



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 15, 2020 – 11:24 PM EST

PDB ID : 6WER  
Title : DENV2 NS1 in complex with neutralizing 2B7 Fab fragment  
Authors : Akey, D.L.; Smith, J.L.  
Deposited on : 2020-04-02  
Resolution : 3.96 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](mailto: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.

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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

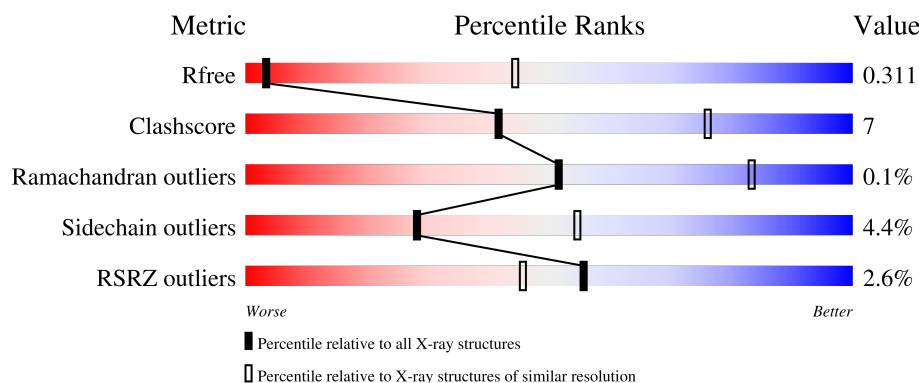
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.96 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	1025 (4.22-3.70)
Clashscore	141614	1085 (4.22-3.70)
Ramachandran outliers	138981	1047 (4.22-3.70)
Sidechain outliers	138945	1039 (4.22-3.70)
RSRZ outliers	127900	1013 (4.28-3.64)

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  $\geq 3$ , 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>2%</div> <div>66%</div> <div>19%</div> <div>14%</div> </div>
1	B	376	<div> <div>0%</div> <div>70%</div> <div>15%</div> <div>14%</div> </div>
2	C	268	<div> <div>0%</div> <div>64%</div> <div>16%</div> <div>20%</div> </div>
2	E	268	<div> <div>5%</div> <div>61%</div> <div>18%</div> <div>20%</div> </div>
3	D	238	<div> <div>0%</div> <div>72%</div> <div>16%</div> <div>10%</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	238	<div><div></div><div>3%</div><div>73%</div><div>16%</div><div>• 10%</div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11710 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	322	Total	C	N	O	S	0	0	0
			2563	1611	444	488	20			
1	B	324	Total	C	N	O	S	0	0	0
			2573	1619	445	489	20			

There are 46 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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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

- Molecule 2 is a protein called 2B7 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	215	Total	C	N	O	S	0	0	0
			1612	1016	258	325	13			
2	E	215	Total	C	N	O	S	0	0	0
			1612	1016	258	325	13			

- Molecule 3 is a protein called 2B7 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	215	Total	C	N	O	S	0	0	0
			1661	1035	281	339	6			
3	F	215	Total	C	N	O	S	0	0	0
			1661	1035	281	339	6			

