



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:47 AM UTC

PDB ID : 8R7C / pdb_00008r7c
Title : MutSbeta bound to compound CHDI-00915542 in the canonical DNA-mismatch bound form
Authors : Thomsen, M.; Thieulin-Pardo, G.; Steinbacher, S.; Brace, G.; Tillack, K.; Johnson, P.; Ritzefeld, M.; Schaertl, S.; Frush, E.; Warfield, B.; Ballantyne, G.; Lee, J.-H.; Witte, D.; Finley, M.; Prasad, B.; Monteagudo, E.; Plotnikov, N.; Pacifici, R.; Maillard, M.; Wilkinson, H.; Iyer, R.; Dominguez, C.; Vogt, T.; Felsenfeld, D.; Haque, T.
Deposited on : 2023-11-24
Resolution : 2.82 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

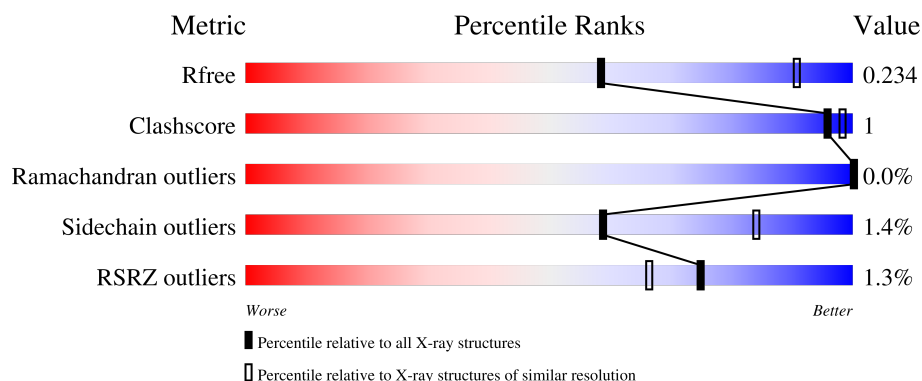
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.82 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	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (2.84-2.80)

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	930	93%
1	E	930	91% 7%
2	B	918	89% 7%

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Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
2	F	918	% 88% 6% 5%
3	C	24	79% 8% 12%
3	G	24	83% . 12%
4	D	24	96% .
5	H	24	96% .

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 29762 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 DNA mismatch repair protein Msh2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	894	Total	C	N	O	S	248	3	0
			7089	4498	1202	1351	38			
1	E	869	Total	C	N	O	S	330	0	0
			6879	4370	1166	1308	35			

- Molecule 2 is a protein called DNA mismatch repair protein Msh3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	852	Total	C	N	O	S	256	1	0
			6826	4354	1166	1274	32			
2	F	868	Total	C	N	O	S	151	1	0
			6958	4437	1193	1297	31			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	217	GLY	-	expression tag	UNP P20585
B	218	PRO	-	expression tag	UNP P20585
B	949	ARG	GLN	conflict	UNP P20585
F	217	GLY	-	expression tag	UNP P20585
F	218	PRO	-	expression tag	UNP P20585
F	949	ARG	GLN	conflict	UNP P20585

- Molecule 3 is a DNA chain called DNA (5'-D(P*CP*TP*AP*TP*CP*TP*GP*AP*AP*GP*CP*CP*GP*AP*TP*CP*GP*AP*TP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	21	Total	C	N	O	P	0	0	0
			432	205	80	126	21			
3	G	21	Total	C	N	O	P	0	0	0
			432	205	80	126	21			

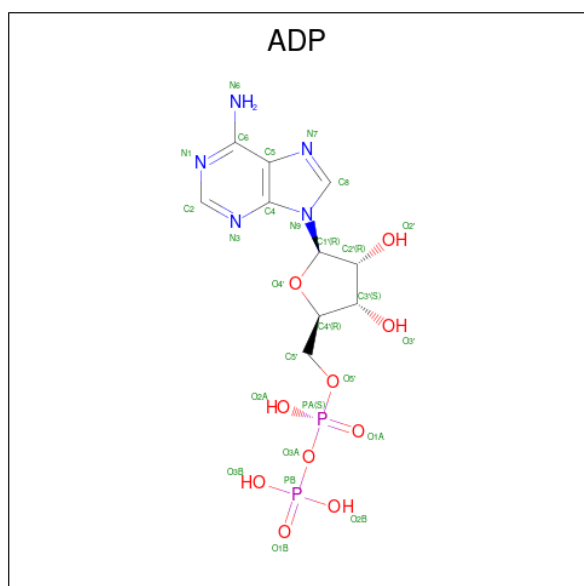
- Molecule 4 is a DNA chain called DNA (5'-D(*CP*CP*AP*TP*CP*GP*AP*TP*CP*GP*CP*AP*GP*CP*TP*TP*CP*AP*GP*AP*TP*AP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	23	Total	C	N	O	P	0	0	0
			466	223	86	135	22			

- Molecule 5 is a DNA chain called DNA (5'-D(P*CP*AP*TP*CP*GP*AP*TP*CP*GP*CP*AP*GP*CP*TP*TP*CP*AP*GP*AP*TP*AP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	H	23	Total	C	N	O	P	0	0	0
			472	224	88	137	23			

