



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:03 AM UTC

PDB ID : 4UT9 / pdb_00004ut9
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 Full wwPDB X-ray Structure Validation 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 types of validation reports are described at

<http://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)
Validation Pipeline (wwPDB-VP)	:	2.49

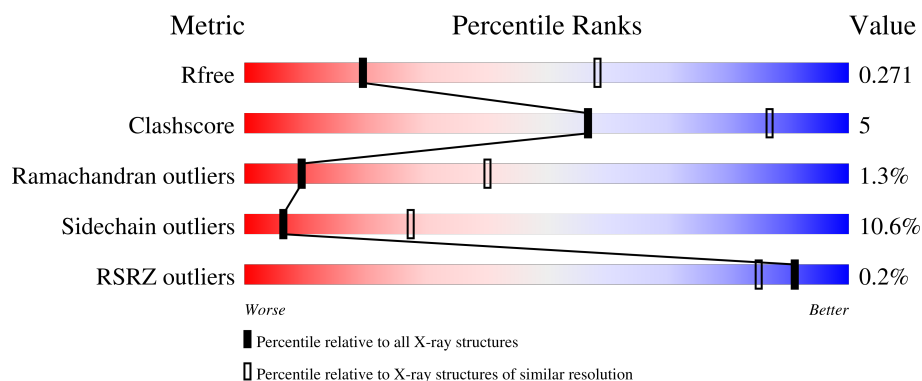
1 Overall quality at a glance

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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (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 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	425	 66% 20% • 11%
1	B	425	 69% 20% • 10%
1	C	425	 64% 22% • 11%
1	D	425	 68% 18% • 11%

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Mol	Chain	Length	Quality of chain
2	H	144	 71% 17% • 12%
2	I	144	 72% 15% • 12%
2	J	144	 71% 16% • 12%
2	K	144	 75% 11% • 12%
3	L	154	 61% 8% • 29%
3	M	154	 60% 10% • 29%
3	N	154	 62% 8% • 29%
3	O	154	 62% 8% • 30%

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

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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

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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

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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			

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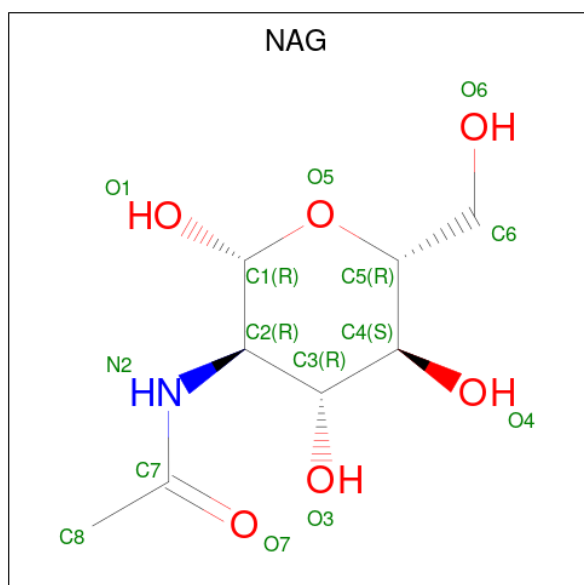
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	127	Total	C	N	O	S	0	0	0
			1021	650	169	197	5			
2	J	127	Total	C	N	O	S	0	0	0
			1021	650	169	197	5			
2	K	127	Total	C	N	O	S	0	0	0
			1021	650	169	197	5			

- 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 (CCD ID: 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		

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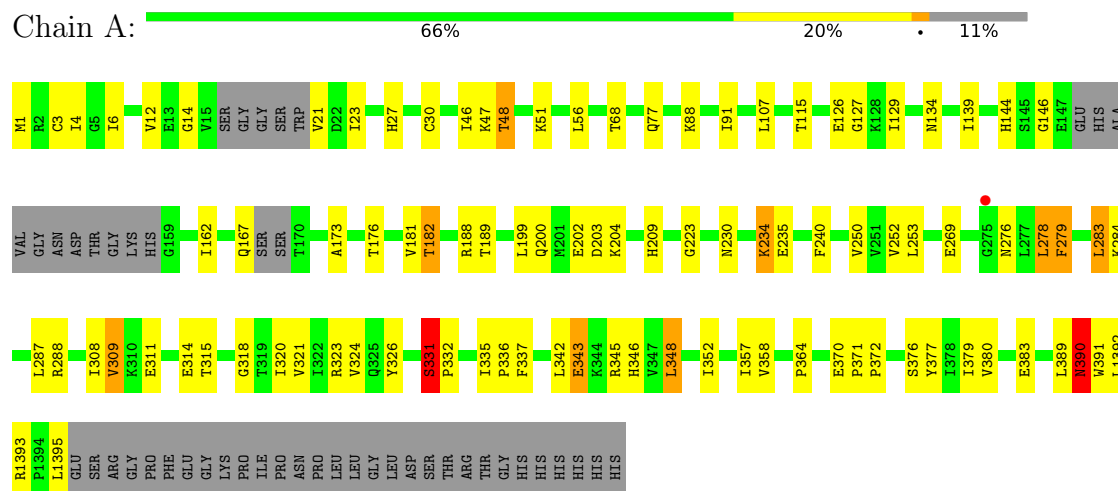
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		