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

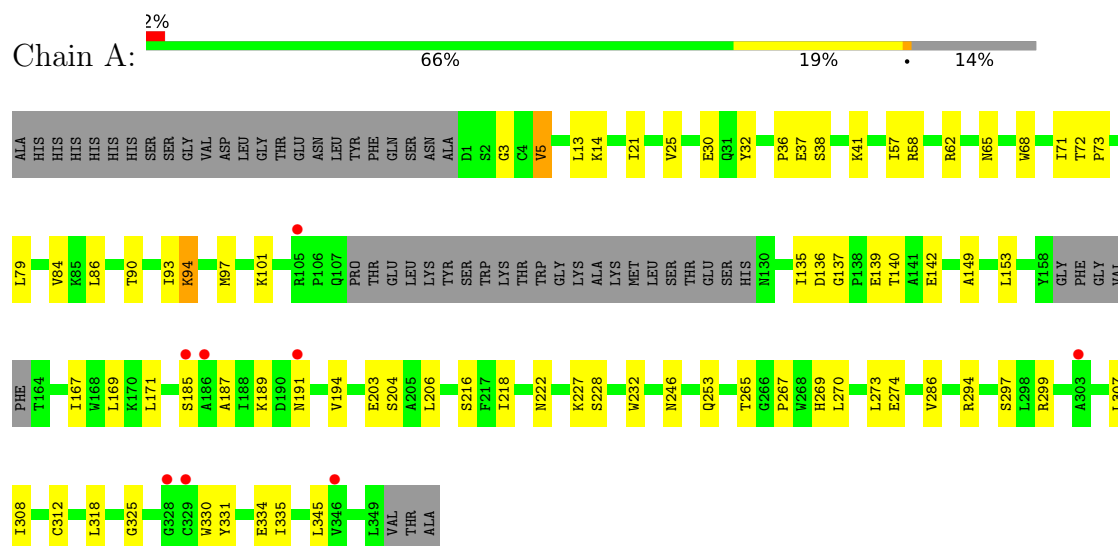


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

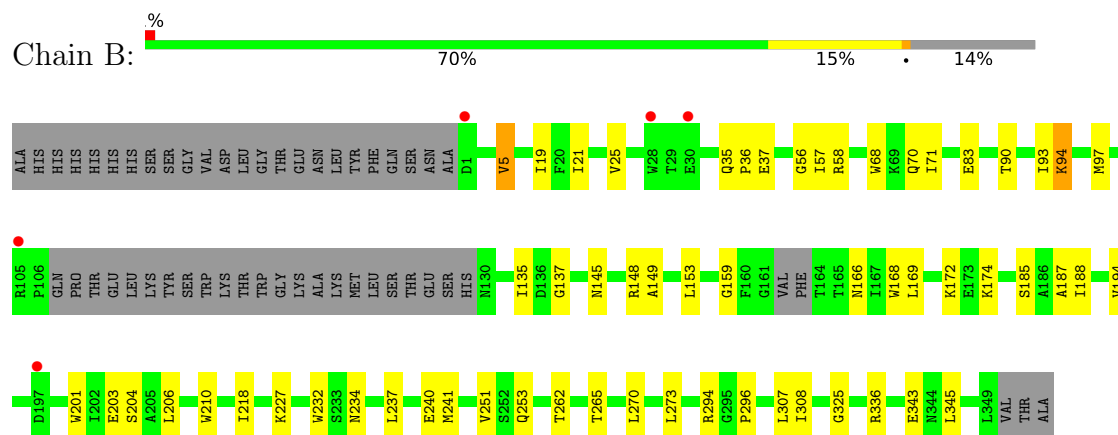
### 3 Residue-property plots [i](#)

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.

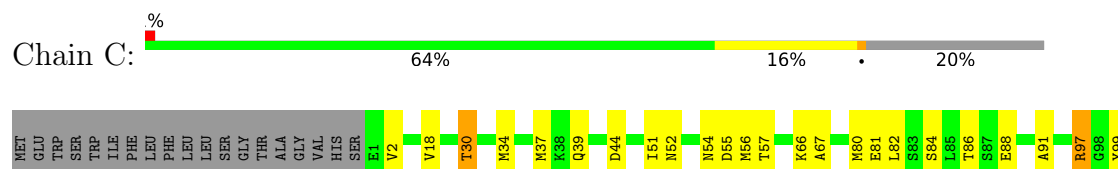
#### • Molecule 1: Non-structural protein 1



#### • Molecule 1: Non-structural protein 1



#### • Molecule 2: 2B7 Fab heavy chain







## 4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	148.47Å 148.47Å 517.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.80 – 3.96 29.80 – 3.96	Depositor EDS
% Data completeness (in resolution range)	99.1 (29.80-3.96) 83.5 (29.80-3.96)	Depositor EDS
$R_{merge}$	0.22	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.62 (at 3.98Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.276 , 0.311 0.274 , 0.311	Depositor DCC
$R_{free}$ test set	1277 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	158.6	Xtriage
Anisotropy	0.474	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 155.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	11710	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	252.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.10% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.26	0/2622	0.50	0/3551
1	B	0.26	0/2633	0.48	0/3565
2	C	0.26	0/1652	0.46	0/2251
2	E	0.26	0/1652	0.49	0/2251
3	D	0.26	0/1699	0.48	0/2312
3	F	0.26	0/1699	0.48	0/2312
All	All	0.26	0/11957	0.48	0/16242

