Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:14 PM GMT

PDB ID	:	4O6C
Title	:	West Nile Virus Non-structural protein 1 (NS1) Form 2 crystal
Authors	:	Akey, D.L.; Smith, J.L.
Deposited on	:	2013-12-20
Resolution	:	2.75 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

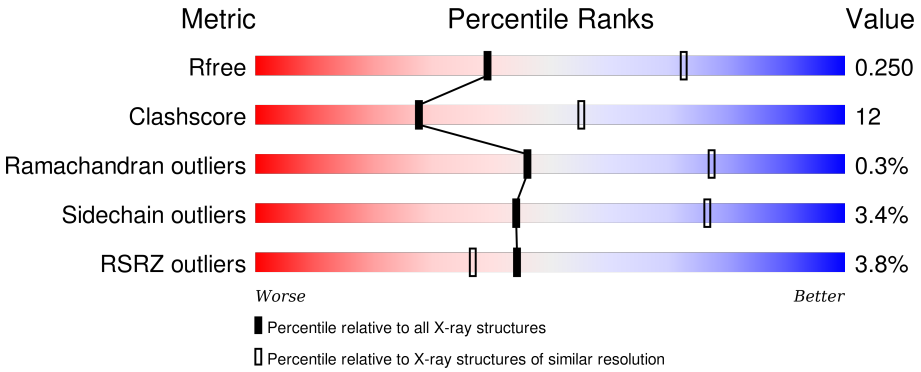
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	3340 (2.80-2.72)
Clashscore	102246	3829 (2.80-2.72)
Ramachandran outliers	100387	3767 (2.80-2.72)
Sidechain outliers	100360	3770 (2.80-2.72)
RSRZ outliers	91569	3352 (2.80-2.72)

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 <=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	377	% 64% 24% • 10%
1	B	377	% 63% 25% • 10%
1	C	377	4% 64% 24% • 10%
1	D	377	3% 65% 24% • 10%
1	E	377	7% 58% 30% • 10%

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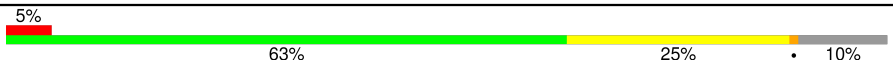
Mol	Chain	Length	Quality of chain
1	F	377	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16113 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 NS1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	S	0	0	0
			2669	1657	472	523	17			
1	B	338	Total	C	N	O	S	0	0	0
			2669	1657	472	523	17			
1	C	338	Total	C	N	O	S	0	0	0
			2669	1657	472	523	17			
1	D	338	Total	C	N	O	S	0	0	0
			2669	1657	472	523	17			
1	E	338	Total	C	N	O	S	0	0	0
			2669	1657	472	523	17			
1	F	338	Total	C	N	O	S	0	0	0
			2669	1657	472	523	17			

There are 138 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-24	ALA	-	EXPRESSION TAG	UNP U3N977
A	-23	GLU	-	EXPRESSION TAG	UNP U3N977
A	-22	HIS	-	EXPRESSION TAG	UNP U3N977
A	-21	HIS	-	EXPRESSION TAG	UNP U3N977
A	-20	HIS	-	EXPRESSION TAG	UNP U3N977
A	-19	HIS	-	EXPRESSION TAG	UNP U3N977
A	-18	HIS	-	EXPRESSION TAG	UNP U3N977
A	-16	SER	-	EXPRESSION TAG	UNP U3N977
A	-15	SER	-	EXPRESSION TAG	UNP U3N977
A	-14	GLY	-	EXPRESSION TAG	UNP U3N977
A	-13	VAL	-	EXPRESSION TAG	UNP U3N977
A	-12	ASP	-	EXPRESSION TAG	UNP U3N977
A	-11	LEU	-	EXPRESSION TAG	UNP U3N977
A	-10	GLY	-	EXPRESSION TAG	UNP U3N977
A	-9	THR	-	EXPRESSION TAG	UNP U3N977
A	-8	GLU	-	EXPRESSION TAG	UNP U3N977
A	-7	ASN	-	EXPRESSION TAG	UNP U3N977

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	LEU	-	EXPRESSION TAG	UNP U3N977
A	-5	TYR	-	EXPRESSION TAG	UNP U3N977
A	-4	PHE	-	EXPRESSION TAG	UNP U3N977
A	-3	GLN	-	EXPRESSION TAG	UNP U3N977
A	-2	SER	-	EXPRESSION TAG	UNP U3N977
A	-1	ASN	-	EXPRESSION TAG	UNP U3N977
B	-24	ALA	-	EXPRESSION TAG	UNP U3N977
B	-23	GLU	-	EXPRESSION TAG	UNP U3N977
B	-22	HIS	-	EXPRESSION TAG	UNP U3N977
B	-21	HIS	-	EXPRESSION TAG	UNP U3N977
B	-20	HIS	-	EXPRESSION TAG	UNP U3N977
B	-19	HIS	-	EXPRESSION TAG	UNP U3N977
B	-18	HIS	-	EXPRESSION TAG	UNP U3N977
B	-16	SER	-	EXPRESSION TAG	UNP U3N977
B	-15	SER	-	EXPRESSION TAG	UNP U3N977
B	-14	GLY	-	EXPRESSION TAG	UNP U3N977
B	-13	VAL	-	EXPRESSION TAG	UNP U3N977
B	-12	ASP	-	EXPRESSION TAG	UNP U3N977
B	-11	LEU	-	EXPRESSION TAG	UNP U3N977
B	-10	GLY	-	EXPRESSION TAG	UNP U3N977
B	-9	THR	-	EXPRESSION TAG	UNP U3N977
B	-8	GLU	-	EXPRESSION TAG	UNP U3N977
B	-7	ASN	-	EXPRESSION TAG	UNP U3N977
B	-6	LEU	-	EXPRESSION TAG	UNP U3N977
B	-5	TYR	-	EXPRESSION TAG	UNP U3N977
B	-4	PHE	-	EXPRESSION TAG	UNP U3N977
B	-3	GLN	-	EXPRESSION TAG	UNP U3N977
B	-2	SER	-	EXPRESSION TAG	UNP U3N977
B	-1	ASN	-	EXPRESSION TAG	UNP U3N977
C	-24	ALA	-	EXPRESSION TAG	UNP U3N977
C	-23	GLU	-	EXPRESSION TAG	UNP U3N977
C	-22	HIS	-	EXPRESSION TAG	UNP U3N977
C	-21	HIS	-	EXPRESSION TAG	UNP U3N977
C	-20	HIS	-	EXPRESSION TAG	UNP U3N977
C	-19	HIS	-	EXPRESSION TAG	UNP U3N977
C	-18	HIS	-	EXPRESSION TAG	UNP U3N977
C	-16	SER	-	EXPRESSION TAG	UNP U3N977
C	-15	SER	-	EXPRESSION TAG	UNP U3N977
C	-14	GLY	-	EXPRESSION TAG	UNP U3N977
C	-13	VAL	-	EXPRESSION TAG	UNP U3N977
C	-12	ASP	-	EXPRESSION TAG	UNP U3N977
C	-11	LEU	-	EXPRESSION TAG	UNP U3N977

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-10	GLY	-	EXPRESSION TAG	UNP U3N977
C	-9	THR	-	EXPRESSION TAG	UNP U3N977
C	-8	GLU	-	EXPRESSION TAG	UNP U3N977
C	-7	ASN	-	EXPRESSION TAG	UNP U3N977
C	-6	LEU	-	EXPRESSION TAG	UNP U3N977
C	-5	TYR	-	EXPRESSION TAG	UNP U3N977
C	-4	PHE	-	EXPRESSION TAG	UNP U3N977
C	-3	GLN	-	EXPRESSION TAG	UNP U3N977
C	-2	SER	-	EXPRESSION TAG	UNP U3N977
C	-1	ASN	-	EXPRESSION TAG	UNP U3N977
D	-24	ALA	-	EXPRESSION TAG	UNP U3N977
D	-23	GLU	-	EXPRESSION TAG	UNP U3N977
D	-22	HIS	-	EXPRESSION TAG	UNP U3N977
D	-21	HIS	-	EXPRESSION TAG	UNP U3N977
D	-20	HIS	-	EXPRESSION TAG	UNP U3N977
D	-19	HIS	-	EXPRESSION TAG	UNP U3N977
D	-18	HIS	-	EXPRESSION TAG	UNP U3N977
D	-16	SER	-	EXPRESSION TAG	UNP U3N977
D	-15	SER	-	EXPRESSION TAG	UNP U3N977
D	-14	GLY	-	EXPRESSION TAG	UNP U3N977
D	-13	VAL	-	EXPRESSION TAG	UNP U3N977
D	-12	ASP	-	EXPRESSION TAG	UNP U3N977
D	-11	LEU	-	EXPRESSION TAG	UNP U3N977
D	-10	GLY	-	EXPRESSION TAG	UNP U3N977
D	-9	THR	-	EXPRESSION TAG	UNP U3N977
D	-8	GLU	-	EXPRESSION TAG	UNP U3N977
D	-7	ASN	-	EXPRESSION TAG	UNP U3N977
D	-6	LEU	-	EXPRESSION TAG	UNP U3N977
D	-5	TYR	-	EXPRESSION TAG	UNP U3N977
D	-4	PHE	-	EXPRESSION TAG	UNP U3N977
D	-3	GLN	-	EXPRESSION TAG	UNP U3N977
D	-2	SER	-	EXPRESSION TAG	UNP U3N977
D	-1	ASN	-	EXPRESSION TAG	UNP U3N977
E	-24	ALA	-	EXPRESSION TAG	UNP U3N977
E	-23	GLU	-	EXPRESSION TAG	UNP U3N977
E	-22	HIS	-	EXPRESSION TAG	UNP U3N977
E	-21	HIS	-	EXPRESSION TAG	UNP U3N977
E	-20	HIS	-	EXPRESSION TAG	UNP U3N977
E	-19	HIS	-	EXPRESSION TAG	UNP U3N977
E	-18	HIS	-	EXPRESSION TAG	UNP U3N977
E	-16	SER	-	EXPRESSION TAG	UNP U3N977
E	-15	SER	-	EXPRESSION TAG	UNP U3N977

