



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 06:42 PM UTC

PDB ID : 3LMM / pdb_00003lmm
Title : Crystal Structure of the DIP2311 protein from Corynebacterium diphtheriae, Northeast Structural Genomics Consortium Target Cdr35
Authors : Forouhar, F.; Lew, S.; Seetharaman, J.; Mao, M.; Xiao, R.; Ciccocanti, C.; Buchwald, W.A.; Maglaqui, M.; Everett, J.K.; Nair, R.; Acton, T.B.; Rost, B.; Montelione, G.T.; Hunt, J.F.; Tong, L.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2010-01-31
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<https://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)

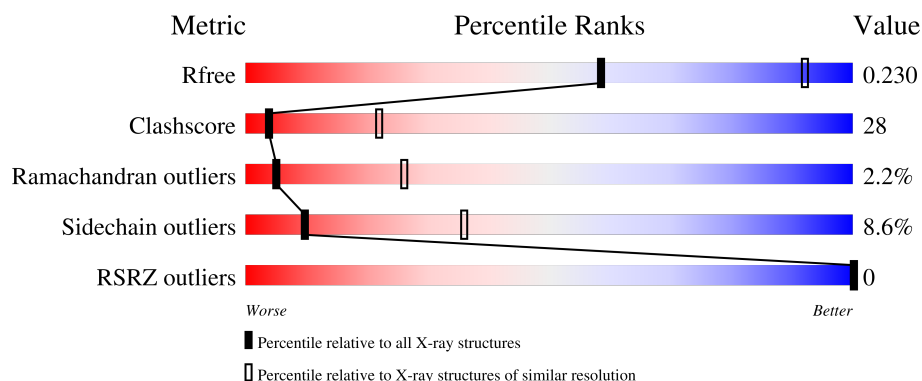
1 Overall quality at a glance

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))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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 of 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	583	
1	B	583	
1	C	583	
1	D	583	

Validation Pipeline (wwPDB-VP) : 2.49

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16408 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 Uncharacterized protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	492	Total	C	N	O	S	Se	0	0	0
			3798	2390	682	716	4	6			
1	B	555	Total	C	N	O	S	Se	0	0	0
			4262	2673	766	808	6	9			
1	C	477	Total	C	N	O	S	Se	0	0	0
			3676	2312	659	695	4	6			
1	D	556	Total	C	N	O	S	Se	0	0	0
			4271	2678	767	811	6	9			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	VAL	-	expression tag	UNP Q6NEG3
A	576	LEU	-	expression tag	UNP Q6NEG3
A	577	GLU	-	expression tag	UNP Q6NEG3
A	578	HIS	-	expression tag	UNP Q6NEG3
A	579	HIS	-	expression tag	UNP Q6NEG3
A	580	HIS	-	expression tag	UNP Q6NEG3
A	581	HIS	-	expression tag	UNP Q6NEG3
A	582	HIS	-	expression tag	UNP Q6NEG3
A	583	HIS	-	expression tag	UNP Q6NEG3
B	1	VAL	-	expression tag	UNP Q6NEG3
B	576	LEU	-	expression tag	UNP Q6NEG3
B	577	GLU	-	expression tag	UNP Q6NEG3
B	578	HIS	-	expression tag	UNP Q6NEG3
B	579	HIS	-	expression tag	UNP Q6NEG3
B	580	HIS	-	expression tag	UNP Q6NEG3
B	581	HIS	-	expression tag	UNP Q6NEG3
B	582	HIS	-	expression tag	UNP Q6NEG3
B	583	HIS	-	expression tag	UNP Q6NEG3
C	1	VAL	-	expression tag	UNP Q6NEG3
C	576	LEU	-	expression tag	UNP Q6NEG3
C	577	GLU	-	expression tag	UNP Q6NEG3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	578	HIS	-	expression tag	UNP Q6NEG3
C	579	HIS	-	expression tag	UNP Q6NEG3
C	580	HIS	-	expression tag	UNP Q6NEG3
C	581	HIS	-	expression tag	UNP Q6NEG3
C	582	HIS	-	expression tag	UNP Q6NEG3
C	583	HIS	-	expression tag	UNP Q6NEG3
D	1	VAL	-	expression tag	UNP Q6NEG3
D	576	LEU	-	expression tag	UNP Q6NEG3
D	577	GLU	-	expression tag	UNP Q6NEG3
D	578	HIS	-	expression tag	UNP Q6NEG3
D	579	HIS	-	expression tag	UNP Q6NEG3
D	580	HIS	-	expression tag	UNP Q6NEG3
D	581	HIS	-	expression tag	UNP Q6NEG3
D	582	HIS	-	expression tag	UNP Q6NEG3
D	583	HIS	-	expression tag	UNP Q6NEG3

- Molecule 2 is COBALT (II) ION (CCD ID: CO) (formula: Co).

