



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 05:07 am GMT

PDB ID : 1MQT  
Title : Swine Vesicular Disease Virus coat protein  
Authors : Verdaguer, N.; Jimenez-Clavero, M.A.; Fita, I.; Ley, V.  
Deposited on : 2002-09-17  
Resolution : 3.30 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

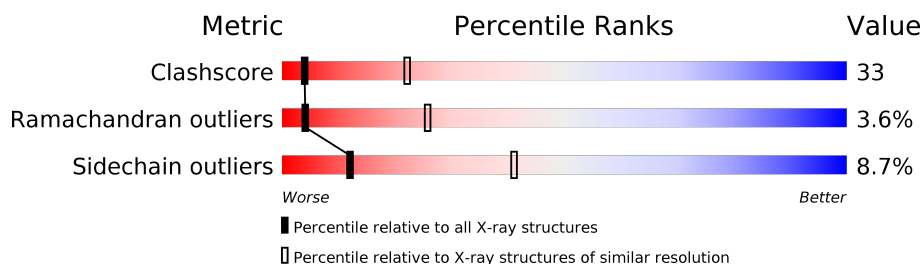
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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	112137	1100 (3.36-3.24)
Ramachandran outliers	110173	1081 (3.36-3.24)
Sidechain outliers	110143	1080 (3.36-3.24)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	283	
2	B	261	
3	C	238	
4	D	68	

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
5	SPL	A	284	X	-	-	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6393 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 Polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	271	Total	C	N	O	S	44	0	0
			2134	1347	372	404	11			

- Molecule 2 is a protein called Polyprotein Capsid Protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	254	Total	C	N	O	S	0	0	0
			1949	1233	329	370	17			

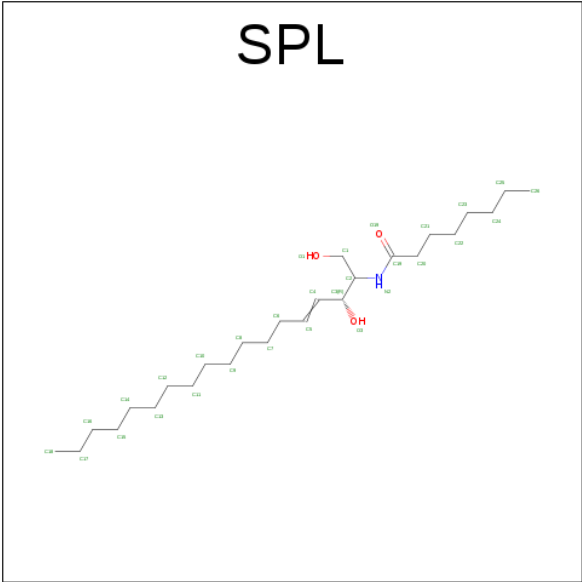
- Molecule 3 is a protein called Polyprotein Capsid Protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	238	Total	C	N	O	S	0	0	0
			1822	1162	291	353	16			

- Molecule 4 is a protein called Polyprotein Capsid Protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	55	Total	C	N	O	S	0	0	0
			428	265	74	87	2			

- Molecule 5 is OCTANOIC ACID (2-HYDROXY-1-HYDROXYMETHYL-HEPTADEC-3-E NYL)-AMIDE (three-letter code: SPL) (formula: C<sub>26</sub>H<sub>51</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			30	26	1	3		

- Molecule 6 is water.

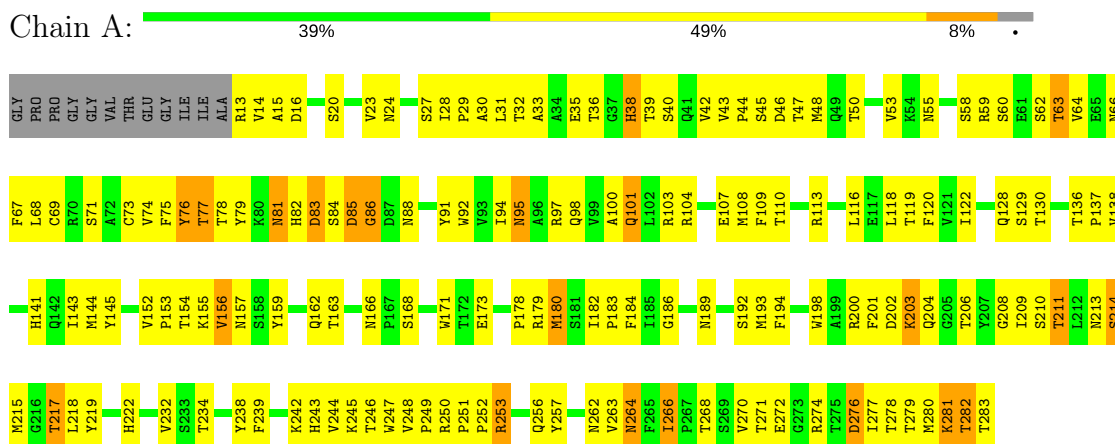
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	13	Total	O	0	0
			13	13		
6	B	6	Total	O	0	0
			6	6		
6	C	10	Total	O	0	0
			10	10		
6	D	1	Total	O	0	0
			1	1		

### 3 Residue-property plots

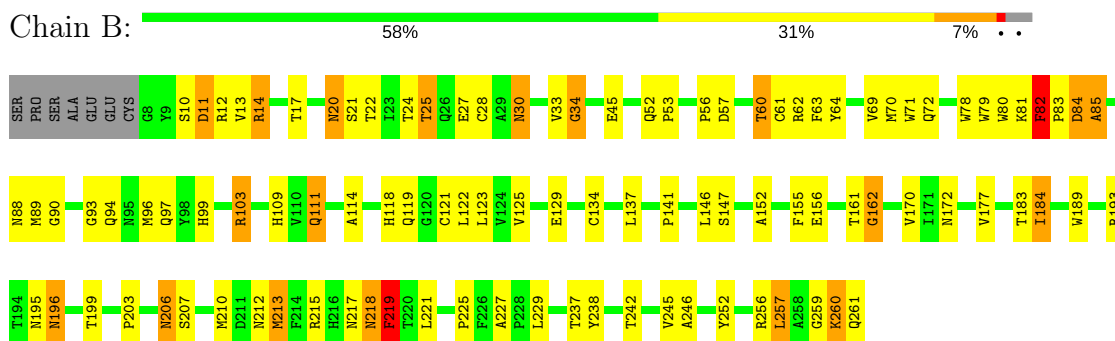
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

