



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:12 PM GMT

PDB ID : 1NY5  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

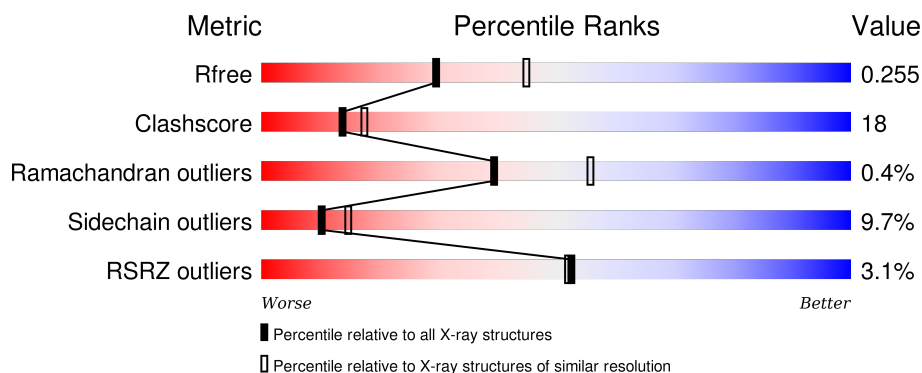
# 1 Overall quality at a glance

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))
$R_{free}$	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>3%</div> <div>63%</div> <div>33%</div> <div>• •</div> </div>
1	B	387	<div> <div>3%</div> <div>60%</div> <div>33%</div> <div>6% •</div> </div>

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.

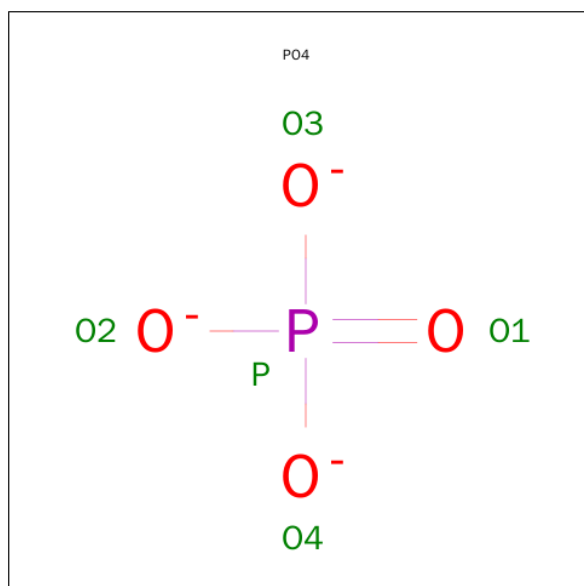
- Molecule 1 is a protein called transcriptional regulator (NtrC family).

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 (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



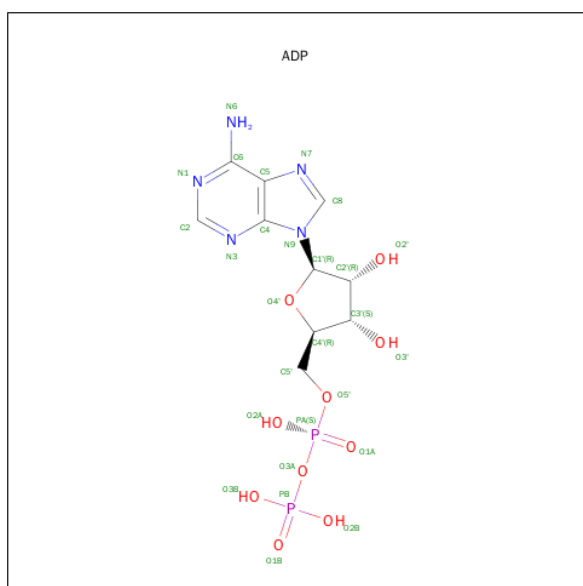
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		

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

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: 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 GLYCEROL (three-letter code: 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		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.77Å 94.77Å 195.01Å 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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.74 (at 2.39Å)	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%)	DCC
Wilson B-factor (Å <sup>2</sup> )	50.8	Xtriage
Anisotropy	0.226	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 52.6	EDS
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 36719 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6545	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, PO4, MG, 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	0.38	0/3139	0.63	0/4210
1	B	0.35	0/3147	0.60	0/4221
All	All	0.37	0/6286	0.61	0/8431

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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	112	0
1	B	3099	0	3217	130	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	235	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 18.

