



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 15, 2020 – 11:26 PM EST

PDB ID : 7K93
Title : DENV2 NS1 in complex with neutralizing 2B7 single chain Fab variable region (scFv)
Authors : Akey, D.L.; Smith, J.L.
Deposited on : 2020-09-28
Resolution : 2.89 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 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 : 2.15.1
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) : 2.15.1

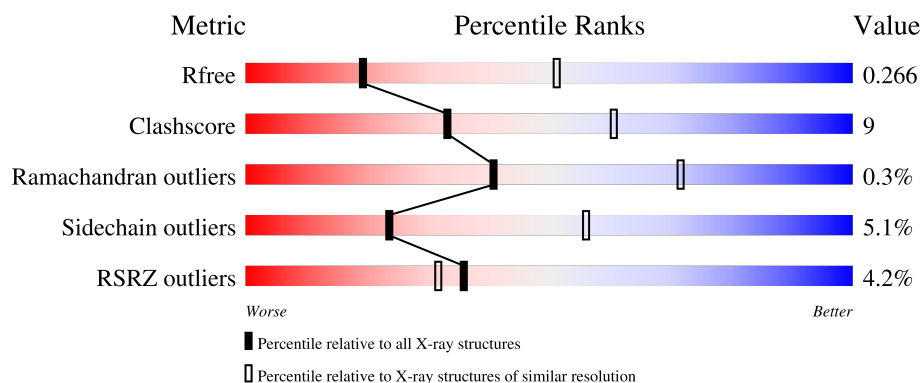
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	376	<div> <div>10%</div> <div>61%</div> <div>25%</div> <div>13%</div> </div>
1	B	376	<div> <div>4%</div> <div>69%</div> <div>18%</div> <div>13%</div> </div>
1	C	376	<div> <div>2%</div> <div>63%</div> <div>25%</div> <div>11%</div> </div>
1	D	376	<div> <div>4%</div> <div>63%</div> <div>22%</div> <div>14%</div> </div>
2	E	251	<div> <div>0%</div> <div>76%</div> <div>15%</div> <div>7%</div> </div>

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Mol	Chain	Length	Quality of chain
2	G	251	<div><div>%</div><div><div></div><div>75%</div><div>15%</div><div>•</div><div>8%</div></div></div>
2	I	251	<div><div>6%</div><div><div></div><div>76%</div><div>16%</div><div>•</div><div>8%</div></div></div>
2	K	251	<div><div>%</div><div><div></div><div>73%</div><div>17%</div><div>•</div><div>8%</div></div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17581 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 Non-structural protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	327	Total	C	N	O	S	0	0	0
			2597	1632	450	495	20			
1	B	328	Total	C	N	O	S	0	0	0
			2600	1635	450	495	20			
1	C	335	Total	C	N	O	S	0	0	0
			2642	1663	457	502	20			
1	D	325	Total	C	N	O	S	0	0	0
			2578	1622	446	490	20			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	ALA	-	expression tag	UNP D0EPS0
A	-22	HIS	-	expression tag	UNP D0EPS0
A	-21	HIS	-	expression tag	UNP D0EPS0
A	-20	HIS	-	expression tag	UNP D0EPS0
A	-19	HIS	-	expression tag	UNP D0EPS0
A	-18	HIS	-	expression tag	UNP D0EPS0
A	-17	HIS	-	expression tag	UNP D0EPS0
A	-16	SER	-	expression tag	UNP D0EPS0
A	-15	SER	-	expression tag	UNP D0EPS0
A	-14	GLY	-	expression tag	UNP D0EPS0
A	-13	VAL	-	expression tag	UNP D0EPS0
A	-12	ASP	-	expression tag	UNP D0EPS0
A	-11	LEU	-	expression tag	UNP D0EPS0
A	-10	GLY	-	expression tag	UNP D0EPS0
A	-9	THR	-	expression tag	UNP D0EPS0
A	-8	GLU	-	expression tag	UNP D0EPS0
A	-7	ASN	-	expression tag	UNP D0EPS0
A	-6	LEU	-	expression tag	UNP D0EPS0
A	-5	TYR	-	expression tag	UNP D0EPS0
A	-4	PHE	-	expression tag	UNP D0EPS0
A	-3	GLN	-	expression tag	UNP D0EPS0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP D0EPS0
A	-1	ASN	-	expression tag	UNP D0EPS0
B	-23	ALA	-	expression tag	UNP D0EPS0
B	-22	HIS	-	expression tag	UNP D0EPS0
B	-21	HIS	-	expression tag	UNP D0EPS0
B	-20	HIS	-	expression tag	UNP D0EPS0
B	-19	HIS	-	expression tag	UNP D0EPS0
B	-18	HIS	-	expression tag	UNP D0EPS0
B	-17	HIS	-	expression tag	UNP D0EPS0
B	-16	SER	-	expression tag	UNP D0EPS0
B	-15	SER	-	expression tag	UNP D0EPS0
B	-14	GLY	-	expression tag	UNP D0EPS0
B	-13	VAL	-	expression tag	UNP D0EPS0
B	-12	ASP	-	expression tag	UNP D0EPS0
B	-11	LEU	-	expression tag	UNP D0EPS0
B	-10	GLY	-	expression tag	UNP D0EPS0
B	-9	THR	-	expression tag	UNP D0EPS0
B	-8	GLU	-	expression tag	UNP D0EPS0
B	-7	ASN	-	expression tag	UNP D0EPS0
B	-6	LEU	-	expression tag	UNP D0EPS0
B	-5	TYR	-	expression tag	UNP D0EPS0
B	-4	PHE	-	expression tag	UNP D0EPS0
B	-3	GLN	-	expression tag	UNP D0EPS0
B	-2	SER	-	expression tag	UNP D0EPS0
B	-1	ASN	-	expression tag	UNP D0EPS0
C	-23	ALA	-	expression tag	UNP D0EPS0
C	-22	HIS	-	expression tag	UNP D0EPS0
C	-21	HIS	-	expression tag	UNP D0EPS0
C	-20	HIS	-	expression tag	UNP D0EPS0
C	-19	HIS	-	expression tag	UNP D0EPS0
C	-18	HIS	-	expression tag	UNP D0EPS0
C	-17	HIS	-	expression tag	UNP D0EPS0
C	-16	SER	-	expression tag	UNP D0EPS0
C	-15	SER	-	expression tag	UNP D0EPS0
C	-14	GLY	-	expression tag	UNP D0EPS0
C	-13	VAL	-	expression tag	UNP D0EPS0
C	-12	ASP	-	expression tag	UNP D0EPS0
C	-11	LEU	-	expression tag	UNP D0EPS0
C	-10	GLY	-	expression tag	UNP D0EPS0
C	-9	THR	-	expression tag	UNP D0EPS0
C	-8	GLU	-	expression tag	UNP D0EPS0
C	-7	ASN	-	expression tag	UNP D0EPS0

