



wwPDB X-ray Structure Validation Summary Report

Mar 1, 2014 – 12:26 AM 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 validation summary report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

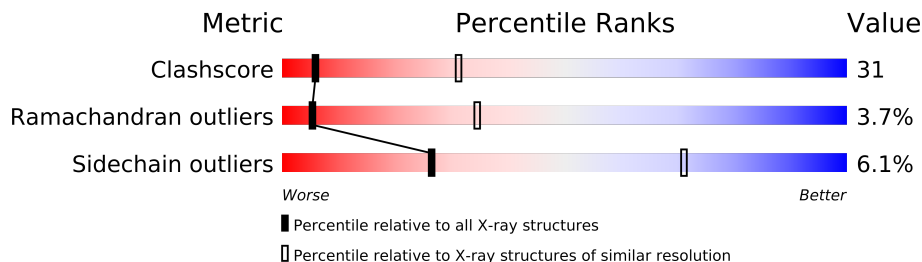
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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	79885	1078 (3.26-3.14)
Ramachandran outliers	78287	1059 (3.26-3.14)
Sidechain outliers	78261	1058 (3.26-3.14)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

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 hydrogen and 0 are deuterium.

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-DINUCLEOTIDEPHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



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.

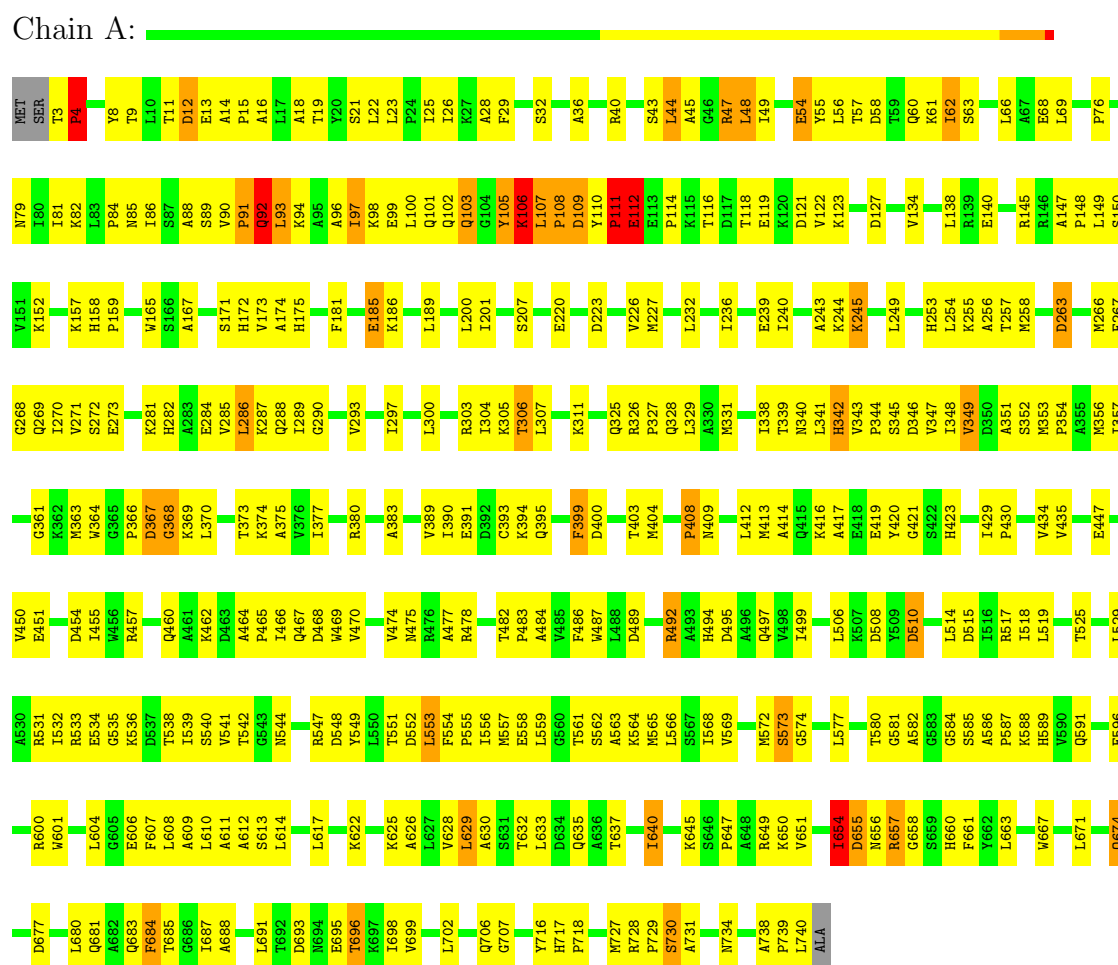
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	123	Total	O	0	0
			123	123		
3	B	101	Total	O	0	0
			101	101		
3	C	99	Total	O	0	0
			99	99		
3	D	122	Total	O	0	0
			122	122		

