



wwPDB X-ray Structure Validation Summary Report ⓘ

May 28, 2020 – 07:53 pm BST

PDB ID : 1HN1
Title : E. COLI (LAC Z) BETA-GALACTOSIDASE (ORTHORHOMBIC)
Authors : Juers, D.H.; Matthews, B.W.
Deposited on : 2000-12-05
Resolution : 3.00 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

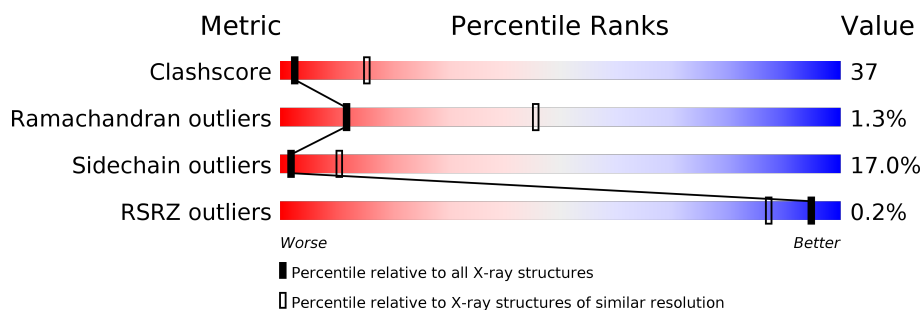
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

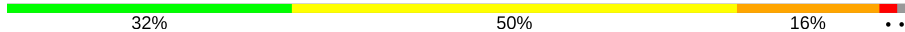
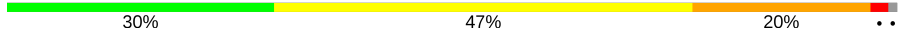

The reported resolution of this entry is 3.00 Å.

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	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1023	 32% 50% 16% ..
1	B	1023	 30% 47% 20% ..
1	C	1023	 33% 48% 16% ..
1	D	1023	 35% 46% 15% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 32954 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 BETA-GALACTOSIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1011	Total	C	N	O	S	0	2	0
			8136	5145	1443	1510	38			
1	B	1011	Total	C	N	O	S	0	2	0
			8136	5145	1443	1510	38			
1	C	1011	Total	C	N	O	S	0	2	0
			8136	5145	1443	1510	38			
1	D	1011	Total	C	N	O	S	0	1	0
			8130	5141	1441	1510	38			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	CLONING ARTIFACT	UNP P00722
A	2	SER	-	CLONING ARTIFACT	UNP P00722
A	3	HIS	-	CLONING ARTIFACT	UNP P00722
A	4	MET	-	CLONING ARTIFACT	UNP P00722
A	5	LEU	-	CLONING ARTIFACT	UNP P00722
A	6	GLU	-	CLONING ARTIFACT	UNP P00722
A	7	ASP	-	CLONING ARTIFACT	UNP P00722
A	8	PRO	-	CLONING ARTIFACT	UNP P00722
B	1	GLY	-	CLONING ARTIFACT	UNP P00722
B	2	SER	-	CLONING ARTIFACT	UNP P00722
B	3	HIS	-	CLONING ARTIFACT	UNP P00722
B	4	MET	-	CLONING ARTIFACT	UNP P00722
B	5	LEU	-	CLONING ARTIFACT	UNP P00722
B	6	GLU	-	CLONING ARTIFACT	UNP P00722
B	7	ASP	-	CLONING ARTIFACT	UNP P00722
B	8	PRO	-	CLONING ARTIFACT	UNP P00722
C	1	GLY	-	CLONING ARTIFACT	UNP P00722
C	2	SER	-	CLONING ARTIFACT	UNP P00722
C	3	HIS	-	CLONING ARTIFACT	UNP P00722
C	4	MET	-	CLONING ARTIFACT	UNP P00722
C	5	LEU	-	CLONING ARTIFACT	UNP P00722