All (235) 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: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:60:LEU:HG	1:A:93:MET:HE2	1.66	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:HD23	1:B:105:LEU:O	1.90	0.72
1:B:18:GLU:O	1:B:22:MET:HG3	1.91	0.71
1:B:201:ARG:HB2	1:B:201:ARG:HH11	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:B:316:ASP:O	1:B:319:PRO:HD2	1.93	0.68
1:A:171:VAL:HG13	1:A:307:ILE:HG22	1.74	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: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:B:189:GLU:HG2	1:B:232:GLY:C	2.18	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:63:LEU:HD23	1:A:93:MET:HE3	1.81	0.62
1:A:153:ILE:HG23	1:A:180:ILE:HG12	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H	1:B:280:ASN:HD22	1.47	0.62
1:A:384:VAL:HA	1:B:365:ARG:HH22	1.65	0.61
1:A:171:VAL:HG13	1:A:307:ILE:CG2	2.29	0.61
1:A:263:LEU:HD13	6:A:747:HOH:O	1.99	0.61
1:A:280:ASN:C	1:A:280:ASN:HD22	2.04	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:299:ARG:O	1:A:302:VAL:HG23	2.03	0.58
1:A:218:GLY:O	1:A:220:VAL:N	2.36	0.58
1:B:285:GLU:O	1:B:289:GLU:HG3	2.04	0.58
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:CB	1:B:201:ARG:HH11	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:B:32:ARG:HB2	1:B:56:ASP:OD1	2.05	0.56
1:A:201:ARG:HB2	1:A:201:ARG:HH11	1.71	0.56
1:A:262:ARG:HG3	1:A:269:ILE:CD1	2.36	0.55
1:A:134:LEU:HD21	1:B:194:LEU:CD2	2.35	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	2.07	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:27:VAL:HG12	1:B:28:GLU:N	2.22	0.55
1:B:201:ARG:CG	1:B:201:ARG:HH11	2.20	0.55
1:B:127:LEU:O	1:B:131:GLU:HG3	2.06	0.54
1:A:77:VAL:O	1:A:98:PHE:HA	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:369:PHE:HE2	1:A:379:GLU:HG2	1.72	0.53
1:B:365:ARG:NE	1:B:383:LEU:HD22	2.13	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: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:B:122:ARG:NH1	6:B:686:HOH:O	2.43	0.52
1:A:165:ILE:O	1:A:278:ALA:HA	2.10	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:346:LEU:HD21	1:B:385:ASN:CB	2.41	0.51
1:B:251:LEU:O	1:B:255:ILE:HG13	2.11	0.51
1:B:257:SER:O	1:B:259:LYS:HG3	2.11	0.51
1:A:51:ASP:HA	1:A:78:ILE:HB	1.92	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:125:ASN:O	1:A:129:ARG:HB2	2.11	0.51
1:A:342:SER:HB3	3:A:603:PO4:O3	2.10	0.51
1:B:365:ARG:NE	1:B:383:LEU:CD2	2.70	0.50
1:A:91:MET:HE3	1:B:110:LEU:HD13	1.92	0.50
1:B:125:ASN:O	1:B:129:ARG:HG3	2.11	0.50
1:A:295:ASP:O	1:A:299:ARG:HG2	2.11	0.50
1:A:7:GLU:OE1	1:A:51:ASP:HB2	2.11	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:168:GLU:O	1:A:171:VAL:HB	2.12	0.49
1:B:341:LYS:HD3	1:B:341:LYS:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:280:ASN:N	1:B:280:ASN:HD22	2.07	0.49
1:A:267:LYS:NZ	5:B:401:GOL:H11	2.27	0.49
1:A:156:ILE:CD1	1:A:305:ILE:HD11	2.43	0.49
1:A:27:VAL:HG12	1:A:28:GLU:N	2.28	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: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
1:A:49:LEU:CD1	1:A:76:ILE:HB	2.44	0.47
1:A:16:LEU:O	1:A:20:LEU:HG	2.15	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:309:PRO:O	1:B:313:ARG:HG2	2.14	0.47
1:B:57:VAL:HG12	1:B:58:ASN:H	1.76	0.47
1:B:3:VAL:HG22	1:B:47:VAL:HB	1.96	0.47