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



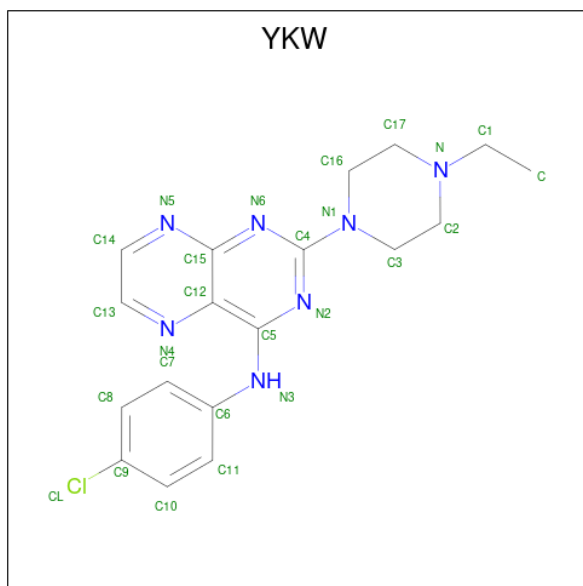
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 7 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 8 is {N}-(4-chlorophenyl)-2-(4-ethylpiperazin-1-yl)pteridin-4-amine (CCD ID: YKW) (formula: $C_{18}H_{20}ClN_7$) (labeled as "Ligand of Interest" by depositor).

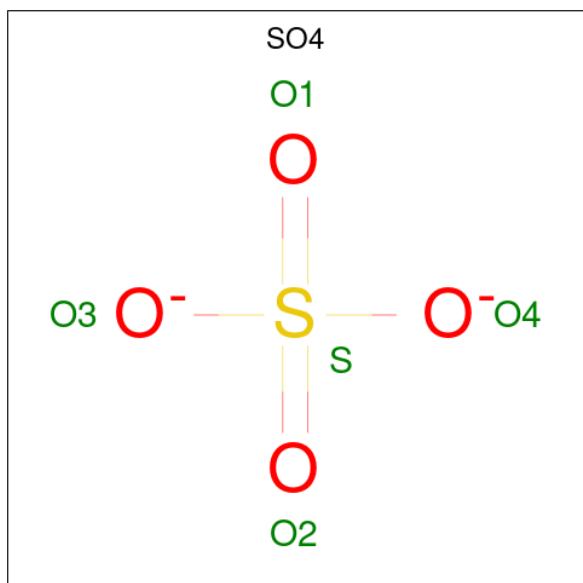


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	Cl	N	1	0
			26	18	1	7		
8	F	1	Total	C	Cl	N	0	0
			26	18	1	7		

- Molecule 9 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total Cl 1 1	0	0
9	F	2	Total Cl 2 2	0	0

- Molecule 10 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total O S 5 4 1	0	0
10	B	1	Total O S 5 4 1	0	0
10	F	1	Total O S 5 4 1	0	0
10	F	1	Total O S 5 4 1	0	0

- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	18	Total O 18 18	0	0
11	B	16	Total O 16 16	0	0
11	E	6	Total O 6 6	0	0

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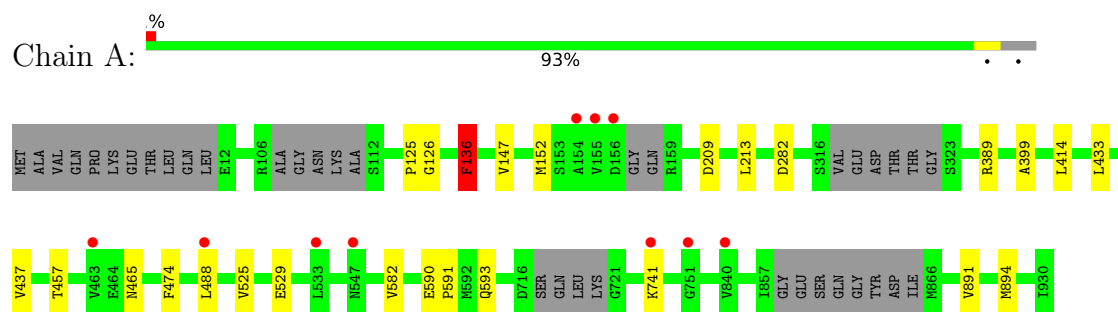
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	F	28	Total 28	O 28	0	0
11	H	1	Total 1	O 1	0	0

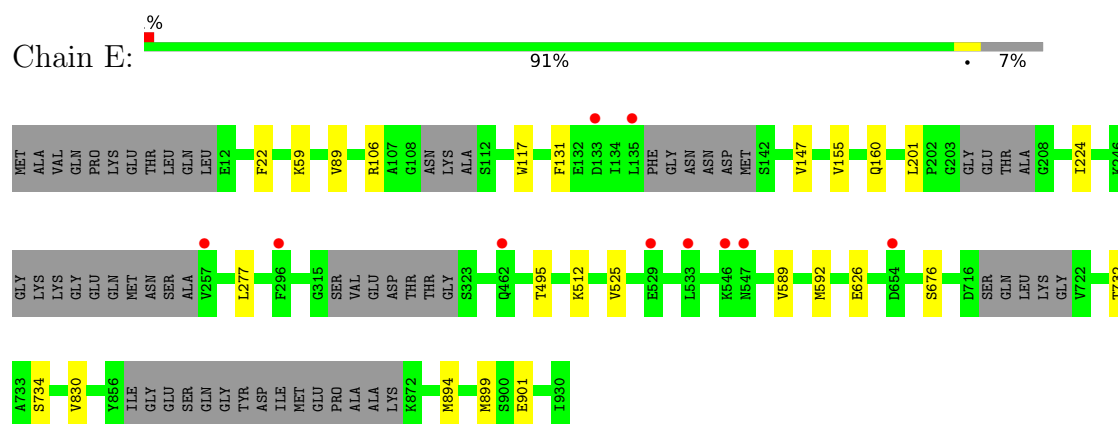
3 Residue-property plots [i](#)

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.

