



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:58 PM GMT

PDB ID : 1ZBA  
Title : Foot-and-Mouth Disease virus serotype A1061 complexed with oligosaccharide receptor.  
Authors : Fry, E.E.; Newman, J.W.; Curry, S.; Najjam, S.; Jackson, T.; Blakemore, W.; Lea, S.M.; Miller, L.; Burman, A.; King, A.M.; Stuart, D.I.  
Deposited on : 2005-04-08  
Resolution : 2.00 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

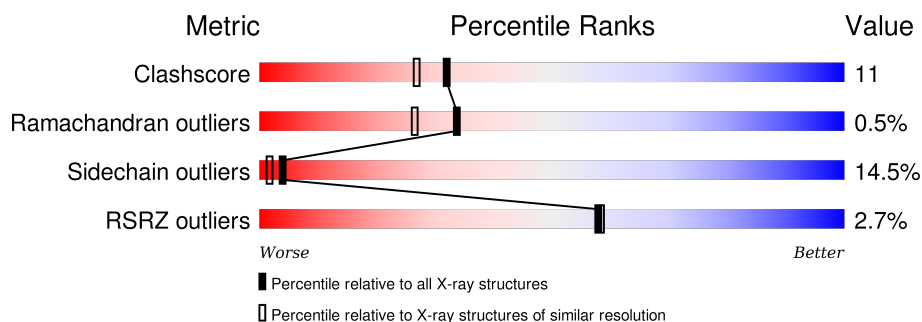
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	212	
2	2	218	
3	3	221	
4	4	85	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5732 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 Coat protein VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	191	Total	C	N	O	S	0	0	0
			1492	944	266	278	4			

- Molecule 2 is a protein called Coat protein VP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	207	Total	C	N	O	S	0	0	0
			1652	1061	280	306	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	14	LEU	ILE	ENGINEERED	UNP Q84769

- Molecule 3 is a protein called Coat protein VP3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	221	Total	C	N	O	S	0	0	0
			1708	1089	277	335	7			

- Molecule 4 is a protein called Coat protein VP4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	4	49	Total	C	N	O	S	0	0	0
			375	235	62	76	2			

- Molecule 5 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	1	3	Total	C	N	O	S	0	0
			55	18	2	30	5		

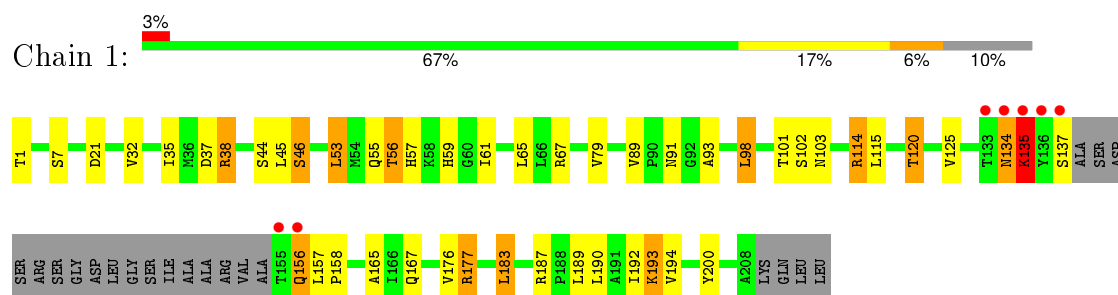
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	1	154	Total 154	O 154	0	0
6	2	109	Total 109	O 109	0	0
6	3	157	Total 157	O 157	0	0
6	4	30	Total 30	O 30	0	0

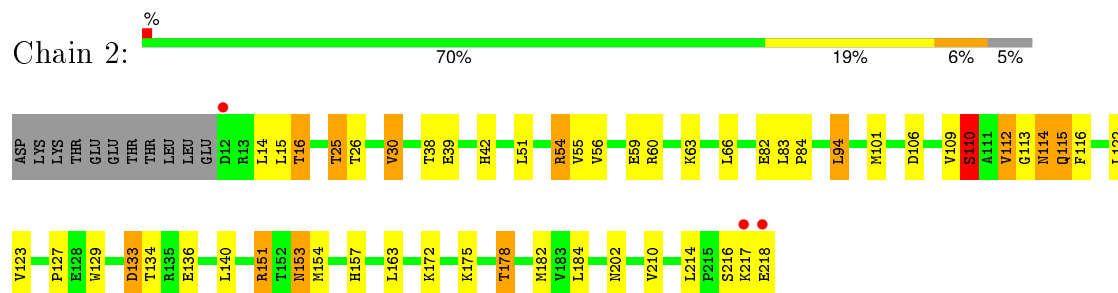
### 3 Residue-property plots [i](#)

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.

