



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 08:10 PM GMT

PDB ID : 1J1W  
Title : Crystal Structure Of The Monomeric Isocitrate Dehydrogenase In Complex With NADP+  
Authors : Yasutake, Y.; Watanabe, S.; Yao, M.; Takada, Y.; Fukunaga, N.; Tanaka, I.  
Deposited on : 2002-12-19  
Resolution : 3.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

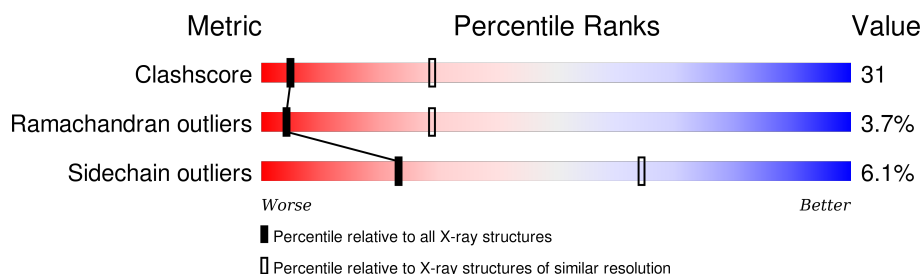
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 Å.


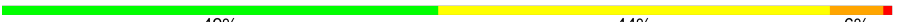
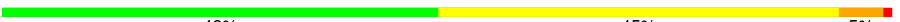
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)

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	741	
1	B	741	
1	C	741	
1	D	741	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 23181 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.

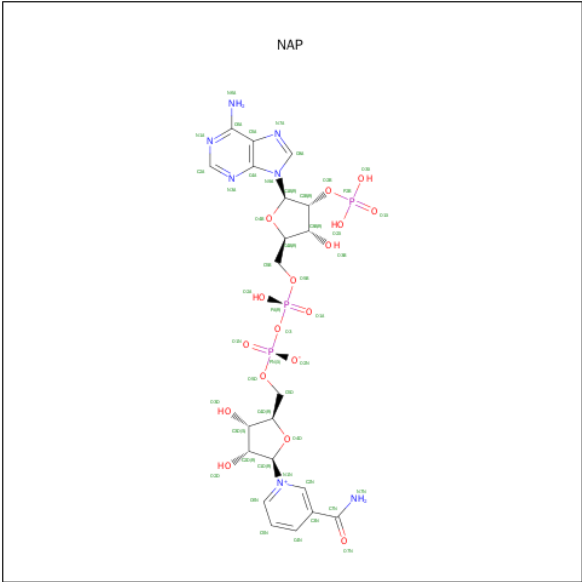
- Molecule 1 is a protein called Isocitrate Dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	738	Total	C	N	O	S	0	0	0
			5636	3562	967	1087	20			
1	B	738	Total	C	N	O	S	0	0	0
			5636	3562	967	1087	20			
1	C	738	Total	C	N	O	S	0	0	0
			5636	3562	967	1087	20			
1	D	738	Total	C	N	O	S	0	0	0
			5636	3562	967	1087	20			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	727	MET	ILE	SEE REMARK 999	UNP P16100
B	727	MET	ILE	SEE REMARK 999	UNP P16100
C	727	MET	ILE	SEE REMARK 999	UNP P16100
D	727	MET	ILE	SEE REMARK 999	UNP P16100

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C<sub>21</sub>H<sub>28</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is water.

