



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 08:33 AM UTC

PDB ID : 4J99 / pdb_00004j99
Title : Crystal Structure of FGF Receptor 2 (FGFR2) Kinase Domain Harboring the Gain-of-Function K659T Mutation.
Authors : Chen, H.; Mohammadi, M.
Deposited on : 2013-02-15
Resolution : 1.85 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

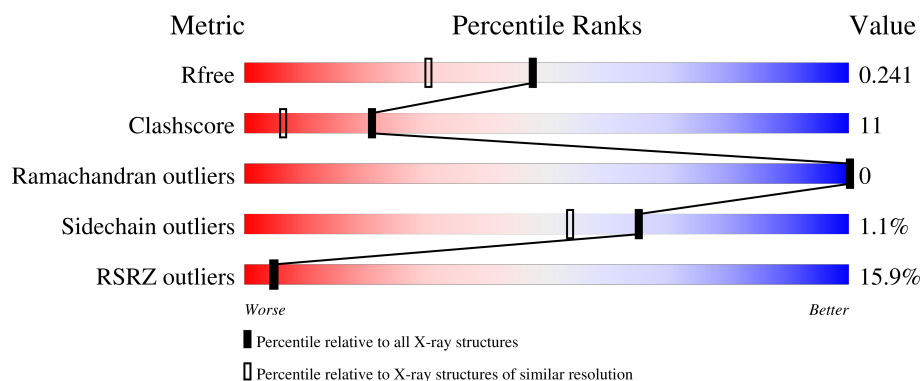
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	1296 (1.84-1.84)
Clashscore	190562	1329 (1.84-1.84)
Ramachandran outliers	187476	1318 (1.84-1.84)
Sidechain outliers	187428	1318 (1.84-1.84)
RSRZ outliers	180081	1296 (1.84-1.84)

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	8% 73% 12% • 14%
1	B	324	8% 76% 14% 10%
1	C	324	16% 79% 11% 10%
1	D	324	24% 69% 17% • 13%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9814 atoms, of which 68 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	280	Total	C	N	O	S	0	4	0
			2241	1434	374	412	21			
1	B	291	Total	C	N	O	S	0	5	0
			2320	1481	385	431	23			
1	C	291	Total	C	N	O	S	0	5	0
			2309	1473	384	429	23			
1	D	281	Total	C	N	O	S	0	2	0
			2229	1425	373	410	21			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	445	MET	-	expression tag	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	491	ALA	CYS	engineered mutation	UNP P21802
A	659	THR	LYS	engineered mutation	UNP P21802
B	445	MET	-	expression tag	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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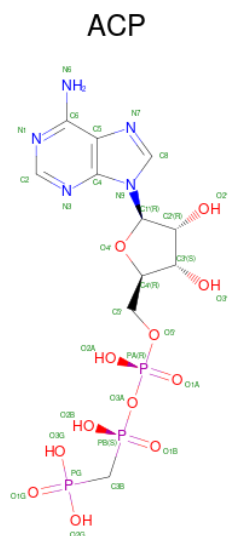
Chain	Residue	Modelled	Actual	Comment	Reference
B	451	HIS	-	expression tag	UNP P21802
B	452	HIS	-	expression tag	UNP P21802
B	453	HIS	-	expression tag	UNP P21802
B	454	HIS	-	expression tag	UNP P21802
B	455	SER	-	expression tag	UNP P21802
B	456	GLN	-	expression tag	UNP P21802
B	457	ASP	-	expression tag	UNP P21802
B	491	ALA	CYS	engineered mutation	UNP P21802
B	659	THR	LYS	engineered mutation	UNP P21802
C	445	MET	-	expression tag	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	491	ALA	CYS	engineered mutation	UNP P21802
C	659	THR	LYS	engineered mutation	UNP P21802
D	445	MET	-	expression tag	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	491	ALA	CYS	engineered mutation	UNP P21802
D	659	THR	LYS	engineered mutation	UNP P21802

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 3 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
3	A	1	Total 48	C 11	H 17	N 5	O 12	P 3	0	0
3	B	1	Total 48	C 11	H 17	N 5	O 12	P 3	0	0
3	C	1	Total 48	C 11	H 17	N 5	O 12	P 3	0	0
3	D	1	Total 48	C 11	H 17	N 5	O 12	P 3	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total Mg 1 1	0	0
4	D	2	Total Mg 2 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	116	Total O 116 116	0	0
5	B	168	Total O 168 168	0	0
5	C	117	Total O 117 117	0	0

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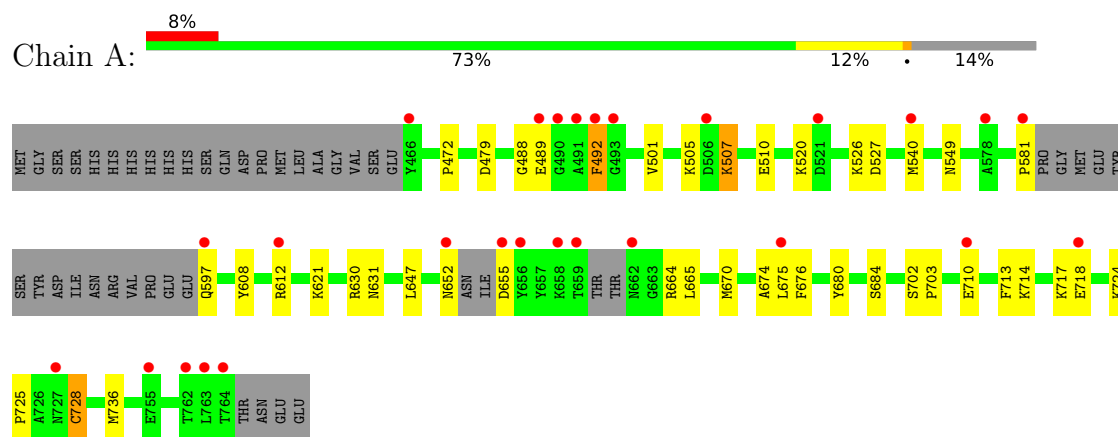
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	84	Total	O	0	0
			84	84		

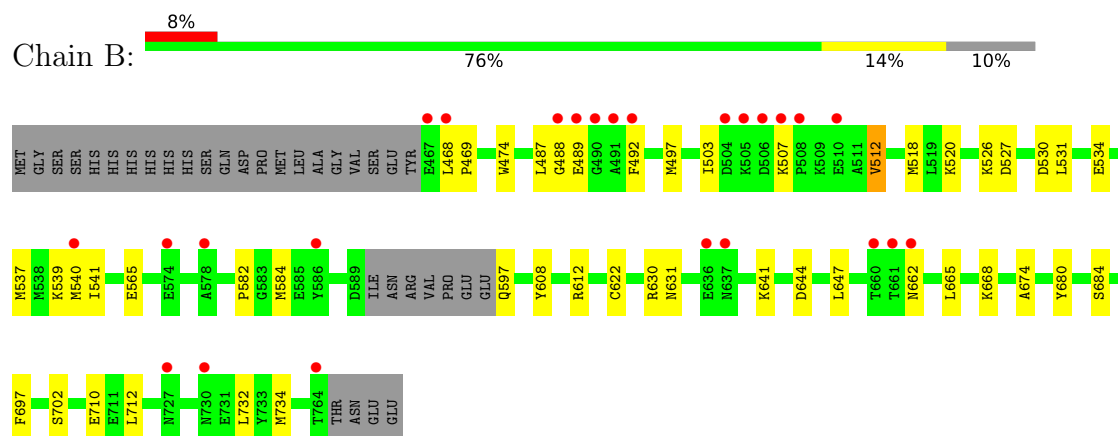
3 Residue-property plots [i](#)

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.