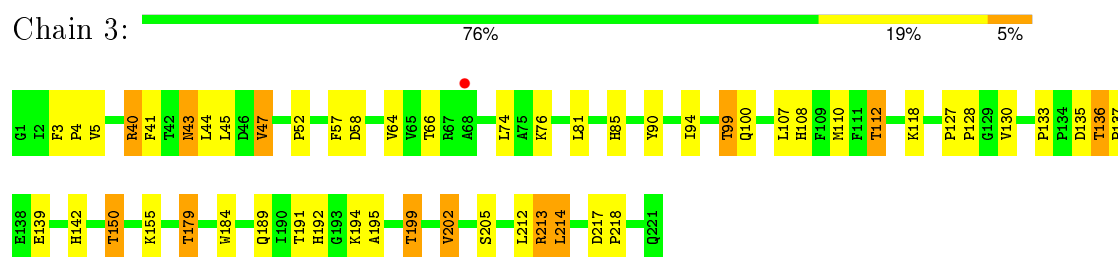
#### • Molecule 1: Coat protein VP1



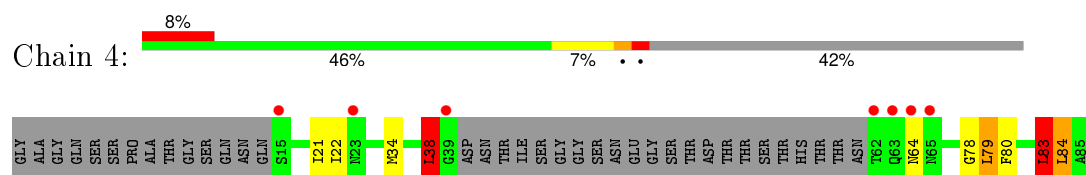
#### • Molecule 2: Coat protein VP2



#### • Molecule 3: Coat protein VP3



#### • Molecule 4: Coat protein VP4



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	307.00Å 307.00Å 715.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.00 24.88 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.00) 26.8 (24.88-2.00)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.10 (at 2.01Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.183 , (Not available) 0.179 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	28.8	Xtriage
Anisotropy	0.172	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 63.3	EDS
Estimated twinning fraction	0.017 for -h,1/3*h-1/3*k-1/3*l,-4/3*h-8/3*k+1/3*l 0.016 for -1/3*h+1/3*k+1/3*l,-k,8/3*h+4/3*k+1/3*l 0.017 for -2/3*h-1/3*k-1/3*l,-1/3*h-2/3*k+1/3*l,-4/3*h+4/3*k+1/3*l 0.017 for 1/3*h+2/3*k-1/3*l,-k,-8/3*h-4/3*k-1/3*l 0.017 for -1/3*h-2/3*k+1/3*l,-2/3*h-1/3*k-1/3*l,4/3*h-4/3*k-1/3*l 0.015 for -h,2/3*h+1/3*k+1/3*l,4/3*h+8/3*k-1/3*l 0.074 for h,-h-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 452651 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5732	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

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	1	0.50	0/1527	0.79	0/2083
2	2	0.49	1/1701 (0.1%)	0.82	4/2322 (0.2%)
3	3	0.51	1/1757 (0.1%)	0.79	0/2405
4	4	0.53	0/381	0.86	2/513 (0.4%)
All	All	0.50	2/5366 (0.0%)	0.81	6/7323 (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
2	2	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	182	MET	SD-CE	-6.00	1.44	1.77
3	3	110	MET	SD-CE	-5.09	1.49	1.77

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	4	38	LEU	CA-CB-CG	6.61	130.51	115.30
2	2	110	SER	O-C-N	-6.09	112.96	122.70
4	4	83	LEU	CA-CB-CG	5.61	128.20	115.30
2	2	113	GLY	N-CA-C	-5.39	99.61	113.10
2	2	109	VAL	C-N-CA	5.29	134.93	121.70
2	2	109	VAL	O-C-N	-5.01	114.68	122.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	2	110	SER	Mainchain

## 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	1	1492	0	1485	44	0
2	2	1652	0	1607	37	0
3	3	1708	0	1631	32	0
4	4	375	0	348	6	1
5	1	55	0	29	1	0
6	1	154	0	0	5	2
6	2	109	0	0	5	3
6	3	157	0	0	2	0
6	4	30	0	0	2	0
All	All	5732	0	5100	110	3

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.

