



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 24, 2018 – 02:55 PM EDT

PDB ID : 5Z0R
Title : Structural insight into the Zika virus capsid encapsulating the viral genome
Authors : Li, T.; Zhao, Q.; Yang, X.; Chen, C.; Yang, K.; Wu, C.; Zhang, T.; Duan, Y.;
Xue, X.; Mi, K.; Ji, X.; Wang, Z.; Yang, H.
Deposited on : 2017-12-20
Resolution : 2.05 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : rb-20031021
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20031021

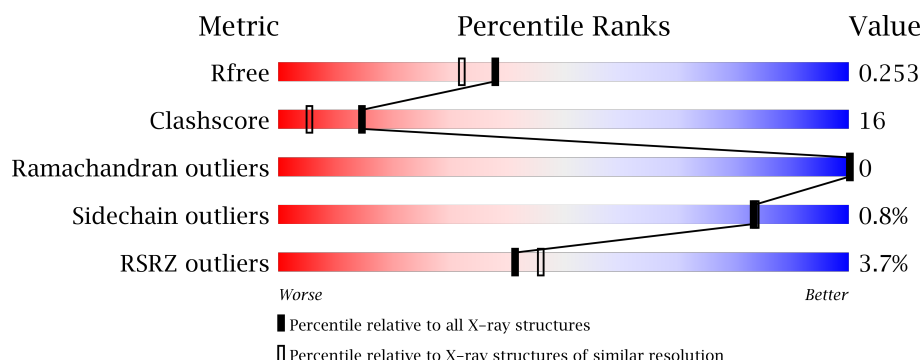
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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}	111664	1449 (2.04-2.04)
Clashscore	122126	1524 (2.04-2.04)
Ramachandran outliers	120053	1512 (2.04-2.04)
Sidechain outliers	120020	1512 (2.04-2.04)
RSRZ outliers	108989	1429 (2.04-2.04)

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 $\leq 5\%$. 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	A	445	<div> <div>6%</div> <div>69%</div> <div>30%</div> <div>.</div> </div>
1	B	445	<div> <div>2%</div> <div>75%</div> <div>25%</div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7342 atoms, of which 44 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.

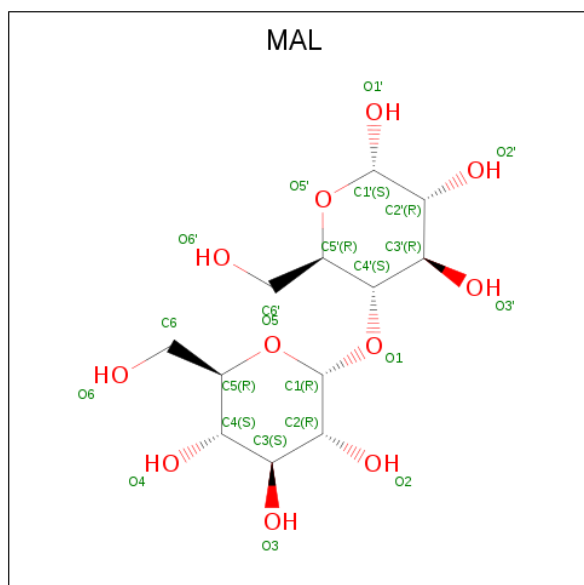
- Molecule 1 is a protein called Extracellular solute-binding protein family 1,viral genome protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	442	Total	C	N	O	S	0	0	0
			3425	2215	569	632	9			
1	B	445	Total	C	N	O	S	0	0	0
			3454	2234	573	637	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A0A140NCD0
A	268	ASP	ASN	engineered mutation	UNP A0A140NCD0
B	1	MET	-	initiating methionine	UNP A0A140NCD0
B	268	ASP	ASN	engineered mutation	UNP A0A140NCD0

- Molecule 2 is MALTOSE (three-letter code: MAL) (formula: C₁₂H₂₂O₁₁).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 45	C 12	H 22	O 11	0	0
2	B	1	Total 45	C 12	H 22	O 11	0	0

