



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 16, 2018 – 11:26 am GMT

PDB ID : 1FP6  
Title : THE NITROGENASE FE PROTEIN FROM AZOTOBACTER VINELANDII COMPLEXED WITH MGADP  
Authors : Jang, S.B.; Seefeldt, L.C.; Peters, J.W.  
Deposited on : 2000-08-30  
Resolution : 2.15 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

<https://www.wwpdb.org/validation/2017/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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30686

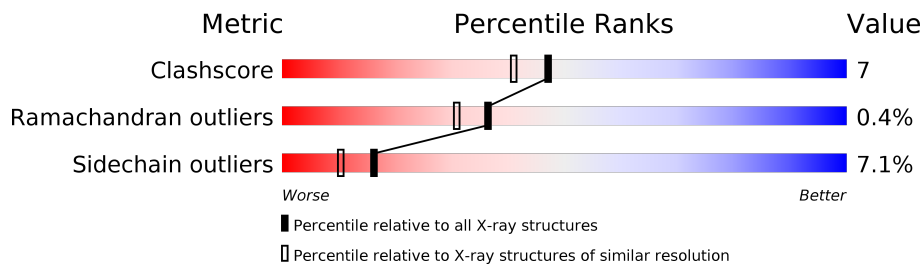
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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))
Clashscore	122078	1390 (2.16-2.16)
Ramachandran outliers	120005	1368 (2.16-2.16)
Sidechain outliers	119972	1367 (2.16-2.16)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	289	
1	B	289	
1	C	289	
1	D	289	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10004 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 NITROGENASE IRON PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	289	Total	C	N	O	S	0	0	0
			2187	1364	369	433	21			
1	B	289	Total	C	N	O	S	0	0	0
			2187	1364	369	433	21			
1	C	285	Total	C	N	O	S	0	0	0
			2156	1346	365	424	21			
1	D	285	Total	C	N	O	S	0	0	0
			2156	1346	365	424	21			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

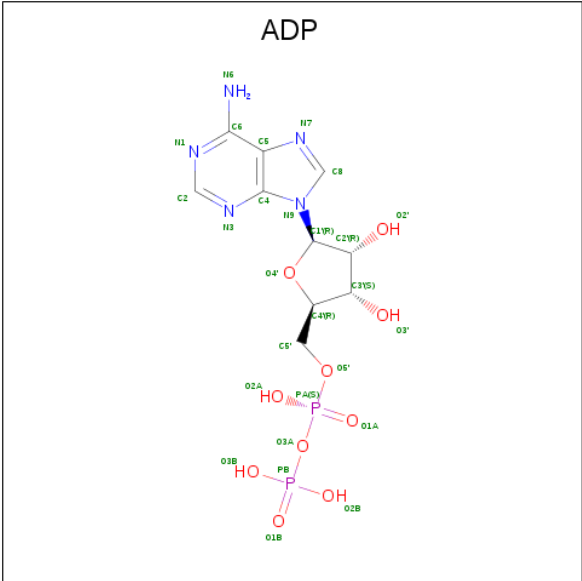
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		

- 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		

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

- Molecule 5 is water.

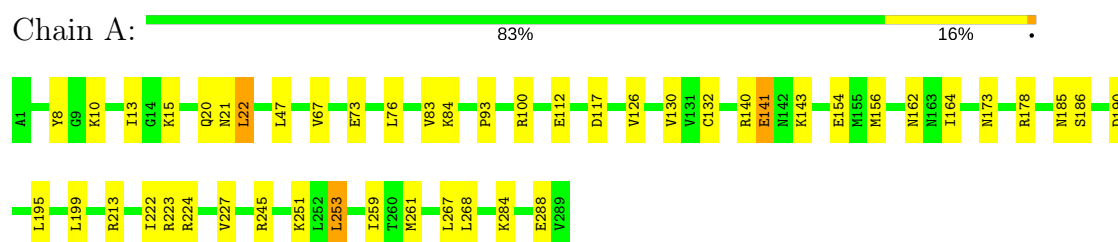
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	304	Total 304	O 304	0	0
5	B	329	Total 329	O 329	0	0
5	C	308	Total 308	O 308	0	0
5	D	249	Total 249	O 249	0	0

