALA	4.3
1	B	748	PRO	4.3
1	D	709	VAL	4.3
1	C	549	ASP	4.3
1	D	684	SER	4.3
1	B	485	LYS	4.3
1	C	488	GLY	4.3
1	D	645	PHE	4.3

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Mol	Chain	Res	Type	RSRZ
1	D	691	VAL	4.3
1	D	476	PHE	4.3
1	B	560	LEU	4.3
1	B	670	MET	4.3
1	D	580	ARG	4.2
1	D	690	GLY	4.2
1	B	539	LYS	4.2
1	B	665	LEU	4.2
1	D	682	HIS	4.2
1	D	738	ASP	4.2
1	D	537	MET	4.2
1	C	716	LEU	4.2
1	D	468	LEU	4.2
1	D	753	LEU	4.2
1	D	515	ALA	4.2
1	D	730	ASN	4.2
1	B	535	MET	4.2
1	D	736	MET	4.2
1	B	503	ILE	4.2
1	B	738	ASP	4.1
1	B	730	ASN	4.1
1	B	645	PHE	4.1
1	A	594	PRO	4.1
1	B	731	GLU	4.1
1	C	745	SER	4.1
1	D	744	PRO	4.1
1	D	733	TYR	4.1
1	D	565	GLU	4.1
1	D	648	ALA	4.1
1	D	548	ILE	4.1
1	D	741	HIS	4.1
1	D	564	VAL	4.1
1	B	690	GLY	4.1
1	D	495	VAL	4.1
1	D	752	GLN	4.0
1	C	588	TYR	4.0
1	B	642	ILE	4.0
1	B	685	ASP	4.0
1	D	493	GLY	4.0
1	B	531	LEU	4.0
1	B	715	LEU	4.0
1	B	492	PHE	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	582	PRO	4.0
1	D	666	PRO	4.0
1	B	567	ALA	4.0
1	D	710	GLU	4.0
1	D	543	LYS	4.0
1	D	535	MET	4.0
1	D	540	MET	4.0
1	B	597	GLN	3.9
1	D	746	GLN	3.9
1	B	629	ALA	3.9
1	D	707	ILE	3.9
1	D	621	LYS	3.9
1	B	521	ASP	3.9
1	B	708	PRO	3.9
1	B	467	GLU	3.9
1	D	751	LYS	3.9
1	A	522	ASP	3.9
1	B	662	ASN	3.9
1	D	631	ASN	3.9
1	B	668	LYS	3.9
1	D	572	LEU	3.9
1	A	506	ASP	3.9
1	B	516	VAL	3.9
1	B	563	ILE	3.9
1	D	628	ALA	3.9
1	D	663	GLY	3.9
1	C	593	VAL	3.9
1	C	504	ASP	3.9
1	D	764	THR	3.8
1	B	741	HIS	3.8
1	B	646	GLY	3.8
1	B	564	VAL	3.8
1	D	602	ASP	3.8
1	B	703	PRO	3.8
1	D	698	THR	3.8
1	B	695	GLU	3.8
1	D	517	LYS	3.8
1	B	617	LEU	3.8
1	D	712	LEU	3.8