All (110) 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)
2:2:129:TRP:HB2	2:2:178:THR:HG21	1.52	0.91
1:1:57:HIS:HD2	1:1:59:HIS:H	1.18	0.88
1:1:156:GLN:HE21	1:1:156:GLN:HA	1.42	0.84
1:1:135:LYS:NZ	1:1:158:PRO:HA	1.93	0.83
2:2:115:GLN:NE2	2:2:115:GLN:H	1.78	0.81
2:2:218:GLU:HB2	3:3:139:GLU:HG2	1.62	0.80
1:1:193:LYS:HE2	5:1:503:SGN:H4	1.64	0.80
1:1:103:ASN:HD21	3:3:217:ASP:H	1.32	0.77
3:3:136:THR:HG22	3:3:139:GLU:H	1.50	0.76
2:2:42:HIS:HB2	6:4:113:HOH:O	1.85	0.76
2:2:115:GLN:HE21	2:2:115:GLN:H	1.32	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:56:THR:HG22	1:1:67:ARG:NH2	2.03	0.73
1:1:165:ALA:HB3	6:1:606:HOH:O	1.88	0.73
1:1:56:THR:HG22	1:1:67:ARG:HH21	1.54	0.72
3:3:43:ASN:HD22	3:3:45:LEU:H	1.38	0.71
1:1:91:ASN:HB3	1:1:120:THR:HG23	1.73	0.71
2:2:16:THR:HB	2:2:25:THR:HB	1.71	0.70
3:3:112:THR:HG22	6:3:373:HOH:O	1.92	0.68
2:2:129:TRP:HB2	2:2:178:THR:CG2	2.22	0.68
1:1:53:LEU:O	1:1:56:THR:HB	1.94	0.68
1:1:57:HIS:CD2	1:1:59:HIS:H	2.07	0.68
1:1:135:LYS:HZ2	1:1:158:PRO:HA	1.57	0.67
2:2:106:ASP:OD2	2:2:157:HIS:HE1	1.79	0.66
1:1:37:ASP:OD2	1:1:177:ARG:HD3	1.98	0.63
1:1:135:LYS:HD2	6:1:624:HOH:O	1.98	0.62
2:2:25:THR:HG21	6:2:235:HOH:O	1.98	0.62
1:1:89:VAL:CG1	1:1:93:ALA:HB3	2.31	0.61
3:3:213:ARG:HD3	3:3:214:LEU:HD22	1.81	0.61
4:4:34:MET:HG3	6:4:100:HOH:O	2.01	0.61
3:3:99:THR:HG22	3:3:100:GLN:HG3	1.83	0.61
3:3:112:THR:HB	3:3:199:THR:HG22	1.81	0.60
2:2:214:LEU:HD23	3:3:127:PRO:HG2	1.83	0.60
1:1:134:ASN:O	1:1:135:LYS:HD3	2.02	0.60
1:1:91:ASN:O	3:3:99:THR:HG21	2.01	0.60
4:4:83:LEU:HD22	4:4:84:LEU:N	2.17	0.59
2:2:101:MET:HG2	2:2:210:VAL:HG12	1.84	0.59
3:3:108:HIS:HE1	3:3:205:SER:OG	1.85	0.59
4:4:21:ILE:HG22	4:4:22:ILE:HD12	1.85	0.59
1:1:135:LYS:O	1:1:135:LYS:HG2	2.03	0.58
1:1:91:ASN:H	1:1:120:THR:CG2	2.17	0.58
3:3:133:PRO:HG3	3:3:184:TRP:CD2	2.39	0.57
2:2:216:SER:HB3	3:3:142:HIS:CD2	2.40	0.57
2:2:63:LYS:HZ3	2:2:202:ASN:HD21	1.52	0.57
3:3:179:THR:HG21	6:3:330:HOH:O	2.05	0.56
2:2:84:PRO:O	2:2:175:LYS:HE3	2.05	0.56
2:2:115:GLN:HE21	2:2:115:GLN:N	2.01	0.56
1:1:55:GLN:HG2	6:1:576:HOH:O	2.06	0.56
1:1:91:ASN:H	1:1:120:THR:HG21	1.70	0.56
1:1:156:GLN:NE2	1:1:156:GLN:HA	2.19	0.56
3:3:99:THR:CG2	3:3:100:GLN:HG3	2.36	0.55
2:2:114:ASN:ND2	2:2:116:PHE:H	2.04	0.55
1:1:35:ILE:O	1:1:38:ARG:HD2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:153:ASN:N	2:2:153:ASN:HD22	2.05	0.55