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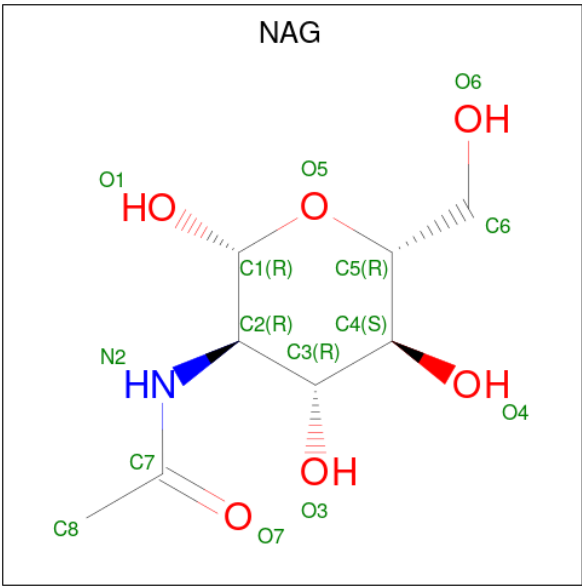
Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	LEU	-	expression tag	UNP D0EPS0
C	-5	TYR	-	expression tag	UNP D0EPS0
C	-4	PHE	-	expression tag	UNP D0EPS0
C	-3	GLN	-	expression tag	UNP D0EPS0
C	-2	SER	-	expression tag	UNP D0EPS0
C	-1	ASN	-	expression tag	UNP D0EPS0
D	-23	ALA	-	expression tag	UNP D0EPS0
D	-22	HIS	-	expression tag	UNP D0EPS0
D	-21	HIS	-	expression tag	UNP D0EPS0
D	-20	HIS	-	expression tag	UNP D0EPS0
D	-19	HIS	-	expression tag	UNP D0EPS0
D	-18	HIS	-	expression tag	UNP D0EPS0
D	-17	HIS	-	expression tag	UNP D0EPS0
D	-16	SER	-	expression tag	UNP D0EPS0
D	-15	SER	-	expression tag	UNP D0EPS0
D	-14	GLY	-	expression tag	UNP D0EPS0
D	-13	VAL	-	expression tag	UNP D0EPS0
D	-12	ASP	-	expression tag	UNP D0EPS0
D	-11	LEU	-	expression tag	UNP D0EPS0
D	-10	GLY	-	expression tag	UNP D0EPS0
D	-9	THR	-	expression tag	UNP D0EPS0
D	-8	GLU	-	expression tag	UNP D0EPS0
D	-7	ASN	-	expression tag	UNP D0EPS0
D	-6	LEU	-	expression tag	UNP D0EPS0
D	-5	TYR	-	expression tag	UNP D0EPS0
D	-4	PHE	-	expression tag	UNP D0EPS0
D	-3	GLN	-	expression tag	UNP D0EPS0
D	-2	SER	-	expression tag	UNP D0EPS0
D	-1	ASN	-	expression tag	UNP D0EPS0

- Molecule 2 is a protein called 2B7 single chain fab variable region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	233	Total	C	N	O	S	0	0	0
			1780	1118	294	355	13			
2	G	232	Total	C	N	O	S	0	0	0
			1776	1116	293	354	13			
2	I	232	Total	C	N	O	S	0	0	0
			1776	1116	293	354	13			
2	K	232	Total	C	N	O	S	0	0	0
			1776	1116	293	354	13			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:

C₈H₁₅NO₆).



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

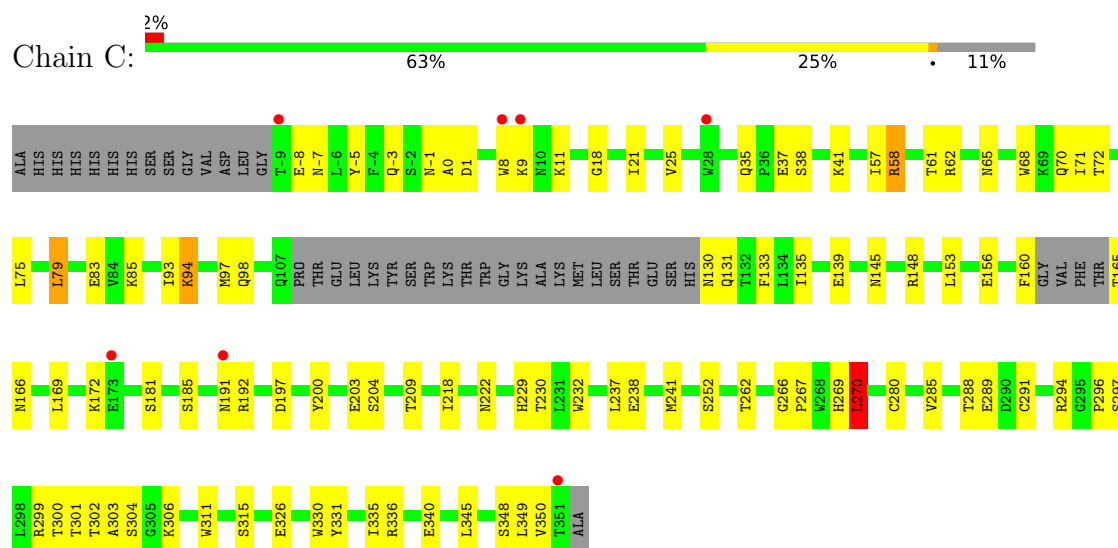
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

[illegible]

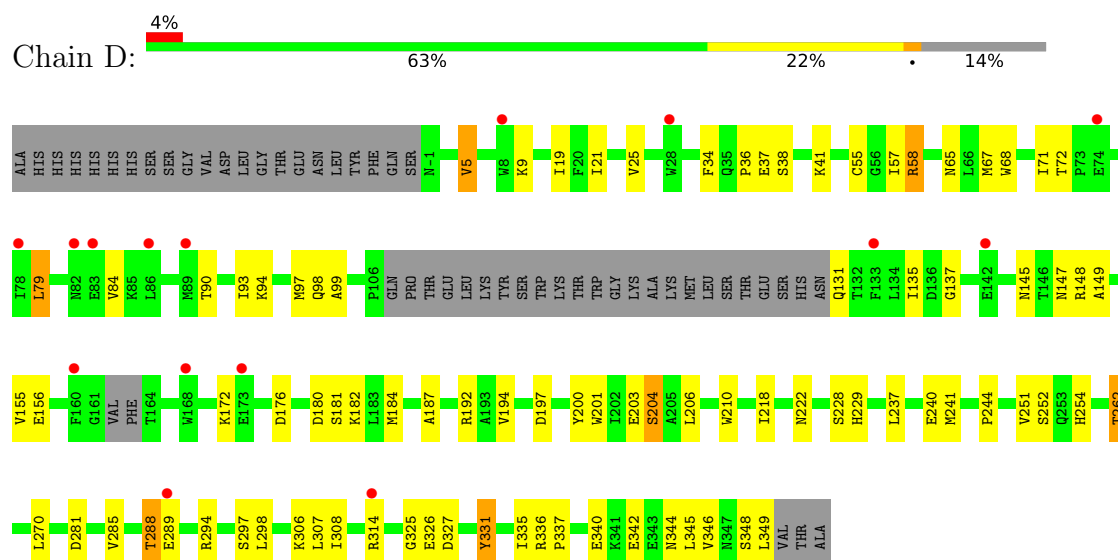
Chain B:

Amino Acid	Category
ALA	Grey
HIS	Green
HIS	Green
HIS	Green
HIS	Green
HIS	Green
HIS	Green
SER	Green
SER	Green
GLY	Green
VAL	Green
ASP	Green
LEU	Green
GLY	Green
THR	Green
GLU	Green
ASN	Green
LEU	Green
THR	Green
PHE	Green
GLN	Green
SER	Green
N-1	Yellow
A0	Green
D1	Green
W8	Green
K9	Green
K14	Green
S17	Green
I21	Green
V25	Green
W28	Green
Q31	Green
Y32	Green
Q35	Green
S38	Green
K41	Green
L42	Green
A43	Green
I46	Green
E51	Green
E52	Green
G53	Green
I57	Green
R58	Orange
W58	Green
K69	Green
Q70	Green
I71	Green
L75	Green
L76	Green
L79	Green
V84	Green
K85	Green
L86	Green
T87	Green
I88	Green
M89	Green
T90	Green
G91	Green
A99	Green
L104	Green
R105	Green
P106	Green
GLN	Green
PRO	Green
THR	Green
GLU	Green
LEU	Green
LYS	Green
TYR	Green
SER	Green
TRP	Green
LYS	Green
THR	Green
TRP	Green
GLY	Green
LYS	Green
ALA	Green
LYS	Green
MET	Green
LEU	Green
SER	Green
THR	Green
GLU	Green
SER	Green
HIS	Green
N130	Green
F133	Green
L134	Green
I135	Green
T140	Green
A141	Green
E142	Green
N145	Green
T146	Green
P146	Green
N147	Green
F147	Green
S204	Green
A205	Green
L206	Green
N207	Green
D208	Green
T209	Green
K210	Green
K211	Green
I218	Green
K221	Green
N222	Green
K227	Green
S228	Green
H229	Green
M241	Green
V251	Green
T262	Green
H269	Green
N293	Green
K294	Green
G295	Green
P296	Green
N147	Green
S207	Green

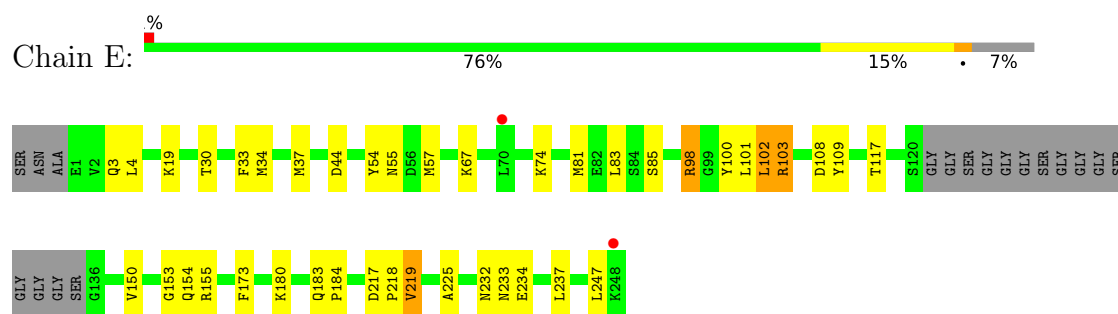
- Molecule 1: Non-structural protein 1



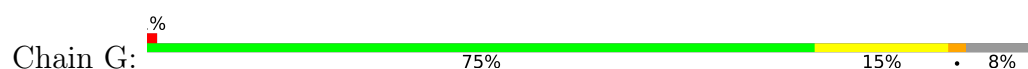
- Molecule 1: Non-structural protein 1

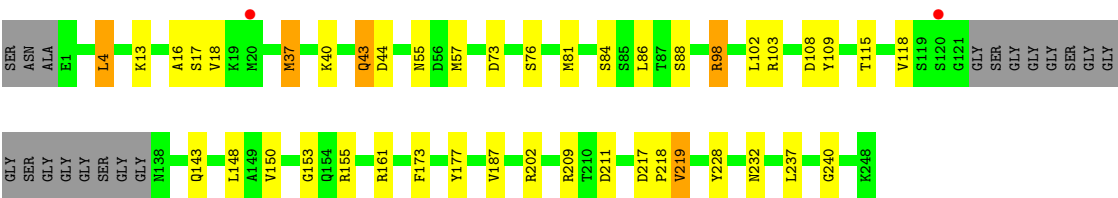


- Molecule 2: 2B7 single chain fab variable region

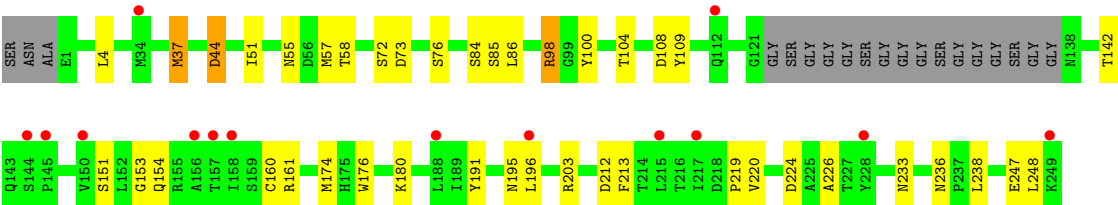


- Molecule 2: 2B7 single chain fab variable region

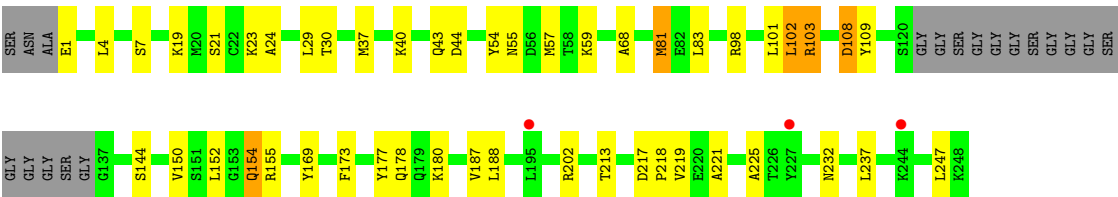




• Molecule 2: 2B7 single chain fab variable region



• Molecule 2: 2B7 single chain fab variable region



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	69.63Å 165.59Å 258.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.38 – 2.89 47.38 – 2.89	Depositor EDS
% Data completeness (in resolution range)	99.0 (47.38-2.89) 89.5 (47.38-2.89)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.64 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, R_{free}	0.223 , 0.269 0.226 , 0.266	Depositor DCC
R_{free} test set	2412 reflections (3.57%)	wwPDB-VP
Wilson B-factor (Å ²)	66.8	Xtriage
Anisotropy	0.428	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 29.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	17581	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% 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

5.1 Standard geometry

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	0.48	0/2657	0.68	1/3599 (0.0%)
1	B	0.50	0/2660	0.67	0/3603
1	C	0.60	0/2703	0.74	2/3663 (0.1%)
1	D	0.55	0/2638	0.67	0/3572
2	E	0.45	0/1820	0.69	0/2467
2	G	0.48	0/1816	0.71	0/2462
2	I	0.50	0/1816	0.69	0/2462
2	K	0.47	0/1816	0.69	1/2462 (0.0%)
All	All	0.51	0/17926	0.69	4/24290 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	152	LEU	CA-CB-CG	6.23	129.62	115.30
1	C	237	LEU	CA-CB-CG	5.41	127.73	115.30
1	C	270	LEU	CA-CB-CG	5.28	127.45	115.30
1	A	237	LEU	CA-CB-CG	5.13	127.11	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2597	0	2518	67	0
1	B	2600	0	2530	46	0
1	C	2642	0	2547	58	0
1	D	2578	0	2508	54	0
2	E	1780	0	1709	22	0
2	G	1776	0	1706	27	0
2	I	1776	0	1706	26	0
2	K	1776	0	1706	27	0
3	A	14	0	13	1	0
3	B	14	0	13	0	0
3	C	14	0	13	0	0
3	D	14	0	13	0	0
All	All	17581	0	16982	296	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 9.