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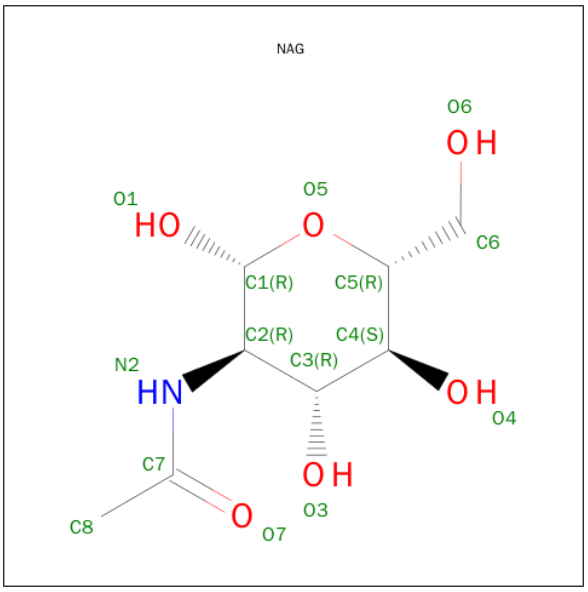
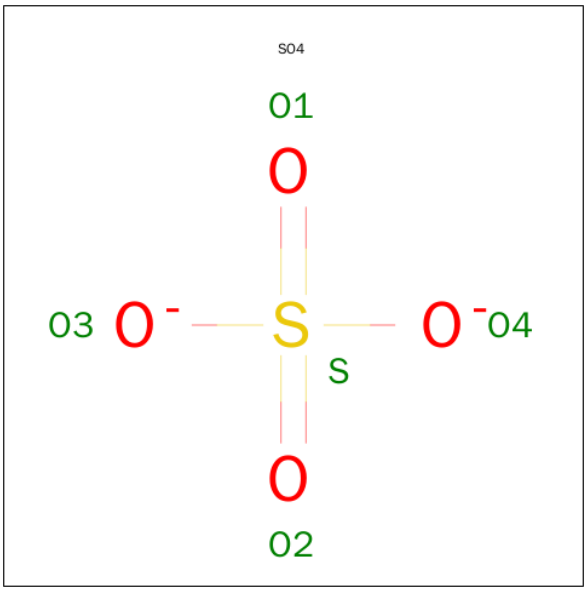
Chain	Residue	Modelled	Actual	Comment	Reference
E	-14	GLY	-	EXPRESSION TAG	UNP U3N977
E	-13	VAL	-	EXPRESSION TAG	UNP U3N977
E	-12	ASP	-	EXPRESSION TAG	UNP U3N977
E	-11	LEU	-	EXPRESSION TAG	UNP U3N977
E	-10	GLY	-	EXPRESSION TAG	UNP U3N977
E	-9	THR	-	EXPRESSION TAG	UNP U3N977
E	-8	GLU	-	EXPRESSION TAG	UNP U3N977
E	-7	ASN	-	EXPRESSION TAG	UNP U3N977
E	-6	LEU	-	EXPRESSION TAG	UNP U3N977
E	-5	TYR	-	EXPRESSION TAG	UNP U3N977
E	-4	PHE	-	EXPRESSION TAG	UNP U3N977
E	-3	GLN	-	EXPRESSION TAG	UNP U3N977
E	-2	SER	-	EXPRESSION TAG	UNP U3N977
E	-1	ASN	-	EXPRESSION TAG	UNP U3N977
F	-24	ALA	-	EXPRESSION TAG	UNP U3N977
F	-23	GLU	-	EXPRESSION TAG	UNP U3N977
F	-22	HIS	-	EXPRESSION TAG	UNP U3N977
F	-21	HIS	-	EXPRESSION TAG	UNP U3N977
F	-20	HIS	-	EXPRESSION TAG	UNP U3N977
F	-19	HIS	-	EXPRESSION TAG	UNP U3N977
F	-18	HIS	-	EXPRESSION TAG	UNP U3N977
F	-16	SER	-	EXPRESSION TAG	UNP U3N977
F	-15	SER	-	EXPRESSION TAG	UNP U3N977
F	-14	GLY	-	EXPRESSION TAG	UNP U3N977
F	-13	VAL	-	EXPRESSION TAG	UNP U3N977
F	-12	ASP	-	EXPRESSION TAG	UNP U3N977
F	-11	LEU	-	EXPRESSION TAG	UNP U3N977
F	-10	GLY	-	EXPRESSION TAG	UNP U3N977
F	-9	THR	-	EXPRESSION TAG	UNP U3N977
F	-8	GLU	-	EXPRESSION TAG	UNP U3N977
F	-7	ASN	-	EXPRESSION TAG	UNP U3N977
F	-6	LEU	-	EXPRESSION TAG	UNP U3N977
F	-5	TYR	-	EXPRESSION TAG	UNP U3N977
F	-4	PHE	-	EXPRESSION TAG	UNP U3N977
F	-3	GLN	-	EXPRESSION TAG	UNP U3N977
F	-2	SER	-	EXPRESSION TAG	UNP U3N977
F	-1	ASN	-	EXPRESSION TAG	UNP U3N977

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



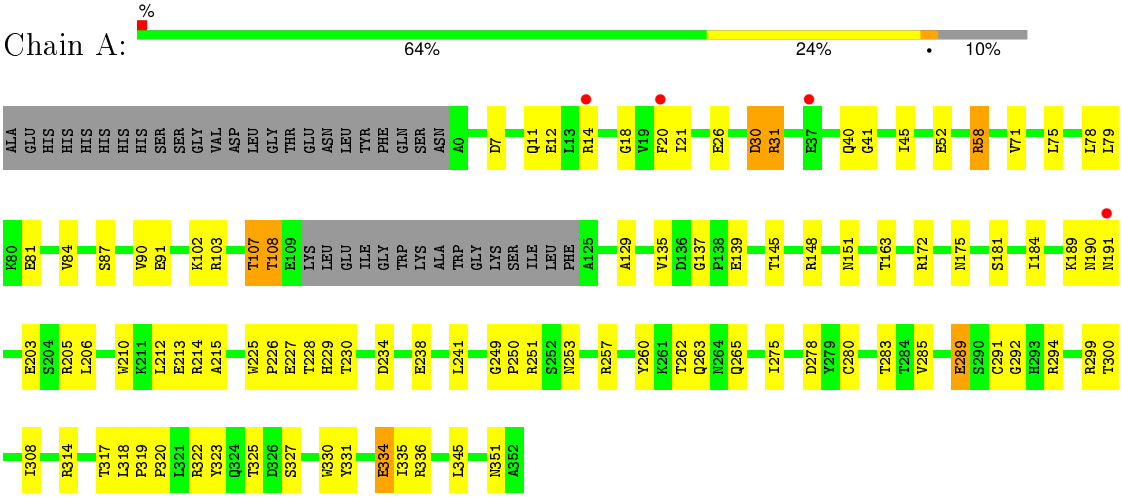
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