3 Residue-property plots

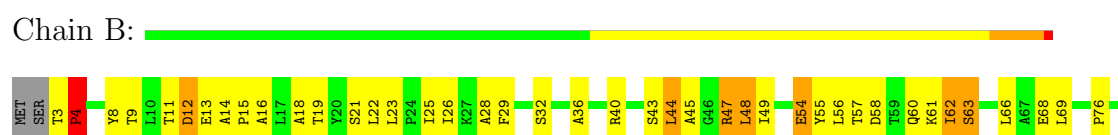
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

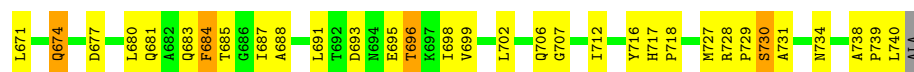
• Molecule 1: Isocitrate Dehydrogenase



• Molecule 1: Isocitrate Dehydrogenase

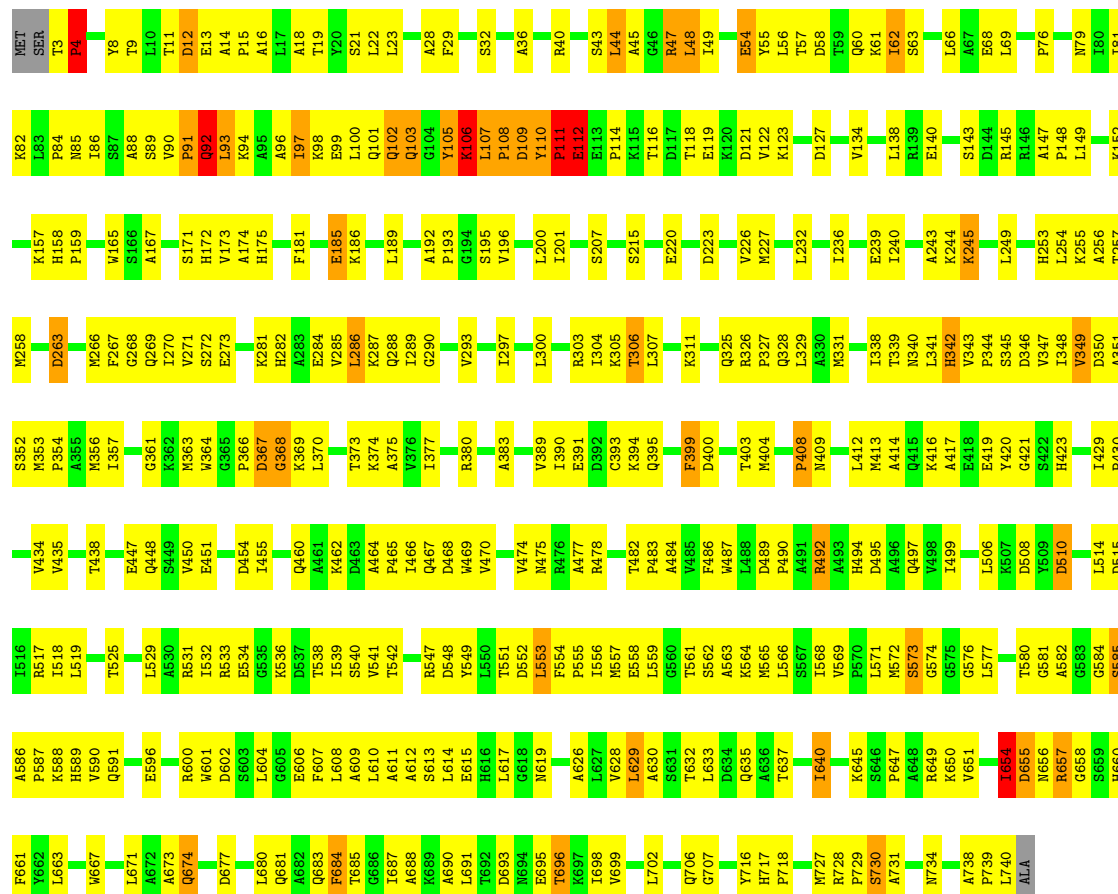


L604	G605	T538	E451	P354	M258	P148	N79
E596	R600	T539	E452	A355	K258	L149	I80
R601	W601	S640	D455	M356	D263	S150	I81
W602	S603	F607	L454	I357	M266	V151	K82
Y604	F608	T542	Q460	G351	F267	K152	L83
L605	A609	V545	A461	G361	C268	K157	P84
L606	L610	L546	K462	W364	Q269	H158	N85
L607	A612	L547	K463	G365	L270	H159	I86
L608	S613	R547	A464	P366	V271	S160	S87
L609	E615	D548	P465	D367	S272	W165	S88
L610	H616	Y549	L466	G368	E273	S166	S89
L611	H617	T551	D468	L370	K281	A167	V90
L612	N619	D552	V469	T373	H282	S171	P91
L613	G625	L553	W470	T374	K283	H172	Q92
L614	A626	F554	A477	K374	E284	V173	K93
L615	L627	P555	R478	A375	V285	A174	A95
L616	L628	I556	T482	V376	L286	H175	A96
L617	L629	M557	P483	I377	K287	F181	I97
L618	A630	E558	F486	C381	Q289	E185	K98
L619	S631	L559	V487	Y382	G290	K186	E99
L620	T632	T561	L488	A383	I297	L189	L100
L621	L633	S562	D489	V389	L300	S195	Q101
L622	D634	K564	P490	I390	K303	E200	I102
L623	Q635	M565	R492	E391	R304	L201	Q103
L624	T637	L566	A493	D392	K305	I201	G104
L625	T638	S567	H494	C393	K306	S207	Y105
L626	L640	P570	A496	K394	T306	L207	I107
L627	K645	L571	Q497	Q395	L307	S207	P108
L628	G646	M572	V498	F399	K311	S215	D109
L629	A648	S573	L499	D400	Q325	E220	Y110
L630	R649	G574	L506	T403	R326	D223	P111
L631	K650	G575	R507	M404	P327	D223	E112
L632	V651	L577	D508	P408	Q328	V226	E113
L633	L654	T580	D510	N409	L329	M227	P114
L634	D655	G581	L514	L412	M331	S228	K115
L635	N656	A582	D515	M413	T338	A231	P116
L636	R657	G583	L516	A414	T339	L232	T117
L637	G658	S584	R517	Q415	K340	L236	T118
L638	S659	G585	L518	K416	L341	I236	E119
L639	H660	A586	L519	A417	H342	E239	K120
L640	F661	P587	T525	E418	V343	I240	D121
L641	Y662	K588	L663	E419	P344	I240	V134
L642	L667	V590	Q591	Y420	D346	K245	L138
L643	L671	E596	L529	G421	V347	K245	R139
L644	Q674	R600	R531	I429	V348	H253	E140
L645	D677	W601	L532	P430	V349	L254	G141
L646	P677	S652	R533	V434	D350	N142	N143
L647	P678	G603	E534	V435	S352	S143	D144
L648	P679	L663	Q674	V436	P587	R145	R146
L649	P680	L664	D677	V437	K589	A147	A147
L650	P681	L665	D678	V438	V590	E239	L138
L651	P682	L666	D679	V439	Q591	I240	R139
L652	P683	L667	D680	V440	G421	K245	E140
L653	P684	L668	D681	V441	I429	H253	G141
L654	P685	L669	D682	V442	P430	L254	N142
