



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:35 PM UTC

PDB ID : 1NY5 / pdb_00001ny5
Title : Crystal structure of sigm54 activator (AAA+ ATPase) in the inactive state
Authors : Lee, S.Y.; de la Torre, A.; Kustu, S.; Nixon, B.T.; Wemmer, D.E.
Deposited on : 2003-02-11
Resolution : 2.40 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

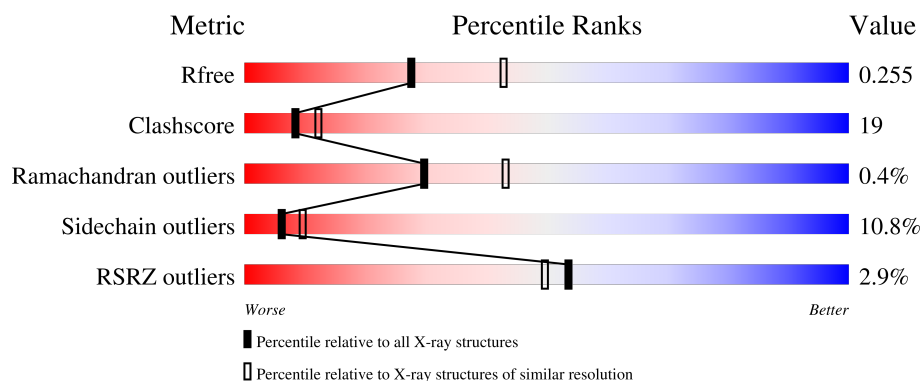
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	387	2% 61% 33% 5% ..
1	B	387	4% 57% 35% 7% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MG	A	500	-	-	-	X
5	GOL	B	400	-	X	-	-
5	GOL	B	401	-	X	-	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6545 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.

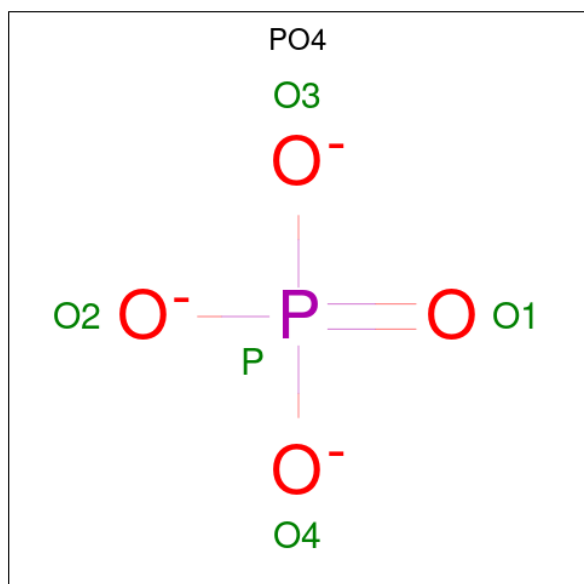
- Molecule 1 is a protein called transcriptional regulator (NtrC family).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	384	Total	C	N	O	S	0	0	0
			3091	1989	519	573	10			
1	B	385	Total	C	N	O	S	0	0	0
			3099	1993	521	575	10			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



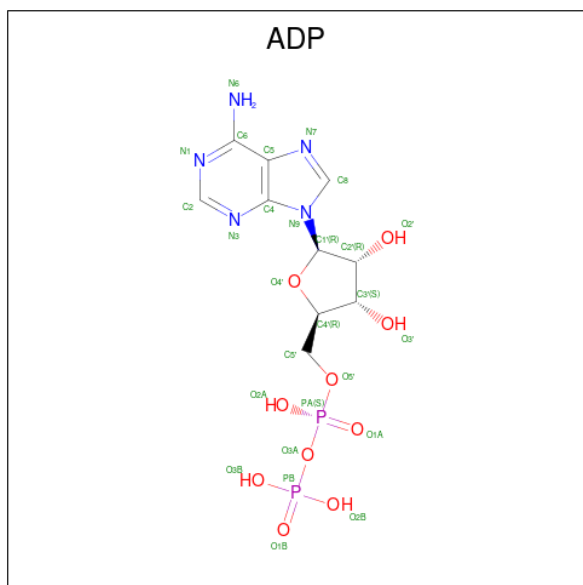
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		

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

- 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 27	C 10	N 5	O 10	P 2	0	0
4	B	1	Total 27	C 10	N 5	O 10	P 2	0	0

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

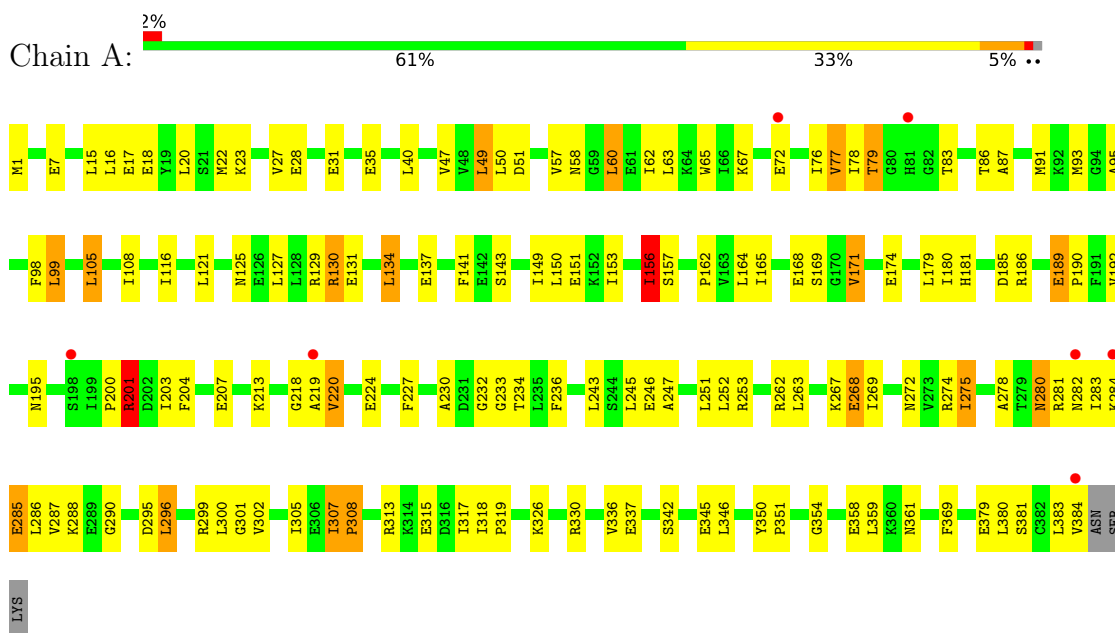
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	173	Total	O	0	0
			173	173		
6	B	95	Total	O	0	0
			95	95		