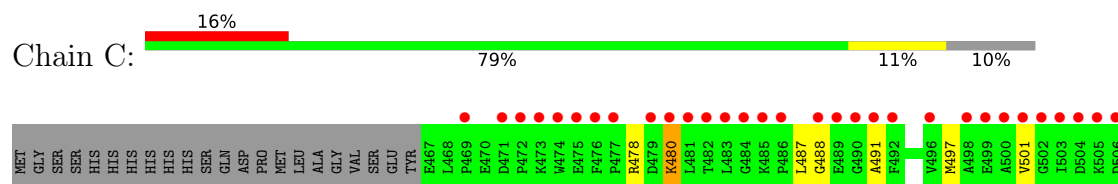
• Molecule 1: Fibroblast growth factor receptor 2

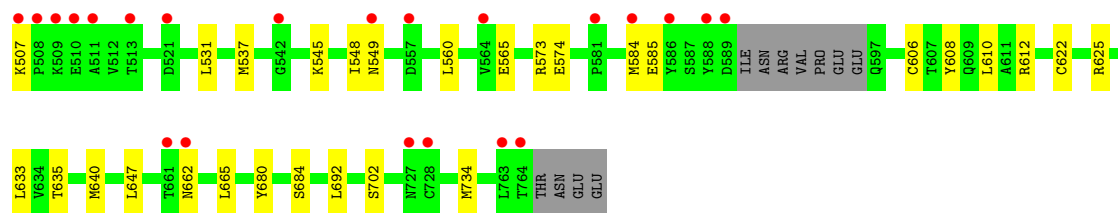


• Molecule 1: Fibroblast growth factor receptor 2

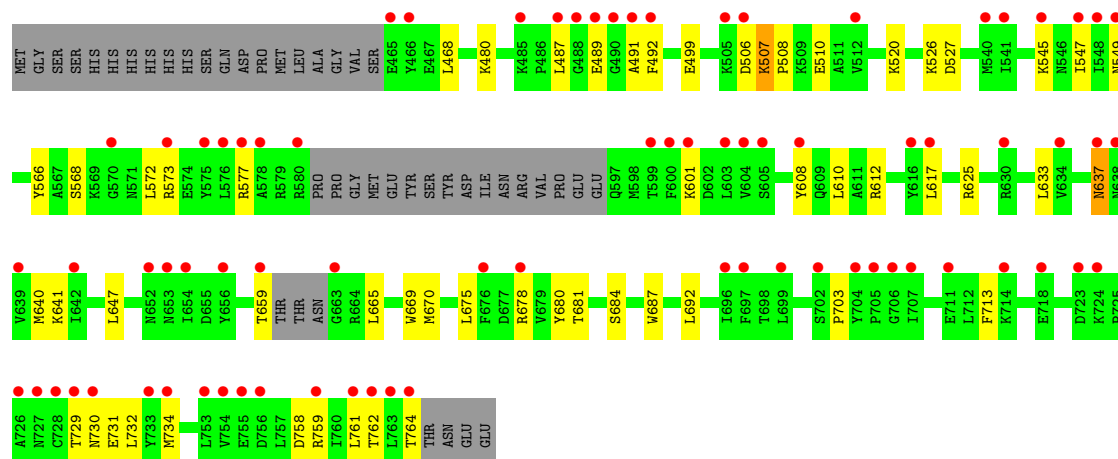


• Molecule 1: Fibroblast growth factor receptor 2





● Molecule 1: Fibroblast growth factor receptor 2



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	278.51Å 78.39Å 73.20Å 90.00° 101.02° 90.00°	Depositor
Resolution (Å)	42.31 – 1.85 42.31 – 1.85	Depositor EDS
% Data completeness (in resolution range)	96.3 (42.31-1.85) 93.1 (42.31-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.03	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.38 (at 1.84Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.206 , 0.240 0.206 , 0.241	Depositor DCC
R_{free} test set	1993 reflections (0.99%)	wwPDB-VP
Wilson B-factor (Å ²)	27.1	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 45.0	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	0.95	EDS
Total number of atoms	9814	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% 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

5.1 Standard geometry

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

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	0.58	0/2297	0.86	3/3104 (0.1%)
1	B	0.58	0/2386	0.83	2/3232 (0.1%)
1	C	0.51	0/2374	0.82	4/3216 (0.1%)
1	D	0.41	0/2281	0.80	3/3083 (0.1%)
All	All	0.52	0/9338	0.83	12/12635 (0.1%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	507	LYS	CA-C-N	8.95	128.68	119.56
1	A	507	LYS	C-N-CA	8.95	128.68	119.56
1	D	507	LYS	CA-C-N	8.85	128.59	119.56
1	D	507	LYS	C-N-CA	8.85	128.59	119.56
1	C	507	LYS	CA-C-N	7.88	127.60	119.56
1	C	507	LYS	C-N-CA	7.88	127.60	119.56
1	C	480	LYS	CG-CD-CE	-6.57	96.19	111.30
1	A	728	CYS	N-CA-C	5.82	119.40	110.20
1	D	487	LEU	N-CA-C	-5.76	106.42	113.50
1	B	507	LYS	CA-C-N	5.54	125.21	119.56
1	B	507	LYS	C-N-CA	5.54	125.21	119.56
1	C	480	LYS	CD-CE-NZ	-5.46	94.44	111.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	2241	0	2229	55	0
1	B	2320	0	2295	66	0
1	C	2309	0	2278	39	0
1	D	2229	0	2214	48	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
2	C	10	0	0	1	0
2	D	5	0	0	0	0
3	A	31	17	14	5	0
3	B	31	17	14	7	0
3	C	31	17	14	4	0
3	D	31	17	14	1	0
4	C	1	0	0	0	0
4	D	2	0	0	0	0
5	A	116	0	0	7	0
5	B	168	0	0	10	0
5	C	117	0	0	5	0
5	D	84	0	0	4	0
All	All	9746	68	9072	201	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 11.

