



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:32 AM GMT

PDB ID : 3P31
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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

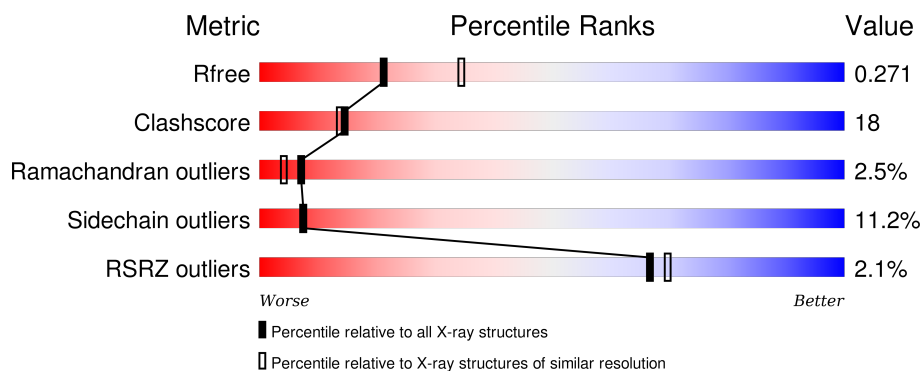
1 Overall quality at a glance ⓘ

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}	91344	4776 (2.50-2.42)
Clashscore	102246	1030 (2.48-2.44)
Ramachandran outliers	100387	1024 (2.48-2.44)
Sidechain outliers	100360	1024 (2.48-2.44)
RSRZ outliers	91569	4787 (2.50-2.42)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>%</div> <div> <div></div> <div>56%</div> <div>18%</div> <div>7%</div> <div>18%</div> </div> </div>
1	B	147	<div> <div>3%</div> <div> <div></div> <div>65%</div> <div>13%</div> <div>•</div> <div>18%</div> </div> </div>
1	C	147	<div> <div>2%</div> <div> <div></div> <div>64%</div> <div>15%</div> <div>•</div> <div>17%</div> </div> </div>
1	D	147	<div> <div>%</div> <div> <div></div> <div>59%</div> <div>17%</div> <div>5%</div> <div>•</div> <div>18%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SCN	A	1	-	-	-	X
2	SCN	B	5	-	-	-	X
2	SCN	B	7	-	-	-	X

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 (three-letter code: 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		

R189	Q194	S201	D202	GLU	ASP	GLY	ARG	LEU	PRO	LEU	PRO	PRO	ASN	GLN	LYS	ARG
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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) 100.0 (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 , 0.271	Depositor DCC
R_{free} test set	1351 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	46.0	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.3	EDS
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 26814 reflections	Xtriage
F_o, F_c correlation	0.94	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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.97	0/964	0.99	0/1303
1	B	0.97	0/972	0.93	3/1314 (0.2%)
1	C	0.95	1/978 (0.1%)	0.87	1/1322 (0.1%)
1	D	0.84	0/973	0.84	0/1315
All	All	0.93	1/3887 (0.0%)	0.91	4/5254 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	137	GLU	CG-CD	5.24	1.59	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	143	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	C	85	LEU	CA-CB-CG	-5.63	102.35	115.30
1	B	143	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	B	161	LEU	C-N-CD	-5.04	109.52	120.60

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	35	0
1	B	955	0	974	34	0
1	C	962	0	975	32	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	138	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 18.