1	B	674	ALA	3.8
1	B	608	TYR	3.8
1	B	710	GLU	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	616	TYR	3.8
1	B	603	LEU	3.8
1	D	576	LEU	3.8
1	B	613	GLY	3.8
1	B	689	PHE	3.8
1	B	666	PRO	3.8
1	D	480	LYS	3.8
1	B	620	GLN	3.8
1	B	711	GLU	3.8
1	D	669	TRP	3.8
1	C	540	MET	3.8
1	D	693	MET	3.8
1	B	476	PHE	3.8
1	D	672	PRO	3.8
1	D	546	ASN	3.7
1	D	529	SER	3.7
1	D	552	GLY	3.7
1	B	621	LYS	3.7
1	B	713	PHE	3.7
1	D	595	GLU	3.7
1	B	633	LEU	3.7
1	B	696	ILE	3.7
1	B	578	ALA	3.7
1	B	520	LYS	3.7
1	A	504	ASP	3.7
1	D	571	ASN	3.7
1	B	502	GLY	3.7
1	D	594	PRO	3.7
1	B	470	GLU	3.7
1	C	585	GLU	3.7
1	D	620	GLN	3.7
1	B	716	LEU	3.7
1	D	763	LEU	3.7
1	B	524	THR	3.7
1	A	728	CYS	3.7
1	B	639	VAL	3.7
1	D	615	GLU	3.7
1	D	509	LYS	3.6
1	D	477	PRO	3.6
1	B	565	GLU	3.6
1	B	660	THR	3.6
1	B	733	TYR	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	722	MET	3.6
1	C	501	VAL	3.6
1	D	721	ARG	3.6
1	B	583	GLY	3.6
1	B	697	PHE	3.6
1	D	705	PRO	3.6
1	B	632	VAL	3.6
1	B	482	THR	3.6
1	A	549	ASP	3.6
1	B	758	ASP	3.6
1	B	581	PRO	3.6
1	B	744	PRO	3.6
1	C	581	PRO	3.6
1	D	680	TYR	3.6
1	D	499	GLU	3.6
1	B	627	LEU	3.6
1	A	521	ASP	3.5
1	B	552	GLY	3.5
1	D	567	ALA	3.5
1	B	486	PRO	3.5
1	D	467	GLU	3.5
1	D	699	LEU	3.5
1	C	533[A]	SER	3.5
1	C	590	ILE	3.5
1	B	764	THR	3.5
1	A	598	MET	3.5
1	B	735	MET	3.5
1	D	469	PRO	3.5
1	D	539	LYS	3.5
1	D	703	PRO	3.5
1	B	550	LEU	3.5
1	B	572	LEU	3.5
1	B	554	CYS	3.5
1	B	762	THR	3.5
1	B	650	VAL	3.5
1	B	678	ARG	3.5
1	D	608	TYR	3.5
1	D	737	ARG	3.5
1	B	684	SER	3.5
1	B	707	ILE	3.5
1	B	598	MET	3.5
1	B	739	CYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	677	ASP	3.5
