



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:35 PM UTC

PDB ID : 2XCM / pdb_00002xcm
Title : COMPLEX OF HSP90 N-TERMINAL, SGT1 CS AND RAR1 CHORD2 DOMAIN
Authors : Zhang, M.; Pearl, L.H.
Deposited on : 2010-04-23
Resolution : 2.20 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

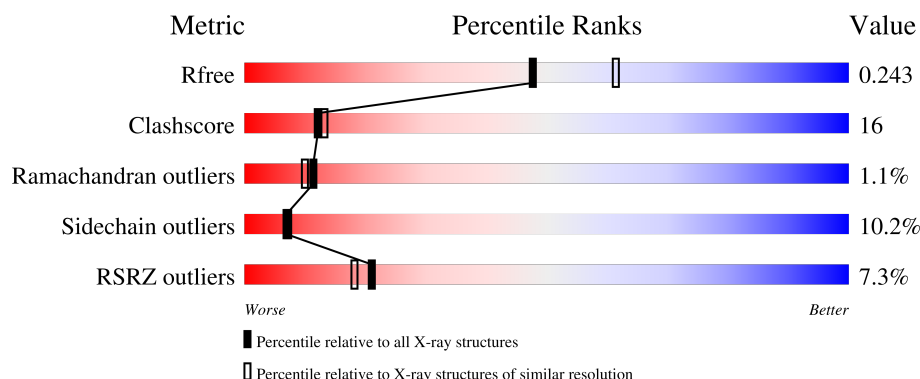
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	214	
1	B	214	
2	C	92	
2	D	92	
3	E	74	

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Mol	Chain	Length	Quality of chain
3	F	74	5% 69% 23% 8%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6330 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 CYTOSOLIC HEAT SHOCK PROTEIN 90.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	213	Total	C	N	O	S	0	0	0
			1675	1061	276	333	5			
1	B	213	Total	C	N	O	S	0	0	0
			1671	1059	276	331	5			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	HIS	-	expression tag	UNP Q7XJ80
A	-1	HIS	-	expression tag	UNP Q7XJ80
A	0	ALA	-	expression tag	UNP Q7XJ80
A	1	ALA	-	expression tag	UNP Q7XJ80
A	211	ALA	-	expression tag	UNP Q7XJ80
B	-2	HIS	-	expression tag	UNP Q7XJ80
B	-1	HIS	-	expression tag	UNP Q7XJ80
B	0	ALA	-	expression tag	UNP Q7XJ80
B	1	ALA	-	expression tag	UNP Q7XJ80
B	211	ALA	-	expression tag	UNP Q7XJ80

- Molecule 2 is a protein called SGT1-LIKE PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	92	Total	C	N	O	S	0	0	0
			743	486	119	136	2			
2	D	92	Total	C	N	O	S	0	0	0
			743	486	119	136	2			

- Molecule 3 is a protein called RAR1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	74	Total	C	N	O	S	0	0	0
			586	363	109	107	7			

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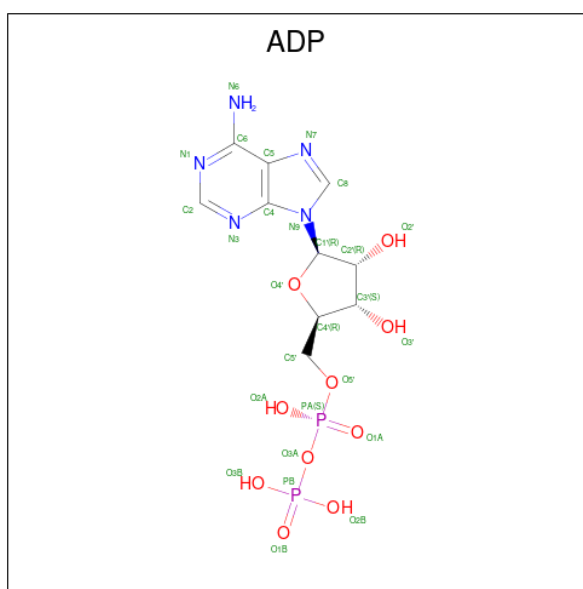
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	74	Total	C	N	O	S	0	0	0
			582	360	108	107	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	148	ALA	-	expression tag	UNP Q9FLI9
F	148	ALA	-	expression tag	UNP Q9FLI9

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

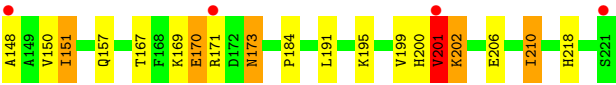
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	B	1	Total	Mg	0	0
			1	1		

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

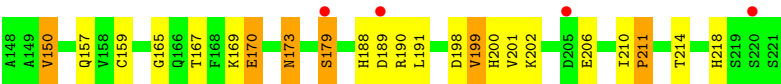
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	2	Total 2	Zn 2	0	0
6	F	2	Total 2	Zn 2	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	82	Total 82	O 82	0	0
7	B	71	Total 71	O 71	0	0
7	C	24	Total 24	O 24	0	0
7	D	26	Total 26	O 26	0	0
7	E	32	Total 32	O 32	0	0
7	F	35	Total 35	O 35	0	0