All (296) 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:289:GLU:HA	1:D:314:ARG:HG3	1.41	0.99
1:C:94:LYS:NZ	1:C:139:GLU:OE2	2.19	0.76
1:C:35:GLN:OE1	1:C:166:ASN:ND2	2.20	0.74
2:I:98:ARG:NH1	2:I:108:ASP:OD2	2.20	0.74
2:I:55:ASN:HB3	2:I:57:MET:HG3	1.67	0.74
1:C:25:VAL:HG13	1:C:218:ILE:HG12	1.70	0.73
1:B:296:PRO:O	1:B:336:ARG:NH1	2.21	0.71
1:A:182:LYS:HG2	1:B:191:ASN:HD21	1.56	0.70
2:G:55:ASN:HB3	2:G:57:MET:HG3	1.74	0.70
1:A:58:ARG:NH1	1:A:137:GLY:O	2.25	0.69
1:A:53:GLY:O	1:A:147:ASN:ND2	2.24	0.69
1:D:331:TYR:HB3	1:D:335:ILE:HB	1.74	0.67
1:D:172:LYS:NZ	1:D:176:ASP:OD1	2.27	0.67
1:D:270:LEU:HD13	1:D:325:GLY:HA3	1.76	0.67
1:D:21:ILE:HG13	1:D:187:ALA:HB2	1.77	0.67
1:A:31:GLN:HE21	1:B:14:LYS:NZ	1.92	0.66
2:I:180:LYS:HD3	2:I:226:ALA:HB2	1.79	0.65
2:G:98:ARG:NH1	2:G:108:ASP:OD2	2.30	0.64
1:B:227:LYS:HE2	1:B:251:VAL:HG11	1.79	0.64
1:A:25:VAL:HG13	1:A:218:ILE:HG12	1.80	0.64
2:E:55:ASN:HB3	2:E:57:MET:HG3	1.78	0.64
2:G:108:ASP:HB3	2:G:109:TYR:CD2	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:PRO:HG3	1:A:262:THR:HG22	1.80	0.63
1:D:58:ARG:HD2	1:D:145:ASN:OD1	1.98	0.63
1:B:69:LYS:NZ	1:B:91:GLY:O	2.32	0.62
1:C:38:SER:HB3	1:C:41:LYS:HB2	1.80	0.62
1:C:58:ARG:HD2	1:C:145:ASN:OD1	2.01	0.61
1:C:296:PRO:O	1:C:336:ARG:NH1	2.27	0.61
1:A:21:ILE:HD12	1:A:185:SER:HB2	1.83	0.61
1:A:38:SER:HB3	1:A:41:LYS:HB2	1.82	0.60
1:D:99:ALA:H	1:D:222:ASN:HD22	1.49	0.60
1:D:308:ILE:HG13	1:D:345:LEU:HD21	1.84	0.60
1:C:267:PRO:HB2	1:C:270:LEU:HD22	1.83	0.59
1:A:31:GLN:HE21	1:B:14:LYS:HZ3	1.49	0.59
1:A:36:PRO:HG3	1:A:71:ILE:HD11	1.84	0.59
1:D:336:ARG:HD3	1:D:342:GLU:OE2	2.03	0.59
1:A:308:ILE:HG13	1:A:345:LEU:HD21	1.84	0.59
1:A:296:PRO:O	1:A:336:ARG:NH1	2.27	0.58
1:A:30:GLU:OE2	1:A:62:ARG:NH1	2.36	0.58
2:G:73:ASP:OD2	2:G:76:SER:HB3	2.02	0.58
2:E:155:ARG:HB2	2:E:217:ASP:OD2	2.04	0.58
2:K:232:ASN:HA	2:K:237:LEU:HD22	1.86	0.58
2:E:54:TYR:HA	2:E:74:LYS:HG2	1.85	0.57
2:K:103:ARG:HB3	2:K:173:PHE:CE2	2.41	0.56
1:C:288:THR:HG23	1:C:291:CYS:HB2	1.88	0.56
1:A:-7:ASN:OD1	1:A:-7:ASN:N	2.36	0.56
1:D:36:PRO:HG3	1:D:71:ILE:HD11	1.87	0.56
1:D:288:THR:O	1:D:314:ARG:HA	2.06	0.55
1:A:341:LYS:HB3	1:A:343:GLU:OE1	2.07	0.55
1:C:153:LEU:HD13	1:C:169:LEU:HD23	1.88	0.55
1:A:269:HIS:HE1	1:A:348:SER:HB3	1.70	0.55
1:A:5:VAL:CG1	1:B:1:ASP:HB3	2.37	0.55
2:G:143:GLN:HG3	2:G:240:GLY:HA3	1.88	0.55
1:D:244:PRO:HG3	1:D:262:THR:HG22	1.89	0.55
2:G:103:ARG:HB3	2:G:173:PHE:CE2	2.42	0.55
1:A:14:LYS:NZ	1:B:31:GLN:HE21	2.04	0.54
1:A:331:TYR:HB3	1:A:335:ILE:HB	1.89	0.54
1:C:197:ASP:HB3	1:C:200:TYR:H	1.72	0.54
1:A:5:VAL:HG11	1:B:1:ASP:HB3	1.90	0.54
2:G:177:TYR:HE2	2:G:187:VAL:HG22	1.71	0.54
1:A:182:LYS:HG2	1:B:191:ASN:ND2	2.23	0.54
1:A:93:ILE:HD13	1:A:97:MET:HE1	1.89	0.54
1:A:174:LYS:HD2	1:A:175:GLN:H	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:57:ILE:HG22	1:D:149:ALA:HB3	1.90	0.53
1:A:197:ASP:HB3	1:A:200:TYR:H	1.74	0.53
1:D:340:GLU:OE1	1:D:344:ASN:ND2	2.41	0.53
1:A:269:HIS:CE1	1:A:348:SER:HB3	2.43	0.53
2:I:44:ASP:N	2:I:44:ASP:OD1	2.35	0.53
1:C:241:MET:O	1:C:262:THR:HG23	2.08	0.53
2:K:108:ASP:HB3	2:K:109:TYR:CD2	2.43	0.53
1:A:207:ASN:HD22	3:A:401:NAG:H83	1.74	0.52
1:D:197:ASP:HB3	1:D:200:TYR:H	1.74	0.52
1:C:266:GLY:HA2	1:C:297:SER:OG	2.10	0.52
1:C:57:ILE:HG23	1:C:133:PHE:CE2	2.43	0.52
2:I:108:ASP:HB3	2:I:109:TYR:CD2	2.44	0.52
2:E:98:ARG:NH1	2:E:100:TYR:OH	2.43	0.52
2:K:1:GLU:HA	2:K:109:TYR:CZ	2.45	0.52
1:A:307:LEU:HD22	2:E:30:THR:HG21	1.92	0.52
1:C:181:SER:HB2	1:C:229:HIS:CE1	2.45	0.52
1:D:38:SER:HB3	1:D:41:LYS:HB2	1.91	0.52
1:D:94:LYS:HE3	1:D:98:GLN:H	1.74	0.52
2:K:55:ASN:HB3	2:K:57:MET:HG3	1.91	0.51
1:C:238:GLU:HA	1:C:241:MET:HG3	1.92	0.51
1:B:68:TRP:HA	1:B:71:ILE:HG22	1.92	0.51
1:A:336:ARG:HD3	1:A:342:GLU:OE1	2.11	0.51
1:C:269:HIS:HE1	1:C:348:SER:HB3	1.75	0.51
1:B:90:THR:HB	1:B:135:ILE:HB	1.92	0.51
2:K:19:LYS:HA	2:K:81:MET:O	2.11	0.51
1:C:37:GLU:OE2	1:C:156:GLU:HG2	2.10	0.51
1:B:86:LEU:HD11	1:B:133:PHE:HB2	1.91	0.50
1:B:21:ILE:HD12	1:B:185:SER:HB2	1.93	0.50
1:D:297:SER:OG	1:D:331:TYR:O	2.29	0.50
1:B:327:ASP:HB3	2:G:102:LEU:HB3	1.94	0.50
2:G:150:VAL:HG13	2:G:219:VAL:HG21	1.93	0.50
1:D:68:TRP:HA	1:D:71:ILE:HG22	1.94	0.50
1:A:173:GLU:HG3	1:A:174:LYS:H	1.77	0.49
1:D:55:CYS:SG	1:D:147:ASN:HB3	2.52	0.49
2:E:180:LYS:HD3	2:E:225:ALA:HB2	1.94	0.49
1:A:68:TRP:HA	1:A:71:ILE:HG22	1.93	0.49
1:A:5:VAL:O	1:A:13:LEU:HD12	2.12	0.49
2:I:191:TYR:O	2:I:195:ASN:HB2	2.13	0.49
1:A:57:ILE:HG22	1:A:149:ALA:HB3	1.93	0.49
2:K:180:LYS:HD3	2:K:225:ALA:HB2	1.93	0.49
1:C:94:LYS:HE3	1:C:98:GLN:H	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:65:ASN:HB3	1:C:93:ILE:HD11	1.95	0.49
1:A:68:TRP:O	1:A:72:THR:OG1	2.22	0.49
1:C:93:ILE:HD13	1:C:97:MET:HE1	1.95	0.49
1:D:348:SER:O	1:D:349:LEU:HG	2.13	0.48
2:G:18:VAL:HG12	2:G:86:LEU:HD11	1.95	0.48
1:C:62:ARG:HD3	1:C:218:ILE:HG22	1.95	0.48
1:C:302:THR:HG22	1:C:304:SER:H	1.79	0.48
2:E:232:ASN:HA	2:E:237:LEU:HD22	1.96	0.48
1:D:34:PHE:HB2	1:D:67:MET:HB2	1.95	0.48
1:D:25:VAL:HG13	1:D:218:ILE:HG13	1.95	0.48
2:E:150:VAL:HG22	2:E:154:GLN:HB2	1.96	0.48
1:C:57:ILE:HD11	1:C:68:TRP:CE2	2.48	0.47
1:A:140:THR:OG1	1:A:142:GLU:HG2	2.14	0.47
1:C:192:ARG:HD2	1:C:203:GLU:OE2	2.15	0.47
1:C:68:TRP:HA	1:C:71:ILE:HG22	1.96	0.47
1:D:37:GLU:OE2	1:D:156:GLU:HG2	2.14	0.47
1:D:194:VAL:HG11	1:D:201:TRP:CH2	2.49	0.47
2:K:155:ARG:HB2	2:K:217:ASP:OD2	2.13	0.47
1:A:14:LYS:HD2	1:A:14:LYS:HA	1.71	0.47
1:A:9:LYS:HE2	1:B:-1:ASN:HA	1.96	0.47
2:I:51:ILE:HD11	2:I:72:SER:HB3	1.96	0.47
1:A:238:GLU:HA	1:A:241:MET:HG3	1.97	0.47
2:E:154:GLN:O	2:E:219:VAL:HG12	2.13	0.47
2:G:161:ARG:HD2	2:G:211:ASP:HA	1.95	0.47
1:D:241:MET:O	1:D:262:THR:HA	2.14	0.47
2:E:183:GLN:HG2	2:E:184:PRO:HD2	1.97	0.47
1:A:36:PRO:HG3	1:A:71:ILE:CD1	2.45	0.47
1:A:42:LEU:HD12	1:A:171:LEU:HD11	1.95	0.47
1:A:94:LYS:HE3	1:A:98:GLN:H	1.80	0.47
1:A:229:HIS:CD2	1:B:188:ILE:HD12	2.50	0.46
1:B:57:ILE:HG12	1:B:135:ILE:HG12	1.96	0.46
2:I:98:ARG:O	2:I:98:ARG:HG3	2.15	0.46
1:B:14:LYS:HA	1:B:14:LYS:HD2	1.64	0.46
1:B:331:TYR:HB3	1:B:335:ILE:HB	1.97	0.46
2:I:233:ASN:HA	2:I:238:LEU:HD22	1.98	0.46
1:A:56:GLY:O	1:A:148:ARG:HA	2.16	0.46
1:B:57:ILE:HG22	1:B:149:ALA:HB3	1.96	0.46
1:C:68:TRP:O	1:C:72:THR:OG1	2.23	0.46
1:C:70:GLN:HA	2:G:16:ALA:HB1	1.98	0.46
1:D:204:SER:OG	1:D:254:HIS:HB3	2.15	0.46
1:C:299:ARG:HA	1:C:330:TRP:HA	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:GLN:HG3	2:G:17:SER:H	1.80	0.46