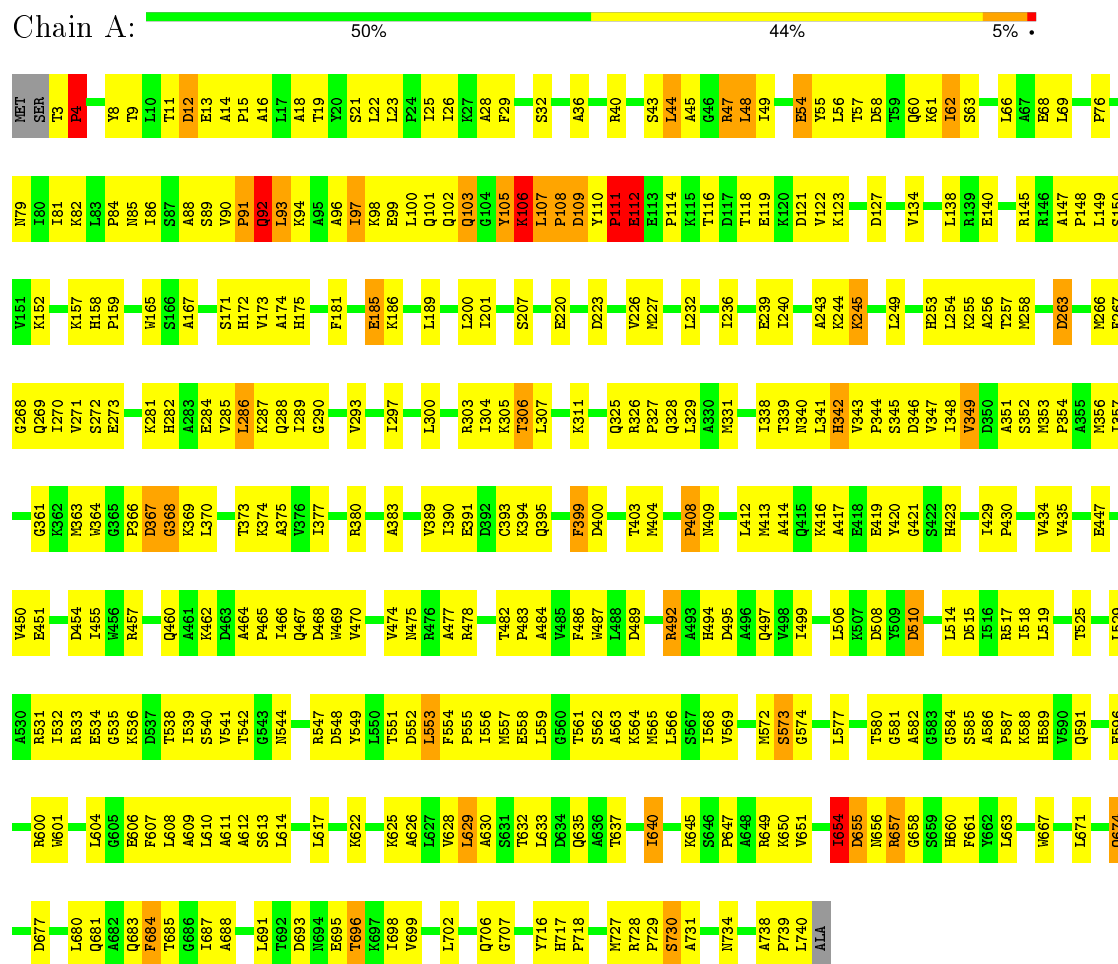
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	123	Total	O	0	0
			123	123		
3	B	101	Total	O	0	0
			101	101		
3	C	99	Total	O	0	0
			99	99		
3	D	122	Total	O	0	0
			122	122		

### 3 Residue-property plots

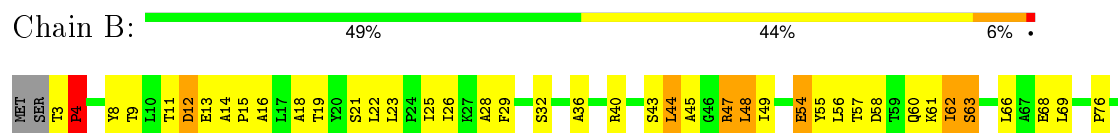
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

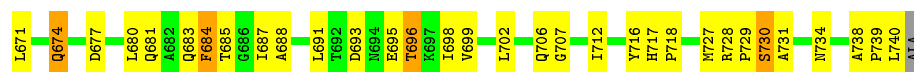
#### • Molecule 1: Isocitrate Dehydrogenase