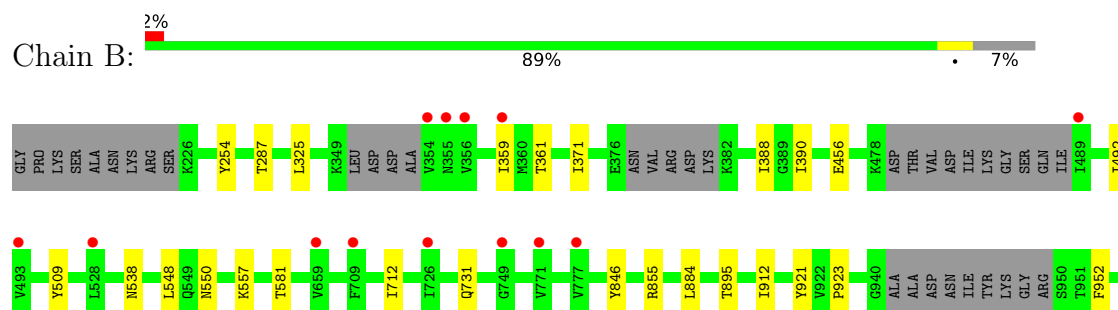
- Molecule 1: DNA mismatch repair protein Msh2

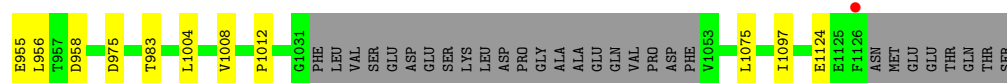


- Molecule 1: DNA mismatch repair protein Msh2

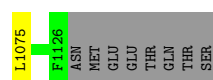
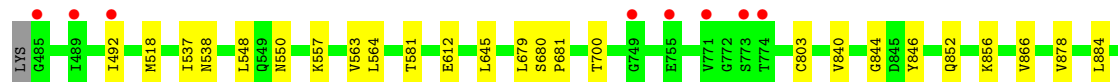
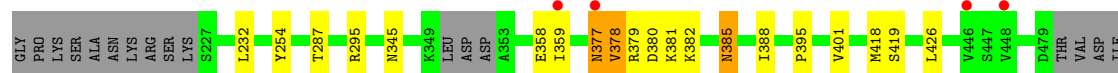
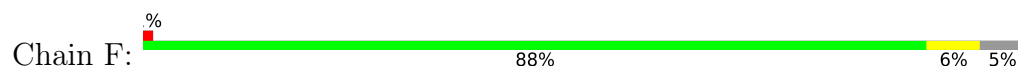


- Molecule 2: DNA mismatch repair protein Msh3

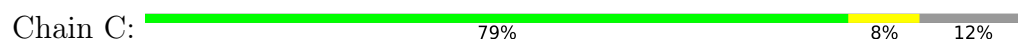




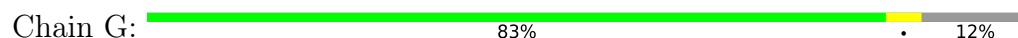
- Molecule 2: DNA mismatch repair protein Msh3



- Molecule 3: DNA (5'-D(P*CP*TP*AP*TP*CP*TP*GP*AP*AP*GP*CP*CP*GP*AP*TP*C P*GP*AP*TP*GP*G)-3')



- Molecule 3: DNA (5'-D(P*CP*TP*AP*TP*CP*TP*GP*AP*AP*GP*CP*CP*GP*AP*TP*C P*GP*AP*TP*GP*G)-3')



- Molecule 4: DNA (5'-D(*CP*CP*AP*TP*CP*GP*AP*TP*CP*GP*CP*AP*GP*CP*TP*TP *CP*AP*GP*AP*TP*AP*G)-3')



- Molecule 5: DNA (5'-D(P*CP*AP*TP*CP*GP*AP*TP*CP*GP*CP*AP*GP*CP*TP*TP*C P*AP*GP*AP*TP*AP*GP*G)-3')





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	101.22Å 104.79Å 121.26Å 110.03° 91.20° 110.50°	Depositor
Resolution (Å)	112.46 – 2.82 112.46 – 2.82	Depositor EDS
% Data completeness (in resolution range)	70.1 (112.46-2.82) 70.2 (112.46-2.82)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.82Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.201 , 0.231 0.205 , 0.234	Depositor DCC
R_{free} test set	3646 reflections (3.49%)	wwPDB-VP
Wilson B-factor (Å ²)	68.5	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 66.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	29762	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.55% 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: CL, PGE, SO4, YKW, ADP