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

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

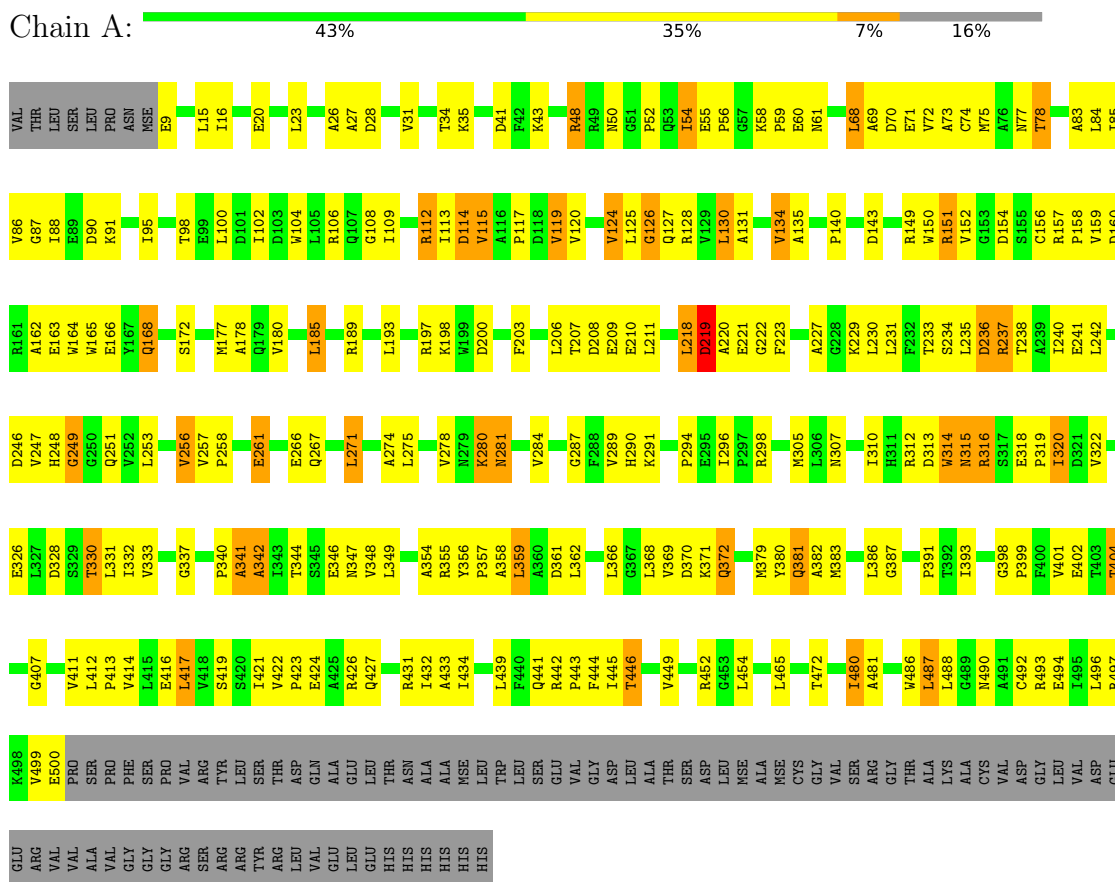
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	128	Total 128	O 128	0	0
4	B	64	Total 64	O 64	0	0
4	C	109	Total 109	O 109	0	0
4	D	90	Total 90	O 90	0	0

