



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:06 PM GMT

PDB ID : 1S48
Title : Crystal structure of RNA-dependent RNA polymerase construct 1 (residues 71-679) from BVDV
Authors : Choi, K.H.; Groarke, J.M.; Young, D.C.; Kuhn, R.J.; Smith, J.L.; Pevear, D.C.; Rossmann, M.G.
Deposited on : 2004-01-15
Resolution : 3.00 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
A user guide is available at
<http://wwpdb.org/validation/2016/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 (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

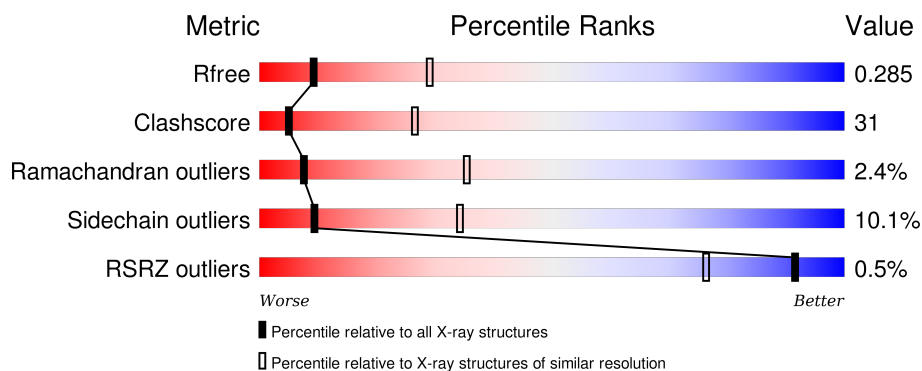
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


The reported resolution of this entry is 3.00 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))
R_{free}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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 ≥ 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	609	 48% 42% 6% ..

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4741 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 RNA-dependent RNA polymerase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	588	Total	C	N	O	S	Se	0	0	0
			4741	3011	837	876	5	12			

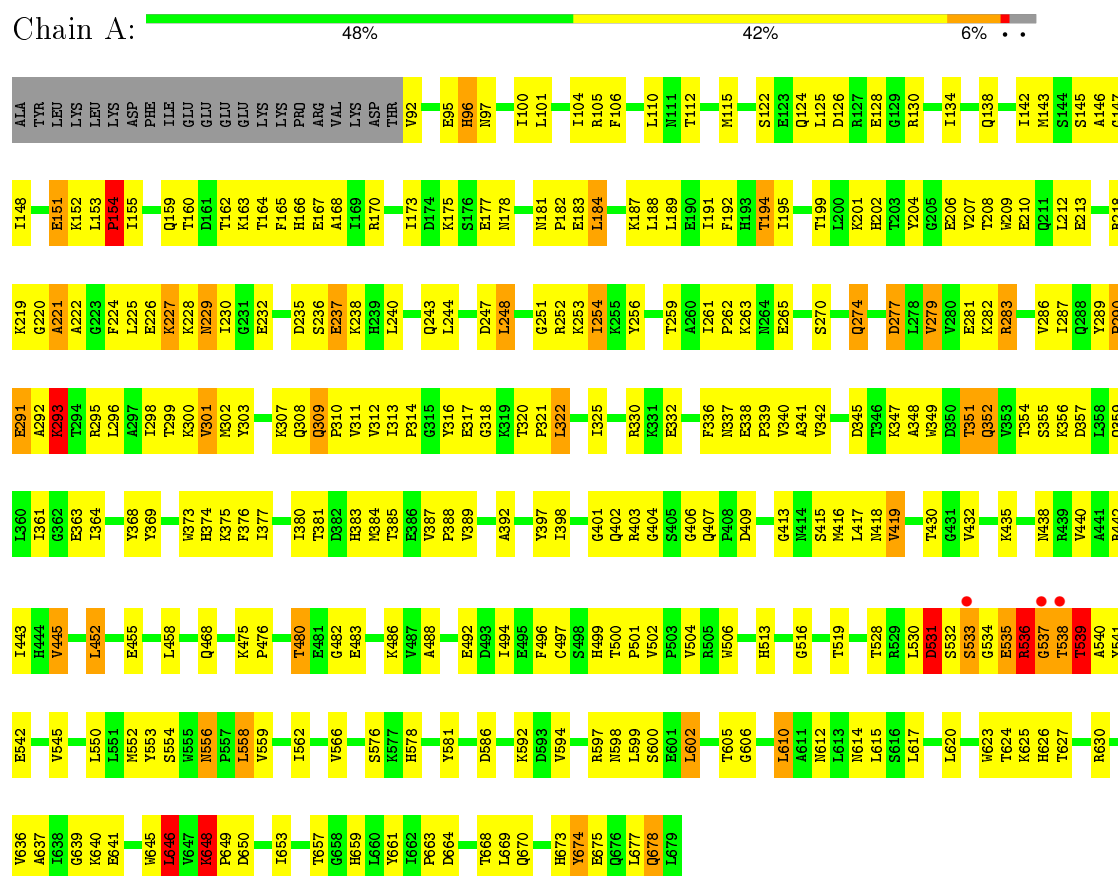
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	115	MSE	MET	MODIFIED RESIDUE	UNP P19711
A	143	MSE	MET	MODIFIED RESIDUE	UNP P19711
A	302	MSE	MET	MODIFIED RESIDUE	UNP P19711
A	384	MSE	MET	MODIFIED RESIDUE	UNP P19711
A	416	MSE	MET	MODIFIED RESIDUE	UNP P19711
A	422	MSE	MET	MODIFIED RESIDUE	UNP P19711
A	423	MSE	MET	MODIFIED RESIDUE	UNP P19711
A	467	MSE	MET	MODIFIED RESIDUE	UNP P19711
A	485	MSE	MET	MODIFIED RESIDUE	UNP P19711
A	514	MSE	MET	MODIFIED RESIDUE	UNP P19711
A	526	MSE	MET	MODIFIED RESIDUE	UNP P19711
A	552	MSE	MET	MODIFIED RESIDUE	UNP P19711