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	1.05	0/7200	1.59	7/9698 (0.1%)
1	E	1.05	0/6985	1.57	0/9410
2	B	1.06	0/6949	1.59	5/9377 (0.1%)
2	F	1.04	0/7084	1.58	7/9560 (0.1%)
3	C	0.31	0/484	0.70	0/745
3	G	0.31	0/484	0.70	0/745
4	D	0.34	0/522	0.71	0/803
5	H	0.35	0/529	0.75	0/814
All	All	1.02	0/30237	1.53	19/41152 (0.0%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	388	ILE	CA-C-N	5.82	126.09	121.61
2	F	388	ILE	C-N-CA	5.82	126.09	121.61
2	F	1012	PRO	N-CA-C	5.70	117.65	110.70
2	B	388	ILE	CA-C-N	5.66	125.97	121.61
2	B	388	ILE	C-N-CA	5.66	125.97	121.61
1	A	209	ASP	CA-CB-CG	5.62	118.22	112.60
2	B	1012	PRO	N-CA-C	5.58	117.50	110.70
2	F	1062	GLY	CA-C-O	-5.52	118.42	122.23
2	F	538	ASN	CA-C-N	5.18	125.84	120.03
2	F	538	ASN	C-N-CA	5.18	125.84	120.03
1	A	125	PRO	CA-C-N	5.13	125.64	120.00
1	A	125	PRO	C-N-CA	5.13	125.64	120.00
2	F	844	GLY	CA-C-O	-5.09	116.64	120.76
2	B	538	ASN	CA-C-N	5.08	125.72	120.03
2	B	538	ASN	C-N-CA	5.08	125.72	120.03
1	A	282	ASP	CA-C-N	5.06	127.31	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	282	ASP	C-N-CA	5.06	127.31	120.38
1	A	136	PHE	CA-C-N	5.04	125.53	119.94
1	A	136	PHE	C-N-CA	5.04	125.53	119.94

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	7089	0	7136	13	0
1	E	6879	0	6935	10	0
2	B	6826	0	6938	13	0
2	F	6958	0	7071	24	0
3	C	432	0	237	1	0
3	G	432	0	237	1	0
4	D	466	0	260	0	0
5	H	472	0	259	0	0
6	A	27	0	12	0	0
6	E	27	0	12	0	0
7	A	10	0	14	0	0
8	B	26	0	0	0	0
8	F	26	0	0	0	0
9	B	1	0	0	0	0
9	F	2	0	0	0	0
10	B	10	0	0	0	0
10	F	10	0	0	0	0
11	A	18	0	0	0	0
11	B	16	0	0	0	0
11	E	6	0	0	0	0
11	F	28	0	0	0	0
11	H	1	0	0	0	0
All	All	29762	0	29111	59	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 1.

All (59) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:741[B]:LYS:CD	1:A:741[B]:LYS:H	2.07	0.67
1:A:741[B]:LYS:H	1:A:741[B]:LYS:HD2	1.67	0.58
2:F:378:VAL:HG13	2:F:379:ARG:HD2	1.87	0.56
2:B:884:LEU:HB3	2:B:1004:LEU:HD22	1.87	0.55
2:B:846:TYR:HB3	2:B:921:TYR:HB3	1.89	0.55
1:E:155:VAL:HG22	1:E:160:GLN:HB2	1.89	0.54
1:A:152:MET:HE1	1:A:213:LEU:HD13	1.90	0.53
1:A:741[B]:LYS:H	1:A:741[B]:LYS:CE	2.22	0.52
1:E:22:PHE:CZ	1:E:117:TRP:HB2	2.45	0.52
1:A:741[B]:LYS:N	1:A:741[B]:LYS:HE3	2.25	0.52
1:A:136:PHE:O	1:A:389:ARG:NH1	2.43	0.52
2:F:846:TYR:HB3	2:F:921:TYR:HB3	1.93	0.51
2:F:899:MET:HE1	2:F:1072:VAL:HG22	1.93	0.50
2:F:295:ARG:NH1	2:F:345:ASN:OD1	2.44	0.49
2:B:952:PHE:CZ	2:B:956:LEU:HD11	2.47	0.48
1:A:741[B]:LYS:H	1:A:741[B]:LYS:HE3	1.78	0.48
2:F:395:PRO:HA	2:F:518:MET:HE1	1.95	0.48
1:A:891:VAL:HA	1:A:894:MET:HE3	1.96	0.48
2:B:975:ASP:HA	2:B:1008:VAL:HB	1.97	0.47
2:F:377:ASN:ND2	2:F:385:ASN:O	2.47	0.47
2:B:550:ASN:ND2	2:B:557:LYS:O	2.46	0.47
2:F:878:VAL:HG21	2:F:1057:TYR:HB2	1.96	0.47
2:B:548:LEU:HD11	2:B:581:THR:HG22	1.97	0.47
2:B:855:ARG:HD2	2:B:1004:LEU:HG	1.96	0.46
3:C:22:DT:H2''	3:C:23:DG:O4'	2.15	0.46
2:F:254:TYR:O	2:F:287:THR:HG23	2.16	0.46
2:B:254:TYR:O	2:B:287:THR:HG23	2.15	0.46
1:E:147:VAL:HG21	1:E:277:LEU:HD21	1.98	0.46
2:F:884:LEU:HD21	2:F:892:MET:HE3	1.97	0.46
2:F:952:PHE:CZ	2:F:956:LEU:HD11	2.50	0.46
1:E:894:MET:HG2	1:E:899:MET:HE1	1.97	0.46
2:F:418:MET:HE3	2:F:426:LEU:HD21	1.96	0.46
2:F:379:ARG:HB2	2:F:382:LYS:HB3	1.99	0.45
2:B:359:ILE:HG22	2:B:361:THR:HG22	1.97	0.45
1:E:589:VAL:HA	1:E:592:MET:HE3	1.99	0.45
1:E:830:VAL:HG12	2:F:956:LEU:HD12	1.98	0.44
1:A:126:GLY:HA3	1:A:147:VAL:HG22	2.00	0.44
1:E:89:VAL:HG11	1:E:131:PHE:CE2	2.53	0.43
1:E:201:LEU:HD12	1:E:224:ILE:HG23	1.99	0.43
2:B:456:GLU:HG2	2:B:509:TYR:CE1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:THR:HG22	1:A:474:PHE:CE1	2.54	0.42
2:B:912:ILE:HG12	2:B:923:PRO:HD2	2.01	0.42
2:F:852:GLN:OE1	2:F:856:LYS:HD3	2.20	0.42
1:A:399:ALA:HB3	1:A:582:VAL:HG13	2.02	0.42
2:F:550:ASN:ND2	2:F:557:LYS:O	2.46	0.42
1:E:155:VAL:O	1:E:155:VAL:HG23	2.20	0.42
1:A:590:GLU:HB3	1:A:591:PRO:HD3	2.02	0.41
1:E:59:LYS:O	2:F:359:ILE:HG21	2.20	0.41
2:F:996:TYR:CE2	2:F:1001:VAL:CG2	3.04	0.41
2:F:645:LEU:HD22	2:F:679:LEU:HD22	2.02	0.41
2:F:680:SER:N	2:F:681:PRO:CD	2.83	0.41
1:A:433:LEU:HA	1:A:437:VAL:HB	2.01	0.41
2:B:952:PHE:CE2	2:B:956:LEU:HD11	2.56	0.41
2:F:700:THR:HA	2:F:803:CYS:SG	2.61	0.41
2:B:371:ILE:HA	2:B:390:ILE:HG22	2.02	0.41
2:F:548:LEU:HD11	2:F:581:THR:HG22	2.02	0.41
2:F:563:VAL:HG21	2:F:866:VAL:HA	2.03	0.41
2:F:232:LEU:HD22	3:G:17:DA:H4'	2.03	0.40
2:F:564:LEU:HA	2:F:840:VAL:HG21	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	885/930 (95%)	841 (95%)	44 (5%)	0	100	100
1	E	853/930 (92%)	816 (96%)	37 (4%)	0	100	100
2	B	841/918 (92%)	806 (96%)	35 (4%)	0	100	100
2	F	859/918 (94%)	824 (96%)	34 (4%)	1 (0%)	48	75
All	All	3438/3696 (93%)	3287 (96%)	150 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	385	ASN

