



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 7, 2020 – 05:41 PM BST

PDB ID : 4UT9
Title : Crystal structure of dengue 2 virus envelope glycoprotein dimer in complex with the ScFv fragment of the broadly neutralizing human antibody EDE1 C10
Authors : Rouvinski, A.; Guardado-Calvo, P.; Barba-Spaeth, G.; Duquerroy, S.; Vaney, M.C.; Rey, F.A.
Deposited on : 2014-07-18
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

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
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
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) : 2.13.1

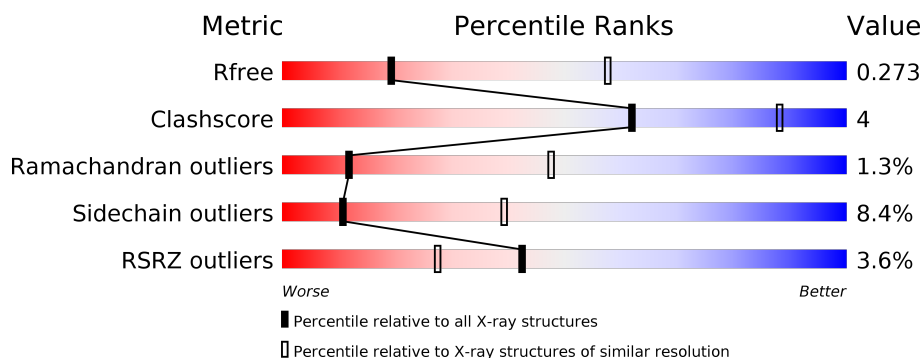
1 Overall quality at a glance

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))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	425	<div> <div>2%</div> <div> <div></div> <div>69%</div> <div>18%</div> <div>•</div> <div>11%</div> </div> </div>
1	B	425	<div> <div>3%</div> <div> <div></div> <div>72%</div> <div>17%</div> <div>•</div> <div>10%</div> </div> </div>
1	C	425	<div> <div>%</div> <div> <div></div> <div>69%</div> <div>19%</div> <div>•</div> <div>11%</div> </div> </div>
1	D	425	<div> <div></div> <div> <div></div> <div>71%</div> <div>17%</div> <div>•</div> <div>11%</div> </div> </div>
2	H	144	<div> <div>4%</div> <div> <div></div> <div>74%</div> <div>13%</div> <div>•</div> <div>12%</div> </div> </div>
2	I	144	<div> <div>11%</div> <div> <div></div> <div>74%</div> <div>14%</div> <div>•</div> <div>12%</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	J	144	<div><div></div><div>13%</div><div>75%</div><div>13%</div><div>12%</div></div>
2	K	144	<div><div></div><div>3%</div><div>78%</div><div>8%</div><div>12%</div></div>
3	L	154	<div><div></div><div>%</div><div>61%</div><div>8%</div><div>29%</div></div>
3	M	154	<div><div></div><div>3%</div><div>62%</div><div>8%</div><div>29%</div></div>
3	N	154	<div><div></div><div>6%</div><div>61%</div><div>10%</div><div>29%</div></div>
3	O	154	<div><div></div><div>%</div><div>62%</div><div>7%</div><div>30%</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 19141 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 ENVELOPE GLYCOPROTEIN E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	377	Total	C	N	O	S	0	0	0
			2940	1858	503	555	24			
1	B	383	Total	C	N	O	S	0	0	0
			2979	1880	512	563	24			
1	C	378	Total	C	N	O	S	0	0	0
			2939	1855	501	559	24			
1	D	380	Total	C	N	O	S	0	0	0
			2959	1870	505	561	23			