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 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: RNA-dependent RNA polymerase



4 Data and refinement statistics

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, α , β , γ	205.73Å 205.73Å 99.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.78 – 3.00 38.88 – 3.00	Depositor EDS
% Data completeness (in resolution range)	95.6 (29.78-3.00) 97.3 (38.88-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.15 (at 3.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.229 , 0.282 0.235 , 0.285	Depositor DCC
R_{free} test set	2395 reflections (9.71%)	DCC
Wilson B-factor (Å ²)	55.3	Xtriage
Anisotropy	0.287	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 51.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 47199 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	4741	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.43	0/4831	0.75	10/6497 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	533	SER	N-CA-C	-10.65	82.24	111.00
1	A	402	GLN	N-CA-C	-7.27	91.37	111.00
1	A	531	ASP	CA-C-N	-7.03	101.73	117.20
1	A	539	THR	N-CA-C	-6.92	92.33	111.00
1	A	673	HIS	N-CA-C	6.47	128.46	111.00
1	A	293	LYS	N-CA-C	-6.45	93.58	111.00
1	A	291	GLU	N-CA-C	6.41	128.29	111.00
1	A	646	LEU	CA-CB-CG	6.31	129.81	115.30
1	A	536	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	A	531	ASP	O-C-N	5.26	131.12	122.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	531	ASP	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	A	4741	0	4781	295	1
All	All	4741	0	4781	295	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 31.

