wwPDB X-ray Structure Validation Summary Report (i)

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PDB ID	:	1EJ6
Title	:	Reovirus core
Authors	:	Reinisch, K.M.; Nibert, M.L.; Harrison, S.C.
Deposited on	:	2000-02-29
Resolution	:	3.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i)) were used in the production of this report:

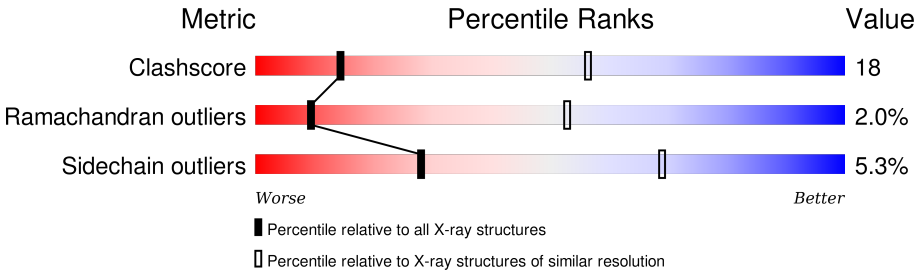
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 3.60 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))
Clashscore	102246	1010 (3.74-3.46)
Ramachandran outliers	100387	1007 (3.76-3.44)
Sidechain outliers	100360	1007 (3.76-3.44)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1289	67% 29% ·
2	B	1275	53% 25% · 19%
2	C	1275	61% 32% · ·
3	D	418	64% 33% ·
3	E	418	61% 34% ·

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 34487 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 LAMBDA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1284	Total	C	N	O	S	0	0	0
			10126	6468	1699	1917	42			

- Molecule 2 is a protein called LAMBDA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1031	Total	C	N	O	S	0	0	0
			8143	5208	1375	1510	50			
2	C	1221	Total	C	N	O	S	0	0	0
			9591	6078	1649	1809	55			

- Molecule 3 is a protein called SIGMA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	417	Total	C	N	O	S	0	0	0
			3313	2092	600	604	17			
3	E	417	Total	C	N	O	S	0	0	0
			3313	2092	600	604	17			