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Chain	Residue	Modelled	Actual	Comment	Reference
C	6	GLU	-	CLONING ARTIFACT	UNP P00722
C	7	ASP	-	CLONING ARTIFACT	UNP P00722
C	8	PRO	-	CLONING ARTIFACT	UNP P00722
D	1	GLY	-	CLONING ARTIFACT	UNP P00722
D	2	SER	-	CLONING ARTIFACT	UNP P00722
D	3	HIS	-	CLONING ARTIFACT	UNP P00722
D	4	MET	-	CLONING ARTIFACT	UNP P00722
D	5	LEU	-	CLONING ARTIFACT	UNP P00722
D	6	GLU	-	CLONING ARTIFACT	UNP P00722
D	7	ASP	-	CLONING ARTIFACT	UNP P00722
D	8	PRO	-	CLONING ARTIFACT	UNP P00722

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

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

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	103	Total O 103 103	0	0

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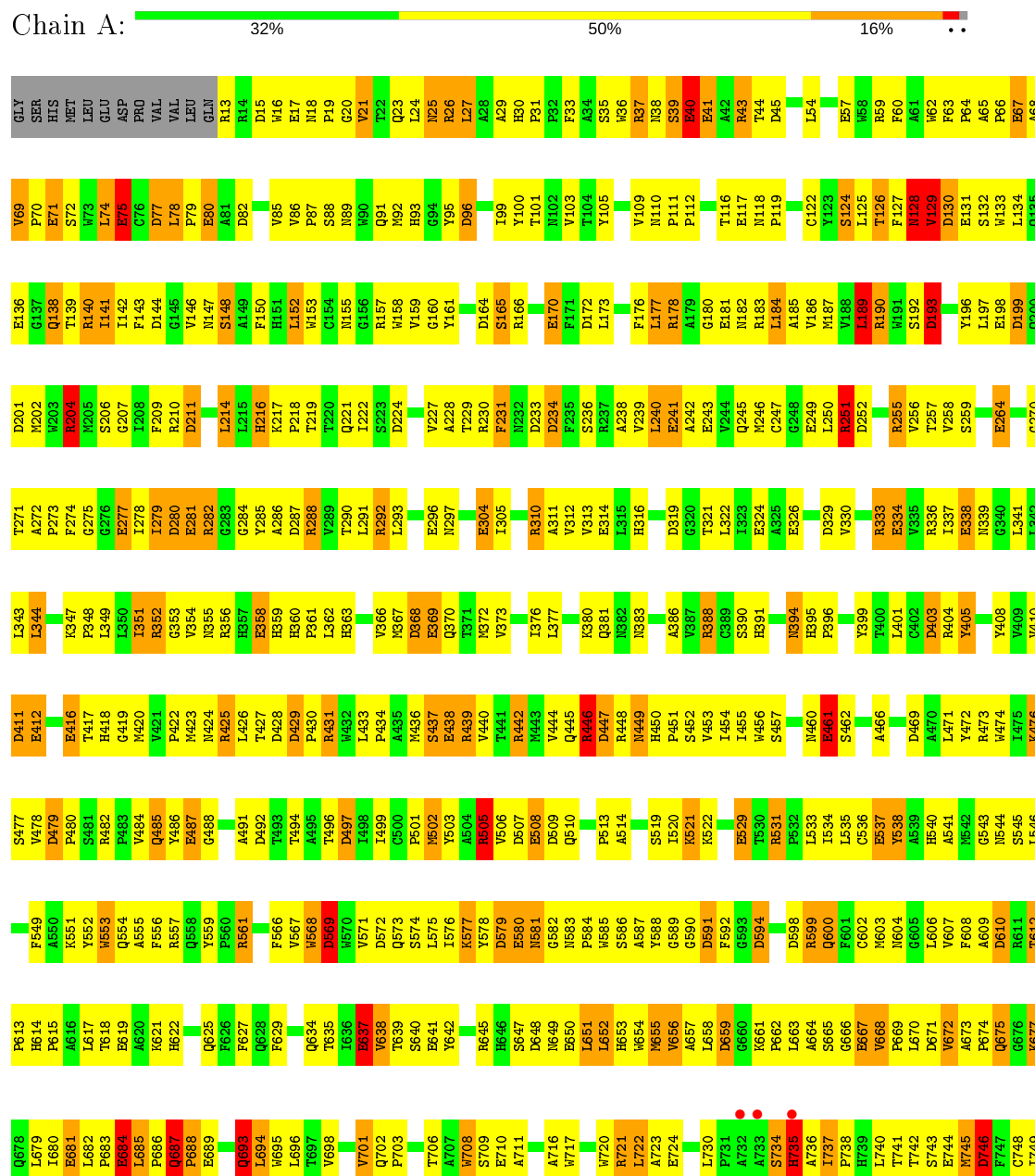
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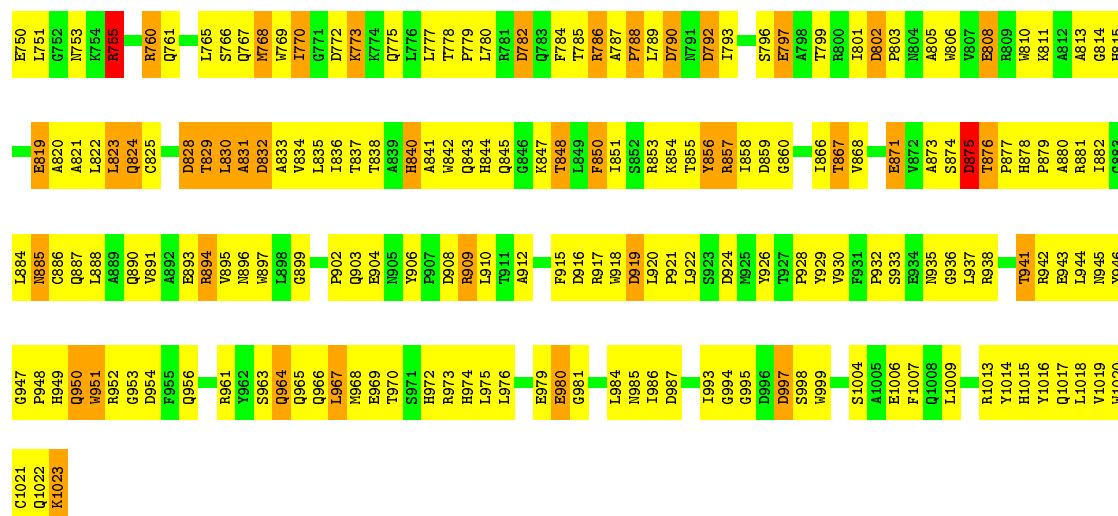
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	92	Total 92	O 92	0	0
4	C	108	Total 108	O 108	0	0
4	D	98	Total 98	O 98	0	0