All (201) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:480:LYS:HE2	1:C:501:VAL:CB	1.69	1.21
1:C:480:LYS:HE2	1:C:501:VAL:HB	1.16	1.13
1:A:665:LEU:HD13	1:A:680[C]:TYR:OH	1.52	1.10
1:C:480:LYS:CE	1:C:501:VAL:HB	1.82	1.10
1:B:665:LEU:HD13	1:B:680[A]:TYR:OH	1.51	1.07
1:A:492:PHE:CD1	1:A:492:PHE:O	2.09	1.05
1:C:480:LYS:HE2	1:C:501:VAL:CG1	1.88	1.01
1:B:597:GLN:NE2	5:B:1021:HOH:O	1.91	1.01
1:A:631:ASN:OD1	3:A:802:ACP:O3G	1.79	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:492:PHE:O	1:A:492:PHE:HD1	1.41	0.99
1:A:675:LEU:HD11	1:A:713:PHE:CE1	2.03	0.94
1:B:630:ARG:NE	5:B:1058:HOH:O	1.84	0.93
1:A:621:LYS:HD2	1:A:652:ASN:HD22	1.35	0.92
1:A:664:ARG:CZ	1:B:526:LYS:HD3	2.00	0.90
1:A:675:LEU:HD11	1:A:713:PHE:HE1	1.35	0.89
3:C:802:ACP:O1B	5:C:959:HOH:O	1.90	0.89
1:B:608:TYR:CZ	1:B:612:ARG:HD2	2.07	0.88
1:C:545:LYS:HD2	5:C:967:HOH:O	1.73	0.87
1:C:491:ALA:HB2	5:D:978:HOH:O	1.74	0.85
1:D:729:THR:HG23	1:D:732:LEU:H	1.41	0.84
1:A:540:MET:HG3	5:A:979:HOH:O	1.79	0.83
3:A:802:ACP:O3G	5:A:970:HOH:O	1.95	0.82
1:C:488:GLY:HA3	3:C:802:ACP:H4'	1.61	0.82
1:C:585:GLU:OE1	5:C:902:HOH:O	2.00	0.79
1:D:761:LEU:O	1:D:764:THR:HG22	1.80	0.79
1:A:492:PHE:HB2	1:A:527:ASP:OD1	1.82	0.79
1:B:488:GLY:HA3	3:B:802:ACP:H4'	1.64	0.79
1:A:505:LYS:HE3	5:A:940:HOH:O	1.83	0.79
1:D:665:LEU:HD12	1:D:670:MET:HE3	1.65	0.77
1:A:526:LYS:HD3	1:B:662:ASN:HB3	1.64	0.77
1:B:665:LEU:CD1	1:B:680[A]:TYR:OH	2.33	0.77
1:A:581:PRO:HG3	1:A:597:GLN:NE2	2.00	0.76
1:A:526:LYS:NZ	1:B:662:ASN:HD22	1.84	0.76
1:C:480:LYS:HE2	1:C:501:VAL:HG12	1.66	0.76
1:B:630:ARG:NH2	5:B:1032:HOH:O	2.16	0.75
1:D:659:THR:CG2	1:D:678:ARG:HB3	2.17	0.74
1:C:537:MET:CE	1:C:622[A]:CYS:SG	2.76	0.74
1:A:621:LYS:HD2	1:A:652:ASN:ND2	2.02	0.74
1:B:492:PHE:CE2	5:B:1016:HOH:O	2.41	0.73
1:B:468:LEU:HD12	1:B:469:PRO:HD2	1.71	0.73
1:A:549:ASN:OD1	5:A:990:HOH:O	2.06	0.73
1:C:480:LYS:CE	1:C:501:VAL:CB	2.52	0.72
1:A:665:LEU:HD13	1:A:680[C]:TYR:CZ	2.23	0.72
1:D:489:GLU:HG3	1:D:520:LYS:HD3	1.69	0.72
1:C:635:THR:OG1	2:C:804:SO4:O2	2.02	0.71
1:D:608:TYR:CZ	1:D:612:ARG:HD2	2.25	0.71
1:A:676:PHE:CE1	1:A:717:LYS:HE3	2.25	0.70
1:B:582:PRO:O	5:B:1020:HOH:O	2.09	0.70
1:B:503:ILE:HG22	1:B:512:VAL:CG1	2.21	0.70
1:B:665:LEU:HD13	1:B:680[A]:TYR:CZ	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:537:MET:HE2	1:C:622[A]:CYS:SG	2.32	0.70
1:A:526:LYS:HZ2	1:B:662:ASN:HD22	1.41	0.69
1:C:487:LEU:HD21	1:C:497:MET:HE2	1.76	0.67
1:C:662:ASN:O	5:C:1012:HOH:O	2.11	0.67
1:A:724:LYS:HE2	1:A:728:CYS:O	1.94	0.67
1:D:637:ASN:OD1	1:D:637:ASN:N	2.25	0.66
1:D:659:THR:HG23	1:D:678:ARG:HB3	1.77	0.66
1:B:630:ARG:NH1	5:B:1058:HOH:O	2.29	0.65
1:B:565:GLU:OE2	1:B:641:LYS:HE3	1.95	0.65
3:B:802:ACP:H3B1	3:B:802:ACP:O1A	1.96	0.65
3:A:802:ACP:O2'	5:A:972:HOH:O	2.15	0.64
1:A:492:PHE:CD1	1:A:492:PHE:C	2.74	0.64
1:B:608:TYR:OH	1:B:612:ARG:HD2	1.98	0.64
1:B:630:ARG:CZ	5:B:1058:HOH:O	2.35	0.63
1:A:608:TYR:CZ	1:A:612:ARG:HD2	2.33	0.63
1:D:731:GLU:OE2	1:D:759:ARG:NH1	2.32	0.62
1:B:537:MET:HE1	1:B:622[B]:CYS:SG	2.40	0.62
1:A:664:ARG:NH2	1:B:526:LYS:HD3	2.13	0.62
1:A:540:MET:HE3	5:A:946:HOH:O	1.99	0.62
1:B:518:MET:HB2	5:B:1023:HOH:O	1.99	0.62
1:C:549:ASN:HD22	1:C:565:GLU:CD	2.09	0.61
1:A:664:ARG:CZ	1:B:526:LYS:CD	2.76	0.61
1:B:584:MET:SD	1:C:584:MET:HE1	2.42	0.60
1:B:612:ARG:HD3	5:B:937:HOH:O	2.02	0.59
1:D:729:THR:HG22	1:D:732:LEU:HD12	1.84	0.59
1:C:625:ARG:HD3	1:C:647:LEU:O	2.02	0.59
1:B:680[B]:TYR:CE1	1:B:684:SER:HB2	2.38	0.59
1:B:492:PHE:CD1	1:B:492:PHE:O	2.56	0.59
1:A:489:GLU:HG3	1:A:520:LYS:HD3	1.85	0.58
1:A:655:ASP:N	1:A:655:ASP:OD1	2.35	0.58
1:B:647:LEU:HD13	1:B:665:LEU:HD23	1.85	0.58
1:A:680[A]:TYR:CE1	1:A:684:SER:HB2	2.37	0.58
1:A:664:ARG:NH1	1:B:526:LYS:CE	2.67	0.57
3:C:802:ACP:H3B2	3:C:802:ACP:O2A	2.04	0.57
1:B:631:ASN:OD1	3:B:802:ACP:PG	2.63	0.57
1:C:608:TYR:OH	1:C:612:ARG:HD2	2.04	0.57
1:A:665:LEU:CD1	1:A:680[C]:TYR:CE2	2.87	0.57
1:A:675:LEU:HD11	1:A:713:PHE:CD1	2.40	0.57
1:A:488:GLY:HA3	3:A:802:ACP:H4'	1.87	0.56
1:B:503:ILE:HG22	1:B:512:VAL:HG13	1.88	0.56
1:C:537:MET:HE1	1:C:622[A]:CYS:SG	2.44	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:491:ALA:N	3:D:802:ACP:O2G	2.38	0.56
1:C:480:LYS:HG3	1:C:480:LYS:O	2.04	0.56
1:D:659:THR:CG2	1:D:678:ARG:CB	2.84	0.56
1:D:669:TRP:CZ2	1:D:703:PRO:HG2	2.41	0.56
1:B:644:ASP:OD2	3:B:802:ACP:O2G	2.24	0.55
1:D:573:ARG:NH2	1:D:577:ARG:NH2	2.55	0.55
1:A:526:LYS:NZ	1:B:662:ASN:ND2	2.52	0.54
1:B:487:LEU:HD21	1:B:497:MET:HG3	1.90	0.54
1:B:734:MET:HA	1:B:734:MET:HE2	1.90	0.54
1:C:734:MET:HE2	1:C:734:MET:HA	1.91	0.53
1:D:491:ALA:HB3	1:D:492:PHE:CE2	2.42	0.53
1:A:664:ARG:NH1	1:B:526:LYS:HE3	2.23	0.53
1:C:573:ARG:NH1	1:C:574:GLU:OE2	2.42	0.53
1:D:758:ASP:O	1:D:762:THR:HG23	2.09	0.53
1:D:659:THR:HG22	1:D:678:ARG:C	2.33	0.53
1:A:676:PHE:CZ	1:A:717:LYS:HG3	2.43	0.53
1:D:573:ARG:NH2	1:D:577:ARG:HH22	2.06	0.53
1:D:601:LYS:HG3	1:D:764:THR:HG23	1.90	0.53
1:D:734:MET:HA	1:D:734:MET:HE2	1.91	0.53
1:B:537:MET:HA	1:B:540:MET:HE3	1.90	0.53
1:D:659:THR:HG22	1:D:678:ARG:CA	2.40	0.52
1:C:665:LEU:HD22	1:C:680[B]:TYR:OH	2.09	0.52
1:C:480:LYS:CD	1:C:501:VAL:HB	2.38	0.52
1:B:474:TRP:CD1	1:B:539:LYS:HE2	2.45	0.52
1:C:610:LEU:HD13	1:C:692:LEU:HD21	1.92	0.51
3:A:802:ACP:O2B	3:A:802:ACP:O1G	2.29	0.51
1:D:608:TYR:OH	1:D:612:ARG:HD2	2.10	0.51
1:A:714:LYS:NZ	1:A:718:GLU:OE2	2.31	0.51
1:D:659:THR:HG22	1:D:678:ARG:HB3	1.91	0.51
1:D:675:LEU:HD11	1:D:713:PHE:CE1	2.46	0.51
1:C:680[A]:TYR:CE1	1:C:684:SER:HB2	2.46	0.51
1:D:680:TYR:CE1	1:D:684:SER:HB2	2.45	0.50
1:A:674:ALA:HB1	1:A:680[C]:TYR:CE2	2.46	0.50
1:D:675:LEU:HD11	1:D:713:PHE:HE1	1.76	0.50
1:A:526:LYS:HZ2	1:B:662:ASN:ND2	2.07	0.50
1:D:547:ILE:O	1:D:549:ASN:ND2	2.45	0.50
1:D:491:ALA:HB3	1:D:492:PHE:CD2	2.47	0.49
1:D:492:PHE:HB3	1:D:527:ASP:OD1	2.12	0.49
1:D:566:TYR:CZ	1:D:568:SER:HA	2.46	0.49
1:C:625:ARG:HA	1:C:680[A]:TYR:OH	2.13	0.49
1:B:665:LEU:CD1	1:B:680[A]:TYR:CZ	2.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:674:ALA:HB1	1:B:680[A]:TYR:CE2	2.47	0.49
1:A:665:LEU:CD1	1:A:680[C]:TYR:CZ	2.96	0.48
1:B:492:PHE:O	1:B:492:PHE:HD1	1.95	0.48
1:B:489:GLU:OE2	1:B:520:LYS:NZ	2.36	0.48
1:B:537:MET:HE3	1:B:541:ILE:HG13	1.96	0.48
1:B:503:ILE:HG22	1:B:512:VAL:HG11	1.96	0.48
1:B:584:MET:HE1	1:C:584:MET:SD	2.54	0.48
1:B:487:LEU:HD21	1:B:497:MET:CG	2.44	0.47
1:D:610:LEU:HD13	1:D:692:LEU:HD21	1.96	0.47
1:A:472:PRO:HD2	5:A:916:HOH:O	2.14	0.47
1:D:681:THR:HB	5:D:926:HOH:O	2.14	0.47
1:C:480:LYS:CE	1:C:501:VAL:HG12	2.40	0.47
1:B:644:ASP:OD2	3:B:802:ACP:PG	2.73	0.47
1:A:507:LYS:HD2	1:A:510:GLU:OE2	2.15	0.46
1:B:489:GLU:HG3	1:B:520:LYS:HE3	1.98	0.46
1:B:631:ASN:OD1	3:B:802:ACP:O2G	2.34	0.46
1:C:480:LYS:HZ3	1:C:480:LYS:HG2	1.26	0.46
1:B:489:GLU:CG	1:B:520:LYS:NZ	2.79	0.46
1:B:492:PHE:HB2	1:B:527:ASP:OD1	2.15	0.46
1:B:665:LEU:CD1	1:B:680[A]:TYR:CE2	2.99	0.45
1:A:647:LEU:HD13	1:A:665:LEU:HD23	1.98	0.45
3:C:802:ACP:O2A	3:C:802:ACP:C3B	2.64	0.45
1:D:507:LYS:HD2	1:D:510:GLU:OE1	2.17	0.45
1:A:676:PHE:CZ	1:A:717:LYS:HE3	2.52	0.45
1:A:675:LEU:HD21	1:A:713:PHE:HD1	1.81	0.45
1:D:506:ASP:C	1:D:508:PRO:HD3	2.42	0.45
1:C:625:ARG:HA	1:C:680[A]:TYR:CZ	2.52	0.45
1:D:659:THR:HG22	1:D:678:ARG:O	2.17	0.45
1:A:675:LEU:HD23	1:A:676:PHE:CZ	2.52	0.45
1:B:489:GLU:HG2	1:B:520:LYS:HZ2	1.82	0.45
1:D:572:LEU:HD13	1:D:640:MET:SD	2.57	0.45
1:A:675:LEU:HD21	1:A:713:PHE:CD1	2.52	0.45
1:B:608:TYR:CE2	1:B:612:ARG:HD2	2.49	0.44
1:A:608:TYR:OH	1:A:612:ARG:HD2	2.18	0.44
1:D:480:LYS:NZ	5:D:951:HOH:O	2.49	0.44
1:D:625:ARG:HD3	1:D:647:LEU:O	2.18	0.44
1:B:489:GLU:CD	1:B:520:LYS:HZ1	2.21	0.44
1:A:501:VAL:HG21	1:D:499:GLU:OE2	2.18	0.43
1:D:507:LYS:N	1:D:508:PRO:HD3	2.33	0.43
1:A:581:PRO:CG	1:A:597:GLN:NE2	2.76	0.43
1:D:489:GLU:CG	1:D:520:LYS:HD3	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:491:ALA:HA	5:D:978:HOH:O	2.18	0.43
1:B:492:PHE:HE1	1:B:531:LEU:HB2	1.83	0.43
1:B:503:ILE:CG2	1:B:512:VAL:CG1	2.95	0.43
1:B:668:LYS:HG2	1:B:712:LEU:HD22	2.01	0.43
1:A:665:LEU:HD12	1:A:670:MET:HE3	2.01	0.42
1:B:526:LYS:NZ	1:B:530:ASP:OD2	2.52	0.42
1:C:491:ALA:N	5:C:959:HOH:O	1.99	0.42
1:C:480:LYS:HZ2	1:C:501:VAL:N	2.07	0.42
1:D:545:LYS:O	1:D:641:LYS:HE2	2.20	0.42
1:A:725:PRO:HG2	1:A:736:MET:HE1	2.01	0.42
1:C:548:ILE:HG13	1:C:633:LEU:HD12	2.01	0.42
1:B:492:PHE:HZ	1:B:534:GLU:OE1	2.02	0.42
1:B:680[B]:TYR:CD1	1:B:684:SER:HB2	2.55	0.42
1:C:531:LEU:HD23	1:C:560:LEU:HD23	2.02	0.42
1:C:606[B]:CYS:SG	1:C:640:MET:HE3	2.60	0.42
1:B:697:PHE:CZ	1:B:732:LEU:HD13	2.55	0.41
1:D:687:TRP:CD1	1:D:687:TRP:C	2.99	0.41
1:A:676:PHE:CE2	1:A:717:LYS:HG2	2.56	0.41
1:A:702[A]:SER:HA	1:A:703:PRO:HD3	1.91	0.41
1:B:487:LEU:CD2	1:B:497:MET:HG3	2.50	0.41
1:C:662:ASN:CB	1:D:526:LYS:HD3	2.51	0.41
1:A:710:GLU:CD	5:B:967:HOH:O	2.64	0.41
1:A:665:LEU:CD1	1:A:680[C]:TYR:OH	2.44	0.40
1:B:631:ASN:OD1	3:B:802:ACP:O1G	2.39	0.40
1:C:478:ARG:C	1:C:480:LYS:H	2.28	0.40
1:D:659:THR:CG2	1:D:678:ARG:CA	2.99	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	276/324 (85%)	274 (99%)	2 (1%)	0	100	100
1	B	292/324 (90%)	289 (99%)	3 (1%)	0	100	100
1	C	292/324 (90%)	287 (98%)	5 (2%)	0	100	100
1	D	277/324 (86%)	273 (99%)	4 (1%)	0	100	100
All	All	1137/1296 (88%)	1123 (99%)	14 (1%)	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	242/284 (85%)	239 (99%)	3 (1%)	63	51
1	B	252/284 (89%)	248 (98%)	4 (2%)	55	39
1	C	249/284 (88%)	248 (100%)	1 (0%)	84	78
1	D	239/284 (84%)	235 (98%)	4 (2%)	53	37
All	All	982/1136 (86%)	970 (99%)	12 (1%)	65	51