● Molecule 3: RAR1



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	88.89Å 88.89Å 117.82Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.78 – 2.20 46.78 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.2 (46.78-2.20) 99.1 (46.78-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.22 (at 2.20Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.5_2)	Depositor
R, R_{free}	0.198 , 0.242 0.203 , 0.243	Depositor DCC
R_{free} test set	2675 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	29.8	Xtriage
Anisotropy	0.238	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 39.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l 0.477 for h,-h-k,-l 0.017 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6330	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% 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: ZN, ADP, MG

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	0.53	0/1704	0.84	2/2303 (0.1%)
1	B	0.51	0/1700	0.83	0/2298
2	C	0.54	1/760 (0.1%)	0.83	2/1029 (0.2%)
2	D	0.49	0/760	0.89	4/1029 (0.4%)
3	E	0.60	1/604 (0.2%)	1.09	6/816 (0.7%)
3	F	0.54	0/600	0.93	2/812 (0.2%)
All	All	0.53	2/6128 (0.0%)	0.88	16/8287 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	148	ALA	C-N	-7.64	1.22	1.33
2	C	239	HIS	C-O	-5.25	1.17	1.23

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	201	VAL	N-CA-C	10.56	120.99	112.12
3	E	148	ALA	O-C-N	9.18	137.69	123.00
2	D	172	ILE	N-CA-C	8.15	116.00	107.76
3	E	148	ALA	CA-C-N	-7.28	107.41	122.03
3	E	148	ALA	C-N-CA	-7.28	107.41	122.03
1	A	4	GLU	CA-C-O	6.77	121.87	117.94
2	C	172	ILE	N-CA-C	6.36	114.18	107.76
3	F	211	PRO	CA-C-N	6.18	126.20	119.90
3	F	211	PRO	C-N-CA	6.18	126.20	119.90
2	D	170	LYS	N-CA-C	5.98	118.95	111.24
1	A	4	GLU	CB-CA-C	-5.74	108.80	117.07
2	D	192	VAL	CA-C-N	5.51	126.73	119.84
2	D	192	VAL	C-N-CA	5.51	126.73	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	210	ILE	CA-C-N	5.39	123.54	119.66
3	E	210	ILE	C-N-CA	5.39	123.54	119.66
2	C	195	GLU	N-CA-C	5.04	114.94	108.34

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	1675	0	1648	72	0
1	B	1671	0	1644	46	0
2	C	743	0	757	19	0
2	D	743	0	757	41	0
3	E	586	0	539	18	0
3	F	582	0	528	18	0
4	A	27	0	12	2	0
4	B	27	0	12	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	E	2	0	0	0	0
6	F	2	0	0	0	0
7	A	82	0	0	5	0
7	B	71	0	0	8	0
7	C	24	0	0	0	0
7	D	26	0	0	0	0
7	E	32	0	0	1	0
7	F	35	0	0	0	0
All	All	6330	0	5897	187	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 16.

