



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:16 AM UTC

PDB ID : 3P31 / pdb_00003p31
Title : Crystal structure of the NS1 effector domain from influenza A/Vietnam/1203/2004 (H5N1) virus
Authors : Chen, S.; Xiao, Y.B.; Ponnusamy, R.; Hilgenfeld, R.
Deposited on : 2010-10-04
Resolution : 2.45 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

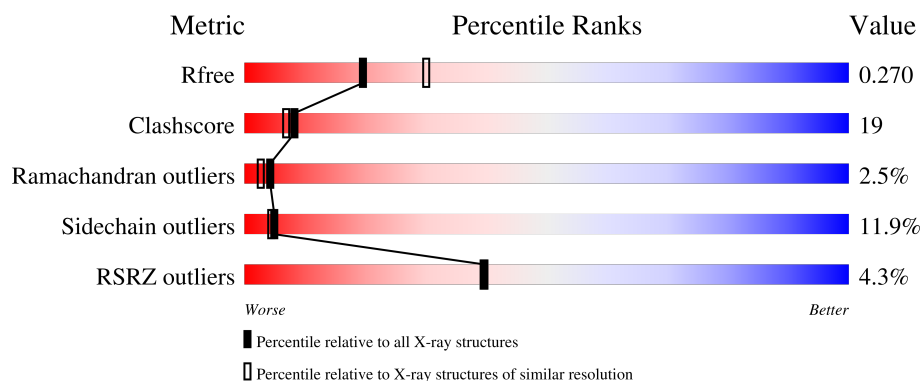
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	147	
1	B	147	
1	C	147	
1	D	147	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3936 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 Nonstructural protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	120	Total	C	N	O	S	0	0	0
			947	606	159	175	7			
1	B	121	Total	C	N	O	S	0	0	0
			955	610	161	177	7			
1	C	122	Total	C	N	O	S	0	0	0
			962	612	162	181	7			
1	D	121	Total	C	N	O	S	0	0	0
			957	609	161	180	7			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	69	GLY	-	expression tag	UNP D1LP63
A	70	PRO	-	expression tag	UNP D1LP63
A	71	LEU	-	expression tag	UNP D1LP63
A	72	GLY	-	expression tag	UNP D1LP63
B	69	GLY	-	expression tag	UNP D1LP63
B	70	PRO	-	expression tag	UNP D1LP63
B	71	LEU	-	expression tag	UNP D1LP63
B	72	GLY	-	expression tag	UNP D1LP63
C	69	GLY	-	expression tag	UNP D1LP63
C	70	PRO	-	expression tag	UNP D1LP63
C	71	LEU	-	expression tag	UNP D1LP63
C	72	GLY	-	expression tag	UNP D1LP63
D	69	GLY	-	expression tag	UNP D1LP63
D	70	PRO	-	expression tag	UNP D1LP63
D	71	LEU	-	expression tag	UNP D1LP63
D	72	GLY	-	expression tag	UNP D1LP63

- Molecule 2 is THIOCYANATE ION (CCD ID: SCN) (formula: CNS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	S	0	0
			3	1	1	1		
2	B	1	Total	C	N	S	0	0
			3	1	1	1		
2	B	1	Total	C	N	S	0	0
			3	1	1	1		
2	B	1	Total	C	N	S	0	0
			3	1	1	1		
2	B	1	Total	C	N	S	0	0
			3	1	1	1		
2	C	1	Total	C	N	S	0	0
			3	1	1	1		
2	D	1	Total	C	N	S	0	0
			3	1	1	1		