All (138) 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:CA	1:D:83:ARG:HH11	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:D:161:LEU:CB	1:D:162:PRO:HD2	1.85	1.06
1:B:200:ASN:HD22	1:B:200:ASN:C	1.60	1.02
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
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:D:83:ARG:CA	1:D:83:ARG:NH1	2.30	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:ARG:HG3	1:C:84:TYR:N	1.89	0.86
1:C:160:SER:O	1:C:162:PRO:CD	2.26	0.84
1:B:200:ASN:ND2	1:B:200:ASN:C	2.30	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:A:132:ILE:O	1:A:133:PHE:CB	2.34	0.75
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:B:159:PRO:C	1:B:161:LEU:H	1.92	0.71
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: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: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:A:134:ASP:OD1	1:A:134:ASP:N	2.29	0.65
1:A:82:SER:HB3	1:A:132:ILE:HG23	1.79	0.64
1:A:136:LEU:C	1:A:136:LEU:HD23	2.18	0.63
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
1:C:116:GLN:NE2	1:D:103:LYS:HE3	2.13	0.62
1:A:167:GLU:HA	1:A:167:GLU:OE1	1.98	0.62
1:A:199:ARG:HB3	3:A:217:HOH:O	1.99	0.62
1:C:160:SER:C	1:C:162:PRO:HD2	2.19	0.61
1:C:161:LEU:HD12	1:C:161:LEU:C	2.22	0.60
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:B:161:LEU:C	1:B:163:GLY:HA2	2.24	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:199:ARG:HG3	3:B:57:HOH:O	2.04	0.57
1:A:194:GLN:CG	3:A:217:HOH:O	2.41	0.57
1:A:167:GLU:CA	1:A:167:GLU:OE1	2.52	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:HH11	1:B:188:ARG:HG2	1.68	0.57
1:C:201:SER:O	1:C:202:ASP:CG	2.43	0.57
1:A:158:LEU:CD1	3:A:218:HOH:O	2.53	0.56
1:D:160:SER:OG	1:D:161:LEU:N	2.37	0.56
1:B:122:THR:HG22	1:B:147:GLU:HG2	1.86	0.56
1:D:158:LEU:O	1:D:160:SER:N	2.38	0.56
1:A:161:LEU:HD13	1:A:162:PRO:HD3	1.88	0.54
1:C:103:LYS:HE2	1:D:182:TRP:CD2	2.43	0.53
1:D:98:PHE:CD2	1:D:98:PHE:C	2.83	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:D:161:LEU:CG	1:D:162:PRO:HD3	2.41	0.51
1:B:87:ASP:CB	1:B:126:LYS:HB3	2.40	0.51
1:B:188:ARG:NH1	1:B:188:ARG:HG2	2.26	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:B:136:LEU:C	1:B:136:LEU:HD23	2.31	0.50
1:B:198:TRP:CZ2	1:B:200:ASN:HB3	2.47	0.50
1:D:162:PRO:O	1:D:163:GLY:O	2.30	0.50
1:C:201:SER:O	1:C:202:ASP:OD2	2.30	0.49
1:A:82:SER:CB	1:A:132:ILE:HG23	2.41	0.49
1:A:194:GLN:CD	3:A:217:HOH:O	2.51	0.49
1:B:118:ILE:HG13	1:B:152:VAL:CG1	2.41	0.49
1:B:159:PRO:C	1:B:161:LEU:N	2.61	0.48
1:A:114:MET:HE3	1:A:180:LEU:HD23	1.95	0.48
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:D:160:SER:O	1:D:161:LEU:C	2.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:82:SER:HA	1:D:131:VAL:O	2.16	0.46
1:D:161:LEU:CG	1:D:162:PRO:CD	2.93	0.46
1:C:161:LEU:CG	1:C:162:PRO:N	2.71	0.46
1:A:91:GLU:OE2	1:A:95:ARG:CG	2.63	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:C:160:SER:O	1:C:161:LEU:C	2.54	0.45
1:D:134:ASP:O	1:D:135:ARG:HG2	2.16	0.45
1:A:164:HIS:HA	1:A:168:ASP:OD2	2.15	0.45
1:C:105:LYS:HB2	1:C:105:LYS:HE3	1.67	0.45
1:A:125:LEU:HD22	1:A:144:ALA:HB2	1.99	0.45
1:D:142:LEU:C	1:D:142:LEU:HD23	2.36	0.44
1:D:98:PHE:C	1:D:98:PHE:HD2	2.19	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:A:119:MET:HG2	1:A:183:ASN:HB3	2.00	0.43
1:B:199:ARG:O	1:B:200:ASN:HB2	2.19	0.43
1:A:132:ILE:HD12	1:A:132:ILE:O	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:N	1:A:133:PHE:CD1	2.86	0.42
1:C:104:GLN:HA	1:C:112:ILE:O	2.20	0.42
1:D:188:ARG:HG2	1:D:188:ARG:HH11	1.85	0.41
1:B:161:LEU:HA	1:B:161:LEU:HD13	1.43	0.41
1:A:136:LEU:O	1:A:136:LEU:HD23	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:A:104:GLN:HG2	1:A:113:LYS:HG2	2.03	0.41
1:B:121:LYS:HZ2	1:B:121:LYS:HG3	1.73	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%)	11	10
1	B	119/147 (81%)	112 (94%)	2 (2%)	5 (4%)	3	1
1	C	120/147 (82%)	112 (93%)	7 (6%)	1 (1%)	24	28
1	D	119/147 (81%)	113 (95%)	2 (2%)	4 (3%)	5	2
All	All	476/588 (81%)	444 (93%)	20 (4%)	12 (2%)	7	4

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
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%)	90 (86%)	14 (14%)	5	4
1	B	105/127 (83%)	94 (90%)	11 (10%)	8	9
1	C	106/127 (84%)	96 (91%)	10 (9%)	11	13
1	D	106/127 (84%)	94 (89%)	12 (11%)	7	7
All	All	421/508 (83%)	374 (89%)	47 (11%)	7	7