All (295) 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:532:SER:C	1:A:534:GLY:H	1.29	1.13
1:A:538:THR:HB	1:A:540:ALA:H	1.16	1.08
1:A:178:ASN:HD21	1:A:352:GLN:HG3	1.17	1.07
1:A:336:PHE:HB2	1:A:339:PRO:HG3	1.33	1.06
1:A:106:PHE:HB3	1:A:151:GLU:HG2	1.36	1.06
1:A:380:ILE:HG12	1:A:384:MSE:HE2	1.35	1.04
1:A:678:GLN:O	1:A:678:GLN:HG2	1.56	1.03
1:A:532:SER:C	1:A:534:GLY:N	2.07	1.01
1:A:227:LYS:H	1:A:227:LYS:HD2	1.25	1.01
1:A:175:LYS:HD3	1:A:351:THR:HG23	1.43	0.98
1:A:283:ARG:CD	1:A:283:ARG:H	1.78	0.93
1:A:313:ILE:HG12	1:A:416:MSE:HE2	1.50	0.91
1:A:227:LYS:H	1:A:227:LYS:CD	1.82	0.87
1:A:536:ARG:HD3	1:A:536:ARG:O	1.74	0.87
1:A:229:ASN:HD21	1:A:232:GLU:HG3	1.39	0.86
1:A:536:ARG:CD	1:A:536:ARG:O	2.26	0.84
1:A:227:LYS:HD3	1:A:228:LYS:H	1.40	0.84
1:A:381:THR:HA	1:A:384:MSE:HE3	1.59	0.83
1:A:178:ASN:ND2	1:A:352:GLN:HG3	1.93	0.83
1:A:237:GLU:HB3	1:A:240:LEU:HD12	1.60	0.83
1:A:229:ASN:HD22	1:A:229:ASN:C	1.82	0.82
1:A:494:ILE:O	1:A:500:THR:HG22	1.78	0.82
1:A:277:ASP:OD1	1:A:279:VAL:HG12	1.83	0.79
1:A:243:GLN:HG3	1:A:247:ASP:OD2	1.83	0.79
1:A:531:ASP:HB3	1:A:541:TYR:CE1	2.17	0.79
1:A:492:GLU:HA	1:A:501:PRO:HG2	1.64	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:ARG:H	1:A:283:ARG:HD3	1.49	0.76
1:A:540:ALA:O	1:A:576:SER:N	2.18	0.76
1:A:349:TRP:CZ3	1:A:475:LYS:HD2	2.20	0.75
1:A:229:ASN:ND2	1:A:232:GLU:HG3	2.02	0.75
1:A:538:THR:HB	1:A:540:ALA:N	1.99	0.74
1:A:254:ILE:HG23	1:A:383:HIS:NE2	2.02	0.74
1:A:536:ARG:HA	1:A:536:ARG:HH11	1.52	0.74
1:A:661:TYR:O	1:A:663:PRO:HD3	1.89	0.72
1:A:648:LYS:HB3	1:A:648:LYS:HZ2	1.56	0.70
1:A:354:THR:HG22	1:A:356:LYS:H	1.56	0.70
1:A:283:ARG:H	1:A:283:ARG:HD2	1.56	0.70
1:A:292:ALA:HB2	1:A:295:ARG:NH2	2.06	0.70
1:A:354:THR:HG22	1:A:355:SER:N	2.06	0.70
1:A:209:TRP:O	1:A:213:GLU:HG3	1.91	0.69
1:A:531:ASP:OD2	1:A:533:SER:N	2.25	0.69
1:A:419:VAL:HG12	1:A:443:ILE:HD13	1.75	0.69
1:A:152:LYS:O	1:A:154:PRO:HD3	1.93	0.68
1:A:532:SER:CA	1:A:534:GLY:H	2.07	0.68
1:A:648:LYS:HD3	1:A:659:HIS:HB2	1.75	0.67
1:A:165:PHE:CD1	1:A:262:PRO:HB3	2.29	0.67
1:A:218:ARG:C	1:A:220:GLY:H	1.98	0.67
1:A:556:ASN:HD22	1:A:559:VAL:H	1.42	0.67
1:A:648:LYS:N	1:A:649:PRO:CD	2.58	0.67
1:A:209:TRP:CD2	1:A:238:LYS:HE3	2.29	0.67
1:A:173:ILE:HD11	1:A:286:VAL:HG21	1.77	0.67
1:A:316:TYR:CZ	1:A:318:GLY:HA3	2.30	0.66
1:A:639:GLY:HA3	1:A:648:LYS:HE2	1.78	0.66
1:A:648:LYS:N	1:A:649:PRO:HD3	2.11	0.65
1:A:101:LEU:HA	1:A:104:ILE:HD13	1.78	0.65
1:A:404:GLY:O	1:A:407:GLN:HG3	1.96	0.65
1:A:541:TYR:HA	1:A:576:SER:HB3	1.78	0.65
1:A:138:GLN:OE1	1:A:138:GLN:HA	1.97	0.65