1	D	758	ASP	3.5
1	D	618	ALA	3.5
1	B	732	LEU	3.5
1	B	541	ILE	3.4
1	B	702	SER	3.4
1	A	540	MET	3.4
1	B	714	LYS	3.4
1	B	530	ASP	3.4
1	D	471	ASP	3.4
1	D	578	ALA	3.4
1	D	496	VAL	3.4
1	B	740	TRP	3.4
1	D	696	ILE	3.4
1	C	742	ALA	3.4
1	B	683	GLN	3.4
1	B	698	THR	3.4
1	D	489	GLU	3.4
1	B	611	ALA	3.4
1	B	682	HIS	3.4
1	B	759	ARG	3.4
1	C	675	LEU	3.4
1	D	603	LEU	3.4
1	D	530	ASP	3.4
1	B	532	VAL	3.4
1	C	676	PHE	3.4
1	C	505	LYS	3.3
1	B	534	GLU	3.3
1	B	628	ALA	3.3
1	C	493	GLY	3.3
1	A	507	LYS	3.3
1	B	515	ALA	3.3
1	B	473	LYS	3.3
1	C	499	GLU	3.3
1	D	624	HIS	3.3
1	B	644	ASP	3.3
1	D	512	VAL	3.3
1	D	649	ARG	3.3
1	C	702	SER	3.3
1	C	703	PRO	3.3
1	D	574	GLU	3.3
1	B	640	MET	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	570	GLY	3.3
1	B	623	ILE	3.3
1	D	644	ASP	3.3
1	B	694	TRP	3.2
1	D	598	MET	3.2
1	D	523	ALA	3.2
1	D	632	VAL	3.2
1	A	655	ASP	3.2
1	A	489	GLU	3.2
1	D	497	MET	3.2
1	C	672	PRO	3.2
1	B	700	GLY	3.2
1	B	526	LYS	3.2
1	B	595	GLU	3.2
1	B	626	ASP	3.2
1	C	756	ASP	3.2
1	B	543	LYS	3.2
1	D	641	LYS	3.2
1	A	470	GLU	3.2
1	D	761	LEU	3.2
1	B	725	PRO	3.2
1	D	486	PRO	3.2
1	B	669	TRP	3.2
1	C	645	PHE	3.2
1	D	630	ARG	3.1
1	B	734[A]	MET	3.1
1	A	755	GLU	3.1
1	C	594	PRO	3.1
1	A	493	GLY	3.1
1	D	694	TRP	3.1
1	B	664	ARG	3.1
1	B	483	LEU	3.1
1	A	656	TYR	3.1
1	B	575	TYR	3.1
1	B	576	LEU	3.1
1	B	699	LEU	3.1
1	D	626	ASP	3.1
1	B	499	GLU	3.1
1	B	558	GLY	3.1
1	B	648	ALA	3.1
1	C	481	LEU	3.1
1	B	500	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	760	ILE	3.1
1	B	514	VAL	3.1
1	B	604	VAL	3.1
1	C	743	VAL	3.0
1	B	728	CYS	3.0
1	B	624	HIS	3.0