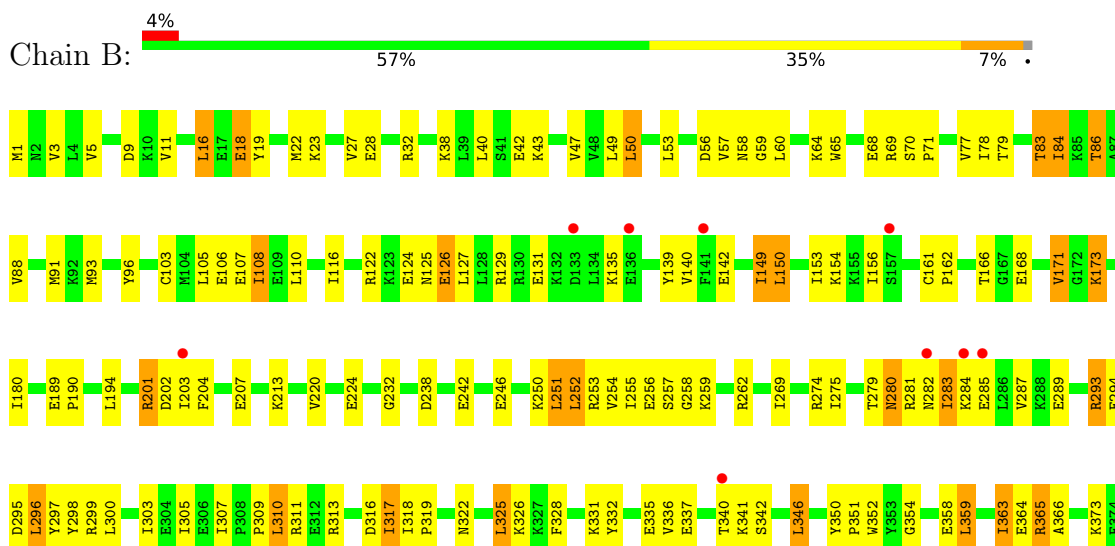
3 Residue-property plots

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: transcriptional regulator (NtrC family)



- Molecule 1: transcriptional regulator (NtrC family)



I375	
D376	
R377	
G378	
E379	
L380	
S381	
C382	
L383	
V384	
N385	
SER	
LYS	

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	94.77 Å 94.77 Å 195.01 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.62 – 2.40 42.62 – 2.40	Depositor EDS
% Data completeness (in resolution range)	90.6 (42.62-2.40) 90.7 (42.62-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.74 (at 2.39 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.213 , 0.257 0.213 , 0.255	Depositor DCC
R_{free} test set	1827 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	50.8	Xtriage
Anisotropy	0.226	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 49.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6545	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% 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: ADP, MG, PO4, GOL

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	0.46	0/3139	0.94	8/4210 (0.2%)
1	B	0.41	0/3147	0.92	8/4221 (0.2%)
All	All	0.43	0/6286	0.93	16/8431 (0.2%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	317	ILE	N-CA-C	8.87	119.67	110.36
1	A	307	ILE	CA-C-N	8.43	125.81	119.66
1	A	307	ILE	C-N-CA	8.43	125.81	119.66
1	B	377	ARG	N-CA-C	-6.74	104.00	111.82
1	A	308	PRO	N-CA-C	5.81	116.04	110.47
1	A	156	ILE	N-CA-C	5.67	116.72	111.45
1	A	204	PHE	N-CA-C	5.54	117.01	110.97
1	B	139	TYR	N-CA-C	5.53	118.64	110.46
1	B	149	ILE	N-CA-C	-5.39	105.12	110.62
1	A	201	ARG	N-CA-C	5.35	117.80	111.33
1	B	204	PHE	N-CA-C	5.33	117.50	111.11
1	B	140	VAL	N-CA-C	5.09	115.18	107.75
1	B	332	TYR	N-CA-C	5.08	118.78	112.59
1	B	380	LEU	N-CA-C	-5.04	107.18	113.38
1	B	262	ARG	N-CA-C	-5.03	104.22	110.41
1	A	268	GLU	N-CA-C	5.00	117.48	110.23

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	3091	0	3211	117	0
1	B	3099	0	3217	133	0
2	A	1	0	0	0	0
3	A	15	0	0	2	0
3	B	5	0	0	0	0
4	A	27	0	12	0	0
4	B	27	0	12	0	0
5	B	12	0	8	2	0
6	A	173	0	0	13	0
6	B	95	0	0	7	0
All	All	6545	0	6460	243	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 19.

