wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 10:12 PM GMT

PDB ID	:	1SID
Title	:	MURINE POLYOMAVIRUS COMPLEXED WITH 3'SIALYL LACTOSE
Authors	:	Stehle, T.; Harrison, S.C.
Deposited on	:	1995-12-12
Resolution	:	3.65 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:

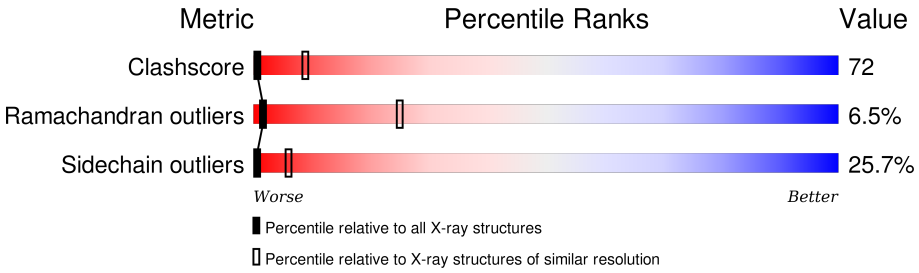
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 3.65 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	1125 (3.82-3.50)
Ramachandran outliers	100387	1079 (3.82-3.50)
Sidechain outliers	100360	1078 (3.82-3.50)

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	383	23% 50% 20%
1	B	383	25% 46% 22%
1	C	383	22% 48% 21% 7%
1	D	383	20% 44% 22% 11%
1	E	383	20% 52% 21%
1	F	383	20% 46% 23% 8%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 17003 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 POLYOMAVIRUS COAT PROTEIN VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	366	Total	C	N	O	S	0	0	0
			2849	1804	479	550	16			
1	B	367	Total	C	N	O	S	0	0	0
			2857	1808	481	552	16			
1	C	357	Total	C	N	O	S	0	0	0
			2784	1761	468	539	16			
1	D	340	Total	C	N	O	S	0	0	0
			2645	1674	445	511	15			
1	E	367	Total	C	N	O	S	0	0	0
			2857	1808	481	552	16			
1	F	354	Total	C	N	O	S	0	0	0
			2753	1740	461	536	16			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	6	ALA	SER	CONFLICT	UNP P49302
B	6	ALA	SER	CONFLICT	UNP P49302
C	6	ALA	SER	CONFLICT	UNP P49302
D	6	ALA	SER	CONFLICT	UNP P49302
E	6	ALA	SER	CONFLICT	UNP P49302
F	6	ALA	SER	CONFLICT	UNP P49302

- Molecule 2 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	3	Total	C	N	O	0	0
			43	23	1	19		
2	B	3	Total	C	N	O	0	0
			43	23	1	19		
2	C	3	Total	C	N	O	0	0
			43	23	1	19		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	D	3	Total	C	N	O	0	0
			43	23	1	19		
2	E	3	Total	C	N	O	0	0
			43	23	1	19		
2	F	3	Total	C	N	O	0	0
			43	23	1	19		

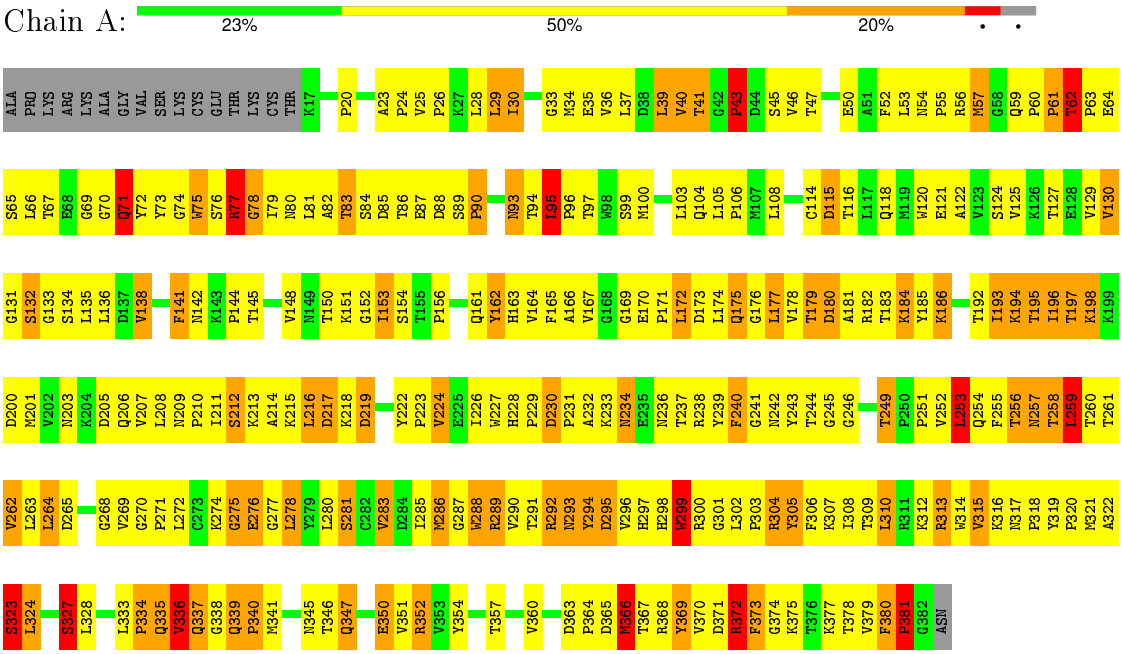
3 Residue-property plots (i)