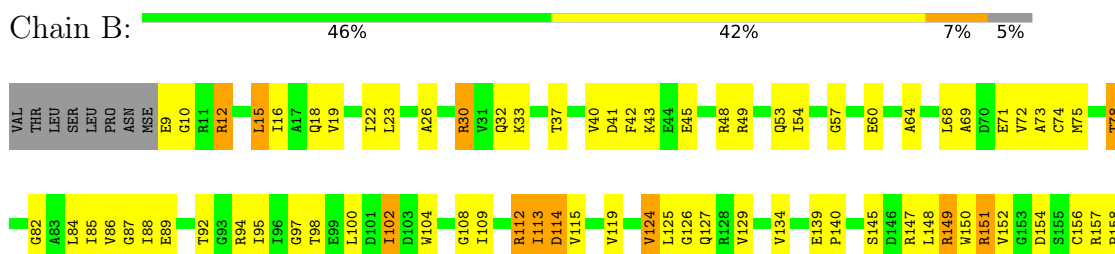
3 Residue-property plots

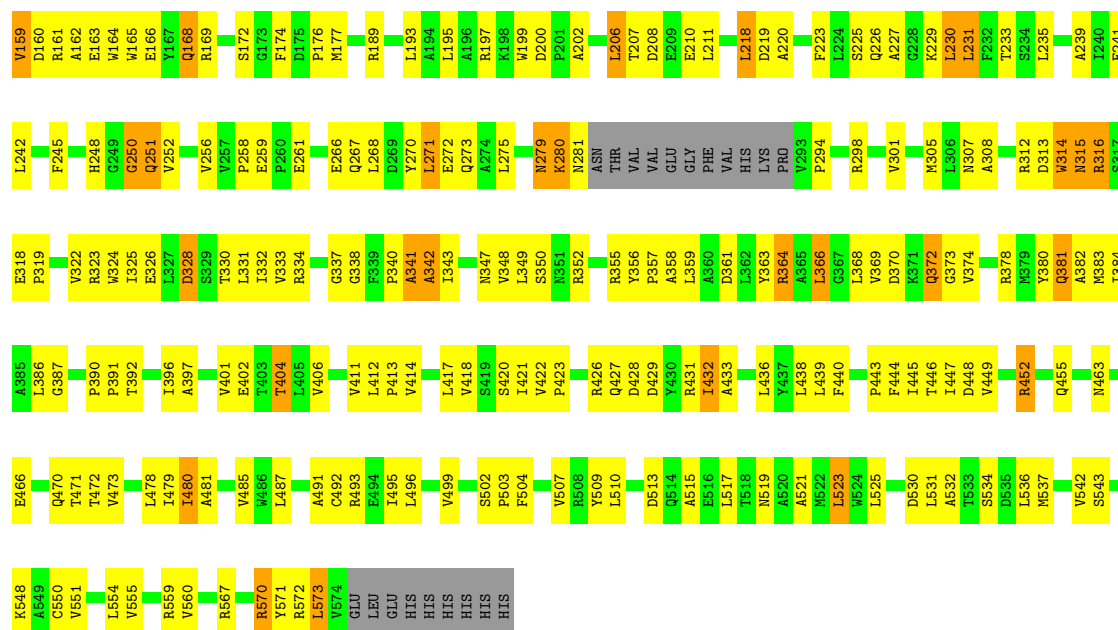
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: Uncharacterized protein





S505	P506	V507	R508	Y509	D513	Q514	A515	E516	L517	T518	M519	M522	L523	W524	L525	S526	E527	D530	L531	S534	D535	L536	M537	A538	M539	C540	G541	V551	L554	V560	R569	R570	Y571	R572	L573	W574	E575	LEU	HIS	HIS	HIS	HIS	HIS								
E402	T403	T404	V411	L412	P413	V414	L417	S420	I421	V422	P423	E424	A425	R426	Q427	I432	L436	R442	P443	F444	I445	T446	I447	D448	V449	L454	E459	E466	T472	V473	L478	L487	N490	A491	C492	R493	E494	T495	L496	R497	K498	V499	S502	P503	F504						
T330	L331	I332	V333	R334	G337	P340	A341	A342	T344	S345	E346	N347	V348	R352	R355	Y356	P357	A358	L359	A360	D361	L362	Y363	L366	G367	L368	V369	Q372	G373	V376	M379	Y380	Q381	A382	M383	I384	G387	N390	A391	C392	R393	E394	E395	I396	A397	F400	V401				
P260	E261	E266	Q267	L268	D269	Y270	L271	E272	Q273	A274	L275	V278	N279	K280	N281	ASN	THR	VAL	VAL	GLU	GLY	PRO	V293	P294	E295	L296	R302	E303	A304	M305	L306	N307	A308	M309	R312	D313	W314	N315	R316	S317	E318	P319	I320	D321	Q322	R323	K324	I325	D328	S329	
P158	V159	D160	R161	E162	L163	W164	W165	Y166	Q168	M177	R189	L190	D191	I192	D193	W194	K198	W199	L206	T207	D208	E209	E210	L218	D219	A220	E221	G222	F223	Q226	A227	G228	K229	T233	S234	L235	D236	R237	I240	E241	L242	S243	T244	G245	G250	W251	V252	V256	V257	C156	E259
L84	I85	V86	G87	I88	E89	D90	K91	T92	G93	R94	I95	T98	E99	L100	D101	I102	D103	W104	L105	R106	Q107	G108	I109	F110	T111	R112	I113	D114	V115	A116	V119	V124	L125	G126	Q127	L130	V134	P140	D143	D146	R147	L148	R149	W150	R151	V152	G153	D154	S155	R157	
VAL	THR	LEU	SER	LEU	PRO	ASN	MSE	E9	G10	R91	R12	E13	Q14	L15	Q18	V19	L23	A24	S25	A26	V31	T34	K35	E36	T37	D41	F42	K43	E44	A45	A46	G57	K58	P59	E60	N61	A64	L68	A69	D70	E71	V72	A73	C74	M75	T78	G81	G82	A83		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	147.31Å 102.03Å 164.51Å 90.00° 116.00° 90.00°	Depositor
Resolution (Å)	19.99 – 3.00 19.99 – 3.00	Depositor EDS
% Data completeness (in resolution range)	81.4 (19.99-3.00) 93.0 (19.99-3.00)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.82 (at 3.00Å)	Xtriage
Refinement program	CNS 1.2 & XtalView, REFMAC	Depositor
R, R_{free}	0.183 , 0.231 0.203 , 0.230	Depositor DCC
R_{free} test set	8526 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	42.4	Xtriage
Anisotropy	0.366	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 14.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.056 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16408	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.53	0/3860	0.94	7/5239 (0.1%)
1	B	0.47	0/4325	0.90	4/5862 (0.1%)
1	C	0.52	0/3734	0.93	5/5067 (0.1%)
1	D	0.46	0/4334	0.89	3/5874 (0.1%)
All	All	0.49	0/16253	0.91	19/22042 (0.1%)