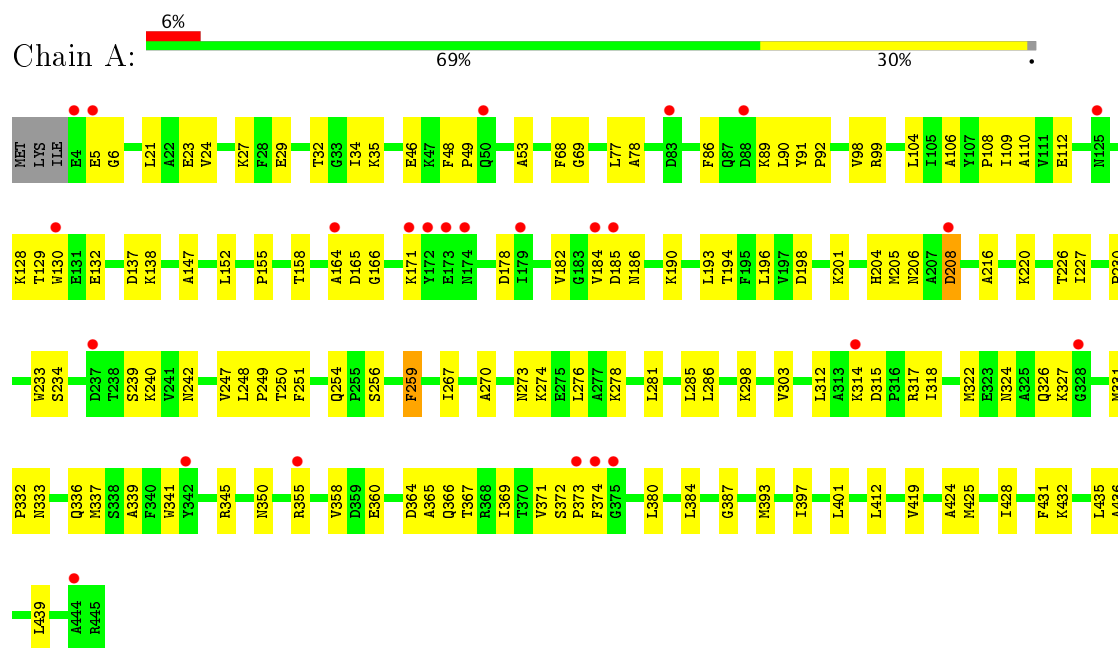
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	154	Total 154	O 154	0	0
3	B	219	Total 219	O 219	0	0

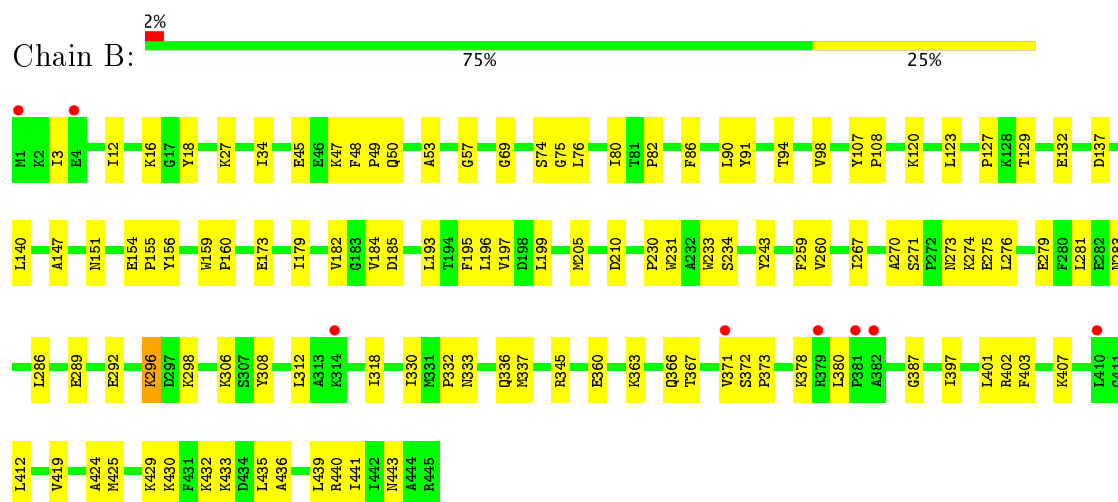
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

- Molecule 1: Extracellular solute-binding protein family 1, viral genome protein



