



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 06:24 am BST

PDB ID : 3ES5
Title : Crystal Structure of Partitivirus (PsV-F)
Authors : Pan, J.; Dong, L.; Lin, L.; Ochoa, W.F.; Sinkovits, R.S.; Havens, W.M.;
Nibert, M.L.; Baker, T.S.; Ghabrial, S.A.; Tao, Y.J.
Deposited on : 2008-10-03
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

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
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

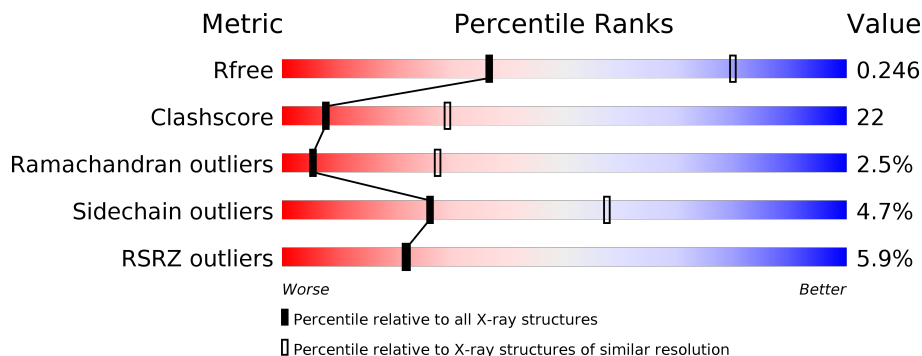
1 Overall quality at a glance

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))
R_{free}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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 respectively. 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	420	 5% 56% 31% 10%
1	B	420	 5% 49% 36% 5% 10%

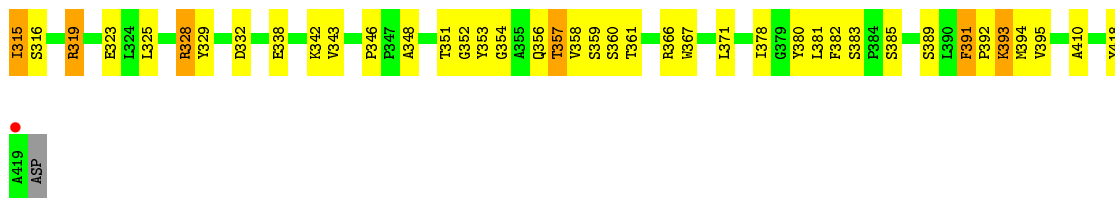
2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5919 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 Putative capsid protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	379	Total 2964	C 1884	N 492	O 578	S 10	0	0	0
1	B	378	Total 2955	C 1880	N 491	O 574	S 10	0	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	F 2 3	Depositor
Cell constants a, b, c, α , β , γ	459.27Å 459.27Å 459.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.96 – 3.30 77.63 – 3.30	Depositor EDS
% Data completeness (in resolution range)	74.9 (48.96-3.30) 74.9 (77.63-3.30)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 3.33Å)	Xtrriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.248 , 0.267 0.241 , 0.246	Depositor DCC
R_{free} test set	4540 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	61.6	Xtrriage
Anisotropy	0.000	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 57.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.020 for k,h,-l	Xtrriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	5919	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.09% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.40	0/3032	0.65	0/4119
1	B	0.41	0/3023	0.67	1/4108 (0.0%)
All	All	0.40	0/6055	0.66	1/8227 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	342	LYS	N-CA-C	-5.31	96.67	111.00

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	2964	0	2908	131	1
1	B	2955	0	2904	145	2
All	All	5919	0	5812	256	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 22.