1:B:207:ASN:HB3	1:B:211:LYS:HZ1	1.81	0.46
1:D:281:ASP:OD1	2:K:29:LEU:HD21	2.16	0.45
1:C:-1:ASN:HA	1:D:9:LYS:HE2	1.99	0.45
1:C:21:ILE:HD12	1:C:185:SER:HB2	1.98	0.45
2:I:174:MET:HG2	2:I:213:PHE:CD2	2.50	0.45
1:D:346:VAL:HG13	2:K:169:TYR:CG	2.52	0.45
1:B:181:SER:HA	1:B:184:MET:HG2	1.99	0.45
1:D:192:ARG:HD2	1:D:203:GLU:OE2	2.15	0.45
2:E:103:ARG:HB3	2:E:173:PHE:CE2	2.52	0.45
1:B:153:LEU:HD13	1:B:169:LEU:HD23	1.99	0.45
1:A:0:ALA:HB1	1:A:18:GLY:O	2.17	0.45
1:B:53:GLY:O	1:B:147:ASN:ND2	2.49	0.45
1:C:241:MET:O	1:C:262:THR:HA	2.16	0.45
2:G:143:GLN:OE1	2:G:228:TYR:HA	2.17	0.45
1:D:57:ILE:HG12	1:D:135:ILE:HG12	1.99	0.45
2:K:29:LEU:HA	2:K:54:TYR:HD2	1.82	0.45
1:C:70:GLN:HG3	2:G:16:ALA:HB1	1.99	0.45
1:A:182:LYS:HE3	1:B:191:ASN:ND2	2.32	0.45
1:B:38:SER:HB3	1:B:41:LYS:HB2	1.98	0.45
2:K:177:TYR:CE2	2:K:187:VAL:HG22	2.52	0.45
1:A:106:PRO:HA	1:A:171:LEU:HD22	1.99	0.45
2:I:153:GLY:HA2	2:I:219:PRO:HB2	1.98	0.45
1:C:85:LYS:HG2	1:C:85:LYS:H	1.40	0.44
2:G:88:SER:HA	2:G:118:VAL:HB	1.99	0.44
1:B:241:MET:O	1:B:262:THR:HA	2.18	0.44
1:D:68:TRP:O	1:D:72:THR:OG1	2.27	0.44
1:D:327:ASP:HA	2:K:102:LEU:H	1.82	0.44
2:K:103:ARG:HB3	2:K:173:PHE:CZ	2.53	0.44
1:A:230:THR:HG21	1:A:251:VAL:O	2.17	0.44
1:C:-7:ASN:C	1:C:-5:TYR:H	2.21	0.44
1:C:326:GLU:OE2	2:I:236:ASN:ND2	2.50	0.44
1:D:326:GLU:OE2	2:K:59:LYS:HD3	2.18	0.44
2:E:19:LYS:HA	2:E:81:MET:O	2.18	0.44
2:I:151:SER:HB2	2:I:154:GLN:HG3	2.00	0.44
2:I:84:SER:HB3	2:I:85:SER:H	1.54	0.44
1:C:0:ALA:HB1	1:C:18:GLY:O	2.17	0.44
2:E:67:LYS:NZ	2:E:85:SER:O	2.48	0.44
2:I:37:MET:HE2	2:I:37:MET:HB3	1.63	0.44
2:K:83:LEU:HA	2:K:83:LEU:HD23	1.79	0.44
1:A:241:MET:O	1:A:262:THR:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:THR:O	1:A:314:ARG:HA	2.18	0.44
1:D:298:LEU:HD12	1:D:337:PRO:HD3	2.00	0.44
2:G:37:MET:HB3	2:G:37:MET:HE2	1.62	0.44
2:K:101:LEU:HD23	2:K:101:LEU:HA	1.80	0.44
1:C:230:THR:HG22	1:C:252:SER:HB2	2.00	0.43
1:C:57:ILE:HG12	1:C:135:ILE:HG12	2.01	0.43
1:D:307:LEU:HD22	2:K:30:THR:HG21	1.99	0.43
2:K:202:ARG:HD3	2:K:218:PRO:O	2.18	0.43
1:B:206:LEU:HD13	1:B:210:TRP:CD1	2.53	0.43
2:G:153:GLY:HA2	2:G:218:PRO:HB2	1.99	0.43
2:I:55:ASN:HB3	2:I:57:MET:H	1.83	0.43
1:B:207:ASN:O	1:B:208:ASP:HB2	2.19	0.43
1:B:90:THR:CB	1:B:135:ILE:HB	2.49	0.43
1:C:1:ASP:HB3	1:D:5:VAL:HG11	2.01	0.43
2:I:180:LYS:CD	2:I:226:ALA:HB2	2.46	0.43
2:K:178:GLN:HB2	2:K:188:LEU:HD11	2.01	0.43
1:A:184:MET:H	1:A:184:MET:HG2	1.62	0.43
1:A:260:TYR:OH	1:A:320:PRO:HA	2.18	0.43
1:B:172:LYS:NZ	1:B:176:ASP:OD1	2.41	0.43
2:E:101:LEU:HD23	2:E:101:LEU:HA	1.77	0.43
1:C:8:TRP:O	1:C:11:LYS:HG3	2.19	0.43
1:B:58:ARG:HD2	1:B:145:ASN:OD1	2.18	0.43
2:G:86:LEU:HD23	2:G:86:LEU:HA	1.83	0.43
1:C:340:GLU:HG2	1:C:345:LEU:HD11	2.00	0.43
1:C:75:LEU:O	1:C:79:LEU:HD22	2.19	0.43
1:A:64:GLU:HG2	1:A:68:TRP:HE1	1.84	0.42
1:C:1:ASP:HB3	1:D:5:VAL:CG1	2.49	0.42
2:I:100:TYR:HB2	2:I:104:THR:HB	2.01	0.42
1:B:155:VAL:HG23	1:B:180:ASP:OD2	2.20	0.42
1:B:32:TYR:HB2	1:B:198:MET:HE2	2.01	0.42
2:G:177:TYR:CE2	2:G:187:VAL:HG22	2.52	0.42
1:A:301:THR:HA	1:A:306:LYS:O	2.19	0.42
1:A:327:ASP:HB3	2:E:102:LEU:HB3	2.01	0.42
1:D:79:LEU:HA	1:D:79:LEU:HD12	1.76	0.42
2:G:155:ARG:NE	2:G:217:ASP:OD2	2.45	0.42
1:A:90:THR:HG22	1:A:135:ILE:HB	2.00	0.42
2:E:217:ASP:HA	2:E:218:PRO:HA	1.79	0.42
2:E:233:ASN:O	2:E:234:GLU:HG3	2.19	0.42
2:E:83:LEU:HA	2:E:83:LEU:HD23	1.88	0.42
2:G:232:ASN:HA	2:G:237:LEU:HD22	2.01	0.42
1:C:191:ASN:ND2	1:D:182:LYS:HG2	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:153:GLY:HA2	2:E:218:PRO:HB2	2.02	0.42
1:C:131:GLN:HG2	1:C:131:GLN:H	1.67	0.42
1:B:269:HIS:HE1	1:B:348:SER:HB3	1.84	0.42
1:C:160:PHE:O	1:C:165:THR:HG22	2.20	0.42
1:D:206:LEU:HB2	1:D:210:TRP:CE2	2.54	0.42
2:I:160:CYS:HB2	2:I:176:TRP:CH2	2.55	0.42
1:A:62:ARG:HD3	1:A:218:ILE:HG22	2.01	0.42
1:A:184:MET:HB2	1:A:229:HIS:CD2	2.55	0.42
1:A:32:TYR:CD1	1:A:167:ILE:HD11	2.54	0.41
1:B:140:THR:OG1	1:B:142:GLU:HG2	2.20	0.41
1:D:58:ARG:HG2	1:D:148:ARG:HD2	2.00	0.41
1:D:181:SER:HB2	1:D:229:HIS:CE1	2.55	0.41
2:I:51:ILE:HG13	2:I:58:THR:HG22	2.02	0.41
2:K:217:ASP:HA	2:K:218:PRO:HA	1.85	0.41
1:A:101:LYS:HA	1:A:101:LYS:HD3	1.84	0.41
1:A:-2:SER:O	1:B:9:LYS:NZ	2.34	0.41
1:A:60:VAL:HG22	1:A:150:TRP:CD1	2.54	0.41
1:C:57:ILE:HD13	1:C:57:ILE:HG21	1.62	0.41
2:G:4:LEU:HD12	2:G:4:LEU:HA	1.91	0.41
1:A:9:LYS:CG	1:B:-1:ASN:HA	2.50	0.41
1:C:58:ARG:HG2	1:C:148:ARG:HD2	2.01	0.41
1:D:65:ASN:HB3	1:D:93:ILE:HD11	2.01	0.41
2:E:30:THR:O	2:E:33:PHE:HE1	2.02	0.41
2:G:202:ARG:HD3	2:G:218:PRO:O	2.20	0.41
1:B:293:ASN:O	1:B:336:ARG:HD2	2.21	0.41
1:C:269:HIS:CE1	1:C:348:SER:HB3	2.55	0.41
1:D:237:LEU:HD13	1:D:240:GLU:HG3	2.01	0.41
2:E:108:ASP:HB3	2:E:109:TYR:CD2	2.55	0.41
2:E:150:VAL:O	2:E:247:LEU:HD23	2.21	0.41
2:G:209:ARG:CZ	2:G:209:ARG:HB3	2.51	0.41
2:K:150:VAL:HG22	2:K:154:GLN:HB2	2.02	0.41
1:A:9:LYS:HG2	1:B:-1:ASN:HA	2.02	0.41
1:B:99:ALA:H	1:B:222:ASN:HD22	1.69	0.41
2:I:161:ARG:HD2	2:I:212:ASP:OD1	2.20	0.41
2:I:203:ARG:NH1	2:I:224:ASP:OD1	2.53	0.41
1:D:155:VAL:HG23	1:D:180:ASP:OD2	2.21	0.41
1:D:57:ILE:HD11	1:D:68:TRP:CE2	2.56	0.41
2:I:247:GLU:HG2	2:I:248:LEU:N	2.36	0.41
2:I:86:LEU:HD23	2:I:86:LEU:HA	1.91	0.41
1:C:280:CYS:HB3	1:C:300:THR:HG21	2.03	0.41
2:K:7:SER:HB3	2:K:21:SER:OG	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:VAL:HG13	1:B:218:ILE:HG13	2.02	0.41
1:C:232:TRP:CG	1:D:228:SER:HA	2.56	0.41
2:K:68:ALA:HA	2:K:83:LEU:HD23	2.03	0.41
1:C:331:TYR:HB3	1:C:335:ILE:HB	2.03	0.41
1:C:349:LEU:HA	1:C:349:LEU:HD23	1.76	0.41
1:C:71:ILE:HG21	1:C:71:ILE:HD13	1.74	0.41
1:B:327:ASP:HA	2:G:102:LEU:H	1.85	0.41
1:A:102:ARG:O	1:A:149:ALA:HA	2.21	0.41
1:D:58:ARG:NH1	1:D:137:GLY:O	2.54	0.41
1:D:36:PRO:HG3	1:D:71:ILE:CD1	2.51	0.41
2:K:40:LYS:HB2	2:K:43:GLN:CB	2.50	0.41
2:G:40:LYS:HB2	2:G:43:GLN:CB	2.51	0.41
2:K:221:ALA:HA	2:K:247:LEU:HD11	2.03	0.41
1:A:192:ARG:HD2	1:A:203:GLU:OE2	2.22	0.40
1:D:285:VAL:HG11	1:D:335:ILE:HD12	2.03	0.40
1:B:184:MET:HB2	1:B:229:HIS:CD2	2.55	0.40
1:C:302:THR:HG22	1:C:303:ALA:N	2.35	0.40
2:I:55:ASN:CB	2:I:57:MET:HG3	2.45	0.40
1:C:301:THR:HA	1:C:306:LYS:O	2.22	0.40
1:C:285:VAL:HG22	1:C:311:TRP:HB2	2.04	0.40
2:K:23:LYS:NZ	2:K:24:ALA:O	2.47	0.40
1:A:155:VAL:HG23	1:A:180:ASP:OD2	2.22	0.40
1:A:241:MET:HA	1:A:255:ASN:O	2.21	0.40
1:A:345:LEU:HA	1:A:345:LEU:HD23	1.72	0.40
1:B:181:SER:HA	1:B:184:MET:CG	2.52	0.40
1:D:184:MET:HB2	1:D:229:HIS:CD2	2.56	0.40
2:I:73:ASP:OD2	2:I:76:SER:HB3	2.20	0.40
1:D:345:LEU:HA	1:D:345:LEU:HD23	1.93	0.40