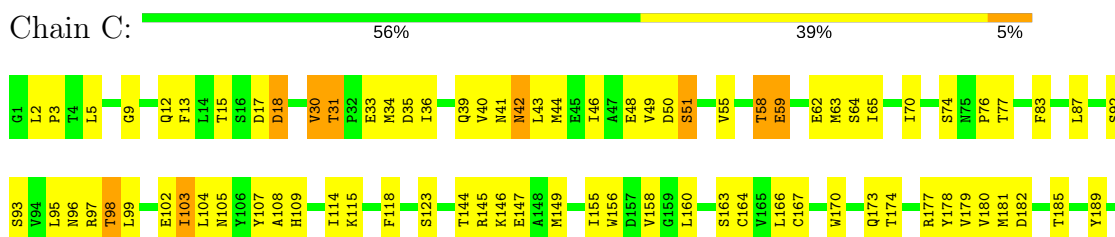
#### • Molecule 1: Polyprotein



#### • Molecule 2: Polyprotein Capsid Protein

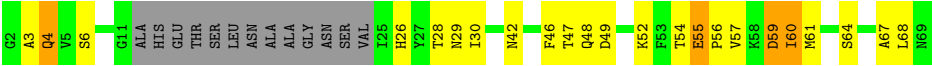


#### • Molecule 3: Polyprotein Capsid Protein





● Molecule 4: Polyprotein Capsid Protein



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	318.35Å 349.96Å 371.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.30	Depositor
% Data completeness (in resolution range)	62.6 (30.00-3.30)	Depositor
$R_{merge}$	0.20	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.257 , 0.279	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6393	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.50	0/2194	0.70	1/2991 (0.0%)
2	B	0.49	0/2000	0.73	2/2730 (0.1%)
3	C	0.44	0/1871	0.69	0/2555
4	D	0.72	0/435	0.68	0/585
All	All	0.50	0/6500	0.71	3/8861 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	82	PHE	N-CA-C	5.88	126.86	111.00
2	B	162	GLY	N-CA-C	5.55	126.98	113.10
1	A	86	GLY	N-CA-C	-5.25	99.97	113.10

There are no chirality outliers.

There are no planarity outliers.

### 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	2134	0	2070	208	0
2	B	1949	0	1878	119	0
3	C	1822	0	1748	128	0
4	D	428	0	411	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	30	0	50	7	0
6	A	13	0	0	2	0
6	B	6	0	0	0	0
6	C	10	0	0	0	0
6	D	1	0	0	0	0
All	All	6393	0	6157	412	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 33.