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	Zn	0	0
			1	1		

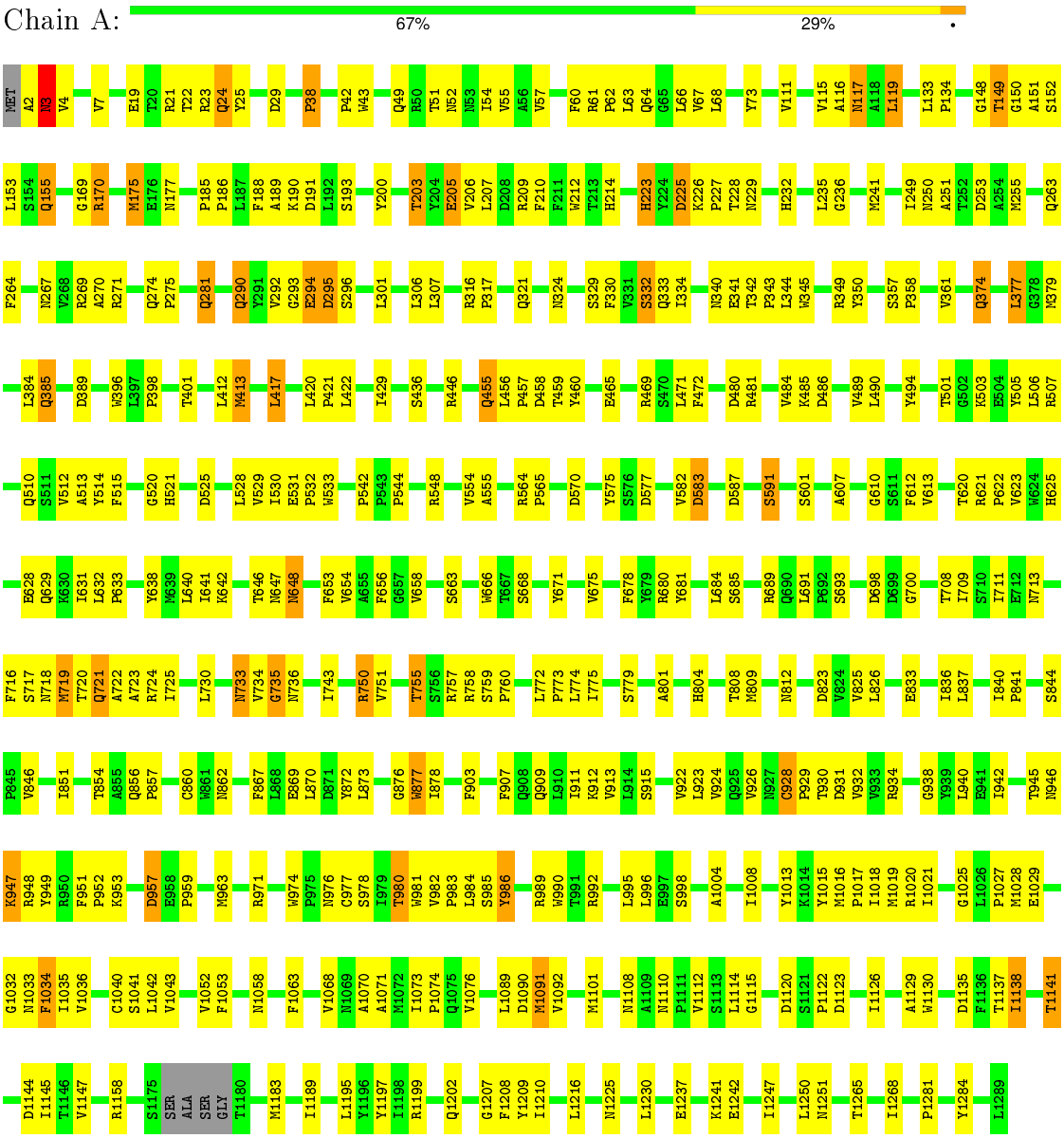
3 Residue-property plots (i)

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.

Note EDS was not executed.