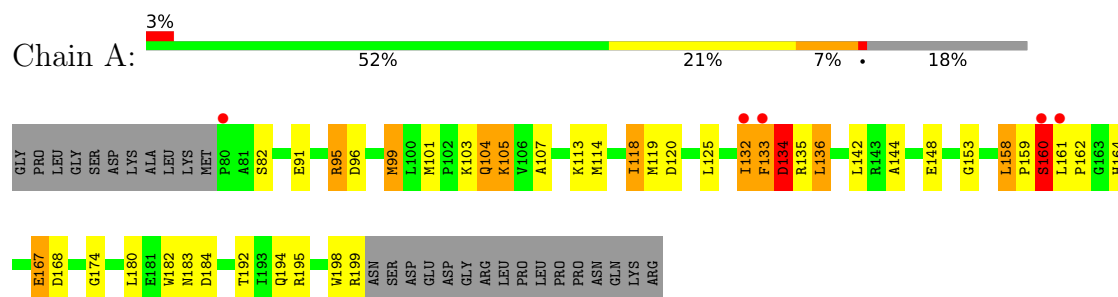
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	21	Total	O	0	0
			21	21		
3	B	22	Total	O	0	0
			22	22		
3	C	36	Total	O	0	0
			36	36		
3	D	12	Total	O	0	0
			12	12		

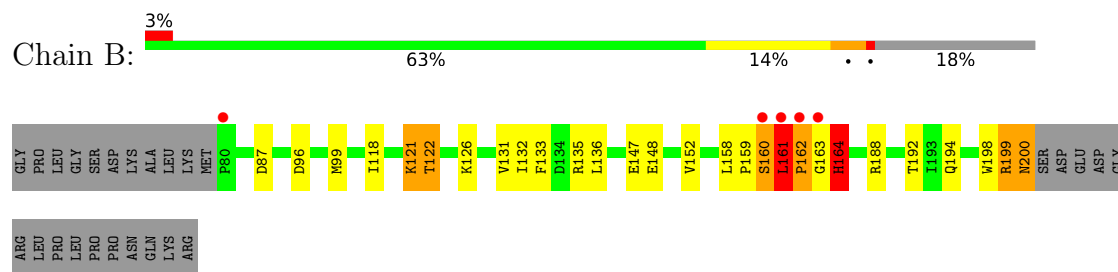
3 Residue-property plots

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.

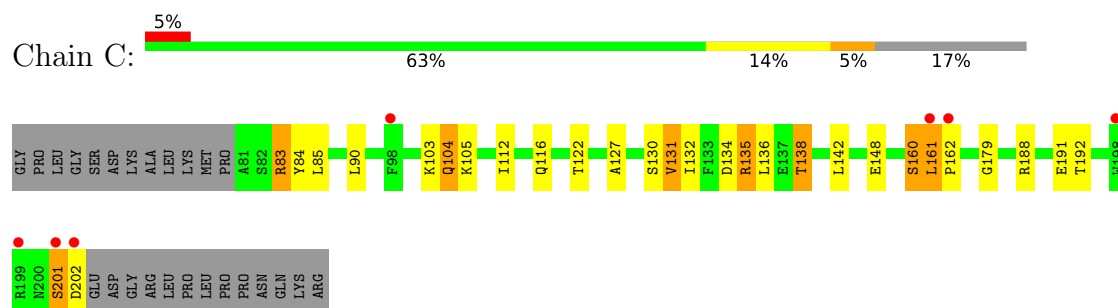
• Molecule 1: Nonstructural protein 1



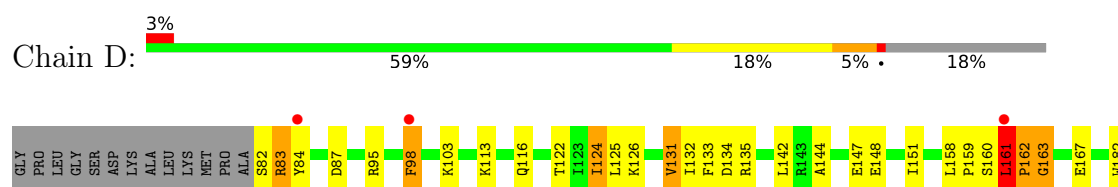
• Molecule 1: Nonstructural protein 1

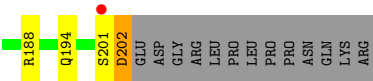


• Molecule 1: Nonstructural protein 1



• Molecule 1: Nonstructural protein 1





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	99.54Å 133.50Å 55.97Å 90.00° 91.38° 90.00°	Depositor
Resolution (Å)	37.63 – 2.45 37.63 – 2.45	Depositor EDS
% Data completeness (in resolution range)	100.0 (37.63-2.45) 99.9 (37.63-2.45)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.68 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.197 , 0.266 0.212 , 0.270	Depositor DCC
R_{free} test set	1351 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	46.0	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 43.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3936	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.43% 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: SCN