L655	P686	L670	D683	V443	D350	S143	D144
L656	P687	L671	D684	V444	S352	R145	R146
L657	P688	L672	D685	V445	P587	A147	A147
L658	P689	L673	D686	V446	K589	E239	L138
L659	P690	L674	D687	V447	V590	I240	R139
L660	P691	L675	D688	V448	Q591	K245	E140
L661	P692	L676	D689	V449	G421	H253	G141
L662	P693	L677	D690	V450	I429	L254	N142
L663	P694	L678	D691	V451	P430	S143	D144
L664	P695	L679	D692	V452	D350	R145	R146
L665	P696	L680	D693	V453	S352	A147	A147
L666	P697	L681	D694	V454	P587	E239	L138
L667	P698	L682	D695	V455	K589	I240	R139
L668	P699	L683	D696	V456	V590	K245	E140
L669	P700	L684	D697	V457	Q591	H253	G141
L670	P701	L685	D698	V458	G421	L254	N142
L671	P702	L686	D699	V459	I429	S143	D144
L672	P703	L687	D700	V460	P430	R145	R146
L673	P704	L688	D701	V461	D350	A147	A147
L674	P705	L689	D702	V462	S352	E239	L138
L675	P706	L690	D703	V463	P587	I240	R139
L676	P707	L691	D704	V464	K589	K245	E140
L677	P708	L692	D705	V465	V590	H253	G141
L678	P709	L693	D706	V466	Q591	L254	N142
L679	P710	L694	D707	V467	G421	S143	D144
L680	P711	L695	D708	V468	I429	R145	R146
L681	P712	L696	D709	V469	P430	A147	A147
L682	P713	L697	D710	V470	D350	E239	L138
L683	P714	L698	D711	V471	S352	I240	R139
L684	P715	L699	D712	V472	P587	K245	E140
L685	P716	L700	D713	V473	K589	H253	G141
L686	P717	L701	D714	V474	V590	L254	N142
L687	P718	L702	D715	V475	Q591	S143	D144
L688	P719	L703	D716	V476	I429	R145	R146
L689	P720	L704	D717	V477	P430	A147	A147
L690	P721	L705	D718	V478	D350	E239	L138
L691	P722	L706	D719	V479	S352	I240	R139
L692	P723	L707	D720	V480	P587	K245	E140
L693	P724	L708	D721	V481	K589	H253	G141
L694	P725	L709	D722	V482	V590	L254	N142
L695	P726	L710	D723	V483	Q591	S143	D144
L696	P727	L711	D724	V484	I429	R145	R146
L697	P728	L712	D725	V485	P430	A147	A147
L698	P729	L713	D726	V486	D350	E239	L138
L699	P730	L714	D727	V487	S352	I240	R139
L700	P731	L715	D728	V488	P587	K245	E140
L701	P732	L716	D729	V489	K589	H253	G141
L702	P733	L717	D730	V490	V590	L254	N142
L703	P734	L718	D731	V491	Q591	S143	D144
L704	P735	L719	D732	V492	I429	R145	R146
L705	P736	L720	D733	V493	P430	A147	A147
L706	P737	L721	D734	V494	D350	E239	L138
L707	P738	L722	D735	V495	S352	I240	R139
L708	P739	L723	D736	V496	P587	K245	E140
L709	P740	L724	D737	V497	K589	H253	G141
L710	P741	L725	D738	V498	V590	L254	N142
L711	P742	L726	D739	V499	Q591	S143	D144
L712	P743	L727	D740	V500	I429	R145	R146
L713	P744	L728	D741	V501	P430	A147	A147
L714	P745	L729	D742	V502	D350	E239	L138
L715	P746	L730	D743	V503	S352	I240	R139