1:A:291:GLU:O	1:A:291:GLU:CG	2.45	0.65
1:A:531:ASP:HB3	1:A:541:TYR:CZ	2.32	0.64
1:A:226:GLU:OE2	1:A:293:LYS:HG3	1.97	0.64
1:A:291:GLU:O	1:A:291:GLU:HG2	1.97	0.64
1:A:354:THR:CG2	1:A:355:SER:N	2.61	0.64
1:A:230:ILE:HG12	1:A:296:LEU:HD11	1.79	0.63
1:A:220:GLY:HA3	1:A:230:ILE:HD12	1.79	0.63
1:A:154:PRO:CG	1:A:620:LEU:HD13	2.29	0.63
1:A:302:MSE:HA	1:A:369:TYR:OH	1.97	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:ALA:O	1:A:226:GLU:OE1	2.17	0.62
1:A:164:THR:HA	1:A:167:GLU:HG3	1.80	0.62
1:A:227:LYS:HD3	1:A:228:LYS:N	2.13	0.62
1:A:480:THR:CG2	1:A:482:GLY:H	2.13	0.61
1:A:143:MSE:O	1:A:148:ILE:HB	1.99	0.61
1:A:212:LEU:HD13	1:A:300:LYS:HA	1.83	0.61
1:A:138:GLN:HE21	1:A:539:THR:CG2	2.12	0.60
1:A:648:LYS:HZ3	1:A:648:LYS:HA	1.66	0.60
1:A:164:THR:HG22	1:A:167:GLU:OE2	2.02	0.60
1:A:592:LYS:HB2	1:A:598:ASN:ND2	2.16	0.60
1:A:298:ILE:HG12	1:A:380:ILE:HD12	1.83	0.59
1:A:227:LYS:N	1:A:227:LYS:CD	2.55	0.59
1:A:183:GLU:HB2	1:A:187:LYS:HE2	1.85	0.59
1:A:146:ALA:HB1	1:A:627:THR:HA	1.83	0.59
1:A:229:ASN:C	1:A:229:ASN:ND2	2.52	0.59
1:A:303:TYR:O	1:A:307:LYS:HB2	2.02	0.59
1:A:336:PHE:CB	1:A:339:PRO:HG3	2.22	0.58
1:A:138:GLN:HG3	1:A:539:THR:HG22	1.85	0.58
1:A:354:THR:HB	1:A:357:ASP:OD1	2.03	0.58
1:A:173:ILE:CD1	1:A:286:VAL:HG21	2.33	0.58
1:A:674:TYR:N	1:A:674:TYR:CD2	2.70	0.58
1:A:261:ILE:HG22	1:A:392:ALA:HB2	1.86	0.57
1:A:352:GLN:HG2	1:A:476:PRO:HD2	1.85	0.57
1:A:226:GLU:OE1	1:A:291:GLU:O	2.22	0.57
1:A:251:GLY:HA3	1:A:375:LYS:HE2	1.87	0.57
1:A:192:PHE:CE1	1:A:364:ILE:HG23	2.40	0.56
1:A:322:LEU:O	1:A:325:ILE:HG22	2.06	0.56
1:A:146:ALA:CB	1:A:627:THR:HG23	2.36	0.56
1:A:163:LYS:O	1:A:167:GLU:HG3	2.06	0.55
1:A:160:THR:O	1:A:160:THR:HG22	2.06	0.55
1:A:221:ALA:O	1:A:295:ARG:NH2	2.39	0.55
1:A:227:LYS:N	1:A:227:LYS:HD2	2.08	0.55
1:A:648:LYS:CB	1:A:648:LYS:NZ	2.70	0.55
1:A:201:LYS:HG2	1:A:202:HIS:CD2	2.41	0.55
1:A:309:GLN:HB2	1:A:310:PRO:CD	2.36	0.55
1:A:640:LYS:HB2	1:A:640:LYS:NZ	2.21	0.55
1:A:432:VAL:HG21	1:A:440:VAL:HG21	1.89	0.55
1:A:354:THR:CG2	1:A:355:SER:H	2.20	0.54
1:A:166:HIS:HB3	1:A:170:ARG:HH12	1.72	0.54
1:A:92:VAL:O	1:A:92:VAL:HG23	2.07	0.54
1:A:586:ASP:HB3	1:A:664:ASP:O	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:ALA:HB1	1:A:627:THR:HG23	1.90	0.54
1:A:309:GLN:HB2	1:A:310:PRO:HD3	1.90	0.54
1:A:330:ARG:HD2	1:A:330:ARG:O	2.07	0.53
1:A:670:GLN:HE22	1:A:677:LEU:N	2.06	0.53
1:A:648:LYS:HE3	1:A:657:THR:OG1	2.09	0.53
1:A:165:PHE:O	1:A:168:ALA:HB3	2.09	0.53
1:A:639:GLY:HA2	1:A:645:TRP:CD1	2.43	0.53
1:A:224:PHE:HB2	1:A:259:THR:HG23	1.90	0.52
1:A:648:LYS:CB	1:A:648:LYS:HZ2	2.22	0.52