1:A:280:ASN:C	1:A:280:ASN:ND2	2.67	0.47
1:B:352:TRP:CH2	1:B:359:LEU:HD23	2.49	0.47
1:A:350:TYR:CD1	1:A:351:PRO:HD2	2.50	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:337:GLU:CG	1:B:373:LYS:HG2	2.41	0.47
1:B:295:ASP:N	1:B:295:ASP:OD1	2.47	0.47
1:B:294:GLU:HG2	6:B:693:HOH:O	2.15	0.47
1:A:83:THR:HG22	1:A:86:THR:CG2	2.44	0.47
1:B:350:TYR:HD2	1:B:352:TRP:CD2	2.33	0.47
1:B:293:ARG:HG2	1:B:295:ASP:OD1	2.14	0.47
1:A:281:ARG:NH2	1:A:286:LEU:HD21	2.29	0.46
1:B:341:LYS:H	1:B:341:LYS:CE	2.29	0.46
1:B:325:LEU:HD21	1:B:336:VAL:HG12	1.97	0.46
1:A:31:GLU:OE1	1:A:31:GLU:N	2.48	0.46
1:B:299:ARG:HD2	1:B:299:ARG:HA	1.79	0.46
1:B:328:PHE:CE1	1:B:364:GLU:HB2	2.49	0.46
1:B:293:ARG:CG	1:B:293:ARG:HH11	2.27	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:LEU:HA	1:B:108:ILE:HG13	1.98	0.46
1:A:105:LEU:O	1:A:105:LEU:HD13	2.15	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:B:316:ASP:C	1:B:319:PRO:HD2	2.37	0.45
1:B:340:THR:HG22	1:B:341:LYS:N	2.32	0.45
1:B:43:LYS:HE2	6:B:668:HOH:O	2.16	0.45
1:A:63:LEU:HD23	1:A:93:MET:CE	2.45	0.45
1:B:251:LEU:HD21	1:B:275:ILE:HD13	1.98	0.45
1:B:65:TRP:O	1:B:69:ARG:HD3	2.17	0.45
1:B:310:LEU:HD22	1:B:317:ILE:HG12	1.99	0.45
1:A:67:LYS:CE	1:A:67:LYS:HA	2.41	0.44
1:B:350:TYR:CD1	1:B:351:PRO:HD2	2.52	0.44
1:A:189:GLU:HG2	1:A:232:GLY:C	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
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: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:B:202:ASP:OD1	1:B:203:ILE:HG13	2.19	0.43
1:A:99:LEU:HD21	1:A:108:ILE:HA	2.00	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: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: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:CD	1:B:341:LYS:N	2.80	0.42
1:A:20:LEU:HD13	1:A:27:VAL:HG22	2.01	0.42
1:A:127:LEU:O	1:A:131:GLU:HG3	2.19	0.42
1:A:302:VAL:HG21	6:A:630:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:ARG:HG3	1:A:269:ILE:HD12	2.01	0.42
1:A:224:GLU:OE1	1:B:122:ARG:NH2	2.52	0.42
1:A:224:GLU:OE2	1:B:126:GLU:OE2	2.38	0.42
1:B:50:LEU:O	1:B:77:VAL:HA	2.20	0.42
1:A:143:SER:HA	1:A:315:GLU:HB2	2.02	0.42
1:B:366:ALA:CA	1:B:383:LEU:HD11	2.50	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:350:TYR:HA	1:B:351:PRO:HD3	1.80	0.41
1:B:84:ILE:O	1:B:88:VAL:HG23	2.20	0.41
1:A:283:ILE:O	1:A:287:VAL:HG23	2.19	0.41
1:B:171:VAL:HG11	1:B:307:ILE:HB	2.01	0.41
1:B:27:VAL:CG1	1:B:28:GLU:N	2.83	0.41
1:B:259:LYS:HA	1:B:269:ILE:O	2.21	0.41
1:A:141:PHE:CE1	1:A:179:LEU:HD11	2.56	0.41
1:B:253:ARG:HH11	1:B:253:ARG:HG3	1.86	0.41
1:B:70:SER:HA	1:B:71:PRO:HD2	1.96	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:B:173:LYS:NZ	1:B:280:ASN:HB3	2.36	0.41
1:B:341:LYS:H	1:B:341:LYS:HE2	1.86	0.41
1:A:213:LYS:HG3	1:A:220:VAL:O	2.20	0.41
1:B:322:ASN:O	1:B:326:LYS:HG3	2.21	0.41
1:B:366:ALA:HA	1:B:383:LEU:HD11	2.02	0.41
1:A:263:LEU:HB2	6:A:747:HOH:O	2.19	0.41
1:B:156:ILE:CD1	1:B:305:ILE:HD11	2.51	0.41
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: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:195:ASN:HB2	6:A:633:HOH:O	2.21	0.40
1:A:301:GLY:O	1:A:302:VAL:C	2.59	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%)	46	63
1	B	383/387 (99%)	366 (96%)	15 (4%)	2 (0%)	34	48
All	All	765/774 (99%)	731 (96%)	31 (4%)	3 (0%)	39	56