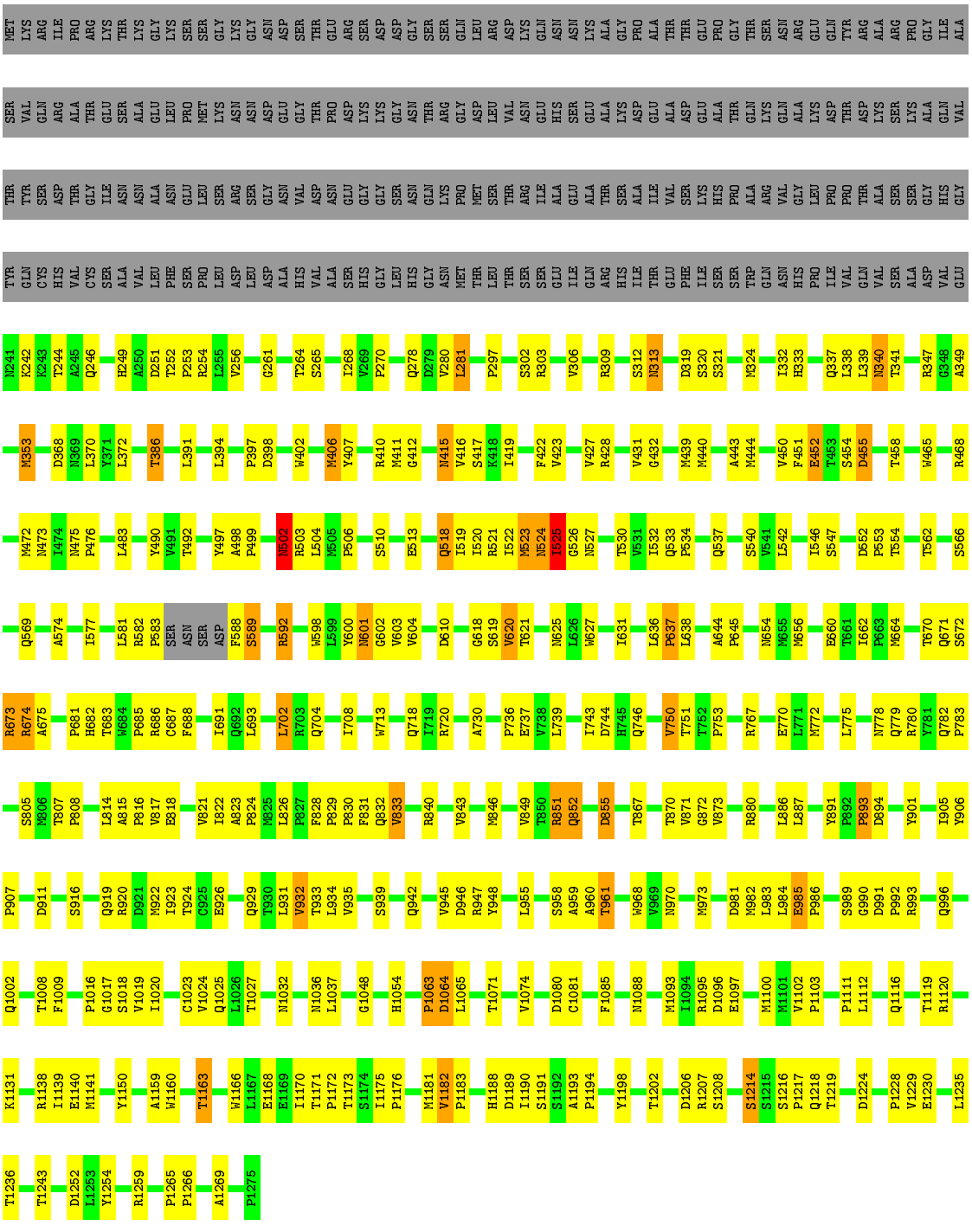
- Molecule 1: LAMBDA2

Chain A:



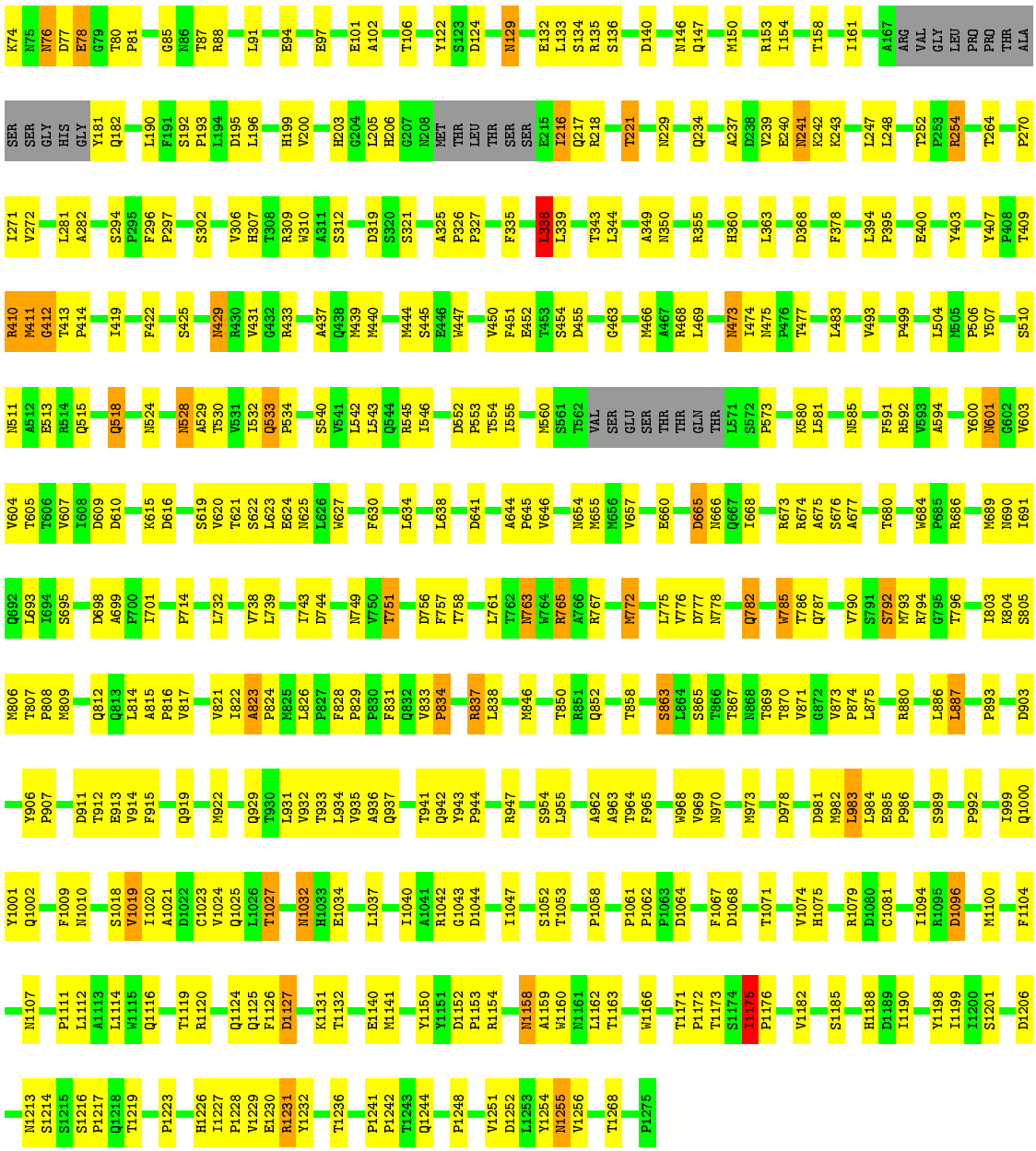
- Molecule 2: LAMBDA1

Chain B:



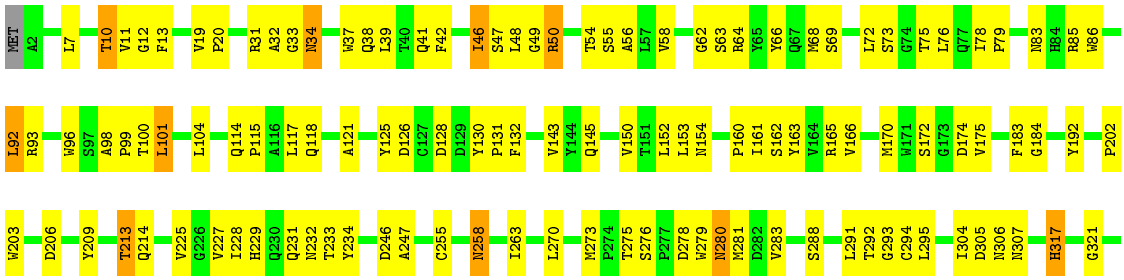
- Molecule 2: LAMBDA1

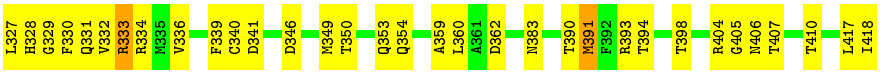
Chain C:



- Molecule 3: SIGMA2

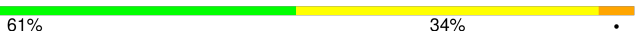
Chain D:

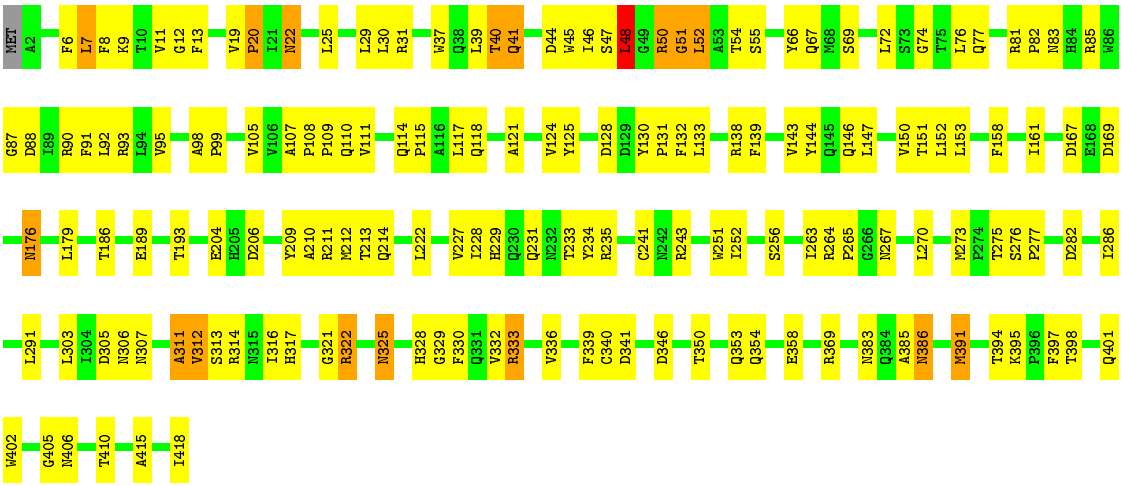




- Molecule 3: SIGMA2

Chain E:





4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	F 4 3 2	Depositor
Cell constants a, b, c, α, β, γ	1255.00Å 1255.00Å 1255.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.60	Depositor
% Data completeness (in resolution range)	88.5 (20.00-3.60)	Depositor
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.206 , 0.208	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	34487	wwPDB-VP
Average B, all atoms (Å^2)	14.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.42	0/10384	0.62	0/14170
2	B	0.47	0/8363	0.66	0/11454
2	C	0.46	0/9833	0.65	0/13437
3	D	0.45	0/3398	0.62	0/4626
3	E	0.44	0/3398	0.63	0/4626
All	All	0.45	0/35376	0.64	0/48313

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	10126	0	9906	315	0
2	B	8143	0	8063	302	0
2	C	9591	0	9453	358	0
3	D	3313	0	3215	139	0
3	E	3313	0	3215	143	0
4	C	1	0	0	0	0
All	All	34487	0	33852	1231	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.

The worst 5 of 1231 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:1171:THR:HG22	2:C:1173:THR:H	1.08	1.16
1:A:1138:ILE:H	1:A:1138:ILE:HD12	1.21	1.05
2:C:106:THR:HG22	2:C:122:TYR:H	1.15	1.04
1:A:149:THR:HG22	1:A:151:ALA:H	1.22	1.01
2:B:1171:THR:HG22	2:B:1173:THR:H	1.22	1.01

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	1280/1289 (99%)	1131 (88%)	125 (10%)	24 (2%)	10	53
2	B	1027/1275 (80%)	872 (85%)	135 (13%)	20 (2%)	10	53
2	C	1211/1275 (95%)	1063 (88%)	127 (10%)	21 (2%)	11	55
3	D	415/418 (99%)	359 (86%)	46 (11%)	10 (2%)	7	49
3	E	415/418 (99%)	361 (87%)	41 (10%)	13 (3%)	5	43
All	All	4348/4675 (93%)	3786 (87%)	474 (11%)	88 (2%)	9	53

5 of 88 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	149	THR
1	A	193	SER
1	A	717	SER
1	A	735	GLY
1	A	945	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	1118/1121 (100%)	1062 (95%)	56 (5%)	30	70
2	B	911/1115 (82%)	857 (94%)	54 (6%)	24	66
2	C	1070/1115 (96%)	1013 (95%)	57 (5%)	28	69
3	D	352/353 (100%)	336 (96%)	16 (4%)	34	74
3	E	352/353 (100%)	335 (95%)	17 (5%)	31	72
All	All	3803/4057 (94%)	3603 (95%)	200 (5%)	28	69

5 of 200 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	852	GLN
2	C	56	ARG
3	E	22	ASN
2	B	939	SER
2	B	1081	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 120 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	1116	GLN
2	C	390	ASN
3	E	176	ASN
2	B	1149	HIS
2	C	129	ASN

5.3.3 RNA (i)

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.