3:3:90:TYR:CE1	3:3:94:ILE:HD11	2.42	0.55
1:1:89:VAL:HB	6:1:606:HOH:O	2.07	0.55
1:1:7:SER:HA	2:2:30:VAL:HG13	1.90	0.54
1:1:56:THR:CG2	1:1:67:ARG:HH21	2.21	0.53
1:1:187:ARG:NH2	2:2:127:PRO:O	2.41	0.53
2:2:122:LEU:HB2	2:2:184:LEU:HD22	1.90	0.52
3:3:118:LYS:HA	3:3:150:THR:HG21	1.90	0.52
2:2:129:TRP:HH2	6:2:230:HOH:O	1.92	0.52
1:1:134:ASN:O	1:1:135:LYS:HB3	2.09	0.52
1:1:135:LYS:HZ3	1:1:158:PRO:HA	1.72	0.51
1:1:46:SER:HB2	6:1:580:HOH:O	2.11	0.50
2:2:217:LYS:HD2	2:2:217:LYS:N	2.27	0.50
2:2:133:ASP:HB2	2:2:136:GLU:HG3	1.94	0.50
1:1:194:VAL:HG22	1:1:200:TYR:HB2	1.94	0.49
3:3:43:ASN:ND2	3:3:45:LEU:H	2.07	0.49
2:2:63:LYS:NZ	2:2:202:ASN:ND2	2.61	0.49
1:1:98:LEU:HG	1:1:167:GLN:HB2	1.93	0.49
2:2:151:ARG:HD3	6:2:327:HOH:O	2.13	0.48
2:2:114:ASN:HD22	2:2:114:ASN:C	2.16	0.48
2:2:63:LYS:NZ	2:2:202:ASN:HD21	2.11	0.48
2:2:157:HIS:HD2	6:2:237:HOH:O	1.95	0.48
1:1:44:SER:O	1:1:45:LEU:HD23	2.14	0.47
3:3:108:HIS:HB3	3:3:155:LYS:HE3	1.97	0.47
2:2:94:LEU:HG	2:2:210:VAL:HG11	1.97	0.47
1:1:89:VAL:CG1	1:1:93:ALA:CB	2.92	0.46
2:2:153:ASN:H	2:2:153:ASN:HD22	1.62	0.46
2:2:82:GLU:HA	2:2:178:THR:HB	1.95	0.46
2:2:175:LYS:HE2	6:2:277:HOH:O	2.15	0.46
3:3:136:THR:HB	3:3:139:GLU:OE1	2.16	0.46
4:4:83:LEU:HD22	4:4:84:LEU:H	1.80	0.46
3:3:40:ARG:HG3	3:3:41:PHE:N	2.31	0.45
3:3:57:PHE:CE2	3:3:202:VAL:HG13	2.52	0.45
2:2:54:ARG:NH1	2:2:59:GLU:OE2	2.48	0.45
1:1:135:LYS:HG3	1:1:158:PRO:HG3	1.99	0.45
2:2:54:ARG:NH1	2:2:59:GLU:OE1	2.51	0.44
1:1:79:VAL:HG22	1:1:114:ARG:HG3	1.99	0.44
4:4:38:LEU:O	4:4:38:LEU:HD12	2.18	0.44
1:1:91:ASN:CB	1:1:120:THR:HG23	2.46	0.43
3:3:192:HIS:HB2	3:3:195:ALA:HB3	1.99	0.43
3:3:47:VAL:HG22	3:3:90:TYR:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:32:VAL:HG13	1:1:183:LEU:HD22	2.00	0.43
1:1:91:ASN:CB	1:1:120:THR:CG2	2.97	0.43
1:1:56:THR:O	1:1:67:ARG:NH2	2.52	0.43
1:1:91:ASN:HB3	1:1:120:THR:CG2	2.45	0.43
3:3:136:THR:HA	3:3:137:PRO:HD3	1.95	0.42
3:3:213:ARG:O	3:3:214:LEU:HB2	2.19	0.42
3:3:85:HIS:H	3:3:85:HIS:CD2	2.37	0.42
2:2:202:ASN:HA	2:2:202:ASN:HD22	1.70	0.42
3:3:66:THR:HB	3:3:189:GLN:OE1	2.19	0.42
2:2:110:SER:HA	2:2:154:MET:O	2.19	0.42
1:1:1:THR:HG23	4:4:79:LEU:HA	2.01	0.42
3:3:3:PHE:HA	3:3:4:PRO:HD3	1.82	0.42
1:1:102:SER:HB2	3:3:217:ASP:OD2	2.20	0.41
3:3:127:PRO:HB2	3:3:128:PRO:HD2	2.02	0.41
1:1:35:ILE:HD11	1:1:61:ILE:HD11	2.03	0.40
3:3:52:PRO:HB3	3:3:205:SER:HB3	2.04	0.40
2:2:112:VAL:HB	2:2:154:MET:SD	2.61	0.40