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%)	301 (90%)	35 (10%)	9	12
1	B	337/339 (99%)	307 (91%)	30 (9%)	12	18
All	All	673/678 (99%)	608 (90%)	65 (10%)	10	15

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	GLU
1	A	35	GLU
1	A	49	LEU

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Mol	Chain	Res	Type
1	A	60	LEU
1	A	69	ARG
1	A	72	GLU
1	A	77	VAL
1	A	79	THR
1	A	92	LYS
1	A	99	LEU
1	A	121	LEU
1	A	130	ARG
1	A	134	LEU
1	A	137	GLU
1	A	164	LEU
1	A	169	SER
1	A	171	VAL
1	A	185	ASP
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	253	ARG
1	A	274	ARG
1	A	280	ASN
1	A	285	GLU
1	A	296	LEU
1	A	336	VAL
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	126	GLU

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Mol	Chain	Res	Type
1	B	142	GLU
1	B	150	LEU
1	B	166	THR
1	B	171	VAL
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
1	B	293	ARG
1	B	296	LEU
1	B	310	LEU
1	B	325	LEU
1	B	346	LEU
1	B	359	LEU
1	B	363	ILE
1	B	365	ARG
1	B	376	ASP

Some 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 ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates 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	1.18	0	6,6,6	0.27	0
3	PO4	A	602	-	4,4,4	1.04	0	6,6,6	0.27	0
3	PO4	A	603	-	4,4,4	1.08	0	6,6,6	0.27	0
4	ADP	A	604	2	22,29,29	1.40	6 (27%)	27,45,45	2.94	4 (14%)
5	GOL	B	400	-	5,5,5	4.75	5 (100%)	5,5,5	5.71	3 (60%)
5	GOL	B	401	-	5,5,5	4.91	5 (100%)	5,5,5	5.79	3 (60%)
3	PO4	B	601	-	4,4,4	1.12	0	6,6,6	0.27	0
4	ADP	B	602	-	22,29,29	1.56	3 (13%)	27,45,45	2.89	3 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PO4	A	600	-	-	0/0/0/0	0/0/0/0
3	PO4	A	602	-	-	0/0/0/0	0/0/0/0
3	PO4	A	603	-	-	0/0/0/0	0/0/0/0
4	ADP	A	604	2	-	0/12/32/32	0/3/3/3
5	GOL	B	400	-	-	0/4/4/4	0/0/0/0
5	GOL	B	401	-	-	0/4/4/4	0/0/0/0
3	PO4	B	601	-	-	0/0/0/0	0/0/0/0
4	ADP	B	602	-	-	0/12/32/32	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	401	GOL	C3-C2	-8.40	1.20	1.52
5	B	400	GOL	C3-C2	-8.18	1.21	1.52
5	B	400	GOL	C1-C2	-3.36	1.39	1.52
5	B	401	GOL	C1-C2	-3.21	1.40	1.52
5	B	401	GOL	O2-C2	-2.67	1.35	1.43
5	B	400	GOL	O2-C2	-2.59	1.35	1.43
4	A	604	ADP	C5-N7	-2.42	1.31	1.39
4	B	602	ADP	C5-N7	-2.32	1.31	1.39
4	A	604	ADP	PA-O2A	-2.05	1.46	1.54
4	A	604	ADP	O4'-C1'	2.03	1.43	1.41
4	A	604	ADP	C4-N3	2.04	1.38	1.35
4	A	604	ADP	C2-N1	2.22	1.38	1.33
4	A	604	ADP	C2-N3	2.24	1.36	1.32
4	B	602	ADP	C2-N3	2.40	1.36	1.32
5	B	400	GOL	O3-C3	3.37	1.56	1.42
5	B	401	GOL	O3-C3	3.53	1.57	1.42
4	B	602	ADP	O4'-C1'	3.84	1.46	1.41
5	B	400	GOL	O1-C1	4.07	1.59	1.42
5	B	401	GOL	O1-C1	4.50	1.61	1.42