1:A:519:THR:HG21	1:A:617:LEU:HD11	1.91	0.52
1:A:309:GLN:O	1:A:311:VAL:N	2.42	0.52
1:A:209:TRP:CG	1:A:238:LYS:HE3	2.44	0.52
1:A:502:VAL:HG23	1:A:516:GLY:HA3	1.92	0.52
1:A:187:LYS:O	1:A:191:ILE:HG13	2.09	0.52
1:A:626:HIS:O	1:A:630:ARG:HG3	2.09	0.52
1:A:320:THR:HG22	1:A:321:PRO:O	2.10	0.52
1:A:535:GLU:C	1:A:537:GLY:H	2.12	0.52
1:A:506:TRP:CD2	1:A:597:ARG:HD3	2.45	0.52
1:A:322:LEU:HD23	1:A:325:ILE:HG21	1.92	0.51
1:A:355:SER:HB3	1:A:385:THR:HG23	1.91	0.51
1:A:610:LEU:HD22	1:A:614:ASN:ND2	2.26	0.51
1:A:528:THR:O	1:A:530:LEU:HD12	2.11	0.51
1:A:332:GLU:OE2	1:A:442:ARG:HD2	2.10	0.51
1:A:648:LYS:NZ	1:A:653:ILE:HG22	2.25	0.51
1:A:230:ILE:HD11	1:A:295:ARG:NH1	2.26	0.51
1:A:389:VAL:HG11	1:A:397:TYR:CZ	2.45	0.51
1:A:256:TYR:OH	1:A:290:PRO:HG3	2.11	0.50
1:A:497:CYS:O	1:A:499:HIS:HD2	1.94	0.50
1:A:352:GLN:HG2	1:A:476:PRO:CD	2.41	0.50
1:A:354:THR:HG22	1:A:356:LYS:N	2.26	0.50
1:A:292:ALA:H	1:A:295:ARG:HE	1.59	0.50
1:A:212:LEU:CD1	1:A:299:THR:HG22	2.42	0.50
1:A:536:ARG:CG	1:A:536:ARG:O	2.59	0.50
1:A:218:ARG:C	1:A:220:GLY:N	2.65	0.50
1:A:361:ILE:HD11	1:A:417:LEU:HB2	1.93	0.50
1:A:322:LEU:HB3	1:A:552:MSE:SE	2.61	0.50
1:A:415:SER:O	1:A:419:VAL:HG22	2.12	0.49
1:A:668:THR:O	1:A:669:LEU:HD23	2.12	0.49
1:A:506:TRP:CE2	1:A:597:ARG:HD2	2.47	0.49
1:A:208:THR:C	1:A:210:GLU:N	2.62	0.49
1:A:227:LYS:HE2	1:A:293:LYS:NZ	2.27	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:VAL:HG22	1:A:302:MSE:HG3	1.92	0.49
1:A:173:ILE:HD11	1:A:286:VAL:CG2	2.41	0.49
1:A:138:GLN:HG2	1:A:542:GLU:OE1	2.13	0.49
1:A:224:PHE:HD2	1:A:225:LEU:HD23	1.78	0.49
1:A:322:LEU:HD13	1:A:552:MSE:HE1	1.94	0.49
1:A:292:ALA:HB2	1:A:295:ARG:HH21	1.78	0.49
1:A:438:ASN:OD1	1:A:442:ARG:NH1	2.46	0.49
1:A:338:GLU:N	1:A:339:PRO:HD3	2.28	0.49
1:A:556:ASN:ND2	1:A:559:VAL:H	2.10	0.49
1:A:380:ILE:HG23	1:A:381:THR:N	2.28	0.48
1:A:126:ASP:HB2	1:A:130:ARG:HB2	1.94	0.48
1:A:452:LEU:O	1:A:452:LEU:HD23	2.14	0.48
1:A:531:ASP:OD2	1:A:532:SER:N	2.46	0.48
1:A:218:ARG:O	1:A:220:GLY:N	2.46	0.48
1:A:541:TYR:HA	1:A:576:SER:CB	2.43	0.48
1:A:204:TYR:HB2	1:A:368:TYR:O	2.14	0.48
1:A:347:LYS:O	1:A:352:GLN:NE2	2.47	0.48
1:A:112:THR:HG21	1:A:115:MSE:HE3	1.96	0.48
1:A:480:THR:HG23	1:A:482:GLY:H	1.78	0.47
1:A:341:ALA:HB3	1:A:488:ALA:HB3	1.96	0.47
1:A:162:THR:HA	1:A:165:PHE:HB3	1.95	0.47
1:A:207:VAL:HG22	1:A:300:LYS:O	2.14	0.47
1:A:418:ASN:HD22	1:A:445:VAL:HG22	1.79	0.47
1:A:227:LYS:HE2	1:A:293:LYS:HZ1	1.79	0.47
1:A:277:ASP:CG	1:A:279:VAL:HG12	2.34	0.47
1:A:581:TYR:OH	1:A:677:LEU:CD1	2.63	0.47
1:A:533:SER:HB2	1:A:578:HIS:CD2	2.50	0.46