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

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	2563	0	2496	43	0
1	B	2573	0	2503	36	0
2	C	1612	0	1560	22	1
2	E	1612	0	1560	28	0
3	D	1661	0	1590	23	2
3	F	1661	0	1590	22	0
4	A	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	14	0	13	0	0
All	All	11710	0	11325	160	2

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 7.

All (160) 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)
2:C:129:PRO:HD3	2:C:214:LYS:HE2	1.68	0.75
1:A:307:LEU:HD22	2:C:30:THR:HG21	1.70	0.74
2:E:97:ARG:NH1	2:E:99:TYR:OH	2.27	0.67
2:C:125:PRO:HB3	2:C:151:TYR:HB3	1.77	0.67
3:D:2:ILE:HG12	3:D:27:GLU:HB3	1.77	0.67
2:E:104:GLY:O	3:F:95:ASN:ND2	2.29	0.66
1:A:58:ARG:NH1	1:A:137:GLY:O	2.30	0.64
1:A:191:ASN:HB3	1:A:206:LEU:HB3	1.79	0.64
1:B:21:ILE:HD12	1:B:185:SER:HB2	1.80	0.64
1:B:237:LEU:HD13	1:B:240:GLU:HG3	1.80	0.63
3:D:46:GLN:HG2	3:D:47:PRO:HD2	1.80	0.63
3:F:2:ILE:HG12	3:F:27:GLU:HB3	1.78	0.63
1:B:194:VAL:HG22	1:B:203:GLU:HG2	1.80	0.63
1:A:90:THR:HG22	1:A:135:ILE:HB	1.81	0.63
1:A:79:LEU:HG	1:A:84:VAL:HG13	1.81	0.62
3:D:186:THR:OG1	3:D:189:GLU:OE2	2.17	0.61
1:A:30:GLU:OE2	1:A:62:ARG:NH1	2.33	0.61
1:A:68:TRP:HA	1:A:71:ILE:HG22	1.83	0.60
1:B:36:PRO:HG3	1:B:71:ILE:HD12	1.83	0.60
3:F:187:LYS:NZ	3:F:191:GLU:OE2	2.30	0.60
2:C:2:VAL:HB	2:C:108:TYR:HD2	1.66	0.60
2:E:125:PRO:HB3	2:E:151:TYR:HB3	1.82	0.60
1:A:331:TYR:HB3	1:A:335:ILE:HB	1.84	0.59
1:A:21:ILE:HD12	1:A:185:SER:HB2	1.84	0.59
3:F:16:GLY:HA2	3:F:81:PRO:HB2	1.85	0.59
2:E:54:ASN:HB3	2:E:56:MET:HG3	1.84	0.58
3:F:46:GLN:HG2	3:F:47:PRO:HD2	1.84	0.58
2:C:97:ARG:NH1	2:C:99:TYR:OH	2.37	0.58
1:B:296:PRO:O	1:B:336:ARG:NH1	2.23	0.58
1:A:194:VAL:HG22	1:A:203:GLU:HG2	1.86	0.57
2:C:54:ASN:HB3	2:C:56:MET:HG3	1.86	0.57
3:F:199:GLU:HG2	3:F:210:VAL:HG22	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:270:LEU:HD13	1:B:325:GLY:HA3	1.87	0.56
3:F:186:THR:OG1	3:F:189:GLU:OE2	2.24	0.56
3:D:153:LYS:HB2	3:D:197:THR:HB	1.87	0.55
1:B:307:LEU:HD13	2:E:30:THR:HG21	1.89	0.55
1:A:21:ILE:HG13	1:A:187:ALA:HB2	1.89	0.55
1:B:90:THR:HG22	1:B:135:ILE:HB	1.88	0.55
2:E:2:VAL:HB	2:E:108:TYR:HD2	1.71	0.55
1:B:21:ILE:HG13	1:B:187:ALA:HB2	1.87	0.54
2:E:75:SER:OG	2:E:77:THR:OG1	2.25	0.54
1:B:68:TRP:HA	1:B:71:ILE:HG22	1.90	0.54
3:D:199:GLU:HG2	3:D:210:VAL:HG22	1.89	0.54
3:F:153:LYS:HB2	3:F:197:THR:HB	1.90	0.54
1:B:25:VAL:HG13	1:B:218:ILE:HG13	1.91	0.53
1:B:343:GLU:OE1	1:B:343:GLU:N	2.41	0.53
1:B:93:ILE:HD13	1:B:97:MET:HE1	1.89	0.53