All (412) 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:201:PHE:HB2	2:B:261:GLN:HG2	1.35	1.05
2:B:20:ASN:H	2:B:20:ASN:ND2	1.46	1.00
2:B:20:ASN:N	2:B:20:ASN:HD22	1.55	0.99
1:A:95:ASN:HD21	1:A:98:GLN:HE21	1.15	0.93
3:C:42:ASN:HD22	3:C:44:MET:H	1.06	0.93
2:B:155:PHE:HB3	2:B:170:VAL:HG22	1.49	0.93
2:B:83:PRO:HG2	2:B:217:ASN:HA	1.52	0.92
3:C:173:GLN:HG2	3:C:174:THR:HG23	1.51	0.92
2:B:257:LEU:HD23	2:B:257:LEU:H	1.36	0.91
3:C:166:LEU:HD12	3:C:167:CYS:H	1.33	0.91
1:A:39:THR:HB	4:D:54:THR:HB	1.55	0.89
2:B:70:MET:HE1	2:B:238:TYR:HB3	1.55	0.89
3:C:182:ASP:HB3	3:C:185:THR:HG22	1.55	0.87
1:A:144:MET:SD	1:A:163:THR:HG22	2.15	0.86
2:B:25:THR:HG21	2:B:28:CYS:HB3	1.58	0.85
1:A:144:MET:CE	1:A:166:ASN:HD22	1.90	0.84
2:B:10:SER:HB3	2:B:13:VAL:HG23	1.61	0.83
2:B:83:PRO:HG2	2:B:218:ASN:H	1.44	0.82
1:A:63:THR:CG2	1:A:66:ASN:HD22	1.93	0.82
1:A:184:PHE:HA	6:A:289:HOH:O	1.78	0.82
3:C:58:THR:HG23	3:C:59:GLU:HG2	1.61	0.81
3:C:144:THR:HG22	3:C:146:LYS:H	1.45	0.81
1:A:14:VAL:HG13	3:C:219:ASP:HA	1.61	0.80
1:A:159:TYR:O	1:A:162:GLN:HG3	1.81	0.80
1:A:14:VAL:CG1	3:C:219:ASP:HA	2.13	0.79
1:A:97:ARG:HH22	1:A:213:ASN:HB2	1.47	0.78
2:B:156:GLU:O	2:B:170:VAL:HG23	1.83	0.78
1:A:16:ASP:HB3	1:A:55:ASN:H	1.46	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:20:ASN:N	2:B:20:ASN:ND2	2.21	0.77
2:B:83:PRO:CG	2:B:217:ASN:HA	2.15	0.77
4:D:60:ILE:H	4:D:60:ILE:HD12	1.50	0.77
1:A:268:THR:H	2:B:172:ASN:HD21	1.34	0.76
1:A:208:GLY:O	1:A:211:THR:HG23	1.87	0.75
1:A:108:MET:CE	1:A:252:PRO:HG3	2.17	0.74
1:A:108:MET:HE2	1:A:252:PRO:HG3	1.68	0.74
1:A:201:PHE:HB2	2:B:261:GLN:CG	2.17	0.74
1:A:95:ASN:ND2	1:A:98:GLN:HE21	1.83	0.74
2:B:134:CYS:HB2	2:B:141:PRO:HD3	1.69	0.74
1:A:43:VAL:HG23	1:A:45:SER:H	1.53	0.73
3:C:146:LYS:O	3:C:147:GLU:HB2	1.88	0.73
2:B:218:ASN:O	2:B:219:PHE:HB3	1.89	0.73
2:B:12:ARG:HD3	4:D:68:LEU:HD22	1.69	0.72
2:B:256:ARG:HG3	2:B:256:ARG:HH11	1.55	0.72
2:B:82:PHE:O	2:B:83:PRO:C	2.26	0.72
3:C:166:LEU:HD12	3:C:167:CYS:N	2.04	0.72
2:B:14:ARG:HB3	2:B:25:THR:OG1	1.90	0.71
1:A:272:GLU:OE1	1:A:283:THR:HG21	1.90	0.71
1:A:16:ASP:CB	1:A:55:ASN:H	2.03	0.71
3:C:237:PHE:O	3:C:238:GLN:HG3	1.91	0.71
1:A:94:ILE:HG21	5:A:284:SPL:H101	1.72	0.70
1:A:27:SER:HB2	4:D:64:SER:HB3	1.73	0.70
4:D:49:ASP:HB3	4:D:52:LYS:NZ	2.07	0.69
3:C:44:MET:O	3:C:48:GLU:HG3	1.92	0.69
1:A:279:THR:CG2	1:A:281:LYS:HG2	2.21	0.69
1:A:35:GLU:HA	2:B:189:TRP:HB2	1.74	0.69
2:B:25:THR:CG2	2:B:28:CYS:HB3	2.22	0.69
3:C:42:ASN:ND2	3:C:44:MET:H	1.87	0.69
2:B:83:PRO:HG2	2:B:218:ASN:N	2.08	0.68
3:C:108:ALA:HA	3:C:179:VAL:CG1	2.24	0.67
3:C:170:TRP:CH2	3:C:177:ARG:HG3	2.30	0.67
1:A:249:PRO:HG3	3:C:40:VAL:HG21	1.77	0.66
1:A:63:THR:HG21	1:A:66:ASN:HD22	1.59	0.66
2:B:119:GLN:NE2	3:C:205:GLN:HB3	2.11	0.66
3:C:55:VAL:HB	3:C:70:ILE:HD11	1.76	0.66
2:B:83:PRO:HG2	2:B:217:ASN:CA	2.25	0.66
2:B:20:ASN:H	2:B:20:ASN:HD22	0.75	0.66
3:C:155:ILE:HD13	3:C:195:GLN:NE2	2.09	0.66
3:C:170:TRP:HH2	3:C:177:ARG:HG3	1.60	0.66
1:A:60:SER:O	1:A:63:THR:HG22	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:ILE:CG2	1:A:31:LEU:HB2	2.27	0.65
2:B:10:SER:C	2:B:12:ARG:H	2.00	0.65
3:C:36:ILE:N	3:C:36:ILE:HD12	2.12	0.65
1:A:81:ASN:HD22	1:A:81:ASN:N	1.95	0.64
2:B:14:ARG:HB3	2:B:25:THR:CB	2.27	0.64
2:B:83:PRO:CG	2:B:218:ASN:H	2.11	0.64
1:A:36:THR:CG2	4:D:57:VAL:HG11	2.26	0.64
1:A:39:THR:HG23	3:C:50:ASP:OD2	1.98	0.64
1:A:249:PRO:HB3	3:C:46:ILE:CD1	2.28	0.64
2:B:206:ASN:HD22	2:B:207:SER:H	1.46	0.64
4:D:67:ALA:O	4:D:68:LEU:HD23	1.99	0.63
1:A:256:GLN:OE1	3:C:231:ILE:HD13	1.99	0.63
3:C:36:ILE:HD12	3:C:36:ILE:H	1.63	0.63
1:A:276:ASP:HB2	1:A:278:THR:HG22	1.80	0.62
1:A:16:ASP:HB2	1:A:53:VAL:O	1.99	0.62
2:B:27:GLU:HB2	2:B:196:ASN:CB	2.29	0.62
2:B:21:SER:CB	2:B:63:PHE:HB2	2.30	0.61
3:C:9:GLY:O	3:C:12:GLN:HB3	1.99	0.61
3:C:44:MET:HE2	3:C:220:PHE:HD1	1.65	0.61
1:A:68:LEU:HD12	1:A:244:VAL:HG11	1.81	0.61
1:A:282:THR:HG21	3:C:92:SER:HA	1.80	0.61
1:A:279:THR:HG23	1:A:281:LYS:HG2	1.83	0.60
1:A:40:SER:HB3	1:A:42:VAL:HG23	1.83	0.60
2:B:193:ARG:NH2	3:C:158:VAL:HG12	2.16	0.60
2:B:12:ARG:HE	4:D:68:LEU:HD13	1.66	0.60
1:A:74:VAL:O	1:A:75:PHE:HB2	2.02	0.60
2:B:27:GLU:HB2	2:B:196:ASN:HB2	1.84	0.60
1:A:282:THR:O	1:A:282:THR:HG22	2.01	0.60
1:A:81:ASN:H	1:A:81:ASN:HD22	1.49	0.60
3:C:200:VAL:HG13	3:C:201:PRO:HD2	1.83	0.60
1:A:144:MET:HE3	1:A:166:ASN:HD22	1.67	0.60
2:B:99:HIS:CD2	2:B:252:TYR:HB3	2.37	0.59
3:C:146:LYS:O	3:C:147:GLU:CB	2.49	0.59
3:C:200:VAL:HG12	3:C:201:PRO:O	2.02	0.59
3:C:200:VAL:CG1	3:C:204:ALA:HB3	2.33	0.59