- Molecule 1: Extracellular solute-binding protein family 1, viral genome protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.30 Å 81.42 Å 77.19 Å 90.00° 104.79° 90.00°	Depositor
Resolution (Å)	48.29 – 2.05 48.29 – 2.05	Depositor EDS
% Data completeness (in resolution range)	95.0 (48.29-2.05) 88.9 (48.29-2.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 2.05 Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575)	Depositor
R, R_{free}	0.221 , 0.254 0.221 , 0.253	Depositor DCC
R_{free} test set	1912 reflections (3.60%)	wwPDB-VP
Wilson B-factor (Å ²)	30.6	Xtriage
Anisotropy	0.286	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 36.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.021 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7342	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.97% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: MAL

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	0.23	0/3505	0.40	0/4749
1	B	0.24	0/3534	0.43	0/4786
All	All	0.23	0/7039	0.41	0/9535

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3425	0	3464	127	0
1	B	3454	0	3504	112	0
2	A	23	22	22	2	0
2	B	23	22	22	3	0
3	A	154	0	0	16	2
3	B	219	0	0	13	1
All	All	7298	44	7012	229	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 16.

All (229) 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:B:151:ASN:HB2	3:B:601:HOH:O	1.34	1.23
1:A:226:THR:C	3:A:601:HOH:O	1.84	1.14
1:B:151:ASN:ND2	3:B:601:HOH:O	1.84	1.10
1:B:185:ASP:HB2	1:B:366:GLN:HG3	1.36	1.08
1:A:185:ASP:HB2	1:A:366:GLN:HG3	1.11	1.05
1:B:306:LYS:NZ	3:B:602:HOH:O	1.88	1.04
1:A:226:THR:O	3:A:601:HOH:O	1.80	0.98
1:A:227:ILE:HG13	3:A:601:HOH:O	1.67	0.93
1:B:185:ASP:CB	1:B:366:GLN:HG3	2.03	0.89
1:B:205:MET:SD	3:B:808:HOH:O	2.32	0.88
1:A:6:GLY:H	1:A:273:ASN:HD21	1.24	0.86
1:B:151:ASN:CB	3:B:601:HOH:O	2.00	0.86
1:B:185:ASP:HB2	1:B:366:GLN:CG	2.08	0.83
1:B:360:GLU:OE1	3:B:603:HOH:O	1.95	0.83
1:A:254:GLN:O	3:A:602:HOH:O	1.96	0.81
1:A:90:LEU:HD23	1:A:108:PRO:HG2	1.62	0.81
1:B:34:ILE:HD13	1:B:276:LEU:HD22	1.63	0.80
1:A:190:LYS:O	1:A:194:THR:HG23	1.81	0.79
1:A:155:PRO:HG3	1:A:345:ARG:HA	1.63	0.79
1:A:248:LEU:HB2	1:A:256:SER:OG	1.82	0.79
1:A:46:GLU:OE2	3:A:605:HOH:O	2.01	0.79