All (3) 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)
6:1:525:HOH:O	6:2:235:HOH:O[2_555]	0.77	1.43
4:4:80:PHE:O	6:2:236:HOH:O[2_555]	1.93	0.27
6:1:653:HOH:O	6:2:221:HOH:O[2_555]	2.12	0.08

## 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	1	187/212 (88%)	179 (96%)	7 (4%)	1 (0%)	34 26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	2	205/218 (94%)	195 (95%)	10 (5%)	0	100	100
3	3	219/221 (99%)	208 (95%)	10 (5%)	1 (0%)	34	26
4	4	45/85 (53%)	41 (91%)	3 (7%)	1 (2%)	8	3
All	All	656/736 (89%)	623 (95%)	30 (5%)	3 (0%)	34	26

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	4	78	GLY
1	1	135	LYS
3	3	58	ASP

### 5.3.2 Protein sidechains ⓘ

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	1	161/176 (92%)	137 (85%)	24 (15%)	4	1
2	2	181/192 (94%)	153 (84%)	28 (16%)	3	1
3	3	183/183 (100%)	158 (86%)	25 (14%)	4	2
4	4	40/68 (59%)	35 (88%)	5 (12%)	6	3
All	All	565/619 (91%)	483 (86%)	82 (14%)	4	2

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	21	ASP
1	1	38	ARG
1	1	46	SER
1	1	53	LEU
1	1	56	THR
1	1	65	LEU
1	1	98	LEU
1	1	101	THR

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Mol	Chain	Res	Type
1	1	114	ARG
1	1	115	LEU
1	1	120	THR
1	1	125	VAL
1	1	134	ASN
1	1	135	LYS
1	1	137	SER
1	1	156	GLN
1	1	157	LEU
1	1	176	VAL
1	1	177	ARG
1	1	183	LEU
1	1	189	LEU
1	1	190	LEU
1	1	192	ILE
1	1	193	LYS
2	2	14	LEU
2	2	15	LEU
2	2	16	THR
2	2	25	THR
2	2	26	THR
2	2	30	VAL
2	2	38	THR
2	2	39	GLU
2	2	51	LEU
2	2	54	ARG
2	2	55	VAL
2	2	56	VAL
2	2	60	ARG
2	2	66	LEU
2	2	83	LEU
2	2	94	LEU
2	2	112	VAL
2	2	114	ASN
2	2	115	GLN
2	2	123	VAL
2	2	133	ASP
2	2	134	THR
2	2	140	LEU
2	2	151	ARG
2	2	153	ASN
2	2	163	LEU