All (256) 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:253:GLN:H	1:A:253:GLN:NE2	1.67	0.90
1:B:163:MET:HA	1:B:351:THR:HG23	1.54	0.90
1:A:94:VAL:HB	1:A:340:ILE:HG23	1.54	0.89
1:B:231:GLN:HE22	1:B:268:ASN:HD22	1.21	0.89
1:A:253:GLN:H	1:A:253:GLN:HE21	0.91	0.88
1:A:253:GLN:N	1:A:253:GLN:HE21	1.73	0.87
1:B:100:LEU:HD22	1:B:105:LYS:HA	1.61	0.83
1:B:299:ASP:HA	1:B:302:THR:HG22	1.61	0.82
1:A:245:VAL:HG22	1:A:246:SER:H	1.46	0.80
1:A:263:PRO:HG2	1:A:266:ALA:HB2	1.64	0.79
1:A:299:ASP:HA	1:A:302:THR:HG22	1.65	0.79
1:B:236:THR:OG1	1:B:242:VAL:HG12	1.84	0.78
1:B:278:ALA:HA	1:B:281:MET:HG3	1.65	0.78
1:B:119:LYS:HG3	1:B:346:PRO:HB3	1.63	0.78
1:B:285:GLN:HE22	1:B:292:PRO:HG3	1.49	0.78
1:B:219:ARG:O	1:B:223:GLU:HG2	1.84	0.77
1:B:65:VAL:HA	1:B:394:MET:HE2	1.66	0.77
1:A:356:GLN:O	1:A:385:SER:HB3	1.85	0.77
1:B:180:LYS:HD3	1:B:315:ILE:HD11	1.66	0.76
1:B:98:ILE:HG22	1:B:99:GLN:H	1.49	0.76
1:B:229:VAL:HG13	1:B:247:MET:O	1.85	0.75
1:A:115:LEU:HD23	1:A:149:ILE:HG22	1.67	0.75
1:A:247:MET:SD	1:A:248:PRO:HD2	2.30	0.72
1:B:356:GLN:O	1:B:385:SER:HB3	1.91	0.71
1:A:163:MET:HA	1:A:351:THR:HG23	1.75	0.67
1:B:85:LYS:HB3	1:B:86:PRO:HD3	1.75	0.67
1:B:232:ARG:HH11	1:B:232:ARG:HB2	1.60	0.67
1:A:232:ARG:HD3	1:B:248:PRO:HB3	1.75	0.67
1:B:92:THR:HA	1:B:105:LYS:HD3	1.77	0.66
1:B:57:PHE:HB2	1:B:58:PRO:HD2	1.76	0.66
1:B:137:GLN:HB3	1:B:138:PRO:HD3	1.78	0.66
1:B:201:LEU:HD22	1:B:307:LEU:HD13	1.76	0.66
1:A:338:GLU:HG2	1:A:343:VAL:HG21	1.77	0.66
1:B:213:SER:O	1:B:217:ILE:HG12	1.96	0.66
1:B:119:LYS:HG2	1:B:149:ILE:HD13	1.78	0.65
1:B:225:ILE:HD11	1:B:275:LEU:CB	2.27	0.65
1:A:56:ILE:HG13	1:A:57:PHE:HD1	1.60	0.65
1:B:50:LEU:HD12	1:B:51:PRO:HD2	1.79	0.65
1:B:164:LYS:HD3	1:B:169:ASP:OD1	1.97	0.64
1:B:231:GLN:HE22	1:B:268:ASN:ND2	1.92	0.64
1:A:229:VAL:HG13	1:A:247:MET:O	1.98	0.63
1:A:190:PHE:HB3	1:A:325:LEU:HD22	1.79	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:SER:O	1:A:273:ARG:HG3	1.99	0.63
1:B:55:THR:HG22	1:B:56:ILE:N	2.13	0.63
1:A:245:VAL:HG21	1:B:245:VAL:CG2	2.29	0.63
1:B:98:ILE:HG22	1:B:99:GLN:N	2.14	0.63
1:B:351:THR:HG22	1:B:352:GLY:O	1.99	0.62
1:A:229:VAL:HG12	1:A:229:VAL:O	1.99	0.62