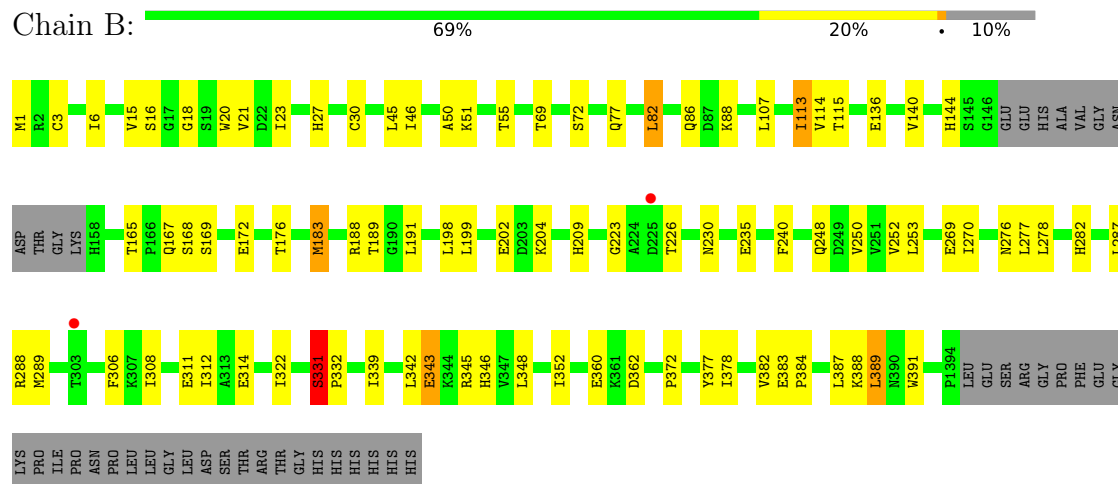
3 Residue-property plots

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

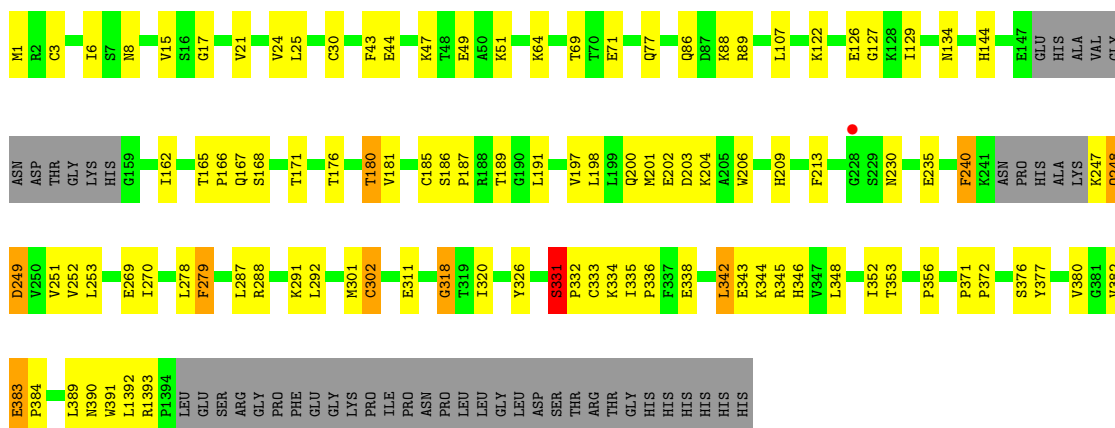


• Molecule 1: ENVELOPE GLYCOPROTEIN E



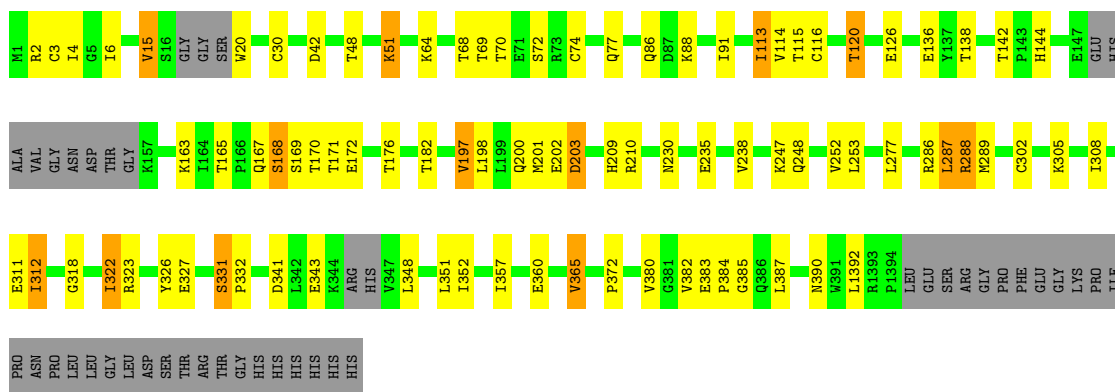
• Molecule 1: ENVELOPE GLYCOPROTEIN E





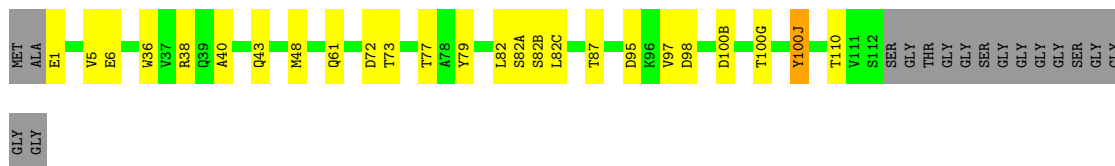
• Molecule 1: ENVELOPE GLYCOPROTEIN E

Chain D: 68% 18% 11%



• Molecule 2: BROADLY NEUTRALIZING HUMAN ANTIBODY EDE1 C10

Chain H: 71% 17% 12%



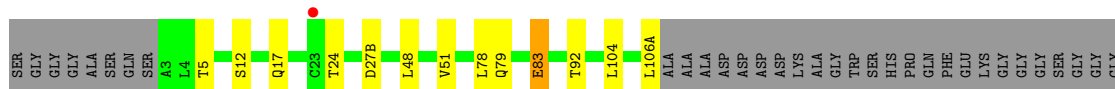
• Molecule 2: BROADLY NEUTRALIZING HUMAN ANTIBODY EDE1 C10