### 3 Residue-property plots [i](#)

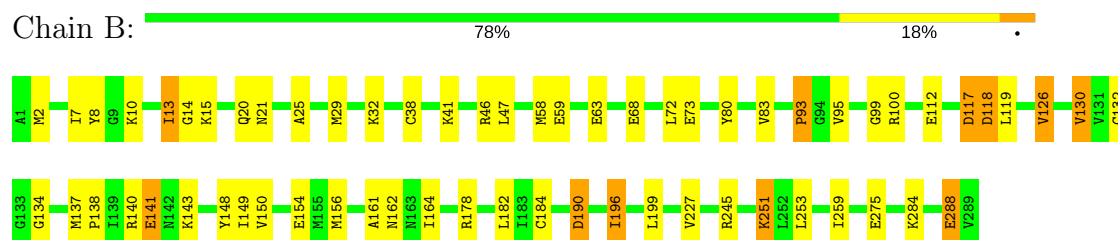
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

Note EDS was not executed.

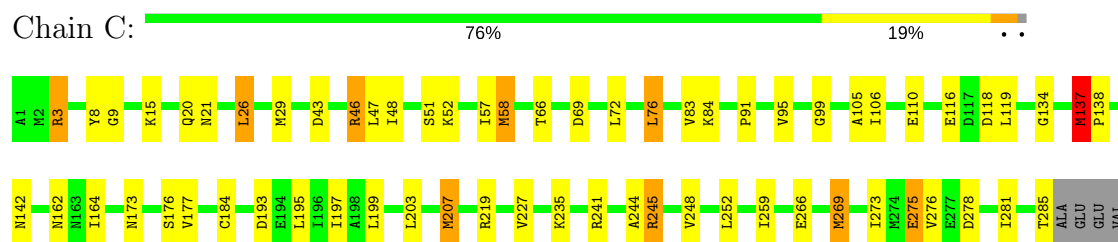
#### • Molecule 1: NITROGENASE IRON PROTEIN



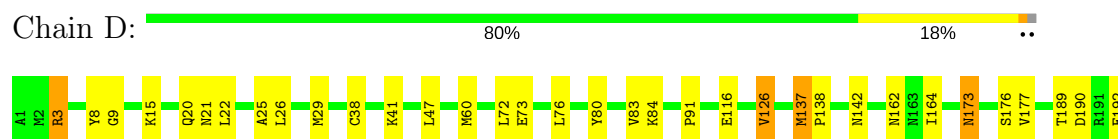
#### • Molecule 1: NITROGENASE IRON PROTEIN



#### • Molecule 1: NITROGENASE IRON PROTEIN



#### • Molecule 1: NITROGENASE IRON PROTEIN



L195	L199	M207	L208	H209	D214	I222	M225	T226	V227	K235	Q236	R241	A242	L243	V248	L252	I259	E263	L267	E275	D278	E279	S280	I281	T285	ALA	GLU	GLU	VAL
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## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.25Å 119.53Å 120.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.15	Depositor
% Data completeness (in resolution range)	88.8 (30.00-2.15)	Depositor
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.200 , 0.268	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10004	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, 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	0.60	0/2211	1.19	8/2977 (0.3%)
1	B	0.62	0/2211	1.19	8/2977 (0.3%)
1	C	0.64	0/2180	1.20	11/2936 (0.4%)
1	D	0.60	0/2180	1.17	6/2936 (0.2%)
All	All	0.61	0/8782	1.18	33/11826 (0.3%)