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.

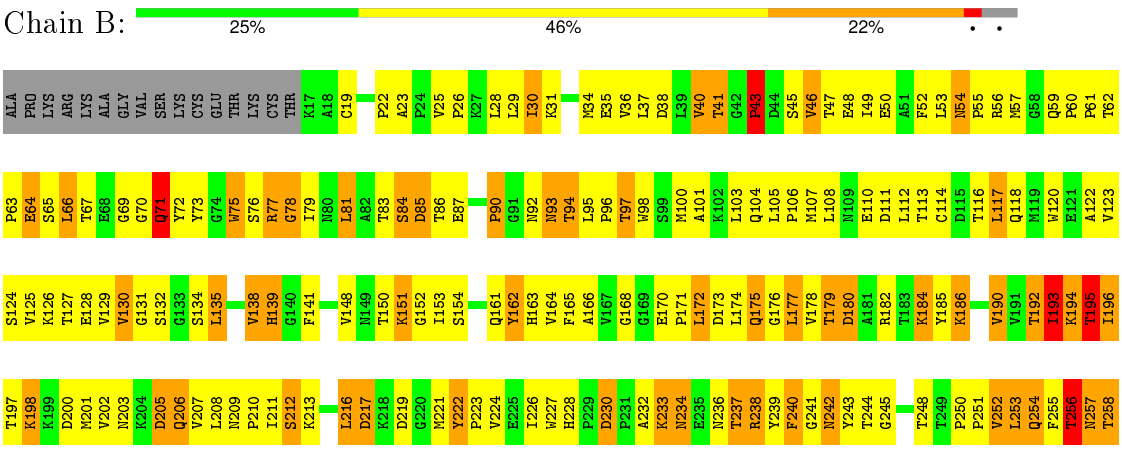
- Molecule 1: POLYOMAVIRUS COAT PROTEIN VP1

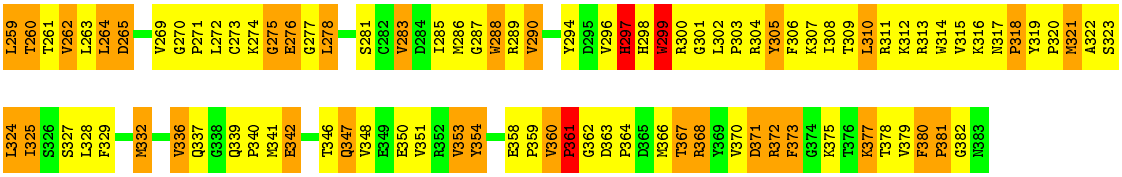
Chain A:



- Molecule 1: POLYOMAVIRUS COAT PROTEIN VP1

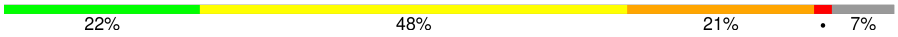
Chain B:

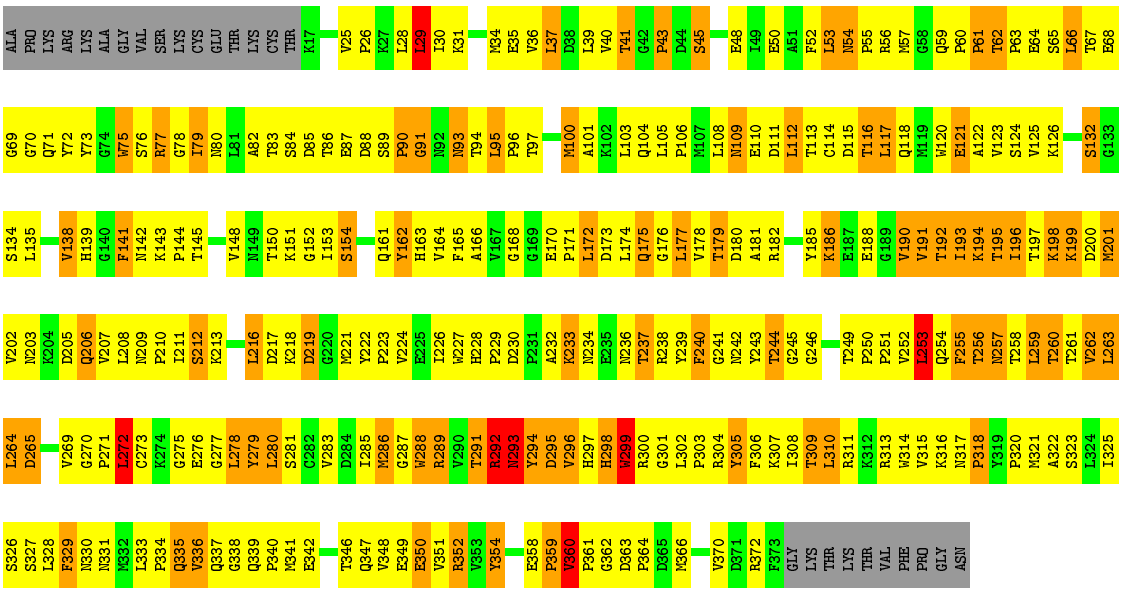




• Molecule 1: POLYOMAVIRUS COAT PROTEIN VP1

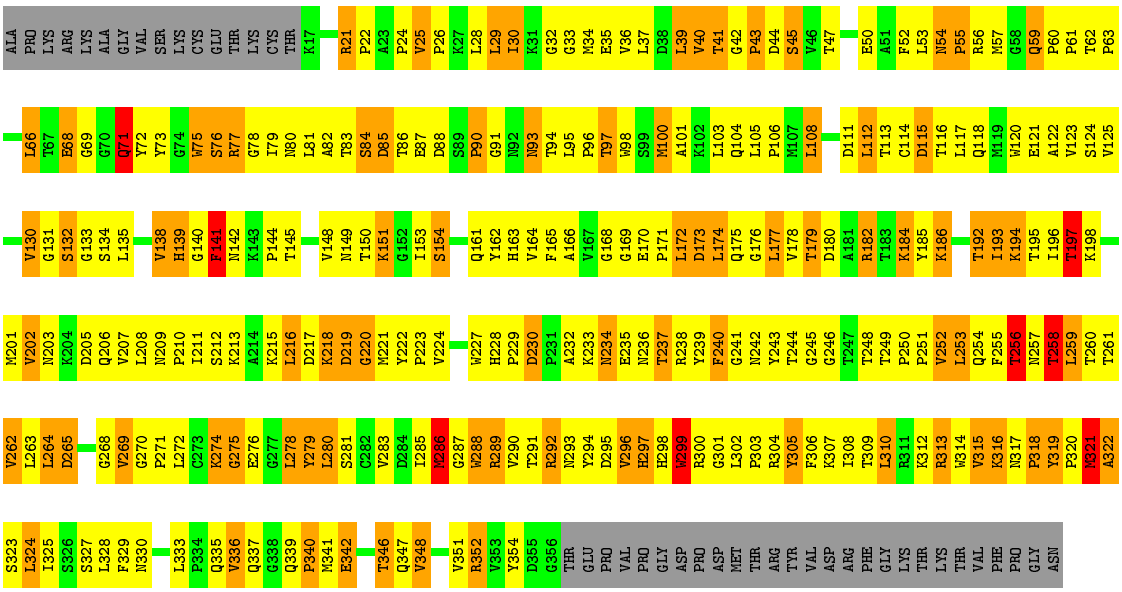
Chain C:





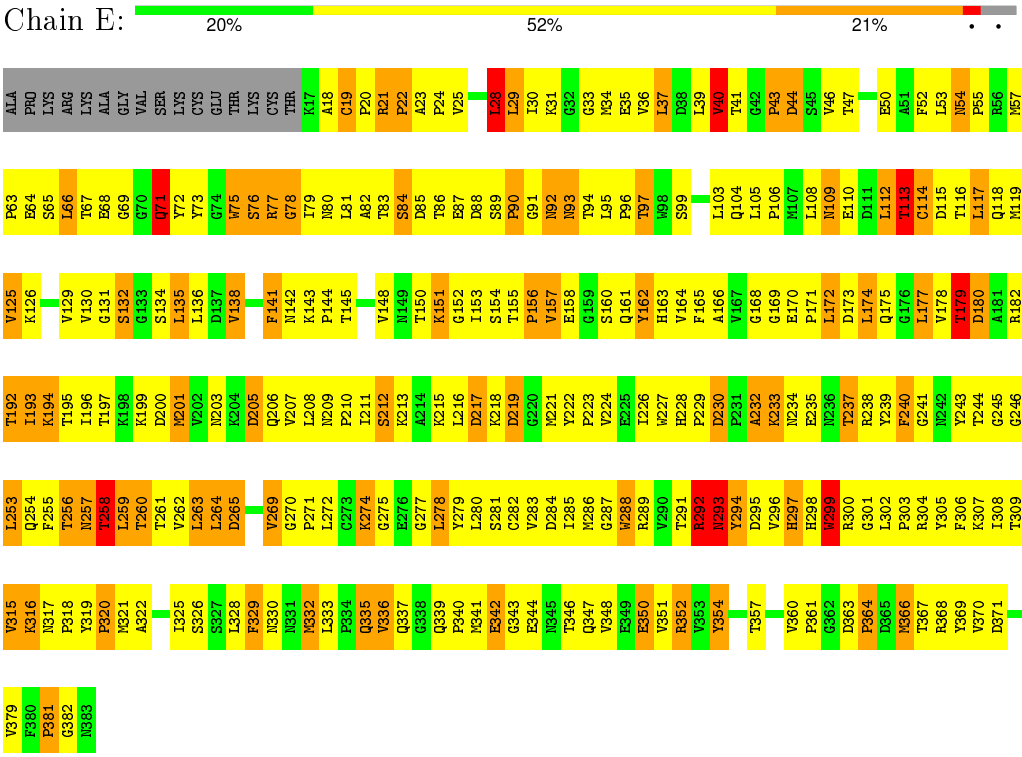
• Molecule 1: POLYOMAVIRUS COAT PROTEIN VP1

Chain D:



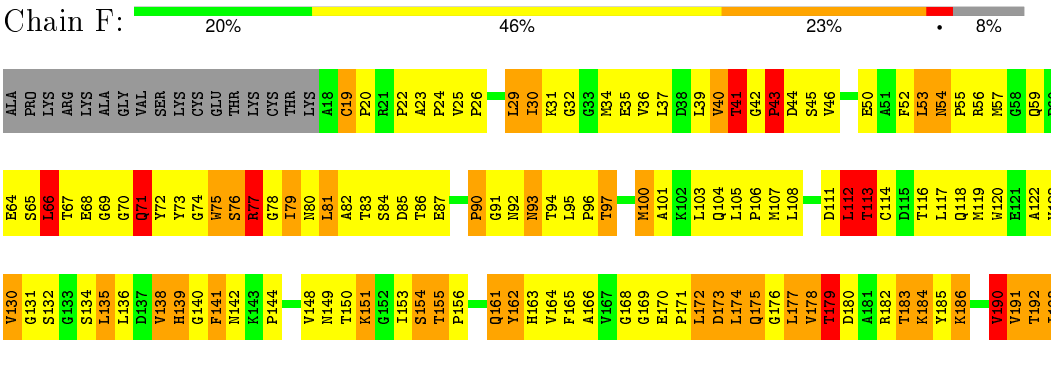
• Molecule 1: POLYOMAVIRUS COAT PROTEIN VP1

Chain E:



• Molecule 1: POLYOMAVIRUS COAT PROTEIN VP1

Chain F:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α, β, γ	570.00Å 570.00Å 570.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 3.65	Depositor
% Data completeness (in resolution range)	73.0 (12.00-3.65)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.236 , 0.253	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	17003	wwPDB-VP
Average B, all atoms (Å^2)	77.0	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: SIA, BGC, GAL