1:A:120:PHE:O	1:A:178:PRO:HD2	2.03	0.59
1:A:63:THR:HG23	1:A:66:ASN:HB2	1.85	0.59
1:A:143:ILE:O	1:A:168:SER:HB2	2.03	0.59
1:A:76:TYR:C	1:A:76:TYR:CD1	2.76	0.58
3:C:108:ALA:HA	3:C:179:VAL:HG11	1.84	0.58
4:D:49:ASP:HB3	4:D:52:LYS:HZ1	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:206:ASN:ND2	2:B:207:SER:H	2.01	0.58
1:A:109:PHE:CD2	1:A:246:THR:HB	2.39	0.58
1:A:95:ASN:HD21	1:A:98:GLN:NE2	1.94	0.58
3:C:55:VAL:HB	3:C:70:ILE:CD1	2.33	0.57
1:A:264:ASN:HD22	2:B:137:LEU:HA	1.70	0.57
2:B:64:TYR:CD1	2:B:89:MET:HB3	2.39	0.57
2:B:12:ARG:NH1	2:B:27:GLU:HG2	2.20	0.57
2:B:21:SER:HB2	2:B:63:PHE:HB2	1.86	0.57
3:C:200:VAL:HG13	3:C:204:ALA:HB3	1.86	0.57
3:C:182:ASP:HB3	3:C:185:THR:CG2	2.31	0.57
1:A:23:VAL:HG12	1:A:24:ASN:N	2.19	0.57
1:A:79:TYR:OH	1:A:141:HIS:HD2	1.88	0.57
1:A:253:ARG:NH2	1:A:263:VAL:O	2.37	0.57
1:A:74:VAL:HG11	1:A:239:PHE:CD2	2.40	0.57
2:B:82:PHE:CZ	2:B:245:VAL:HG21	2.40	0.57
2:B:14:ARG:HB3	2:B:25:THR:HB	1.87	0.57
3:C:95:LEU:O	3:C:97:ARG:N	2.38	0.56
3:C:173:GLN:CG	3:C:174:THR:HG23	2.32	0.56
1:A:118:LEU:HD21	1:A:239:PHE:HE1	1.71	0.56
1:A:38:HIS:CE1	4:D:55:GLU:HG2	2.39	0.56
1:A:217:THR:HB	1:A:219:TYR:HE1	1.69	0.56
3:C:87:LEU:HD11	3:C:114:ILE:HD12	1.87	0.56
2:B:12:ARG:CD	4:D:68:LEU:HD22	2.35	0.56
1:A:271:THR:CG2	3:C:97:ARG:HB2	2.35	0.56
1:A:14:VAL:CG1	1:A:15:ALA:N	2.69	0.56
1:A:82:HIS:O	1:A:83:ASP:HB2	2.06	0.56
1:A:249:PRO:HB3	3:C:46:ILE:HD11	1.86	0.56
2:B:13:VAL:O	2:B:14:ARG:HB2	2.05	0.56
1:A:266:ILE:HD13	1:A:266:ILE:C	2.26	0.56
2:B:71:TRP:HD1	2:B:72:GLN:N	2.03	0.56
1:A:14:VAL:HG12	1:A:15:ALA:N	2.20	0.56
1:A:84:SER:O	1:A:85:ASP:HB2	2.05	0.56
1:A:28:ILE:HG21	1:A:31:LEU:HB2	1.87	0.55
3:C:144:THR:HG22	3:C:146:LYS:N	2.19	0.55
2:B:84:ASP:O	2:B:85:ALA:HB2	2.04	0.55
4:D:60:ILE:H	4:D:60:ILE:CD1	2.12	0.55
1:A:144:MET:HE2	1:A:166:ASN:HD22	1.69	0.55
3:C:180:VAL:HG12	3:C:181:MET:H	1.70	0.55
3:C:44:MET:CE	3:C:220:PHE:HD1	2.19	0.55
1:A:249:PRO:HG3	3:C:40:VAL:CG2	2.36	0.55
2:B:122:LEU:HD23	2:B:225:PRO:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:PHE:HA	3:C:236:PHE:CE1	2.42	0.54
1:A:103:ARG:O	1:A:107:GLU:HG3	2.07	0.54
1:A:270:VAL:O	1:A:271:THR:HG23	2.07	0.54
2:B:193:ARG:HG3	2:B:193:ARG:HH11	1.71	0.54
1:A:83:ASP:HB3	1:A:88:ASN:HD22	1.73	0.54
3:C:103:ILE:HG22	3:C:104:LEU:N	2.21	0.54
4:D:3:ALA:HB2	4:D:30:ILE:CG1	2.38	0.54
1:A:39:THR:HB	4:D:54:THR:CB	2.33	0.54
3:C:118:PHE:O	3:C:163:SER:HA	2.08	0.54
4:D:6:SER:O	4:D:26:HIS:HB3	2.08	0.54
1:A:145:TYR:HB2	5:A:284:SPL:H161	1.90	0.54
3:C:198:ILE:O	3:C:198:ILE:HG22	2.07	0.54
2:B:256:ARG:HG3	2:B:256:ARG:NH1	2.22	0.54
1:A:97:ARG:HA	1:A:103:ARG:HD2	1.89	0.54
2:B:114:ALA:HB1	2:B:118:HIS:HB2	1.90	0.54
2:B:12:ARG:HH21	3:C:160:LEU:HD11	1.73	0.54
3:C:156:TRP:CD1	3:C:164:CYS:HB2	2.43	0.54
1:A:86:GLY:HA2	1:A:156:VAL:HG23	1.90	0.54
1:A:171:TRP:CH2	1:A:173:GLU:HA	2.43	0.53
1:A:276:ASP:HB2	1:A:278:THR:H	1.73	0.53
2:B:93:GLY:O	2:B:97:GLN:HG3	2.07	0.53
4:D:60:ILE:N	4:D:60:ILE:HD12	2.22	0.53
1:A:47:THR:O	1:A:48:MET:HB3	2.07	0.53
3:C:36:ILE:CD1	3:C:36:ILE:H	2.20	0.53
3:C:65:ILE:O	3:C:65:ILE:HG12	2.09	0.53
3:C:83:PHE:C	3:C:83:PHE:CD1	2.81	0.53
1:A:214:SER:H	1:A:215:MET:CE	2.22	0.53
2:B:71:TRP:CD1	2:B:72:GLN:N	2.77	0.53
1:A:81:ASN:HA	1:A:222:HIS:ND1	2.24	0.52
1:A:13:ARG:HA	1:A:58:SER:HA	1.90	0.52
3:C:2:LEU:HD12	3:C:3:PRO:CD	2.38	0.52
1:A:279:THR:HG22	1:A:281:LYS:HG2	1.92	0.52
2:B:193:ARG:HG3	2:B:193:ARG:NH1	2.24	0.52
3:C:180:VAL:HG12	3:C:181:MET:N	2.24	0.52
1:A:28:ILE:HG22	1:A:31:LEU:HB2	1.90	0.52
4:D:3:ALA:HB2	4:D:30:ILE:HD11	1.91	0.52
1:A:116:LEU:HD11	1:A:239:PHE:HB3	1.92	0.52
3:C:109:HIS:CD2	3:C:223:ARG:HH21	2.28	0.52
2:B:62:ARG:HH11	2:B:62:ARG:HG3	1.74	0.52
1:A:282:THR:CG2	3:C:93:SER:H	2.22	0.52
4:D:3:ALA:HB2	4:D:30:ILE:HG13	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:ALA:CB	4:D:67:ALA:HB3	2.40	0.52
2:B:80:TRP:CZ2	2:B:152:ALA:HB2	2.45	0.52
1:A:214:SER:H	1:A:215:MET:HE2	1.75	0.51
4:D:55:GLU:N	4:D:56:PRO:CD	2.74	0.51
1:A:271:THR:HG22	3:C:97:ARG:HB2	1.92	0.51
1:A:27:SER:C	1:A:29:PRO:HD3	2.30	0.51
4:D:47:THR:HG22	4:D:48:GLN:N	2.24	0.51
1:A:86:GLY:CA	1:A:156:VAL:HG23	2.41	0.51
2:B:81:LYS:HG3	2:B:147:SER:HB2	1.92	0.51
2:B:121:CYS:HB3	2:B:227:ALA:HB3	1.93	0.51
1:A:277:ILE:O	1:A:277:ILE:HG12	2.10	0.51
2:B:33:VAL:O	2:B:34:GLY:C	2.49	0.51
3:C:98:THR:O	3:C:102:GLU:HG2	2.11	0.51
3:C:146:LYS:HA	3:C:149:MET:CG	2.40	0.50
1:A:97:ARG:HH22	1:A:213:ASN:CB	2.20	0.50
2:B:122:LEU:CD2	2:B:225:PRO:HB3	2.41	0.50