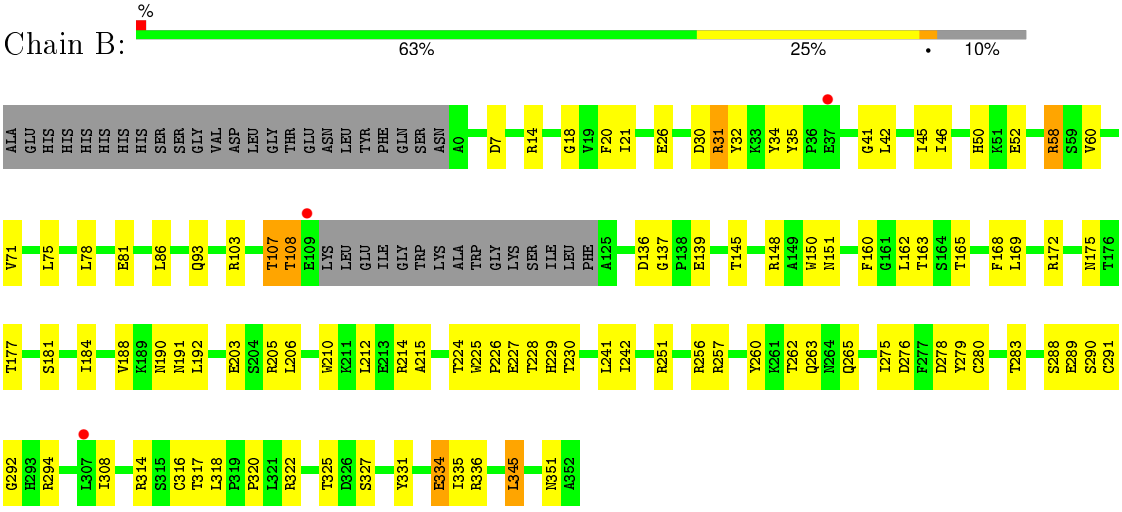
- Molecule 1: NS1

Chain A:



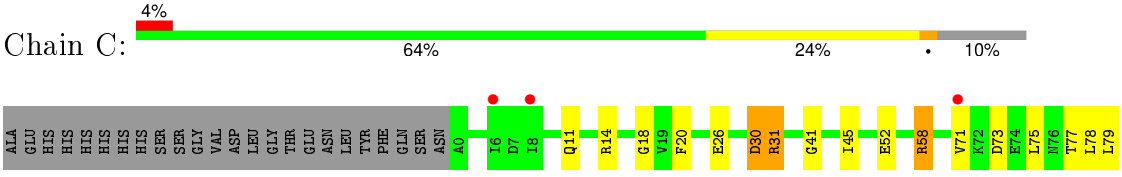
- Molecule 1: NS1

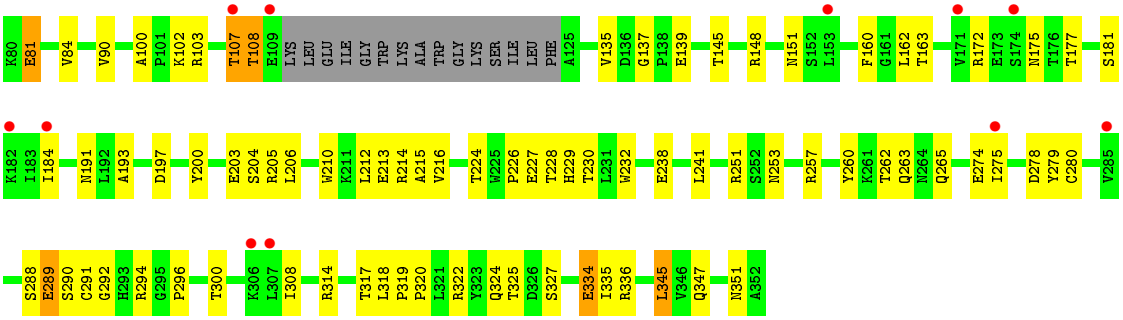
Chain B:



- Molecule 1: NS1

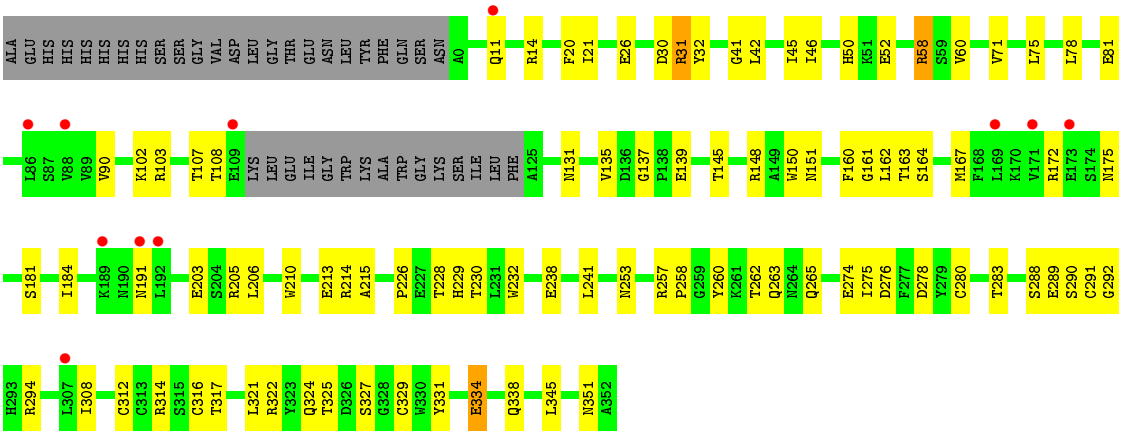
Chain C:





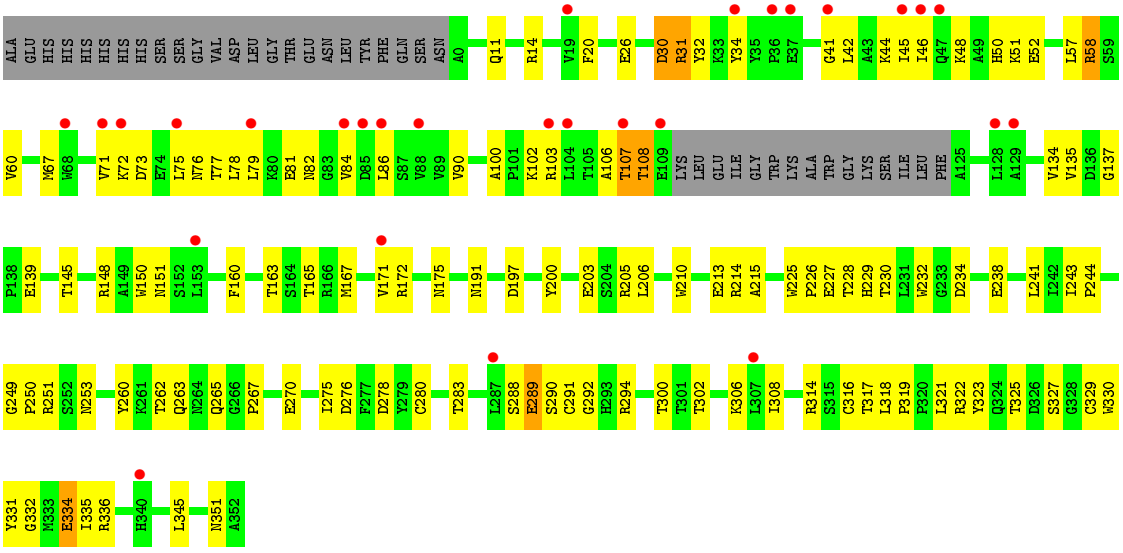
• Molecule 1: NS1

Chain D:



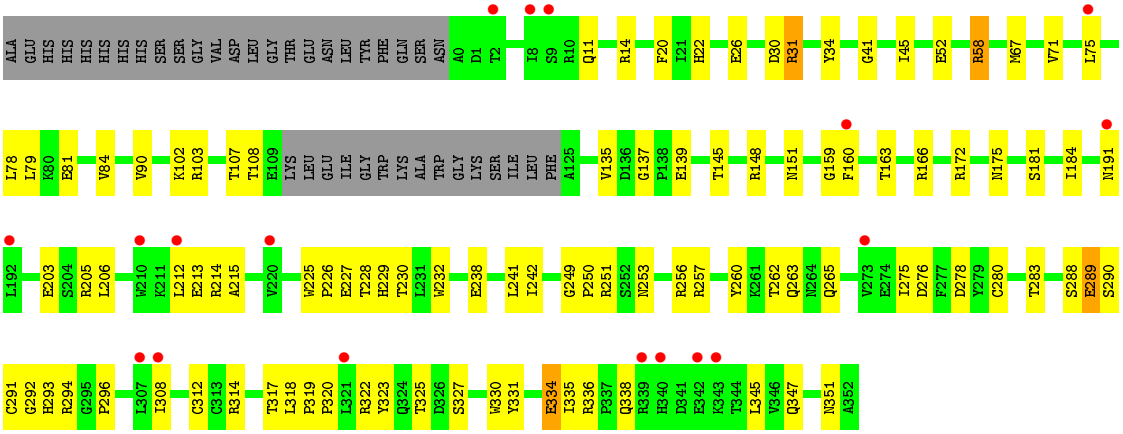
• Molecule 1: NS1

Chain E:



• Molecule 1: NS1

Chain F:


ALA GLU HIS HIS HIS HIS HIS SER SER GLY VAL ASP LEU GLY THR GLU ASN LEU TYR PHE GLN SER ASN
A0 D1 T2 I8 S9 R10 Q11 R14 F20 I21 H22 E26 D30 R31 Y34 G41 I45 E52 R58 W67 V71 L75
L78 L79 K80 E81 V84 V90 K102 R103 T107 T108 E109 LYS LEU GLU ILE GLY TRP LYS ALA TRP GLY LYS SER ILE LEU PHE A125 V135 D136 G137 P138 E139 T145 R148 N151 G159 F160 T163 R166 R172 N175 S181 I184 N191
L192 E203 S204 R205 L206 W210 K211 L212 E213 R214 A215 V220 W225 P226 E227 T228 H229 T230 L231 W232 E238 L241 I242 G249 P250 R251 S252 N253 R256 R257 Y260 K261 T262 Q263 N264 Q265 V273 E274 I275 D276 F277 D278 Y279 C280 T283 S288 E289 S290
C291 G292 H293 R294 G295 P296 L307 I308 C312 C313 R314 T317 I318 P319 P320 L321 R322 Y323 Q324 T325 D326 S327 W330 Y331 E334 I335 R336 P337 Q338 R339 H340 D341 E342 K343 T344 L345 V346 Q347 N351 A352

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α, β, γ	186.88Å 186.88Å 81.77Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.98 – 2.75 48.98 – 2.75	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.98-2.75) 100.0 (48.98-2.75)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.78 (at 2.77Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.215 , 0.232 0.229 , 0.250	Depositor DCC
R_{free} test set	2007 reflections (2.42%)	DCC
Wilson B-factor (Å^2)	50.9	Xtriage
Anisotropy	0.655	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 37.4	EDS
Estimated twinning fraction	0.520 for -h,-k,l 0.449 for -h,-k,l 0.156 for h,-h-k,-l 0.156 for -k,-h,-l	Xtriage
Reported twinning fraction	0.520 for -h,-k,l	Depositor
L-test for twinning[2]	$< \|L\| > = 0.36$, $< L^2 > = 0.19$	Xtriage
Outliers	0 of 82983 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	16113	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 4.67% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: NAG, SO4

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	0.30	0/2726	0.48	0/3700
1	B	0.29	0/2726	0.47	0/3700
1	C	0.27	0/2726	0.46	0/3700
1	D	0.27	0/2726	0.46	0/3700
1	E	0.27	0/2726	0.46	0/3700
1	F	0.26	0/2726	0.46	0/3700
All	All	0.27	0/16356	0.47	0/22200

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	2669	0	2577	65	0
1	B	2669	0	2577	67	0
1	C	2669	0	2577	62	0
1	D	2669	0	2577	56	0
1	E	2669	0	2577	79	0
1	F	2669	0	2577	59	0
2	A	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	14	0	13	0	0
2	C	14	0	13	0	0
2	D	14	0	13	0	0
2	E	14	0	13	0	0
2	F	14	0	13	0	0
3	A	5	0	0	0	0
3	C	5	0	0	0	0
3	F	5	0	0	0	0
All	All	16113	0	15540	372	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 12.

