wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 01:05 PM GMT

PDB ID	:	3SLD
Title	:	Structural characterization of a GII.4 2004 norovirus variant (TCH05) bound to A trisaccharide
Authors	:	Shanker, S.; Choi, J.-M.; Sankaran, B.; Atmar, R.L.; Estes, M.K.; Prasad, B.V.V.
Deposited on	:	2011-06-24
Resolution	:	2.68 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 (1)) were used in the production of this report:

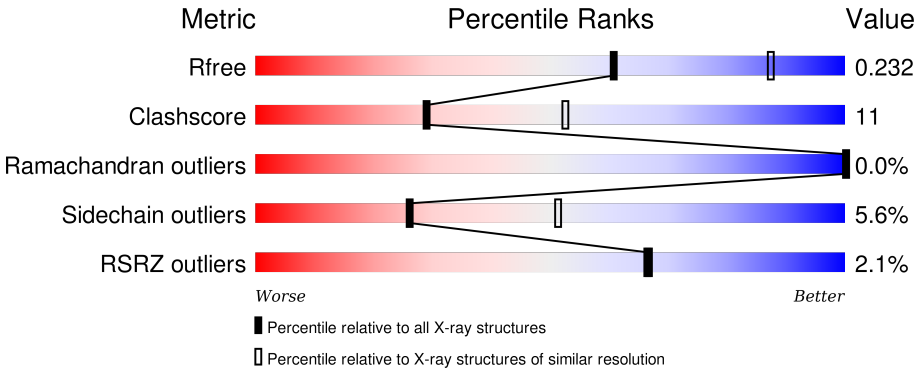
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.68 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	2780 (2.70-2.66)
Clashscore	102246	3138 (2.70-2.66)
Ramachandran outliers	100387	3089 (2.70-2.66)
Sidechain outliers	100360	3089 (2.70-2.66)
RSRZ outliers	91569	2789 (2.70-2.66)

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	311	81% 16%
1	B	311	81% 15%
1	C	311	84% 14%
1	D	311	77% 20%
1	E	311	80% 17%

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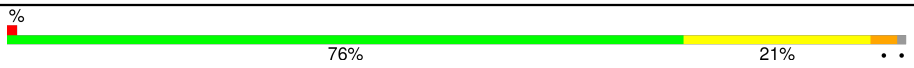
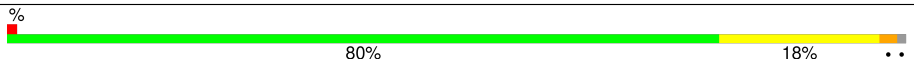
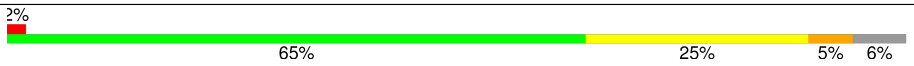
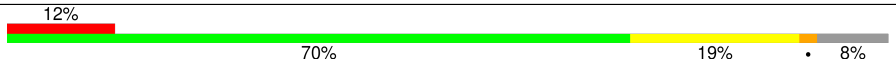
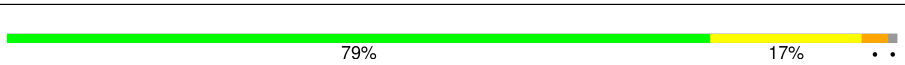
Mol	Chain	Length	Quality of chain
1	F	311	
1	G	311	
1	H	311	
1	I	311	
1	J	311	