All (187) 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:-1:HIS:NE2	2:D:214:LYS:CD	1.85	1.39
1:A:-1:HIS:CD2	2:D:214:LYS:HD2	1.67	1.27
1:A:-1:HIS:NE2	2:D:214:LYS:HD2	1.43	1.26
1:A:-1:HIS:NE2	2:D:214:LYS:CE	2.02	1.21
2:D:240:GLY:O	2:D:241:LYS:HG2	1.44	1.14
3:E:201:VAL:O	3:E:202:LYS:HB2	1.58	1.03
1:A:-1:HIS:CD2	2:D:214:LYS:CD	2.35	0.99
1:A:-1:HIS:CD2	2:D:214:LYS:CG	2.49	0.95
1:A:-1:HIS:NE2	2:D:214:LYS:HE2	1.80	0.94
1:A:87:THR:HG22	1:A:90:ASP:H	1.35	0.88
2:D:220:THR:HG23	2:D:221:LYS:HG2	1.57	0.87
2:C:158:GLN:HE22	2:C:234:TRP:H	1.23	0.85
3:E:169:LYS:O	3:E:170:GLU:CB	2.26	0.82
1:A:184:MET:HE3	1:A:187:LEU:HD11	1.60	0.82
1:A:-1:HIS:CD2	2:D:214:LYS:HG3	2.16	0.80
3:E:199:VAL:HG21	3:E:210:ILE:HG21	1.62	0.80
3:F:169:LYS:O	3:F:170:GLU:CB	2.27	0.80
1:A:147:GLN:HE22	1:A:169:LEU:H	1.29	0.80
1:B:3:THR:HG21	1:B:162:ARG:HH21	1.47	0.80
3:F:169:LYS:O	3:F:170:GLU:HB2	1.80	0.80
1:B:20:LEU:O	1:B:24:THR:HG23	1.83	0.79
1:A:146:GLU:OE1	1:A:162:ARG:HD2	1.82	0.79
1:A:87:THR:HG21	2:D:155:GLU:OE1	1.84	0.77
3:E:170:GLU:HA	3:E:173:ASN:HB2	1.68	0.76
1:B:3:THR:O	1:B:3:THR:HG23	1.85	0.76
2:D:240:GLY:O	2:D:241:LYS:CG	2.30	0.75
1:A:-1:HIS:NE2	2:D:214:LYS:CG	2.50	0.74
2:C:192:VAL:HB	2:C:195:GLU:HG2	1.69	0.74
1:A:173:THR:HG23	7:A:2031:HOH:O	1.87	0.74
2:C:220:THR:HG23	2:C:221:LYS:HG2	1.69	0.74
2:D:158:GLN:HE22	2:D:234:TRP:H	1.34	0.73
1:B:3:THR:HG21	1:B:162:ARG:NH2	2.03	0.73
1:B:123:GLY:HA2	4:B:1211:ADP:O2B	1.87	0.73
3:E:169:LYS:O	3:E:170:GLU:HB3	1.90	0.72
2:D:240:GLY:C	2:D:241:LYS:HG2	2.15	0.72
1:A:3:THR:HG21	1:A:162:ARG:NE	2.04	0.71
1:A:-1:HIS:HD2	2:D:214:LYS:HB3	1.56	0.71
2:C:158:GLN:HE21	2:C:228:LYS:NZ	1.89	0.71
1:A:193:LYS:HD2	1:A:209:LEU:HD12	1.74	0.70
2:C:158:GLN:HE21	2:C:228:LYS:HZ1	1.39	0.69
1:A:146:GLU:HG3	2:D:220:THR:HG21	1.75	0.69
2:D:158:GLN:HE21	2:D:228:LYS:NZ	1.90	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:ILE:HD11	1:B:130:TYR:HB3	1.74	0.69
1:B:147:GLN:HE22	1:B:169:LEU:H	1.41	0.68
1:B:78:THR:HG21	7:B:2024:HOH:O	1.93	0.68
1:A:115:ASP:OD2	1:A:117:SER:HB2	1.94	0.67
1:A:-1:HIS:CE1	2:D:214:LYS:CE	2.77	0.67
3:E:201:VAL:O	3:E:202:LYS:CB	2.40	0.67
3:F:199:VAL:HG22	3:F:210:ILE:HD13	1.77	0.66
3:E:199:VAL:CG2	3:E:210:ILE:HG21	2.24	0.66
1:A:-1:HIS:HD2	2:D:214:LYS:CG	2.05	0.65
2:D:169:ALA:HB1	2:D:172:ILE:HD13	1.79	0.65
1:A:-1:HIS:HD2	2:D:214:LYS:CB	2.10	0.65
1:A:184:MET:HE3	1:A:187:LEU:CD1	2.25	0.65
2:D:158:GLN:HE21	2:D:228:LYS:HZ1	1.45	0.64
1:B:18:LEU:O	1:B:22:ILE:HG12	1.97	0.64
1:A:139:THR:HG23	7:A:2045:HOH:O	1.98	0.63
2:D:240:GLY:C	2:D:241:LYS:CG	2.71	0.63
1:A:123:GLY:HA2	4:A:1211:ADP:O2B	1.98	0.63
1:A:149:VAL:HG23	1:A:163:ASP:HB2	1.80	0.62
1:A:28:ASN:H	1:A:28:ASN:HD22	1.44	0.62
3:E:173:ASN:HD21	3:E:218:HIS:H	1.47	0.61
3:E:199:VAL:HG21	3:E:210:ILE:CG2	2.31	0.61
1:B:101:SER:O	1:B:105:GLU:HG3	2.00	0.60
1:A:167:GLU:O	1:A:168:GLN:HB2	2.01	0.60
1:B:146:GLU:HG3	2:C:220:THR:HG21	1.81	0.60
1:B:189:GLU:HG3	1:B:190:ARG:N	2.17	0.60
1:A:75:SER:HB3	1:A:184:MET:HE1	1.84	0.59
3:F:173:ASN:HD21	3:F:218:HIS:H	1.50	0.59
2:D:192:VAL:HB	2:D:195:GLU:HG3	1.85	0.59
1:B:75:SER:CB	1:B:184:MET:HE1	2.34	0.58
1:B:139:THR:HG23	7:B:2039:HOH:O	2.04	0.57
2:C:201:GLN:OE1	3:E:151:ILE:HD13	2.05	0.57
1:A:31:ILE:HD13	1:A:117:SER:HA	1.87	0.57
3:F:201:VAL:HG21	3:F:206:GLU:CD	2.29	0.57
2:D:218:LEU:HD12	2:D:221:LYS:HE3	1.87	0.56
3:E:169:LYS:O	3:E:170:GLU:HB2	2.05	0.56
1:A:101:SER:O	1:A:105:GLU:HG3	2.06	0.56
1:B:146:GLU:OE1	1:B:162:ARG:HD2	2.04	0.56
1:B:3:THR:O	1:B:3:THR:CG2	2.54	0.56
3:F:170:GLU:HA	3:F:173:ASN:HB2	1.86	0.56
2:C:186:LEU:O	2:C:201:GLN:HA	2.07	0.55
1:B:164:THR:O	1:B:165:SER:CB	2.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:THR:HG21	7:A:2037:HOH:O	2.06	0.55
1:A:164:THR:O	1:A:165:SER:HB3	2.06	0.55
1:A:85:GLY:HA2	1:A:173:THR:HG22	1.87	0.55
1:B:80:VAL:HG22	1:B:174:LYS:HG3	1.89	0.54
2:C:169:ALA:HB1	2:C:172:ILE:HD13	1.90	0.53
1:B:184:MET:HE3	1:B:187:LEU:HD12	1.91	0.53
1:B:22:ILE:CD1	1:B:130:TYR:HB3	2.38	0.53
1:A:61:GLN:C	1:A:61:GLN:HE21	2.17	0.53
3:E:199:VAL:HG23	3:E:210:ILE:HD13	1.91	0.53
2:C:240:GLY:C	2:C:241:LYS:HG2	2.34	0.52
1:A:-1:HIS:CD2	2:D:214:LYS:HB3	2.41	0.52
1:A:92:VAL:O	1:A:97:THR:HB	2.10	0.52
1:A:3:THR:O	1:A:3:THR:HG22	2.09	0.52
1:B:97:THR:HG21	7:B:2034:HOH:O	2.10	0.52