All (372) 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:31:ARG:NH1	1:B:163:THR:O	2.07	0.87
1:E:14:ARG:HH22	1:F:31:ARG:HB3	1.41	0.85
1:D:31:ARG:NH1	1:D:163:THR:O	2.11	0.83
1:F:31:ARG:NH1	1:F:163:THR:O	2.13	0.82
1:E:31:ARG:NH1	1:E:163:THR:O	2.12	0.82
1:E:160:PHE:HB2	1:F:11:GLN:HG2	1.63	0.81
1:A:31:ARG:NH1	1:A:163:THR:O	2.13	0.81
1:A:58:ARG:NH1	1:A:137:GLY:O	2.14	0.80
1:D:103:ARG:NH2	1:D:175:ASN:OD1	2.16	0.78
1:C:26:GLU:OE2	1:C:214:ARG:NH2	2.17	0.78
1:B:103:ARG:NH2	1:B:175:ASN:OD1	2.17	0.77
1:A:103:ARG:NH2	1:A:175:ASN:OD1	2.16	0.76
1:C:263:GLN:NE2	1:C:334:GLU:OE1	2.18	0.75
1:C:291:CYS:O	1:C:314:ARG:NH2	2.20	0.75
1:B:291:CYS:O	1:B:314:ARG:NH2	2.21	0.74
1:C:14:ARG:HH22	1:D:31:ARG:HB3	1.53	0.73
1:F:103:ARG:NH2	1:F:175:ASN:OD1	2.21	0.72
1:C:31:ARG:NH1	1:C:163:THR:O	2.22	0.72
1:B:145:THR:HA	1:B:148:ARG:HD2	1.71	0.72
1:E:265:GLN:HE21	1:E:351:ASN:HD21	1.37	0.72
1:E:78:LEU:HA	1:E:81:GLU:HG2	1.70	0.72
1:B:26:GLU:OE2	1:B:214:ARG:NH2	2.23	0.71
1:A:31:ARG:HB3	1:B:14:ARG:HH22	1.56	0.71
1:A:14:ARG:HH22	1:B:31:ARG:HB3	1.55	0.70
1:D:78:LEU:HA	1:D:81:GLU:HG2	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:GLU:OE2	1:C:145:THR:OG1	2.06	0.70
1:D:263:GLN:NE2	1:D:334:GLU:OE1	2.24	0.69
1:F:58:ARG:NH1	1:F:137:GLY:O	2.26	0.69
1:C:78:LEU:HA	1:C:81:GLU:HG2	1.74	0.69
1:B:139:GLU:OE2	1:B:145:THR:OG1	2.09	0.68
1:E:260:TYR:HE1	1:E:317:THR:HG22	1.58	0.68
1:C:274:GLU:HB3	1:C:324:GLN:HB2	1.75	0.68
1:D:58:ARG:NH1	1:D:137:GLY:O	2.27	0.68
1:F:26:GLU:OE2	1:F:214:ARG:NH2	2.26	0.67
1:B:260:TYR:HE1	1:B:317:THR:HG22	1.59	0.67
1:C:325:THR:HG22	1:C:327:SER:H	1.60	0.67
1:E:58:ARG:NH1	1:E:137:GLY:O	2.27	0.67
1:F:263:GLN:NE2	1:F:334:GLU:OE1	2.28	0.66
1:E:325:THR:HG22	1:E:327:SER:H	1.60	0.66
1:C:103:ARG:NH2	1:C:175:ASN:OD1	2.28	0.66
1:D:260:TYR:HE1	1:D:317:THR:HG22	1.59	0.66
1:D:145:THR:HA	1:D:148:ARG:HD2	1.77	0.66
1:C:58:ARG:NH1	1:C:137:GLY:O	2.29	0.66
1:D:26:GLU:OE2	1:D:214:ARG:NH2	2.28	0.66
1:F:78:LEU:HA	1:F:81:GLU:HG2	1.78	0.66
1:D:325:THR:HG22	1:D:327:SER:H	1.61	0.66
1:F:226:PRO:O	1:F:230:THR:OG1	2.13	0.65
1:B:288:SER:HG	1:B:290:SER:HG	1.45	0.65
1:B:78:LEU:HA	1:B:81:GLU:HG2	1.77	0.65
1:E:103:ARG:NH2	1:E:175:ASN:OD1	2.29	0.65
1:F:151:ASN:OD1	1:F:172:ARG:NH2	2.30	0.65
1:F:139:GLU:OE2	1:F:145:THR:OG1	2.11	0.64
1:D:139:GLU:OE2	1:D:145:THR:OG1	2.13	0.64
1:C:100:ALA:O	1:C:103:ARG:NH1	2.30	0.64
1:C:160:PHE:HB2	1:D:11:GLN:HG2	1.79	0.63
1:F:260:TYR:HE1	1:F:317:THR:HG22	1.63	0.63
1:C:288:SER:HG	1:C:290:SER:HG	1.46	0.63
1:E:11:GLN:HG2	1:F:160:PHE:HB2	1.78	0.62
1:A:228:THR:HG1	1:A:229:HIS:HD1	1.48	0.62
1:A:139:GLU:OE2	1:A:145:THR:OG1	2.12	0.62
1:D:226:PRO:O	1:D:230:THR:OG1	2.18	0.62
1:A:263:GLN:NE2	1:A:334:GLU:OE1	2.32	0.62
1:A:11:GLN:HG2	1:B:160:PHE:HB2	1.81	0.62
1:B:263:GLN:NE2	1:B:334:GLU:OE1	2.33	0.62
1:A:265:GLN:HE21	1:A:351:ASN:HD21	1.46	0.62
1:E:26:GLU:OE2	1:E:214:ARG:NH2	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:191:ASN:HB3	1:C:206:LEU:HB3	1.82	0.62
1:F:215:ALA:HB3	1:F:275:ILE:HB	1.81	0.61
1:F:191:ASN:HB3	1:F:206:LEU:HB3	1.81	0.61
1:F:228:THR:HG1	1:F:229:HIS:HD1	1.48	0.61
1:F:325:THR:HG22	1:F:327:SER:H	1.66	0.61
1:D:291:CYS:O	1:D:314:ARG:NH2	2.34	0.61
1:D:191:ASN:HB3	1:D:206:LEU:HB3	1.81	0.61
1:F:291:CYS:O	1:F:314:ARG:NH2	2.34	0.60
1:E:139:GLU:OE2	1:E:145:THR:OG1	2.14	0.60
1:A:26:GLU:OE2	1:A:214:ARG:NH2	2.35	0.60
1:C:212:LEU:O	1:C:257:ARG:NH1	2.34	0.59
1:A:325:THR:HG22	1:A:327:SER:H	1.67	0.59
1:C:260:TYR:HE1	1:C:317:THR:HG22	1.66	0.59
1:E:145:THR:HA	1:E:148:ARG:HD2	1.83	0.59
1:B:191:ASN:HB3	1:B:206:LEU:HB3	1.83	0.59
1:C:215:ALA:HB3	1:C:275:ILE:HB	1.84	0.59
1:C:145:THR:HA	1:C:148:ARG:HD2	1.83	0.59
1:E:288:SER:HG	1:E:290:SER:HG	1.50	0.59
1:A:78:LEU:HA	1:A:81:GLU:HG2	1.83	0.59
1:C:203:GLU:OE2	1:C:205:ARG:NH2	2.35	0.58
1:E:151:ASN:OD1	1:E:172:ARG:NH2	2.37	0.58
1:C:228:THR:HG1	1:C:229:HIS:HD1	1.51	0.58
1:C:31:ARG:HB3	1:D:14:ARG:HH22	1.69	0.58
1:B:283:THR:OG1	1:B:331:TYR:OH	2.12	0.58
1:B:151:ASN:OD1	1:B:172:ARG:NH2	2.36	0.58
1:E:263:GLN:NE2	1:E:334:GLU:OE1	2.35	0.58
1:D:151:ASN:OD1	1:D:172:ARG:NH2	2.37	0.57
1:A:145:THR:HA	1:A:148:ARG:HD2	1.86	0.57
1:A:215:ALA:HB3	1:A:275:ILE:HB	1.86	0.57
1:B:325:THR:HG22	1:B:327:SER:H	1.70	0.57
1:D:288:SER:OG	1:D:290:SER:OG	2.20	0.56
1:E:90:VAL:HA	1:E:135:VAL:HB	1.88	0.56
1:C:151:ASN:OD1	1:C:172:ARG:NH2	2.38	0.56
1:F:205:ARG:HB2	1:F:213:GLU:HG3	1.88	0.56
1:E:31:ARG:HB3	1:F:14:ARG:HH22	1.71	0.55
1:B:265:GLN:HE21	1:B:351:ASN:HD21	1.55	0.55
1:A:12:GLU:OE2	1:B:165:THR:OG1	2.21	0.55
1:B:31:ARG:O	1:B:165:THR:N	2.36	0.55
1:B:288:SER:OG	1:B:290:SER:OG	2.18	0.55
1:D:265:GLN:HE21	1:D:351:ASN:HD21	1.55	0.55
1:B:58:ARG:NH1	1:B:137:GLY:O	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:ASN:OD1	1:A:172:ARG:NH2	2.40	0.55
1:E:215:ALA:HB3	1:E:275:ILE:HB	1.89	0.54
1:A:291:CYS:O	1:A:314:ARG:NH2	2.40	0.54
1:C:265:GLN:HE21	1:C:351:ASN:HD21	1.53	0.54
1:A:206:LEU:HB2	1:A:210:TRP:CE2	2.43	0.54
1:B:226:PRO:O	1:B:230:THR:OG1	2.24	0.54
1:C:79:LEU:O	1:C:84:VAL:N	2.40	0.54
1:F:145:THR:HA	1:F:148:ARG:HD2	1.90	0.53
1:E:278:ASP:HB3	1:E:322:ARG:HE	1.72	0.53
1:B:203:GLU:OE2	1:B:205:ARG:NH2	2.41	0.53
1:A:7:ASP:OD2	1:A:190:ASN:ND2	2.40	0.53
1:A:226:PRO:O	1:A:230:THR:OG1	2.27	0.53
1:E:71:VAL:HG22	1:E:75:LEU:HG	1.91	0.53
1:F:203:GLU:HB3	1:F:214:ARG:HB3	1.91	0.53
1:D:215:ALA:HB3	1:D:275:ILE:HB	1.91	0.53
1:C:226:PRO:O	1:C:230:THR:OG1	2.27	0.53
1:A:280:CYS:HB2	1:A:331:TYR:CZ	2.43	0.53
1:A:79:LEU:O	1:A:84:VAL:N	2.41	0.53