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	321/376 (85%)	306 (95%)	15 (5%)	0	100	100
1	B	322/376 (86%)	308 (96%)	14 (4%)	0	100	100
1	C	329/376 (88%)	308 (94%)	17 (5%)	4 (1%)	13	40
1	D	319/376 (85%)	305 (96%)	14 (4%)	0	100	100
2	E	229/251 (91%)	217 (95%)	11 (5%)	1 (0%)	34	66
2	G	228/251 (91%)	216 (95%)	11 (5%)	1 (0%)	34	66
2	I	228/251 (91%)	215 (94%)	13 (6%)	0	100	100
2	K	228/251 (91%)	214 (94%)	13 (6%)	1 (0%)	34	66
All	All	2204/2508 (88%)	2089 (95%)	108 (5%)	7 (0%)	41	71

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	-3	GLN
1	C	-8	GLU
2	G	84	SER
1	C	94	LYS
2	E	102	LEU
2	K	102	LEU
1	C	350	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	288/331 (87%)	271 (94%)	17 (6%)	19	49
1	B	289/331 (87%)	275 (95%)	14 (5%)	25	58
1	C	289/331 (87%)	275 (95%)	14 (5%)	25	58
1	D	286/331 (86%)	270 (94%)	16 (6%)	21	52
2	E	196/203 (97%)	187 (95%)	9 (5%)	27	60
2	G	196/203 (97%)	186 (95%)	10 (5%)	24	56
2	I	196/203 (97%)	189 (96%)	7 (4%)	35	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	K	196/203 (97%)	185 (94%)	11 (6%)	21	52
All	All	1936/2136 (91%)	1838 (95%)	98 (5%)	24	56