1:A:94:ASN:ND2	1:A:100:ARG:HH21	2.08	0.52
2:C:199:TYR:CD1	3:E:150:VAL:HG22	2.45	0.52
1:B:0:ALA:O	1:B:1:ALA:HB3	2.10	0.52
1:B:78:THR:HG23	7:B:2022:HOH:O	2.10	0.51
2:C:175:GLN:NE2	2:C:175:GLN:H	2.08	0.51
1:B:135:ARG:HD2	1:B:153:GLN:HE21	1.75	0.51
1:B:184:MET:HE3	1:B:187:LEU:CD1	2.41	0.51
1:B:76:THR:HG22	7:B:2022:HOH:O	2.11	0.51
2:D:175:GLN:NE2	2:D:175:GLN:H	2.09	0.50
2:D:151:LYS:HZ1	2:D:192:VAL:HG11	1.76	0.50
3:F:201:VAL:HG22	3:F:202:LYS:H	1.76	0.50
1:A:94:ASN:ND2	1:A:100:ARG:NH2	2.59	0.50
1:A:28:ASN:H	1:A:28:ASN:ND2	2.09	0.50
1:A:28:ASN:HD22	1:A:28:ASN:N	2.06	0.50
1:B:139:THR:HB	1:B:149:VAL:HG22	1.92	0.50
2:C:175:GLN:H	2:C:175:GLN:HE21	1.58	0.50
1:A:68:ILE:O	1:A:209:LEU:O	2.30	0.49
1:A:-1:HIS:NE2	2:D:214:LYS:HG3	2.23	0.49
1:A:94:ASN:HD22	1:A:100:ARG:HH21	1.60	0.49
3:F:189:ASP:O	3:F:190:ARG:HB2	2.13	0.48
1:B:177:LEU:N	1:B:177:LEU:HD23	2.27	0.48
1:A:-1:HIS:CE1	2:D:214:LYS:HE3	2.48	0.48
1:A:199:HIS:HB2	7:A:2074:HOH:O	2.13	0.48
1:A:86:MET:HE3	4:A:1211:ADP:H1'	1.94	0.48
1:A:6:GLU:HB3	1:A:8:PHE:CE1	2.49	0.48
1:B:92:VAL:O	1:B:97:THR:HB	2.13	0.48
1:A:80:VAL:HG22	1:A:174:LYS:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:175:GLN:H	2:D:175:GLN:HE21	1.62	0.47
2:D:170:LYS:O	2:D:219:SER:O	2.31	0.47
1:A:3:THR:HG21	1:A:162:ARG:CZ	2.44	0.47
1:A:-1:HIS:NE2	2:D:214:LYS:HE3	2.18	0.47
1:B:70:PRO:HG3	1:B:192:ILE:CD1	2.44	0.47
1:B:104:LYS:O	1:B:108:GLU:HG3	2.15	0.47
2:D:241:LYS:HE2	2:D:241:LYS:HB3	1.47	0.47
1:B:-2:HIS:CE1	2:C:217:VAL:H	2.34	0.46
1:B:199:HIS:HB2	7:B:2065:HOH:O	2.16	0.46
2:D:186:LEU:O	2:D:201:GLN:HA	2.15	0.46
3:F:169:LYS:O	3:F:170:GLU:HB3	2.16	0.46
1:A:94:ASN:HD22	1:A:100:ARG:NH2	2.15	0.45
1:B:6:GLU:HB3	1:B:8:PHE:CE1	2.51	0.45
1:A:87:THR:HG22	1:A:90:ASP:N	2.17	0.45
1:B:149:VAL:HG23	1:B:163:ASP:HB2	1.98	0.45
1:A:18:LEU:HD12	1:A:18:LEU:HA	1.84	0.45
2:C:192:VAL:HB	2:C:195:GLU:CG	2.44	0.45
2:D:188:VAL:O	2:D:199:TYR:HA	2.17	0.45
2:D:179:ILE:HD12	2:D:215:TYR:CD2	2.52	0.45
2:C:214:LYS:HB3	2:C:214:LYS:HE3	1.63	0.44
1:A:97:THR:CG2	7:A:2037:HOH:O	2.64	0.44
3:E:184:PRO:HD2	3:E:195:LYS:HB3	1.98	0.44
2:D:199:TYR:CE1	3:F:150:VAL:HG22	2.53	0.44
3:E:201:VAL:HG11	3:E:206:GLU:HB3	2.00	0.43
1:A:-1:HIS:CD2	2:D:214:LYS:CB	2.91	0.43
1:A:164:THR:O	1:A:165:SER:CB	2.66	0.43
3:F:157:GLN:O	3:F:167:THR:HA	2.17	0.43
1:A:20:LEU:O	1:A:24:THR:HG23	2.19	0.43
3:E:157:GLN:O	3:E:167:THR:HA	2.17	0.43
1:B:75:SER:HB3	1:B:184:MET:HE1	2.00	0.43
1:A:195:LEU:HD12	1:A:195:LEU:HA	1.78	0.43
1:A:-2:HIS:HA	2:D:215:TYR:O	2.17	0.43
1:A:32:PHE:CG	1:A:33:LEU:N	2.85	0.43
1:A:110:LEU:HD23	1:A:114:ALA:O	2.19	0.43
1:B:32:PHE:CG	1:B:33:LEU:N	2.87	0.43
1:A:209:LEU:O	1:A:210:TRP:O	2.36	0.43
1:B:76:THR:CG2	7:B:2022:HOH:O	2.66	0.43
2:C:151:LYS:HE2	2:C:152:TYR:CZ	2.54	0.42
1:B:164:THR:O	1:B:165:SER:HB2	2.18	0.42
3:F:198:ASP:OD1	3:F:200:HIS:HE1	2.01	0.42
3:F:201:VAL:HG22	3:F:202:LYS:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:201:VAL:CG2	3:F:206:GLU:CD	2.92	0.42
1:B:31:ILE:HD13	1:B:117:SER:HA	2.02	0.42
1:A:75:SER:OG	1:A:184:MET:HE2	2.20	0.42
1:A:133:ALA:HB2	1:A:177:LEU:HB3	2.01	0.42
3:F:159:CYS:O	3:F:165:GLY:HA2	2.19	0.42
3:F:210:ILE:HA	3:F:211:PRO:HD3	1.83	0.42
1:B:86:MET:HB3	1:B:90:ASP:HB2	2.00	0.41
2:C:179:ILE:HD12	2:C:215:TYR:CD2	2.55	0.41
1:A:147:GLN:HE22	1:A:169:LEU:N	2.06	0.41
1:B:189:GLU:HG3	1:B:190:ARG:H	1.84	0.41
1:B:133:ALA:HB2	1:B:177:LEU:HB3	2.03	0.41
1:A:47:ILE:HD12	1:A:47:ILE:HA	1.95	0.41
3:F:179:SER:HA	3:F:214:THR:O	2.20	0.41
1:A:30:GLU:HB2	1:A:195:LEU:HD21	2.01	0.41
1:A:70:PRO:HG3	1:A:192:ILE:CD1	2.51	0.41
1:B:-2:HIS:HA	2:C:215:TYR:O	2.21	0.41
3:F:188:HIS:CE1	3:F:189:ASP:OD1	2.74	0.41
1:A:139:THR:HB	1:A:149:VAL:HG22	2.02	0.40
1:B:75:SER:HA	1:B:184:MET:HE1	2.03	0.40
3:E:201:VAL:CG1	3:E:206:GLU:HB3	2.51	0.40
3:E:200:HIS:HD2	7:E:2023:HOH:O	2.04	0.40
1:B:97:THR:CG2	7:B:2034:HOH:O	2.66	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	211/214 (99%)	195 (92%)	13 (6%)	3 (1%)	9	7
1	B	211/214 (99%)	198 (94%)	12 (6%)	1 (0%)	24	27
2	C	90/92 (98%)	85 (94%)	4 (4%)	1 (1%)	11	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	90/92 (98%)	85 (94%)	5 (6%)	0	100	100
3	E	72/74 (97%)	68 (94%)	2 (3%)	2 (3%)	4	2
3	F	72/74 (97%)	69 (96%)	2 (3%)	1 (1%)	9	7
All	All	746/760 (98%)	700 (94%)	38 (5%)	8 (1%)	11	10