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	1.29	2/964 (0.2%)	1.28	4/1303 (0.3%)
1	B	1.19	0/972	1.14	2/1314 (0.2%)
1	C	1.14	0/978	1.09	1/1322 (0.1%)
1	D	1.05	0/973	1.02	0/1315
All	All	1.17	2/3887 (0.1%)	1.14	7/5254 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	101	MET	C-O	-6.29	1.20	1.25
1	A	182	TRP	C-O	-5.07	1.18	1.24

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	134	ASP	N-CA-C	-7.10	102.73	112.03
1	A	160	SER	N-CA-C	5.62	122.78	110.80
1	A	118	ILE	CB-CA-C	5.35	118.11	111.15
1	C	179	GLY	N-CA-C	-5.23	106.08	112.77
1	B	158	LEU	CA-C-N	5.13	124.85	119.82
1	B	158	LEU	C-N-CA	5.13	124.85	119.82
1	A	174	GLY	N-CA-C	-5.04	106.68	112.73

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	947	0	968	39	0
1	B	955	0	974	38	0
1	C	962	0	975	35	0
1	D	957	0	970	43	0
2	A	3	0	0	0	0
2	B	15	0	0	1	0
2	C	3	0	0	0	0
2	D	3	0	0	0	0
3	A	21	0	0	5	0
3	B	22	0	0	2	0
3	C	36	0	0	1	0
3	D	12	0	0	1	0
All	All	3936	0	3887	149	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 19.