#### • Molecule 1: Isocitrate Dehydrogenase

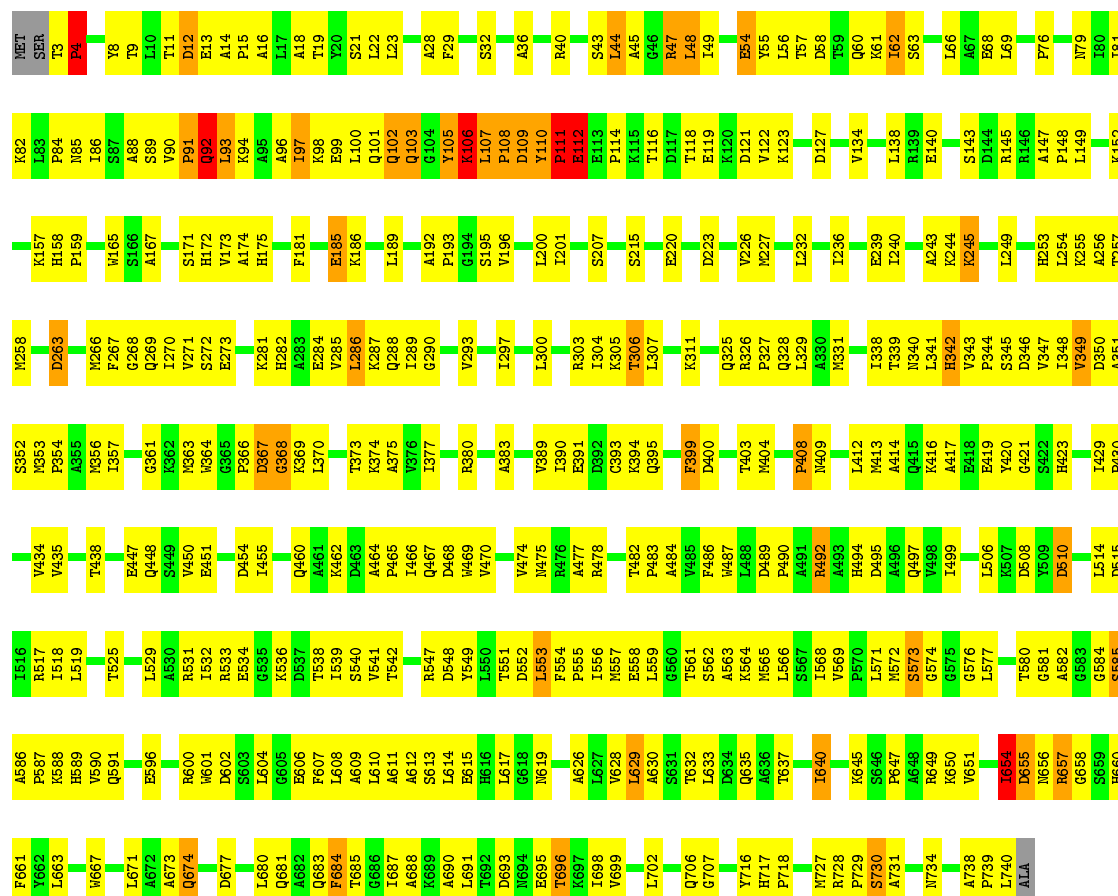


L604	G605	T538	D537	E451	P354	K258	P148	N79
G606	T539	T538	T538	D454	A355	D263	L149	L80
F607	S540	A682	S540	T455	I357		S150	L81
L608	F541	F684	T542		G351		V151	K82
A609	L610	T685	V545	Q460			K152	L83
A611	A612	G686	V545	A461				P84
S613	S613	A688	L546	K462			K157	N85
L614	S614	R547	R547	D463			H158	L86
S615	S615	L614	D548	A464			P159	S87
A616	S616	L615	Y549	P465				A88
H616	H616	D682	Y549	A466			W165	S89
L617	L617	D683	L550	Q467			S166	V90
L618	L618	D684	T551	D468			A167	P91
L619	L619	E695	D552	W469				Q92
L620	L620	T696	L553	V470			S171	L93
L621	L621	F687	F554				H173	K94
L622	L622	V699	P555	A477			V173	A95
L623	L623	L702	I556	R478			A174	A96
L624	L624	Q706	E558	T482			H175	I97
L625	L625	G707	L559	P483				K98
L626	L626		G560	F486			F181	E99
L627	L627	Y716	S562	H487			E185	L100
L628	L628	F718	A563	L488			K186	Q101
L629	L629	P718	R564	D489				Q102
L630	L630		M565				L189	G104
L631	L631	M727	L566	R492			S195	Y105
L632	L632	W737	S567	A493			L200	L107
L633	L633	T640	I568	H494			I201	P108
L634	L634	K645	P569	D495				D109
L635	L635	S730	P570	A496			S207	Y110
L636	L636	A731	L571	Q497				P111
L637	L637	N734	M572	V498			S215	E112
L638	L638		S573	L499			E220	P114
L639	L639	A738	G574	L506				K115
L640	L640	P739	G575	R507			D223	T116
L641	L641	L740	L577	B508			D226	D117
L642	L642	ALA		Y509			V226	E118
L643	L643		T580	D510				E119
L644	L644		G581	D511			M227	K120
L645	L645		A582	D512			S228	D121
L646	L646		G583	D513				V122
L647	L647		G584	D514			A231	K123
L648	L648		G585	D515				
L649	L649		G586	D516			I236	D127
L650	L650		G587	D517				V134
L651	L651		G588	D518			E239	L138
L652	L652		G589	D519			I240	R139
L653	L653		G590	D520			K245	E140
L654	L654		G591	D521				G141
L655	L655		G592	D522			H253	N142
L656	L656		G593	D523			L254	S143
L657	L657		G594	D524			K255	D144
L658	L658		G595	D525			R145	R146