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	165	SER
1	B	165	SER
3	E	170	GLU
3	E	202	LYS
1	A	1	ALA
1	A	168	GLN
3	F	170	GLU
2	C	170	LYS

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	183/184 (100%)	165 (90%)	18 (10%)	7	8
1	B	182/184 (99%)	161 (88%)	21 (12%)	5	5
2	C	81/81 (100%)	71 (88%)	10 (12%)	4	4
2	D	81/81 (100%)	73 (90%)	8 (10%)	7	8
3	E	65/65 (100%)	60 (92%)	5 (8%)	12	13
3	F	64/65 (98%)	59 (92%)	5 (8%)	11	13
All	All	656/660 (99%)	589 (90%)	67 (10%)	7	7

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LEU
1	A	28	ASN
1	A	61	GLN
1	A	63	GLU
1	A	77	LEU
1	A	87	THR
1	A	97	THR
1	A	107	MET
1	A	117	SER
1	A	137	VAL
1	A	139	THR
1	A	169	LEU
1	A	173	THR
1	A	177	LEU
1	A	184	MET
1	A	193	LYS
1	A	203	ILE
1	A	209	LEU
1	B	3	THR
1	B	18	LEU
1	B	24	THR
1	B	61	GLN
1	B	63	GLU
1	B	76	THR
1	B	77	LEU
1	B	78	THR
1	B	89	SER
1	B	97	THR
1	B	100	ARG
1	B	104	LYS
1	B	137	VAL
1	B	139	THR
1	B	169	LEU
1	B	177	LEU
1	B	193	LYS
1	B	197	LYS
1	B	203	ILE
1	B	204	SER
1	B	209	LEU
2	C	151	LYS
2	C	162	GLU
2	C	174	LYS
2	C	175	GLN