1:A:83:ILE:O	1:A:86:PRO:HD2	2.00	0.62
1:B:236:THR:HA	1:B:242:VAL:HA	1.82	0.62
1:B:225:ILE:HD11	1:B:275:LEU:HB3	1.81	0.62
1:A:119:LYS:HD2	1:A:346:PRO:HB3	1.81	0.61
1:A:274:VAL:HA	1:A:295:GLU:HG2	1.81	0.61
1:B:125:TYR:HA	1:B:128:MET:HG3	1.82	0.61
1:B:47:ILE:HG12	1:B:48:ASP:N	2.15	0.61
1:B:55:THR:HG22	1:B:56:ILE:H	1.66	0.60
1:A:245:VAL:HG22	1:A:246:SER:N	2.15	0.60
1:A:231:GLN:NE2	1:A:267:PRO:HB2	2.17	0.59
1:A:194:ASP:O	1:A:196:ASP:N	2.35	0.59
1:B:147:THR:O	1:B:346:PRO:HG3	2.02	0.59
1:A:232:ARG:HD3	1:B:248:PRO:CB	2.33	0.59
1:A:351:THR:HG22	1:A:352:GLY:O	2.02	0.59
1:B:299:ASP:HA	1:B:302:THR:CG2	2.34	0.58
1:A:271:GLN:H	1:A:271:GLN:CD	2.07	0.58
1:B:180:LYS:CD	1:B:315:ILE:HD11	2.33	0.57
1:A:112:ILE:HG23	1:A:153:MET:HE3	1.86	0.57
1:A:354:GLY:HA3	1:A:371:LEU:HD22	1.86	0.57
1:B:83:ILE:O	1:B:86:PRO:HD2	2.05	0.57
1:A:122:ARG:NH1	1:A:143:TYR:O	2.38	0.56
1:A:237:ASP:OD1	1:A:238:ALA:N	2.38	0.56
1:A:360:SER:HB2	1:A:383:SER:HB2	1.87	0.56
1:B:100:LEU:CD2	1:B:105:LYS:HA	2.33	0.56
1:A:85:LYS:HB3	1:A:86:PRO:HD3	1.86	0.56
1:A:273:ARG:HG2	1:A:273:ARG:HH11	1.71	0.56
1:A:237:ASP:HA	1:B:237:ASP:OD2	2.06	0.56
1:A:56:ILE:C	1:A:58:PRO:HD2	2.26	0.56
1:B:75:LEU:HD21	1:B:356:GLN:HG2	1.87	0.55
1:A:199:TRP:CZ3	1:A:312:ALA:O	2.60	0.55
1:B:299:ASP:CA	1:B:302:THR:HG22	2.35	0.55
1:B:285:GLN:NE2	1:B:292:PRO:HG3	2.21	0.55
1:A:285:GLN:OE1	1:A:292:PRO:HD3	2.08	0.54
1:B:129:LEU:HB2	1:B:132:GLU:HG3	1.90	0.54
1:B:260:ASP:O	1:B:262:ILE:N	2.39	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:ASP:CA	1:A:302:THR:HG22	2.36	0.53
1:A:180:LYS:HD3	1:A:315:ILE:HD11	1.91	0.53
1:B:107:ASN:HB3	1:B:193:ILE:HD12	1.90	0.53
1:A:164:LYS:O	1:A:164:LYS:HG3	2.09	0.53
1:A:194:ASP:C	1:A:196:ASP:H	2.12	0.52
1:B:251:THR:H	1:B:253:GLN:HE21	1.57	0.52
1:B:47:ILE:HG12	1:B:48:ASP:H	1.75	0.52
1:A:231:GLN:HE22	1:A:268:ASN:ND2	2.07	0.52
1:B:354:GLY:O	1:B:357:THR:HB	2.10	0.52
1:A:281:MET:HE2	1:A:300:LEU:HD21	1.92	0.52
1:A:47:ILE:HG12	1:A:48:ASP:N	2.25	0.52
1:A:245:VAL:HG21	1:B:245:VAL:HG21	1.91	0.52
1:A:299:ASP:HA	1:A:302:THR:CG2	2.39	0.52
1:B:278:ALA:HA	1:B:281:MET:CG	2.38	0.52
1:A:251:THR:N	1:A:253:GLN:HE22	2.09	0.51