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	3	ARG	NE-CZ-NH1	10.45	125.52	120.30
1	C	3	ARG	NE-CZ-NH2	-8.51	116.05	120.30
1	D	3	ARG	NE-CZ-NH1	8.01	124.30	120.30
1	B	140	ARG	NE-CZ-NH1	7.41	124.00	120.30
1	D	241	ARG	NE-CZ-NH1	6.77	123.69	120.30
1	C	241	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	D	241	ARG	NE-CZ-NH2	-6.49	117.06	120.30
1	C	137	MET	CA-CB-CG	6.38	124.14	113.30
1	A	140	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	A	140	ARG	NE-CZ-NH1	6.05	123.32	120.30
1	C	46	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	D	3	ARG	NE-CZ-NH2	-5.97	117.31	120.30
1	C	245	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	C	46	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	B	178	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	D	137	MET	CA-CB-CG	5.80	123.16	113.30
1	A	22	LEU	CA-CB-CG	5.71	128.44	115.30
1	A	224	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	C	219	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	A	223	ARG	NE-CZ-NH2	-5.47	117.56	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	224	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	C	245	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	B	46	ARG	NE-CZ-NH1	5.43	123.01	120.30
1	B	140	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	D	22	LEU	CA-CB-CG	5.41	127.73	115.30
1	C	269	MET	CA-CB-CG	5.40	122.48	113.30
1	B	58	MET	CA-CB-CG	5.25	122.22	113.30
1	A	253	LEU	CA-CB-CG	5.24	127.34	115.30
1	A	178	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	B	190	ASP	N-CA-C	5.21	125.06	111.00
1	C	29	MET	CA-CB-CG	5.18	122.10	113.30
1	B	126	VAL	O-C-N	5.03	130.75	122.70
1	B	178	ARG	CA-CB-CG	5.02	124.44	113.40

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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	2187	0	2196	24	0
1	B	2187	0	2196	36	0
1	C	2156	0	2171	37	0
1	D	2156	0	2171	29	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	8	0	0	0	0
3	C	8	0	0	0	0
4	A	27	0	12	2	0
4	B	27	0	12	2	0
4	C	27	0	12	0	0
4	D	27	0	12	0	0
5	A	304	0	0	1	0
5	B	329	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	308	0	0	5	0
5	D	249	0	0	2	0
All	All	10004	0	8782	118	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 7.