1:E:14:ARG:HD2	1:F:22:HIS:CG	2.44	0.52
1:D:276:ASP:OD2	1:D:322:ARG:NH2	2.42	0.52
1:A:260:TYR:HE1	1:A:317:THR:HG22	1.74	0.52
1:C:11:GLN:HG2	1:D:160:PHE:HB2	1.90	0.52
1:B:228:THR:HG1	1:B:229:HIS:HD1	1.47	0.52
1:E:79:LEU:O	1:E:84:VAL:N	2.42	0.52
1:C:238:GLU:HA	1:C:241:LEU:HD12	1.91	0.52
1:F:181:SER:HA	1:F:184:ILE:HD12	1.92	0.52
1:E:276:ASP:OD2	1:E:322:ARG:NH2	2.43	0.51
1:A:278:ASP:HB3	1:A:322:ARG:HE	1.75	0.51
1:C:90:VAL:HA	1:C:135:VAL:HB	1.92	0.51
1:F:323:TYR:HB2	1:F:330:TRP:HB2	1.90	0.51
1:B:228:THR:HG1	1:B:229:HIS:CE1	2.28	0.51
1:D:203:GLU:OE2	1:D:205:ARG:NH2	2.43	0.51
1:B:50:HIS:CE1	1:B:86:LEU:HD13	2.46	0.51
1:A:228:THR:OG1	1:A:229:HIS:ND1	2.37	0.51
1:E:50:HIS:CE1	1:E:86:LEU:HD13	2.46	0.51
1:A:238:GLU:HA	1:A:241:LEU:HD12	1.92	0.51
1:A:212:LEU:O	1:A:257:ARG:NH1	2.41	0.51
1:B:41:GLY:O	1:B:45:ILE:HG12	2.11	0.50
1:A:41:GLY:O	1:A:45:ILE:HG12	2.12	0.50
1:E:205:ARG:HB2	1:E:213:GLU:HG3	1.92	0.50
1:E:191:ASN:HB3	1:E:206:LEU:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:288:SER:HG	1:D:290:SER:HG	1.54	0.50
1:A:191:ASN:HB3	1:A:206:LEU:HB3	1.93	0.50
1:A:280:CYS:N	1:A:331:TYR:OH	2.42	0.50
1:A:181:SER:HA	1:A:184:ILE:HD12	1.94	0.50
1:E:203:GLU:OE2	1:E:205:ARG:NH2	2.44	0.50
1:C:41:GLY:O	1:C:45:ILE:HG12	2.12	0.50
1:F:288:SER:OG	1:F:290:SER:OG	2.29	0.50
1:E:41:GLY:O	1:E:45:ILE:HG12	2.12	0.50
1:E:265:GLN:NE2	1:E:351:ASN:HD21	2.07	0.49
1:F:79:LEU:O	1:F:84:VAL:N	2.45	0.49
1:D:274:GLU:HB3	1:D:324:GLN:HB2	1.94	0.49
1:E:280:CYS:HB3	1:E:300:THR:HG21	1.93	0.49
1:A:203:GLU:HB3	1:A:214:ARG:HB3	1.95	0.49
1:C:227:GLU:OE2	1:C:251:ARG:HD3	2.12	0.49
1:A:228:THR:HG1	1:A:229:HIS:CE1	2.31	0.49
1:F:278:ASP:HB3	1:F:322:ARG:HE	1.76	0.49
1:A:206:LEU:HD13	1:A:210:TRP:CD1	2.47	0.49
1:B:215:ALA:HB3	1:B:275:ILE:HB	1.94	0.49
1:C:228:THR:HG1	1:C:229:HIS:CE1	2.31	0.49
1:C:30:ASP:N	1:C:30:ASP:OD1	2.45	0.49
1:E:283:THR:HG22	1:E:308:ILE:O	2.13	0.49
1:B:291:CYS:SG	1:B:292:GLY:N	2.85	0.48
1:F:212:LEU:O	1:F:257:ARG:NH1	2.41	0.48
1:B:192:LEU:HD11	1:B:203:GLU:HG3	1.95	0.48
1:A:265:GLN:NE2	1:A:351:ASN:HD21	2.11	0.48
1:D:205:ARG:HB2	1:D:213:GLU:HG3	1.94	0.48
1:D:291:CYS:SG	1:D:292:GLY:N	2.86	0.48
1:A:71:VAL:HG22	1:A:75:LEU:HG	1.96	0.48
1:B:227:GLU:OE2	1:B:251:ARG:HD3	2.13	0.48
1:D:283:THR:OG1	1:D:331:TYR:OH	2.12	0.48
1:F:228:THR:HG1	1:F:229:HIS:CE1	2.32	0.48
1:B:206:LEU:HB2	1:B:210:TRP:CE2	2.49	0.48
1:D:232:TRP:CD2	1:D:253:ASN:HB2	2.49	0.48
1:E:206:LEU:HB2	1:E:210:TRP:CE2	2.49	0.48
1:D:42:LEU:O	1:D:46:ILE:HG13	2.13	0.47
1:E:291:CYS:SG	1:E:292:GLY:N	2.87	0.47
1:E:226:PRO:O	1:E:230:THR:OG1	2.30	0.47
1:D:181:SER:HA	1:D:184:ILE:HD12	1.96	0.47
1:E:60:VAL:HG22	1:E:150:TRP:NE1	2.29	0.47
1:E:30:ASP:OD1	1:E:30:ASP:N	2.48	0.47
1:D:260:TYR:CE2	1:D:321:LEU:HB2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:41:GLY:O	1:D:45:ILE:HG12	2.14	0.47
1:A:291:CYS:SG	1:A:292:GLY:N	2.87	0.47
1:A:280:CYS:HB3	1:A:300:THR:HG21	1.96	0.47
1:A:107:THR:O	1:A:108:THR:OG1	2.32	0.47
1:A:285:VAL:HG11	1:A:335:ILE:HD12	1.96	0.47
1:F:90:VAL:HA	1:F:135:VAL:HB	1.97	0.47
1:F:265:GLN:HE21	1:F:351:ASN:HD21	1.62	0.47
1:E:107:THR:O	1:E:108:THR:OG1	2.30	0.47
1:E:206:LEU:HD13	1:E:210:TRP:CD1	2.49	0.47
1:C:291:CYS:SG	1:C:292:GLY:N	2.88	0.46
1:E:205:ARG:NH1	1:E:213:GLU:HB3	2.30	0.46
1:E:73:ASP:O	1:E:77:THR:HG23	2.15	0.46
1:D:90:VAL:HA	1:D:135:VAL:HB	1.97	0.46
1:E:260:TYR:CZ	1:E:316:CYS:HB2	2.50	0.46
1:F:291:CYS:SG	1:F:292:GLY:N	2.88	0.46
1:D:241:LEU:O	1:D:262:THR:HA	2.15	0.46
1:E:225:TRP:HA	1:E:226:PRO:HD3	1.82	0.46
1:C:205:ARG:HB2	1:C:213:GLU:HG3	1.97	0.46
1:F:225:TRP:HA	1:F:226:PRO:HD3	1.80	0.46
1:E:280:CYS:HB2	1:E:331:TYR:CZ	2.51	0.46
1:E:72:LYS:O	1:E:76:ASN:ND2	2.49	0.46
1:B:335:ILE:O	1:B:336:ARG:NE	2.46	0.46
1:D:60:VAL:HG22	1:D:150:TRP:NE1	2.31	0.46
1:C:181:SER:HA	1:C:184:ILE:HD12	1.98	0.46
1:F:238:GLU:HA	1:F:241:LEU:HD12	1.98	0.46
1:B:203:GLU:HB3	1:B:214:ARG:HB3	1.98	0.46
1:E:100:ALA:O	1:E:103:ARG:NH1	2.48	0.46
1:F:276:ASP:OD2	1:F:322:ARG:NH2	2.48	0.46
1:C:71:VAL:HG22	1:C:75:LEU:HG	1.98	0.45
1:C:73:ASP:O	1:C:77:THR:HG23	2.17	0.45
1:D:280:CYS:HB2	1:D:331:TYR:CZ	2.51	0.45
1:E:228:THR:HG1	1:E:229:HIS:CE1	2.34	0.45
1:F:227:GLU:OE2	1:F:251:ARG:HD3	2.15	0.45
1:D:203:GLU:HB3	1:D:214:ARG:HB3	1.97	0.45
1:E:280:CYS:N	1:E:331:TYR:OH	2.46	0.45
1:F:34:TYR:HB2	1:F:67:MET:HB2	1.98	0.45
1:A:289:GLU:HG2	1:A:289:GLU:H	1.49	0.45
1:E:197:ASP:OD2	1:E:200:TYR:HB2	2.15	0.45
1:F:296:PRO:HB2	1:F:347:GLN:HB3	1.99	0.45
1:E:42:LEU:O	1:E:46:ILE:HG13	2.17	0.45
1:B:241:LEU:O	1:B:262:THR:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:335:ILE:O	1:E:336:ARG:NE	2.48	0.45
1:C:107:THR:O	1:C:108:THR:OG1	2.32	0.45
1:A:318:LEU:HD23	1:A:320:PRO:HD3	1.99	0.45
1:F:241:LEU:O	1:F:262:THR:HA	2.17	0.45
1:E:228:THR:OG1	1:E:229:HIS:ND1	2.40	0.45
1:E:32:TYR:HB3	1:E:167:MET:HE1	1.99	0.45
1:E:44:LYS:HD2	1:E:108:THR:HG21	1.99	0.45
1:B:212:LEU:O	1:B:257:ARG:NH1	2.46	0.45
1:E:260:TYR:CE2	1:E:321:LEU:HB2	2.52	0.44
1:B:280:CYS:HB2	1:B:331:TYR:CZ	2.51	0.44
1:E:291:CYS:O	1:E:314:ARG:NH2	2.50	0.44
1:B:188:VAL:HA	1:B:192:LEU:O	2.18	0.44
1:B:160:PHE:CZ	1:B:162:LEU:HD23	2.52	0.44
1:F:278:ASP:HB3	1:F:322:ARG:NE	2.32	0.44
1:E:238:GLU:HA	1:E:241:LEU:HD12	1.99	0.44
1:D:161:GLY:HA3	1:D:164:SER:O	2.17	0.44
1:B:32:TYR:CD2	1:B:165:THR:HB	2.52	0.44
1:E:81:GLU:HG3	1:E:82:ASN:N	2.31	0.44
1:C:216:VAL:HG22	1:C:274:GLU:HG3	1.98	0.44
1:C:160:PHE:CZ	1:C:162:LEU:HD23	2.52	0.44
1:F:30:ASP:N	1:F:30:ASP:OD1	2.50	0.44
1:F:335:ILE:O	1:F:336:ARG:NE	2.48	0.44