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	A2G	A	1	-	-	-	X
2	FUC	A	3	-	-	-	X
2	A2G	B	1	-	-	-	X
2	FUC	B	3	-	-	-	X
2	FUC	C	3	-	-	-	X
2	FUC	D	3	-	-	-	X
2	FUC	E	3	-	-	-	X
2	FUC	F	3	-	-	-	X
2	FUC	G	3	-	-	-	X
2	A2G	J	1	-	-	-	X
2	FUC	J	3	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 24607 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 Capsid.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	309	Total	C	N	O	S	0	0	0
			2404	1517	415	462	10			
1	B	308	Total	C	N	O	S	0	0	0
			2392	1510	411	461	10			
1	C	311	Total	C	N	O	S	0	0	0
			2403	1514	413	466	10			
1	D	307	Total	C	N	O	S	0	0	0
			2385	1507	410	458	10			
1	E	309	Total	C	N	O	S	0	0	0
			2406	1518	415	463	10			
1	F	308	Total	C	N	O	S	0	0	0
			2393	1511	411	461	10			
1	G	308	Total	C	N	O	S	0	0	0
			2380	1505	407	458	10			
1	H	293	Total	C	N	O	S	0	0	0
			2274	1445	386	434	9			
1	I	286	Total	C	N	O	S	0	0	0
			2189	1391	376	414	8			
1	J	307	Total	C	N	O	S	0	0	0
			2386	1507	410	459	10			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	228	THR	SER	SEE REMARK 999	UNP Q5EGK8
A	271	ALA	VAL	SEE REMARK 999	UNP Q5EGK8
A	282	ASP	ASN	SEE REMARK 999	UNP Q5EGK8
B	228	THR	SER	SEE REMARK 999	UNP Q5EGK8
B	271	ALA	VAL	SEE REMARK 999	UNP Q5EGK8
B	282	ASP	ASN	SEE REMARK 999	UNP Q5EGK8
C	228	THR	SER	SEE REMARK 999	UNP Q5EGK8
C	271	ALA	VAL	SEE REMARK 999	UNP Q5EGK8
C	282	ASP	ASN	SEE REMARK 999	UNP Q5EGK8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	228	THR	SER	SEE REMARK 999	UNP Q5EGK8
D	271	ALA	VAL	SEE REMARK 999	UNP Q5EGK8
D	282	ASP	ASN	SEE REMARK 999	UNP Q5EGK8
E	228	THR	SER	SEE REMARK 999	UNP Q5EGK8
E	271	ALA	VAL	SEE REMARK 999	UNP Q5EGK8
E	282	ASP	ASN	SEE REMARK 999	UNP Q5EGK8
F	228	THR	SER	SEE REMARK 999	UNP Q5EGK8
F	271	ALA	VAL	SEE REMARK 999	UNP Q5EGK8
F	282	ASP	ASN	SEE REMARK 999	UNP Q5EGK8
G	228	THR	SER	SEE REMARK 999	UNP Q5EGK8
G	271	ALA	VAL	SEE REMARK 999	UNP Q5EGK8
G	282	ASP	ASN	SEE REMARK 999	UNP Q5EGK8
H	228	THR	SER	SEE REMARK 999	UNP Q5EGK8
H	271	ALA	VAL	SEE REMARK 999	UNP Q5EGK8
H	282	ASP	ASN	SEE REMARK 999	UNP Q5EGK8
I	228	THR	SER	SEE REMARK 999	UNP Q5EGK8
I	271	ALA	VAL	SEE REMARK 999	UNP Q5EGK8
I	282	ASP	ASN	SEE REMARK 999	UNP Q5EGK8
J	228	THR	SER	SEE REMARK 999	UNP Q5EGK8
J	271	ALA	VAL	SEE REMARK 999	UNP Q5EGK8
J	282	ASP	ASN	SEE REMARK 999	UNP Q5EGK8

- 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
			36	20	1	15		
2	B	3	Total	C	N	O	0	0
			36	20	1	15		
2	C	3	Total	C	N	O	0	0
			36	20	1	15		
2	D	3	Total	C	N	O	0	0
			36	20	1	15		
2	E	3	Total	C	N	O	0	0
			36	20	1	15		
2	F	3	Total	C	N	O	0	0
			36	20	1	15		
2	G	3	Total	C	N	O	0	0
			36	20	1	15		
2	J	3	Total	C	N	O	0	0
			36	20	1	15		

- Molecule 3 is water.