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-7	ASN
1	A	-5	TYR
1	A	-3	GLN
1	A	5	VAL
1	A	58	ARG
1	A	84	VAL
1	A	97	MET
1	A	181	SER
1	A	204	SER
1	A	209	THR
1	A	222	ASN
1	A	246	ASN
1	A	270	LEU
1	A	289	GLU
1	A	294	ARG
1	A	297	SER
1	A	331	TYR
1	B	17	SER
1	B	35	GLN
1	B	51	GLU
1	B	58	ARG
1	B	70	GLN
1	B	79	LEU
1	B	84	VAL
1	B	90	THR
1	B	188	ILE
1	B	204	SER
1	B	221	LYS
1	B	294	ARG
1	B	297	SER
1	B	349	LEU
1	C	9	LYS
1	C	58	ARG
1	C	61	THR
1	C	79	LEU
1	C	83	GLU

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Mol	Chain	Res	Type
1	C	130	ASN
1	C	172	LYS
1	C	204	SER
1	C	209	THR
1	C	222	ASN
1	C	270	LEU
1	C	289	GLU
1	C	294	ARG
1	C	315	SER
1	D	5	VAL
1	D	19	ILE
1	D	58	ARG
1	D	79	LEU
1	D	84	VAL
1	D	90	THR
1	D	97	MET
1	D	131	GLN
1	D	204	SER
1	D	251	VAL
1	D	252	SER
1	D	262	THR
1	D	288	THR
1	D	294	ARG
1	D	306	LYS
1	D	331	TYR
2	E	3	GLN
2	E	4	LEU
2	E	34	MET
2	E	37	MET
2	E	44	ASP
2	E	98	ARG
2	E	103	ARG
2	E	117	THR
2	E	219	VAL
2	G	4	LEU
2	G	13	LYS
2	G	37	MET
2	G	43	GLN
2	G	44	ASP
2	G	81	MET
2	G	98	ARG
2	G	115	THR