Chain I: 72% 15% 12%



• Molecule 2: BROADLY NEUTRALIZING HUMAN ANTIBODY EDE1 C10

Chain J: 71% 16% 12%



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 20.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	95.3 (20.00-3.20) 94.9 (20.00-3.20)	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 0.220 , 0.271	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)	0.28 , 89.2	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	0.92	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	0.75	0/2995	1.25	10/4045 (0.2%)
1	B	0.76	0/3039	1.24	9/4108 (0.2%)
1	C	0.82	0/2995	1.29	15/4046 (0.4%)
1	D	0.79	0/3016	1.25	8/4075 (0.2%)
2	H	0.66	0/1050	1.13	3/1427 (0.2%)
2	I	0.65	0/1050	1.14	2/1427 (0.1%)
2	J	0.65	0/1050	1.13	4/1427 (0.3%)
2	K	0.68	0/1050	1.13	2/1427 (0.1%)
3	L	0.69	0/820	1.10	0/1113
3	M	0.68	0/820	1.11	1/1113 (0.1%)
3	N	0.68	0/811	1.11	1/1101 (0.1%)
3	O	0.67	0/805	1.08	0/1093
All	All	0.74	0/19501	1.21	55/26402 (0.2%)

There are no bond length outliers.

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	17	GLY	CA-C-N	7.67	127.89	120.98
1	C	17	GLY	C-N-CA	7.67	127.89	120.98
1	D	352	ILE	N-CA-C	-7.52	105.34	111.81
1	B	352	ILE	N-CA-C	-7.49	103.56	110.82
2	J	98	ASP	CA-CB-CG	7.02	119.62	112.60
1	A	309	VAL	N-CA-C	-6.89	103.95	110.42
1	C	279	PHE	CA-CB-CG	6.84	120.64	113.80
1	C	89	ARG	N-CA-C	-6.31	105.71	113.41
2	I	98	ASP	CA-CB-CG	6.04	118.64	112.60
1	D	360	GLU	CB-CG-CD	5.76	122.39	112.60
1	A	279	PHE	CA-CB-CG	5.75	119.55	113.80
1	B	45	LEU	CA-C-N	5.74	127.88	120.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	45	LEU	C-N-CA	5.74	127.88	120.88
1	D	15	VAL	CA-C-N	5.66	131.89	121.70
1	D	15	VAL	C-N-CA	5.66	131.89	121.70
3	M	27(B)	ASP	CA-CB-CG	5.62	118.22	112.60
1	A	390	ASN	CA-CB-CG	5.57	118.17	112.60
1	D	48	THR	N-CA-C	-5.56	100.64	109.76
2	H	100(J)	TYR	N-CA-CB	5.47	117.87	110.10
1	B	50	ALA	CA-C-N	5.47	131.99	121.54
1	B	50	ALA	C-N-CA	5.47	131.99	121.54
1	C	247	LYS	CA-C-N	5.46	131.97	121.54
1	C	247	LYS	C-N-CA	5.46	131.97	121.54
2	I	100(J)	TYR	N-CA-CB	5.46	117.86	110.10
2	J	100(J)	TYR	N-CA-CB	5.41	117.78	110.10
1	C	352	ILE	N-CA-C	-5.41	105.84	111.58
1	C	134	ASN	CA-CB-CG	5.40	118.00	112.60
2	K	100(J)	TYR	N-CA-CB	5.40	117.77	110.10
1	D	203	ASP	CA-CB-CG	5.35	117.95	112.60
1	C	318	GLY	CA-C-N	5.31	128.62	120.82
1	C	318	GLY	C-N-CA	5.31	128.62	120.82
1	C	249	ASP	CA-CB-CG	5.30	117.90	112.60
2	K	98	ASP	CA-CB-CG	5.28	117.88	112.60
1	A	134	ASN	CA-CB-CG	5.28	117.88	112.60
1	C	383	GLU	CB-CG-CD	5.17	121.39	112.60
1	A	223	GLY	CA-C-N	5.16	127.72	120.28
1	A	223	GLY	C-N-CA	5.16	127.72	120.28
1	A	234	LYS	CA-C-N	5.14	128.82	120.60
1	A	234	LYS	C-N-CA	5.14	128.82	120.60
1	B	226	THR	CA-C-N	5.13	127.41	120.38
1	B	226	THR	C-N-CA	5.13	127.41	120.38
1	D	238	VAL	N-CA-C	5.10	115.25	108.11
1	A	331	SER	CA-C-O	-5.09	113.19	120.16
1	B	223	GLY	CA-C-N	5.06	127.57	120.28
1	B	223	GLY	C-N-CA	5.06	127.57	120.28
2	H	61	GLN	CA-C-N	5.05	127.56	120.28
2	H	61	GLN	C-N-CA	5.05	127.56	120.28
3	N	72	SER	N-CA-C	5.05	116.65	108.26
1	A	189	THR	N-CA-C	-5.05	105.48	111.69
1	D	42	ASP	CA-CB-CG	5.04	117.64	112.60
1	C	8	ASN	CA-CB-CG	5.01	117.61	112.60
1	C	391	TRP	CA-C-N	5.01	129.26	122.19
1	C	391	TRP	C-N-CA	5.01	129.26	122.19
2	J	97	VAL	CA-C-N	5.01	127.97	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	97	VAL	C-N-CA	5.01	127.97	120.90

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	39	0
1	B	2979	0	2987	27	0
1	C	2939	0	2947	33	0
1	D	2959	0	2966	34	0
2	H	1021	0	960	7	0
2	I	1021	0	960	9	0
2	J	1021	0	960	11	0
2	K	1021	0	960	7	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	175	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 5.