3 Residue-property plots

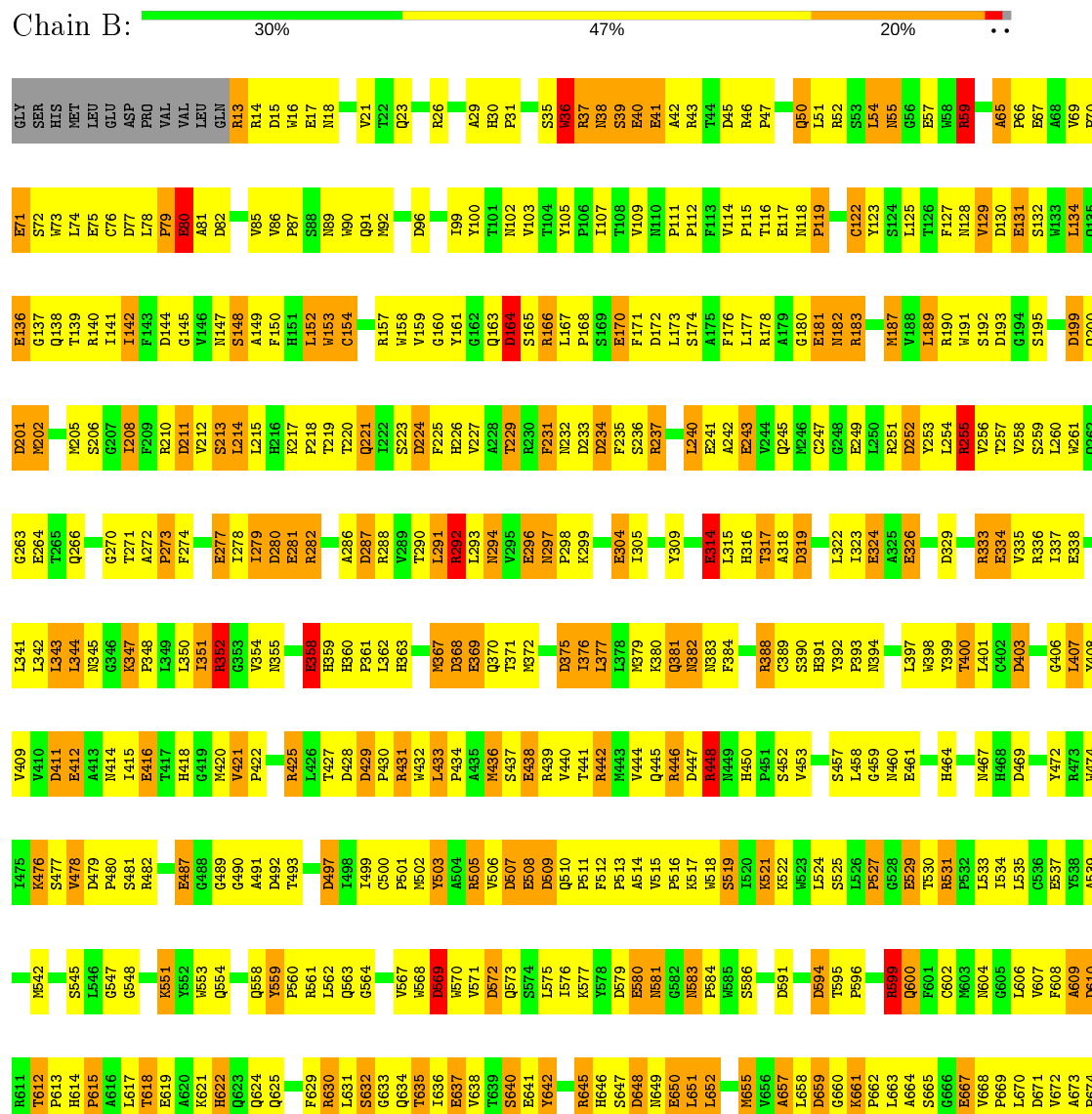
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: BETA-GALACTOSIDASE