1:A:337:ASN:C	1:A:339:PRO:HD3	2.36	0.46
1:A:298:ILE:HD13	1:A:380:ILE:HD11	1.96	0.46
1:A:229:ASN:ND2	1:A:232:GLU:CG	2.76	0.46
1:A:355:SER:HB3	1:A:385:THR:CG2	2.45	0.46
1:A:138:GLN:OE1	1:A:138:GLN:CA	2.64	0.46
1:A:95:GLU:C	1:A:97:ASN:H	2.19	0.46
1:A:283:ARG:CD	1:A:283:ARG:N	2.58	0.46
1:A:206:GLU:HA	1:A:301:VAL:HA	1.98	0.46
1:A:480:THR:HG22	1:A:482:GLY:H	1.78	0.46
1:A:612:ASN:HA	1:A:615:LEU:HG	1.97	0.46
1:A:106:PHE:CB	1:A:151:GLU:HG2	2.25	0.46
1:A:640:LYS:CB	1:A:640:LYS:NZ	2.78	0.46
1:A:430:THR:HB	1:A:458:LEU:HD22	1.97	0.46
1:A:160:THR:O	1:A:160:THR:CG2	2.63	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:PRO:O	1:A:312:VAL:HG13	2.16	0.46
1:A:313:ILE:HB	1:A:316:TYR:HB2	1.97	0.46
1:A:218:ARG:NH2	1:A:235:ASP:OD1	2.49	0.46
1:A:506:TRP:CD2	1:A:597:ARG:CD	2.99	0.46
1:A:181:ASN:HA	1:A:182:PRO:HD3	1.76	0.45
1:A:531:ASP:CB	1:A:541:TYR:CE1	2.95	0.45
1:A:143:MSE:HE2	1:A:148:ILE:HG21	1.99	0.45
1:A:207:VAL:HG11	1:A:303:TYR:HB3	1.99	0.45
1:A:307:LYS:O	1:A:308:GLN:C	2.54	0.45
1:A:110:LEU:HB3	1:A:112:THR:HG23	1.99	0.45
1:A:154:PRO:HG3	1:A:620:LEU:HD13	1.98	0.45
1:A:482:GLY:O	1:A:483:GLU:HB2	2.16	0.45
1:A:502:VAL:CG2	1:A:516:GLY:HA3	2.47	0.45
1:A:605:THR:O	1:A:606:GLY:C	2.55	0.45
1:A:248:LEU:HB3	1:A:376:PHE:CD1	2.52	0.45
1:A:159:GLN:HG2	1:A:281:GLU:CD	2.37	0.45
1:A:243:GLN:O	1:A:247:ASP:OD2	2.33	0.45
1:A:309:GLN:CB	1:A:310:PRO:HD3	2.46	0.45
1:A:531:ASP:CG	1:A:532:SER:N	2.67	0.45
1:A:220:GLY:O	1:A:229:ASN:HB2	2.16	0.45
1:A:192:PHE:O	1:A:195:ILE:HG12	2.17	0.45
1:A:159:GLN:HG2	1:A:281:GLU:OE2	2.17	0.45
1:A:562:ILE:O	1:A:566:VAL:HG23	2.16	0.45
1:A:226:GLU:OE1	1:A:291:GLU:HG3	2.17	0.45
1:A:416:MSE:O	1:A:419:VAL:HG23	2.17	0.45
1:A:330:ARG:HG2	1:A:513:HIS:CE1	2.52	0.45
1:A:558:LEU:O	1:A:562:ILE:HG13	2.17	0.45
1:A:209:TRP:O	1:A:213:GLU:CG	2.63	0.44
1:A:188:LEU:HA	1:A:188:LEU:HD23	1.87	0.44
1:A:403:ARG:HG3	1:A:404:GLY:N	2.32	0.44
1:A:302:MSE:HE3	1:A:377:ILE:HG12	1.99	0.44
1:A:191:ILE:O	1:A:194:THR:HG23	2.16	0.44
1:A:648:LYS:HZ3	1:A:653:ILE:HG22	1.83	0.44
1:A:336:PHE:HB3	1:A:455:GLU:OE1	2.18	0.44
1:A:309:GLN:O	1:A:310:PRO:C	2.52	0.44
1:A:151:GLU:HG3	1:A:151:GLU:H	1.31	0.44
1:A:289:TYR:HA	1:A:290:PRO:HD3	1.84	0.44
1:A:184:LEU:O	1:A:188:LEU:HG	2.18	0.44
1:A:282:LYS:HG2	1:A:283:ARG:HD3	2.00	0.44
1:A:541:TYR:O	1:A:545:VAL:HG23	2.17	0.44
1:A:229:ASN:ND2	1:A:230:ILE:O	2.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:LEU:O	1:A:155:ILE:N	2.50	0.44
1:A:100:ILE:HG23	1:A:101:LEU:N	2.32	0.44
1:A:126:ASP:N	1:A:130:ARG:O	2.28	0.43
1:A:263:LYS:HD3	1:A:265:GLU:OE2	2.18	0.43