There are 140 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1392	LEU	-	expression tag	UNP Q68Y26
A	1393	ARG	-	expression tag	UNP Q68Y26
A	1394	PRO	-	expression tag	UNP Q68Y26
A	1395	LEU	-	expression tag	UNP Q68Y26
A	1396	GLU	-	expression tag	UNP Q68Y26
A	1397	SER	-	expression tag	UNP Q68Y26
A	1398	ARG	-	expression tag	UNP Q68Y26
A	1399	GLY	-	expression tag	UNP Q68Y26
A	1400	PRO	-	expression tag	UNP Q68Y26
A	1401	PHE	-	expression tag	UNP Q68Y26
A	1402	GLU	-	expression tag	UNP Q68Y26
A	1403	GLY	-	expression tag	UNP Q68Y26
A	1404	LYS	-	expression tag	UNP Q68Y26
A	1405	PRO	-	expression tag	UNP Q68Y26
A	1406	ILE	-	expression tag	UNP Q68Y26
A	1407	PRO	-	expression tag	UNP Q68Y26
A	1408	ASN	-	expression tag	UNP Q68Y26
A	1409	PRO	-	expression tag	UNP Q68Y26
A	1410	LEU	-	expression tag	UNP Q68Y26
A	1411	LEU	-	expression tag	UNP Q68Y26
A	1412	GLY	-	expression tag	UNP Q68Y26

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	1413	LEU	-	expression tag	UNP Q68Y26
A	1414	ASP	-	expression tag	UNP Q68Y26
A	1415	SER	-	expression tag	UNP Q68Y26
A	1416	THR	-	expression tag	UNP Q68Y26
A	1417	ARG	-	expression tag	UNP Q68Y26
A	1418	THR	-	expression tag	UNP Q68Y26
A	1419	GLY	-	expression tag	UNP Q68Y26
A	1420	HIS	-	expression tag	UNP Q68Y26
A	1421	HIS	-	expression tag	UNP Q68Y26
A	1422	HIS	-	expression tag	UNP Q68Y26
A	1423	HIS	-	expression tag	UNP Q68Y26
A	1424	HIS	-	expression tag	UNP Q68Y26
A	1425	HIS	-	expression tag	UNP Q68Y26
A	118	LYS	MET	conflict	UNP Q68Y26
B	1392	LEU	-	expression tag	UNP Q68Y26
B	1393	ARG	-	expression tag	UNP Q68Y26
B	1394	PRO	-	expression tag	UNP Q68Y26
B	1395	LEU	-	expression tag	UNP Q68Y26
B	1396	GLU	-	expression tag	UNP Q68Y26
B	1397	SER	-	expression tag	UNP Q68Y26
B	1398	ARG	-	expression tag	UNP Q68Y26
B	1399	GLY	-	expression tag	UNP Q68Y26
B	1400	PRO	-	expression tag	UNP Q68Y26
B	1401	PHE	-	expression tag	UNP Q68Y26
B	1402	GLU	-	expression tag	UNP Q68Y26
B	1403	GLY	-	expression tag	UNP Q68Y26
B	1404	LYS	-	expression tag	UNP Q68Y26
B	1405	PRO	-	expression tag	UNP Q68Y26
B	1406	ILE	-	expression tag	UNP Q68Y26
B	1407	PRO	-	expression tag	UNP Q68Y26
B	1408	ASN	-	expression tag	UNP Q68Y26
B	1409	PRO	-	expression tag	UNP Q68Y26
B	1410	LEU	-	expression tag	UNP Q68Y26
B	1411	LEU	-	expression tag	UNP Q68Y26
B	1412	GLY	-	expression tag	UNP Q68Y26
B	1413	LEU	-	expression tag	UNP Q68Y26
B	1414	ASP	-	expression tag	UNP Q68Y26
B	1415	SER	-	expression tag	UNP Q68Y26
B	1416	THR	-	expression tag	UNP Q68Y26
B	1417	ARG	-	expression tag	UNP Q68Y26
B	1418	THR	-	expression tag	UNP Q68Y26
B	1419	GLY	-	expression tag	UNP Q68Y26