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	479	ASP
1	A	492	PHE
1	A	630	ARG
1	B	512	VAL
1	B	702[A]	SER
1	B	702[B]	SER
1	B	710	GLU
1	C	702	SER
1	D	468	LEU
1	D	633	LEU
1	D	637	ASN
1	D	730	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	549	ASN
1	A	652	ASN
1	A	730	ASN
1	B	556	GLN
1	B	620	GLN
1	B	662	ASN
1	B	746	GLN
1	D	546	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 3 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	$\# Z > 2$
3	ACP	B	802	-	31,33,33	1.77	7 (22%)	47,52,52	1.99	9 (19%)
2	SO4	B	801	-	4,4,4	0.24	0	6,6,6	0.30	0
2	SO4	D	801	-	4,4,4	0.22	0	6,6,6	0.15	0
2	SO4	A	803	-	4,4,4	0.28	0	6,6,6	0.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ACP	D	802	4	31,33,33	1.75	7 (22%)	47,52,52	1.79	9 (19%)
2	SO4	A	801	-	4,4,4	0.22	0	6,6,6	0.17	0
3	ACP	A	802	-	31,33,33	1.85	11 (35%)	47,52,52	1.92	12 (25%)
2	SO4	C	804	-	4,4,4	0.25	0	6,6,6	0.11	0
3	ACP	C	802	4	31,33,33	1.75	7 (22%)	47,52,52	1.91	11 (23%)
2	SO4	B	803	-	4,4,4	0.41	0	6,6,6	0.25	0
2	SO4	C	801	-	4,4,4	0.25	0	6,6,6	0.27	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ACP	C	802	4	-	2/19/38/38	0/3/3/3
3	ACP	A	802	-	-	6/19/38/38	0/3/3/3
3	ACP	B	802	-	-	6/19/38/38	0/3/3/3
3	ACP	D	802	4	-	3/19/38/38	0/3/3/3