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	779/804 (97%)	772 (99%)	7 (1%)	70	89
1	E	757/804 (94%)	748 (99%)	9 (1%)	63	86
2	B	763/818 (93%)	752 (99%)	11 (1%)	59	84
2	F	776/818 (95%)	761 (98%)	15 (2%)	50	79
All	All	3075/3244 (95%)	3033 (99%)	42 (1%)	59	84

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	136	PHE
1	A	414	LEU
1	A	465	ASN
1	A	488	LEU
1	A	525	VAL
1	A	529	GLU
1	A	593	GLN
2	B	325	LEU
2	B	492	ILE
2	B	712	ILE
2	B	731	GLN
2	B	895	THR
2	B	955	GLU
2	B	958	ASP
2	B	983	THR
2	B	1075	LEU
2	B	1097	ILE
2	B	1124	GLU
1	E	106	ARG

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Mol	Chain	Res	Type
1	E	495	THR
1	E	512	LYS
1	E	525	VAL
1	E	626	GLU
1	E	676	SER
1	E	732	THR
1	E	734	SER
1	E	901	GLU
2	F	358	GLU
2	F	377	ASN
2	F	378	VAL
2	F	380	ASP
2	F	381	LYS
2	F	401	VAL
2	F	419	SER
2	F	492	ILE
2	F	537	ILE
2	F	612	GLU
2	F	895	THR
2	F	938	ARG
2	F	958	ASP
2	F	983	THR
2	F	1075	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	160	GLN
1	A	193	GLN
1	A	339	GLN
1	A	428	HIS
1	A	451	GLN
1	A	560	ASN
1	A	662	GLN
1	A	681	GLN
1	A	783	HIS
1	A	793	GLN
2	B	243	HIS
2	B	394	GLN
2	B	470	GLN
2	B	494	ASN
2	B	514	ASN

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Mol	Chain	Res	Type
2	B	544	ASN
1	E	74	ASN
1	E	193	GLN
1	E	429	GLN
1	E	451	GLN
1	E	596	ASN
1	E	610	HIS
1	E	793	GLN
1	E	835	ASN
1	E	885	GLN
1	E	924	ASN
2	F	243	HIS
2	F	377	ASN
2	F	385	ASN
2	F	549	GLN
2	F	743	GLN
2	F	826	HIS

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 12 ligands modelled in this entry, 3 are monoatomic - leaving 9 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
8	YKW	F	1201	-	29,29,29	0.34	0	35,40,40	0.48	0
10	SO4	F	1204	-	4,4,4	0.33	0	6,6,6	0.09	0
7	PGE	A	1002	-	9,9,9	0.29	0	8,8,8	0.16	0
10	SO4	B	1204	-	4,4,4	0.34	0	6,6,6	0.07	0
6	ADP	E	1001	-	28,29,29	0.45	0	43,45,45	0.47	0
10	SO4	F	1202	-	4,4,4	0.35	0	6,6,6	0.12	0
10	SO4	B	1203	-	4,4,4	0.34	0	6,6,6	0.09	0
6	ADP	A	1001	-	28,29,29	0.43	0	43,45,45	0.49	0
8	YKW	B	1201	-	29,29,29	0.48	0	35,40,40	0.55	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
8	YKW	F	1201	-	-	0/10/20/20	0/4/4/4
7	PGE	A	1002	-	-	1/7/7/7	-
6	ADP	E	1001	-	-	0/16/32/32	0/3/3/3
6	ADP	A	1001	-	-	1/16/32/32	0/3/3/3
8	YKW	B	1201	-	-	2/10/20/20	0/4/4/4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