All (243) 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:B:189:GLU:HG3	1:B:190:PRO:HD2	1.30	1.12
1:B:365:ARG:HE	1:B:383:LEU:HD22	1.30	0.94
1:B:150:LEU:HD22	1:B:154:LYS:HE3	1.50	0.93
1:A:63:LEU:HD23	1:A:93:MET:HE3	1.52	0.91
1:A:60:LEU:HG	1:A:93:MET:HE1	1.58	0.85
1:A:280:ASN:ND2	1:A:281:ARG:HG3	1.93	0.84
1:A:67:LYS:HE2	1:A:67:LYS:HA	1.58	0.83
1:B:365:ARG:HE	1:B:383:LEU:CD2	1.93	0.82
1:A:186:ARG:HH22	1:A:272:ASN:HD21	1.31	0.78
1:B:242:GLU:HG2	1:B:281:ARG:HH12	1.48	0.77
1:A:186:ARG:HH22	1:A:272:ASN:ND2	1.83	0.75
1:A:326:LYS:HE2	1:A:330:ARG:HH21	1.51	0.74
1:B:375:ILE:HA	1:B:379:GLU:OE1	1.87	0.74
1:B:337:GLU:HG2	1:B:373:LYS:HG2	1.70	0.73
1:A:47:VAL:HG12	6:A:774:HOH:O	1.87	0.72
1:B:105:LEU:O	1:B:105:LEU:HD23	1.90	0.72
1:B:18:GLU:O	1:B:22:MET:HG3	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:ARG:HH11	1:B:201:ARG:HB2	1.54	0.70
1:B:346:LEU:HD21	1:B:385:ASN:HB2	1.74	0.70
1:B:168:GLU:O	1:B:171:VAL:HB	1.91	0.69
1:A:57:VAL:HG12	1:A:58:ASN:N	2.08	0.69
1:A:60:LEU:HG	1:A:93:MET:CE	2.23	0.68
1:A:1:MET:HE1	1:A:116:ILE:HD11	1.73	0.68
1:B:189:GLU:HG2	1:B:232:GLY:C	2.18	0.68
1:A:171:VAL:HG13	1:A:307:ILE:HG22	1.74	0.68
1:B:316:ASP:O	1:B:319:PRO:HD2	1.93	0.68
1:A:282:ASN:HD22	1:A:285:GLU:H	1.37	0.68
6:A:640:HOH:O	1:B:135:LYS:HD3	1.95	0.67
1:A:189:GLU:HG2	1:A:232:GLY:O	1.95	0.67
1:B:153:ILE:HG23	1:B:180:ILE:HG12	1.77	0.67
1:A:83:THR:O	1:A:86:THR:HG22	1.95	0.66
1:A:280:ASN:C	1:A:280:ASN:HD22	2.04	0.65
1:A:253:ARG:HB3	6:A:760:HOH:O	1.97	0.65
1:B:64:LYS:O	1:B:68:GLU:HG3	1.98	0.64
1:A:358:GLU:OE2	1:B:365:ARG:NH1	2.31	0.63
1:B:103:CYS:HB2	1:B:107:GLU:OE1	1.98	0.63
1:A:280:ASN:HD22	1:A:281:ARG:N	1.96	0.63
1:B:313:ARG:HD2	1:B:316:ASP:OD2	1.99	0.62
1:A:153:ILE:HG23	1:A:180:ILE:HG12	1.81	0.62
1:B:354:GLY:HA3	1:B:358:GLU:HB2	1.80	0.62
1:B:38:LYS:O	1:B:42:GLU:HG3	1.98	0.62
1:B:242:GLU:HG2	1:B:281:ARG:NH1	2.15	0.62
1:B:280:ASN:HD22	1:B:280:ASN:H	1.47	0.62
1:A:171:VAL:HG13	1:A:307:ILE:CG2	2.29	0.61
1:A:384:VAL:HA	1:B:365:ARG:HH22	1.65	0.61
1:A:263:LEU:HD13	6:A:747:HOH:O	1.99	0.61
1:A:50:LEU:HD11	1:A:62:ILE:HD12	1.82	0.60
1:A:308:PRO:HG2	1:A:313:ARG:HD2	1.83	0.60
1:B:5:VAL:HG22	1:B:49:LEU:HD12	1.84	0.60
1:B:340:THR:HG22	1:B:342:SER:H	1.66	0.60
1:B:284:LYS:HE2	1:B:297:TYR:OH	2.02	0.59
1:A:83:THR:HG22	1:A:86:THR:HG22	1.85	0.59
1:B:79:THR:OG1	1:B:83:THR:HB	2.03	0.59
1:B:57:VAL:HG12	1:B:58:ASN:N	2.18	0.58
1:A:49:LEU:HD22	6:A:774:HOH:O	2.02	0.58
1:A:218:GLY:O	1:A:220:VAL:N	2.36	0.58
1:A:299:ARG:O	1:A:302:VAL:HG23	2.03	0.58
1:B:285:GLU:O	1:B:289:GLU:HG3	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:THR:HG21	1:A:87:ALA:HB2	1.87	0.57
1:A:49:LEU:HD13	6:A:774:HOH:O	2.03	0.57
1:A:282:ASN:ND2	1:A:285:GLU:H	2.03	0.57
1:B:201:ARG:HH11	1:B:201:ARG:CB	2.18	0.57
1:A:379:GLU:O	1:A:383:LEU:HG	2.04	0.57
1:A:203:ILE:O	1:A:207:GLU:HG3	2.04	0.56
1:B:16:LEU:HG	1:B:49:LEU:HD13	1.88	0.56
1:A:149:ILE:O	1:A:153:ILE:HG13	2.05	0.56
1:B:283:ILE:O	1:B:287:VAL:HG23	2.05	0.56
1:A:201:ARG:HB2	1:A:201:ARG:HH11	1.71	0.56
1:B:32:ARG:HB2	1:B:56:ASP:OD1	2.05	0.56
1:A:134:LEU:HD21	1:B:194:LEU:CD2	2.35	0.55
1:A:262:ARG:HG3	1:A:269:ILE:CD1	2.36	0.55
1:A:280:ASN:HD22	1:A:281:ARG:HG3	1.70	0.55
1:B:91:MET:HE3	1:B:96:TYR:O	2.06	0.55
1:B:203:ILE:HG22	1:B:207:GLU:HG3	1.89	0.55
1:B:335:GLU:O	1:B:373:LYS:HA	2.07	0.55
1:B:201:ARG:HH11	1:B:201:ARG:CG	2.20	0.55
1:A:77:VAL:O	1:A:98:PHE:HA	2.06	0.54
1:B:127:LEU:O	1:B:131:GLU:HG3	2.06	0.54
1:B:341:LYS:N	1:B:341:LYS:HD3	2.22	0.54
1:B:161:CYS:HB2	1:B:162:PRO:HD2	1.89	0.54
1:A:318:ILE:HB	1:A:319:PRO:HD3	1.90	0.54