2:B:81:LYS:CG	2:B:147:SER:HB2	2.40	0.50
1:A:43:VAL:HG23	1:A:45:SER:N	2.23	0.50
1:A:78:THR:CG2	1:A:79:TYR:N	2.74	0.50
1:A:118:LEU:HD21	1:A:239:PHE:CE1	2.47	0.50
1:A:202:ASP:O	1:A:204:GLN:N	2.45	0.50
1:A:78:THR:HG23	1:A:232:VAL:HG13	1.92	0.50
2:B:52:GLN:HG3	2:B:53:PRO:HD2	1.94	0.50
3:C:105:ASN:HB3	3:C:228:THR:HG22	1.93	0.50
1:A:201:PHE:HD2	2:B:212:ASN:OD1	1.95	0.49
2:B:257:LEU:H	2:B:257:LEU:CD2	2.13	0.49
1:A:280:MET:HE2	3:C:189:TYR:HB3	1.93	0.49
2:B:69:VAL:HG21	2:B:78:TRP:NE1	2.26	0.49
1:A:81:ASN:ND2	1:A:82:HIS:N	2.60	0.49
2:B:17:THR:OG1	2:B:22:THR:HG23	2.13	0.49
3:C:108:ALA:HA	3:C:179:VAL:HG12	1.93	0.49
4:D:4:GLN:HG3	4:D:29:ASN:O	2.12	0.49
1:A:78:THR:HG22	1:A:79:TYR:N	2.28	0.49
2:B:257:LEU:HD23	2:B:257:LEU:N	2.16	0.49
2:B:71:TRP:HD1	2:B:72:GLN:H	1.59	0.49
1:A:88:ASN:ND2	1:A:156:VAL:HG21	2.27	0.49
2:B:20:ASN:HD21	2:B:62:ARG:HE	1.61	0.49
1:A:186:GLY:O	3:C:31:THR:HG21	2.12	0.49
1:A:118:LEU:HG	1:A:182:ILE:CD1	2.43	0.49
2:B:109:HIS:HD2	2:B:199:THR:OG1	1.96	0.48
2:B:12:ARG:HD3	2:B:28:CYS:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:83:PRO:CD	2:B:217:ASN:HA	2.43	0.48
1:A:36:THR:CG2	1:A:38:HIS:HB3	2.43	0.48
1:A:67:PHE:CD1	3:C:43:LEU:HD11	2.49	0.48
1:A:59:ARG:NH1	3:C:44:MET:HB3	2.28	0.48
1:A:200:ARG:HD3	1:A:204:GLN:O	2.13	0.48
2:B:12:ARG:HB3	2:B:27:GLU:HA	1.95	0.48
3:C:34:MET:HG2	3:C:35:ASP:H	1.78	0.48
1:A:104:ARG:NH1	1:A:253:ARG:O	2.46	0.48
1:A:44:PRO:O	1:A:48:MET:HG2	2.13	0.48
1:A:198:TRP:HZ2	2:B:146:LEU:HD12	1.77	0.48
3:C:42:ASN:HD22	3:C:44:MET:N	1.90	0.48
1:A:108:MET:HE3	1:A:252:PRO:HG3	1.92	0.48
1:A:276:ASP:CB	1:A:278:THR:HG22	2.44	0.48
2:B:111:GLN:HG3	2:B:242:THR:O	2.14	0.48
2:B:69:VAL:HG21	2:B:78:TRP:CD1	2.49	0.48
3:C:109:HIS:HD2	3:C:223:ARG:NH2	2.11	0.48
1:A:81:ASN:HD22	1:A:82:HIS:H	1.61	0.47
1:A:171:TRP:CD1	1:A:178:PRO:HG3	2.48	0.47
2:B:155:PHE:CB	2:B:170:VAL:HG22	2.33	0.47
3:C:36:ILE:N	3:C:36:ILE:CD1	2.77	0.47
1:A:36:THR:HG22	4:D:57:VAL:HG11	1.96	0.47
3:C:144:THR:HG22	3:C:145:ARG:N	2.30	0.47
3:C:17:ASP:O	3:C:18:ASP:HB2	2.13	0.47
4:D:3:ALA:CB	4:D:30:ILE:HG13	2.44	0.47
1:A:20:SER:HB3	1:A:50:THR:H	1.80	0.47
3:C:55:VAL:CB	3:C:70:ILE:HD11	2.44	0.47
3:C:173:GLN:HG2	3:C:174:THR:CG2	2.34	0.47
3:C:2:LEU:HD12	3:C:3:PRO:N	2.28	0.47
1:A:64:VAL:HG23	3:C:41:ASN:C	2.35	0.47
1:A:118:LEU:HG	1:A:182:ILE:HD11	1.96	0.47
1:A:120:PHE:CE2	1:A:180:MET:HE1	2.50	0.47
3:C:196:THR:O	3:C:197:ASN:O	2.32	0.47
1:A:110:THR:O	1:A:193:MET:HB2	2.14	0.46
1:A:244:VAL:HG12	1:A:245:LYS:N	2.31	0.46
1:A:92:TRP:HE1	1:A:98:GLN:NE2	2.13	0.46
4:D:55:GLU:C	4:D:57:VAL:H	2.19	0.46
1:A:155:LYS:C	1:A:157:ASN:H	2.19	0.46
1:A:122:ILE:HB	1:A:171:TRP:CZ3	2.51	0.46
2:B:119:GLN:HE22	3:C:205:GLN:HB3	1.77	0.46
2:B:80:TRP:CE2	2:B:152:ALA:HB2	2.51	0.46
1:A:262:ASN:OD1	1:A:264:ASN:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:THR:HG23	1:A:232:VAL:CG1	2.46	0.46
1:A:251:PRO:HG3	2:B:184:ILE:HD11	1.97	0.46
1:A:250:ARG:NH2	2:B:129:GLU:O	2.49	0.46
1:A:250:ARG:HA	2:B:184:ILE:HD12	1.97	0.46
1:A:215:MET:HG3	5:A:284:SPL:H262	1.98	0.46
2:B:63:PHE:CD1	2:B:246:ALA:HB2	2.51	0.46
1:A:36:THR:HG22	1:A:38:HIS:HB3	1.97	0.45
1:A:38:HIS:ND1	4:D:55:GLU:HA	2.30	0.45
2:B:193:ARG:HH21	3:C:158:VAL:HG12	1.80	0.45
1:A:81:ASN:H	1:A:81:ASN:ND2	2.14	0.45
2:B:83:PRO:HD2	2:B:217:ASN:HA	1.98	0.45
2:B:60:THR:CG2	2:B:61:CYS:N	2.80	0.45
3:C:156:TRP:HB2	3:C:164:CYS:SG	2.57	0.45
3:C:146:LYS:HA	3:C:149:MET:HG3	1.97	0.45
1:A:73:CYS:HB2	1:A:238:TYR:CE2	2.52	0.45
1:A:31:LEU:HD23	3:C:164:CYS:HA	1.99	0.45
3:C:193:TRP:CD1	3:C:193:TRP:N	2.85	0.45
1:A:184:PHE:HB3	3:C:30:VAL:HG21	1.99	0.45
4:D:3:ALA:HB2	4:D:30:ILE:CD1	2.47	0.45
2:B:189:TRP:O	2:B:195:ASN:ND2	2.50	0.45
2:B:259:GLY:C	2:B:260:LYS:HG2	2.37	0.45
4:D:49:ASP:HB3	4:D:52:LYS:HZ2	1.80	0.45
1:A:276:ASP:C	1:A:278:THR:H	2.18	0.45
1:A:67:PHE:CG	3:C:43:LEU:HD11	2.51	0.45
2:B:83:PRO:CG	2:B:218:ASN:N	2.76	0.45
1:A:76:TYR:C	1:A:76:TYR:HD1	2.19	0.44
3:C:115:LYS:HE3	3:C:115:LYS:HB2	1.68	0.44
1:A:71:SER:HA	1:A:239:PHE:O	2.16	0.44
2:B:114:ALA:HB1	2:B:118:HIS:CB	2.47	0.44
2:B:212:ASN:ND2	2:B:213:MET:H	2.16	0.44
1:A:60:SER:CB	4:D:46:PHE:HE1	2.30	0.44
1:A:88:ASN:CG	1:A:156:VAL:HG21	2.38	0.44
3:C:2:LEU:HD12	3:C:2:LEU:C	2.38	0.44
2:B:56:PRO:O	2:B:57:ASP:HB3	2.17	0.44
2:B:119:GLN:HB3	3:C:123:SER:N	2.33	0.44
1:A:280:MET:CE	3:C:189:TYR:HB3	2.48	0.44
1:A:91:TYR:HA	1:A:218:LEU:O	2.18	0.44
1:A:35:GLU:HB3	2:B:195:ASN:HD21	1.83	0.44
1:A:184:PHE:HB3	3:C:30:VAL:CG2	2.48	0.43
2:B:125:VAL:O	2:B:221:LEU:HD12	2.18	0.43