All (175) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:567:NAG:HB2	2:K:65:ASP:HB3	1.67	0.74
1:D:348:LEU:HB3	1:D:372:PRO:HG3	1.70	0.72
1:C:348:LEU:HB3	1:C:372:PRO:HG3	1.69	0.71
1:B:331:SER:HB3	1:B:332:PRO:CD	2.21	0.71
1:A:240:PHE:CE2	1:A:250:VAL:HG12	2.26	0.70
1:D:308:ILE:HD12	1:D:322:ILE:HD11	1.73	0.70
1:B:240:PHE:CE2	1:B:250:VAL:HG12	2.27	0.69
1:C:331:SER:HB3	1:C:332:PRO:CD	2.23	0.68
1:C:331:SER:HB3	1:C:332:PRO:HD3	1.75	0.67
1:B:382:VAL:HG23	1:B:384:PRO:HD2	1.77	0.67
1:B:362:ASP:HB3	3:L:60:SER:HB2	1.76	0.67
1:D:198:LEU:HD21	1:D:277:LEU:HD22	1.78	0.66
1:D:302:CYS:HB3	1:D:326:TYR:CE1	2.30	0.66
1:A:88:LYS:HB2	1:A:230:ASN:HD22	1.61	0.66
1:A:331:SER:HB3	1:A:332:PRO:HD3	1.78	0.65
1:D:70:THR:HG21	2:J:100(D):TRP:HZ3	1.62	0.64
1:C:88:LYS:HB2	1:C:230:ASN:HD22	1.62	0.64
1:B:88:LYS:HB2	1:B:230:ASN:HD22	1.64	0.62
2:I:36:TRP:HB3	2:I:48:MET:HE3	1.82	0.62
2:K:36:TRP:HB3	2:K:48:MET:HE3	1.81	0.62
1:B:348:LEU:HB3	1:B:372:PRO:HG3	1.80	0.62
2:H:36:TRP:HB3	2:H:48:MET:HE3	1.82	0.62
1:C:165:THR:H	1:C:168:SER:HB3	1.65	0.61
1:D:88:LYS:HB2	1:D:230:ASN:HD22	1.63	0.61
2:J:36:TRP:HB3	2:J:48:MET:HE3	1.82	0.61
3:L:78:LEU:HD21	3:L:104:LEU:HD21	1.81	0.60
1:C:343:GLU:HG2	1:C:345:ARG:HG2	1.84	0.60
1:B:165:THR:H	1:B:168:SER:HB3	1.67	0.60
1:A:352:ILE:HD11	1:A:370:GLU:HB2	1.83	0.60
1:B:308:ILE:HG12	1:B:322:ILE:HD11	1.84	0.60
1:D:165:THR:H	1:D:168:SER:HB3	1.67	0.59
1:A:309:VAL:HG21	1:A:364:PRO:HB3	1.83	0.59
1:A:314:GLU:HB2	1:A:391:TRP:CZ2	2.37	0.59
1:B:331:SER:CB	1:B:332:PRO:HD3	2.33	0.59
1:D:331:SER:HB2	1:D:332:PRO:CD	2.29	0.58
1:A:56:LEU:HB2	1:A:129:ILE:HG12	1.85	0.58
3:M:5:THR:HB	3:M:24:THR:HB	1.86	0.58
1:B:189:THR:HG23	1:B:282:HIS:HB3	1.84	0.58
3:L:5:THR:HB	3:L:24:THR:HB	1.86	0.57
2:K:40:ALA:HB3	2:K:43:GLN:HB2	1.86	0.57
3:O:5:THR:HB	3:O:24:THR:HB	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:5:THR:HB	3:N:24:THR:HB	1.86	0.57
1:D:74:CYS:O	1:D:77:GLN:HB2	2.05	0.57
2:H:40:ALA:HB3	2:H:43:GLN:HB2	1.88	0.56
1:A:27:HIS:HE2	2:I:100:TYR:HE1	1.53	0.56
1:A:27:HIS:NE2	2:I:100:TYR:HE1	2.03	0.56
1:B:20:TRP:HA	1:B:287:LEU:O	2.05	0.56
2:I:40:ALA:HB3	2:I:43:GLN:HB2	1.87	0.56
2:J:40:ALA:HB3	2:J:43:GLN:HB2	1.87	0.55
2:H:87:THR:HG23	2:H:110:THR:HA	1.89	0.55
1:A:314:GLU:HB2	1:A:391:TRP:HZ2	1.70	0.55
2:I:87:THR:HG23	2:I:110:THR:HA	1.89	0.55
1:A:320:ILE:HG12	1:A:371:PRO:HG3	1.88	0.55
1:A:127:GLY:HA2	1:A:199:LEU:HA	1.87	0.54
2:J:87:THR:HG23	2:J:110:THR:HA	1.89	0.54
1:B:204:LYS:HE2	1:B:269:GLU:HG2	1.90	0.54
1:C:331:SER:CB	1:C:332:PRO:HD3	2.37	0.54
1:C:204:LYS:HE2	1:C:269:GLU:HG2	1.91	0.53
1:A:331:SER:HB3	1:A:332:PRO:CD	2.39	0.53
2:K:87:THR:HG23	2:K:110:THR:HA	1.90	0.53
1:A:204:LYS:HE2	1:A:269:GLU:HG2	1.90	0.53
1:D:247:LYS:HB3	2:J:100(D):TRP:NE1	2.24	0.53
1:A:4:ILE:HG21	1:A:321:VAL:HG11	1.91	0.52
1:C:269:GLU:O	1:C:270:ILE:HD13	2.10	0.52
1:D:312:ILE:HG13	1:D:322:ILE:CD1	2.40	0.52
1:A:377:TYR:CE2	1:A:390:ASN:HB3	2.45	0.51
1:A:173:ALA:HB3	1:A:181:VAL:HB	1.92	0.51
1:A:326:TYR:HB2	1:A:358:VAL:HG21	1.92	0.51
1:B:23:ILE:HD11	1:B:183:MET:HE1	1.92	0.51
1:D:331:SER:CB	1:D:332:PRO:HD3	2.33	0.50
1:C:25:LEU:HD21	1:C:43:PHE:HB3	1.92	0.50
1:D:20:TRP:HA	1:D:287:LEU:O	2.12	0.50
3:L:4:LEU:HB2	3:L:99:GLY:HA2	1.93	0.50
1:C:201:MET:HB2	1:C:206:TRP:HZ3	1.76	0.50
1:C:301:MET:HG3	1:C:334:LYS:HB2	1.93	0.50
3:N:46:LEU:HD21	3:N:49:TYR:HB3	1.92	0.50
1:C:342:LEU:HA	1:C:377:TYR:CE2	2.47	0.49
1:B:82:LEU:HD12	1:B:114:VAL:HG13	1.94	0.49
1:D:2:ARG:C	1:D:4:ILE:H	2.19	0.49
1:D:51:LYS:HE2	1:D:136:GLU:HB2	1.93	0.49
2:K:95:ASP:OD1	2:K:100(J):TYR:HA	2.12	0.49
1:C:47:LYS:HG3	1:C:278:LEU:HD23	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:286:ARG:HB3	1:D:288:ARG:HH12	1.78	0.49
1:D:380:VAL:HB	1:D:387:LEU:HB2	1.93	0.49
1:B:46:ILE:HG12	1:B:140:VAL:HG22	1.93	0.49