2:C:66:LYS:NZ	2:C:84:SER:O	2.38	0.53
1:A:153:LEU:HD13	1:A:169:LEU:HD23	1.92	0.52
3:F:127:GLU:OE1	3:F:127:GLU:N	2.42	0.52
2:C:102:ARG:HB3	3:D:36:PHE:CZ	2.45	0.52
1:B:57:ILE:HG22	1:B:149:ALA:HB3	1.92	0.51
1:A:228:SER:HA	1:B:232:TRP:CG	2.46	0.51
1:A:270:LEU:HD23	1:A:325:GLY:HA3	1.92	0.50
3:D:16:GLY:HA2	3:D:81:PRO:HB2	1.92	0.50
1:B:159:GLY:HA3	1:B:166:ASN:HB2	1.93	0.50
3:D:53:TYR:O	3:D:57:ASN:HB2	2.12	0.50
1:A:38:SER:HB3	1:A:41:LYS:HB2	1.94	0.49
1:A:57:ILE:HG22	1:A:149:ALA:HB3	1.94	0.49
2:E:174:ALA:HA	2:E:183:MET:HB3	1.93	0.49
1:B:206:LEU:HB2	1:B:210:TRP:CE2	2.48	0.49
2:E:52(A):PRO:HA	2:E:71:SER:HB2	1.95	0.49
2:C:154:GLU:HG2	2:C:155:SER:HB3	1.94	0.48
1:A:189:LYS:HD3	1:B:21:ILE:HD13	1.95	0.48
1:A:3:GLY:HA3	1:B:5:VAL:HA	1.94	0.48
2:C:170:HIS:CE1	3:D:178:SER:HG	2.31	0.48
3:D:127:GLU:OE1	3:D:127:GLU:N	2.44	0.48
1:B:153:LEU:HD13	1:B:169:LEU:HD23	1.95	0.48
3:D:123:PRO:HB3	3:D:213:PHE:CE2	2.49	0.48
1:B:308:ILE:HG13	1:B:345:LEU:HD11	1.94	0.48
2:C:51:ILE:HG13	2:C:57:THR:HG22	1.97	0.47
2:E:154:GLU:HG2	2:E:155:SER:HB3	1.96	0.47
2:E:51:ILE:HG13	2:E:57:THR:HG22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:138:CYS:HB2	3:F:152:TRP:CZ2	2.50	0.47
2:E:12:VAL:HG21	2:E:18:VAL:HB	1.95	0.47
1:A:5:VAL:O	1:A:13:LEU:HD12	2.15	0.47
2:C:67:ALA:HA	2:C:81:GLU:O	2.14	0.47
2:E:29:LEU:HA	2:E:53:TYR:CD2	2.50	0.47
1:A:232:TRP:CD2	1:A:253:GLN:HB2	2.50	0.47
3:D:112:ARG:HD3	3:D:113:ALA:O	2.15	0.47
1:B:227:LYS:HE2	1:B:251:VAL:HG11	1.97	0.46
1:A:299:ARG:HA	1:A:330:TRP:HA	1.97	0.46
3:F:53:TYR:O	3:F:57:ASN:HB2	2.15	0.46
2:E:99:TYR:CD1	2:E:104:GLY:HA3	2.51	0.46
1:B:57:ILE:HG12	1:B:135:ILE:HG12	1.98	0.46
1:A:140:THR:OG1	1:A:142:GLU:HG2	2.16	0.46
1:B:232:TRP:CD2	1:B:253:GLN:HB2	2.51	0.46
3:D:138:CYS:HB2	3:D:152:TRP:CZ2	2.51	0.46
3:D:144:TYR:CD1	3:D:145:PRO:HA	2.51	0.46
1:B:194:VAL:HG11	1:B:201:TRP:CH2	2.51	0.46
3:F:124:PRO:HD3	3:F:136:VAL:HG22	1.97	0.46
1:A:25:VAL:HG13	1:A:218:ILE:HG12	1.98	0.45
3:D:124:PRO:HD3	3:D:136:VAL:HG22	1.98	0.45
2:E:67:ALA:HA	2:E:81:GLU:O	2.17	0.45
3:F:112:ARG:HD3	3:F:113:ALA:O	2.17	0.45
1:A:228:SER:HA	1:B:232:TRP:CD2	2.51	0.45
3:F:123:PRO:HB3	3:F:213:PHE:CE2	2.52	0.45
1:A:41:LYS:HB3	1:A:171:LEU:HD21	1.98	0.45
2:E:50:TYR:CE2	2:E:58:LYS:HB3	2.52	0.45
1:A:216:SER:OG	1:A:274:GLU:OE2	2.28	0.45
1:B:56:GLY:O	1:B:148:ARG:HA	2.18	0.44
3:D:202:HIS:CD2	3:D:203:LYS:H	2.36	0.44
2:E:52:ASN:HB3	2:E:54:ASN:HB2	1.99	0.44
2:E:2:VAL:HG21	2:E:97:ARG:NH2	2.32	0.44
1:A:308:ILE:HG13	1:A:345:LEU:HD21	1.99	0.44