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	802	ACP	C6-N6	4.50	1.45	1.34
3	B	802	ACP	C6-N6	4.43	1.45	1.34
3	A	802	ACP	C6-N6	4.31	1.45	1.34
3	C	802	ACP	C6-N6	4.30	1.45	1.34
3	D	802	ACP	C2'-C3'	-4.23	1.41	1.53
3	C	802	ACP	C2'-C3'	-4.11	1.42	1.53
3	B	802	ACP	C2'-C3'	-3.67	1.43	1.53
3	A	802	ACP	C2'-C3'	-3.62	1.43	1.53
3	B	802	ACP	O4'-C1'	3.52	1.50	1.42
3	B	802	ACP	C5-N7	-3.32	1.33	1.39
3	C	802	ACP	C5-N7	-3.28	1.33	1.39
3	D	802	ACP	C5-N7	-3.13	1.33	1.39
3	D	802	ACP	O4'-C1'	3.12	1.49	1.42
3	C	802	ACP	O4'-C1'	3.08	1.49	1.42
3	A	802	ACP	C5-N7	-2.98	1.33	1.39
3	A	802	ACP	PB-O3A	2.96	1.61	1.58
3	A	802	ACP	O4'-C1'	2.87	1.48	1.42
3	A	802	ACP	C3'-C4'	-2.85	1.45	1.53
3	D	802	ACP	C2'-C1'	-2.70	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	802	ACP	C3'-C4'	-2.69	1.46	1.53
3	D	802	ACP	C3'-C4'	-2.66	1.46	1.53
3	B	802	ACP	C3'-C4'	-2.55	1.46	1.53
3	A	802	ACP	C2'-C1'	-2.40	1.45	1.53
3	C	802	ACP	C2'-C1'	-2.40	1.45	1.53
3	C	802	ACP	C1'-N9	-2.30	1.40	1.46
3	B	802	ACP	C2'-C1'	-2.27	1.46	1.53
3	B	802	ACP	C8-N9	-2.25	1.33	1.37
3	A	802	ACP	PA-O3A	2.18	1.61	1.59
3	D	802	ACP	C1'-N9	-2.14	1.40	1.46
3	A	802	ACP	C8-N9	-2.11	1.34	1.37
3	A	802	ACP	PG-O2G	2.08	1.59	1.55
3	A	802	ACP	C2-N3	2.03	1.37	1.33

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802	ACP	C5-C4-N3	-6.16	118.24	126.72
3	B	802	ACP	C5-C4-N3	-5.99	118.47	126.72
3	C	802	ACP	C5-C4-N3	-5.59	119.02	126.72
3	B	802	ACP	N3-C2-N1	-5.41	120.39	128.58
3	A	802	ACP	N3-C4-N9	5.21	136.03	127.17
3	D	802	ACP	C5-C4-N3	-5.19	119.57	126.72
3	D	802	ACP	N3-C2-N1	-5.12	120.83	128.58
3	C	802	ACP	N3-C2-N1	-5.09	120.88	128.58
3	B	802	ACP	N3-C4-N9	4.59	134.97	127.17
3	C	802	ACP	N3-C4-N9	4.54	134.88	127.17
3	A	802	ACP	N3-C2-N1	-4.32	122.04	128.58
3	D	802	ACP	N3-C4-N9	3.89	133.78	127.17
3	B	802	ACP	C2-N3-C4	3.85	121.23	111.83
3	B	802	ACP	C5-N7-C8	3.69	109.25	103.45
3	D	802	ACP	C5-N7-C8	3.65	109.19	103.45
3	C	802	ACP	C2-N3-C4	3.54	120.47	111.83
3	D	802	ACP	C2-N3-C4	3.40	120.13	111.83
3	C	802	ACP	C5-N7-C8	3.40	108.79	103.45
3	A	802	ACP	C2-N3-C4	3.32	119.94	111.83
3	B	802	ACP	O1G-PG-C3B	-3.28	104.22	111.37
3	B	802	ACP	C4-C5-N7	-3.21	106.91	110.58
3	C	802	ACP	PB-O3A-PA	-3.14	122.11	132.37
3	D	802	ACP	C4-C5-N7	-3.06	107.08	110.58
3	B	802	ACP	O3G-PG-C3B	2.99	113.66	106.40
3	D	802	ACP	C4'-O4'-C1'	-2.96	102.94	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802	ACP	C5-N7-C8	2.92	108.04	103.45
3	C	802	ACP	C4'-O4'-C1'	-2.71	103.49	109.47
3	C	802	ACP	N9-C8-N7	-2.60	110.25	113.94
3	A	802	ACP	O3G-PG-C3B	-2.58	100.14	106.40
3	D	802	ACP	N9-C8-N7	-2.58	110.27	113.94
3	A	802	ACP	C5-C6-N6	-2.52	117.06	123.29
3	C	802	ACP	C4-C5-N7	-2.44	107.79	110.58
3	B	802	ACP	N9-C8-N7	-2.41	110.51	113.94
3	A	802	ACP	C2'-C3'-C4'	2.37	107.19	102.61
3	D	802	ACP	PB-O3A-PA	-2.29	124.89	132.37
3	A	802	ACP	C4-C5-N7	-2.28	107.97	110.58
3	A	802	ACP	C6-C5-C4	2.18	120.16	117.18
3	A	802	ACP	O2G-PG-C3B	2.13	111.58	106.40
3	C	802	ACP	C5-C6-N6	-2.03	118.25	123.29
3	C	802	ACP	O2A-PA-O3A	2.02	112.73	107.27
3	A	802	ACP	N9-C8-N7	-2.01	111.08	113.94

There are no chirality outliers.