1	C	636	GLU	3.0
1	D	482	THR	3.0
1	D	490	GLY	3.0
1	B	679	VAL	3.0
1	B	469	PRO	3.0
1	B	559	PRO	3.0
1	B	752	GLN	3.0
1	D	521	ASP	3.0
1	B	478	ARG	3.0
1	D	614	MET	3.0
1	D	524	THR	3.0
1	B	610	LEU	3.0
1	A	582	PRO	3.0
1	B	736	MET	3.0
1	C	670	MET	3.0
1	B	691	VAL	3.0
1	D	750	PHE	3.0
1	D	601	LYS	2.9
1	B	680	TYR	2.9
1	B	649	ARG	2.9
1	B	709	VAL	2.9
1	D	668	LYS	2.9
1	B	704	TYR	2.9
1	A	511	ALA	2.9
1	B	641	LYS	2.9
1	D	673	GLU	2.9
1	B	518	MET	2.9
1	B	540	MET	2.9
1	C	681	THR	2.9
1	D	479	ASP	2.9
1	D	723	ASP	2.9
1	B	496	VAL	2.9
1	D	483	LEU	2.9
1	B	475	GLU	2.8
1	B	721	ARG	2.8
1	A	488	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	756	ASP	2.8
1	A	588	TYR	2.8
1	C	618	ALA	2.8
1	B	750	PHE	2.8
1	D	731	GLU	2.8
1	C	494	GLN	2.8
1	C	651	ILE	2.8
1	C	524	THR	2.8
1	B	537	MET	2.8
1	B	630	ARG	2.8
1	D	702	SER	2.8
1	B	484	GLY	2.8
1	C	570	GLY	2.8
1	C	758	ASP	2.8
1	A	660	THR	2.8
1	C	511	ALA	2.8
1	A	499	GLU	2.8
1	A	510	GLU	2.8
1	D	573	ARG	2.8
1	B	551	LEU	2.8
1	D	720	HIS	2.8
1	B	489	GLU	2.8
1	C	470	GLU	2.8
1	B	580	ARG	2.8
1	C	466	TYR	2.8
1	C	649	ARG	2.8
1	B	548	ILE	2.7
1	B	495	VAL	2.7
1	B	615	GLU	2.7
1	B	612	ARG	2.7
1	B	477	PRO	2.7
1	D	545	LYS	2.7
1	C	623	ILE	2.7
1	A	662	ASN	2.7
1	C	598	MET	2.7
1	D	612	ARG	2.7
1	C	699	LEU	2.7
1	B	490	GLY	2.7
1	B	706	GLY	2.7
1	B	673	GLU	2.7
1	D	695	GLU	2.7
1	C	515	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	471	ASP	2.7
1	C	714	LYS	2.7
1	D	473	LYS	2.7
1	C	561	TYR	2.7
1	D	706	GLY	2.7
1	C	529	SER	2.7
1	D	534	GLU	2.7
1	A	523	ALA	2.7
1	D	500	ALA	2.7
1	B	549	ASP	2.7
1	C	521	ASP	2.7
1	C	530	ASP	2.7
1	C	525	GLU	2.6