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	1420	HIS	-	expression tag	UNP Q68Y26
B	1421	HIS	-	expression tag	UNP Q68Y26
B	1422	HIS	-	expression tag	UNP Q68Y26
B	1423	HIS	-	expression tag	UNP Q68Y26
B	1424	HIS	-	expression tag	UNP Q68Y26
B	1425	HIS	-	expression tag	UNP Q68Y26
B	118	LYS	MET	conflict	UNP Q68Y26
C	1392	LEU	-	expression tag	UNP Q68Y26
C	1393	ARG	-	expression tag	UNP Q68Y26
C	1394	PRO	-	expression tag	UNP Q68Y26
C	1395	LEU	-	expression tag	UNP Q68Y26
C	1396	GLU	-	expression tag	UNP Q68Y26
C	1397	SER	-	expression tag	UNP Q68Y26
C	1398	ARG	-	expression tag	UNP Q68Y26
C	1399	GLY	-	expression tag	UNP Q68Y26
C	1400	PRO	-	expression tag	UNP Q68Y26
C	1401	PHE	-	expression tag	UNP Q68Y26
C	1402	GLU	-	expression tag	UNP Q68Y26
C	1403	GLY	-	expression tag	UNP Q68Y26
C	1404	LYS	-	expression tag	UNP Q68Y26
C	1405	PRO	-	expression tag	UNP Q68Y26
C	1406	ILE	-	expression tag	UNP Q68Y26
C	1407	PRO	-	expression tag	UNP Q68Y26
C	1408	ASN	-	expression tag	UNP Q68Y26
C	1409	PRO	-	expression tag	UNP Q68Y26
C	1410	LEU	-	expression tag	UNP Q68Y26
C	1411	LEU	-	expression tag	UNP Q68Y26
C	1412	GLY	-	expression tag	UNP Q68Y26
C	1413	LEU	-	expression tag	UNP Q68Y26
C	1414	ASP	-	expression tag	UNP Q68Y26
C	1415	SER	-	expression tag	UNP Q68Y26
C	1416	THR	-	expression tag	UNP Q68Y26
C	1417	ARG	-	expression tag	UNP Q68Y26
C	1418	THR	-	expression tag	UNP Q68Y26
C	1419	GLY	-	expression tag	UNP Q68Y26
C	1420	HIS	-	expression tag	UNP Q68Y26
C	1421	HIS	-	expression tag	UNP Q68Y26
C	1422	HIS	-	expression tag	UNP Q68Y26
C	1423	HIS	-	expression tag	UNP Q68Y26
C	1424	HIS	-	expression tag	UNP Q68Y26
C	1425	HIS	-	expression tag	UNP Q68Y26
C	118	LYS	MET	conflict	UNP Q68Y26

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	1392	LEU	-	expression tag	UNP Q68Y26
D	1393	ARG	-	expression tag	UNP Q68Y26
D	1394	PRO	-	expression tag	UNP Q68Y26
D	1395	LEU	-	expression tag	UNP Q68Y26
D	1396	GLU	-	expression tag	UNP Q68Y26
D	1397	SER	-	expression tag	UNP Q68Y26
D	1398	ARG	-	expression tag	UNP Q68Y26
D	1399	GLY	-	expression tag	UNP Q68Y26
D	1400	PRO	-	expression tag	UNP Q68Y26
D	1401	PHE	-	expression tag	UNP Q68Y26
D	1402	GLU	-	expression tag	UNP Q68Y26
D	1403	GLY	-	expression tag	UNP Q68Y26
D	1404	LYS	-	expression tag	UNP Q68Y26
D	1405	PRO	-	expression tag	UNP Q68Y26
D	1406	ILE	-	expression tag	UNP Q68Y26
D	1407	PRO	-	expression tag	UNP Q68Y26
D	1408	ASN	-	expression tag	UNP Q68Y26
D	1409	PRO	-	expression tag	UNP Q68Y26
D	1410	LEU	-	expression tag	UNP Q68Y26
D	1411	LEU	-	expression tag	UNP Q68Y26
D	1412	GLY	-	expression tag	UNP Q68Y26
D	1413	LEU	-	expression tag	UNP Q68Y26
D	1414	ASP	-	expression tag	UNP Q68Y26
D	1415	SER	-	expression tag	UNP Q68Y26
D	1416	THR	-	expression tag	UNP Q68Y26
D	1417	ARG	-	expression tag	UNP Q68Y26
D	1418	THR	-	expression tag	UNP Q68Y26
D	1419	GLY	-	expression tag	UNP Q68Y26
D	1420	HIS	-	expression tag	UNP Q68Y26
D	1421	HIS	-	expression tag	UNP Q68Y26
D	1422	HIS	-	expression tag	UNP Q68Y26
D	1423	HIS	-	expression tag	UNP Q68Y26
D	1424	HIS	-	expression tag	UNP Q68Y26
D	1425	HIS	-	expression tag	UNP Q68Y26
D	118	LYS	MET	conflict	UNP Q68Y26