L659	L659		G596	D526			T257	A147
L660	L660		G597	D527				
L661	L661		G598	D528				
L662	L662		G599	D529				
L663	L663		G600	D530				
L664	L664		G601	D531				
L665	L665		G602	D532				
L666	L666		G603	D533				
L667	L667		G604	D534				
L668	L668		G605	D535				
L669	L669		G606	D536				
L670	L670		G607	D537				
L671	L671		G608	D538				
L672	L672		G609	D539				
L673	L673		G610	D540				
L674	L674		G611	D541				
L675	L675		G612	D542				
L676	L676		G613	D543				
L677	L677		G614	D544				
L678	L678		G615	D545				
L679	L679		G616	D546				
L680	L680		G617	D547				
L681	L681		G618	D548				
L682	L682		G619	D549				
L683	L683		G620	D550				
L684	L684		G621	D551				
L685	L685		G622	D552				
L686	L686		G623	D553				
L687	L687		G624	D554				
L688	L688		G625	D555				
L689	L689		G626	D556				
L690	L690		G627	D557				
L691	L691		G628	D558				
L692	L692		G629	D559				
L693	L693		G630	D560				
L694	L694		G631	D561				
L695	L695		G632	D562				
L696	L696		G633	D563				
L697	L697		G634	D564				
L698	L698		G635	D565				
L699	L699		G636	D566				
L700	L700		G637	D567				
L701	L701		G638	D568				
L702	L702		G639	D569				
L703	L703		G640	D570				
L704	L704		G641	D571				
L705	L705		G642	D572				
L706	L706		G643	D573				
L707	L707		G644	D574				
L708	L708		G645	D575				
L709	L709		G646	D576				
L710	L710		G647	D577				
L711	L711		G648	D578				
L712	L712		G649	D579				
L713	L713		G650	D580				
L714	L714		G651	D581				
L715	L715		G652	D582				
L716	L716		G653	D583				
L717	L717		G654	D584				
L718	L718		G655	D585				
L719	L719		G656	D586				
L720	L720		G657	D587				
L721	L721		G658	D588				
L722	L722		G659	D589				
L723	L723		G660	D590				
L724	L724		G661	D591				
L725	L725		G662	D592				
L726	L726		G663	D593				
L727	L727		G664	D594				
L728	L728		G665	D595				
L729	L729		G666	D596				
L730	L730		G667	D597				
L731	L731		G668	D598				
L732	L732		G669	D599				
L733	L733		G670	D600				
L734	L734		G671	D601				
L735	L735		G672	D602				