3:C:46:ILE:O	3:C:49:VAL:HB	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:LYS:O	1:A:157:ASN:N	2.51	0.43
1:A:118:LEU:O	1:A:179:ARG:HA	2.17	0.43
1:A:77:THR:O	1:A:234:THR:HA	2.17	0.43
3:C:98:THR:HG22	3:C:99:LEU:H	1.83	0.43
1:A:119:THR:HG21	3:C:13:PHE:CE1	2.54	0.43
1:A:245:LYS:HE3	3:C:33:GLU:OE2	2.18	0.43
1:A:198:TRP:CE3	1:A:203:LYS:HG2	2.54	0.43
1:A:253:ARG:HG3	1:A:257:TYR:CZ	2.53	0.43
2:B:82:PHE:O	2:B:84:ASP:N	2.52	0.43
2:B:84:ASP:O	2:B:85:ALA:CB	2.65	0.43
1:A:81:ASN:HD22	1:A:82:HIS:N	2.16	0.43
1:A:59:ARG:HD3	3:C:44:MET:HG3	2.01	0.43
1:A:33:ALA:HB3	4:D:67:ALA:CB	2.48	0.43
1:A:242:LYS:O	1:A:243:HIS:C	2.57	0.43
2:B:62:ARG:HG3	2:B:62:ARG:NH1	2.34	0.43
1:A:62:SER:HA	3:C:107:TYR:OH	2.18	0.43
2:B:103:ARG:HB3	2:B:210:MET:HG2	2.01	0.43
6:A:297:HOH:O	3:C:63:MET:HB3	2.18	0.43
1:A:94:ILE:CG2	5:A:284:SPL:H101	2.45	0.43
2:B:123:LEU:HB2	2:B:189:TRP:CZ3	2.54	0.43
1:A:31:LEU:HD21	3:C:156:TRP:CD1	2.54	0.42
1:A:271:THR:HG22	3:C:97:ARG:CG	2.48	0.42
1:A:16:ASP:HB3	1:A:55:ASN:N	2.25	0.42
2:B:34:GLY:HA3	2:B:203:PRO:HD3	2.01	0.42
1:A:71:SER:O	3:C:15:THR:HG23	2.19	0.42
2:B:123:LEU:HG	2:B:125:VAL:HG13	2.01	0.42
2:B:71:TRP:CE2	2:B:229:LEU:HB2	2.55	0.42
2:B:121:CYS:CB	2:B:227:ALA:HB3	2.49	0.42
1:A:136:THR:HA	1:A:137:PRO:HD3	1.88	0.42
1:A:182:ILE:HA	1:A:183:PRO:HD3	1.89	0.42
1:A:33:ALA:HB1	1:A:35:GLU:OE1	2.20	0.42
1:A:63:THR:HG23	1:A:66:ASN:HD22	1.82	0.42
1:A:94:ILE:HG21	5:A:284:SPL:C10	2.47	0.42
1:A:189:ASN:CB	3:C:34:MET:HB2	2.49	0.42
1:A:193:MET:O	1:A:209:ILE:HD13	2.19	0.42
1:A:194:PHE:HE1	1:A:250:ARG:HD3	1.84	0.42
1:A:256:GLN:OE1	3:C:231:ILE:CD1	2.67	0.42
3:C:109:HIS:HD2	3:C:223:ARG:HH21	1.65	0.42
1:A:113:ARG:HB3	1:A:245:LYS:HB2	2.01	0.42
1:A:252:PRO:HG2	3:C:102:GLU:HB3	2.02	0.42
3:C:103:ILE:CG2	3:C:104:LEU:N	2.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:144:THR:O	3:C:146:LYS:O	2.38	0.42
3:C:231:ILE:O	3:C:231:ILE:CG2	2.68	0.42
4:D:28:THR:HG22	4:D:29:ASN:N	2.35	0.42
1:A:116:LEU:HD21	1:A:239:PHE:CD1	2.55	0.42
1:A:23:VAL:CG1	1:A:24:ASN:N	2.82	0.42
2:B:256:ARG:HB2	2:B:257:LEU:HD23	2.01	0.42
3:C:202:ALA:O	3:C:203:ASP:HB2	2.20	0.42
3:C:95:LEU:O	3:C:98:THR:OG1	2.37	0.42
1:A:152:VAL:HA	1:A:153:PRO:HD3	1.87	0.41
1:A:215:MET:CG	5:A:284:SPL:H262	2.50	0.41
1:A:35:GLU:HB3	2:B:195:ASN:ND2	2.35	0.41
3:C:225:LEU:HD12	3:C:225:LEU:HA	1.86	0.41
1:A:144:MET:HA	1:A:168:SER:CB	2.50	0.41
1:A:100:ALA:HB1	3:C:231:ILE:HD12	2.02	0.41
1:A:97:ARG:CA	1:A:103:ARG:HD2	2.51	0.41
1:A:245:LYS:HB3	1:A:247:TRP:CH2	2.55	0.41
1:A:263:VAL:HG12	1:A:263:VAL:O	2.20	0.41
1:A:35:GLU:H	1:A:35:GLU:CD	2.23	0.41
1:A:81:ASN:ND2	1:A:81:ASN:N	2.65	0.41
1:A:282:THR:HG23	3:C:93:SER:H	1.86	0.41
2:B:94:GLN:C	2:B:96:MET:N	2.73	0.41
1:A:274:ARG:NH2	3:C:55:VAL:O	2.49	0.41
1:A:33:ALA:HB2	4:D:67:ALA:HB3	2.01	0.41
2:B:30:ASN:CG	4:D:59:ASP:HB2	2.41	0.41
2:B:45:GLU:OE1	2:B:45:GLU:N	2.53	0.41
3:C:178:TYR:HB2	3:C:185:THR:HG21	2.03	0.41
3:C:74:SER:HA	3:C:197:ASN:OD1	2.21	0.41
3:C:64:SER:OG	3:C:65:ILE:N	2.53	0.41
1:A:91:TYR:C	1:A:91:TYR:CD1	2.93	0.41
1:A:39:THR:HG21	3:C:48:GLU:O	2.20	0.41
1:A:189:ASN:ND2	3:C:34:MET:HB2	2.36	0.41
1:A:32:THR:HG23	1:A:33:ALA:N	2.36	0.41
1:A:198:TRP:CZ2	2:B:146:LEU:HD12	2.55	0.41
2:B:14:ARG:O	2:B:24:THR:HA	2.20	0.41
2:B:84:ASP:OD1	2:B:85:ALA:N	2.53	0.41
4:D:57:VAL:HG23	4:D:59:ASP:O	2.21	0.41
1:A:104:ARG:NH2	3:C:102:GLU:OE1	2.47	0.41
1:A:155:LYS:C	1:A:157:ASN:N	2.74	0.41
1:A:280:MET:HE2	3:C:189:TYR:CD2	2.56	0.41
1:A:247:TRP:CD1	3:C:39:GLN:HB2	2.55	0.41
1:A:30:ALA:HB2	1:A:47:THR:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:PHE:CB	2:B:261:GLN:HG2	2.27	0.41
2:B:70:MET:HE1	2:B:238:TYR:CB	2.37	0.41
3:C:44:MET:CE	3:C:220:PHE:CD1	3.02	0.41
1:A:118:LEU:HD12	5:A:284:SPL:H151	2.03	0.40
1:A:206:THR:HG22	1:A:211:THR:HG22	2.03	0.40
1:A:217:THR:HB	1:A:219:TYR:CE1	2.53	0.40
3:C:51:SER:OG	3:C:98:THR:HG22	2.21	0.40
1:A:253:ARG:HG3	1:A:257:TYR:OH	2.21	0.40
2:B:206:ASN:HD22	2:B:207:SER:N	2.14	0.40
2:B:82:PHE:C	2:B:84:ASP:N	2.72	0.40
1:A:282:THR:HG23	3:C:93:SER:OG	2.21	0.40
1:A:36:THR:HG21	4:D:61:MET:SD	2.61	0.40
2:B:172:ASN:HA	2:B:177:VAL:O	2.22	0.40
3:C:109:HIS:HB2	3:C:223:ARG:HB2	2.03	0.40
3:C:42:ASN:HD21	3:C:44:MET:HG2	1.87	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	269/283 (95%)	229 (85%)	28 (10%)	12 (4%)	3	20
2	B	252/261 (97%)	213 (84%)	28 (11%)	11 (4%)	3	20
3	C	236/238 (99%)	208 (88%)	23 (10%)	5 (2%)	8	38
4	D	51/68 (75%)	45 (88%)	5 (10%)	1 (2%)	9	39
All	All	808/850 (95%)	695 (86%)	84 (10%)	29 (4%)	4	26