• Molecule 1: BETA-GALACTOSIDASE





GLY	S481	I415	P348	D211	I142	P70	
	R482	E416	L349	V212	F143	E71	
	Q485	T417	L350	S213	F143	S72	
		H418	E281	L214	V146	W73	
		G419	R282	L215	W147	L74	
	E487	M420	G353	H216	S148	E75	
	G488	V421	V354	K217	C76	C76	
	A491	P422	N355	P218	A149	ASP	
	F566	M423	R356	K218	F150	PRQ	
	V567	M424	R357	D224	L78	VAL	
E568	R425	R358	F225	L152	LEU		
R669	T426	H358	H226	L153	VAL		
W570	T427	H360	T227	W158	GLN		
V571	T428	R361	V227	T83	R13		
D572	D429	L362	T229	V84	R14		
Q573	P430	H363	R230	V85	D15		
S574	R431	G364	F231	Y161	W16		
L575	M432	T297	N332	V86	G20		
L433	L298	D233	N332	P87		V21	
S576	P434	E369	D234	S88		V21	
K577	M435	Q370	F235	R166	T22		
E578	A436	Q371	S236	W90	Q23		
D579	M436	T371	N301	P168	L24		
E580	S437	M372	S302	S169	N25		
H30	E508	E438	W373	A303	E170	N35	
	D609	R439	Q374	E304	F171	R26	
	Q510	V440	D375	I305	G94	H30	
	P511	T441	I376	L173	D96		F33
	W585	R442	L377	N307	S174		W36
	F512	R443	L378	V244	A175	I99	
	P513	M443	L378	V244	F176	Y100	
	A514	V444	M379	Q245	L177	N110	
	V515	Q445	R380	E246	R178	P111	
	P516	R446	Q381	C247	A179	E41	
K517	D447	N382	G248	G180	P112		
G593	R448	L383	E249	L113	R42		
D594	M449	F384	H316	E381	L42		
T595	H450	N385	T317	N382	R43		
Q600	P627	V453	A386	R251	V114	T94	
	G528	I454	A318	D252	P115	D45	
	E529	T530	L184	Y253	L184	R46	
	R539	I455	R388	L254	E117	P47	
	E631	M456	H391	R255	M187	S48	
	P532	S457	Y392	V256	V188	L51	
	L533	L533	P393	T257	L189	R52	
	M603	E461	N394	V258	R190	S53	
	N604	S462	H395	D829	D193	L54	
	G605	G463	P396	W261	G194	F127	
L606	E537	L397	F332	S195	N128		
V607	R538	R398	Q262	S195	G56		
F608	M467	H398	G263	V129	E57		
A609	H468	Y399	E264	E198	W58		
D610	D469	T400	V335	D199	R59		
R611	A470	L401	R336	Q200	S132		
S645	L471	R611	I337	W133	F60		
T612	Y472	T612	I337	D201	L134		
P613	R473	L407	E338	M202	L134		
H614	Y408	Y408	L203	W203	Q135		
P615	K476	V410	L241	R204	P64		
A616	S477	V410	A272	E136	A65		
L617	W553	D411	L343	G137	P66		
T618	E412	D411	L344	S206	E67		
D619	D479	A413	F274	G207	T139		
E620	P480	N414	E377	R340	A68		
E620	E555	E555	E377	I208	W60		