2:C:18:VAL:O	2:C:81:GLU:HA	2.17	0.44
1:A:36:PRO:HG3	1:A:71:ILE:CD1	2.47	0.44
3:F:35:SER:HB2	3:F:55:ALA:HB2	1.99	0.44
2:C:174:ALA:HA	2:C:183:MET:HB3	1.99	0.44
2:E:18:VAL:HG12	2:E:85:LEU:HD11	1.99	0.44
2:C:154:GLU:HA	2:C:155:SER:HA	1.71	0.44
2:E:154:GLU:HA	2:E:155:SER:HA	1.72	0.44
2:E:23:LYS:HG2	2:E:77:THR:OG1	2.18	0.44
2:C:52:ASN:HB3	2:C:54:ASN:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:170:HIS:HD2	3:F:178:SER:OG	2.01	0.43
1:A:286:VAL:O	1:A:312:CYS:HA	2.18	0.43
1:B:241:MET:O	1:B:262:THR:HA	2.18	0.43
2:C:109:TRP:HB2	3:D:47:PRO:HB2	2.00	0.43
1:A:101:LYS:HD3	1:A:101:LYS:HA	1.73	0.43
3:F:23:CYS:HB2	3:F:39:TRP:CH2	2.54	0.43
2:E:86:THR:HG23	2:E:88:GLU:H	1.84	0.43
2:E:39:GLN:O	2:E:91:ALA:HB1	2.18	0.43
1:A:93:ILE:HD13	1:A:97:MET:HE1	2.01	0.43
1:B:58:ARG:NH1	1:B:137:GLY:O	2.51	0.43
1:B:37:GLU:HG3	1:B:168:TRP:HB3	2.01	0.43
3:F:163:VAL:O	3:F:164:LEU:HD23	2.19	0.43
2:E:70:THR:OG1	2:E:79:PHE:HB2	2.19	0.43
1:A:269:HIS:HE2	3:D:32:TYR:HE1	1.67	0.42
3:F:179:MET:HE3	3:F:179:MET:HB2	1.97	0.42
1:A:32:TYR:CD1	1:A:167:ILE:HD11	2.54	0.42
1:B:58:ARG:HD2	1:B:145:ASN:OD1	2.18	0.42
2:C:158:VAL:HG22	2:C:203:VAL:HG22	2.01	0.42
3:F:188:ASP:HB3	3:F:192:ARG:NH2	2.34	0.42
3:D:80:ASP:HA	3:D:81:PRO:HA	1.76	0.42
2:C:194:TRP:CG	2:C:195:PRO:HA	2.55	0.42
2:C:86:THR:HG23	2:C:88:GLU:H	1.85	0.42
1:A:65:ASN:ND2	1:A:136:ASP:OD2	2.38	0.41
1:B:145:ASN:HA	1:B:148:ARG:HG3	2.02	0.41
1:A:267:PRO:HB2	1:A:270:LEU:HD13	2.02	0.41
1:A:14:LYS:HA	1:A:14:LYS:HD2	1.77	0.41
1:A:79:LEU:HG	1:A:84:VAL:CG1	2.49	0.41
3:F:15:LEU:HD12	3:F:111:LYS:O	2.20	0.41
1:A:72:THR:N	1:A:73:PRO:HD2	2.36	0.41
3:D:135:SER:HA	3:D:183:LEU:O	2.21	0.41
3:D:42:GLN:O	3:D:88:ALA:HB1	2.20	0.41
1:B:174:LYS:HD2	1:B:174:LYS:HA	1.78	0.41
1:B:206:LEU:HD13	1:B:210:TRP:CD1	2.56	0.41
2:E:172:PHE:HA	2:E:173:PRO:HD3	1.96	0.41
1:A:94:LYS:NZ	1:A:139:GLU:OE2	2.54	0.41
2:C:82:LEU:HD23	2:C:82:LEU:HA	1.93	0.41
2:C:39:GLN:O	2:C:91:ALA:HB1	2.21	0.41
3:F:191:GLU:HG2	3:F:215:ARG:HH12	1.85	0.41
1:A:345:LEU:HA	1:A:345:LEU:HD23	1.82	0.40
1:A:227:LYS:HD2	1:B:234:ASN:CG	2.41	0.40
3:D:163:VAL:O	3:D:164:LEU:HD23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:LEU:HD23	1:A:86:LEU:O	2.21	0.40
1:B:93:ILE:HG22	1:B:94:LYS:O	2.22	0.40
1:A:269:HIS:NE2	3:D:32:TYR:HE1	2.19	0.40
2:E:12:VAL:O	2:E:117:VAL:HA	2.21	0.40
2:E:152:PHE:HA	2:E:153:PRO:HA	1.91	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:86:THR:OG1	3:D:160:GLN:OE1[8_555]	2.18	0.02
3:D:18:ARG:NH1	3:D:71:SER:OG[15_555]	2.19	0.01