All (149) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:LEU:HB3	1:B:162:PRO:CD	1.42	1.47
1:D:83:ARG:HA	1:D:83:ARG:NH1	1.34	1.40
1:D:161:LEU:HB3	1:D:162:PRO:CD	1.51	1.30
1:C:160:SER:O	1:C:162:PRO:HD2	1.46	1.15
1:D:161:LEU:HD12	1:D:162:PRO:HD3	1.23	1.14
1:D:83:ARG:HH11	1:D:83:ARG:CA	1.65	1.10
1:D:161:LEU:CB	1:D:162:PRO:CD	2.30	1.09
1:C:161:LEU:HB3	1:C:162:PRO:HD3	1.35	1.08
1:B:200:ASN:HD22	1:B:200:ASN:C	1.60	1.07
1:D:161:LEU:CB	1:D:162:PRO:HD2	1.85	1.06
1:B:161:LEU:CB	1:B:162:PRO:CD	2.30	1.02
1:B:161:LEU:HB3	1:B:162:PRO:HD3	1.02	1.01
1:D:161:LEU:CD1	1:D:162:PRO:HD3	1.89	1.01
1:B:161:LEU:HB3	1:B:162:PRO:HD2	1.45	0.99
1:B:161:LEU:CB	1:B:162:PRO:HD3	1.90	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:LEU:O	1:B:163:GLY:HA2	1.66	0.95
1:B:163:GLY:O	1:B:164:HIS:HB3	1.66	0.93
1:A:132:ILE:O	1:A:133:PHE:HB2	1.67	0.92
1:D:201:SER:O	1:D:202:ASP:HB3	1.70	0.90
1:D:161:LEU:HB3	1:D:162:PRO:HD2	0.90	0.89
1:A:194:GLN:HG3	3:A:217:HOH:O	1.73	0.86
1:C:83:ARG:HG3	1:C:84:TYR:N	1.89	0.86
1:D:83:ARG:NH1	1:D:83:ARG:CA	2.30	0.86
1:C:160:SER:O	1:C:162:PRO:CD	2.26	0.84
1:B:161:LEU:O	1:B:163:GLY:CA	2.30	0.80
1:C:201:SER:O	1:C:202:ASP:CB	2.30	0.80
1:C:116:GLN:HE22	1:D:103:LYS:HE3	1.46	0.80
1:D:83:ARG:HA	1:D:83:ARG:HH11	0.82	0.78
1:C:161:LEU:CB	1:C:162:PRO:HD3	2.10	0.78
1:C:201:SER:O	1:C:202:ASP:HB2	1.82	0.77
1:B:159:PRO:C	1:B:161:LEU:H	1.92	0.76
1:A:132:ILE:O	1:A:133:PHE:CB	2.34	0.75
1:B:200:ASN:C	1:B:200:ASN:ND2	2.30	0.74
1:B:163:GLY:O	1:B:164:HIS:CB	2.36	0.73
1:B:194:GLN:OE1	1:B:199:ARG:HB3	1.89	0.72
1:C:85:LEU:CD1	1:C:131:VAL:HG13	2.20	0.72
1:A:95:ARG:HD3	1:D:133:PHE:CE1	2.23	0.71
1:D:201:SER:O	1:D:202:ASP:CB	2.39	0.70
1:C:161:LEU:HB3	1:C:162:PRO:CD	2.19	0.69
1:C:103:LYS:HE2	1:D:182:TRP:CE2	2.28	0.68
1:C:83:ARG:HG3	1:C:84:TYR:H	1.55	0.68
1:A:136:LEU:C	1:A:136:LEU:HD23	2.18	0.68
1:B:87:ASP:HB3	1:B:126:LYS:HB3	1.75	0.68
1:A:159:PRO:O	1:A:160:SER:HB3	1.93	0.67
1:C:161:LEU:HG	1:C:162:PRO:N	2.10	0.67
1:D:124:ILE:HD12	1:D:188:ARG:HG3	1.75	0.67
1:D:116:GLN:HG3	3:D:58:HOH:O	1.96	0.66
1:A:99:MET:HE3	1:A:103:LYS:H	1.61	0.65
1:C:160:SER:C	1:C:162:PRO:HD2	2.19	0.65
1:B:161:LEU:O	1:B:163:GLY:N	2.30	0.65
1:D:161:LEU:CB	1:D:162:PRO:HD3	2.24	0.65