1	B	529	SER	2.6
1	A	479	ASP	2.6
1	B	755	GLU	2.6
1	B	614	MET	2.6
1	B	693	MET	2.6
1	C	616	TYR	2.6
1	C	715	LEU	2.6
1	D	700	GLY	2.6
1	B	472	PRO	2.6
1	C	687	TRP	2.6
1	C	677	ASP	2.6
1	C	610	LEU	2.6
1	C	664	ARG	2.6
1	D	566	TYR	2.6
1	C	717	LYS	2.6
1	D	636	GLU	2.6
1	D	701	GLY	2.6
1	C	650	VAL	2.6
1	A	764	THR	2.5
1	A	557	ASP	2.5
1	D	557	ASP	2.5
1	C	741	HIS	2.5
1	C	680	TYR	2.5
1	D	609	GLN	2.5
1	D	727	ASN	2.5
1	B	497	MET	2.5
1	A	664	ARG	2.5
1	B	724	LYS	2.5
1	C	621	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	544	HIS	2.5
1	B	602	ASP	2.5
1	B	647	LEU	2.5
1	C	483	LEU	2.5
1	C	737	ARG	2.5
1	C	596	GLU	2.5
1	D	488	GLY	2.5
1	A	670[A]	MET	2.5
1	C	709	VAL	2.5
1	C	746	GLN	2.5
1	D	511	ALA	2.5
1	C	482	THR	2.5
1	B	751	LYS	2.5
1	B	761	LEU	2.5
1	C	471	ASP	2.5
1	A	467	GLU	2.5
1	B	574	GLU	2.5
1	B	718	GLU	2.5
1	C	667	VAL	2.5
1	B	726	ALA	2.5
1	C	674	ALA	2.5
1	D	724	LYS	2.4
1	C	528	LEU	2.4
1	C	711	GLU	2.4
1	A	581	PRO	2.4
1	B	556	GLN	2.4
1	A	498	ALA	2.4
1	B	579	ARG	2.4
1	D	729	THR	2.4
1	A	677	ASP	2.4
1	B	677	ASP	2.4
1	B	756	ASP	2.4
1	D	728	CYS	2.4
1	C	467	GLU	2.4
1	C	734	MET	2.4
1	B	600	PHE	2.4
1	B	573	ARG	2.4
1	A	468	LEU	2.4
1	B	587	SER	2.4
1	D	619	SER	2.4
1	C	622[A]	CYS	2.4
1	A	583	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	701	GLY	2.4
1	D	708	PRO	2.4
1	C	726	ALA	2.4
1	C	468	LEU	2.4
1	A	661	THR	2.4
1	B	546	ASN	2.4
1	A	469	PRO	2.4
1	B	719	GLY	2.4
1	D	558	GLY	2.4
1	B	746	GLN	2.4
1	C	648	ALA	2.4
1	C	732	LEU	2.3
1	C	537	MET	2.3
1	C	522	ASP	2.3
1	D	491	CYS	2.3
1	D	559	PRO	2.3
1	D	513	THR	2.3
1	C	637	ASN	2.3
1	C	465	GLU	2.3