All (118) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:285:THR:HG22	1:D:225:MET:SD	2.27	0.75
1:A:130:VAL:HG13	1:A:132:CYS:SG	2.30	0.71
1:B:182:LEU:HB3	1:B:196:ILE:HD11	1.72	0.71
1:C:278:ASP:HB3	1:C:281:ILE:HG12	1.73	0.71
1:A:10:LYS:NZ	1:B:10:LYS:HZ1	1.90	0.70
1:C:142:ASN:HD22	1:C:177:VAL:HG23	1.59	0.68
1:B:38:CYS:HB2	1:B:126:VAL:HG22	1.77	0.66
1:B:80:TYR:O	1:B:83:VAL:HG12	1.95	0.65
1:D:76:LEU:HD22	1:D:84:LYS:HB3	1.78	0.65
1:D:21:ASN:HD21	1:D:227:VAL:H	1.46	0.64
1:B:21:ASN:HD21	1:B:227:VAL:H	1.44	0.64
1:B:184:CYS:HB2	1:B:196:ILE:HG21	1.80	0.62
1:A:8:TYR:CZ	1:A:126:VAL:HG11	2.34	0.62
1:D:142:ASN:HD22	1:D:177:VAL:HG23	1.63	0.62
1:C:106:ILE:O	1:C:110:GLU:HG3	2.00	0.61
1:A:10:LYS:HZ1	1:B:10:LYS:HZ1	1.47	0.61
1:C:142:ASN:HD21	1:C:176:SER:H	1.48	0.61
1:C:193:ASP:O	1:C:197:ILE:HG12	2.00	0.61
1:A:8:TYR:HB3	1:A:164:ILE:HD13	1.84	0.60
1:B:10:LYS:O	1:B:13:ILE:HG13	2.02	0.60
1:D:21:ASN:HD21	1:D:227:VAL:N	1.99	0.59
1:C:76:LEU:HD22	1:C:84:LYS:HB3	1.84	0.59
1:A:20:GLN:HE22	1:A:47:LEU:H	1.51	0.59
1:C:21:ASN:HD21	1:C:227:VAL:H	1.51	0.58
1:A:141:GLU:HB2	1:A:143:LYS:HD3	1.84	0.58
1:B:130:VAL:HG13	1:B:132:CYS:SG	2.44	0.57
1:A:21:ASN:HD21	1:A:227:VAL:H	1.50	0.57
1:C:21:ASN:HD21	1:C:227:VAL:N	2.02	0.57
1:A:162:ASN:HD21	1:A:259:ILE:H	1.51	0.57
1:C:46:ARG:HD2	1:C:51:SER:O	2.04	0.57
1:D:20:GLN:HE22	1:D:47:LEU:H	1.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:142:ASN:ND2	1:D:177:VAL:HG23	2.20	0.56
1:C:162:ASN:HD21	1:C:259:ILE:H	1.54	0.56
1:D:60:MET:HG3	5:D:8494:HOH:O	2.04	0.56
1:A:15:LYS:HG2	4:A:5291:ADP:O1B	2.07	0.55
1:D:8:TYR:HB3	1:D:164:ILE:HD13	1.87	0.55
1:B:20:GLN:HE22	1:B:47:LEU:H	1.53	0.55
1:D:9:GLY:O	1:D:15:LYS:HE3	2.06	0.55
1:B:2:MET:HE2	1:B:119:LEU:HB2	1.88	0.54
1:D:214:ASP:HB3	1:D:236:GLN:HG3	1.90	0.54
1:D:38:CYS:HB2	1:D:126:VAL:HB	1.89	0.54
1:A:8:TYR:CE1	1:A:126:VAL:HG11	2.43	0.53
1:C:8:TYR:HB3	1:C:164:ILE:HD13	1.91	0.53
1:C:9:GLY:O	1:C:15:LYS:HE3	2.09	0.52
1:C:26:LEU:HD13	1:C:244:ALA:HB1	1.91	0.52
1:C:162:ASN:HD22	1:C:203:LEU:HD21	1.75	0.52
1:D:162:ASN:HD21	1:D:259:ILE:H	1.56	0.52
1:C:58:MET:HG2	5:C:7458:HOH:O	2.10	0.52
1:D:80:TYR:O	1:D:83:VAL:HG22	2.11	0.51
1:A:10:LYS:NZ	1:B:10:LYS:NZ	2.59	0.51
1:A:195:LEU:HD21	1:A:268:LEU:HD23	1.93	0.51
1:B:284:LYS:HD3	1:B:288:GLU:HG2	1.93	0.51
1:B:14:GLY:HA2	4:B:6291:ADP:PA	2.50	0.51
1:C:137:MET:HG3	1:C:138:PRO:HD3	1.93	0.50
1:D:142:ASN:HD21	1:D:176:SER:H	1.59	0.50
1:B:7:ILE:HD13	1:B:148:TYR:HB2	1.92	0.50
1:D:189:THR:HB	1:D:192:GLU:HB2	1.93	0.50
1:D:278:ASP:HB3	1:D:281:ILE:HG12	1.93	0.50
1:C:66:THR:HG23	1:C:69:ASP:H	1.77	0.50
1:B:32:LYS:HZ3	1:B:118:ASP:H	1.60	0.50
1:D:263:GLU:O	1:D:267:LEU:HB2	2.13	0.49
1:B:138:PRO:HA	1:B:143:LYS:HB2	1.94	0.48