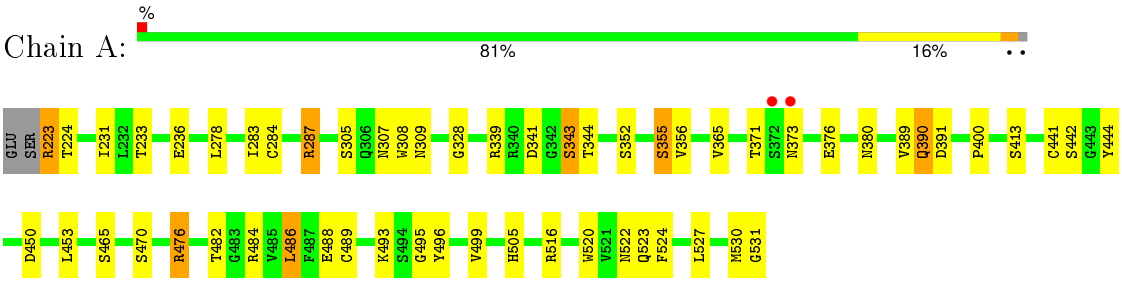
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	105	Total O 105 105	0	0
3	B	100	Total O 100 100	0	0
3	C	93	Total O 93 93	0	0
3	D	83	Total O 83 83	0	0
3	E	80	Total O 80 80	0	0
3	F	50	Total O 50 50	0	0
3	G	50	Total O 50 50	0	0
3	H	48	Total O 48 48	0	0
3	I	30	Total O 30 30	0	0
3	J	68	Total O 68 68	0	0

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.

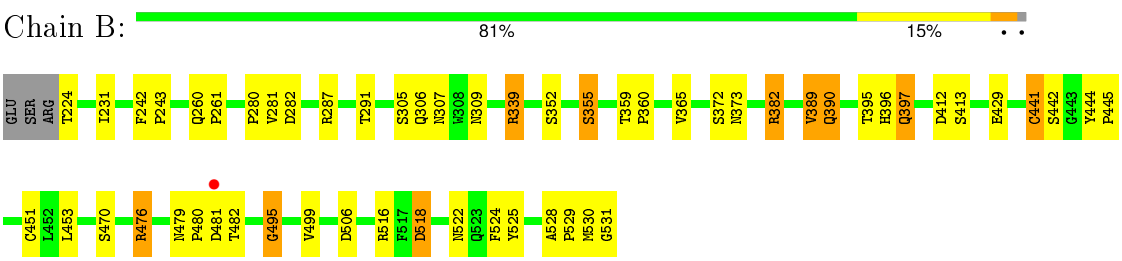
- Molecule 1: Capsid

Chain A:



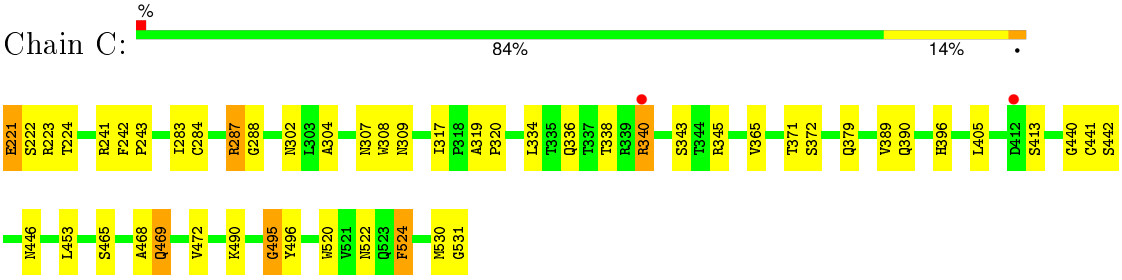
- Molecule 1: Capsid

Chain B:



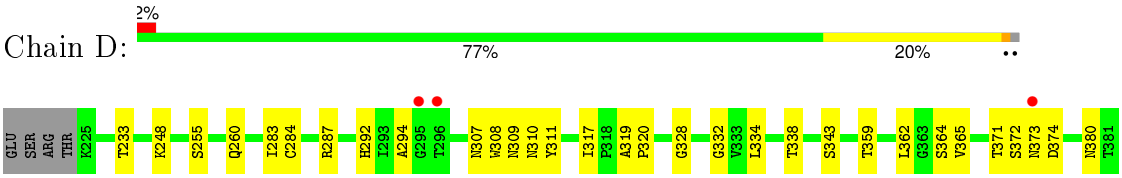
- Molecule 1: Capsid

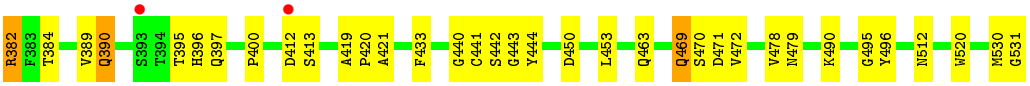
Chain C:



- Molecule 1: Capsid

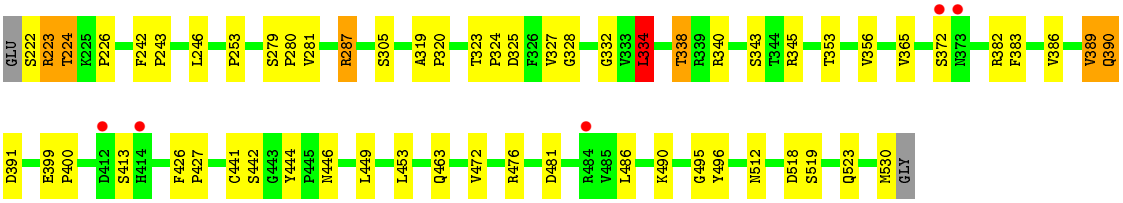
Chain D:





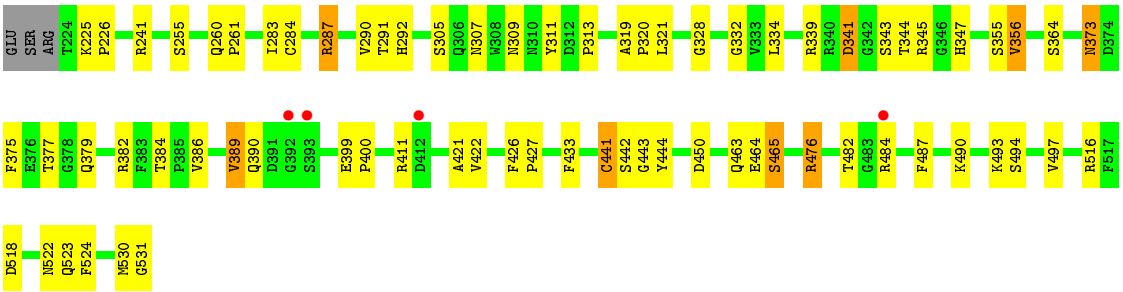
• Molecule 1: Capsid

Chain E:



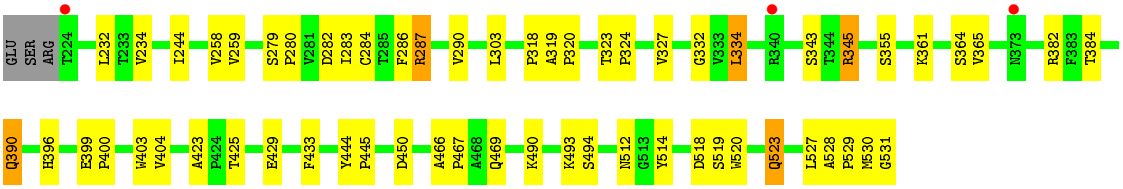
• Molecule 1: Capsid

Chain F:



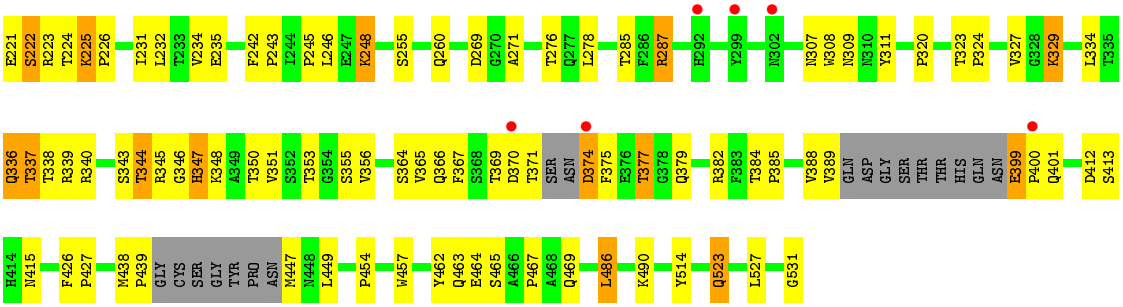
• Molecule 1: Capsid

Chain G:



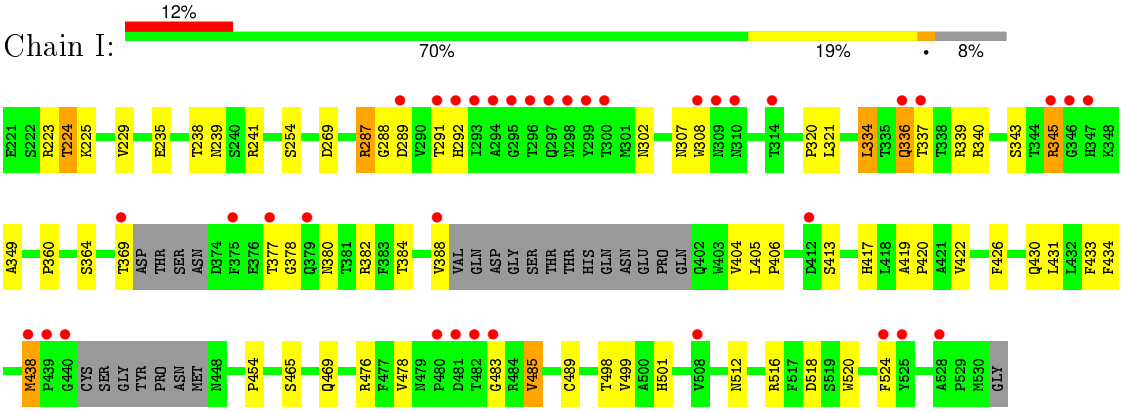
• Molecule 1: Capsid

Chain H:



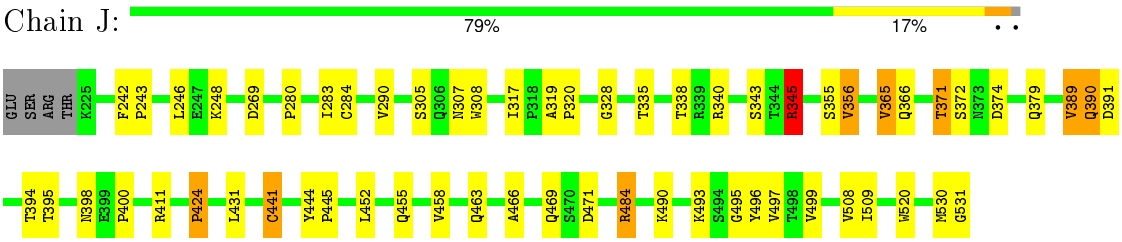
- Molecule 1: Capsid

Chain I:



- Molecule 1: Capsid

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	244.54Å 341.46Å 124.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.66 – 2.68 41.65 – 2.68	Depositor EDS
% Data completeness (in resolution range)	98.1 (41.66-2.68) 98.2 (41.65-2.68)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.46 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.181 , 0.230 0.186 , 0.232	Depositor DCC
R_{free} test set	7203 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	39.1	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 37.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 143407 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	24607	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.30% 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: GAL, FUC, A2G

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	1.14	3/2474 (0.1%)	0.97	5/3385 (0.1%)
1	B	1.09	8/2462 (0.3%)	0.93	1/3369 (0.0%)
1	C	1.01	2/2472 (0.1%)	0.94	4/3384 (0.1%)
1	D	0.99	1/2455 (0.0%)	0.98	3/3360 (0.1%)
1	E	1.03	2/2476 (0.1%)	0.97	6/3388 (0.2%)
1	F	0.93	1/2463 (0.0%)	0.93	3/3371 (0.1%)
1	G	0.93	0/2450	0.91	4/3355 (0.1%)
1	H	0.97	2/2338 (0.1%)	0.98	10/3197 (0.3%)
1	I	0.88	0/2251	0.88	2/3080 (0.1%)
1	J	1.01	4/2456 (0.2%)	0.94	3/3361 (0.1%)
All	All	1.00	23/24297 (0.1%)	0.94	41/33250 (0.1%)

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	E	0	1
1	I	0	1
All	All	0	2

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	441	CYS	CB-SG	-7.31	1.69	1.82
1	A	376	GLU	C-N	7.16	1.50	1.34
1	C	221	GLU	CG-CD	6.94	1.62	1.51
1	H	221	GLU	CG-CD	6.75	1.62	1.51
1	B	518	ASP	CB-CG	6.25	1.64	1.51