1:C:161:LEU:HD12	1:C:161:LEU:C	2.22	0.65
1:A:134:ASP:N	1:A:134:ASP:OD1	2.29	0.65
1:A:82:SER:HB3	1:A:132:ILE:HG23	1.79	0.64
1:C:85:LEU:HD13	1:C:131:VAL:HG13	1.81	0.63
1:B:159:PRO:O	1:B:161:LEU:N	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:LEU:C	1:B:163:GLY:HA2	2.24	0.63
1:A:167:GLU:OE1	1:A:167:GLU:HA	1.98	0.62
1:C:116:GLN:NE2	1:D:103:LYS:HE3	2.13	0.62
1:A:199:ARG:HB3	3:A:217:HOH:O	1.99	0.62
1:C:201:SER:O	1:C:202:ASP:CG	2.43	0.61
1:A:132:ILE:HD11	1:A:135:ARG:NH1	2.17	0.59
2:B:7:SCN:S	2:B:8:SCN:S	3.01	0.59
1:A:104:GLN:OE1	1:A:113:LYS:HE2	2.03	0.59
1:D:131:VAL:HB	1:D:135:ARG:O	2.04	0.58
1:A:105:LYS:HE2	1:A:107:ALA:HB2	1.85	0.58
1:B:199:ARG:O	1:B:200:ASN:CB	2.50	0.57
1:A:167:GLU:OE1	1:A:167:GLU:CA	2.52	0.57
1:A:194:GLN:CG	3:A:217:HOH:O	2.41	0.57
1:B:199:ARG:HG3	3:B:57:HOH:O	2.04	0.57
1:C:85:LEU:HD13	1:C:131:VAL:CG1	2.35	0.57
1:C:135:ARG:HG3	3:C:223:HOH:O	2.03	0.57
1:B:188:ARG:HG2	1:B:188:ARG:HH11	1.68	0.57
1:D:98:PHE:C	1:D:98:PHE:CD2	2.83	0.56
1:A:158:LEU:CD1	3:A:218:HOH:O	2.53	0.56
1:B:122:THR:HG22	1:B:147:GLU:HG2	1.86	0.56
1:D:160:SER:OG	1:D:161:LEU:N	2.37	0.56
1:D:158:LEU:O	1:D:160:SER:N	2.38	0.56
1:B:136:LEU:C	1:B:136:LEU:HD23	2.31	0.55
1:A:161:LEU:HD13	1:A:162:PRO:HD3	1.88	0.54
1:A:194:GLN:CD	3:A:217:HOH:O	2.51	0.54
1:C:103:LYS:HE2	1:D:182:TRP:CD2	2.43	0.53
1:D:160:SER:O	1:D:161:LEU:C	2.52	0.52
1:C:161:LEU:CB	1:C:162:PRO:CD	2.73	0.52
1:D:161:LEU:HD12	1:D:162:PRO:CD	2.16	0.52
1:A:113:LYS:O	1:A:153:GLY:HA2	2.10	0.51
1:B:87:ASP:CB	1:B:126:LYS:HB3	2.40	0.51
1:B:188:ARG:HG2	1:B:188:ARG:NH1	2.26	0.51
1:D:161:LEU:CG	1:D:162:PRO:HD3	2.41	0.51
1:A:198:TRP:O	1:A:199:ARG:HB2	2.11	0.50
1:C:122:THR:HG22	1:C:188:ARG:HH12	1.76	0.50
1:A:91:GLU:OE2	1:A:95:ARG:HG2	2.10	0.50
1:D:83:ARG:HG3	1:D:84:TYR:H	1.77	0.50
1:C:160:SER:O	1:C:161:LEU:C	2.54	0.50
1:B:198:TRP:CZ2	1:B:200:ASN:HB3	2.47	0.50
1:D:98:PHE:C	1:D:98:PHE:HD2	2.19	0.50
1:D:162:PRO:O	1:D:163:GLY:O	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:SER:O	1:C:202:ASP:OD2	2.30	0.49
1:D:142:LEU:C	1:D:142:LEU:HD23	2.36	0.49
1:A:82:SER:CB	1:A:132:ILE:HG23	2.41	0.49
1:B:159:PRO:C	1:B:161:LEU:N	2.61	0.49
1:B:118:ILE:HG13	1:B:152:VAL:CG1	2.41	0.49
1:D:103:LYS:O	1:D:113:LYS:HA	2.13	0.48
1:B:161:LEU:CB	1:B:162:PRO:HD2	2.24	0.48
