wwPDB X-ray Structure Validation Summary Report (i)

Sep 29, 2024 – 08:23 AM EDT

PDB ID	:	3LMM
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.; Ciccosanti, 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.

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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

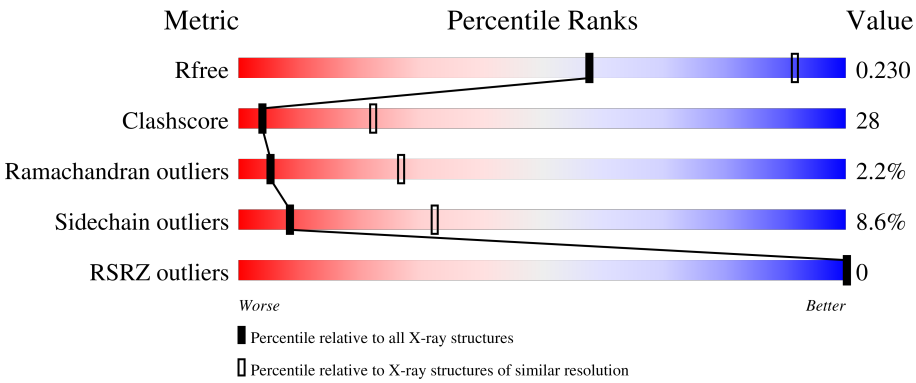
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)

1 Overall quality at a glance (i)

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}	164625	2511 (3.00-3.00)
Clashscore	180529	2866 (3.00-3.00)
Ramachandran outliers	177936	2778 (3.00-3.00)
Sidechain outliers	177891	2781 (3.00-3.00)
RSRZ outliers	164620	2523 (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 <=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	44% 35% 5% 16%
1	B	583	48% 40% 7% 5%
1	C	583	46% 31% 5% 18%
1	D	583	53% 37% 6% 5%

Validation Pipeline (wwPDB-VP) : 2.39

2 Entry composition (i)

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

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 (three-letter code: CO) (formula: Co).

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

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 4 is water.

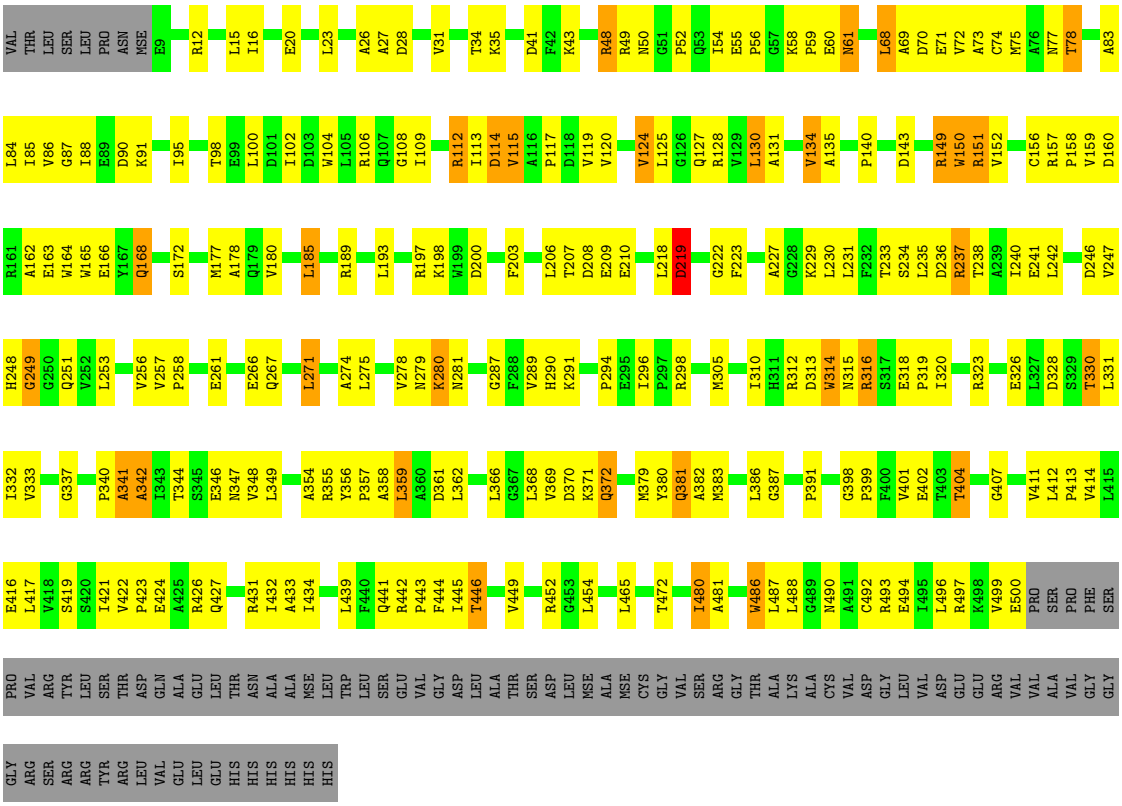
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	128	128	128	0	0
			Total	O		
4	B	64	64	64	0	0
			Total	O		
4	C	109	109	109	0	0
			Total	O		
4	D	90	90	90	0	0

3 Residue-property plots (i)

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.