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	337	THR	O-C-N	11.56	141.20	122.70
1	H	223	ARG	NE-CZ-NH2	-8.95	115.83	120.30
1	I	337	THR	CA-C-N	-8.71	98.04	117.20
1	H	223	ARG	NE-CZ-NH1	7.25	123.92	120.30
1	E	334	LEU	CA-CB-CG	7.21	131.89	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	223	ARG	Sidechain
1	I	223	ARG	Sidechain

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	2404	0	2295	53	0
1	B	2392	0	2278	57	0
1	C	2403	0	2282	45	0
1	D	2385	0	2272	43	0
1	E	2406	0	2297	52	1
1	F	2393	0	2282	62	0
1	G	2380	0	2263	49	0
1	H	2274	0	2173	81	0
1	I	2189	0	2066	61	1
1	J	2386	0	2275	52	0
2	A	36	0	33	2	0
2	B	36	0	33	0	0
2	C	36	0	33	1	0
2	D	36	0	33	1	0
2	E	36	0	33	2	0
2	F	36	0	33	0	0
2	G	36	0	33	2	0
2	J	36	0	33	3	0
3	A	105	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	100	0	0	6	0
3	C	93	0	0	10	0
3	D	83	0	0	5	0
3	E	80	0	0	8	0
3	F	50	0	0	10	0
3	G	50	0	0	8	0
3	H	48	0	0	22	0
3	I	30	0	0	25	0
3	J	68	0	0	5	0
All	All	24607	0	22747	533	1

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 11.

The worst 5 of 533 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:C:453:LEU:HD21	1:C:495:GLY:O	1.33	1.27
1:D:310:ASN:HB3	3:D:555:HOH:O	1.48	1.14
1:B:339:ARG:HG3	1:B:339:ARG:HH11	1.01	1.10
1:A:223:ARG:HG2	1:A:224:THR:H	0.94	1.10
1:H:531:GLY:HA3	3:H:586:HOH:O	1.50	1.08

All (1) 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:E:223:ARG:NH1	1:I:321:LEU:CD2[4_555]	2.11	0.09

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	307/311 (99%)	299 (97%)	8 (3%)	0	100	100
1	B	306/311 (98%)	296 (97%)	10 (3%)	0	100	100
1	C	309/311 (99%)	301 (97%)	8 (3%)	0	100	100
1	D	305/311 (98%)	294 (96%)	11 (4%)	0	100	100
1	E	307/311 (99%)	296 (96%)	11 (4%)	0	100	100
1	F	306/311 (98%)	290 (95%)	16 (5%)	0	100	100
1	G	306/311 (98%)	293 (96%)	13 (4%)	0	100	100
1	H	285/311 (92%)	264 (93%)	21 (7%)	0	100	100
1	I	278/311 (89%)	266 (96%)	11 (4%)	1 (0%)	39	67
1	J	305/311 (98%)	295 (97%)	10 (3%)	0	100	100
All	All	3014/3110 (97%)	2894 (96%)	119 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	483	GLY

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	270/272 (99%)	256 (95%)	14 (5%)	29	55
1	B	269/272 (99%)	254 (94%)	15 (6%)	26	51
1	C	269/272 (99%)	258 (96%)	11 (4%)	37	66
1	D	267/272 (98%)	255 (96%)	12 (4%)	34	62
1	E	271/272 (100%)	259 (96%)	12 (4%)	35	63
1	F	269/272 (99%)	252 (94%)	17 (6%)	22	46
1	G	266/272 (98%)	253 (95%)	13 (5%)	31	58
1	H	254/272 (93%)	228 (90%)	26 (10%)	9	19
1	I	238/272 (88%)	225 (94%)	13 (6%)	27	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	J	268/272 (98%)	254 (95%)	14 (5%)	29 55
All	All	2641/2720 (97%)	2494 (94%)	147 (6%)	26 51

5 of 147 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	290	VAL
1	G	244	ILE
1	J	340	ARG
1	F	334	LEU
1	F	373	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	347	HIS
1	G	523	GLN
1	J	398	ASN
1	F	523	GLN
1	H	297	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)