1:C:181:VAL:HB	1:C:292:LEU:HD13	1.95	0.49
2:I:95:ASP:OD1	2:I:100(J):TYR:HA	2.12	0.49
2:J:95:ASP:OD1	2:J:100(J):TYR:HA	2.13	0.49
2:H:95:ASP:OD1	2:H:100(J):TYR:HA	2.13	0.48
1:D:3:CYS:HA	1:D:6:ILE:HD12	1.94	0.48
2:H:72:ASP:HB2	2:H:79:TYR:HE2	1.79	0.48
3:N:21:ILE:HD12	3:N:73:LEU:HD23	1.95	0.48
1:A:331:SER:CB	1:A:332:PRO:HD3	2.42	0.48
1:A:324:VAL:HG11	1:A:380:VAL:HG11	1.96	0.47
1:C:166:PRO:HA	1:C:187:PRO:HG2	1.94	0.47
1:C:335:ILE:HB	1:C:356:PRO:HB2	1.95	0.47
1:C:318:GLY:HA3	1:C:1393:ARG:HH21	1.80	0.47
1:C:377:TYR:CE1	1:C:390:ASN:HB3	2.50	0.47
1:A:3:CYS:HA	1:A:6:ILE:HD12	1.95	0.47
1:B:312:ILE:HD11	1:B:389:LEU:HD13	1.97	0.47
1:D:305:LYS:HE2	1:D:385:GLY:HA3	1.96	0.47
2:J:72:ASP:HB2	2:J:79:TYR:HE2	1.79	0.47
1:D:138:THR:HG23	1:D:163:LYS:HG2	1.96	0.47
1:A:1:MET:HE3	1:A:146:GLY:HA2	1.96	0.47
1:A:46:ILE:HG22	1:A:47:LYS:HG3	1.96	0.47
2:I:72:ASP:HB2	2:I:79:TYR:HE2	1.80	0.47
1:A:12:VAL:HG21	1:A:23:ILE:HG22	1.96	0.47
1:A:47:LYS:HG2	1:A:278:LEU:HD11	1.97	0.47
1:C:3:CYS:HA	1:C:6:ILE:HD12	1.95	0.47
1:A:309:VAL:HG11	1:A:323:ARG:HD2	1.97	0.46
3:N:12:SER:HB3	3:N:106(A):LEU:HD11	1.97	0.46
1:C:382:VAL:HG23	1:C:384:PRO:HD2	1.97	0.46
1:B:72:SER:HB3	1:B:113:ILE:HD12	1.98	0.46
1:C:180:THR:O	1:C:291:LYS:HB2	2.14	0.46
3:L:12:SER:HB3	3:L:106(A):LEU:HD11	1.97	0.46
3:M:12:SER:HB3	3:M:106(A):LEU:HD11	1.97	0.46
1:A:48:THR:HB	1:A:279:PHE:HB2	1.97	0.46
3:O:12:SER:HB3	3:O:106(A):LEU:HD11	1.97	0.46
1:A:309:VAL:HB	1:A:323:ARG:HB3	1.98	0.46
2:I:6:GLU:CD	2:I:106:GLY:H	2.24	0.45
1:D:72:SER:HB3	1:D:113:ILE:HD12	1.98	0.45
1:C:185:CYS:O	1:C:187:PRO:HD3	2.16	0.45
1:B:339:ILE:HG12	1:B:378:ILE:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:302:CYS:H	1:C:333:CYS:HB2	1.82	0.44
1:C:301:MET:HE2	1:C:336:PRO:HA	1.98	0.44
1:D:247:LYS:CB	2:J:100(D):TRP:NE1	2.81	0.44
1:D:331:SER:CB	1:D:332:PRO:CD	2.95	0.44
1:C:302:CYS:HB3	1:C:326:TYR:CE1	2.53	0.44
1:A:188:ARG:HE	1:C:24:VAL:HB	1.83	0.43
1:A:343:GLU:HB2	1:A:345:ARG:HG2	2.00	0.43
2:J:95:ASP:OD1	2:J:100(G):THR:HG22	2.18	0.43
3:L:27(B):ASP:HB3	3:L:92:THR:HG22	1.99	0.43
1:C:129:ILE:HD11	1:C:197:VAL:HG22	2.01	0.43
2:H:95:ASP:OD1	2:H:100(G):THR:HG22	2.19	0.43
1:C:189:THR:C	1:C:191:LEU:H	2.27	0.43
2:J:98:ASP:HB3	2:J:100(B):ASP:O	2.19	0.43
1:A:182:THR:HB	1:A:288:ARG:HB2	2.01	0.42
2:K:95:ASP:OD1	2:K:100(G):THR:HG22	2.19	0.42
1:A:47:LYS:HA	1:A:278:LEU:HD21	2.00	0.42
1:B:3:CYS:HA	1:B:6:ILE:HD12	2.00	0.42
1:B:314:GLU:HB2	1:B:391:TRP:HZ2	1.84	0.42
4:C:567:NAG:C6	2:K:65:ASP:HB3	2.43	0.42
1:D:171:THR:O	1:D:182:THR:HA	2.20	0.42
1:D:323:ARG:HA	1:D:365:VAL:O	2.17	0.42
1:D:247:LYS:HB3	2:J:100(D):TRP:CD1	2.54	0.42
1:D:305:LYS:HB3	1:D:327:GLU:HB2	2.01	0.42
1:B:306:PHE:O	1:B:387:LEU:HD11	2.20	0.42
1:B:342:LEU:HD23	1:B:377:TYR:CE2	2.55	0.42
1:C:127:GLY:HA3	1:C:213:PHE:CZ	2.55	0.42
1:B:20:TRP:HB3	1:B:288:ARG:HD3	2.02	0.42
1:C:320:ILE:HG12	1:C:371:PRO:HG3	2.02	0.42
2:I:95:ASP:OD1	2:I:100(G):THR:HG22	2.19	0.42
1:A:14:GLY:HA2	1:A:21:VAL:HG11	2.01	0.42
1:A:337:PHE:HA	1:A:379:ILE:O	2.20	0.41
1:B:343:GLU:HB2	1:B:345:ARG:HG2	2.02	0.41
1:D:382:VAL:HG12	1:D:384:PRO:HD2	2.03	0.41
2:H:97:VAL:HG13	2:H:100(B):ASP:O	2.21	0.41
3:M:23:CYS:HB3	3:M:71:ALA:O	2.20	0.41
3:O:27(B):ASP:HB3	3:O:92:THR:HG22	2.02	0.41
1:A:1:MET:SD	1:A:4:ILE:HD12	2.61	0.41
1:A:348:LEU:HB3	1:A:372:PRO:HG3	2.02	0.41
1:B:331:SER:CB	1:B:332:PRO:CD	2.94	0.41
1:C:64:LYS:HB3	1:C:122:LYS:HD2	2.03	0.41
1:D:64:LYS:HG3	1:D:120:THR:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:LEU:HD12	1:A:283:LEU:HA	1.94	0.41
1:A:335:ILE:HA	1:A:336:PRO:HD3	1.99	0.41
1:D:341:ASP:C	1:D:343:GLU:H	2.29	0.41
1:D:68:THR:HA	1:D:116:CYS:O	2.21	0.40
1:D:197:VAL:CG2	1:D:210:ARG:HA	2.51	0.40
1:A:91:ILE:HD13	1:A:234:LYS:HB2	2.03	0.40
1:B:198:LEU:HD21	1:B:277:LEU:HD22	2.02	0.40
1:C:240:PHE:CE1	1:C:248:GLN:HG3	2.56	0.40