1:A:6:GLY:H	1:A:273:ASN:ND2	1.81	0.78
1:A:165:ASP:O	3:A:604:HOH:O	2.01	0.78
1:A:164:ALA:O	3:A:603:HOH:O	2.01	0.78
1:B:90:LEU:HD23	1:B:108:PRO:HG2	1.67	0.76
1:B:279:GLU:OE2	1:B:283:ASN:ND2	2.17	0.76
1:A:185:ASP:CB	1:A:366:GLN:HG3	2.05	0.76
1:A:327:LYS:NZ	3:A:608:HOH:O	2.18	0.74
1:A:185:ASP:HB2	1:A:366:GLN:CG	2.07	0.74
1:B:107:TYR:CD2	1:B:281:LEU:HD13	2.22	0.74
1:B:27:LYS:NZ	1:B:289:GLU:OE2	2.22	0.73
1:B:155:PRO:HG3	1:B:345:ARG:HA	1.72	0.72
1:A:129:THR:HA	1:A:250:THR:HG22	1.70	0.71
1:B:366:GLN:NE2	3:B:605:HOH:O	2.22	0.71
1:B:276:LEU:HG	3:B:636:HOH:O	1.91	0.70
1:B:179:ILE:H	1:B:179:ILE:HD12	1.57	0.70
1:A:332:PRO:HB2	1:A:337:MET:HE3	1.74	0.69
1:B:69:GLY:HA3	1:B:333:ASN:O	1.93	0.69
1:A:435:LEU:HD22	1:B:435:LEU:HD12	1.74	0.68
1:B:156:TYR:HB2	2:B:501:MAL:H6'2	1.76	0.67
1:A:439:LEU:HD11	1:B:425:MET:HG3	1.75	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:VAL:HB	1:A:366:GLN:HG2	1.76	0.67
1:B:12:ILE:HD11	1:B:16:LYS:CB	2.24	0.67
1:A:336:GLN:HA	1:A:374:PHE:CD2	2.29	0.67
1:B:182:VAL:O	1:B:366:GLN:NE2	2.23	0.67
1:A:158:THR:HG23	1:A:196:LEU:HD22	1.76	0.67
1:A:230:PRO:HA	1:A:233:TRP:CE2	2.31	0.66
1:A:34:ILE:HD13	1:A:276:LEU:HD13	1.78	0.66
1:A:112:GLU:OE2	2:A:501:MAL:O2'	2.05	0.66
1:A:182:VAL:O	1:A:366:GLN:NE2	2.28	0.66
1:B:332:PRO:HB2	1:B:337:MET:CE	2.26	0.66
1:A:129:THR:HG22	1:A:250:THR:CG2	2.26	0.66
1:A:248:LEU:CB	1:A:256:SER:OG	2.44	0.66
1:A:425:MET:HE3	1:B:443:ASN:HB2	1.78	0.66
1:B:308:TYR:CE2	1:B:312:LEU:HD11	2.31	0.65
1:B:140:LEU:HD12	1:B:147:ALA:HA	1.79	0.65
1:A:216:ALA:HB1	1:A:220:LYS:NZ	2.12	0.64
1:A:436:ALA:HA	1:B:432:LYS:HZ1	1.63	0.64
1:A:251:PHE:O	3:A:602:HOH:O	2.15	0.63
1:A:69:GLY:HA3	1:A:333:ASN:O	1.98	0.63
1:A:34:ILE:CD1	1:A:276:LEU:HD22	2.29	0.63
1:B:234:SER:HB2	1:B:298:LYS:HD3	1.81	0.63
1:A:339:ALA:HB2	1:A:374:PHE:HE2	1.64	0.63
1:B:184:VAL:HB	1:B:366:GLN:HG2	1.81	0.62
1:A:27:LYS:HD3	3:A:661:HOH:O	1.98	0.62
1:B:184:VAL:H	1:B:366:GLN:HE21	1.46	0.62
1:B:332:PRO:HB2	1:B:337:MET:HE1	1.80	0.62
1:A:254:GLN:HB2	3:A:602:HOH:O	1.98	0.61
1:A:34:ILE:HD13	1:A:276:LEU:CD1	2.30	0.61
1:A:267:ILE:HG21	1:A:274:LYS:HG3	1.83	0.61
1:B:12:ILE:HD11	1:B:16:LYS:HB3	1.83	0.60
1:A:322:MET:O	1:A:326:GLN:HG2	2.02	0.59
1:A:34:ILE:CD1	1:A:276:LEU:CD2	2.81	0.59