## 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	316/376 (84%)	301 (95%)	14 (4%)	1 (0%)	41	74
1	B	318/376 (85%)	299 (94%)	18 (6%)	1 (0%)	41	74
2	C	209/268 (78%)	195 (93%)	14 (7%)	0	100	100
2	E	209/268 (78%)	196 (94%)	13 (6%)	0	100	100
3	D	213/238 (90%)	206 (97%)	7 (3%)	0	100	100
3	F	213/238 (90%)	207 (97%)	6 (3%)	0	100	100
All	All	1478/1764 (84%)	1404 (95%)	72 (5%)	2 (0%)	51	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	94	LYS
1	B	94	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	286/331 (86%)	275 (96%)	11 (4%)	33	58
1	B	286/331 (86%)	275 (96%)	11 (4%)	33	58
2	C	187/233 (80%)	176 (94%)	11 (6%)	19	47
2	E	187/233 (80%)	176 (94%)	11 (6%)	19	47
3	D	188/209 (90%)	181 (96%)	7 (4%)	34	59
3	F	188/209 (90%)	181 (96%)	7 (4%)	34	59
All	All	1322/1546 (86%)	1264 (96%)	58 (4%)	28	54

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	VAL
1	A	37	GLU
1	A	204	SER
1	A	222	ASN
1	A	246	ASN
1	A	265	THR
1	A	273	LEU
1	A	294	ARG
1	A	297	SER
1	A	318	LEU
1	A	334	GLU
1	B	5	VAL
1	B	19	ILE
1	B	35	GLN
1	B	70	GLN
1	B	83	GLU
1	B	172	LYS
1	B	188	ILE
1	B	204	SER
1	B	265	THR
1	B	273	LEU
1	B	294	ARG