All (17) torsion outliers are listed below:

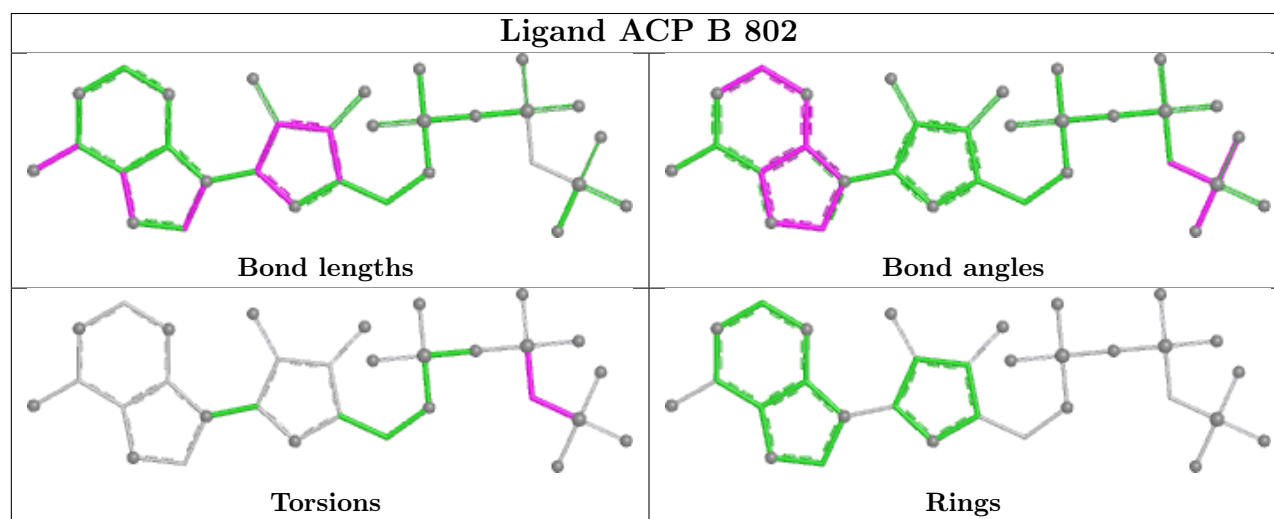
Mol	Chain	Res	Type	Atoms
3	A	802	ACP	PB-C3B-PG-O1G
3	A	802	ACP	PB-C3B-PG-O2G
3	A	802	ACP	PB-C3B-PG-O3G
3	A	802	ACP	PG-C3B-PB-O1B
3	A	802	ACP	PG-C3B-PB-O2B
3	A	802	ACP	PG-C3B-PB-O3A
3	B	802	ACP	PB-C3B-PG-O1G
3	B	802	ACP	PB-C3B-PG-O2G
3	B	802	ACP	PB-C3B-PG-O3G
3	B	802	ACP	PG-C3B-PB-O1B
3	B	802	ACP	PG-C3B-PB-O2B
3	B	802	ACP	PG-C3B-PB-O3A
3	C	802	ACP	C5'-O5'-PA-O3A
3	D	802	ACP	C5'-O5'-PA-O1A
3	D	802	ACP	C5'-O5'-PA-O2A
3	D	802	ACP	C5'-O5'-PA-O3A
3	C	802	ACP	O4'-C4'-C5'-O5'

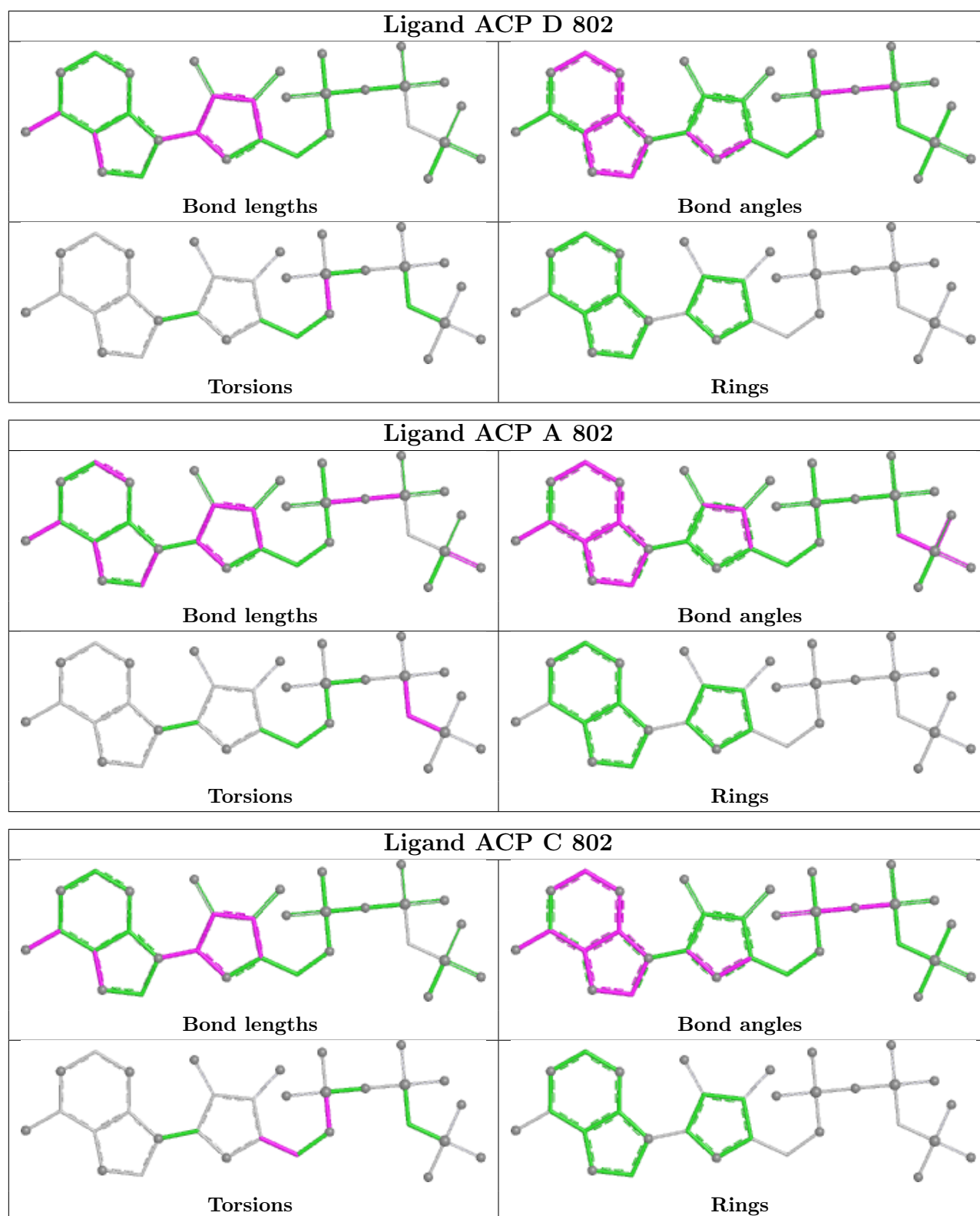
There are no ring outliers.

5 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	802	ACP	7	0
3	D	802	ACP	1	0
3	A	802	ACP	5	0
2	C	804	SO4	1	0
3	C	802	ACP	4	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.