1:A:184:LEU:HD22	1:A:188:LEU:HG	2.00	0.43
1:A:649:PRO:HG3	1:A:661:TYR:CD2	2.54	0.43
1:A:195:ILE:HD12	1:A:314:PRO:CG	2.48	0.43
1:A:115:MSE:HE2	1:A:115:MSE:HB3	1.90	0.43
1:A:290:PRO:HB2	1:A:295:ARG:HG3	2.01	0.43
1:A:309:GLN:CB	1:A:310:PRO:CD	2.96	0.43
1:A:528:THR:O	1:A:530:LEU:CD1	2.67	0.43
1:A:342:VAL:HB	1:A:452:LEU:CD2	2.49	0.43
1:A:636:VAL:O	1:A:637:ALA:C	2.57	0.43
1:A:535:GLU:C	1:A:537:GLY:N	2.71	0.43
1:A:355:SER:CB	1:A:385:THR:HG23	2.48	0.43
1:A:106:PHE:HE1	1:A:122:SER:HA	1.83	0.43
1:A:528:THR:C	1:A:530:LEU:HD12	2.38	0.43
1:A:263:LYS:HD3	1:A:265:GLU:CD	2.39	0.43
1:A:105:ARG:HG3	1:A:122:SER:HB3	2.00	0.43
1:A:678:GLN:O	1:A:678:GLN:CG	2.44	0.43
1:A:533:SER:CB	1:A:578:HIS:CD2	3.01	0.43
1:A:646:LEU:O	1:A:649:PRO:HD2	2.18	0.43
1:A:403:ARG:NH2	1:A:413:GLY:HA3	2.34	0.43
1:A:531:ASP:CB	1:A:541:TYR:CZ	3.01	0.43
1:A:286:VAL:O	1:A:286:VAL:HG23	2.18	0.43
1:A:499:HIS:HE1	1:A:553:TYR:OH	2.02	0.43
1:A:387:VAL:HA	1:A:388:PRO:HD3	1.89	0.43
1:A:289:TYR:HB3	1:A:406:GLY:HA3	2.01	0.42
1:A:147:GLY:HA3	1:A:624:THR:HG23	2.01	0.42
1:A:142:ILE:O	1:A:145:SER:HB2	2.18	0.42
1:A:363:GLU:OE2	1:A:363:GLU:HA	2.18	0.42
1:A:531:ASP:OD2	1:A:532:SER:C	2.58	0.42
1:A:277:ASP:OD1	1:A:279:VAL:CG1	2.59	0.42
1:A:247:ASP:O	1:A:252:ARG:HB2	2.20	0.42
1:A:594:VAL:HG13	1:A:668:THR:HB	2.02	0.42
1:A:398:ILE:HG22	1:A:398:ILE:O	2.20	0.42
1:A:283:ARG:N	1:A:283:ARG:HD3	2.24	0.42
1:A:650:ASP:OD2	1:A:653:ILE:HD13	2.19	0.42
1:A:206:GLU:HB2	1:A:373:TRP:CZ2	2.55	0.42
1:A:648:LYS:NZ	1:A:648:LYS:HA	2.33	0.41
1:A:175:LYS:CD	1:A:351:THR:HG23	2.32	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:PRO:HG2	1:A:620:LEU:CD1	2.50	0.41
1:A:143:MSE:CE	1:A:148:ILE:HG21	2.50	0.41
1:A:624:THR:C	1:A:626:HIS:H	2.24	0.41
1:A:355:SER:O	1:A:359:GLN:HG3	2.20	0.41
1:A:274:GLN:HE21	1:A:620:LEU:HD11	1.85	0.41
1:A:640:LYS:O	1:A:659:HIS:CD2	2.74	0.41
1:A:325:ILE:HD11	1:A:496:PHE:CE2	2.55	0.41
1:A:263:LYS:HG3	1:A:287:ILE:HD11	2.02	0.41
1:A:124:GLN:HG3	1:A:134:ILE:HG12	2.02	0.41
1:A:100:ILE:CG2	1:A:101:LEU:N	2.84	0.41
1:A:452:LEU:HD23	1:A:452:LEU:C	2.40	0.41
1:A:533:SER:C	1:A:535:GLU:H	2.23	0.41
1:A:154:PRO:HB3	1:A:270:SER:HA	2.02	0.41
1:A:165:PHE:CE1	1:A:262:PRO:HD3	2.56	0.41
1:A:204:TYR:HB2	1:A:369:TYR:HA	2.03	0.40
1:A:177:GLU:OE1	1:A:354:THR:HG23	2.21	0.40
1:A:504:VAL:HG11	1:A:602:LEU:CD2	2.52	0.40
1:A:409:ASP:CG	1:A:409:ASP:O	2.60	0.40
1:A:202:HIS:HE1	1:A:374:HIS:HE1	1.70	0.40
1:A:348:ALA:O	1:A:352:GLN:NE2	2.55	0.40
1:A:352:GLN:HE21	1:A:352:GLN:HB2	1.64	0.40
1:A:536:ARG:HA	1:A:536:ARG:NH1	2.29	0.40
1:A:220:GLY:O	1:A:221:ALA:O	2.39	0.40