1:B:27:VAL:HG12	1:B:28:GLU:N	2.22	0.54
1:A:369:PHE:HE2	1:A:379:GLU:HG2	1.72	0.53
1:A:280:ASN:HD21	1:A:281:ARG:HG3	1.70	0.53
1:B:149:ILE:O	1:B:153:ILE:HG13	2.09	0.53
1:B:365:ARG:NE	1:B:383:LEU:HD22	2.13	0.53
1:A:151:GLU:HG2	6:A:773:HOH:O	2.08	0.52
1:B:60:LEU:HD22	1:B:93:MET:SD	2.50	0.52
1:A:380:LEU:O	1:A:384:VAL:HG22	2.09	0.52
1:A:192:VAL:HG21	1:A:230:ALA:HB2	1.91	0.52
1:A:165:ILE:O	1:A:278:ALA:HA	2.10	0.52
1:B:122:ARG:NH1	6:B:686:HOH:O	2.43	0.52
1:A:186:ARG:NH2	1:A:272:ASN:HD21	2.05	0.52
1:B:213:LYS:HG3	1:B:220:VAL:O	2.10	0.52
1:B:250:LYS:HE3	6:B:671:HOH:O	2.09	0.52
1:B:252:LEU:O	1:B:256:GLU:HG3	2.09	0.52
1:A:57:VAL:CG1	1:A:58:ASN:N	2.72	0.51
1:A:189:GLU:HG3	1:A:190:PRO:HD2	1.92	0.51
1:B:251:LEU:O	1:B:255:ILE:HG13	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:346:LEU:HD21	1:B:385:ASN:CB	2.41	0.51
1:B:1:MET:HE1	1:B:116:ILE:HG23	1.93	0.51
1:A:51:ASP:HA	1:A:78:ILE:HB	1.92	0.51
1:B:257:SER:O	1:B:259:LYS:HG3	2.11	0.51
1:A:125:ASN:O	1:A:129:ARG:HB2	2.11	0.51
1:B:189:GLU:CG	1:B:190:PRO:HD2	2.20	0.51
1:B:341:LYS:CD	1:B:341:LYS:H	2.22	0.51
1:B:359:LEU:HD22	1:B:363:ILE:CD1	2.40	0.51
1:A:342:SER:HB3	3:A:603:PO4:O3	2.10	0.51
1:B:125:ASN:O	1:B:129:ARG:HG3	2.11	0.50
1:B:365:ARG:NE	1:B:383:LEU:CD2	2.70	0.50
1:A:7:GLU:OE1	1:A:51:ASP:HB2	2.11	0.50
1:A:295:ASP:O	1:A:299:ARG:HG2	2.11	0.50
1:B:316:ASP:C	1:B:319:PRO:HD2	2.37	0.50
1:A:151:GLU:HG3	6:A:756:HOH:O	2.11	0.50
1:B:359:LEU:HD22	1:B:363:ILE:HD13	1.94	0.50
1:A:200:PRO:HG2	1:A:203:ILE:CG1	2.42	0.50
1:B:311:ARG:HG2	1:B:351:PRO:O	2.11	0.50
1:A:296:LEU:HD22	1:A:300:LEU:HG	1.93	0.50
1:A:125:ASN:HB3	1:A:129:ARG:NH2	2.27	0.49
1:A:1:MET:HE1	1:A:116:ILE:CD1	2.42	0.49
1:A:168:GLU:O	1:A:171:VAL:HB	2.12	0.49
1:A:189:GLU:HG2	1:A:232:GLY:C	2.37	0.49
1:B:341:LYS:HD3	1:B:341:LYS:H	1.77	0.49
1:B:189:GLU:HG2	1:B:232:GLY:O	2.12	0.49
1:B:293:ARG:HG3	1:B:293:ARG:HH11	1.78	0.49
1:A:267:LYS:NZ	5:B:401:GOL:H11	2.27	0.49
1:B:280:ASN:HD22	1:B:280:ASN:N	2.07	0.49
1:A:27:VAL:HG12	1:A:28:GLU:N	2.28	0.49
1:A:156:ILE:CD1	1:A:305:ILE:HD11	2.43	0.49
3:A:600:PO4:O1	1:B:224:GLU:OE2	2.31	0.49
1:A:130:ARG:NH2	1:B:224:GLU:O	2.45	0.48
1:B:319:PRO:HD3	6:B:676:HOH:O	2.13	0.48
1:A:181:HIS:HD2	1:A:234:THR:OG1	1.97	0.48
1:A:280:ASN:ND2	1:A:280:ASN:C	2.67	0.48
1:B:19:TYR:O	1:B:23:LYS:HG2	2.13	0.48
1:B:38:LYS:HE2	6:B:656:HOH:O	2.13	0.48
1:B:280:ASN:H	1:B:280:ASN:ND2	2.11	0.48
1:A:189:GLU:HB3	1:A:233:GLY:HA2	1.96	0.48
1:B:168:GLU:OE1	1:B:309:PRO:HG3	2.13	0.48
1:A:141:PHE:CZ	1:A:179:LEU:HD11	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:LEU:O	1:A:20:LEU:HG	2.15	0.47
1:A:49:LEU:CD1	1:A:76:ILE:HB	2.44	0.47
1:B:325:LEU:HD21	1:B:336:VAL:CG1	2.44	0.47
1:B:378:GLY:O	1:B:381:SER:HB3	2.13	0.47
1:B:3:VAL:HG22	1:B:47:VAL:HB	1.96	0.47
1:B:57:VAL:HG12	1:B:58:ASN:H	1.76	0.47
1:B:309:PRO:O	1:B:313:ARG:HG2	2.14	0.47
1:A:350:TYR:CD1	1:A:351:PRO:HD2	2.50	0.47
1:B:352:TRP:CH2	1:B:359:LEU:HD23	2.49	0.47
1:A:253:ARG:NH2	1:A:268:GLU:OE2	2.48	0.47
1:A:354:GLY:HA3	1:A:358:GLU:HB2	1.97	0.47
1:B:294:GLU:HG2	6:B:693:HOH:O	2.15	0.47
1:B:337:GLU:CG	1:B:373:LYS:HG2	2.41	0.47
1:A:83:THR:HG22	1:A:86:THR:CG2	2.44	0.47
1:B:293:ARG:HG2	1:B:295:ASP:OD1	2.14	0.47
1:B:350:TYR:HD2	1:B:352:TRP:CD2	2.33	0.47
1:A:281:ARG:NH2	1:A:286:LEU:HD21	2.29	0.46
1:A:31:GLU:N	1:A:31:GLU:OE1	2.48	0.46
1:B:299:ARG:HA	1:B:299:ARG:HD2	1.79	0.46
1:B:325:LEU:HD21	1:B:336:VAL:HG12	1.97	0.46
1:B:328:PHE:CE1	1:B:364:GLU:HB2	2.49	0.46
1:B:341:LYS:H	1:B:341:LYS:CE	2.29	0.46
1:B:293:ARG:HH11	1:B:293:ARG:CG	2.27	0.46
1:B:295:ASP:OD1	1:B:295:ASP:N	2.47	0.46