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	280/324 (86%)	0.55	27 (9%)	13 14	12, 30, 60, 88	4 (1%)
1	B	291/324 (89%)	0.43	25 (8%)	16 17	11, 28, 54, 83	5 (1%)
1	C	291/324 (89%)	0.95	53 (18%)	3 3	14, 38, 76, 91	5 (1%)
1	D	281/324 (86%)	1.41	77 (27%)	1 1	21, 46, 71, 90	2 (0%)
All	All	1143/1296 (88%)	0.83	182 (15%)	5 5	11, 35, 68, 91	16 (1%)

All (182) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	492	PHE	7.7
1	A	491	ALA	7.4
1	D	764	THR	6.2
1	B	506	ASP	6.1
1	C	491	ALA	6.0
1	C	511	ALA	5.9
1	B	491	ALA	5.8
1	D	488	GLY	5.6
1	B	492	PHE	5.6
1	D	727	ASN	5.5
1	C	506	ASP	5.5
1	B	488	GLY	5.3
1	A	466	TYR	5.1
1	D	578	ALA	5.1
1	B	467	GLU	5.1
1	C	479	ASP	5.0
1	D	506	ASP	5.0
1	C	480	LYS	4.9
1	C	488	GLY	4.5
1	D	763	LEU	4.4
1	A	656	TYR	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	659	THR	4.2
1	C	662	ASN	4.1
1	D	575	TYR	4.0
1	C	501	VAL	4.0
1	A	581	PRO	4.0
1	A	662	ASN	4.0
1	D	639	VAL	4.0
1	C	508	PRO	3.9
1	C	489	GLU	3.9
1	C	473	LYS	3.9
1	C	492	PHE	3.9
1	A	727	ASN	3.8
1	D	549	ASN	3.7
1	D	699	LEU	3.7
1	C	483	LEU	3.7
1	D	637	ASN	3.6
1	D	540	MET	3.6
1	C	509	LYS	3.6
1	C	498	ALA	3.5
1	D	600	PHE	3.5
1	C	507	LYS	3.5
1	D	762	THR	3.5
1	B	507	LYS	3.5
1	C	661	THR	3.4
1	C	763	LEU	3.4
1	D	729	THR	3.4
1	C	481	LEU	3.4
1	D	466	TYR	3.3
1	D	547	ILE	3.3
1	D	634	VAL	3.3
1	C	510	GLU	3.3
1	D	465	GLU	3.3
1	B	578	ALA	3.3
1	A	597	GLN	3.3
1	D	490	GLY	3.3
1	D	659	THR	3.2
1	B	727	ASN	3.2
1	C	505	LYS	3.2
1	C	764	THR	3.2
1	D	492	PHE	3.2
1	D	726	ALA	3.2
1	C	482	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	601	LYS	3.2
1	C	502	GLY	3.2
1	A	763	LEU	3.1
1	D	663	GLY	3.1
1	D	505	LYS	3.1
1	D	638	ASN	3.1
1	D	723	ASP	3.1
1	C	727	ASN	3.1
1	D	724	LYS	3.0
1	D	754	VAL	3.0
1	D	654	ILE	3.0
1	D	761	LEU	2.9
1	C	588	TYR	2.9
1	B	574	GLU	2.9
1	C	485	LYS	2.9
1	D	733	TYR	2.9
1	A	540	MET	2.9
1	D	541	ILE	2.9
1	D	696	ILE	2.9
1	A	655	ASP	2.9
1	B	636	GLU	2.9
1	A	764	THR	2.8
1	C	500	ALA	2.8
1	C	586	TYR	2.8
1	D	605	SER	2.8
1	D	617	LEU	2.8
1	C	513	THR	2.8
1	C	476	PHE	2.8
1	D	706	GLY	2.8
1	D	577	ARG	2.7
1	D	580	ARG	2.7
1	D	728	CYS	2.7
1	C	542	GLY	2.7
1	B	661	THR	2.7
1	C	477	PRO	2.7
1	D	702	SER	2.7
1	B	637	ASN	2.7
1	C	557	ASP	2.7
1	A	710	GLU	2.7
1	A	658	LYS	2.6
1	B	662	ASN	2.6
1	B	489	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	581	PRO	2.6
1	D	718	GLU	2.6
1	C	499	GLU	2.5
1	B	504	ASP	2.5
1	D	604	VAL	2.5
1	C	472	PRO	2.5
1	B	586	TYR	2.5
1	D	603	LEU	2.5
1	D	570	GLY	2.5
1	D	599	THR	2.5
1	D	705	PRO	2.5
1	C	475	GLU	2.5
1	B	505	LYS	2.5
1	C	728	CYS	2.4
1	A	490	GLY	2.4
1	A	493	GLY	2.4
1	D	678	ARG	2.4
1	B	764	THR	2.4
1	C	496	VAL	2.4
1	C	564	VAL	2.4
1	C	484	GLY	2.4
1	D	704	TYR	2.4
1	A	506	ASP	2.4
1	D	573	ARG	2.4
1	B	508	PRO	2.4
1	B	660	THR	2.4
1	D	714	LYS	2.4
1	C	504	ASP	2.3
1	C	589	ASP	2.3
1	D	707	ILE	2.3
1	D	653	ASN	2.3
1	B	468	LEU	2.3
1	A	675	LEU	2.3
1	A	762	THR	2.3
1	D	676	PHE	2.3
1	C	503	ILE	2.3
1	D	616	TYR	2.2
1	B	510	GLU	2.2
1	D	576	LEU	2.2
1	B	490	GLY	2.2
1	D	608	TYR	2.2
1	D	485	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	753	LEU	2.2
1	C	521	ASP	2.2
1	D	656	TYR	2.2
1	D	642	ILE	2.2
1	D	630	ARG	2.2
1	D	759	ARG	2.2
1	A	755	GLU	2.2
1	D	491	ALA	2.2
1	A	612	ARG	2.2
1	D	652	ASN	2.1
1	D	548	ILE	2.1
1	D	756	ASP	2.1
1	B	540	MET	2.1
1	C	584	MET	2.1
1	D	489	GLU	2.1
1	D	734	MET	2.1
1	A	578	ALA	2.1
1	A	521	ASP	2.1
1	C	474	TRP	2.1
1	D	512	VAL	2.1
1	A	489	GLU	2.1
1	D	755	GLU	2.1
1	C	471	ASP	2.1
1	B	730	ASN	2.1
1	D	487	LEU	2.1
1	D	711	GLU	2.0
1	C	490	GLY	2.0
1	D	730	ASN	2.0
1	C	469	PRO	2.0
1	A	718	GLU	2.0
1	D	545	LYS	2.0
1	D	697	PHE	2.0
1	A	652	ASN	2.0
1	C	549	ASN	2.0
1	C	486	PRO	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 ⓘ