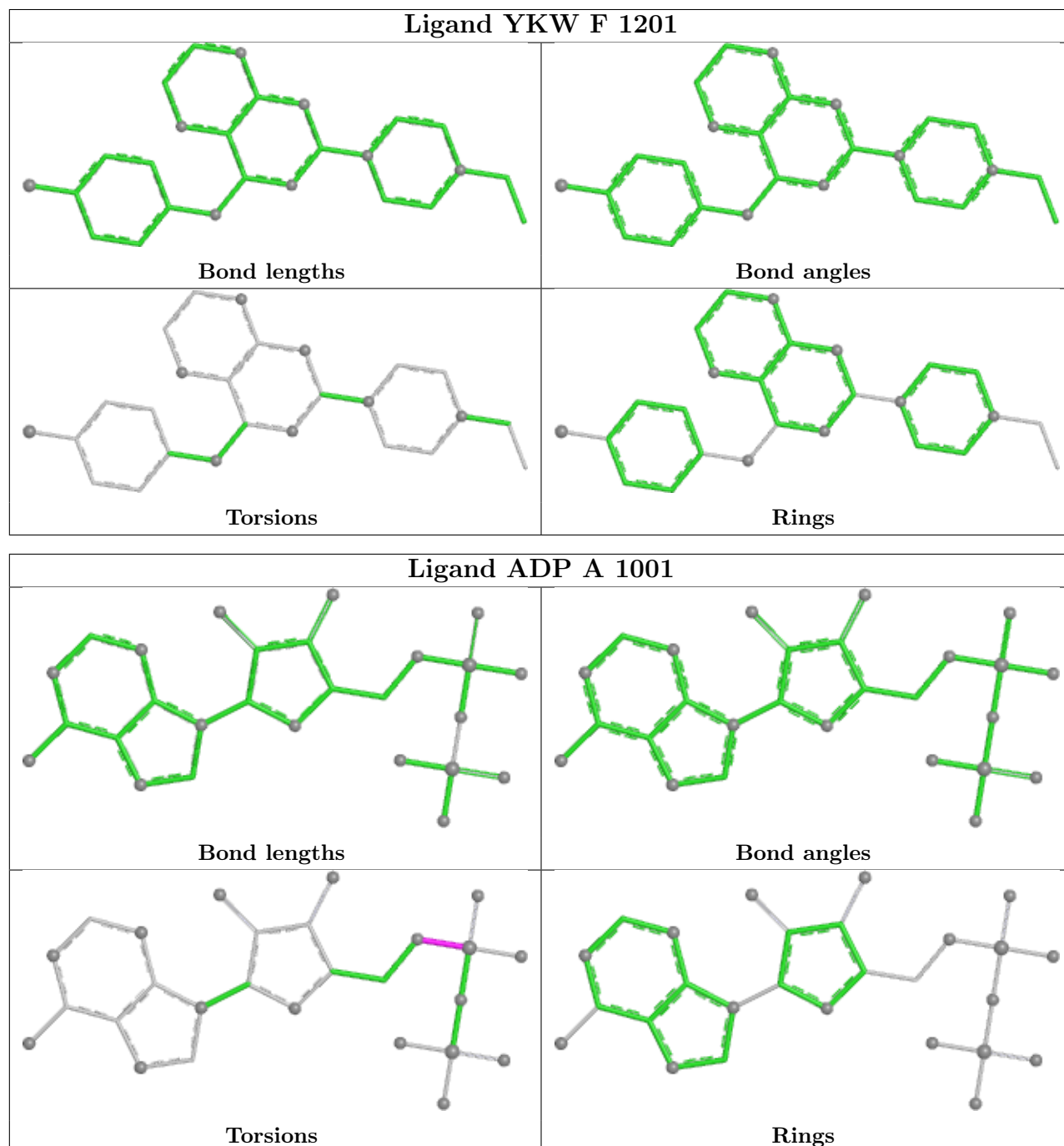
Mol	Chain	Res	Type	Atoms
6	A	1001	ADP	C5'-O5'-PA-O1A
8	B	1201	YKW	C12-C5-N3-C6
8	B	1201	YKW	N2-C5-N3-C6
7	A	1002	PGE	O2-C3-C4-O3