There are no bond length outliers.

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	154	ASP	N-CA-C	-9.57	101.61	113.38
1	D	154	ASP	N-CA-C	-9.13	102.28	113.97
1	C	154	ASP	N-CA-C	-8.62	102.89	113.41
1	A	220	ALA	N-CA-C	-7.59	104.25	113.97
1	A	290	HIS	CB-CA-C	-7.43	97.49	109.75

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	3798	0	3826	225	0
1	B	4262	0	4290	267	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3676	0	3699	201	0
1	D	4271	0	4296	236	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	3	0	0	2	0
3	B	1	0	0	1	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	128	0	0	11	0
4	B	64	0	0	3	0
4	C	109	0	0	9	0
4	D	90	0	0	5	0
All	All	16408	0	16111	913	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 28.

The worst 5 of 913 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:446:THR:HG22	1:B:449:VAL:HG23	1.19	1.19
1:C:271:LEU:HD12	1:C:305:MSE:HE1	1.32	1.10
1:D:446:THR:HG22	1:D:449:VAL:HG23	1.32	1.07
1:C:78:THR:HG23	1:C:150:TRP:HB2	1.42	1.01
1:B:177:MSE:HG2	1:B:359:LEU:HB2	1.51	0.93

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	490/583 (84%)	432 (88%)	46 (9%)	12 (2%)	4	24
1	B	551/583 (94%)	488 (89%)	51 (9%)	12 (2%)	5	26
1	C	473/583 (81%)	431 (91%)	30 (6%)	12 (2%)	4	23
1	D	552/583 (95%)	492 (89%)	51 (9%)	9 (2%)	7	34
All	All	2066/2332 (89%)	1843 (89%)	178 (9%)	45 (2%)	5	26

5 of 45 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	341	ALA
1	A	342	ALA
1	B	280	LYS
1	B	341	ALA
1	B	342	ALA

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	396/462 (86%)	357 (90%)	39 (10%)	7	30
1	B	445/462 (96%)	407 (92%)	38 (8%)	10	36
1	C	382/462 (83%)	352 (92%)	30 (8%)	11	39
1	D	446/462 (96%)	409 (92%)	37 (8%)	10	37
All	All	1669/1848 (90%)	1525 (91%)	144 (9%)	10	36

5 of 144 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	146	ASP
1	D	573	LEU
1	D	206	LEU
1	D	368	LEU
1	B	151	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	279	ASN
1	D	18	GLN
1	D	519	ASN
1	C	381	GLN
1	C	463	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 10 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 ⓘ

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](#)

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	486/583 (83%)	-1.81	0 100 100	9, 29, 65, 98	0
1	B	546/583 (93%)	-1.72	0 100 100	14, 45, 85, 119	0
1	C	471/583 (80%)	-1.79	0 100 100	9, 34, 74, 103	0
1	D	547/583 (93%)	-1.69	0 100 100	14, 47, 88, 126	0
All	All	2050/2332 (87%)	-1.75	0 100 100	9, 39, 82, 126	0

There are no RSRZ outliers to report.

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 oligosaccharides 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(Å ²)	Q<0.9
3	CL	A	585	1/1	0.99	0.08	71,71,71,71	0
3	CL	A	586	1/1	0.99	0.04	58,58,58,58	0
2	CO	C	601	1/1	1.00	0.03	106,106,106,106	0
2	CO	D	601	1/1	1.00	0.02	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CL	A	584	1/1	1.00	0.02	28,28,28,28	0
2	CO	A	601	1/1	1.00	0.03	93,93,93,93	0
2	CO	B	601	1/1	1.00	0.02	88,88,88,88	0
3	CL	B	584	1/1	1.00	0.02	40,40,40,40	0
3	CL	C	584	1/1	1.00	0.03	37,37,37,37	0
3	CL	D	584	1/1	1.00	0.02	47,47,47,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.