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Mol	Chain	Res	Type
2	C	192	VAL
2	C	195	GLU
2	C	214	LYS
2	C	232	ILE
2	C	237	LEU
2	C	241	LYS
2	D	162	GLU
2	D	175	GLN
2	D	191	GLU
2	D	192	VAL
2	D	195	GLU
2	D	232	ILE
2	D	237	LEU
2	D	241	LYS
3	E	151	ILE
3	E	171	ARG
3	E	173	ASN
3	E	191	LEU
3	E	201	VAL
3	F	150	VAL
3	F	173	ASN
3	F	179	SER
3	F	191	LEU
3	F	199	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	16	GLN
1	A	23	ASN
1	A	28	ASN
1	A	61	GLN
1	A	94	ASN
1	A	121	GLN
1	A	147	GLN
1	A	183	GLN
1	B	-2	HIS
1	B	-1	HIS
1	B	11	GLN
1	B	16	GLN
1	B	23	ASN

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Mol	Chain	Res	Type
1	B	61	GLN
1	B	94	ASN
1	B	121	GLN
1	B	147	GLN
1	B	153	GLN
1	B	183	GLN
2	C	158	GLN
2	C	175	GLN
2	C	178	ASN
2	D	158	GLN
2	D	175	GLN
3	E	157	GLN
3	E	173	ASN
3	E	174	HIS
3	E	180	HIS
3	E	200	HIS
3	F	157	GLN
3	F	173	ASN
3	F	174	HIS
3	F	200	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 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 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
4	ADP	A	1211	5	28,29,29	1.58	5 (17%)	43,45,45	1.69	8 (18%)
4	ADP	B	1211	5	28,29,29	1.62	5 (17%)	43,45,45	1.64	8 (18%)

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
4	ADP	A	1211	5	-	3/16/32/32	0/3/3/3
4	ADP	B	1211	5	-	2/16/32/32	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1211	ADP	C5-C4	5.22	1.48	1.39
4	A	1211	ADP	C5-C4	4.97	1.48	1.39
4	B	1211	ADP	PA-O3A	3.47	1.63	1.59
4	A	1211	ADP	PA-O3A	3.38	1.63	1.59
4	B	1211	ADP	C5-C6	2.94	1.49	1.41
4	A	1211	ADP	C8-N7	2.92	1.37	1.31
4	A	1211	ADP	C5-C6	2.92	1.49	1.41
4	B	1211	ADP	C8-N7	2.82	1.37	1.31
4	B	1211	ADP	C5-N7	-2.10	1.35	1.39
4	A	1211	ADP	C5-N7	-2.00	1.35	1.39

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1211	ADP	C5-C4-N3	-5.64	118.94	126.72
4	B	1211	ADP	C5-C4-N3	-5.31	119.41	126.72
4	A	1211	ADP	N3-C4-N9	4.07	134.08	127.17
4	B	1211	ADP	N3-C4-N9	3.81	133.65	127.17
4	A	1211	ADP	C2-N3-C4	3.65	120.75	111.83
4	A	1211	ADP	C4-C5-N7	-3.61	106.46	110.58
4	B	1211	ADP	C4-C5-N7	-3.56	106.51	110.58
4	B	1211	ADP	C2-N3-C4	3.38	120.08	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1211	ADP	N3-C2-N1	-3.09	123.91	128.58
4	B	1211	ADP	N3-C2-N1	-2.98	124.08	128.58
4	A	1211	ADP	C5-N7-C8	2.46	107.32	103.45
4	B	1211	ADP	C5-N7-C8	2.33	107.11	103.45
4	A	1211	ADP	C6-C5-N7	2.26	136.45	132.09
4	B	1211	ADP	C6-C5-N7	2.16	136.26	132.09
4	A	1211	ADP	C4-N9-C8	2.09	107.94	105.74
4	B	1211	ADP	C2-N1-C6	2.06	122.12	118.73

There are no chirality outliers.

All (5) torsion outliers are listed below:

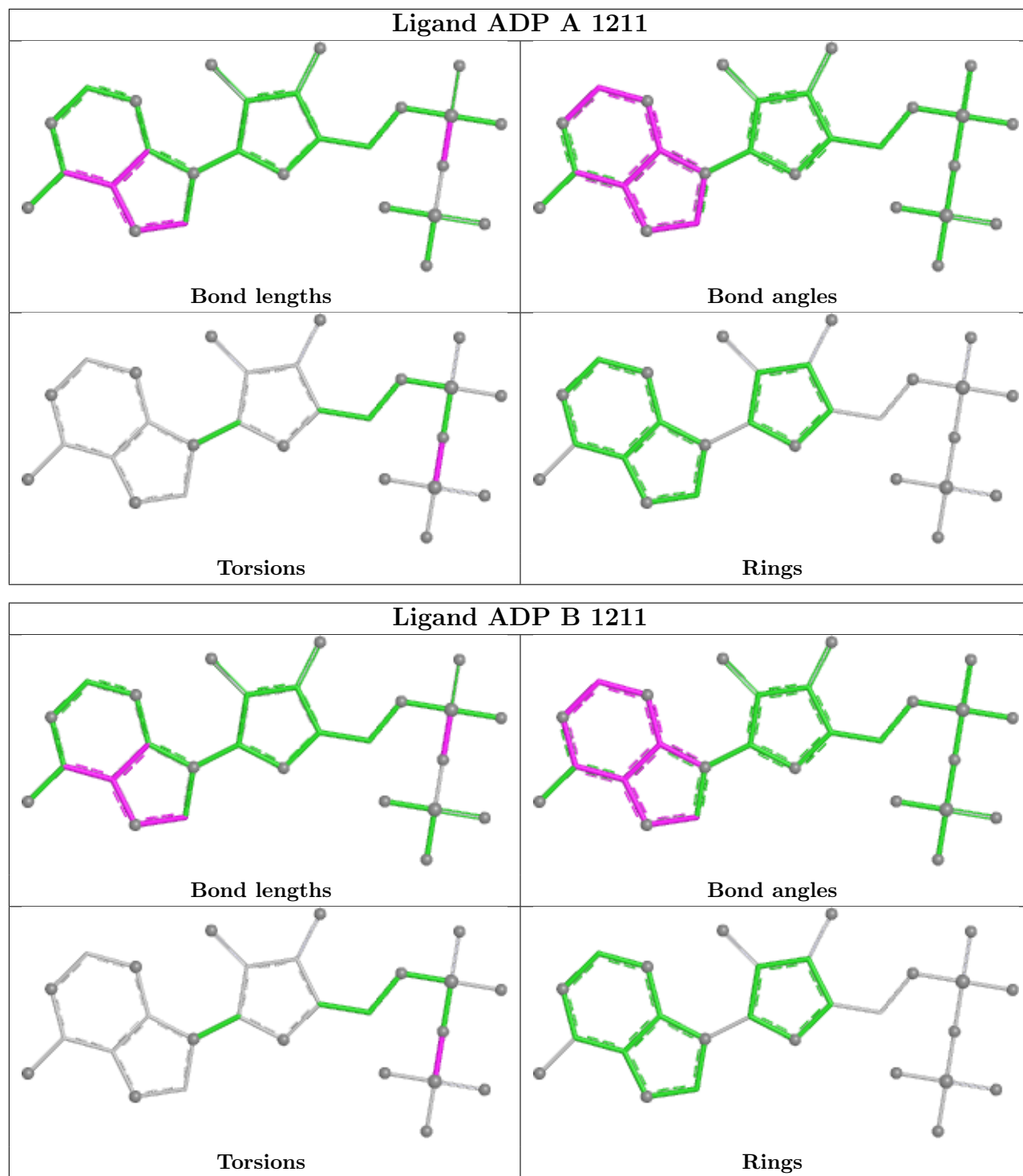
Mol	Chain	Res	Type	Atoms
4	A	1211	ADP	PA-O3A-PB-O2B
4	A	1211	ADP	PA-O3A-PB-O3B
4	B	1211	ADP	PA-O3A-PB-O2B
4	B	1211	ADP	PA-O3A-PB-O3B
4	A	1211	ADP	PA-O3A-PB-O1B

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1211	ADP	2	0
4	B	1211	ADP	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.



5.7 Other polymers [i](#)

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	213/214 (99%)	0.28	17 (7%) 18 16	17, 30, 58, 70	0
1	B	213/214 (99%)	0.21	15 (7%) 22 19	17, 30, 57, 70	0
2	C	92/92 (100%)	0.12	6 (6%) 25 22	20, 29, 56, 77	0
2	D	92/92 (100%)	0.22	9 (9%) 13 10	20, 30, 58, 79	0
3	E	74/74 (100%)	0.06	4 (5%) 31 28	21, 27, 43, 53	0
3	F	74/74 (100%)	0.13	4 (5%) 31 28	21, 27, 45, 53	0
All	All	758/760 (99%)	0.20	55 (7%) 21 18	17, 29, 56, 79	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	-1	HIS	7.8
1	B	2	ALA	6.3
1	A	210	TRP	5.7
2	D	193	PRO	5.5
1	A	2	ALA	5.2
1	B	-1	HIS	5.2
2	C	193	PRO	4.6
2	D	194	GLY	4.2
1	A	1	ALA	4.2
1	B	1	ALA	4.0
1	B	0	ALA	4.0
1	B	210	TRP	3.7
2	D	171	GLY	3.7
2	D	192	VAL	3.7
1	A	164	THR	3.4
1	B	189	GLU	3.3
1	A	0	ALA	3.3
2	C	192	VAL	3.2
1	A	4	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	164	THR	3.2
2	D	240	GLY	3.1
2	C	194	GLY	3.1
1	A	105	GLU	3.0
1	B	-2	HIS	3.0
1	A	-2	HIS	2.9
2	C	171	GLY	2.8
3	F	189	ASP	2.8
1	A	112	ALA	2.7
3	F	205	ASP	2.7
3	E	201	VAL	2.6
1	B	109	ALA	2.6
2	C	150	ALA	2.5
2	D	241	LYS	2.4
2	D	195	GLU	2.4
1	B	105	GLU	2.4
3	E	171	ARG	2.3
1	B	4	GLU	2.3
1	A	109	ALA	2.3
1	A	166	GLY	2.2
2	C	195	GLU	2.2
1	A	3	THR	2.2
1	A	200	SER	2.1
3	E	148	ALA	2.1
1	B	3	THR	2.1
1	B	112	ALA	2.1
1	B	114	ALA	2.1
3	E	221	SER	2.1
1	A	118	MET	2.1
1	B	165	SER	2.1
3	F	220	SER	2.1
1	A	203	ILE	2.1
2	D	172	ILE	2.1
3	F	179	SER	2.0
1	A	25	PHE	2.0
2	D	150	ALA	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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