- Molecule 2 is a protein called BROADLY NEUTRALIZING HUMAN ANTIBODY EDE1 C10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	127	Total	C	N	O	S	0	0	0
			1021	650	169	197	5			

Continued on next page...

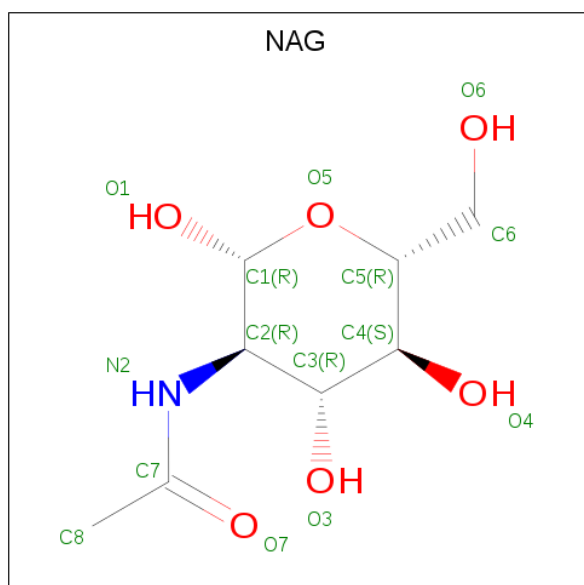
Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	127	Total	C	N	O	S	0	0	0
			1021	650	169	197	5			
2	J	127	Total	C	N	O	S	0	0	0
			1021	650	169	197	5			
2	K	127	Total	C	N	O	S	0	0	0
			1021	650	169	197	5			

- Molecule 3 is a protein called BROADLY NEUTRALIZING HUMAN ANTIBODY EDE1 C10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	110	Total	C	N	O	S	0	0	0
			802	496	137	166	3			
3	M	110	Total	C	N	O	S	0	0	0
			802	496	137	166	3			
3	N	109	Total	C	N	O	S	0	0	0
			793	491	135	164	3			
3	O	108	Total	C	N	O	S	0	0	0
			787	488	134	162	3			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

Continued on next page...