1:A:222:ILE:HG21	1:B:275:GLU:HG3	1.95	0.48
1:B:32:LYS:HG2	1:B:119:LEU:HD23	1.95	0.47
1:C:57:ILE:HD12	1:C:105:ALA:HA	1.96	0.47
1:C:76:LEU:CD2	1:C:84:LYS:HB3	2.43	0.47
1:A:156:MET:CE	1:B:41:LYS:HD2	2.44	0.47
1:A:21:ASN:HD21	1:A:227:VAL:N	2.12	0.47
1:C:46:ARG:HH11	1:C:52:LYS:HA	1.80	0.47
1:C:48:ILE:HG21	1:C:83:VAL:HG23	1.97	0.47
1:C:245:ARG:HD2	5:C:7313:HOH:O	2.15	0.47
1:A:185:ASN:HD21	4:A:5291:ADP:HN61	1.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:TYR:HB3	1:B:164:ILE:HD13	1.98	0.46
1:B:13:ILE:HD13	1:B:150:VAL:HB	1.98	0.46
1:B:245:ARG:HD3	5:B:6572:HOH:O	2.15	0.45
1:B:59:GLU:O	1:B:63:GLU:HG2	2.16	0.45
1:A:245:ARG:HG3	5:C:7293:HOH:O	2.16	0.45
1:B:15:LYS:HG2	4:B:6291:ADP:O1B	2.17	0.45
1:C:269:MET:HG2	1:C:275:GLU:O	2.17	0.45
1:D:3:ARG:NH2	1:D:248:VAL:HA	2.31	0.45
1:A:8:TYR:CE1	1:A:126:VAL:CG1	3.00	0.45
1:C:173:ASN:H	1:C:173:ASN:ND2	2.15	0.44
5:A:5301:HOH:O	1:B:156:MET:HE3	2.18	0.44
1:B:99:GLY:O	1:B:134:GLY:HA3	2.17	0.44
1:C:20:GLN:HE22	1:C:47:LEU:H	1.64	0.44
1:C:142:ASN:ND2	1:C:177:VAL:HG23	2.30	0.44
1:B:2:MET:CE	1:B:119:LEU:HB2	2.47	0.44
1:B:162:ASN:HD21	1:B:259:ILE:H	1.66	0.43
1:B:21:ASN:HD21	1:B:227:VAL:N	2.15	0.43
5:C:7391:HOH:O	1:D:279:GLU:HG3	2.19	0.43
1:C:99:GLY:O	1:C:134:GLY:HA3	2.18	0.43
1:C:184:CYS:HB2	1:C:207:MET:HE2	2.01	0.43
1:C:43:ASP:HB2	1:C:46:ARG:HG3	2.01	0.43
1:A:10:LYS:HZ3	1:B:10:LYS:NZ	2.17	0.43
1:C:3:ARG:HH22	1:C:248:VAL:HA	1.83	0.42
1:B:149:ILE:HG21	1:B:161:ALA:HA	2.02	0.42
1:D:162:ASN:HD21	1:D:259:ILE:N	2.15	0.42
1:D:41:LYS:HE2	5:D:8448:HOH:O	2.18	0.42
1:D:25:ALA:O	1:D:29:MET:HG2	2.20	0.42
1:A:186:SER:O	1:A:213:ARG:HB2	2.20	0.42
1:B:251:LYS:HA	1:B:251:LYS:HD2	1.79	0.42
1:D:173:ASN:H	1:D:173:ASN:HD22	1.68	0.42
1:C:142:ASN:ND2	1:C:176:SER:H	2.17	0.41
1:D:214:ASP:CB	1:D:236:GLN:HG3	2.50	0.41
1:B:141:GLU:HB2	1:B:143:LYS:HD3	2.02	0.41
1:A:20:GLN:NE2	1:A:47:LEU:H	2.17	0.41
1:C:173:ASN:H	1:C:173:ASN:HD22	1.67	0.41
1:A:76:LEU:HD11	1:A:84:LYS:HB3	2.03	0.41
1:B:32:LYS:HZ1	1:B:117:ASP:HB3	1.85	0.41
1:D:76:LEU:CD2	1:D:84:LYS:HB3	2.47	0.41
1:D:137:MET:HG3	1:D:138:PRO:HD3	2.03	0.41
1:D:209:HIS:HB3	1:D:243:LEU:HD13	2.03	0.41
1:C:273:ILE:HD11	5:C:7509:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:ALA:O	1:B:29:MET:HG2	2.20	0.41
1:C:266:GLU:HA	1:C:269:MET:SD	2.61	0.41
1:A:284:LYS:HA	1:A:284:LYS:HE2	2.03	0.40
1:C:269:MET:HE3	1:C:276:VAL:HA	2.02	0.40
1:C:275:GLU:HG2	1:D:222:ILE:HG21	2.03	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	287/289 (99%)	274 (96%)	12 (4%)	1 (0%)	43	39
1	B	287/289 (99%)	274 (96%)	12 (4%)	1 (0%)	43	39
1	C	283/289 (98%)	272 (96%)	10 (4%)	1 (0%)	36	31
1	D	283/289 (98%)	271 (96%)	11 (4%)	1 (0%)	36	31
All	All	1140/1156 (99%)	1091 (96%)	45 (4%)	4 (0%)	36	31