1:C:130:SER:OG	1:C:138:THR:HB	2.13	0.47
1:A:132:ILE:CD1	1:A:135:ARG:NH1	2.77	0.47
1:C:103:LYS:HG2	1:D:182:TRP:CZ2	2.50	0.47
1:D:82:SER:HA	1:D:131:VAL:O	2.16	0.46
1:A:91:GLU:OE2	1:A:95:ARG:CG	2.63	0.46
1:C:161:LEU:CG	1:C:162:PRO:N	2.71	0.46
1:D:161:LEU:CG	1:D:162:PRO:CD	2.93	0.46
1:D:87:ASP:HB3	1:D:126:LYS:HB3	1.98	0.46
1:D:95:ARG:HD2	1:D:151:ILE:HD12	1.98	0.46
1:D:82:SER:O	1:D:83:ARG:NH1	2.48	0.46
1:A:99:MET:HE3	1:A:103:LYS:N	2.29	0.45
1:A:164:HIS:HA	1:A:168:ASP:OD2	2.15	0.45
1:D:134:ASP:O	1:D:135:ARG:HG2	2.16	0.45
1:A:114:MET:HE3	1:A:180:LEU:HD23	1.98	0.45
1:C:105:LYS:HE3	1:C:105:LYS:HB2	1.67	0.45
1:A:125:LEU:HD22	1:A:144:ALA:HB2	1.99	0.45
1:C:160:SER:C	1:C:162:PRO:CD	2.85	0.44
1:C:160:SER:O	1:C:160:SER:OG	2.35	0.44
1:B:161:LEU:C	1:B:163:GLY:CA	2.89	0.44
1:A:104:GLN:HE21	1:A:104:GLN:HB3	1.50	0.44
1:C:127:ALA:HB2	1:C:142:LEU:HD12	1.99	0.43
1:B:161:LEU:O	1:B:162:PRO:C	2.61	0.43
1:A:119:MET:HG2	1:A:183:ASN:HB3	2.00	0.43
1:A:136:LEU:C	1:A:136:LEU:CD2	2.90	0.43
1:B:121:LYS:HZ2	1:B:121:LYS:HG3	1.71	0.43
1:C:136:LEU:HD23	1:C:136:LEU:C	2.44	0.43
1:B:199:ARG:O	1:B:200:ASN:HB2	2.19	0.43
1:A:132:ILE:O	1:A:132:ILE:HD12	2.19	0.43
1:B:122:THR:HG23	1:B:147:GLU:OE1	2.19	0.42
1:C:188:ARG:HH11	1:C:188:ARG:HG2	1.84	0.42
1:D:124:ILE:HG13	1:D:125:LEU:N	2.33	0.42
1:D:125:LEU:HD22	1:D:144:ALA:HB2	2.01	0.42
1:A:133:PHE:CD1	1:A:133:PHE:N	2.86	0.42
1:C:104:GLN:HA	1:C:112:ILE:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:LEU:C	1:A:142:LEU:HD23	2.45	0.42
1:D:188:ARG:HH11	1:D:188:ARG:HG2	1.85	0.41
1:B:161:LEU:HA	1:B:161:LEU:HD13	1.43	0.41
1:A:136:LEU:HD23	1:A:136:LEU:O	2.21	0.41
1:B:122:THR:CG2	1:B:147:GLU:CG	2.98	0.41
1:B:147:GLU:HG2	3:B:37:HOH:O	2.21	0.41
1:B:160:SER:O	1:B:161:LEU:C	2.63	0.41
1:A:104:GLN:HG2	1:A:113:LYS:HG2	2.03	0.41
1:B:99:MET:HE3	1:B:99:MET:HB2	1.82	0.41
1:A:120:ASP:HA	1:A:184:ASP:O	2.22	0.40
1:A:118:ILE:HD11	1:D:135:ARG:HH21	1.86	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	118/147 (80%)	107 (91%)	9 (8%)	2 (2%)	7	6
1	B	119/147 (81%)	112 (94%)	2 (2%)	5 (4%)	2	0
1	C	120/147 (82%)	112 (93%)	7 (6%)	1 (1%)	16	20
1	D	119/147 (81%)	113 (95%)	2 (2%)	4 (3%)	3	1
All	All	476/588 (81%)	444 (93%)	20 (4%)	12 (2%)	4	3