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	369/425 (87%)	333 (90%)	32 (9%)	4 (1%)	11	43
1	B	379/425 (89%)	342 (90%)	29 (8%)	8 (2%)	5	31
1	C	372/425 (88%)	341 (92%)	26 (7%)	5 (1%)	9	40
1	D	372/425 (88%)	346 (93%)	20 (5%)	6 (2%)	7	36
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%)	6	33
3	M	108/154 (70%)	103 (95%)	3 (3%)	2 (2%)	6	33
3	N	107/154 (70%)	102 (95%)	3 (3%)	2 (2%)	6	33
3	O	106/154 (69%)	100 (94%)	4 (4%)	2 (2%)	6	33
All	All	2421/2892 (84%)	2215 (92%)	175 (7%)	31 (1%)	9	40

All (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
1	C	331	SER
1	D	51	LYS
1	D	331	SER
1	B	16	SER
1	B	18	GLY
1	B	188	ARG
1	C	15	VAL
1	C	302	CYS
3	L	83	GLU
1	B	51	LYS
1	B	169	SER
1	D	202	GLU
3	M	83	GLU
3	N	83	GLU
1	A	202	GLU
1	B	15	VAL
1	D	168	SER
1	D	169	SER
1	A	318	GLY
3	O	83	GLU
1	C	202	GLU
1	D	318	GLY
3	L	51	VAL
3	M	51	VAL
3	N	51	VAL
3	O	51	VAL