1	C	701	GLY	2.3
1	A	491	CYS	2.3
1	B	606[A]	CYS	2.3
1	C	491	CYS	2.3
1	D	556	GLN	2.3
1	A	501	VAL	2.3
1	A	514	VAL	2.3
1	C	707	ILE	2.3
1	C	720	HIS	2.3
1	B	635	THR	2.3
1	C	749	THR	2.3
1	B	480	LYS	2.3
1	B	584	MET	2.3
1	B	637	ASN	2.3
1	B	727	ASN	2.3
1	B	619	SER	2.3
1	D	527	ASP	2.3
1	D	759	ARG	2.3
1	B	488	GLY	2.3
1	C	646	GLY	2.3
1	C	679	VAL	2.3
1	A	715	LEU	2.3
1	B	538	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	637	ASN	2.3
1	A	703	PRO	2.3
1	B	605	SER	2.3
1	D	542	GLY	2.3
1	A	726	ALA	2.2
1	C	503	ILE	2.2
1	C	489	GLU	2.2
1	C	595	GLU	2.2
1	B	631	ASN	2.2
1	C	592	ARG	2.2
1	C	469	PRO	2.2
1	B	609	GLN	2.2
1	C	683	GLN	2.2
1	D	502	GLY	2.2
1	A	732	LEU	2.2
1	C	559	PRO	2.2
1	B	487	LEU	2.2
1	C	560	LEU	2.2
1	A	717	LYS	2.2
1	A	741	HIS	2.2
1	A	553	ALA	2.2
1	A	654	ILE	2.2
1	A	720	HIS	2.2
1	C	696	ILE	2.2
1	B	596	GLU	2.2
1	C	762	THR	2.2
1	D	762	THR	2.2
1	A	573	ARG	2.2
1	A	652	ASN	2.2
1	A	725	PRO	2.2
1	C	724	LYS	2.2
1	D	538	MET	2.2
1	C	532	VAL	2.2
1	C	605	SER	2.2
1	C	684	SER	2.2
1	D	605	SER	2.2
1	C	628	ALA	2.1
1	D	711	GLU	2.1
1	A	658	LYS	2.1
1	D	520	LYS	2.1
1	C	531	LEU	2.1
1	A	711	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	727	ASN	2.1
1	C	591	ASN	2.1
1	D	522	ASP	2.1
1	C	578	ALA	2.1
1	C	694	TRP	2.1
1	D	478	ARG	2.1
1	A	659	LYS	2.1
1	B	569	LYS	2.1
1	A	472	PRO	2.1
1	C	708	PRO	2.1
1	D	640	MET	2.1
1	A	586	TYR	2.1
1	C	492	PHE	2.1
1	B	737	ARG	2.1
1	D	577	ARG	2.1
1	A	763	LEU	2.1
1	A	490	GLY	2.1
1	C	527	ASP	2.0
1	C	612	ARG	2.0
1	A	611	ALA	2.0
1	C	740	TRP	2.0
1	A	761	LEU	2.0
1	D	570	GLY	2.0
1	B	510	GLU	2.0
1	C	534	GLU	2.0
1	A	520	LYS	2.0