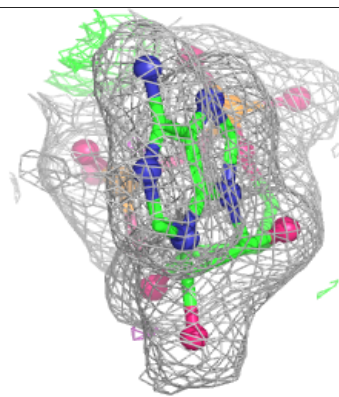
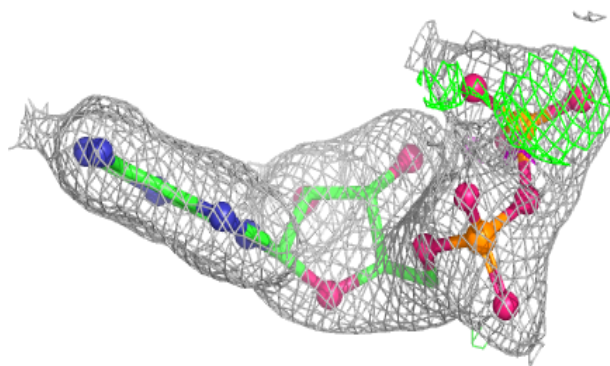
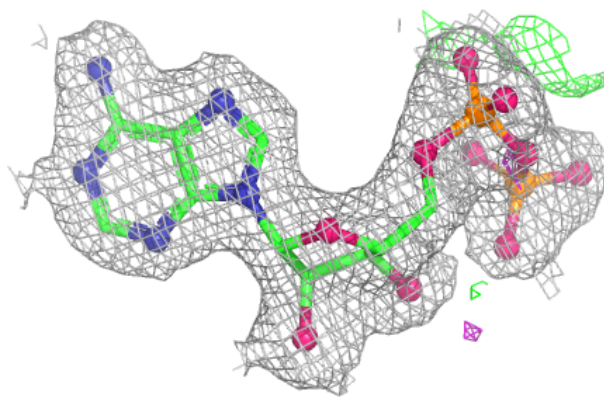
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	MG	A	1212	1/1	0.95	0.12	23,23,23,23	0
5	MG	B	1212	1/1	0.95	0.14	22,22,22,22	0
4	ADP	B	1211	27/27	0.97	0.06	17,23,27,33	0
4	ADP	A	1211	27/27	0.98	0.05	20,23,27,28	0
6	ZN	E	1222	1/1	1.00	0.01	20,20,20,20	0
6	ZN	E	1223	1/1	1.00	0.01	22,22,22,22	0
6	ZN	F	1222	1/1	1.00	0.01	21,21,21,21	0
6	ZN	F	1223	1/1	1.00	0.01	22,22,22,22	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.

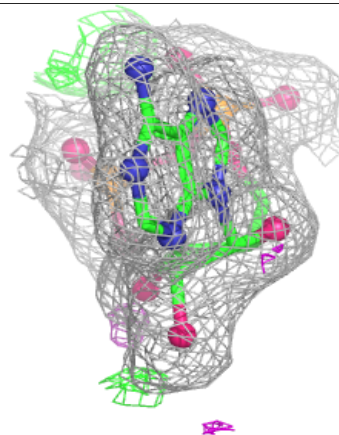
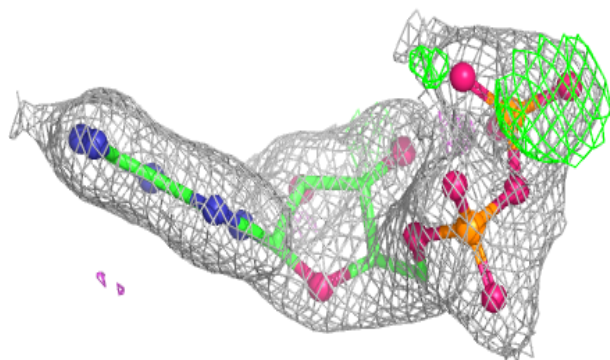
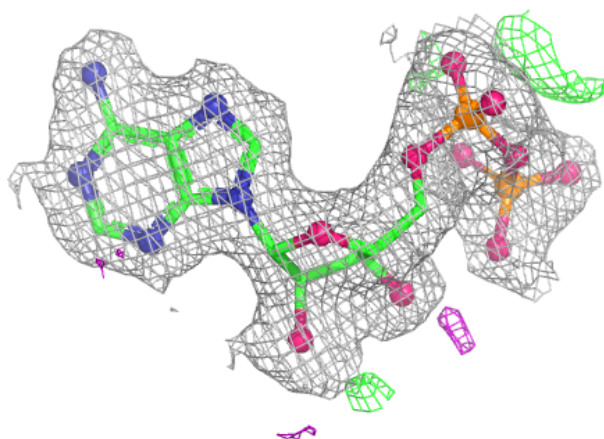
Electron density around ADP B 1211:

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



Electron density around ADP A 1211:

$2mF_o-DF_c$ (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.