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	0.96	2/2920 (0.1%)	1.26	22/3981 (0.6%)
1	B	0.95	0/2927	1.25	19/3989 (0.5%)
1	C	0.97	0/2852	1.26	21/3888 (0.5%)
1	D	1.01	2/2708 (0.1%)	1.27	23/3690 (0.6%)
1	E	1.00	1/2928 (0.0%)	1.34	23/3992 (0.6%)
1	F	0.96	2/2820 (0.1%)	1.25	21/3847 (0.5%)
All	All	0.98	7/17155 (0.0%)	1.27	129/23387 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	3
1	C	0	4
1	D	0	5
1	E	0	2
1	F	0	3
All	All	0	22

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	336	VAL	C-N	13.07	1.64	1.34
1	D	342	GLU	CD-OE2	6.37	1.32	1.25
1	A	336	VAL	C-N	-5.83	1.20	1.34
1	D	299	TRP	CB-CG	5.46	1.60	1.50
1	F	234	ASN	CB-CG	5.37	1.63	1.51

The worst 5 of 129 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	336	VAL	O-C-N	21.97	157.85	122.70
1	A	336	VAL	O-C-N	-17.79	94.24	122.70
1	E	336	VAL	CA-C-N	-16.45	81.00	117.20
1	C	29	LEU	CA-CB-CG	-11.50	88.85	115.30
1	F	264	LEU	CA-CB-CG	-11.09	89.80	115.30

There are no chirality outliers.

5 of 22 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	162	TYR	Sidechain
1	A	305	TYR	Sidechain
1	A	336	VAL	Mainchain,Peptide
1	A	71	GLN	Mainchain
1	B	71	GLN	Mainchain

5.2 Too-close contacts (i)

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	2849	0	2814	457	2
1	B	2857	0	2820	454	0
1	C	2784	0	2743	441	0
1	D	2645	0	2616	404	0
1	E	2857	0	2821	472	0
1	F	2753	0	2710	420	0
2	A	43	0	37	1	0
2	B	43	0	37	5	0
2	C	43	0	37	3	0
2	D	43	0	37	1	0
2	E	43	0	37	3	0
2	F	43	0	37	5	0
All	All	17003	0	16746	2434	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 72.

The worst 5 of 2434 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:A:328:LEU:CD2	1:A:333:LEU:HD21	1.37	1.52
1:A:328:LEU:HD21	1:A:333:LEU:CD2	1.40	1.50
1:A:175:GLN:HB2	1:A:230:ASP:HB2	1.26	1.11
1:F:175:GLN:HB2	1:F:230:ASP:HB2	1.33	1.10
1:B:336:VAL:HA	1:B:337:GLN:N	1.68	1.09

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:LYS:CD	1:A:328:LEU:O[2_555]	1.75	0.45
1:A:217:ASP:O	1:A:336:VAL:O[2_555]	2.05	0.15

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	364/383 (95%)	270 (74%)	67 (18%)	27 (7%)	1	20
1	B	363/383 (95%)	280 (77%)	62 (17%)	21 (6%)	2	27
1	C	353/383 (92%)	275 (78%)	60 (17%)	18 (5%)	2	30
1	D	336/383 (88%)	264 (79%)	58 (17%)	14 (4%)	3	36
1	E	365/383 (95%)	278 (76%)	62 (17%)	25 (7%)	1	23
1	F	350/383 (91%)	271 (77%)	45 (13%)	34 (10%)	1	13
All	All	2131/2298 (93%)	1638 (77%)	354 (17%)	139 (6%)	1	25

5 of 139 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	PRO
1	A	62	THR
1	A	148	VAL
1	A	183	THR
1	A	276	GLU

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	321/335 (96%)	244 (76%)	77 (24%)	1	7
1	B	322/335 (96%)	237 (74%)	85 (26%)	0	5
1	C	314/335 (94%)	238 (76%)	76 (24%)	1	7
1	D	298/335 (89%)	214 (72%)	84 (28%)	0	4
1	E	322/335 (96%)	241 (75%)	81 (25%)	1	6
1	F	311/335 (93%)	228 (73%)	83 (27%)	0	5
All	All	1888/2010 (94%)	1402 (74%)	486 (26%)	0	6