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Mol	Chain	Res	Type
2	2	172	LYS
2	2	178	THR
3	3	5	VAL
3	3	40	ARG
3	3	43	ASN
3	3	44	LEU
3	3	47	VAL
3	3	64	VAL
3	3	74	LEU
3	3	76	LYS
3	3	81	LEU
3	3	99	THR
3	3	107	LEU
3	3	112	THR
3	3	130	VAL
3	3	135	ASP
3	3	136	THR
3	3	150	THR
3	3	179	THR
3	3	191	THR
3	3	194	LYS
3	3	199	THR
3	3	202	VAL
3	3	212	LEU
3	3	213	ARG
3	3	214	LEU
3	3	218	PRO
4	4	38	LEU
4	4	64	ASN
4	4	79	LEU
4	4	83	LEU
4	4	84	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	28	HIS
1	1	57	HIS
1	1	103	ASN
1	1	156	GLN
1	1	169	GLN
2	2	114	ASN

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Mol	Chain	Res	Type
2	2	115	GLN
2	2	153	ASN
2	2	157	HIS
2	2	166	ASN
2	2	202	ASN
3	3	36	ASN
3	3	43	ASN
3	3	85	HIS
3	3	108	HIS
3	3	153	ASN
3	3	180	ASN
4	4	17	ASN
4	4	64	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 ⓘ

3 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	$\# Z  > 2$
5	SGN	1	501	5	18,20,20	2.67	3 (16%)	20,31,31	0.72	1 (5%)
5	IDS	1	502	5	12,15,17	2.10	2 (16%)	12,22,26	1.78	2 (16%)
5	SGN	1	503	5	18,20,20	2.59	3 (16%)	20,31,31	0.73	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
5	SGN	1	501	5	-	0/11/31/31	0/1/1/1
5	IDS	1	502	5	-	0/5/22/29	0/1/1/1
5	SGN	1	503	5	-	0/11/31/31	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	1	502	IDS	O2-C2	-2.99	1.42	1.47
5	1	503	SGN	O6-S2	6.02	1.76	1.57
5	1	503	SGN	O1S-S1	6.06	1.48	1.42
5	1	502	IDS	O2-S	6.26	1.77	1.57
5	1	501	SGN	O1S-S1	6.32	1.48	1.42
5	1	501	SGN	O2S-S1	6.41	1.48	1.42
5	1	503	SGN	O2S-S1	6.44	1.48	1.42
5	1	501	SGN	O6-S2	6.45	1.77	1.57

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	1	503	SGN	C6-C5-C4	-2.02	107.45	112.03
5	1	501	SGN	O5-C5-C6	2.20	111.10	106.61
5	1	502	IDS	O5-C5-C4	3.46	115.95	110.56
5	1	502	IDS	C1-O5-C5	4.55	120.86	113.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	1	503	SGN	1	0

## 5.6 Ligand geometry

There are no ligands in this entry.



## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	1	191/212 (90%)	-0.62	7 (3%) 45 47	13, 21, 59, 151	0
2	2	207/218 (94%)	-0.90	3 (1%) 78 78	14, 21, 44, 104	0
3	3	221/221 (100%)	-0.82	1 (0%) 91 92	14, 20, 48, 86	0
4	4	49/85 (57%)	0.48	7 (14%) 4 4	17, 43, 109, 138	0
All	All	668/736 (90%)	-0.69	18 (2%) 58 58	13, 21, 61, 151	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1	136	TYR	13.8
1	1	137	SER	12.0
1	1	134	ASN	7.9
4	4	62	THR	6.8
1	1	135	LYS	6.0
4	4	64	ASN	5.6
4	4	63	GLN	5.2
1	1	155	THR	4.8
4	4	15	SER	4.1
2	2	218	GLU	3.8
2	2	217	LYS	3.7
4	4	65	ASN	3.5
2	2	12	ASP	3.1
4	4	39	GLY	2.8
3	3	68	ALA	2.7
1	1	133	THR	2.7
1	1	156	GLN	2.5
4	4	23	ASN	2.4

## 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](#)

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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
5	SGN	1	503	20/20	0.90	0.21	-	10,42,81,86	20
5	SGN	1	501	20/20	0.68	0.57	-	66,78,118,125	20
5	IDS	1	502	15/17	0.79	0.37	-	34,57,83,91	15

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.