L736	L736		G673	D603				
L737	L737		G674	D604				
L738	L738		G675	D605				
L739	L739		G676	D606				
L740	L740		G677	D607				
L741	L741		G678	D608				
L742	L742		G679	D609				
L743	L743		G680	D610				
L744	L744		G681	D611				
L745	L745		G682	D612				
L746	L746		G683	D613				
L747	L747		G684	D614				
L748	L748		G685	D615				
L749	L749		G686	D616				
L750	L750		G687	D617				
L751	L751		G688	D618				
L752	L752		G689	D619				
L753	L753		G690	D620				
L754	L754		G691	D621				
L755	L755		G692	D622				
L756	L756		G693	D623				
L757	L757		G694	D624				
L758	L758		G695	D625				
L759	L759		G696	D626				
L760	L760		G697	D627				
L761	L761		G698	D628				
L762	L762		G699	D629				
L763	L763		G700	D630				
L764	L764		G701	D631				
L765	L765		G702	D632				
L766	L766		G703	D633				
L767	L767		G704	D634				
L768	L768		G705	D635				
L769	L769		G706	D636				
L770	L770		G707	D637				
L771	L771		G708	D638				
L772	L772		G709	D639				
L773	L773		G710	D640				
L774	L774		G711	D641				
L775	L775		G712	D642				
L776	L776		G713	D643				
L777	L777		G714	D644				
L778	L778		G715	D645				
L779	L779		G716	D646				
L780	L780		G717	D647				
L781	L781		G718	D648				
L782	L782		G719	D649				
L783	L783		G720	D650				
L784	L784		G721	D651				
L785	L785		G722	D652				
L786	L786		G723	D653				
L787	L787		G724	D654				
L788	L788		G725	D655				
L789	L789		G726	D656				
L790	L790		G727	D657				
L791	L791		G728	D658				
L792	L792		G729	D659				
L793	L793		G730	D660				
L794	L794		G731	D661				
L795	L795		G732	D662				
L796	L796		G733	D663				
L797	L797		G734	D664				
L798	L798		G735	D665				
L799	L799		G736	D666				
L800	L800		G737	D667				
L801	L801		G738	D668				
L802	L802		G739	D669				
L803	L803		G740	D670				
L804	L804		G741	D671				
L805	L805		G742	D672				
L806	L806		G743	D673				
L807	L807		G744	D674				
L808	L808		G745	D675				
L809	L809		G746	D676				
L810	L810		G747	D677				
L811	L811		G748	D678				