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%)	291 (88%)	39 (12%)	5	23
1	B	334/369 (90%)	297 (89%)	37 (11%)	6	25
1	C	330/369 (89%)	286 (87%)	44 (13%)	4	19
1	D	332/369 (90%)	295 (89%)	37 (11%)	6	25
2	H	107/112 (96%)	96 (90%)	11 (10%)	7	28
2	I	107/112 (96%)	98 (92%)	9 (8%)	10	38
2	J	107/112 (96%)	97 (91%)	10 (9%)	8	33
2	K	107/112 (96%)	97 (91%)	10 (9%)	8	33
3	L	90/116 (78%)	84 (93%)	6 (7%)	15	47
3	M	90/116 (78%)	81 (90%)	9 (10%)	7	30
3	N	89/116 (77%)	84 (94%)	5 (6%)	19	52
3	O	88/116 (76%)	82 (93%)	6 (7%)	14	46
All	All	2111/2388 (88%)	1888 (89%)	223 (11%)	6	27

All (223) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	CYS
1	A	48	THR
1	A	68	THR
1	A	77	GLN
1	A	107	LEU
1	A	115	THR
1	A	126	GLU
1	A	139	ILE
1	A	144	HIS
1	A	162	ILE
1	A	167	GLN
1	A	176	THR
1	A	182	THR
1	A	200	GLN
1	A	203	ASP
1	A	209	HIS
1	A	235	GLU
1	A	252	VAL
1	A	253	LEU
1	A	276	ASN
1	A	278	LEU
1	A	283	LEU

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Mol	Chain	Res	Type
1	A	284	LYS
1	A	287	LEU
1	A	308	ILE
1	A	311	GLU
1	A	315	THR
1	A	342	LEU
1	A	343	GLU
1	A	346	HIS
1	A	348	LEU
1	A	357	ILE
1	A	376	SER
1	A	383	GLU
1	A	389	LEU
1	A	390	ASN
1	A	1392	LEU
1	A	1393	ARG
1	A	1395	LEU
1	B	1	MET
1	B	21	VAL
1	B	27	HIS
1	B	30	CYS
1	B	55	THR
1	B	69	THR
1	B	77	GLN
1	B	82	LEU
1	B	86	GLN
1	B	107	LEU
1	B	113	ILE
1	B	115	THR
1	B	136	GLU
1	B	144	HIS
1	B	167	GLN
1	B	172	GLU
1	B	176	THR
1	B	183	MET
1	B	191	LEU
1	B	199	LEU
1	B	209	HIS
1	B	235	GLU
1	B	248	GLN
1	B	252	VAL
1	B	253	LEU

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Mol	Chain	Res	Type
1	B	270	ILE
1	B	276	ASN
1	B	278	LEU
1	B	289	MET
1	B	311	GLU
1	B	331	SER
1	B	343	GLU
1	B	346	HIS
1	B	360	GLU
1	B	383	GLU
1	B	388	LYS
1	B	389	LEU
1	C	1	MET
1	C	21	VAL
1	C	30	CYS
1	C	44	GLU
1	C	49	GLU
1	C	69	THR
1	C	71	GLU
1	C	77	GLN
1	C	86	GLN
1	C	107	LEU
1	C	126	GLU
1	C	144	HIS
1	C	162	ILE
1	C	167	GLN
1	C	171	THR
1	C	176	THR
1	C	180	THR
1	C	186	SER
1	C	198	LEU
1	C	200	GLN
1	C	203	ASP
1	C	209	HIS
1	C	235	GLU
1	C	240	PHE
1	C	248	GLN
1	C	249	ASP
1	C	251	VAL
1	C	252	VAL
1	C	253	LEU
1	C	279	PHE

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Mol	Chain	Res	Type
1	C	287	LEU
1	C	288	ARG
1	C	311	GLU
1	C	331	SER
1	C	338	GLU
1	C	342	LEU
1	C	344	LYS
1	C	346	HIS
1	C	353	THR
1	C	376	SER
1	C	380	VAL
1	C	383	GLU
1	C	389	LEU
1	C	1392	LEU
1	D	15	VAL
1	D	30	CYS
1	D	69	THR
1	D	86	GLN
1	D	91	ILE
1	D	113	ILE
1	D	114	VAL
1	D	115	THR
1	D	120	THR
1	D	126	GLU
1	D	142	THR
1	D	144	HIS
1	D	167	GLN
1	D	170	THR
1	D	172	GLU
1	D	176	THR
1	D	197	VAL
1	D	200	GLN
1	D	201	MET
1	D	203	ASP
1	D	209	HIS
1	D	235	GLU
1	D	248	GLN
1	D	252	VAL
1	D	253	LEU
1	D	287	LEU
1	D	288	ARG
1	D	289	MET