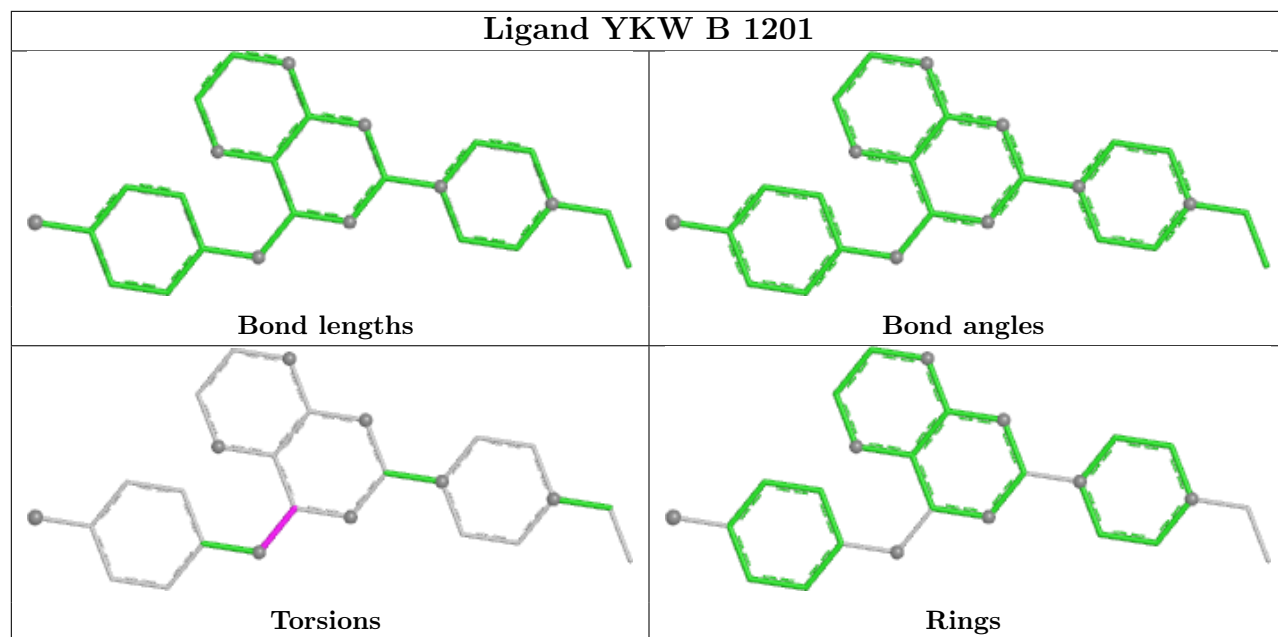
There are no ring outliers.

No monomer is involved in short contacts.

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 [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	894/930 (96%)	0.03	10 (1%) 78 70	28, 67, 112, 144	77 (8%)
1	E	869/930 (93%)	0.11	10 (1%) 76 68	28, 73, 117, 154	92 (10%)
2	B	852/918 (92%)	0.17	14 (1%) 70 61	24, 75, 118, 167	80 (9%)
2	F	868/918 (94%)	-0.14	12 (1%) 73 64	26, 56, 102, 160	48 (5%)
3	C	21/24 (87%)	-0.20	0 100 100	56, 96, 183, 192	0
3	G	21/24 (87%)	-0.14	0 100 100	40, 81, 153, 163	0
4	D	23/24 (95%)	-0.30	0 100 100	47, 87, 157, 195	0
5	H	23/24 (95%)	-0.33	0 100 100	41, 77, 128, 161	0
All	All	3571/3792 (94%)	0.04	46 (1%) 75 66	24, 68, 117, 195	297 (8%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	547	ASN	4.5
1	A	547	ASN	3.7
2	B	771	VAL	3.5
1	E	296	PHE	3.4
1	A	751	GLY	3.3
2	F	359	ILE	3.2
2	F	773	SER	3.1
1	E	135	LEU	3.0
2	F	749	GLY	2.7
2	F	377	ASN	2.7
2	B	777	VAL	2.7
1	E	462	GLN	2.6
2	F	771	VAL	2.5
2	F	774	THR	2.5
1	A	154	ALA	2.5
2	B	356	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	529	GLU	2.5
2	F	755	GLU	2.5
2	B	489	ILE	2.5
2	F	485	GLY	2.5
1	A	155	VAL	2.5
1	E	133	ASP	2.4
2	B	659	VAL	2.4
1	E	533	LEU	2.4
2	F	489	ILE	2.4
2	B	359	ILE	2.4
1	A	741[A]	LYS	2.3
2	B	355	ASN	2.3
1	E	257	VAL	2.3
2	F	446	VAL	2.2
2	F	492	ILE	2.2
2	B	1126	PHE	2.2
2	B	528	LEU	2.2
2	B	709	PHE	2.2
1	E	654	ASP	2.1
1	A	533	LEU	2.1
2	B	354	VAL	2.1
2	B	493	VAL	2.1
1	A	156	ASP	2.1
2	B	726	ILE	2.1
1	A	463	VAL	2.1
2	B	749	GLY	2.1
1	A	840	VAL	2.0
2	F	448	VAL	2.0
1	E	546	LYS	2.0
1	A	488	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