• Molecule 1: Isocitrate Dehydrogenase

Chain D: 49% 45% 5%



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	113.50Å 110.41Å 133.70Å 90.00° 90.16° 90.00°	Depositor
Resolution (Å)	10.00 – 3.20	Depositor
% Data completeness (in resolution range)	88.8 (10.00-3.20)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.260 , 0.297	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	23181	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAP

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	0.41	0/5742	0.70	6/7783 (0.1%)
1	B	0.41	0/5742	0.70	6/7783 (0.1%)
1	C	0.40	0/5742	0.70	6/7783 (0.1%)
1	D	0.41	0/5742	0.70	6/7783 (0.1%)
All	All	0.41	0/22968	0.70	24/31132 (0.1%)

There are no bond length outliers.

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	111	PRO	N-CA-C	8.39	133.92	112.10
1	C	111	PRO	N-CA-C	8.35	133.80	112.10
1	D	111	PRO	N-CA-C	8.28	133.64	112.10
1	B	111	PRO	N-CA-C	8.28	133.62	112.10
1	B	654	ILE	N-CA-C	7.84	132.17	111.00

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	5636	0	5687	365	0
1	B	5636	0	5687	351	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	5636	0	5687	362	0
1	D	5636	0	5687	352	0
2	A	48	0	25	4	0
2	B	48	0	25	4	0
2	C	48	0	25	2	0
2	D	48	0	25	5	0
3	A	123	0	0	2	0
3	B	101	0	0	1	0
3	C	99	0	0	2	0
3	D	122	0	0	5	0
All	All	23181	0	22848	1424	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 31.

The worst 5 of 1424 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:622:LYS:NZ	1:C:441:SER:HB3	1.69	1.07
1:D:561:THR:HG22	1:D:563:ALA:H	1.24	0.99
1:A:622:LYS:HZ1	1:C:441:SER:HB3	1.25	0.98
1:C:478:ARG:HH12	1:C:510:ASP:HB3	1.29	0.96
1:C:561:THR:HG22	1:C:563:ALA:H	1.27	0.96

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	736/741 (99%)	591 (80%)	119 (16%)	26 (4%)	4	31
1	B	736/741 (99%)	587 (80%)	122 (17%)	27 (4%)	4	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	736/741 (99%)	590 (80%)	119 (16%)	27 (4%)	4	29
1	D	736/741 (99%)	588 (80%)	120 (16%)	28 (4%)	4	28
All	All	2944/2964 (99%)	2356 (80%)	480 (16%)	108 (4%)	4	29

5 of 108 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	PRO
1	A	103	GLN
1	A	108	PRO
1	A	573	SER
1	B	91	PRO

### 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	599/601 (100%)	563 (94%)	36 (6%)	24	65
1	B	599/601 (100%)	563 (94%)	36 (6%)	24	65
1	C	599/601 (100%)	562 (94%)	37 (6%)	23	64
1	D	599/601 (100%)	563 (94%)	36 (6%)	24	65
All	All	2396/2404 (100%)	2251 (94%)	145 (6%)	23	64

5 of 145 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	654	ILE
1	C	97	ILE
1	D	585	SER
1	B	657	ARG
1	C	11	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 72 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	660	HIS
1	C	282	HIS
1	D	591	GLN
1	B	669	GLN
1	C	175	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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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	$\# Z  > 2$
2	NAP	A	1000	-	42,52,52	1.72	9 (21%)	54,80,80	1.88	11 (20%)
2	NAP	B	1001	-	42,52,52	1.75	8 (19%)	54,80,80	1.84	11 (20%)
2	NAP	C	1002	-	42,52,52	1.77	11 (26%)	54,80,80	1.90	11 (20%)
2	NAP	D	1003	-	42,52,52	1.73	8 (19%)	54,80,80	1.88	10 (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
2	NAP	A	1000	-	-	0/27/67/67	0/5/5/5
2	NAP	B	1001	-	-	0/27/67/67	0/5/5/5
2	NAP	C	1002	-	-	0/27/67/67	0/5/5/5
2	NAP	D	1003	-	-	0/27/67/67	0/5/5/5

The worst 5 of 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1003	NAP	PA-O1A	-3.11	1.39	1.51
2	A	1000	NAP	PA-O1A	-2.93	1.40	1.51
2	C	1002	NAP	PA-O1A	-2.90	1.40	1.51
2	B	1001	NAP	PA-O1A	-2.82	1.40	1.51
2	A	1000	NAP	C4A-N3A	2.02	1.38	1.35

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1003	NAP	N3A-C2A-N1A	-7.91	122.84	128.89
2	C	1002	NAP	N3A-C2A-N1A	-7.90	122.84	128.89
2	A	1000	NAP	N3A-C2A-N1A	-7.71	122.99	128.89
2	B	1001	NAP	N3A-C2A-N1A	-7.66	123.03	128.89
2	C	1002	NAP	O4D-C1D-N1N	-5.26	102.35	108.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1000	NAP	4	0
2	B	1001	NAP	4	0
2	C	1002	NAP	2	0
2	D	1003	NAP	5	0

## 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](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.