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	604	ADP	N3-C2-N1	-14.19	118.03	128.89
4	B	602	ADP	N3-C2-N1	-13.93	118.23	128.89
4	B	602	ADP	C4-C5-N7	-2.30	107.36	109.48
4	A	604	ADP	C4-C5-N7	-2.07	107.57	109.48
4	A	604	ADP	C4'-O4'-C1'	2.30	112.25	109.72
4	B	602	ADP	O3A-PA-O5'	2.40	109.31	102.94
4	A	604	ADP	O3A-PA-O5'	2.42	109.36	102.94
5	B	400	GOL	O1-C1-C2	2.94	124.42	110.18
5	B	401	GOL	O1-C1-C2	3.30	126.17	110.18
5	B	401	GOL	O2-C2-C3	6.53	138.58	108.65
5	B	400	GOL	O2-C2-C3	6.81	139.87	108.65
5	B	400	GOL	O3-C3-C2	10.38	160.50	110.18
5	B	401	GOL	O3-C3-C2	10.67	161.94	110.18

There are no chirality outliers.

There are no torsion outliers.

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
3	A	603	PO4	1	0
5	B	400	GOL	1	0
5	B	401	GOL	1	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	384/387 (99%)	-0.04	11 (2%) 55 54	29, 52, 89, 111	0
1	B	385/387 (99%)	0.05	13 (3%) 49 49	36, 63, 93, 110	0
All	All	769/774 (99%)	0.01	24 (3%) 52 52	29, 57, 92, 111	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	382	CYS	9.4
1	A	54	LEU	5.1
1	A	34	LYS	3.8
1	B	383	LEU	3.7
1	B	141	PHE	3.3
1	B	353	TYR	3.2
1	B	348	LEU	3.0
1	A	32	ARG	2.9
1	B	311	ARG	2.8
1	A	369	PHE	2.8
1	A	371	GLU	2.7
1	A	55	PRO	2.7
1	A	56	ASP	2.5
1	B	381	SER	2.5
1	B	32	ARG	2.3
1	B	285	GLU	2.3
1	B	282	ASN	2.3
1	B	217	THR	2.3
1	A	38	LYS	2.2
1	B	385	ASN	2.2
1	A	36	ALA	2.2
1	B	384	VAL	2.1
1	A	35	GLU	2.1
1	A	57	VAL	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	MG	A	500	1/1	0.90	0.52	12.89	69,69,69,69	0
5	GOL	B	400	6/6	0.85	0.19	1.88	73,76,77,78	0
4	ADP	A	604	27/27	0.97	0.19	0.25	29,34,38,40	0
3	PO4	A	602	5/5	0.98	0.14	-0.11	53,55,57,58	0
3	PO4	A	603	5/5	0.96	0.12	-0.46	68,71,72,73	0
3	PO4	A	600	5/5	0.97	0.13	-0.51	73,73,76,78	0
3	PO4	B	601	5/5	0.99	0.11	-0.84	37,39,46,46	0
4	ADP	B	602	27/27	0.97	0.13	-0.89	39,45,53,54	0
5	GOL	B	401	6/6	0.90	0.30	-	75,76,78,79	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.