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	91	PRO
1	D	91	PRO
1	A	190	ASP
1	B	93	PRO

### 5.3.2 Protein sidechains [i](#)

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	233/233 (100%)	215 (92%)	18 (8%)	14	8
1	B	233/233 (100%)	213 (91%)	20 (9%)	11	6
1	C	230/233 (99%)	215 (94%)	15 (6%)	19	12
1	D	230/233 (99%)	217 (94%)	13 (6%)	23	17
All	All	926/932 (99%)	860 (93%)	66 (7%)	16	10

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ILE
1	A	22	LEU
1	A	67	VAL
1	A	73	GLU
1	A	83	VAL
1	A	93	PRO
1	A	100	ARG
1	A	112	GLU
1	A	117	ASP
1	A	141	GLU
1	A	154	GLU
1	A	173	ASN
1	A	199	LEU
1	A	251	LYS
1	A	253	LEU
1	A	261	MET
1	A	267	LEU
1	A	288	GLU
1	B	13	ILE
1	B	68	GLU
1	B	72	LEU
1	B	73	GLU
1	B	93	PRO
1	B	95	VAL
1	B	100	ARG
1	B	112	GLU
1	B	117	ASP
1	B	118	ASP
1	B	130	VAL
1	B	137	MET

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Mol	Chain	Res	Type
1	B	141	GLU
1	B	154	GLU
1	B	190	ASP
1	B	196	ILE
1	B	199	LEU
1	B	251	LYS
1	B	253	LEU
1	B	288	GLU
1	C	26	LEU
1	C	58	MET
1	C	72	LEU
1	C	76	LEU
1	C	95	VAL
1	C	116	GLU
1	C	118	ASP
1	C	119	LEU
1	C	137	MET
1	C	195	LEU
1	C	199	LEU
1	C	207	MET
1	C	235	LYS
1	C	252	LEU
1	C	275	GLU
1	D	26	LEU
1	D	72	LEU
1	D	73	GLU
1	D	116	GLU
1	D	126	VAL
1	D	173	ASN
1	D	190	ASP
1	D	195	LEU
1	D	199	LEU
1	D	207	MET
1	D	235	LYS
1	D	252	LEU
1	D	275	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	21	ASN

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Mol	Chain	Res	Type
1	A	107	ASN
1	A	162	ASN
1	A	163	ASN
1	A	185	ASN
1	A	201	ASN
1	B	20	GLN
1	B	21	ASN
1	B	145	GLN
1	B	162	ASN
1	B	163	ASN
1	B	185	ASN
1	B	218	GLN
1	C	20	GLN
1	C	21	ASN
1	C	55	ASN
1	C	142	ASN
1	C	162	ASN
1	C	163	ASN
1	C	173	ASN
1	C	209	HIS
1	D	20	GLN
1	D	21	ASN
1	D	50	HIS
1	D	142	ASN
1	D	162	ASN
1	D	163	ASN
1	D	173	ASN
1	D	215	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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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	SF4	A	5290	1	0,12,12	0.00	-	0,24,24	0.00	-
4	ADP	A	5291	2	25,29,29	1.87	3 (12%)	25,45,45	1.45	4 (16%)
4	ADP	B	6291	2	25,29,29	1.87	3 (12%)	25,45,45	1.38	4 (16%)
3	SF4	C	7290	1	0,12,12	0.00	-	0,24,24	0.00	-
4	ADP	C	7291	2	25,29,29	1.88	4 (16%)	25,45,45	1.51	6 (24%)
4	ADP	D	8291	2	25,29,29	1.84	4 (16%)	25,45,45	1.53	6 (24%)