1:A:105:LEU:HD13	1:A:105:LEU:O	2.15	0.46
1:B:105:LEU:HA	1:B:108:ILE:HG13	1.98	0.46
1:A:57:VAL:HG12	1:A:58:ASN:H	1.79	0.46
1:A:282:ASN:HD21	1:A:284:LYS:HB2	1.81	0.46
1:B:352:TRP:CZ3	1:B:359:LEU:HA	2.51	0.46
1:A:326:LYS:HE2	1:A:330:ARG:NH2	2.26	0.46
1:A:301:GLY:O	1:A:302:VAL:C	2.59	0.45
1:B:43:LYS:HE2	6:B:668:HOH:O	2.16	0.45
1:B:340:THR:HG22	1:B:341:LYS:N	2.32	0.45
1:B:65:TRP:O	1:B:69:ARG:HD3	2.17	0.45
1:B:251:LEU:HD21	1:B:275:ILE:HD13	1.98	0.45
1:B:310:LEU:HD22	1:B:317:ILE:HG12	1.99	0.45
1:A:67:LYS:HA	1:A:67:LYS:CE	2.41	0.44
1:B:350:TYR:CD1	1:B:351:PRO:HD2	2.52	0.44
1:A:60:LEU:CG	1:A:93:MET:HE1	2.37	0.44
1:B:279:THR:HG21	1:B:283:ILE:HG13	1.99	0.44
1:B:296:LEU:HD22	1:B:300:LEU:HG	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:THR:HG22	1:B:86:THR:OG1	2.18	0.44
1:B:298:TYR:HB2	6:B:640:HOH:O	2.16	0.44
1:B:105:LEU:HD23	1:B:105:LEU:C	2.42	0.44
1:B:161:CYS:SG	1:B:303:ILE:HD11	2.57	0.44
1:B:9:ASP:OD1	1:B:11:VAL:HB	2.18	0.44
1:A:156:ILE:HG22	1:A:157:SER:N	2.32	0.43
1:B:150:LEU:O	1:B:154:LYS:HG3	2.18	0.43
1:A:162:PRO:HA	1:A:275:ILE:O	2.18	0.43
1:A:49:LEU:HD12	1:A:76:ILE:HB	1.99	0.43
1:A:18:GLU:O	1:A:22:MET:HG3	2.18	0.43
1:A:99:LEU:HD21	1:A:108:ILE:HA	2.00	0.43
1:B:202:ASP:OD1	1:B:203:ILE:HG13	2.19	0.43
1:A:57:VAL:CG1	1:A:58:ASN:H	2.32	0.43
1:A:83:THR:O	1:A:83:THR:HG22	2.18	0.43
1:A:213:LYS:HG3	1:A:220:VAL:C	2.44	0.43
1:B:50:LEU:O	1:B:78:ILE:N	2.50	0.43
1:A:91:MET:HA	1:A:95:ALA:HB3	2.01	0.43
1:A:91:MET:HE3	1:B:110:LEU:HD13	2.01	0.43
1:A:156:ILE:HD12	1:A:305:ILE:HD11	2.01	0.43
1:A:174:GLU:HG3	1:A:236:PHE:CE2	2.54	0.42
1:A:361:ASN:HB3	6:A:705:HOH:O	2.19	0.42
1:B:318:ILE:HB	1:B:319:PRO:HD3	2.01	0.42
1:B:341:LYS:N	1:B:341:LYS:CD	2.80	0.42
1:A:20:LEU:HD13	1:A:27:VAL:HG22	2.01	0.42
1:A:91:MET:HE2	1:A:98:PHE:CD2	2.53	0.42
1:A:127:LEU:O	1:A:131:GLU:HG3	2.19	0.42
1:A:224:GLU:OE2	1:B:126:GLU:OE2	2.38	0.42
1:A:224:GLU:OE1	1:B:122:ARG:NH2	2.52	0.42
1:A:262:ARG:HG3	1:A:269:ILE:HD12	2.01	0.42
1:A:302:VAL:HG21	6:A:630:HOH:O	2.20	0.42
1:A:143:SER:HA	1:A:315:GLU:HB2	2.02	0.42
1:B:50:LEU:O	1:B:77:VAL:HA	2.20	0.42
1:A:15:LEU:HD22	1:A:105:LEU:HD23	2.01	0.42
1:A:345:GLU:HG2	6:A:750:HOH:O	2.20	0.42
1:B:366:ALA:CA	1:B:383:LEU:HD11	2.50	0.42
1:B:350:TYR:HA	1:B:351:PRO:HD3	1.80	0.41
1:A:283:ILE:O	1:A:287:VAL:HG23	2.19	0.41
1:A:288:LYS:C	1:A:290:GLY:H	2.27	0.41
1:B:84:ILE:O	1:B:88:VAL:HG23	2.20	0.41
1:A:141:PHE:CE1	1:A:179:LEU:HD11	2.56	0.41
1:B:27:VAL:CG1	1:B:28:GLU:N	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:SER:HA	1:B:71:PRO:HD2	1.96	0.41
1:B:171:VAL:HG11	1:B:307:ILE:HB	2.01	0.41
1:B:253:ARG:HG3	1:B:253:ARG:HH11	1.86	0.41
1:B:259:LYS:HA	1:B:269:ILE:O	2.21	0.41
1:A:318:ILE:N	1:A:319:PRO:CD	2.83	0.41
1:B:156:ILE:HD11	1:B:305:ILE:HD11	2.03	0.41
1:A:213:LYS:HG3	1:A:220:VAL:O	2.20	0.41
1:B:173:LYS:NZ	1:B:280:ASN:HB3	2.36	0.41
1:B:322:ASN:O	1:B:326:LYS:HG3	2.21	0.41
1:B:341:LYS:H	1:B:341:LYS:HE2	1.86	0.41
1:A:263:LEU:HB2	6:A:747:HOH:O	2.19	0.41
1:B:366:ALA:HA	1:B:383:LEU:HD11	2.02	0.41
1:B:156:ILE:CD1	1:B:305:ILE:HD11	2.51	0.41
1:B:58:ASN:O	1:B:59:GLY:C	2.64	0.40
1:B:238:ASP:OD2	5:B:400:GOL:O1	2.39	0.40
1:A:243:LEU:HD22	1:A:247:ALA:HB1	2.03	0.40
1:A:195:ASN:HB2	6:A:633:HOH:O	2.21	0.40
1:B:161:CYS:SG	1:B:303:ILE:CD1	3.10	0.40
1:B:296:LEU:CD2	1:B:300:LEU:HG	2.52	0.40
1:A:40:LEU:HB3	1:A:65:TRP:CZ3	2.56	0.40
1:B:254:VAL:O	1:B:258:GLY:N	2.53	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	382/387 (99%)	365 (96%)	16 (4%)	1 (0%)	36	50
1	B	383/387 (99%)	366 (96%)	15 (4%)	2 (0%)	24	37
All	All	765/774 (99%)	731 (96%)	31 (4%)	3 (0%)	30	43