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	161	LEU
1	B	162	PRO
1	B	164	HIS
1	C	161	LEU

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Mol	Chain	Res	Type
1	D	161	LEU
1	D	163	GLY
1	A	133	PHE
1	A	160	SER
1	B	160	SER
1	D	162	PRO
1	D	159	PRO
1	B	133	PHE

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	104/127 (82%)	91 (88%)	13 (12%)	4	4
1	B	105/127 (83%)	93 (89%)	12 (11%)	5	5
1	C	106/127 (84%)	93 (88%)	13 (12%)	4	4
1	D	106/127 (84%)	94 (89%)	12 (11%)	5	5
All	All	421/508 (83%)	371 (88%)	50 (12%)	5	4

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	ARG
1	A	96	ASP
1	A	99	MET
1	A	104	GLN
1	A	105	LYS
1	A	132	ILE
1	A	134	ASP
1	A	136	LEU
1	A	148	GLU
1	A	158	LEU
1	A	167	GLU
1	A	192	THR
1	A	195	ARG

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Mol	Chain	Res	Type
1	B	96	ASP
1	B	121	LYS
1	B	122	THR
1	B	131	VAL
1	B	132	ILE
1	B	135	ARG
1	B	148	GLU
1	B	161	LEU
1	B	164	HIS
1	B	192	THR
1	B	199	ARG
1	B	200	ASN
1	C	83	ARG
1	C	90	LEU
1	C	104	GLN
1	C	131	VAL
1	C	132	ILE
1	C	134	ASP
1	C	135	ARG
1	C	138	THR
1	C	148	GLU
1	C	160	SER
1	C	191	GLU
1	C	192	THR
1	C	201	SER
1	D	83	ARG
1	D	98	PHE
1	D	122	THR
1	D	124	ILE
1	D	131	VAL
1	D	132	ILE
1	D	147	GLU
1	D	148	GLU
1	D	161	LEU
1	D	167	GLU
1	D	194	GLN
1	D	202	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	GLN

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Mol	Chain	Res	Type
1	A	116	GLN
1	B	200	ASN
1	C	104	GLN
1	C	116	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](#)

8 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	$\# Z > 2$
2	SCN	A	1	-	1,2,2	1.13	0	0,1,1	-	-
2	SCN	B	4	-	1,2,2	0.69	0	0,1,1	-	-
2	SCN	B	5	-	1,2,2	1.06	0	0,1,1	-	-
2	SCN	B	6	-	1,2,2	1.23	0	0,1,1	-	-
2	SCN	D	3	-	1,2,2	0.89	0	0,1,1	-	-
2	SCN	B	8	-	1,2,2	0.68	0	0,1,1	-	-
2	SCN	B	7	-	1,2,2	0.93	0	0,1,1	-	-
2	SCN	C	2	-	1,2,2	0.98	0	0,1,1	-	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	8	SCN	1	0
2	B	7	SCN	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	120/147 (81%)	-0.03	5 (4%)	40	40	26, 46, 90, 120	0
1	B	121/147 (82%)	-0.06	5 (4%)	41	41	26, 46, 73, 105	0
1	C	122/147 (82%)	-0.16	7 (5%)	29	26	25, 42, 76, 105	0
1	D	121/147 (82%)	0.13	4 (3%)	49	50	31, 54, 87, 107	0
All	All	484/588 (82%)	-0.03	21 (4%)	40	39	25, 48, 85, 120	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	162	PRO	5.6
1	A	161	LEU	5.5
1	B	161	LEU	4.7
1	D	161	LEU	4.3
1	C	161	LEU	4.2
1	A	133	PHE	3.3
1	C	199	ARG	3.0
1	C	98	PHE	2.7
1	B	80	PRO	2.7
1	C	198	TRP	2.7
1	A	132	ILE	2.6
1	D	84	TYR	2.5
1	D	201	SER	2.3
1	A	160	SER	2.3
1	C	162	PRO	2.2
1	C	202	ASP	2.2
1	A	80	PRO	2.2
1	D	98	PHE	2.2
1	B	163	GLY	2.1
1	C	201	SER	2.1
1	B	160	SER	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 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
2	SCN	B	5	3/3	0.73	0.23	83,83,83,84	0
2	SCN	B	6	3/3	0.79	0.19	76,76,77,78	0
2	SCN	B	7	3/3	0.80	0.16	90,90,90,90	0
2	SCN	C	2	3/3	0.81	0.19	79,79,80,80	0
2	SCN	B	4	3/3	0.82	0.22	90,90,90,91	0
2	SCN	D	3	3/3	0.86	0.15	76,76,77,79	0
2	SCN	A	1	3/3	0.87	0.15	74,74,75,75	0
2	SCN	B	8	3/3	0.89	0.15	83,83,83,84	0

6.5 Other polymers [i](#)

There are no such residues in this entry.