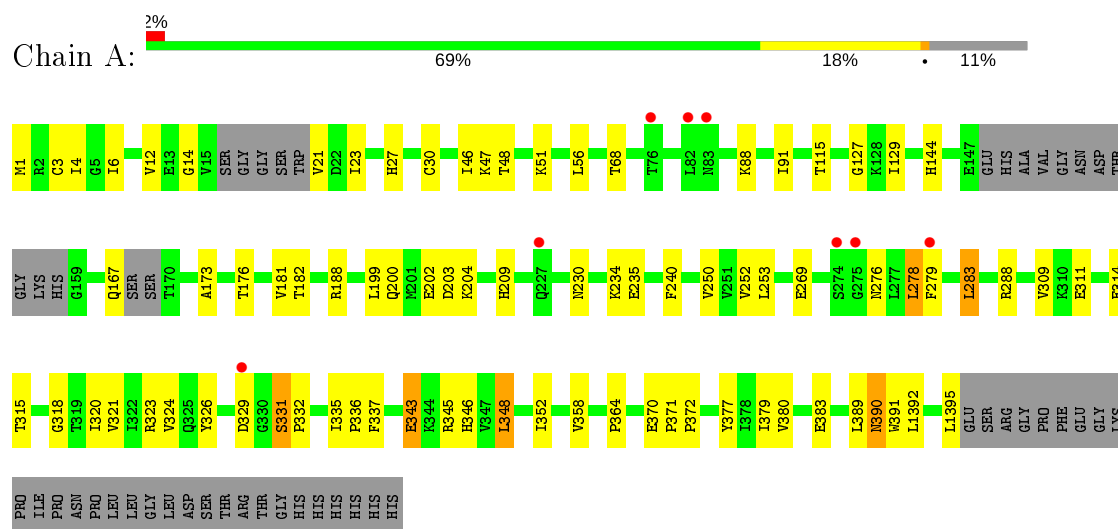
Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		

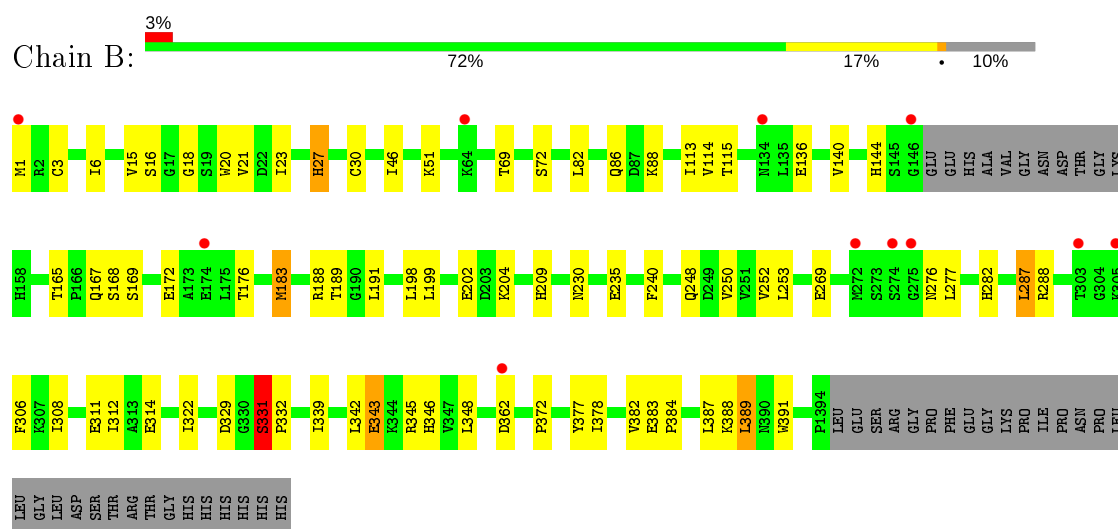
3 Residue-property plots [i](#)

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: ENVELOPE GLYCOPROTEIN E

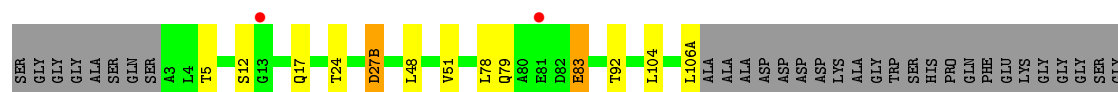


• Molecule 1: ENVELOPE GLYCOPROTEIN E



• Molecule 1: ENVELOPE GLYCOPROTEIN E





GLY
GLY
SER
GLY
GLY
GLY
SER
TRP
SER
HIS
PRO
GLN
PHE
GLU
LYS

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	57.52Å 102.23Å 131.09Å 88.52° 85.69° 83.90°	Depositor
Resolution (Å)	20.00 – 3.20 29.29 – 3.20	Depositor EDS
% Data completeness (in resolution range)	95.3 (20.00-3.20) 95.3 (29.29-3.20)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 3.18Å)	Xtriage
Refinement program	BUSTER 2.11.4	Depositor
R, R_{free}	0.198 , 0.249 0.221 , 0.273	Depositor DCC
R_{free} test set	2347 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	75.7	Xtriage
Anisotropy	0.382	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 69.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	19141	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.20% 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: NAG