S960	G488	L696	Q761	A827	L898	S960
R961	G489	T697	S762	D828	G899	R961
E969	F666	V698	L765	T829	L900	E969
T970	V567	R699	S766	L830	G901	T970
S971	W568	Q700	Q767	A831	P902	S971
H972	D569	V701	W768	D832	Q903	H972
R973	T493	Q702	W769	A833	E904	R973
H974	T494	P703	L770	L836	N905	H974
L975	D497	T706	G771	T837	P907	L975
A978	I498	A707	K773	T838	D908	A978
E979	C500	W708	S709	A839	R909	E979
E880	P501	S709	K774	H840	L910	E880
G981	M502	E710	Q775	A841	T911	G981
T982	Y503	A711	L776	W842	A912	T982
W983	A504	L777	T778	Q843	Q913	W983
L984	R505	H713	T779	H844	C914	L984
N985	V506	W714	W779	Q845	F915	N985
I986	V507	L750	R781	F850	D916	I986
D987	E508	W717	D782	R853	R917	D987
G988	D509	Q718	Q783	R854	W918	G988
F989	Q510	W719	F784	T855	D919	F989
H990	P511	W720	T785	W856	L920	H990
N991	F512	R721	R786	A857	P921	N991
D996	W515	L722	A787	I858	D924	D996
D997	P516	E724	P788	T859	N925	D997
S998	K517	N725	L789	G860	Y926	S998
A1004	K521	W726	W791	I866	T927	A1004
A1005	K522	S727	T792	T867	P928	A1005
F1007	L524	W728	T793	W868	Y929	F1007
A1011	G528	T729	G794	D869	V930	A1011
G1012	E529	L730	W795	V870	F931	G1012
R1013	T530	P731	S796	E871	S932	R1013
Y1014	E531	W734	E797	V872	S933	Y1014
Q1017	P532	H735	A798	D875	N935	Q1017
L1018	L533	I737	R800	T876	G936	L1018
V1019	I534	P738	I801	P877	L937	V1019
H1020	E537	H739	D802	H878	R938	H1020
C1021	G543	L740	P803	P879	C939	C1021
Q1022	M544	T741	N804	A880	T941	Q1022
G947	S545	W742	A805	R881	R942	G947
H949	L546	S743	W806	I882	E943	H949
Q950	G547	E744	E808	G883	Y946	Q950
W951	K551	D746	R809	L884	G947	W951
R952	Y552	F747	C748	Q887	P948	R952
G953	W553	E750	Y816	L888	H949	G953
D954	F556	L751	A818	A889	Q950	D954
F955	Q558	R755	E820	Q890	W951	F955
Q956	Y559	W756	A821	W891	G953	Q956
F957	R557	Q757	A821	A892	D954	F957
N958	F626	W758	Q824	R894	F955	N958
I959	P627	R760	G825	W895	I959	I959
L562	L617	L617	T826	W897		L562
F666	T618	T618				F666
W567	E619	E619				W567
W568	A620	A620				W568
D569	K621	K621				D569
T493	R557	R557				T493
T494	Q558	Q558				T494
D497	Y559	Y559				D497
D572	P560	P560				D572
Q573	R561	R561				Q573
I576						I576
K577						K577
Y578						Y578
D579						D579
E580						E580
A584						A584
R581						R581
V582						V582
N583						N583
E588						E588
P584						P584
W585						W585
S586						S586
A587						A587
Y588						Y588
G589						G589
C590						C590
D591						D591
F592						F592
G593						G593
D594						D594
T595						T595
P596						P596
N597						N597
D598						D598
R599						R599
Q600						Q600
F601						F601
C602						C602
G605						G605
L606						L606
V607						V607
F608						F608
A609						A609
D610						D610
R611						R611
T612						T612
P613						P613
H614						H614
L617						L617
Y618						Y618
W619						W619
A620						A620
K621						K621
R622						R622
F626						F626
P627						P627
Q693						Q693
L694						L694
W695						W695

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	153.90 Å 171.40 Å 204.50 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.00 29.96 – 2.99	Depositor EDS
% Data completeness (in resolution range)	94.0 (15.00-3.00) 88.8 (29.96-2.99)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 3.00 Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.148 , 0.299 0.134 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	31.4	Xtriage
Anisotropy	0.253	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 132.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	32954	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.90 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.2078e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	1.08	58/8387 (0.7%)	1.66	166/11442 (1.5%)
1	B	1.07	55/8387 (0.7%)	1.65	170/11442 (1.5%)
1	C	1.07	56/8387 (0.7%)	1.65	157/11442 (1.4%)
1	D	1.09	58/8376 (0.7%)	1.65	168/11427 (1.5%)
All	All	1.08	227/33537 (0.7%)	1.65	661/45753 (1.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	1	0
1	D	1	0
All	All	2	0

The worst 5 of 227 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	314	GLU	CD-OE2	8.73	1.35	1.25
1	D	304	GLU	CD-OE2	8.61	1.35	1.25
1	D	334	GLU	CD-OE2	8.13	1.34	1.25
1	A	304	GLU	CD-OE2	8.00	1.34	1.25
1	C	461	GLU	CD-OE2	7.99	1.34	1.25

The worst 5 of 661 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	685	LEU	C-N-CD	-21.41	73.50	120.60
1	B	730	LEU	C-N-CD	-21.06	74.26	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	987	ASP	CB-CG-OD2	-13.47	106.18	118.30
1	A	687	GLN	C-N-CD	-12.61	92.86	120.60
1	D	166	ARG	NE-CZ-NH2	-12.33	114.13	120.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	37	ARG	CA
1	D	951	TRP	CA

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	8136	0	7723	593	0
1	B	8136	0	7723	660	0
1	C	8136	0	7723	548	0
1	D	8130	0	7720	550	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	1	0	0	0	0
4	A	103	0	0	2	0
4	B	92	0	0	9	0
4	C	108	0	0	8	0
4	D	98	0	0	6	0
All	All	32954	0	30889	2319	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 37.