1:B:177:THR:O	1:B:224:THR:N	2.46	0.44
1:E:227:GLU:OE2	1:E:251:ARG:HD3	2.18	0.44
1:A:189:LYS:HE2	1:A:190:ASN:HD21	1.83	0.44
1:B:181:SER:HA	1:B:184:ILE:HD12	1.99	0.43
1:B:7:ASP:OD2	1:B:190:ASN:ND2	2.48	0.43
1:C:197:ASP:OD2	1:C:200:TYR:HB2	2.17	0.43
1:A:283:THR:HG22	1:A:308:ILE:O	2.18	0.43
1:E:34:TYR:HB2	1:E:67:MET:HB2	2.00	0.43
1:C:203:GLU:HB3	1:C:214:ARG:HB3	2.00	0.43
1:E:323:TYR:HB2	1:E:330:TRP:HB2	2.00	0.43
1:F:325:THR:HB	1:F:330:TRP:HE1	1.83	0.43
1:D:278:ASP:HB3	1:D:322:ARG:HE	1.84	0.43
1:A:21:ILE:O	1:B:18:GLY:HA3	2.17	0.43
1:B:278:ASP:HB3	1:B:322:ARG:HE	1.83	0.43
1:E:57:LEU:N	1:E:134:VAL:O	2.44	0.43
1:B:71:VAL:HG22	1:B:75:LEU:HG	2.00	0.43
1:E:302:THR:HG22	1:E:306:LYS:HB3	2.00	0.43
1:E:278:ASP:HB3	1:E:322:ARG:NE	2.34	0.43
1:B:50:HIS:ND1	1:B:86:LEU:HD13	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:228:THR:HG1	1:D:229:HIS:CE1	2.35	0.43
1:D:260:TYR:CZ	1:D:316:CYS:HB2	2.54	0.43
1:B:278:ASP:HB3	1:B:322:ARG:NE	2.33	0.43
1:E:318:LEU:HA	1:E:319:PRO:C	2.39	0.43
1:C:278:ASP:OD1	1:C:279:TYR:N	2.45	0.43
1:F:280:CYS:N	1:F:331:TYR:OH	2.50	0.43
1:A:102:LYS:HB2	1:A:148:ARG:O	2.19	0.43
1:D:283:THR:HG22	1:D:308:ILE:O	2.19	0.43
1:C:232:TRP:CD2	1:C:253:ASN:HB2	2.54	0.43
1:C:18:GLY:HA3	1:D:21:ILE:O	2.18	0.43
1:E:31:ARG:O	1:E:165:THR:N	2.47	0.42
1:D:312:CYS:HB3	1:D:338:GLN:OE1	2.19	0.42
1:B:30:ASP:N	1:B:30:ASP:OD1	2.50	0.42
1:B:103:ARG:NE	1:B:150:TRP:O	2.50	0.42
1:D:102:LYS:HB2	1:D:148:ARG:O	2.19	0.42
1:C:206:LEU:HD13	1:C:210:TRP:CD1	2.53	0.42
1:B:308:ILE:HD13	1:B:345:LEU:HD23	2.01	0.42
1:A:30:ASP:OD1	1:A:30:ASP:N	2.53	0.42
1:C:102:LYS:HB2	1:C:148:ARG:O	2.20	0.42
1:B:318:LEU:HD23	1:B:320:PRO:HD3	2.00	0.42
1:A:58:ARG:HG2	1:A:148:ARG:HD3	2.01	0.42
1:A:335:ILE:O	1:A:336:ARG:NE	2.49	0.42
1:F:289:GLU:HG2	1:F:289:GLU:H	1.51	0.42
1:E:48:LYS:HA	1:E:51:LYS:HB2	2.01	0.42
1:C:260:TYR:CE1	1:C:317:THR:HG22	2.52	0.42
1:C:265:GLN:NE2	1:C:351:ASN:HD21	2.17	0.42
1:E:241:LEU:O	1:E:262:THR:HA	2.20	0.42
1:B:34:TYR:CE1	1:B:169:LEU:HD21	2.55	0.42
1:F:232:TRP:CD2	1:F:253:ASN:HB2	2.55	0.42
1:C:280:CYS:HB3	1:C:300:THR:HG21	2.02	0.42
1:A:91:GLU:HG2	1:A:137:GLY:HA3	2.02	0.42
1:A:241:LEU:O	1:A:262:THR:HA	2.19	0.42
1:A:205:ARG:HB2	1:A:213:GLU:HG3	2.01	0.42
1:C:177:THR:O	1:C:224:THR:N	2.40	0.42
1:E:232:TRP:CG	1:E:253:ASN:HB2	2.55	0.42
1:A:318:LEU:HA	1:A:319:PRO:C	2.38	0.42
1:C:278:ASP:HB3	1:C:322:ARG:HE	1.85	0.42
1:E:102:LYS:HB2	1:E:148:ARG:O	2.20	0.42
1:F:293:HIS:O	1:F:336:ARG:HD2	2.20	0.42
1:C:318:LEU:HD23	1:C:320:PRO:HD3	2.02	0.42
1:F:283:THR:HG22	1:F:308:ILE:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:ALA:HB3	1:C:204:SER:OG	2.20	0.42
1:A:249:GLY:HA2	1:A:250:PRO:HD3	1.86	0.42
1:F:260:TYR:CE1	1:F:317:THR:HG22	2.50	0.42
1:D:238:GLU:HA	1:D:241:LEU:HD12	2.01	0.42
1:A:323:TYR:HB2	1:A:330:TRP:HB2	2.02	0.42
1:A:225:TRP:HA	1:A:226:PRO:HD3	1.79	0.41
1:C:335:ILE:O	1:C:336:ARG:NE	2.53	0.41
1:C:289:GLU:HG2	1:C:289:GLU:H	1.59	0.41
1:B:280:CYS:N	1:B:331:TYR:OH	2.50	0.41
1:A:87:SER:HB3	1:A:129:ALA:HB3	2.02	0.41
1:F:318:LEU:HD23	1:F:320:PRO:HD3	2.02	0.41
1:F:318:LEU:HA	1:F:319:PRO:C	2.41	0.41
1:D:30:ASP:OD1	1:D:30:ASP:N	2.52	0.41
1:A:278:ASP:HB3	1:A:322:ARG:NE	2.34	0.41
1:C:308:ILE:HD13	1:C:345:LEU:HD23	2.03	0.41
1:B:42:LEU:O	1:B:46:ILE:HG13	2.20	0.41
1:E:289:GLU:HG2	1:E:289:GLU:H	1.57	0.41
1:C:296:PRO:HB2	1:C:347:GLN:HB3	2.03	0.41
1:D:206:LEU:HB2	1:D:210:TRP:CE2	2.56	0.41
1:D:160:PHE:CZ	1:D:162:LEU:HD23	2.55	0.41
1:B:276:ASP:OD2	1:B:322:ARG:NH2	2.51	0.41
1:B:308:ILE:CD1	1:B:345:LEU:HD23	2.51	0.41
1:A:18:GLY:HA3	1:B:21:ILE:O	2.21	0.41
1:F:71:VAL:HG22	1:F:75:LEU:HG	2.02	0.41
1:F:249:GLY:HA2	1:F:250:PRO:HD3	1.93	0.41
1:B:93:GLN:HB2	1:B:136:ASP:HB3	2.03	0.41
1:E:323:TYR:HE2	1:E:332:GLY:HA2	1.85	0.41
1:A:299:ARG:NH1	1:A:327:SER:HB2	2.36	0.41
1:C:241:LEU:O	1:C:262:THR:HA	2.20	0.41
1:F:312:CYS:HB3	1:F:338:GLN:OE1	2.21	0.41
1:A:234:ASP:O	1:A:253:ASN:ND2	2.54	0.41
1:F:41:GLY:O	1:F:45:ILE:HG12	2.20	0.41
1:D:50:HIS:HE1	1:D:131:ASN:HD22	1.69	0.41
1:F:159:GLY:N	1:F:166:ARG:O	2.43	0.41
1:B:60:VAL:HG22	1:B:150:TRP:NE1	2.36	0.41
1:B:260:TYR:CZ	1:B:316:CYS:HB2	2.56	0.41
1:B:278:ASP:OD1	1:B:279:TYR:N	2.45	0.41
1:C:318:LEU:HA	1:C:319:PRO:C	2.41	0.41
1:A:40:GLN:N	1:A:40:GLN:OE1	2.53	0.41
1:E:325:THR:HB	1:E:330:TRP:HE1	1.86	0.40
1:E:249:GLY:HA2	1:E:250:PRO:HD3	1.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:267:PRO:HB2	1:E:270:GLU:HG3	2.02	0.40
1:B:242:ILE:HG12	1:B:256:ARG:HA	2.02	0.40
1:D:32:TYR:HB3	1:D:167:MET:SD	2.61	0.40
1:A:227:GLU:OE2	1:A:251:ARG:HD3	2.21	0.40
1:F:102:LYS:HB2	1:F:148:ARG:O	2.22	0.40
1:D:232:TRP:CG	1:D:253:ASN:HB2	2.57	0.40
1:E:234:ASP:O	1:E:253:ASN:ND2	2.54	0.40
1:E:243:ILE:HA	1:E:244:PRO:HD3	1.93	0.40
1:D:71:VAL:HG22	1:D:75:LEU:HG	2.02	0.40
1:D:257:ARG:HG3	1:D:258:PRO:HD2	2.03	0.40
1:A:90:VAL:HA	1:A:135:VAL:HB	2.03	0.40
1:E:106:ALA:HB2	1:E:171:VAL:HB	2.04	0.40
1:E:330:TRP:CD1	1:E:330:TRP:N	2.89	0.40
1:C:206:LEU:HB2	1:C:210:TRP:CE2	2.56	0.40
1:B:225:TRP:HA	1:B:226:PRO:HD3	1.77	0.40
1:D:228:THR:OG1	1:D:229:HIS:ND1	2.42	0.40
1:B:35:TYR:O	1:B:168:PHE:HA	2.21	0.40
1:F:242:ILE:HG12	1:F:256:ARG:HA	2.03	0.40
1:B:107:THR:O	1:B:108:THR:OG1	2.34	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	334/377 (89%)	323 (97%)	10 (3%)	1 (0%)	46	77
1	B	334/377 (89%)	323 (97%)	10 (3%)	1 (0%)	46	77
1	C	334/377 (89%)	323 (97%)	10 (3%)	1 (0%)	46	77
1	D	334/377 (89%)	322 (96%)	11 (3%)	1 (0%)	46	77
1	E	334/377 (89%)	322 (96%)	11 (3%)	1 (0%)	46	77