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	0.42	0/2995	0.69	0/4045
1	B	0.42	0/3039	0.68	0/4108
1	C	0.45	0/2995	0.71	0/4046
1	D	0.44	0/3016	0.70	0/4075
2	H	0.38	0/1050	0.63	0/1427
2	I	0.37	0/1050	0.64	0/1427
2	J	0.36	0/1050	0.62	0/1427
2	K	0.39	0/1050	0.64	0/1427
3	L	0.37	0/820	0.56	0/1113
3	M	0.36	0/820	0.56	0/1113
3	N	0.37	0/811	0.57	0/1101
3	O	0.37	0/805	0.55	0/1093
All	All	0.41	0/19501	0.66	0/26402

There are no bond length outliers.

There are no bond angle outliers.

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	2940	0	2959	38	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2979	0	2987	28	0
1	C	2939	0	2947	31	0
1	D	2959	0	2966	33	0
2	H	1021	0	960	7	0
2	I	1021	0	960	8	0
2	J	1021	0	960	10	0
2	K	1021	0	960	6	0
3	L	802	0	766	6	0
3	M	802	0	766	3	0
3	N	793	0	755	4	0
3	O	787	0	750	3	0
4	A	14	0	13	0	0
4	B	14	0	13	0	0
4	C	14	0	13	2	0
4	D	14	0	13	0	0
All	All	19141	0	18788	168	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 4.

The worst 5 of 168 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:331:SER:HB2	1:D:332:PRO:HD3	1.50	0.93
1:B:331:SER:HB3	1:B:332:PRO:HD3	1.69	0.75
1:D:312:ILE:HG13	1:D:322:ILE:HD13	1.70	0.74
4:C:567:NAG:H62	2:K:65:ASP:HB3	1.67	0.74
1:D:348:LEU:HB3	1:D:372:PRO:HG3	1.70	0.72

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	369/425 (87%)	333 (90%)	32 (9%)	4 (1%)	14	51
1	B	379/425 (89%)	342 (90%)	29 (8%)	8 (2%)	7	37
1	C	372/425 (88%)	341 (92%)	26 (7%)	5 (1%)	12	47
1	D	372/425 (88%)	346 (93%)	20 (5%)	6 (2%)	9	43
2	H	125/144 (87%)	111 (89%)	14 (11%)	0	100	100
2	I	125/144 (87%)	112 (90%)	13 (10%)	0	100	100
2	J	125/144 (87%)	111 (89%)	14 (11%)	0	100	100
2	K	125/144 (87%)	112 (90%)	13 (10%)	0	100	100
3	L	108/154 (70%)	102 (94%)	4 (4%)	2 (2%)	8	39
3	M	108/154 (70%)	103 (95%)	3 (3%)	2 (2%)	8	39
3	N	107/154 (70%)	102 (95%)	3 (3%)	2 (2%)	8	39
3	O	106/154 (69%)	100 (94%)	4 (4%)	2 (2%)	8	39
All	All	2421/2892 (84%)	2215 (92%)	175 (7%)	31 (1%)	12	47

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	51	LYS
1	A	331	SER
1	B	202	GLU
1	B	331	SER
1	C	51	LYS

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	330/369 (89%)	304 (92%)	26 (8%)	12	43
1	B	334/369 (90%)	304 (91%)	30 (9%)	9	34
1	C	330/369 (89%)	298 (90%)	32 (10%)	8	31
1	D	332/369 (90%)	303 (91%)	29 (9%)	10	37