L716	P747	L731	D744	V504	P587	K245	E140
L717	P748	L732	D745	V505	K589	H253	G141
L718	P749	L733	D746	V506	V590	L254	N142
L719	P750	L734	D747	V507	Q591	S143	D144
L720	P751	L735	D748	V508	I429	R145	R146
L721	P752	L736	D749	V509	P430	A147	A147
L722	P753	L737	D750	V510	D350	E239	L138
L723	P754	L738	D751	V511	S352	I240	R139
L724	P755	L739	D752	V512	P587	K245	E140
L725	P756	L740	D753	V513	K589	H253	G141
L726	P757	L741	D754	V514	V590	L254	N142
L727	P758	L742	D755	V515	Q591	S143	D144
L728	P759	L743	D756	V516	I429	R145	R146
L729	P760	L744	D757	V517	P430	A147	A147
L730	P761	L745	D758	V518	D350	E239	L138
L731	P762	L746	D759	V519	S352	I240	R139
L732	P763	L747	D760	V520	P587	K245	E140
L733	P764	L748	D761	V521	K589	H253	G141
L734	P765	L749	D762	V522	V590	L254	N142
L735	P766	L750	D763	V523	Q591	S143	D144
L736	P767	L751	D764	V524	I429	R145	R146
L737	P768	L752	D765	V525	P430	A147	A147
L738	P769	L753	D766	V526	D350	E239	L138
L739	P770	L754	D767	V527	S352	I240	R139
L740	P771	L755	D768	V528	P587	K245	E140
L741	P772	L756	D769	V529	K589	H253	G141
L742	P773	L757	D770	V530	V590	L254	N142
L743	P774	L758	D771	V531	Q591	S143	D144
L744	P775	L759	D772	V532	I429	R145	R146
L745	P776	L760	D773	V533	P430	A147	A147
L746	P777	L761	D774	V534	D350	E239	L138
L747	P778	L762	D775	V535	S352	I240	R139
L748	P779	L763	D776	V536	P587	K245	E140
L749	P780	L764	D777	V537	K589	H253	G141
L750	P781	L765	D778	V538	V590	L254	N142
L751	P782	L766	D779	V539	Q591	S143	D144
L752	P783	L767	D780	V540	I429	R145	R146
L753	P784	L768	D781	V541	P430	A147	A147
L754	P785	L769	D782	V542	D350	E239	L138
L755	P786	L770	D783	V543	S352	I240	R139
L756	P787	L771	D784	V544	P587	K245	E140
L757	P788	L772	D785	V545	K589	H253	G141
L758	P789	L773	D786	V546	V590	L254	N142
L759	P790	L774	D787	V547	Q591	S143	D144
L760	P791	L775	D788	V548	I429	R145	R146
L761	P792	L776	D789	V549	P430	A147	A147
L762	P793	L777	D790	V550	D350	E239	L138
L763	P794	L778	D791	V551	S352	I240	R139
L764	P795	L779	D792	V552	P587	K245	E140
L765	P796	L780	D793	V553	K589	H253	G141
L766	P797	L781	D794	V554	V590	L254	N142
L767	P798	L782	D795	V555	Q591	S143	D144
L768	P799	L783	D796	V556	I429	R145	R146
L769	P800	L784	D797	V557	P430	A147	A147
L770	P801	L785	D798	V558	D350	E239	L138
L771	P802	L786	D799	V559	S352	I240	R139
L772	P803	L787	D800	V560	P587	K245	E140
L773	P804	L788	D801	V561	K589	H253	G141
L774	P805	L789	D802	V562	V590	L254	N142
L775	P806	L790	D803	V563	Q591	S143	D144
L776	P807	L791	D804	V564	I429	R145	R146
L777	P80						