1	A	482	THR	2.0
1	D	518	MET	2.0
1	A	699	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands

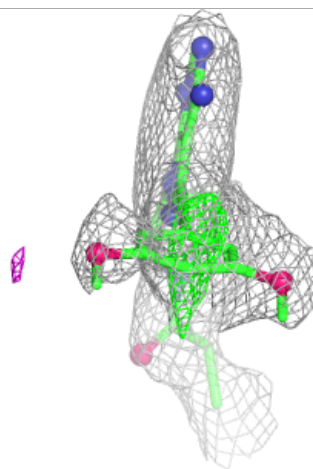
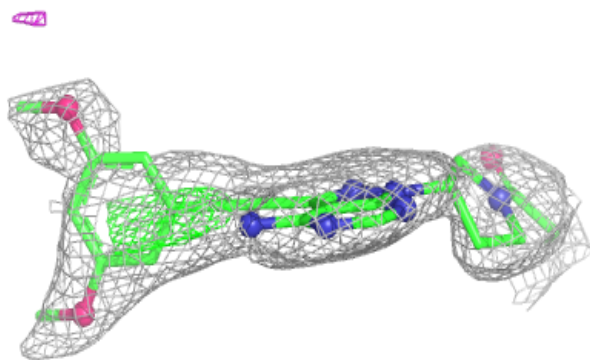
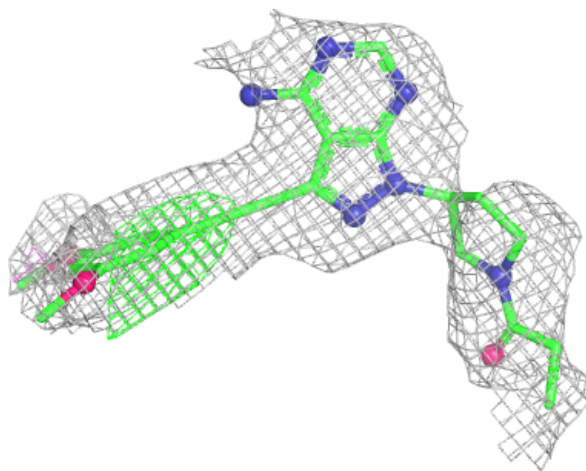
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	B	803	5/5	0.47	0.31	146,147,148,149	0
3	SO4	B	802	5/5	0.48	0.44	168,169,172,173	0
3	SO4	B	804	5/5	0.54	0.40	167,169,170,172	0
3	SO4	C	802	5/5	0.54	0.27	131,131,131,132	0
3	SO4	C	804	5/5	0.65	0.33	150,150,151,153	0
3	SO4	C	803	5/5	0.66	0.31	161,162,164,165	0
3	SO4	A	802	5/5	0.72	0.47	210,214,216,217	0
2	TZ0	D	800	31/31	0.82	0.21	66,66,68,68	0
2	TZ0	B	801	31/31	0.85	0.18	66,70,71,72	0
2	TZ0	A	801	31/31	0.90	0.13	39,43,44,45	0
2	TZ0	C	801	31/31	0.90	0.15	36,37,39,39	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.

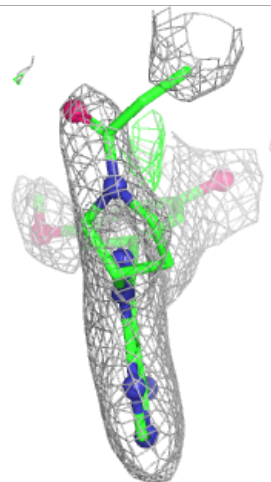
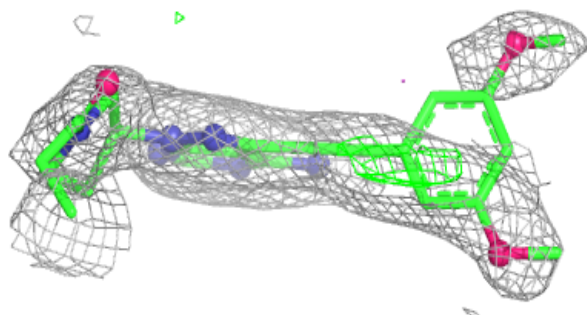
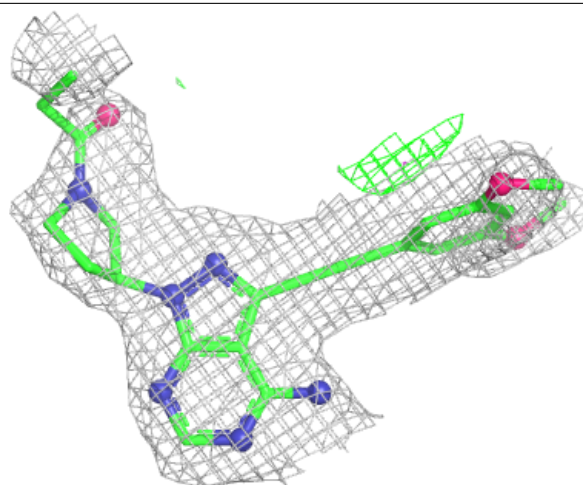
Electron density around TZ0 D 800:

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



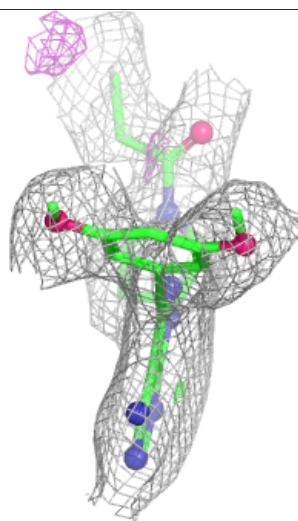
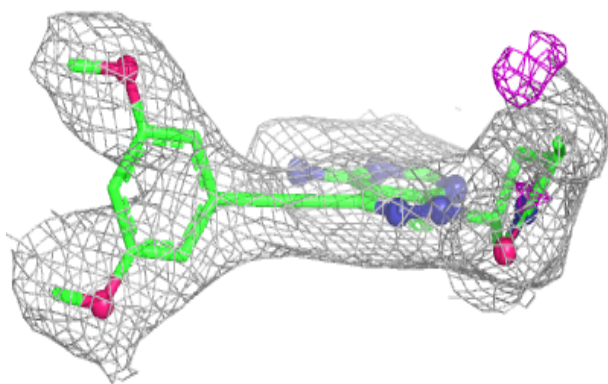
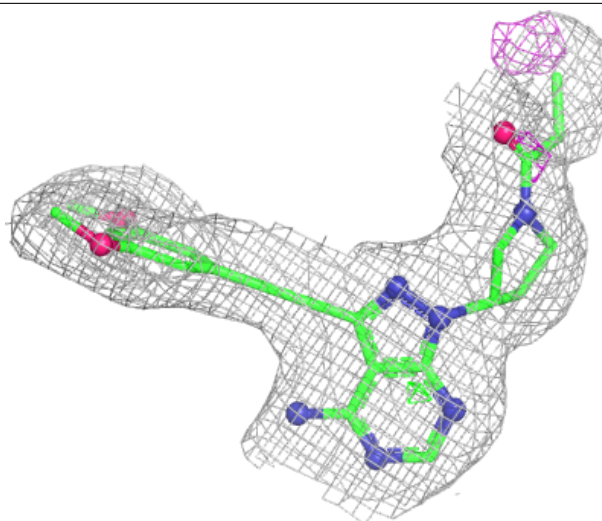
Electron density around TZ0 B 801:

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



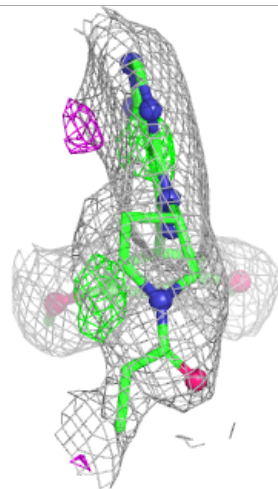
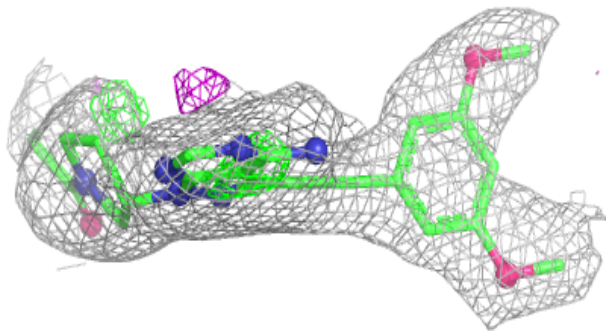
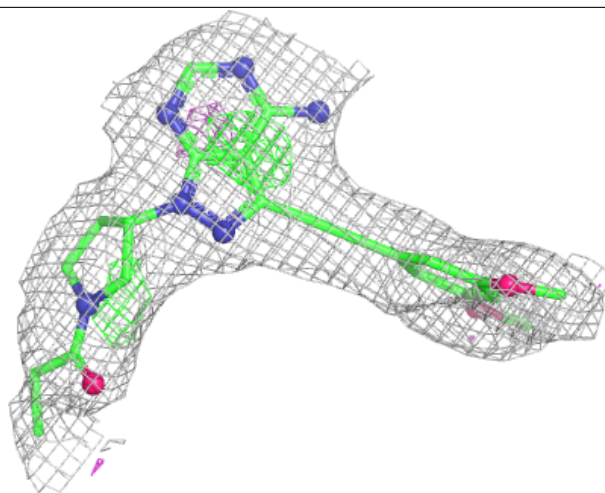
Electron density around TZ0 A 801:

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



Electron density around TZ0 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.