1:B:231:TRP:O	1:B:298:LYS:HD2	2.03	0.59
1:A:198:ASP:HA	1:A:201:LYS:HG2	1.85	0.58
1:A:21:LEU:O	1:A:24:VAL:HG22	2.02	0.58
1:B:173:GLU:OE1	3:B:604:HOH:O	2.16	0.58
1:A:129:THR:OG1	1:A:132:GLU:HG3	2.04	0.58
1:B:234:SER:CB	1:B:298:LYS:HD3	2.34	0.57
1:A:256:SER:N	3:A:606:HOH:O	2.09	0.57
1:B:184:VAL:N	1:B:366:GLN:HE21	2.02	0.57
1:A:155:PRO:HD3	1:A:345:ARG:HG3	1.85	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:THR:HG21	1:A:34:ILE:HD12	1.87	0.56
1:A:109:ILE:CD1	1:A:286:LEU:HD11	2.35	0.56
1:A:32:THR:CG2	1:A:34:ILE:HD12	2.35	0.56
1:A:6:GLY:N	1:A:273:ASN:HD21	1.99	0.56
1:A:193:LEU:HD23	1:A:358:VAL:HG13	1.89	0.55
1:B:53:ALA:HA	1:B:270:ALA:HB3	1.87	0.55
1:A:98:VAL:CG2	1:A:106:ALA:HB3	2.37	0.55
1:A:339:ALA:CB	1:A:374:PHE:HE2	2.20	0.55
1:A:98:VAL:HG21	1:A:106:ALA:HB3	1.89	0.55
1:A:206:ASN:OD1	1:A:208:ASP:HB2	2.07	0.55
1:B:419:VAL:HG21	1:B:424:ALA:HB2	1.88	0.54
1:A:332:PRO:HB2	1:A:337:MET:CE	2.38	0.54
1:B:234:SER:HB2	1:B:298:LYS:CD	2.37	0.54
1:B:123:LEU:HD21	1:B:127:PRO:HD3	1.90	0.54
1:B:12:ILE:CD1	1:B:16:LYS:HB2	2.37	0.53
1:A:384:LEU:HD13	1:A:393:MET:HG2	1.90	0.53
1:A:312:LEU:C	1:A:314:LYS:H	2.12	0.53
1:A:312:LEU:O	1:A:318:ILE:HD12	2.09	0.53
1:B:182:VAL:C	1:B:366:GLN:HE22	2.09	0.53
1:A:129:THR:HG22	1:A:250:THR:HG22	1.90	0.52
1:B:372:SER:OG	1:B:373:PRO:HD3	2.09	0.52
1:B:230:PRO:HA	1:B:233:TRP:CE2	2.43	0.52
1:A:439:LEU:HD22	1:B:432:LYS:HE2	1.92	0.52
1:A:341:TRP:CD1	2:A:501:MAL:H4	2.45	0.52
1:B:12:ILE:CD1	1:B:16:LYS:CB	2.87	0.52
1:A:68:PHE:HD2	1:A:77:LEU:HD11	1.74	0.52
1:B:367:THR:O	1:B:371:VAL:HG23	2.10	0.52
1:A:234:SER:HB3	1:A:298:LYS:HD3	1.91	0.52
1:B:137:ASP:HA	1:B:147:ALA:HB2	1.92	0.52
1:B:140:LEU:CD1	1:B:147:ALA:HA	2.40	0.51
1:A:130:TRP:CD1	1:A:249:PRO:HB2	2.45	0.51
1:A:367:THR:O	1:A:371:VAL:HG23	2.10	0.51
1:B:156:TYR:HB2	2:B:501:MAL:C6'	2.41	0.51
1:A:155:PRO:HG3	1:A:345:ARG:CA	2.37	0.51
1:B:234:SER:HB2	1:B:298:LYS:NZ	2.26	0.50
1:A:339:ALA:HB2	1:A:374:PHE:CE2	2.46	0.50
1:A:34:ILE:HD12	1:A:276:LEU:HD22	1.95	0.49
1:A:365:ALA:O	1:A:369:ILE:HG13	2.12	0.49
1:B:48:PHE:N	1:B:49:PRO:HD2	2.28	0.49
1:A:273:ASN:HB3	1:A:276:LEU:HD12	1.94	0.48
1:A:234:SER:CB	1:A:298:LYS:HD3	2.43	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:ASP:HB2	1:B:366:GLN:CD	2.34	0.48