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Mol	Chain	Res	Type
1	D	311	GLU
1	D	312	ILE
1	D	322	ILE
1	D	351	LEU
1	D	357	ILE
1	D	365	VAL
1	D	383	GLU
1	D	390	ASN
1	D	1392	LEU
2	H	1	GLU
2	H	5	VAL
2	H	6	GLU
2	H	38	ARG
2	H	73	THR
2	H	77	THR
2	H	82	LEU
2	H	82(A)	SER
2	H	82(B)	SER
2	H	82(C)	LEU
2	H	98	ASP
2	I	1	GLU
2	I	5	VAL
2	I	38	ARG
2	I	77	THR
2	I	82	LEU
2	I	82(A)	SER
2	I	82(B)	SER
2	I	82(C)	LEU
2	I	98	ASP
2	J	1	GLU
2	J	5	VAL
2	J	38	ARG
2	J	69	ILE
2	J	73	THR
2	J	77	THR
2	J	82	LEU
2	J	82(A)	SER
2	J	82(B)	SER
2	J	82(C)	LEU
2	K	1	GLU
2	K	5	VAL
2	K	6	GLU

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Mol	Chain	Res	Type
2	K	38	ARG
2	K	65	ASP
2	K	82	LEU
2	K	82(A)	SER
2	K	82(B)	SER
2	K	82(C)	LEU
2	K	98	ASP
3	L	17	GLN
3	L	48	LEU
3	L	78	LEU
3	L	79	GLN
3	L	83	GLU
3	L	104	LEU
3	M	1	GLN
3	M	17	GLN
3	M	48	LEU
3	M	73	LEU
3	M	78	LEU
3	M	79	GLN
3	M	83	GLU
3	M	85	ASP
3	M	104	LEU
3	N	17	GLN
3	N	48	LEU
3	N	72	SER
3	N	73	LEU
3	N	79	GLN
3	O	17	GLN
3	O	48	LEU
3	O	78	LEU
3	O	79	GLN
3	O	83	GLU
3	O	104	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	GLN
1	A	124	ASN
1	A	131	GLN
1	A	134	ASN
1	A	144	HIS

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Mol	Chain	Res	Type
1	A	167	GLN
1	A	209	HIS
1	A	230	ASN
1	A	248	GLN
1	A	256	GLN
1	A	276	ASN
1	A	282	HIS
1	A	325	GLN
1	A	346	HIS
1	B	77	GLN
1	B	124	ASN
1	B	131	GLN
1	B	134	ASN
1	B	230	ASN
1	B	256	GLN
1	B	271	GLN
1	B	276	ASN
1	B	325	GLN
1	B	346	HIS
1	C	8	ASN
1	C	27	HIS
1	C	77	GLN
1	C	124	ASN
1	C	131	GLN
1	C	134	ASN
1	C	209	HIS
1	C	230	ASN
1	C	256	GLN
1	C	271	GLN
1	C	325	GLN
1	C	366	ASN
1	C	386	GLN
1	D	8	ASN
1	D	131	GLN
1	D	134	ASN
1	D	209	HIS
1	D	230	ASN
1	D	256	GLN
1	D	366	ASN
2	H	52	ASN
2	H	56	ASN
2	I	52	ASN

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Mol	Chain	Res	Type
2	I	56	ASN
2	J	52	ASN
2	J	56	ASN
2	K	52	ASN
2	K	56	ASN
2	K	61	GLN
2	K	64	GLN
3	L	37	GLN
3	M	37	GLN
3	N	31	ASN
3	N	37	GLN
3	O	37	GLN

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](#)

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	C	567	1	14,14,15	0.34	0	17,19,21	0.63	0
4	NAG	D	567	1	14,14,15	0.34	0	17,19,21	0.70	1 (5%)

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	0.31	0	17,19,21	0.70	1 (5%)
4	NAG	B	567	1	14,14,15	0.31	0	17,19,21	0.57	0

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

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	2.38	115.38	112.19
4	A	567	NAG	C1-O5-C5	2.23	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%)	-0.08	1 (0%) 90 81	44, 103, 144, 169	0
1	B	383/425 (90%)	-0.08	2 (0%) 87 76	51, 99, 139, 170	0
1	C	378/425 (88%)	-0.31	1 (0%) 90 81	37, 75, 116, 168	0
1	D	380/425 (89%)	-0.39	0 100 100	36, 71, 103, 130	0
2	H	127/144 (88%)	-0.06	0 100 100	48, 93, 132, 157	0
2	I	127/144 (88%)	0.15	0 100 100	69, 137, 208, 228	0
2	J	127/144 (88%)	0.06	0 100 100	66, 135, 176, 200	0
2	K	127/144 (88%)	-0.15	1 (0%) 82 67	45, 85, 114, 134	0
3	L	110/154 (71%)	-0.04	0 100 100	53, 99, 154, 166	0
3	M	110/154 (71%)	-0.01	0 100 100	82, 111, 175, 208	0
3	N	109/154 (70%)	0.04	0 100 100	58, 109, 154, 202	0
3	O	108/154 (70%)	-0.16	1 (0%) 81 64	54, 92, 144, 181	0
All	All	2463/2892 (85%)	-0.14	6 (0%) 91 85	36, 94, 157, 228	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	228	GLY	2.9
1	B	225	ASP	2.7
1	B	303	THR	2.2
3	O	23	CYS	2.1
1	A	275	GLY	2.0
2	K	29	PHE	2.0

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 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($\text{\AA}^2$)	Q<0.9
4	NAG	A	567	14/15	0.26	0.11	123,124,124,125	0
4	NAG	C	567	14/15	0.71	0.10	89,100,102,104	0
4	NAG	B	567	14/15	0.72	0.10	139,140,141,142	0
4	NAG	D	567	14/15	0.77	0.09	100,103,108,108	0

6.5 Other polymers [i](#)

There are no such residues in this entry.