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	83	ASP
1	A	203	LYS
1	A	214	SER
2	B	162	GLY
2	B	260	LYS
3	C	96	ASN
3	C	197	ASN
1	A	69	CYS
1	A	130	THR
1	A	282	THR
2	B	34	GLY
2	B	85	ALA
3	C	18	ASP
1	A	101	GLN
1	A	156	VAL
1	A	210	SER
2	B	14	ARG
2	B	219	PHE
3	C	59	GLU
1	A	129	SER
2	B	11	ASP
2	B	183	THR
2	B	196	ASN
3	C	224	MET
1	A	248	VAL
1	A	264	ASN
2	B	82	PHE
4	D	55	GLU
2	B	90	GLY

### 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	A	238/245 (97%)	218 (92%)	20 (8%)	13	43
2	B	211/217 (97%)	191 (90%)	20 (10%)	10	35
3	C	203/205 (99%)	186 (92%)	17 (8%)	13	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	47/56 (84%)	43 (92%)	4 (8%)	12	42
All	All	699/723 (97%)	638 (91%)	61 (9%)	12	41

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	HIS
1	A	46	ASP
1	A	63	THR
1	A	76	TYR
1	A	77	THR
1	A	81	ASN
1	A	85	ASP
1	A	95	ASN
1	A	101	GLN
1	A	128	GLN
1	A	138	VAL
1	A	154	THR
1	A	180	MET
1	A	192	SER
1	A	211	THR
1	A	217	THR
1	A	253	ARG
1	A	266	ILE
1	A	276	ASP
1	A	281	LYS
2	B	11	ASP
2	B	20	ASN
2	B	25	THR
2	B	30	ASN
2	B	60	THR
2	B	79	TRP
2	B	82	PHE
2	B	84	ASP
2	B	88	ASN
2	B	103	ARG
2	B	111	GLN
2	B	161	THR
2	B	184	ILE
2	B	206	ASN
2	B	213	MET
2	B	215	ARG