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	107/112 (96%)	98 (92%)	9 (8%)	11	39
2	I	107/112 (96%)	97 (91%)	10 (9%)	9	33
2	J	107/112 (96%)	99 (92%)	8 (8%)	13	45
2	K	107/112 (96%)	99 (92%)	8 (8%)	13	45
3	L	90/116 (78%)	84 (93%)	6 (7%)	16	50
3	M	90/116 (78%)	83 (92%)	7 (8%)	12	43
3	N	89/116 (77%)	84 (94%)	5 (6%)	21	57
3	O	88/116 (76%)	81 (92%)	7 (8%)	12	42
All	All	2111/2388 (88%)	1934 (92%)	177 (8%)	11	39

5 of 177 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	331	SER
1	D	172	GLU
3	M	85	ASP
1	C	344	LYS
1	D	30	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	230	ASN
1	D	230	ASN
1	B	325	GLN
1	A	230	ASN
1	B	276	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 [i](#)

There are no monosaccharides 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	$\# Z > 2$
4	NAG	A	567	1	14,14,15	0.29	0	17,19,21	0.68	1 (5%)
4	NAG	B	567	1	14,14,15	0.30	0	17,19,21	0.55	0
4	NAG	C	567	1	14,14,15	0.32	0	17,19,21	0.62	0
4	NAG	D	567	1	14,14,15	0.33	0	17,19,21	0.68	1 (5%)

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
4	NAG	A	567	1	-	0/6/23/26	0/1/1/1
4	NAG	B	567	1	-	0/6/23/26	0/1/1/1
4	NAG	C	567	1	-	0/6/23/26	0/1/1/1
4	NAG	D	567	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	567	NAG	C1-O5-C5	2.35	115.38	112.19
4	A	567	NAG	C1-O5-C5	2.20	115.17	112.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	567	NAG	2	0

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	377/425 (88%)	0.04	8 (2%) 63 49	44, 103, 144, 169	0
1	B	383/425 (90%)	0.11	11 (2%) 51 36	51, 99, 139, 170	0
1	C	378/425 (88%)	-0.23	6 (1%) 72 59	37, 75, 116, 168	0
1	D	380/425 (89%)	-0.32	2 (0%) 91 86	36, 71, 103, 130	0
2	H	127/144 (88%)	0.26	6 (4%) 31 19	48, 93, 132, 157	0
2	I	127/144 (88%)	0.75	16 (12%) 3 2	69, 137, 208, 228	0
2	J	127/144 (88%)	0.73	19 (14%) 2 1	66, 135, 176, 200	0
2	K	127/144 (88%)	0.02	4 (3%) 49 32	45, 85, 114, 134	0
3	L	110/154 (71%)	-0.01	1 (0%) 84 75	53, 99, 154, 166	0
3	M	110/154 (71%)	0.32	5 (4%) 33 21	82, 111, 175, 208	0
3	N	109/154 (70%)	0.48	9 (8%) 11 6	58, 109, 154, 202	0
3	O	108/154 (70%)	0.04	2 (1%) 66 53	54, 92, 144, 181	0
All	All	2463/2892 (85%)	0.06	89 (3%) 42 27	36, 94, 157, 228	0

The worst 5 of 89 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	11	VAL	5.2
2	J	26	GLY	4.6
3	N	106(A)	LEU	4.6
2	I	1	GLU	4.5
1	A	275	GLY	4.4

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

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(\AA^2)	Q<0.9
4	NAG	D	567	14/15	0.78	0.24	100,103,108,108	0
4	NAG	C	567	14/15	0.80	0.24	89,100,102,104	0
4	NAG	B	567	14/15	0.81	0.36	139,140,141,142	0
4	NAG	A	567	14/15	0.82	0.33	123,124,124,125	0

6.5 Other polymers [i](#)

There are no such residues in this entry.