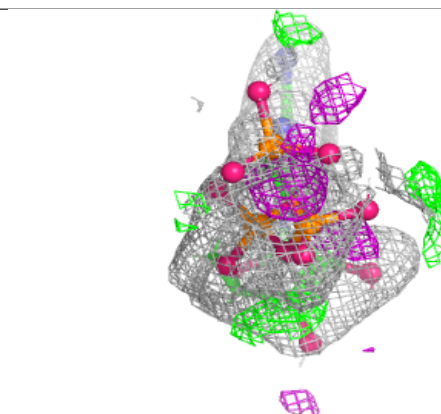
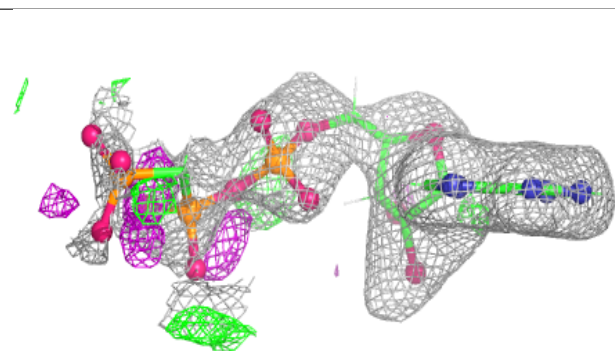
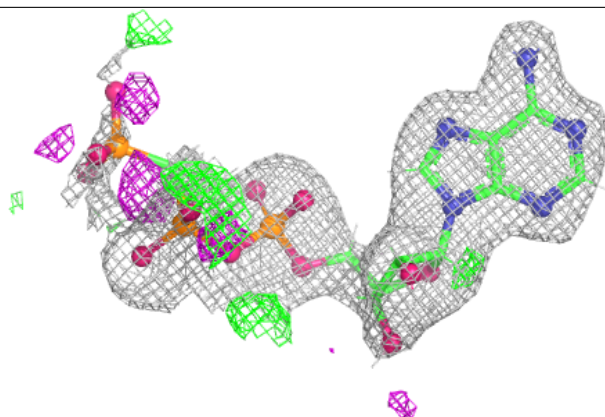
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MG	C	803	1/1	0.76	0.22	65,65,65,65	0
2	SO4	C	804	5/5	0.78	0.14	97,100,101,104	0
2	SO4	D	801	5/5	0.79	0.16	73,74,77,83	0
3	ACP	C	802	31/31	0.79	0.15	31,69,109,120	0
2	SO4	A	803	5/5	0.79	0.13	66,71,80,81	0
4	MG	D	804	1/1	0.82	0.18	46,46,46,46	0
3	ACP	B	802	31/31	0.84	0.15	25,47,64,93	0
3	ACP	D	802	31/31	0.86	0.14	39,57,97,116	0
3	ACP	A	802	31/31	0.87	0.13	23,43,64,93	0
2	SO4	A	801	5/5	0.89	0.10	49,55,61,72	0
4	MG	D	803	1/1	0.90	0.08	51,51,51,51	0
2	SO4	B	801	5/5	0.97	0.09	36,37,39,42	0
2	SO4	B	803	5/5	0.97	0.14	28,33,34,39	0
2	SO4	C	801	5/5	0.97	0.09	33,36,39,40	0

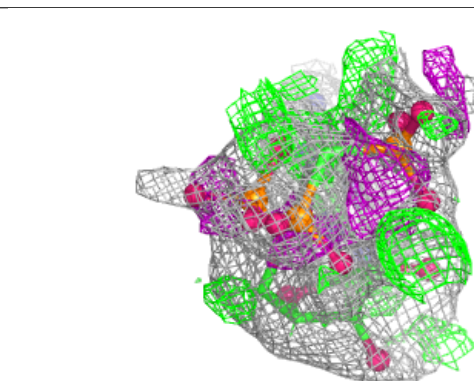
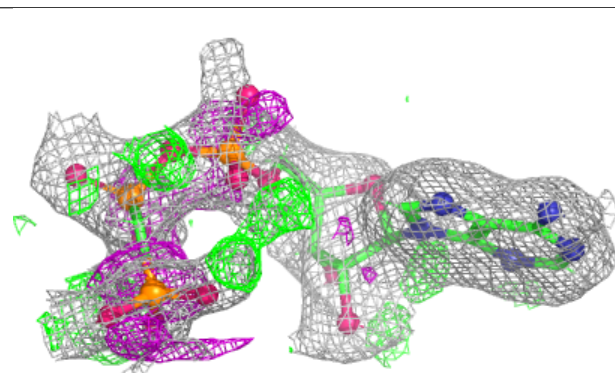
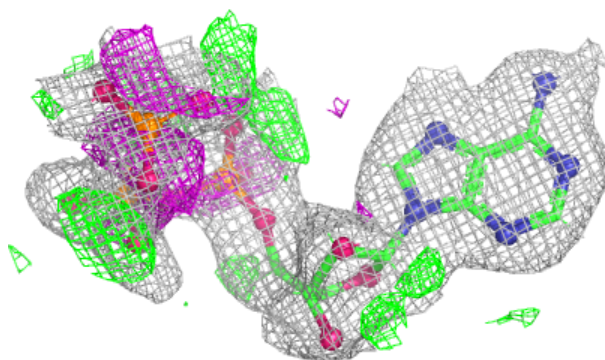
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ACP C 802:

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

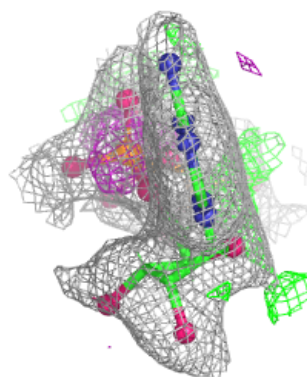
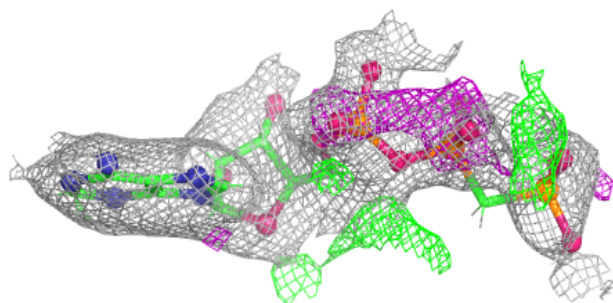
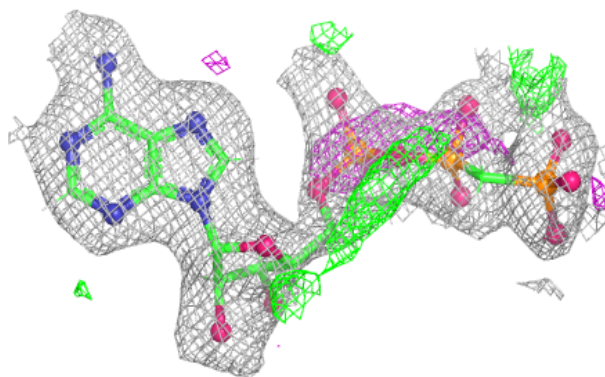
**Electron density around ACP B 802:**

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

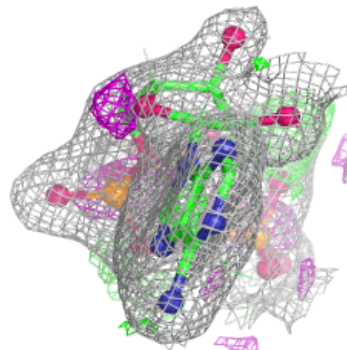
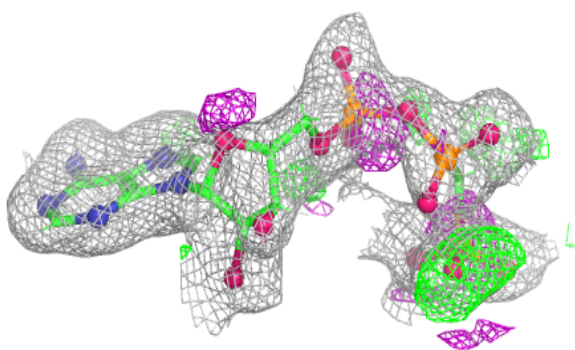
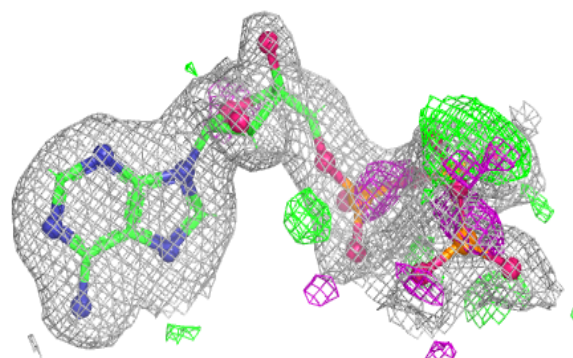


Electron density around ACP D 802:

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

**Electron density around ACP A 802:**

$2mF_o-DF_c$ (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.