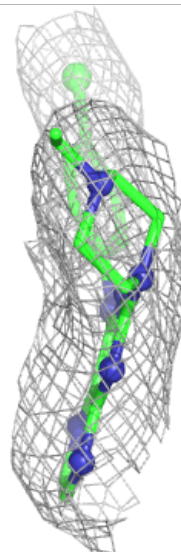
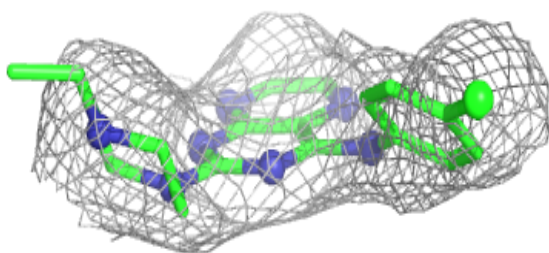
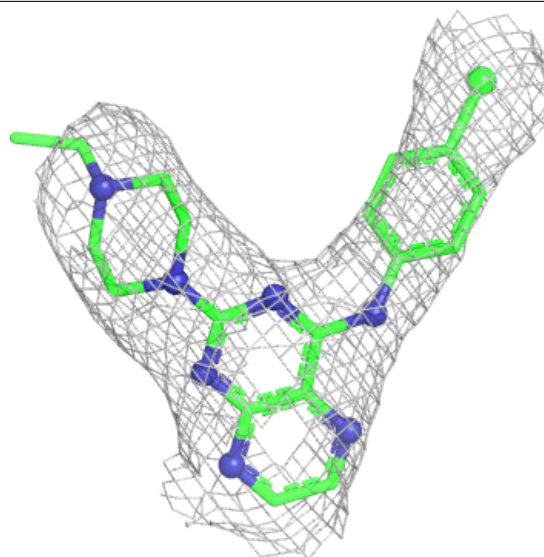
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
10	SO4	B	1203	5/5	0.81	0.09	120,122,124,126	0
7	PGE	A	1002	10/10	0.89	0.12	55,62,64,65	0
10	SO4	B	1204	5/5	0.90	0.09	121,121,123,128	0
8	YKW	B	1201	26/26	0.93	0.10	77,85,95,97	1
10	SO4	F	1204	5/5	0.93	0.11	92,94,97,98	0
10	SO4	F	1202	5/5	0.94	0.11	64,66,68,72	0
8	YKW	F	1201	26/26	0.95	0.07	47,49,61,68	0
6	ADP	E	1001	27/27	0.96	0.06	50,59,64,65	0
6	ADP	A	1001	27/27	0.96	0.06	48,59,64,68	0
9	CL	F	1203	1/1	0.97	0.07	58,58,58,58	0
9	CL	B	1202	1/1	0.99	0.03	41,41,41,41	0
9	CL	F	1205	1/1	0.99	0.02	44,44,44,44	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.

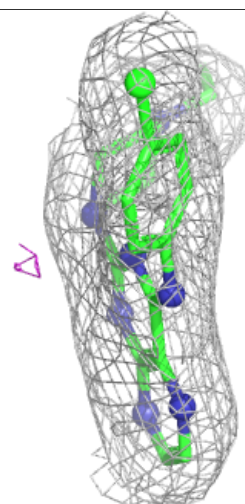
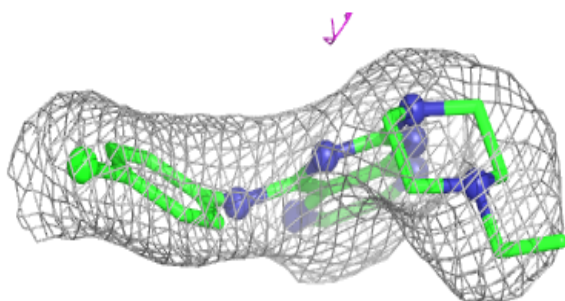
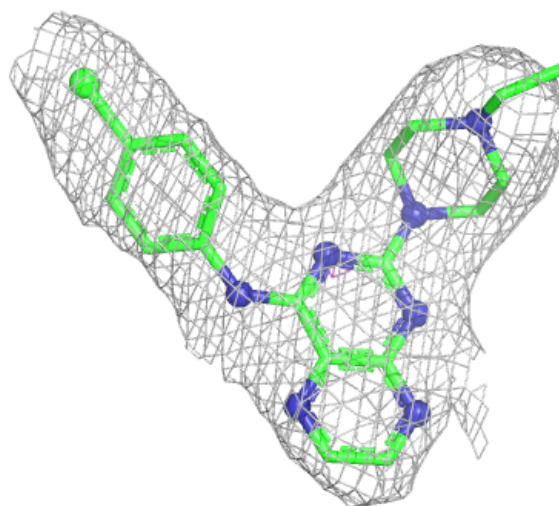
Electron density around YKW B 1201:

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



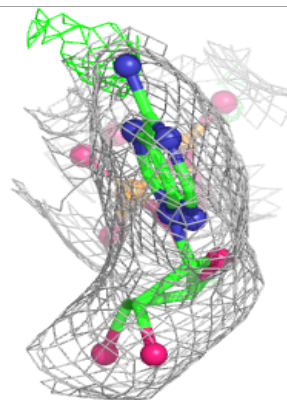
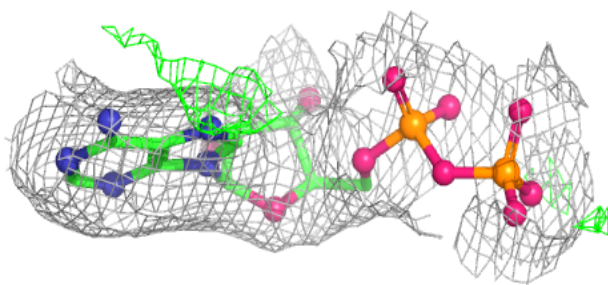
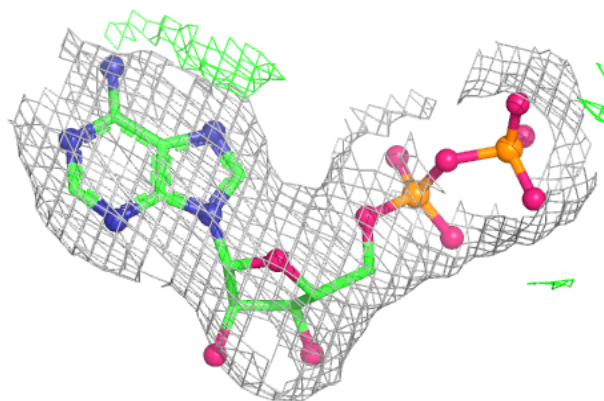
Electron density around YKW F 1201:

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



Electron density around ADP A 1001:

$2mF_o-DF_c$ (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.