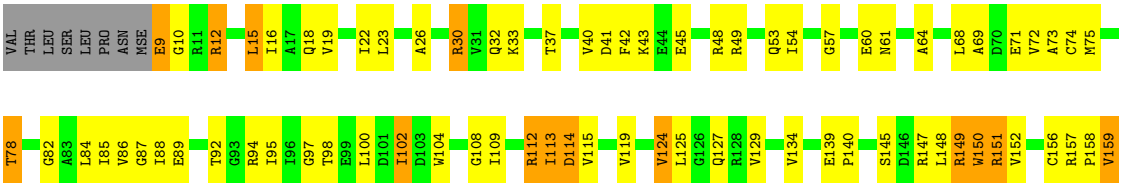
• Molecule 1: Uncharacterized protein

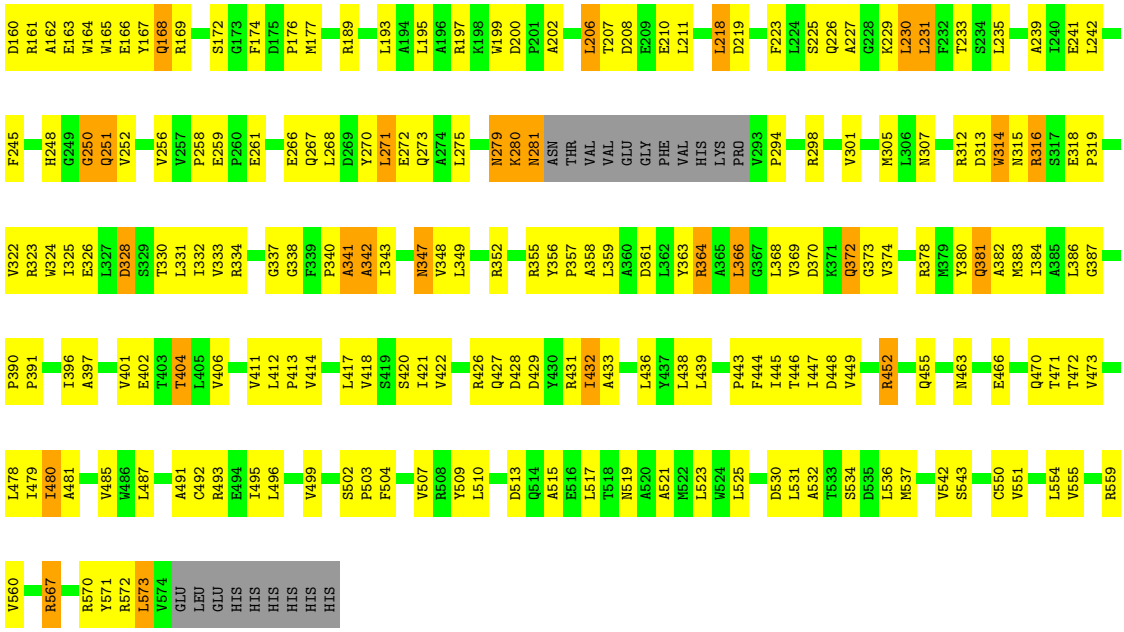
Chain A:



• Molecule 1: Uncharacterized protein

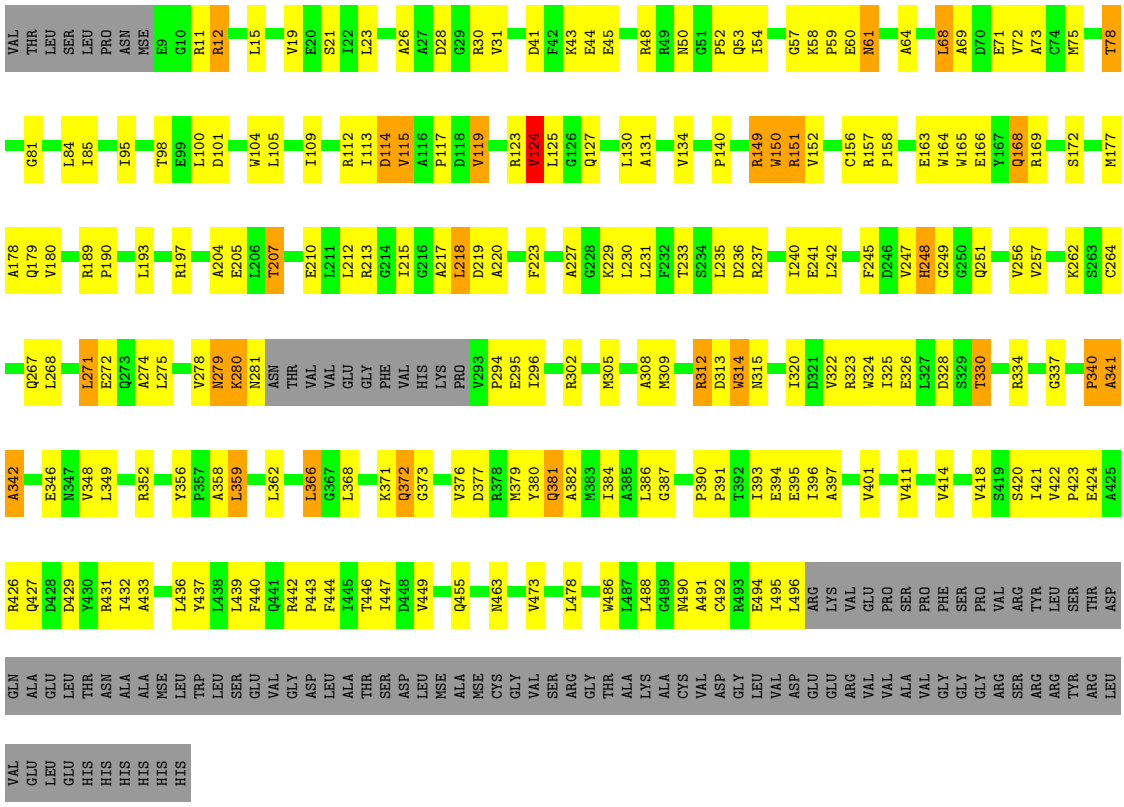
Chain B:





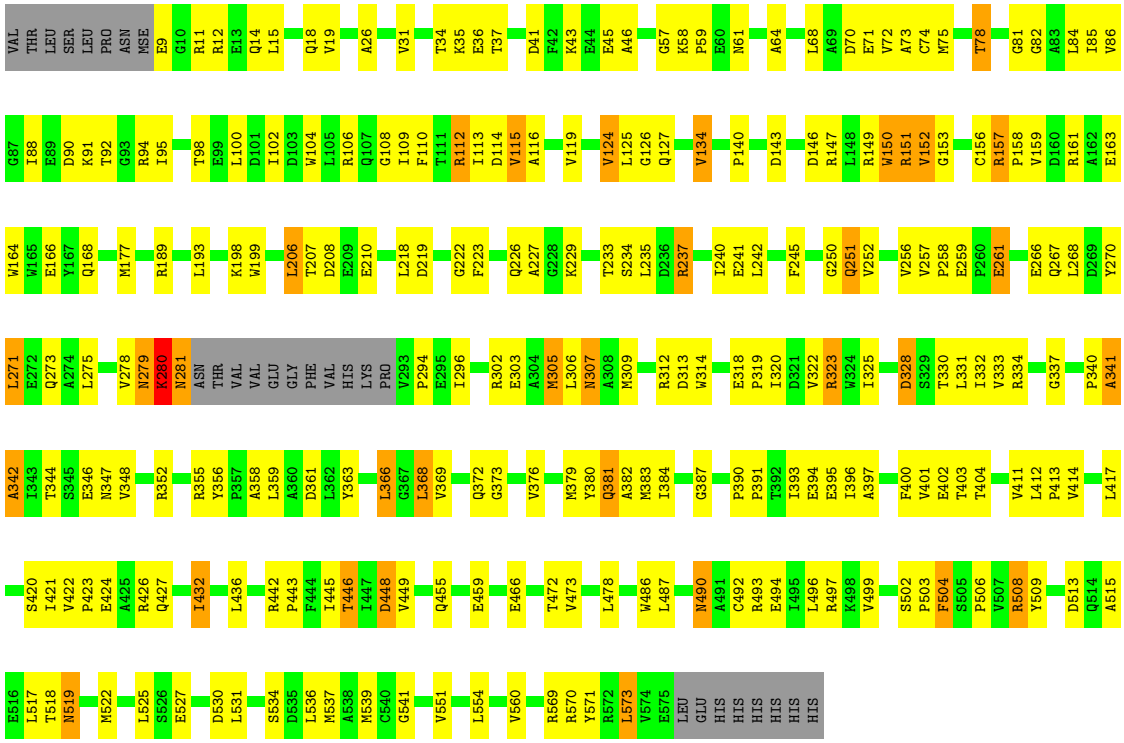
• Molecule 1: Uncharacterized protein

Chain C:



• Molecule 1: Uncharacterized protein

Chain D:


VAL THR LEU SER LEU PRO ASN MSE E9 G10 R11 R12 E13 Q14 L15 Q18 V19 A26 V31 T34 K35 E36 T37 D41 F42 K43 E44 E45 A46 G57 K58 P59 E60 N61 A64 L68 A69 D70 E71 V72 A73 C74 M75 T78 G81 G82 A83 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 V134 P140 D143 D146 R147 L148 R149 W150 R151 V152 G153 C156 R157 P158 V159 D160 R161 A162 E163
W164 W165 E166 Y167 Q168 M177 R189 L193 K198 W199 L206 T207 D208 E209 E210 L218 D219 G222 F223 Q226 A227 G228 K229 T233 S234 L235 D236 R237 I240 E241 L242 F245 G250 Q251 V252 V256 V257 P258 E259 P260 E261 E266 Q267 L268 D269 Y270
L271 E272 Q273 A274 L275 V278 N279 K280 N281 ASN THR VAL VAL GLU GLY PHE VAL HIS LYS PRO V293 P294 E295 I296 R302 E303 A304 M305 L306 N307 A308 M309 R312 D313 W314 E318 P319 I320 D321 V322 R323 W324 I325 D328 S329 T330 L331 I332 V333 R334 G337 P340 A341
A342 I343 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 P390 P391 T392 I393 E394 E395 I396 A397 F400 V401 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 Q455 E459 E466 T472 V473 L478 W486 L487 N490 A491 C492 R493 E494 I495 L496 R497 K498 V499 S502 P503 F504 S505 P506 V507 R508 Y509 D513 Q514 A515
E516 L517 T518 N519 M522 L525 S526 E527 D530 L531 S534 D535 L536 M537 A538 M539 C540 G541 V551 L554 V560 R569 R570 Y571 R572 L573 V574 E575 LEU GLU HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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	4078 reflections (4.99%)	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 , 14.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: CL, CO

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	0/3860	0.62	1/5239 (0.0%)
1	B	0.37	0/4325	0.58	0/5862
1	C	0.40	0/3734	0.60	0/5067
1	D	0.36	0/4334	0.57	0/5874
All	All	0.39	0/16253	0.59	1/22042 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	290	HIS	CB-CA-C	-6.45	97.49	110.40

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	3798	0	3826	221	0
1	B	4262	0	4290	257	0
1	C	3676	0	3699	196	0
1	D	4271	0	4296	227	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	885	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 885 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%)	5 25
1	B	551/583 (94%)	488 (89%)	51 (9%)	12 (2%)	5 27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	473/583 (81%)	431 (91%)	30 (6%)	12 (2%)	4	24
1	D	552/583 (95%)	492 (89%)	51 (9%)	9 (2%)	8	34
All	All	2066/2332 (89%)	1843 (89%)	178 (9%)	45 (2%)	5	27

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 (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	396/462 (86%)	363 (92%)	33 (8%)	9	34
1	B	445/462 (96%)	405 (91%)	40 (9%)	8	30
1	C	382/462 (83%)	352 (92%)	30 (8%)	10	35
1	D	446/462 (96%)	406 (91%)	40 (9%)	8	30
All	All	1669/1848 (90%)	1526 (91%)	143 (9%)	8	32

5 of 143 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	157	ARG
1	D	261	GLU
1	D	403	THR
1	B	168	GLN
1	B	167	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	490	ASN
1	D	107	GLN
1	D	14	GLN
1	D	50	ASN
1	D	279	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

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 (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	486/583 (83%)	-1.95	0	100	100	9, 29, 65, 98	0
1	B	546/583 (93%)	-1.86	0	100	100	14, 45, 85, 119	0
1	C	471/583 (80%)	-1.93	0	100	100	9, 34, 74, 103	0
1	D	547/583 (93%)	-1.84	0	100	100	14, 47, 88, 126	0
All	All	2050/2332 (87%)	-1.89	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 monosaccharides 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	0.03	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(Å^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.