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Mol	Chain	Res	Type
2	B	218	ASN
2	B	219	PHE
2	B	237	THR
2	B	257	LEU
3	C	5	LEU
3	C	30	VAL
3	C	31	THR
3	C	42	ASN
3	C	51	SER
3	C	58	THR
3	C	62	GLU
3	C	76	PRO
3	C	77	THR
3	C	98	THR
3	C	103	ILE
3	C	206	SER
3	C	207	ASP
3	C	225	LEU
3	C	228	THR
3	C	231	ILE
3	C	234	ASP
4	D	4	GLN
4	D	42	ASN
4	D	59	ASP
4	D	60	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	ASN
1	A	81	ASN
1	A	88	ASN
1	A	98	GLN
1	A	101	GLN
1	A	141	HIS
1	A	162	GLN
1	A	166	ASN
1	A	264	ASN
2	B	20	ASN
2	B	30	ASN
2	B	55	GLN
2	B	109	HIS

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Mol	Chain	Res	Type
2	B	119	GLN
2	B	172	ASN
2	B	195	ASN
2	B	206	ASN
2	B	212	ASN
3	C	39	GLN
3	C	42	ASN
3	C	73	GLN
3	C	81	GLN
3	C	109	HIS
4	D	31	ASN
4	D	69	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](#)

1 ligand is 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	SPL	A	284	-	28,29,29	1.36	5 (17%)	28,31,31	3.34	10 (35%)



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	SPL	A	284	-	1/1/3/6	2/32/32/32	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	284	SPL	C21-C20	2.12	1.60	1.52
5	A	284	SPL	C11-C10	2.57	1.66	1.51
5	A	284	SPL	C10-C9	2.76	1.67	1.51
5	A	284	SPL	O3-C3	3.10	1.49	1.43
5	A	284	SPL	O19-C19	3.21	1.30	1.23

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	284	SPL	C3-C4-C5	-6.80	116.08	125.22
5	A	284	SPL	O3-C3-C2	-5.79	92.31	107.90
5	A	284	SPL	O3-C3-C4	-5.62	96.39	110.79
5	A	284	SPL	O19-C19-N2	-3.78	116.44	122.97
5	A	284	SPL	C6-C5-C4	-3.39	112.17	125.66
5	A	284	SPL	O19-C19-C20	-2.08	118.10	122.01
5	A	284	SPL	C21-C20-C19	4.18	125.06	113.32
5	A	284	SPL	O1-C1-C2	4.43	122.38	111.12
5	A	284	SPL	C20-C19-N2	5.48	125.46	115.82
5	A	284	SPL	C1-C2-N2	9.85	126.61	109.38

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	284	SPL	C2

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	284	SPL	C20-C19-N2-C2
5	A	284	SPL	C3-C2-N2-C19

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	284	SPL	7	0

## 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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.