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	SF4	A	5290	1	-	0/0/48/48	0/6/5/5
4	ADP	A	5291	2	-	0/12/32/32	0/3/3/3
4	ADP	B	6291	2	-	0/12/32/32	0/3/3/3
3	SF4	C	7290	1	-	0/0/48/48	0/6/5/5
4	ADP	C	7291	2	-	0/12/32/32	0/3/3/3
4	ADP	D	8291	2	-	0/12/32/32	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	5291	ADP	PB-O3A	-6.91	1.49	1.60
4	B	6291	ADP	PB-O3A	-6.59	1.50	1.60
4	C	7291	ADP	PB-O3A	-6.33	1.50	1.60
4	D	8291	ADP	PB-O3A	-6.08	1.50	1.60
4	D	8291	ADP	C8-N7	-2.21	1.30	1.34
4	C	7291	ADP	C8-N7	-2.07	1.30	1.34
4	A	5291	ADP	O4'-C1'	2.34	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	8291	ADP	O4'-C1'	2.62	1.44	1.41
4	C	7291	ADP	O4'-C1'	2.87	1.45	1.41
4	B	6291	ADP	O4'-C1'	3.15	1.45	1.41
4	A	5291	ADP	PB-O3B	4.00	1.71	1.54
4	B	6291	ADP	PB-O3B	4.17	1.71	1.54
4	D	8291	ADP	PB-O3B	4.73	1.73	1.54
4	C	7291	ADP	PB-O3B	4.81	1.74	1.54

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	8291	ADP	C2'-C3'-C4'	-4.13	94.70	102.62
4	C	7291	ADP	C2'-C3'-C4'	-3.82	95.28	102.62
4	A	5291	ADP	C2'-C3'-C4'	-3.73	95.45	102.62
4	B	6291	ADP	C2'-C3'-C4'	-3.15	96.58	102.62
4	C	7291	ADP	O3B-PB-O1B	-2.92	99.19	110.60
4	B	6291	ADP	O3B-PB-O1B	-2.75	99.88	110.60
4	D	8291	ADP	C4'-O4'-C1'	-2.68	107.04	109.83
4	A	5291	ADP	C4'-O4'-C1'	-2.61	107.10	109.83
4	C	7291	ADP	C4'-O4'-C1'	-2.36	107.37	109.83
4	D	8291	ADP	O3B-PB-O1B	-2.33	101.52	110.60
4	B	6291	ADP	O5'-PA-O1A	-2.30	100.06	109.07
4	C	7291	ADP	O5'-PA-O1A	-2.12	100.80	109.07
4	D	8291	ADP	O3B-PB-O2B	-2.06	99.43	107.59
4	C	7291	ADP	O3B-PB-O2B	-2.06	99.44	107.59
4	D	8291	ADP	O5'-PA-O1A	-2.01	101.20	109.07
4	A	5291	ADP	C5-C6-N6	2.16	124.87	120.47
4	C	7291	ADP	O5'-C5'-C4'	2.61	118.06	109.00
4	A	5291	ADP	O5'-C5'-C4'	2.73	118.48	109.00
4	D	8291	ADP	O5'-C5'-C4'	2.75	118.55	109.00
4	B	6291	ADP	O5'-C5'-C4'	2.91	119.11	109.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	5291	ADP	2	0
4	B	6291	ADP	2	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

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.