5 of 486 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	291	THR
1	D	179	THR
1	F	217	ASP
1	C	305	TYR
1	D	59	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 79 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	206	GLN
1	D	118	GLN
1	F	118	GLN
1	C	228	HIS

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Mol	Chain	Res	Type
1	D	54	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

18 carbohydrates 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	SIA	A	384	2	16,20,21	0.50	0	18,28,31	0.91	1 (5%)
2	GAL	A	385	2	11,11,12	0.35	0	14,15,17	1.32	1 (7%)
2	BGC	A	386	2	12,12,12	0.67	0	17,17,17	0.86	1 (5%)
2	SIA	B	384	2	16,20,21	0.58	0	18,28,31	0.77	0
2	GAL	B	385	2	11,11,12	0.55	0	14,15,17	1.77	1 (7%)
2	BGC	B	386	2	12,12,12	0.72	0	17,17,17	0.75	0
2	SIA	C	384	2	16,20,21	0.50	0	18,28,31	1.04	1 (5%)
2	GAL	C	385	2	11,11,12	0.38	0	14,15,17	1.96	1 (7%)
2	BGC	C	386	2	12,12,12	0.71	0	17,17,17	0.82	1 (5%)
2	SIA	D	384	2	16,20,21	0.73	0	18,28,31	1.30	2 (11%)
2	GAL	D	385	2	11,11,12	0.23	0	14,15,17	1.65	1 (7%)
2	BGC	D	386	2	12,12,12	0.70	0	17,17,17	0.84	1 (5%)
2	SIA	E	384	2	16,20,21	0.59	0	18,28,31	1.18	2 (11%)
2	GAL	E	385	2	11,11,12	0.24	0	14,15,17	1.67	1 (7%)
2	BGC	E	386	2	12,12,12	0.83	0	17,17,17	1.06	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SIA	F	384	2	16,20,21	0.79	0	18,28,31	1.09	1 (5%)
2	GAL	F	385	2	11,11,12	0.35	0	14,15,17	1.24	1 (7%)
2	BGC	F	386	2	12,12,12	0.83	0	17,17,17	0.88	1 (5%)

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	SIA	A	384	2	-	0/14/34/38	0/1/1/1
2	GAL	A	385	2	-	0/2/19/22	0/1/1/1
2	BGC	A	386	2	-	0/2/22/22	0/1/1/1
2	SIA	B	384	2	-	0/14/34/38	0/1/1/1
2	GAL	B	385	2	-	0/2/19/22	0/1/1/1
2	BGC	B	386	2	-	0/2/22/22	0/1/1/1
2	SIA	C	384	2	-	0/14/34/38	0/1/1/1
2	GAL	C	385	2	-	0/2/19/22	0/1/1/1
2	BGC	C	386	2	-	0/2/22/22	0/1/1/1
2	SIA	D	384	2	-	0/14/34/38	0/1/1/1
2	GAL	D	385	2	-	0/2/19/22	0/1/1/1
2	BGC	D	386	2	-	0/2/22/22	0/1/1/1
2	SIA	E	384	2	-	0/14/34/38	0/1/1/1
2	GAL	E	385	2	-	0/2/19/22	0/1/1/1
2	BGC	E	386	2	-	0/2/22/22	0/1/1/1
2	SIA	F	384	2	-	0/14/34/38	0/1/1/1
2	GAL	F	385	2	-	0/2/19/22	0/1/1/1
2	BGC	F	386	2	-	0/2/22/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	385	GAL	C1-C2-C3	-6.46	101.90	109.54
2	B	385	GAL	C1-C2-C3	-5.88	102.59	109.54
2	D	385	GAL	C1-C2-C3	-5.85	102.62	109.54
2	E	385	GAL	C1-C2-C3	-5.67	102.84	109.54
2	A	385	GAL	C1-C2-C3	-4.56	104.15	109.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	384	SIA	1	0
2	B	384	SIA	2	0
2	B	385	GAL	4	0
2	C	384	SIA	1	0
2	C	385	GAL	3	0
2	D	384	SIA	1	0
2	D	385	GAL	1	0
2	E	384	SIA	2	0
2	E	385	GAL	2	0
2	F	384	SIA	2	0
2	F	385	GAL	4	0

5.6 Ligand geometry (i)

There are no ligands in this entry.

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

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.