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	F	334/377 (89%)	323 (97%)	10 (3%)	1 (0%)	46 77
All	All	2004/2262 (89%)	1936 (97%)	62 (3%)	6 (0%)	46 77

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	108	THR
1	F	108	THR
1	A	108	THR
1	B	108	THR
1	C	108	THR
1	E	108	THR

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	296/329 (90%)	286 (97%)	10 (3%)	44 76
1	B	296/329 (90%)	287 (97%)	9 (3%)	48 80
1	C	296/329 (90%)	285 (96%)	11 (4%)	41 74
1	D	296/329 (90%)	286 (97%)	10 (3%)	44 76
1	E	296/329 (90%)	285 (96%)	11 (4%)	41 74
1	F	296/329 (90%)	287 (97%)	9 (3%)	48 80
All	All	1776/1974 (90%)	1716 (97%)	60 (3%)	44 76

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	PHE
1	A	30	ASP
1	A	31	ARG
1	A	52	GLU
1	A	58	ARG

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Mol	Chain	Res	Type
1	A	107	THR
1	A	289	GLU
1	A	294	ARG
1	A	334	GLU
1	A	345	LEU
1	B	20	PHE
1	B	31	ARG
1	B	52	GLU
1	B	58	ARG
1	B	107	THR
1	B	289	GLU
1	B	294	ARG
1	B	334	GLU
1	B	345	LEU
1	C	20	PHE
1	C	30	ASP
1	C	31	ARG
1	C	52	GLU
1	C	58	ARG
1	C	81	GLU
1	C	107	THR
1	C	289	GLU
1	C	294	ARG
1	C	334	GLU
1	C	345	LEU
1	D	20	PHE
1	D	31	ARG
1	D	52	GLU
1	D	58	ARG
1	D	107	THR
1	D	289	GLU
1	D	294	ARG
1	D	329	CYS
1	D	334	GLU
1	D	345	LEU
1	E	20	PHE
1	E	30	ASP
1	E	31	ARG
1	E	52	GLU
1	E	58	ARG
1	E	107	THR
1	E	289	GLU

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Mol	Chain	Res	Type
1	E	294	ARG
1	E	329	CYS
1	E	334	GLU
1	E	345	LEU
1	F	20	PHE
1	F	31	ARG
1	F	52	GLU
1	F	58	ARG
1	F	107	THR
1	F	289	GLU
1	F	294	ARG
1	F	334	GLU
1	F	345	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	351	ASN
1	B	351	ASN
1	C	50	HIS
1	C	351	ASN
1	D	50	HIS
1	D	351	ASN
1	E	50	HIS
1	E	351	ASN
1	F	351	ASN

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)

9 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	NAG	A	401	1	14,14,15	0.21	0	15,19,21	0.46	0
3	SO4	A	402	-	4,4,4	0.34	0	6,6,6	0.14	0
2	NAG	B	401	1	14,14,15	0.35	0	15,19,21	0.45	0
2	NAG	C	401	1	14,14,15	0.16	0	15,19,21	0.47	0
3	SO4	C	402	-	4,4,4	0.26	0	6,6,6	0.12	0
2	NAG	D	401	1	14,14,15	0.15	0	15,19,21	0.37	0
2	NAG	E	401	1	14,14,15	0.33	0	15,19,21	0.56	0
2	NAG	F	401	1	14,14,15	0.16	0	15,19,21	0.52	0
3	SO4	F	402	-	4,4,4	0.32	0	6,6,6	0.16	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	NAG	A	401	1	-	0/6/23/26	0/1/1/1
3	SO4	A	402	-	-	0/0/0/0	0/0/0/0
2	NAG	B	401	1	-	0/6/23/26	0/1/1/1
2	NAG	C	401	1	-	0/6/23/26	0/1/1/1
3	SO4	C	402	-	-	0/0/0/0	0/0/0/0
2	NAG	D	401	1	-	0/6/23/26	0/1/1/1
2	NAG	E	401	1	-	0/6/23/26	0/1/1/1
2	NAG	F	401	1	-	0/6/23/26	0/1/1/1
3	SO4	F	402	-	-	0/0/0/0	0/0/0/0

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.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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^{th} 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	338/377 (89%)	0.08	4 (1%)	81	76	22, 57, 101, 140	0
1	B	338/377 (89%)	0.01	3 (0%)	85	82	25, 63, 109, 136	0
1	C	338/377 (89%)	0.20	14 (4%)	41	34	56, 88, 130, 144	0
1	D	338/377 (89%)	0.21	11 (3%)	50	43	55, 90, 128, 142	0
1	E	338/377 (89%)	0.50	28 (8%)	14	9	57, 96, 135, 170	0
1	F	338/377 (89%)	0.23	18 (5%)	30	23	60, 91, 123, 158	0
All	All	2028/2262 (89%)	0.20	78 (3%)	44	37	22, 83, 127, 170	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	109	GLU	9.9
1	D	109	GLU	8.1
1	C	109	GLU	6.0
1	E	84	VAL	5.2
1	A	37	GLU	4.8
1	E	86	LEU	4.8
1	F	191	ASN	4.7
1	E	72	LYS	4.3
1	E	45	ILE	4.3
1	F	8	ILE	4.2
1	E	103	ARG	4.1
1	C	184	ILE	4.0
1	F	160	PHE	4.0
1	E	47	GLN	3.8
1	D	86	LEU	3.8
1	C	182	LYS	3.7
1	F	343	LYS	3.5
1	E	79	LEU	3.4
1	D	307	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	F	308	ILE	3.2
1	E	287	LEU	3.2
1	E	75	LEU	3.1
1	C	307	LEU	3.1
1	E	104	LEU	3.1
1	E	19	VAL	3.1
1	C	306	LYS	3.0
1	E	128	LEU	3.0
1	F	307	LEU	3.0
1	E	85	ASP	3.0
1	E	71	VAL	2.9
1	A	14	ARG	2.9
1	D	173	GLU	2.9
1	E	107	THR	2.8
1	B	37	GLU	2.8
1	C	8	ILE	2.7
1	F	321	LEU	2.7
1	C	285	VAL	2.7
1	C	153	LEU	2.7
1	E	68	TRP	2.7
1	E	307	LEU	2.6
1	F	2	THR	2.6
1	B	307	LEU	2.5
1	E	153	LEU	2.5
1	F	339	ARG	2.5
1	F	75	LEU	2.5
1	D	192	LEU	2.4
1	F	340	HIS	2.4
1	D	191	ASN	2.4
1	E	41	GLY	2.4
1	F	212	LEU	2.4
1	D	171	VAL	2.4
1	D	189	LYS	2.4
1	C	71	VAL	2.4
1	E	88	VAL	2.3
1	E	129	ALA	2.3
1	F	210	TRP	2.3
1	E	46	ILE	2.3
1	C	171	VAL	2.3
1	F	273	VAL	2.3
1	C	275	ILE	2.3
1	A	191	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	107	THR	2.2
1	C	6	ILE	2.2
1	D	169	LEU	2.2
1	E	36	PRO	2.2
1	F	220	VAL	2.2
1	E	37	GLU	2.1
1	C	174	SER	2.1
1	F	9	SER	2.1
1	B	109	GLU	2.1
1	D	88	VAL	2.0
1	F	342	GLU	2.0
1	E	340	HIS	2.0
1	F	192	LEU	2.0
1	A	20	PHE	2.0
1	D	11	GLN	2.0
1	E	34	TYR	2.0
1	E	171	VAL	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 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, 95^{th} 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
3	SO4	F	402	5/5	0.97	0.20	0.79	92,93,93,93	0
3	SO4	A	402	5/5	0.99	0.16	0.22	87,88,89,89	0
3	SO4	C	402	5/5	0.97	0.10	-1.97	97,98,98,98	0
2	NAG	F	401	14/15	0.95	0.10	-	75,78,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	NAG	E	401	14/15	0.91	0.17	-	76,78,80,81	0
2	NAG	C	401	14/15	0.96	0.10	-	77,81,82,82	0
2	NAG	B	401	14/15	0.96	0.13	-	66,69,72,72	0
2	NAG	A	401	14/15	0.95	0.11	-	56,58,61,61	0
2	NAG	D	401	14/15	0.96	0.15	-	69,75,80,80	0

6.5 Other polymers

There are no such residues in this entry.