1:B:282:SER:OG	1:B:285:GLN:HG3	2.09	0.51
1:B:225:ILE:HD11	1:B:275:LEU:HB2	1.92	0.51
1:A:125:TYR:HA	1:A:128:MET:HG3	1.92	0.50
1:B:119:LYS:HA	1:B:119:LYS:HE3	1.93	0.50
1:A:122:ARG:HE	1:A:348:ALA:HB2	1.77	0.50
1:A:122:ARG:NE	1:A:348:ALA:HB2	2.26	0.50
1:A:202:ASP:OD2	1:A:205:LYS:HE3	2.11	0.50
1:A:260:ASP:O	1:A:262:ILE:N	2.41	0.50
1:B:264:ASP:N	1:B:264:ASP:OD2	2.45	0.50
1:A:248:PRO:HB3	1:B:232:ARG:HD3	1.93	0.50
1:A:249:GLN:NE2	1:B:249:GLN:NE2	2.60	0.50
1:B:338:GLU:HG2	1:B:343:VAL:HG21	1.93	0.50
1:A:72:GLU:N	1:A:170:VAL:HG13	2.26	0.50
1:B:351:THR:HG22	1:B:352:GLY:N	2.26	0.50
1:A:111:SER:O	1:A:115:LEU:HB2	2.12	0.50
1:B:263:PRO:HG2	1:B:266:ALA:HB2	1.94	0.50
1:B:291:LEU:HD11	1:B:297:ARG:HA	1.94	0.50
1:A:231:GLN:HE21	1:A:267:PRO:HB2	1.77	0.49
1:A:131:HIS:O	1:A:134:ALA:HB3	2.11	0.49
1:B:360:SER:HB2	1:B:383:SER:HB2	1.94	0.49
1:B:255:LEU:HB2	1:B:256:PRO:HD3	1.93	0.49
1:A:382:PHE:O	1:A:383:SER:C	2.51	0.49
1:B:201:LEU:HD12	1:B:313:TYR:CE1	2.47	0.49
1:A:291:LEU:HD11	1:A:297:ARG:HA	1.94	0.49
1:B:140:LYS:HG2	1:B:144:TYR:CE1	2.47	0.49
1:B:260:ASP:C	1:B:262:ILE:H	2.17	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:ILE:HA	1:B:356:GLN:OE1	2.13	0.48
1:B:190:PHE:HB3	1:B:325:LEU:HD22	1.96	0.48
1:A:274:VAL:O	1:A:277:ALA:HB3	2.14	0.48
1:A:377:ASN:ND2	1:B:56:ILE:HD12	2.28	0.48
1:A:231:GLN:HE22	1:A:268:ASN:HD22	1.60	0.48
1:A:165:THR:C	1:A:167:VAL:H	2.17	0.48
1:B:147:THR:HG21	1:B:329:TYR:CE2	2.49	0.48
1:B:86:PRO:O	1:B:90:THR:HG23	2.14	0.48
1:B:163:MET:HE3	1:B:353:TYR:O	2.13	0.48
1:B:201:LEU:HD12	1:B:313:TYR:CD1	2.49	0.47
1:A:281:MET:CE	1:A:300:LEU:HD21	2.44	0.47
1:A:405:ALA:HB1	1:B:381:LEU:HD21	1.96	0.47
1:B:224:LYS:O	1:B:228:LEU:HG	2.14	0.47
1:A:63:PRO:HB3	1:B:367:TRP:HZ2	1.78	0.47
1:A:243:TYR:O	1:A:245:VAL:N	2.47	0.47
1:A:377:ASN:HD22	1:B:56:ILE:HD12	1.78	0.47
1:B:199:TRP:CZ3	1:B:312:ALA:O	2.67	0.47
1:B:382:PHE:O	1:B:383:SER:C	2.53	0.47
1:A:112:ILE:HG23	1:A:153:MET:CE	2.44	0.47
1:A:266:ALA:O	1:A:269:SER:HB2	2.15	0.47
1:B:137:GLN:O	1:B:140:LYS:HB2	2.14	0.47
1:B:391:PHE:N	1:B:392:PRO:HD3	2.29	0.47
1:A:174:ASP:OD1	1:A:219:ARG:NH2	2.48	0.47