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:A:128:GLU:OE1	1:A:128:GLU:OE1[4_675]	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	586/609 (96%)	525 (90%)	47 (8%)	14 (2%)	7 35

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	221	ALA
1	A	309	GLN
1	A	219	LYS
1	A	277	ASP
1	A	401	GLY
1	A	537	GLY
1	A	154	PRO
1	A	237	GLU
1	A	535	GLU
1	A	646	LEU
1	A	625	LYS
1	A	96	HIS
1	A	293	LYS
1	A	648	LYS

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	516/524 (98%)	464 (90%)	52 (10%)	9 34

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	HIS
1	A	125	LEU
1	A	151	GLU
1	A	154	PRO
1	A	184	LEU
1	A	189	LEU
1	A	194	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	199	THR
1	A	227	LYS
1	A	229	ASN
1	A	236	SER
1	A	244	LEU
1	A	248	LEU
1	A	253	LYS
1	A	254	ILE
1	A	274	GLN
1	A	279	VAL
1	A	283	ARG
1	A	290	PRO
1	A	301	VAL
1	A	317	GLU
1	A	322	LEU
1	A	340	VAL
1	A	345	ASP
1	A	351	THR
1	A	352	GLN
1	A	419	VAL
1	A	435	LYS
1	A	445	VAL
1	A	452	LEU
1	A	468	GLN
1	A	480	THR
1	A	486	LYS
1	A	531	ASP
1	A	536	ARG
1	A	538	THR
1	A	539	THR
1	A	550	LEU
1	A	554	SER
1	A	556	ASN
1	A	558	LEU
1	A	599	LEU
1	A	600	SER
1	A	602	LEU
1	A	610	LEU
1	A	623	TRP
1	A	641	GLU
1	A	646	LEU
1	A	648	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	674	TYR
1	A	675	GLU
1	A	678	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	ASN
1	A	117	ASN
1	A	159	GLN
1	A	202	HIS
1	A	229	ASN
1	A	274	GLN
1	A	352	GLN
1	A	365	GLN
1	A	418	ASN
1	A	468	GLN
1	A	499	HIS
1	A	513	HIS
1	A	556	ASN
1	A	598	ASN
1	A	670	GLN
1	A	673	HIS

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 ⓘ

There are no carbohydrates in this entry.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	576/609 (94%)	-0.30	3 (0%) 91 76	18, 44, 83, 101	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	537	GLY	2.7
1	A	533	SER	2.7
1	A	538	THR	2.3

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.