• Molecule 1: Isocitrate Dehydrogenase

Chain D:



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, α , β , γ	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 ²)	36.0	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: 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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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
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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 31.

The worst 5 of 1424 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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

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	736/741 (99%)	591 (80%)	119 (16%)	26 (4%)	6	37
1	B	736/741 (99%)	587 (80%)	122 (17%)	27 (4%)	5	34
1	C	736/741 (99%)	590 (80%)	119 (16%)	27 (4%)	5	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	736/741 (99%)	588 (80%)	120 (16%)	28 (4%)	5	34
All	All	2944/2964 (99%)	2356 (80%)	480 (16%)	108 (4%)	5	34

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%)	27	72
1	B	599/601 (100%)	563 (94%)	36 (6%)	27	72
1	C	599/601 (100%)	562 (94%)	37 (6%)	26	70
1	D	599/601 (100%)	563 (94%)	36 (6%)	27	72
All	All	2396/2404 (100%)	2251 (94%)	145 (6%)	26	71

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 ⓘ

There are no RNA chains 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 ⓘ

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	-	52,52,52	1.79	9 (17%)	80,80,80	1.77	15 (18%)
2	NAP	B	1001	-	52,52,52	1.80	11 (21%)	80,80,80	1.75	18 (22%)
2	NAP	C	1002	-	52,52,52	1.83	13 (25%)	80,80,80	1.80	16 (20%)
2	NAP	D	1003	-	52,52,52	1.78	11 (21%)	80,80,80	1.77	16 (20%)

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	-	-	0/35/67/67	0/3/5/5
2	NAP	B	1001	-	-	0/35/67/67	0/3/5/5
2	NAP	C	1002	-	-	0/35/67/67	0/3/5/5
2	NAP	D	1003	-	-	0/35/67/67	0/3/5/5

The worst 5 of 44 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1000	NAP	C2N-N1N	6.55	1.43	1.35
2	B	1001	NAP	C2N-N1N	6.38	1.43	1.35
2	D	1003	NAP	C2N-N1N	6.14	1.43	1.35
2	C	1002	NAP	C2N-N1N	5.99	1.43	1.35
2	C	1002	NAP	C4N-C3N	4.84	1.47	1.39

The worst 5 of 65 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1003	NAP	N3A-C2A-N1A	-7.02	122.84	128.71
2	C	1002	NAP	N3A-C2A-N1A	-7.02	122.84	128.71
2	A	1000	NAP	N3A-C2A-N1A	-6.84	122.99	128.71
2	B	1001	NAP	N3A-C2A-N1A	-6.79	123.03	128.71
2	C	1002	NAP	O4D-C1D-N1N	-5.48	102.35	107.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

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

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

6.3 Carbohydrates ⓘ

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

6.4 Ligands ⓘ

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

6.5 Other polymers ⓘ

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