1:A:171:LYS:HB3	1:A:178:ASP:HB3	1.94	0.48
1:B:433:LYS:HB2	1:B:433:LYS:HE3	1.57	0.48
1:A:387:GLY:HA2	1:A:412:LEU:HD13	1.94	0.48
1:A:138:LYS:HE2	1:A:204:HIS:HE1	1.78	0.48
1:B:436:ALA:O	1:B:440:ARG:HG3	2.14	0.48
1:B:425:MET:O	1:B:429:LYS:HD3	2.14	0.48
1:B:80:ILE:HG22	1:B:82:PRO:HD3	1.95	0.47
1:A:431:PHE:CE1	1:B:403:PHE:HB3	2.49	0.47
1:A:432:LYS:HE3	3:B:708:HOH:O	2.13	0.47
1:A:278:LYS:HE2	3:A:614:HOH:O	2.14	0.47
1:B:179:ILE:HG23	1:B:336:GLN:HG2	1.95	0.47
1:B:195:PHE:O	1:B:199:LEU:HG	2.15	0.47
1:B:306:LYS:NZ	3:B:619:HOH:O	2.44	0.47
1:A:371:VAL:HG12	1:A:371:VAL:O	2.15	0.47
1:A:419:VAL:HG21	1:A:424:ALA:HB2	1.97	0.46
1:A:86:PHE:HZ	1:A:286:LEU:HD22	1.80	0.46
1:A:336:GLN:HG3	1:A:374:PHE:HB2	1.98	0.46
1:A:439:LEU:CD1	1:B:425:MET:HG3	2.43	0.46
1:B:154:GLU:HA	1:B:155:PRO:HD3	1.80	0.46
1:B:419:VAL:CG2	1:B:424:ALA:HB2	2.45	0.46
1:B:129:THR:OG1	1:B:132:GLU:HG3	2.16	0.46
1:B:273:ASN:HB3	1:B:276:LEU:HD12	1.97	0.46
1:B:332:PRO:HB2	1:B:337:MET:HE3	1.94	0.45
1:B:407:LYS:HE3	1:B:407:LYS:HB2	1.83	0.45
1:A:129:THR:CA	1:A:250:THR:HG22	2.42	0.45
1:A:350:ASN:ND2	1:A:355:ARG:HD2	2.31	0.45
1:B:260:VAL:O	1:B:330:ILE:HD12	2.16	0.45
1:A:78:ALA:HB1	1:A:274:LYS:HD3	1.98	0.45
1:B:182:VAL:C	1:B:366:GLN:NE2	2.69	0.45
1:A:254:GLN:C	3:A:602:HOH:O	2.48	0.45
1:B:292:GLU:O	1:B:296:LYS:HB2	2.17	0.45
1:B:312:LEU:O	1:B:318:ILE:HD12	2.17	0.45
1:B:397:ILE:O	1:B:401:LEU:HG	2.17	0.45
1:B:98:VAL:HG21	1:B:108:PRO:HD3	1.99	0.45
1:A:129:THR:HA	1:A:250:THR:H	1.81	0.45
1:A:53:ALA:HA	1:A:270:ALA:HB3	1.98	0.45
1:B:274:LYS:HB2	1:B:274:LYS:HE3	1.75	0.45
1:A:216:ALA:HB1	1:A:220:LYS:HZ1	1.82	0.45
1:A:34:ILE:HD13	1:A:276:LEU:CD2	2.48	0.44
1:B:107:TYR:HD2	1:B:281:LEU:HD13	1.77	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:LEU:HD21	1:A:205:MET:HE1	1.99	0.44
1:A:98:VAL:HG22	1:A:98:VAL:O	2.17	0.44
1:A:384:LEU:CD1	1:A:393:MET:HG2	2.47	0.44
1:B:120:LYS:HE3	1:B:243:TYR:O	2.17	0.44
1:B:185:ASP:CA	1:B:366:GLN:HG3	2.47	0.44
1:A:281:LEU:O	1:A:286:LEU:HD13	2.18	0.44
1:A:137:ASP:HA	1:A:147:ALA:HB2	2.00	0.44
1:A:91:TYR:HA	1:A:92:PRO:HD3	1.90	0.44
1:B:159:TRP:N	1:B:160:PRO:CD	2.80	0.44
1:A:184:VAL:H	1:A:366:GLN:HE21	1.64	0.43
1:A:314:LYS:HE3	1:A:314:LYS:HB2	1.82	0.43
1:A:110:ALA:HA	1:A:303:VAL:HA	2.00	0.43