All (47) 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	132	ILE
1	A	134	ASP
1	A	135	ARG
1	A	136	LEU
1	A	148	GLU
1	A	158	LEU
1	A	167	GLU
1	A	192	THR
1	A	195	ARG
1	A	199	ARG
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	161	LEU
1	B	164	HIS
1	B	192	THR
1	B	199	ARG
1	B	200	ASN
1	C	90	LEU
1	C	104	GLN
1	C	131	VAL
1	C	132	ILE
1	C	134	ASP
1	C	160	SER
1	C	191	GLU
1	C	192	THR

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Mol	Chain	Res	Type
1	C	195	ARG
1	C	201	SER
1	D	83	ARG
1	D	98	PHE
1	D	124	ILE
1	D	131	VAL
1	D	132	ILE
1	D	134	ASP
1	D	147	GLU
1	D	148	GLU
1	D	161	LEU
1	D	167	GLU
1	D	194	GLN
1	D	202	ASP

Some 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
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 carbohydrates 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	-	2,2,2	2.06	1 (50%)	1,1,1	0.14	0
2	SCN	B	4	-	2,2,2	1.76	1 (50%)	1,1,1	0.37	0
2	SCN	B	5	-	2,2,2	2.02	1 (50%)	1,1,1	0.24	0
2	SCN	B	6	-	2,2,2	2.11	1 (50%)	1,1,1	0.30	0
2	SCN	B	7	-	2,2,2	1.97	1 (50%)	1,1,1	0.38	0
2	SCN	B	8	-	2,2,2	1.97	1 (50%)	1,1,1	0.17	0
2	SCN	C	2	-	2,2,2	2.03	1 (50%)	1,1,1	0.44	0
2	SCN	D	3	-	2,2,2	2.01	1 (50%)	1,1,1	0.26	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
2	SCN	A	1	-	-	0/0/0/0	0/0/0/0
2	SCN	B	4	-	-	0/0/0/0	0/0/0/0
2	SCN	B	5	-	-	0/0/0/0	0/0/0/0
2	SCN	B	6	-	-	0/0/0/0	0/0/0/0
2	SCN	B	7	-	-	0/0/0/0	0/0/0/0
2	SCN	B	8	-	-	0/0/0/0	0/0/0/0
2	SCN	C	2	-	-	0/0/0/0	0/0/0/0
2	SCN	D	3	-	-	0/0/0/0	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	4	SCN	C-S	2.47	1.79	1.63
2	B	7	SCN	C-S	2.74	1.81	1.63
2	B	8	SCN	C-S	2.77	1.81	1.63
2	B	5	SCN	C-S	2.80	1.81	1.63
2	D	3	SCN	C-S	2.81	1.81	1.63
2	C	2	SCN	C-S	2.82	1.81	1.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	SCN	C-S	2.84	1.81	1.63
2	B	6	SCN	C-S	2.92	1.82	1.63

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	7	SCN	1	0
2	B	8	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.21	1 (0%) 87 89	26, 46, 90, 120	0
1	B	121/147 (82%)	-0.24	4 (3%) 50 53	26, 46, 73, 105	0
1	C	122/147 (82%)	-0.06	3 (2%) 61 63	25, 42, 76, 105	0
1	D	121/147 (82%)	-0.11	2 (1%) 73 75	31, 54, 87, 107	0
All	All	484/588 (82%)	-0.16	10 (2%) 67 70	25, 48, 85, 120	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	161	LEU	7.2
1	C	161	LEU	6.9
1	B	162	PRO	5.9
1	A	161	LEU	4.3
1	B	161	LEU	3.7
1	D	108	GLY	3.0
1	C	198	TRP	3.0
1	C	199	ARG	2.9
1	B	200	ASN	2.8
1	B	108	GLY	2.3

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	SCN	A	1	3/3	0.89	0.23	7.55	74,74,75,75	0
2	SCN	B	7	3/3	0.79	0.17	2.33	90,90,90,90	0
2	SCN	B	5	3/3	0.80	0.22	2.04	83,83,83,84	0
2	SCN	B	8	3/3	0.93	0.24	-	83,83,83,84	0
2	SCN	B	6	3/3	0.81	0.19	-	76,76,77,78	0
2	SCN	C	2	3/3	0.69	0.20	-	79,79,80,80	0
2	SCN	D	3	3/3	0.82	0.17	-	76,76,77,79	0
2	SCN	B	4	3/3	0.82	0.13	-	90,90,90,91	0

6.5 Other polymers [i](#)

There are no such residues in this entry.