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Mol	Chain	Res	Type
2	C	30	THR
2	C	34	MET
2	C	37	MET
2	C	44	ASP
2	C	55	ASP
2	C	80	MET
2	C	97	ARG
2	C	116	THR
2	C	193	THR
2	C	201	CYS
2	C	211	THR
3	D	54	LEU
3	D	112	ARG
3	D	179	MET
3	D	183	LEU
3	D	186	THR
3	D	189	GLU
3	D	204	THR
2	E	30	THR
2	E	34	MET
2	E	37	MET
2	E	44	ASP
2	E	55	ASP
2	E	97	ARG
2	E	116	THR
2	E	170	HIS
2	E	193	THR
2	E	201	CYS
2	E	211	THR
3	F	54	LEU
3	F	112	ARG
3	F	179	MET
3	F	183	LEU
3	F	186	THR
3	F	189	GLU
3	F	204	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	35	GLN
1	B	70	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

2 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	401	1	14,14,15	0.31	0	17,19,21	0.45	0
4	NAG	B	401	1	14,14,15	0.34	0	17,19,21	0.49	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	A	401	1	-	2/6/23/26	0/1/1/1
4	NAG	B	401	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	401	NAG	C8-C7-N2-C2
4	A	401	NAG	O7-C7-N2-C2
4	B	401	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	322/376 (85%)	-0.12	8 (2%) 57 47	200, 224, 273, 339	0
1	B	324/376 (86%)	-0.17	5 (1%) 73 64	212, 245, 302, 385	0
2	C	215/268 (80%)	-0.02	3 (1%) 75 66	202, 246, 286, 295	0
2	E	215/268 (80%)	0.26	14 (6%) 18 15	237, 292, 330, 354	0
3	D	215/238 (90%)	-0.22	2 (0%) 84 77	201, 234, 282, 292	0
3	F	215/238 (90%)	0.04	7 (3%) 46 37	234, 270, 327, 336	0
All	All	1506/1764 (85%)	-0.05	39 (2%) 56 46	200, 247, 317, 385	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	146	CYS	8.2
3	F	120	SER	4.6
2	E	144	LEU	4.5
2	E	185	SER	3.8
1	A	105	ARG	3.5
2	E	137	THR	3.4
1	B	28	TRP	3.4
2	C	131	ALA	3.1
1	A	185	SER	3.0
2	C	132	PRO	2.9
2	C	146	CYS	2.8
3	F	118	THR	2.8
3	F	146	LYS	2.8
3	F	41	GLN	2.7
2	E	145	GLY	2.6
2	E	131	ALA	2.6
2	E	187	VAL	2.6
3	D	110	LEU	2.6
1	B	1	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	105	ARG	2.5
3	F	138	CYS	2.5
1	A	191	ASN	2.4
3	F	42	GLN	2.4
1	B	197	ASP	2.4
2	E	34	MET	2.4
2	E	219	SER	2.4
2	E	196	SER	2.3
1	A	303	ALA	2.3
3	F	212	SER	2.3
1	A	186	ALA	2.2
3	D	190	TYR	2.2
2	E	167	SER	2.2
1	B	30	GLU	2.2
1	A	346	VAL	2.1
2	E	160	TRP	2.1
2	E	195	PRO	2.1
1	A	328	GLY	2.1
1	A	329	CYS	2.0
2	E	36	TRP	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	B	401	14/15	0.90	0.16	234,234,234,234	0
4	NAG	A	401	14/15	0.93	0.28	243,243,243,243	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.