1:A:48:PHE:N	1:A:49:PRO:HD2	2.33	0.43
1:A:397:ILE:O	1:A:401:LEU:HG	2.18	0.43
1:B:179:ILE:HD12	1:B:179:ILE:N	2.28	0.43
1:B:193:LEU:O	1:B:197:VAL:HG23	2.19	0.43
1:B:155:PRO:HG3	1:B:345:ARG:CA	2.44	0.43
1:B:12:ILE:HG12	1:B:16:LYS:HB2	2.00	0.43
1:A:239:SER:O	1:A:240:LYS:HB2	2.19	0.43
1:A:29:GLU:OE2	1:A:35:LYS:HG2	2.19	0.43
1:A:166:GLY:O	1:A:186:ASN:ND2	2.52	0.43
1:A:315:ASP:OD1	1:A:317:ARG:N	2.45	0.43
1:A:380:LEU:HG	1:B:380:LEU:CD1	2.49	0.43
1:A:436:ALA:CA	1:B:432:LYS:HZ1	2.30	0.43
1:B:47:LYS:O	1:B:50:GLN:HB3	2.19	0.43
1:A:128:LYS:O	1:A:250:THR:HG22	2.19	0.42
1:B:185:ASP:N	1:B:366:GLN:HG3	2.34	0.42
1:A:27:LYS:HB2	1:A:27:LYS:HE3	1.69	0.42
1:B:151:ASN:HB3	1:B:210:ASP:C	2.39	0.42
1:A:345:ARG:HH11	1:A:345:ARG:HB3	1.83	0.42
1:B:12:ILE:HG21	1:B:18:TYR:HB3	2.00	0.42
1:A:424:ALA:O	1:A:428:ILE:HG13	2.20	0.42
1:B:260:VAL:HB	1:B:330:ILE:HA	2.01	0.42
1:A:285:LEU:HG	1:A:286:LEU:HD12	2.01	0.42
1:A:336:GLN:HA	1:A:374:PHE:CE2	2.54	0.42
1:B:275:GLU:CD	1:B:275:GLU:H	2.23	0.42
1:B:371:VAL:O	1:B:371:VAL:HG12	2.20	0.42
1:A:425:MET:HG3	1:B:439:LEU:HD11	2.01	0.42
1:B:196:LEU:HA	1:B:199:LEU:HD12	2.01	0.42
1:B:91:TYR:O	1:B:94:THR:OG1	2.28	0.42
1:B:271:SER:O	1:B:274:LYS:HE3	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:GLY:O	1:B:441:ILE:HG23	2.19	0.42
1:B:3:ILE:HG23	1:B:57:GLY:O	2.19	0.42
1:A:5:GLU:HA	1:A:273:ASN:HD21	1.84	0.42
1:B:402:ARG:NH2	3:B:628:HOH:O	2.52	0.42
1:B:179:ILE:CG2	1:B:336:GLN:HG2	2.49	0.42
1:A:227:ILE:CG1	3:A:601:HOH:O	2.43	0.42
1:B:156:TYR:CB	2:B:501:MAL:H6'2	2.48	0.42
1:B:267:ILE:HG21	1:B:274:LYS:HG3	2.02	0.41
1:A:23:GLU:HG3	3:A:689:HOH:O	2.21	0.41
1:B:12:ILE:CG2	1:B:18:TYR:HB3	2.50	0.41
1:B:372:SER:N	1:B:373:PRO:CD	2.84	0.41
1:B:387:GLY:HA2	1:B:412:LEU:HD13	2.03	0.41
1:B:378:LYS:HD2	1:B:378:LYS:HA	1.79	0.41
1:B:363:LYS:CE	3:B:603:HOH:O	2.69	0.41
1:B:74:SER:HB2	1:B:76:LEU:HG	2.02	0.41
1:B:45:GLU:OE1	1:B:45:GLU:N	2.46	0.40
1:A:360:GLU:O	1:A:364:ASP:HB2	2.22	0.40
1:A:259:PHE:CD1	1:A:331:MET:HG2	2.56	0.40
1:A:86:PHE:O	1:A:89:LYS:HB2	2.21	0.40
1:A:99:ARG:NH1	1:A:104:LEU:HD21	2.36	0.40
1:B:86:PHE:HZ	1:B:286:LEU:CD1	2.34	0.40
1:A:274:LYS:HE3	1:A:274:LYS:HB2	1.95	0.40
1:A:247:VAL:HA	1:A:324:ASN:HD21	1.87	0.40
1:A:372:SER:HA	1:A:373:PRO:HD3	1.74	0.40