The worst 5 of 2319 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:D:502:MET:HB2	1:D:537:GLU:HB2	1.25	1.18
1:D:734:SER:HB3	1:D:860:GLY:HA3	1.20	1.11
1:B:18:ASN:HD22	1:B:21:VAL:HG23	1.09	1.10
1:B:737:ILE:HD12	1:B:738:PRO:HD2	1.26	1.09
1:A:737:ILE:HG13	1:A:832:ASP:HA	1.35	1.08

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	1011/1023 (99%)	902 (89%)	99 (10%)	10 (1%)	15	53
1	B	1011/1023 (99%)	901 (89%)	96 (10%)	14 (1%)	11	43
1	C	1011/1023 (99%)	904 (89%)	93 (9%)	14 (1%)	11	43
1	D	1010/1023 (99%)	904 (90%)	93 (9%)	13 (1%)	12	45
All	All	4043/4092 (99%)	3611 (89%)	381 (9%)	51 (1%)	12	45

5 of 51 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	129	VAL
1	A	425	ARG
1	A	688	PRO
1	B	201	ASP
1	B	647	SER

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	866/875 (99%)	723 (84%)	143 (16%)	2	11
1	B	866/875 (99%)	699 (81%)	167 (19%)	1	8
1	C	866/875 (99%)	732 (84%)	134 (16%)	2	13
1	D	865/875 (99%)	721 (83%)	144 (17%)	2	11
All	All	3463/3500 (99%)	2875 (83%)	588 (17%)	2	10

5 of 588 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	766	SER
1	C	189	LEU
1	D	749	ILE
1	B	797	GLU
1	B	952	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 85 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	687	GLN
1	B	1022	GLN
1	D	804	ASN
1	B	702	GLN
1	B	735	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](#)

Of 15 ligands modelled in this entry, 15 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1011/1023 (98%)	-0.82	3 (0%) 94 84	10, 35, 92, 211	0
1	B	1011/1023 (98%)	-0.78	0 100 100	8, 38, 101, 212	0
1	C	1011/1023 (98%)	-0.79	4 (0%) 92 79	14, 34, 91, 214	0
1	D	1011/1023 (98%)	-0.83	0 100 100	5, 34, 93, 210	0
All	All	4044/4092 (98%)	-0.81	7 (0%) 95 87	5, 35, 94, 214	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	689	GLU	3.0
1	A	735	HIS	2.7
1	A	733	ALA	2.6
1	C	733	ALA	2.4
1	C	732	ALA	2.1

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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NA	B	3102	1/1	0.93	0.21	32,32,32,32	0
3	NA	C	3101	1/1	0.94	0.43	49,49,49,49	0
2	MG	B	3002	1/1	0.94	0.12	30,30,30,30	0
3	NA	A	3101	1/1	0.95	0.25	52,52,52,52	0
3	NA	B	3103	1/1	0.96	0.13	45,45,45,45	0
3	NA	A	3102	1/1	0.96	0.38	24,24,24,24	0
2	MG	A	3001	1/1	0.96	0.26	29,29,29,29	0
3	NA	C	3102	1/1	0.96	0.23	24,24,24,24	0
2	MG	C	3001	1/1	0.97	0.26	25,25,25,25	0
3	NA	D	3102	1/1	0.98	0.30	47,47,47,47	0
2	MG	D	3001	1/1	0.98	0.28	26,26,26,26	0
2	MG	A	3002	1/1	0.98	0.08	29,29,29,29	0
2	MG	D	3002	1/1	0.98	0.22	30,30,30,30	0
2	MG	B	3001	1/1	0.99	0.15	13,13,13,13	0
2	MG	C	3002	1/1	0.99	0.18	25,25,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.