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Mol	Chain	Res	Type
2	G	148	LEU
2	G	219	VAL
2	I	4	LEU
2	I	37	MET
2	I	44	ASP
2	I	98	ARG
2	I	142	THR
2	I	196	LEU
2	I	220	VAL
2	K	4	LEU
2	K	37	MET
2	K	44	ASP
2	K	81	MET
2	K	98	ARG
2	K	103	ARG
2	K	108	ASP
2	K	144	SER
2	K	154	GLN
2	K	213	THR
2	K	219	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	70	GLN
1	A	191	ASN
1	A	222	ASN
1	A	246	ASN
1	A	269	HIS
1	B	-1	ASN
1	B	31	GLN
1	B	35	GLN
1	B	70	GLN
1	B	191	ASN
1	B	222	ASN
1	B	269	HIS
1	C	31	GLN
1	C	191	ASN
1	C	222	ASN
1	C	269	HIS
1	D	-1	ASN

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Mol	Chain	Res	Type
1	D	131	GLN
1	D	222	ASN
1	D	269	HIS
2	E	39	GLN
2	E	179	GLN
2	K	154	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 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	$\# Z > 2$
3	NAG	B	401	1	14,14,15	0.83	1 (7%)	17,19,21	0.46	0
3	NAG	A	401	1	14,14,15	0.37	0	17,19,21	0.61	1 (5%)
3	NAG	D	401	1	14,14,15	0.96	2 (14%)	17,19,21	0.72	0
3	NAG	C	401	1	14,14,15	0.88	1 (7%)	17,19,21	0.66	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
3	NAG	B	401	1	-	2/6/23/26	0/1/1/1
3	NAG	A	401	1	-	4/6/23/26	0/1/1/1
3	NAG	D	401	1	-	1/6/23/26	0/1/1/1
3	NAG	C	401	1	-	3/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	NAG	O5-C1	2.77	1.48	1.43
3	C	401	NAG	O5-C1	2.76	1.48	1.43
3	D	401	NAG	C1-C2	2.54	1.56	1.52
3	D	401	NAG	O5-C1	2.42	1.47	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	401	NAG	C1-O5-C5	2.27	115.27	112.19
3	A	401	NAG	C1-O5-C5	2.05	114.97	112.19

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	401	NAG	O5-C5-C6-O6
3	A	401	NAG	O5-C5-C6-O6
3	A	401	NAG	C8-C7-N2-C2
3	A	401	NAG	O7-C7-N2-C2
3	C	401	NAG	C8-C7-N2-C2
3	C	401	NAG	O7-C7-N2-C2
3	A	401	NAG	C4-C5-C6-O6
3	B	401	NAG	C4-C5-C6-O6
3	C	401	NAG	O5-C5-C6-O6
3	D	401	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	NAG	1	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	327/376 (86%)	0.73	36 (11%) 5 4	64, 90, 155, 173	0
1	B	328/376 (87%)	0.39	16 (4%) 29 26	67, 82, 114, 125	0
1	C	335/376 (89%)	0.22	7 (2%) 63 61	55, 66, 94, 115	0
1	D	325/376 (86%)	0.41	15 (4%) 32 29	57, 81, 107, 122	0
2	E	233/251 (92%)	0.21	2 (0%) 84 84	68, 85, 110, 120	0
2	G	232/251 (92%)	0.17	2 (0%) 84 84	64, 78, 90, 99	0
2	I	232/251 (92%)	0.48	14 (6%) 21 18	66, 81, 131, 152	0
2	K	232/251 (92%)	0.23	3 (1%) 77 77	67, 83, 105, 119	0
All	All	2244/2508 (89%)	0.37	95 (4%) 36 32	55, 80, 123, 173	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	134	LEU	7.0
1	D	160	PHE	6.7
1	C	8	TRP	6.6
1	B	8	TRP	5.6
1	A	142	GLU	5.5
1	A	28	TRP	5.3
1	A	105	ARG	5.2
1	D	8	TRP	4.4
1	A	78	ILE	4.4
1	A	8	TRP	4.3
1	A	106	PRO	4.3
1	A	57	ILE	4.2
1	A	88	ILE	4.1
1	A	54	ILE	4.0
1	D	142	GLU	4.0
1	A	132	THR	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	-5	TYR	3.8
1	A	24	ASN	3.8
1	C	28	TRP	3.7
1	A	87	THR	3.7
1	A	149	ALA	3.6
1	D	82	ASN	3.6
1	A	175	GLN	3.6
1	B	87	THR	3.6
1	D	28	TRP	3.5
1	D	314	ARG	3.5
1	A	82	ASN	3.4
1	A	73	PRO	3.3
1	D	78	ILE	3.3
1	A	143	CYS	3.3
1	A	133	PHE	3.3
2	I	217	ILE	3.2
1	B	134	LEU	3.2
1	A	104	LEU	3.1
1	A	144	PRO	3.1
1	A	141	ALA	3.1
2	I	144	SER	3.0
2	I	158	ILE	2.9
2	G	120	SER	2.9
1	A	56	GLY	2.9
2	I	249	LYS	2.9
2	G	20	MET	2.9
1	A	86	LEU	2.8
1	C	173	GLU	2.8
1	D	83	GLU	2.8
1	B	88	ILE	2.8
1	D	89	MET	2.8
1	C	-9	THR	2.7
2	E	248	LYS	2.7
1	A	173	GLU	2.6
2	I	196	LEU	2.6
1	A	85	LYS	2.6
1	A	103	SER	2.6
2	I	157	THR	2.6
2	K	195	LEU	2.6
1	B	68	TRP	2.5
1	B	42	LEU	2.5
1	A	89	MET	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	191	ASN	2.5
1	B	46	ILE	2.5
1	D	168	TRP	2.4
1	D	289	GLU	2.4
1	A	140	THR	2.4
1	C	9	LYS	2.4
1	D	173	GLU	2.4
1	B	86	LEU	2.4
2	I	150	VAL	2.3
2	I	156	ALA	2.3
2	K	227	TYR	2.3
1	B	90	THR	2.3
1	A	153	LEU	2.3
1	B	43	ALA	2.3
1	B	75	LEU	2.3
1	B	78	ILE	2.2
1	D	74	GLU	2.2
1	D	133	PHE	2.2
1	B	326	GLU	2.2
2	I	112	GLN	2.1
1	A	75	LEU	2.1
1	A	71	ILE	2.1
1	D	86	LEU	2.1
1	C	351	THR	2.1
1	A	37	GLU	2.1
1	B	104	LEU	2.1
2	I	228	TYR	2.1
1	B	28	TRP	2.1
1	A	47	GLN	2.0
2	I	34	MET	2.0
1	A	191	ASN	2.0
2	I	145	PRO	2.0
1	B	135	ILE	2.0
2	K	244	LYS	2.0
2	E	70	LEU	2.0
2	I	188	LEU	2.0
2	I	215	LEU	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 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
3	NAG	C	401	14/15	0.83	0.16	89,89,89,89	0
3	NAG	A	401	14/15	0.85	0.14	91,91,91,91	0
3	NAG	B	401	14/15	0.90	0.12	91,91,91,91	0
3	NAG	D	401	14/15	0.91	0.17	87,87,87,87	0

6.5 Other polymers [i](#)

There are no such residues in this entry.