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)
3:A:697:HOH:O	3:B:696:HOH:O[2_746]	1.91	0.29
3:A:667:HOH:O	3:A:693:HOH:O[2_855]	2.14	0.06

5.3 Torsion angles

5.3.1 Protein backbone

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	440/445 (99%)	429 (98%)	11 (2%)	0	100	100
1	B	443/445 (100%)	438 (99%)	5 (1%)	0	100	100
All	All	883/890 (99%)	867 (98%)	16 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	352/356 (99%)	349 (99%)	3 (1%)	81	81
1	B	356/356 (100%)	353 (99%)	3 (1%)	83	84
All	All	708/712 (99%)	702 (99%)	6 (1%)	83	84

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	208	ASP
1	A	242	ASN
1	A	259	PHE
1	B	259	PHE
1	B	296	LYS
1	B	430	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	125	ASN
1	A	204	HIS
1	A	254	GLN
1	A	273	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	350	ASN
1	B	235	ASN
1	B	366	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](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

2 ligands 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	MAL	A	501	-	24,24,24	1.53	4 (16%)	35,35,35	1.04	2 (5%)
2	MAL	B	501	-	24,24,24	0.57	0	35,35,35	1.93	11 (31%)

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	MAL	A	501	-	-	0/8/48/48	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAL	B	501	-	-	0/8/48/48	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	MAL	O1-C4'	2.32	1.50	1.43
2	A	501	MAL	C1'-C2'	2.67	1.58	1.52
2	A	501	MAL	C3'-C2'	2.74	1.59	1.52
2	A	501	MAL	C4-C5	3.06	1.59	1.53

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	MAL	C1-O1-C4'	-3.47	109.30	117.97
2	B	501	MAL	C2'-C3'-C4'	-3.11	102.53	109.68
2	B	501	MAL	C3-C4-C5	-2.76	105.30	110.24
2	B	501	MAL	O1-C1-O5	-2.69	103.04	110.66
2	A	501	MAL	C4-C3-C2	-2.46	106.51	110.83
2	B	501	MAL	O5'-C5'-C4'	-2.08	105.35	109.76
2	B	501	MAL	O1-C4'-C3'	2.02	112.69	107.27
2	A	501	MAL	O5'-C5'-C6'	2.06	111.61	106.43
2	B	501	MAL	O5'-C1'-C2'	2.69	115.15	110.31
2	B	501	MAL	C1'-O5'-C5'	2.87	119.22	113.69
2	B	501	MAL	C1-O5-C5	3.84	121.28	113.71
2	B	501	MAL	O5-C1-C2	3.87	118.65	110.34
2	B	501	MAL	O1-C4'-C5'	4.31	121.36	109.42

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	MAL	2	0
2	B	501	MAL	3	0

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, 95th 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	442/445 (99%)	0.45	25 (5%) 24 26	26, 41, 62, 104	0
1	B	445/445 (100%)	0.07	8 (1%) 68 72	24, 33, 47, 68	0
All	All	887/890 (99%)	0.26	33 (3%) 41 46	24, 37, 57, 104	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	374	PHE	10.5
1	A	375	GLY	9.5
1	A	173	GLU	5.2
1	A	174	ASN	4.9
1	A	355	ARG	4.2
1	B	1	MET	3.8
1	A	184	VAL	3.6
1	A	314	LYS	3.1
1	A	50	GLN	3.0
1	A	237	ASP	2.9
1	B	314	LYS	2.9
1	A	171	LYS	2.9
1	A	83	ASP	2.8
1	A	125	ASN	2.7
1	A	164	ALA	2.7
1	A	4	GLU	2.7
1	A	342	TYR	2.7
1	B	382	ALA	2.7
1	A	5	GLU	2.6
1	B	410	LEU	2.5
1	A	185	ASP	2.4
1	A	208	ASP	2.3
1	A	328	GLY	2.3
1	B	381	PRO	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	179	ILE	2.3
1	A	130	TRP	2.2
1	B	4	GLU	2.1
1	B	371	VAL	2.1
1	B	379	ARG	2.1
1	A	444	ALA	2.1
1	A	373	PRO	2.1
1	A	88	ASP	2.1
1	A	172	TYR	2.1

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](#)

There are no carbohydrates in this entry.

6.4 Ligands [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. The B-factors column lists the minimum, median, 95th 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	B-factors(\AA^2)	Q<0.9
2	MAL	B	501	23/23	0.82	0.18	28,38,54,62	0
2	MAL	A	501	23/23	0.92	0.13	33,45,64,77	0

6.5 Other polymers [i](#)

There are no such residues in this entry.