24 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	A2G	A	1	2	14,14,15	0.52	0	15,19,21	0.86	1 (6%)
2	GAL	A	2	2	11,11,12	0.64	0	15,15,17	0.97	1 (6%)
2	FUC	A	3	2	11,11,11	0.54	0	16,16,16	0.84	1 (6%)
2	A2G	B	1	2	14,14,15	0.53	0	15,19,21	0.87	1 (6%)
2	GAL	B	2	2	11,11,12	0.64	0	15,15,17	0.97	1 (6%)
2	FUC	B	3	2	11,11,11	0.53	0	16,16,16	0.84	1 (6%)
2	A2G	C	1	2	14,14,15	0.53	0	15,19,21	0.86	1 (6%)
2	GAL	C	2	2	11,11,12	0.64	0	15,15,17	0.97	1 (6%)
2	FUC	C	3	2	11,11,11	0.54	0	16,16,16	0.84	1 (6%)
2	A2G	D	1	2	14,14,15	0.53	0	15,19,21	0.86	1 (6%)
2	GAL	D	2	2	11,11,12	0.63	0	15,15,17	0.99	1 (6%)
2	FUC	D	3	2	11,11,11	0.54	0	16,16,16	0.83	1 (6%)
2	A2G	E	1	2	14,14,15	0.53	0	15,19,21	0.86	1 (6%)
2	GAL	E	2	2	11,11,12	0.64	0	15,15,17	0.98	1 (6%)
2	FUC	E	3	2	11,11,11	0.53	0	16,16,16	0.84	1 (6%)
2	A2G	F	1	2	14,14,15	0.52	0	15,19,21	0.87	1 (6%)
2	GAL	F	2	2	11,11,12	0.63	0	15,15,17	0.99	1 (6%)
2	FUC	F	3	2	11,11,11	0.52	0	16,16,16	0.83	1 (6%)
2	A2G	G	1	2	14,14,15	0.52	0	15,19,21	0.86	1 (6%)
2	GAL	G	2	2	11,11,12	0.64	0	15,15,17	0.98	1 (6%)
2	FUC	G	3	2	11,11,11	0.53	0	16,16,16	0.84	1 (6%)
2	A2G	J	1	2	14,14,15	0.52	0	15,19,21	0.86	1 (6%)
2	GAL	J	2	2	11,11,12	0.64	0	15,15,17	0.99	1 (6%)
2	FUC	J	3	2	11,11,11	0.54	0	16,16,16	0.84	1 (6%)

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	A2G	A	1	2	-	0/6/23/26	0/1/1/1
2	GAL	A	2	2	-	0/2/18/22	0/1/1/1
2	FUC	A	3	2	-	0/0/20/20	0/1/1/1
2	A2G	B	1	2	-	0/6/23/26	0/1/1/1
2	GAL	B	2	2	-	0/2/18/22	0/1/1/1
2	FUC	B	3	2	-	0/0/20/20	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A2G	C	1	2	-	0/6/23/26	0/1/1/1
2	GAL	C	2	2	-	0/2/18/22	0/1/1/1
2	FUC	C	3	2	-	0/0/20/20	0/1/1/1
2	A2G	D	1	2	-	0/6/23/26	0/1/1/1
2	GAL	D	2	2	-	0/2/18/22	0/1/1/1
2	FUC	D	3	2	-	0/0/20/20	0/1/1/1
2	A2G	E	1	2	-	0/6/23/26	0/1/1/1
2	GAL	E	2	2	-	0/2/18/22	0/1/1/1
2	FUC	E	3	2	-	0/0/20/20	0/1/1/1
2	A2G	F	1	2	-	0/6/23/26	0/1/1/1
2	GAL	F	2	2	-	0/2/18/22	0/1/1/1
2	FUC	F	3	2	-	0/0/20/20	0/1/1/1
2	A2G	G	1	2	-	0/6/23/26	0/1/1/1
2	GAL	G	2	2	-	0/2/18/22	0/1/1/1
2	FUC	G	3	2	-	0/0/20/20	0/1/1/1
2	A2G	J	1	2	-	0/6/23/26	0/1/1/1
2	GAL	J	2	2	-	0/2/18/22	0/1/1/1
2	FUC	J	3	2	-	0/0/20/20	0/1/1/1

There are no bond length outliers.