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	219	ALA
1	B	317	ILE
1	B	384	VAL

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	336/339 (99%)	298 (89%)	38 (11%)	5	8
1	B	337/339 (99%)	302 (90%)	35 (10%)	7	10
All	All	673/678 (99%)	600 (89%)	73 (11%)	6	9

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	GLU
1	A	23	LYS
1	A	35	GLU
1	A	49	LEU
1	A	60	LEU
1	A	72	GLU
1	A	77	VAL
1	A	79	THR
1	A	99	LEU
1	A	105	LEU
1	A	121	LEU
1	A	130	ARG
1	A	134	LEU
1	A	137	GLU
1	A	150	LEU
1	A	156	ILE
1	A	164	LEU
1	A	169	SER
1	A	171	VAL
1	A	185	ASP

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Mol	Chain	Res	Type
1	A	189	GLU
1	A	201	ARG
1	A	220	VAL
1	A	227	PHE
1	A	245	LEU
1	A	246	GLU
1	A	251	LEU
1	A	252	LEU
1	A	274	ARG
1	A	275	ILE
1	A	280	ASN
1	A	285	GLU
1	A	296	LEU
1	A	336	VAL
1	A	337	GLU
1	A	346	LEU
1	A	359	LEU
1	A	381	SER
1	B	16	LEU
1	B	18	GLU
1	B	40	LEU
1	B	50	LEU
1	B	53	LEU
1	B	83	THR
1	B	84	ILE
1	B	86	THR
1	B	106	GLU
1	B	108	ILE
1	B	124	GLU
1	B	126	GLU
1	B	142	GLU
1	B	150	LEU
1	B	166	THR
1	B	171	VAL
1	B	173	LYS
1	B	201	ARG
1	B	246	GLU
1	B	251	LEU
1	B	252	LEU
1	B	274	ARG
1	B	280	ASN
1	B	282	ASN

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Mol	Chain	Res	Type
1	B	283	ILE
1	B	293	ARG
1	B	296	LEU
1	B	310	LEU
1	B	325	LEU
1	B	331	LYS
1	B	346	LEU
1	B	359	LEU
1	B	363	ILE
1	B	365	ARG
1	B	376	ASP

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	181	HIS
1	A	272	ASN
1	A	280	ASN
1	A	282	ASN
1	A	361	ASN
1	B	280	ASN
1	B	323	HIS
1	B	361	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 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 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	PO4	A	600	-	4,4,4	1.78	1 (25%)	6,6,6	0.50	0
5	GOL	B	400	-	5,5,5	4.72	5 (100%)	5,5,5	6.15	3 (60%)
3	PO4	B	601	-	4,4,4	1.71	1 (25%)	6,6,6	0.47	0
3	PO4	A	602	-	4,4,4	1.60	0	6,6,6	0.45	0
5	GOL	B	401	-	5,5,5	4.89	5 (100%)	5,5,5	6.23	3 (60%)
4	ADP	B	602	-	28,29,29	1.62	5 (17%)	43,45,45	2.01	9 (20%)
4	ADP	A	604	2	28,29,29	1.56	5 (17%)	43,45,45	2.04	8 (18%)
3	PO4	A	603	-	4,4,4	1.66	1 (25%)	6,6,6	0.47	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
4	ADP	B	602	-	-	7/16/32/32	0/3/3/3
5	GOL	B	400	-	-	2/4/4/4	-
4	ADP	A	604	2	-	7/16/32/32	0/3/3/3
5	GOL	B	401	-	-	2/4/4/4	-

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	401	GOL	C3-C2	-8.28	1.20	1.51
5	B	400	GOL	C3-C2	-8.05	1.21	1.51
5	B	401	GOL	O1-C1	4.60	1.61	1.42
4	A	604	ADP	C5-N7	-4.33	1.31	1.39
5	B	400	GOL	O1-C1	4.17	1.59	1.42
4	B	602	ADP	C5-N7	-4.13	1.31	1.39
5	B	401	GOL	O3-C3	3.61	1.57	1.42
5	B	400	GOL	O3-C3	3.44	1.56	1.42
4	B	602	ADP	C4-N9	-3.38	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	400	GOL	C1-C2	-3.23	1.39	1.51
5	B	401	GOL	C1-C2	-3.08	1.40	1.51
4	A	604	ADP	C4-N9	-2.94	1.31	1.37
5	B	401	GOL	O2-C2	-2.70	1.35	1.43
5	B	400	GOL	O2-C2	-2.62	1.35	1.43
4	A	604	ADP	C2-N1	2.35	1.38	1.33
4	A	604	ADP	C4-N3	2.25	1.38	1.34
3	B	601	PO4	P-O3	-2.23	1.48	1.54
4	A	604	ADP	PA-O3A	-2.22	1.57	1.59
4	B	602	ADP	C5-C4	2.20	1.43	1.39
4	B	602	ADP	C5'-C4'	2.16	1.58	1.51
4	B	602	ADP	C4-N3	2.15	1.38	1.34
3	A	603	PO4	P-O3	-2.10	1.48	1.54
3	A	600	PO4	P-O4	-2.09	1.48	1.54