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	3	FUC	C1-O5-C5	-2.20	109.45	113.57
2	G	1	A2G	C1-O-C5	-2.20	109.45	112.25
2	J	1	A2G	C1-O-C5	-2.20	109.46	112.25
2	C	3	FUC	C1-O5-C5	-2.19	109.47	113.57
2	E	3	FUC	C1-O5-C5	-2.18	109.48	113.57

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2	GAL	1	0
2	A	3	FUC	1	0
2	C	3	FUC	1	0
2	D	3	FUC	1	0
2	E	3	FUC	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	3	FUC	2	0
2	J	3	FUC	3	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

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	309/311 (99%)	-0.41	2 (0%) 90 91	16, 26, 50, 69	0
1	B	308/311 (99%)	-0.49	1 (0%) 94 95	16, 28, 51, 74	0
1	C	311/311 (100%)	-0.33	2 (0%) 90 91	16, 30, 53, 79	0
1	D	307/311 (98%)	-0.34	5 (1%) 74 74	16, 29, 56, 75	0
1	E	309/311 (99%)	-0.34	5 (1%) 74 74	18, 29, 53, 72	0
1	F	308/311 (99%)	-0.24	4 (1%) 79 79	20, 37, 64, 86	0
1	G	308/311 (99%)	-0.45	3 (0%) 84 84	22, 35, 58, 85	0
1	H	293/311 (94%)	-0.33	6 (2%) 68 68	22, 41, 70, 81	0
1	I	286/311 (91%)	0.37	37 (12%) 5 3	34, 57, 81, 106	0
1	J	307/311 (98%)	-0.44	0 100 100	17, 29, 54, 69	0
All	All	3046/3110 (97%)	-0.30	65 (2%) 67 66	16, 33, 66, 106	0

The worst 5 of 65 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	336	GLN	7.2
1	I	524	PHE	5.6
1	I	375	PHE	5.2
1	I	295	GLY	4.5
1	I	296	THR	4.4

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

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

6.3 Carbohydrates (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
2	A2G	A	1	14/15	0.64	0.50	11.90	102,104,105,105	0
2	FUC	F	3	11/11	0.82	0.34	5.96	83,89,93,100	0
2	FUC	A	3	11/11	0.86	0.34	5.86	62,67,74,83	0
2	A2G	J	1	14/15	0.71	0.43	5.69	91,97,100,101	0
2	A2G	B	1	14/15	0.80	0.42	5.54	93,95,96,96	0
2	FUC	B	3	11/11	0.74	0.32	5.40	50,54,64,75	0
2	FUC	G	3	11/11	0.81	0.36	4.04	86,91,96,102	0
2	FUC	E	3	11/11	0.78	0.32	3.84	65,73,81,89	0
2	FUC	C	3	11/11	0.81	0.30	3.48	67,71,79,87	0
2	FUC	D	3	11/11	0.86	0.32	3.30	76,79,85,93	0
2	FUC	J	3	11/11	0.81	0.27	2.57	65,69,74,81	0
2	GAL	J	2	11/12	0.82	0.33	-	88,91,92,93	0
2	GAL	A	2	11/12	0.53	0.45	-	86,93,95,99	0
2	GAL	F	2	11/12	0.80	0.40	-	103,108,110,113	0
2	GAL	G	2	11/12	0.75	0.42	-	104,109,110,114	0
2	GAL	B	2	11/12	0.82	0.44	-	83,87,89,90	0
2	A2G	D	1	14/15	0.64	0.58	-	112,114,118,118	0
2	A2G	G	1	14/15	0.73	0.44	-	114,116,117,117	0
2	GAL	E	2	11/12	0.69	0.44	-	97,101,102,105	0
2	GAL	C	2	11/12	0.62	0.44	-	90,98,98,102	0
2	GAL	D	2	11/12	0.77	0.58	-	100,103,105,110	0
2	A2G	F	1	14/15	0.70	0.53	-	108,115,120,121	0
2	A2G	E	1	14/15	0.72	0.68	-	110,111,112,112	0
2	A2G	C	1	14/15	0.72	0.54	-	105,109,110,110	0

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.