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	401	GOL	O3-C3-C2	11.45	161.94	110.38
5	B	400	GOL	O3-C3-C2	11.13	160.50	110.38
5	B	400	GOL	O2-C2-C3	7.41	139.87	109.18
5	B	401	GOL	O2-C2-C3	7.10	138.58	109.18
4	A	604	ADP	N3-C2-N1	-6.97	118.03	128.58
4	B	602	ADP	N3-C2-N1	-6.84	118.23	128.58
4	A	604	ADP	C5-C4-N3	-5.21	119.55	126.72
4	B	602	ADP	C5-C4-N3	-5.02	119.80	126.72
4	A	604	ADP	C2-N3-C4	4.40	122.59	111.83
4	B	602	ADP	C2-N3-C4	4.34	122.42	111.83
4	A	604	ADP	N3-C4-N9	4.09	134.12	127.17
4	B	602	ADP	N3-C4-N9	3.74	133.52	127.17
5	B	401	GOL	O1-C1-C2	3.51	126.17	110.38
4	A	604	ADP	C5-N7-C8	3.23	108.53	103.45
4	B	602	ADP	C5-N7-C8	3.16	108.41	103.45
5	B	400	GOL	O1-C1-C2	3.12	124.42	110.38
4	B	602	ADP	N9-C8-N7	-3.07	109.58	113.94
4	A	604	ADP	N9-C8-N7	-2.98	109.71	113.94
4	B	602	ADP	C4-C5-N7	-2.81	107.36	110.58
4	A	604	ADP	C4-C5-N7	-2.63	107.57	110.58
4	B	602	ADP	C4-N9-C8	2.12	107.97	105.74
4	B	602	ADP	C2-N1-C6	2.06	122.11	118.73
4	A	604	ADP	C4-N9-C8	2.02	107.86	105.74

There are no chirality outliers.

All (18) torsion outliers are listed below:

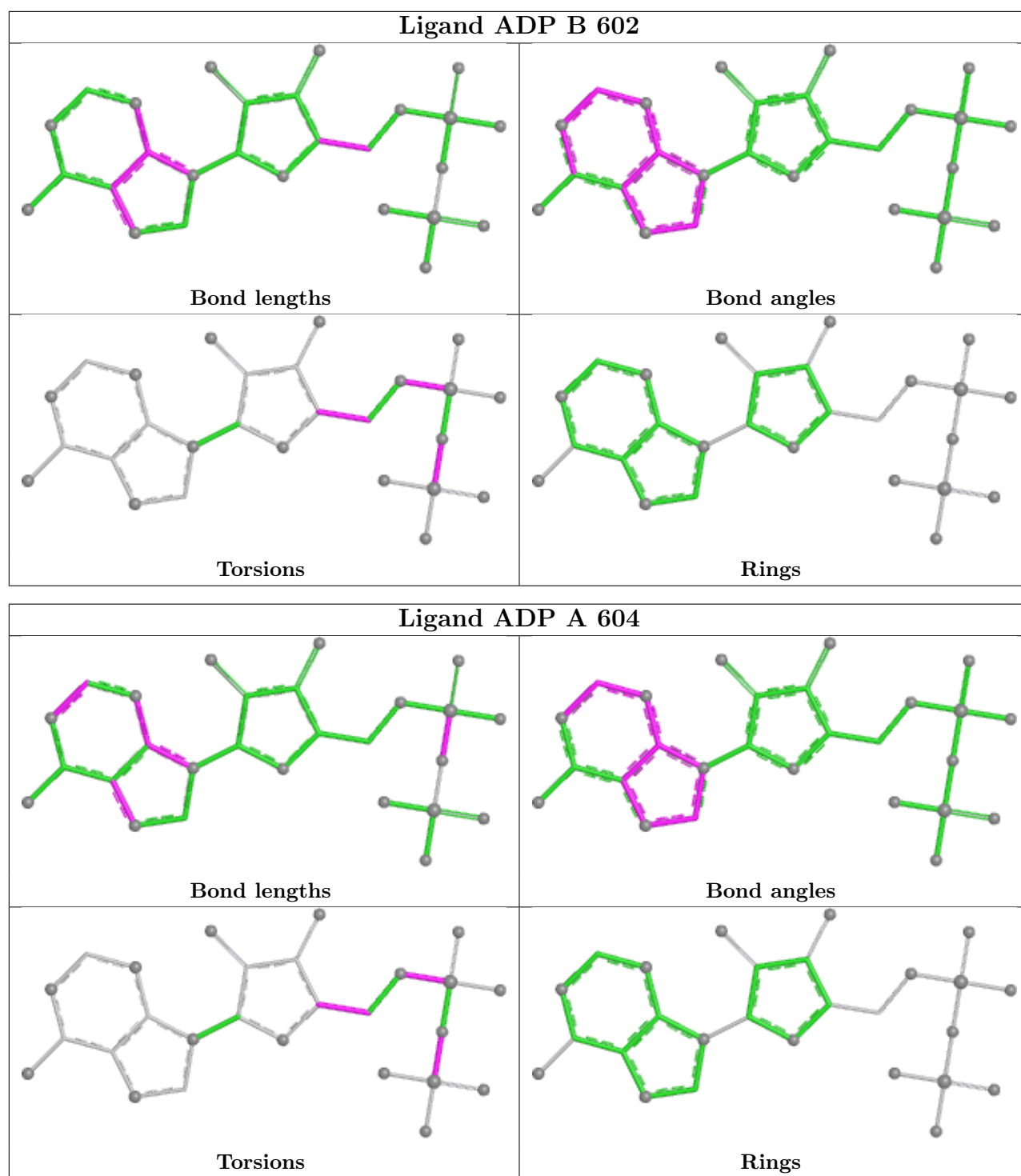
Mol	Chain	Res	Type	Atoms
4	A	604	ADP	PA-O3A-PB-O2B
4	A	604	ADP	C5'-O5'-PA-O1A
4	A	604	ADP	C5'-O5'-PA-O2A
4	A	604	ADP	C5'-O5'-PA-O3A
4	B	602	ADP	PA-O3A-PB-O2B
4	B	602	ADP	C5'-O5'-PA-O1A
4	B	602	ADP	C5'-O5'-PA-O2A
4	B	602	ADP	C5'-O5'-PA-O3A
5	B	400	GOL	C1-C2-C3-O3
5	B	401	GOL	O1-C1-C2-O2
5	B	401	GOL	C1-C2-C3-O3
4	A	604	ADP	O4'-C4'-C5'-O5'
4	A	604	ADP	C3'-C4'-C5'-O5'
4	B	602	ADP	O4'-C4'-C5'-O5'
4	B	602	ADP	C3'-C4'-C5'-O5'
5	B	400	GOL	O1-C1-C2-O2
4	B	602	ADP	PA-O3A-PB-O1B
4	A	604	ADP	PA-O3A-PB-O1B

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	600	PO4	1	0
5	B	400	GOL	1	0
5	B	401	GOL	1	0
3	A	603	PO4	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 ⓘ

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	384/387 (99%)	0.03	7 (1%) 67 63	29, 52, 89, 111	0
1	B	385/387 (99%)	0.31	15 (3%) 43 39	36, 63, 93, 110	0
All	All	769/774 (99%)	0.17	22 (2%) 53 50	29, 57, 92, 111	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	285	GLU	2.9
1	A	284	LYS	2.8
1	B	383	LEU	2.8
1	B	284	LYS	2.8
1	B	203	ILE	2.7
1	B	282	ASN	2.6
1	B	385	ASN	2.6
1	A	384	VAL	2.6
1	B	141	PHE	2.5
1	B	382	CYS	2.5
1	B	340	THR	2.5
1	B	384	VAL	2.4
1	A	219	ALA	2.4
1	B	381	SER	2.3
1	A	72	GLU	2.2
1	A	81	HIS	2.2
1	A	198	SER	2.1
1	B	157	SER	2.1
1	A	282	ASN	2.1
1	B	378	GLY	2.1
1	B	136	GLU	2.1
1	B	133	ASP	2.1

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 ⓘ

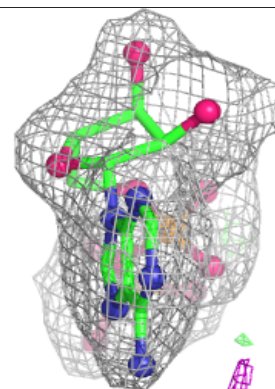
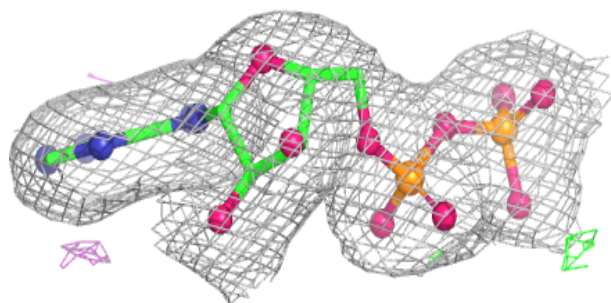
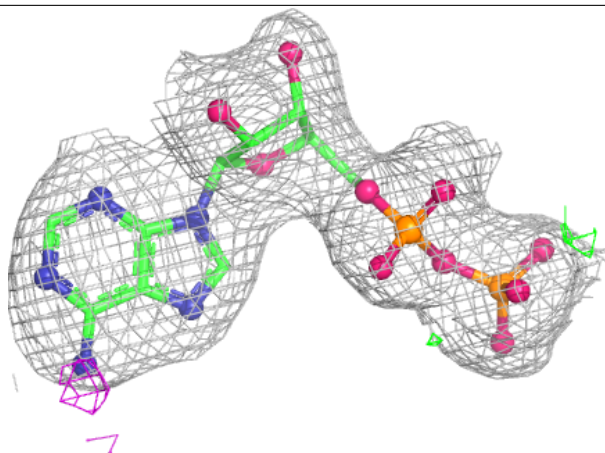
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MG	A	500	1/1	0.78	0.43	69,69,69,69	0
5	GOL	B	401	6/6	0.79	0.20	75,76,78,79	0
5	GOL	B	400	6/6	0.86	0.10	73,76,77,78	0
3	PO4	A	600	5/5	0.87	0.09	73,73,76,78	0
3	PO4	A	603	5/5	0.90	0.10	68,71,72,73	0
4	ADP	B	602	27/27	0.96	0.06	39,45,53,54	0
4	ADP	A	604	27/27	0.97	0.06	29,34,38,40	0
3	PO4	A	602	5/5	0.97	0.11	53,55,57,58	0
3	PO4	B	601	5/5	0.99	0.03	37,39,46,46	0

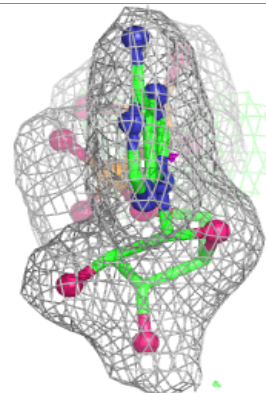
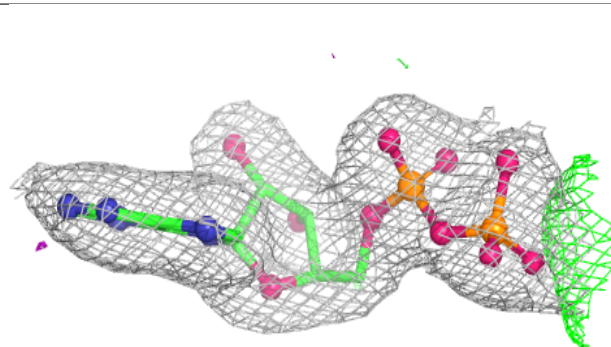
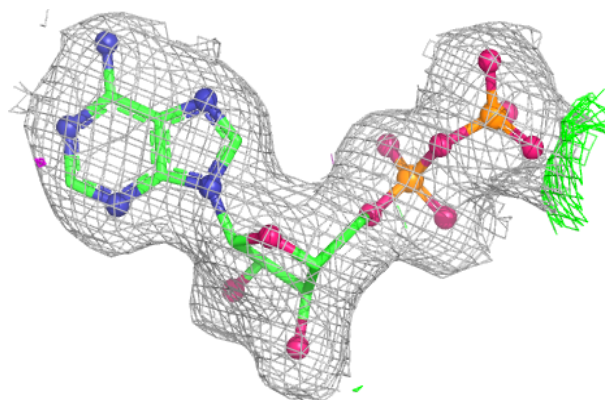
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP B 602:

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

**Electron density around ADP A 604:**

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



6.5 Other polymers ⓘ

There are no such residues in this entry.