1:B:263:PRO:HB2	1:B:265:VAL:HG12	1.97	0.47
1:A:352:GLY:HA3	1:A:356:GLN:NE2	2.30	0.47
1:B:259:TYR:CE1	1:B:273:ARG:HB3	2.50	0.47
1:B:280:GLN:HE22	1:B:293:HIS:CD2	2.33	0.47
1:B:66:GLU:HB2	1:B:395:VAL:HG23	1.97	0.47
1:A:150:PRO:HB2	1:A:153:MET:HB3	1.95	0.47
1:B:85:LYS:CB	1:B:86:PRO:HD3	2.44	0.47
1:A:278:ALA:O	1:A:281:MET:HG2	2.15	0.46
1:B:71:GLY:O	1:B:170:VAL:HA	2.14	0.46
1:A:243:TYR:O	1:A:244:SER:C	2.53	0.46
1:B:296:ASP:HB2	1:B:299:ASP:OD2	2.16	0.46
1:B:50:LEU:HD12	1:B:51:PRO:CD	2.44	0.46
1:A:351:THR:HG22	1:A:352:GLY:N	2.31	0.46
1:B:393:LYS:HE3	1:B:393:LYS:HB2	1.68	0.46
1:A:73:VAL:HG22	1:A:388:PHE:CD1	2.50	0.46
1:B:101:VAL:HG12	1:B:102:ASP:N	2.30	0.46
1:B:328:ARG:HG3	1:B:328:ARG:HH11	1.81	0.46
1:A:203:CYS:HA	1:A:206:LEU:HG	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:ILE:HG13	1:A:57:PHE:H	1.81	0.46
1:B:243:TYR:HB3	1:B:244:SER:H	1.60	0.45
1:B:79:LEU:N	1:B:80:PRO:HD2	2.31	0.45
1:A:54:ASP:HA	1:A:57:PHE:CD1	2.51	0.45
1:A:207:VAL:HG11	1:A:306:LEU:HD13	1.98	0.45
1:B:101:VAL:HG12	1:B:102:ASP:H	1.82	0.45
1:A:273:ARG:NH1	1:A:273:ARG:HG2	2.31	0.45
1:B:42:MET:O	1:B:166:LYS:NZ	2.49	0.45
1:A:225:ILE:HD11	1:A:275:LEU:HB3	1.99	0.45
1:B:122:ARG:NH1	1:B:348:ALA:HB2	2.32	0.45
1:A:128:MET:HB3	1:A:132:GLU:HB2	1.99	0.45
1:A:229:VAL:CG1	1:A:229:VAL:O	2.63	0.45
1:A:370:PRO:O	1:B:46:TRP:CZ3	2.69	0.45
1:A:165:THR:HG22	1:B:47:ILE:HG13	1.98	0.45
1:A:199:TRP:CE2	1:A:321:GLN:HG2	2.52	0.45
1:B:115:LEU:HD11	1:B:329:TYR:CZ	2.51	0.45
1:B:259:TYR:CE2	1:B:293:HIS:HB3	2.51	0.45
1:B:65:VAL:HG22	1:B:394:MET:HE1	1.99	0.45
1:B:69:PRO:HB3	1:B:171:LEU:CD1	2.47	0.45
1:A:128:MET:HA	1:A:162:HIS:CD2	2.52	0.44
1:B:258:TYR:O	1:B:262:ILE:HG13	2.16	0.44
1:B:358:VAL:HG12	1:B:359:SER:N	2.31	0.44
1:B:128:MET:HB3	1:B:132:GLU:HB2	1.98	0.44
1:A:405:ALA:CB	1:B:381:LEU:HD21	2.47	0.44
1:B:225:ILE:C	1:B:227:GLN:H	2.21	0.44
1:B:161:GLY:N	1:B:356:GLN:OE1	2.48	0.44
1:A:278:ALA:CB	1:A:281:MET:HE2	2.47	0.44
1:B:269:SER:O	1:B:273:ARG:HG3	2.18	0.44
1:A:249:GLN:NE2	1:B:249:GLN:HE21	2.16	0.44
1:A:221:ALA:HA	1:A:275:LEU:HD22	1.99	0.44
1:B:240:GLY:O	1:B:241:HIS:O	2.35	0.44
1:B:57:PHE:CB	1:B:58:PRO:HD2	2.46	0.44
1:B:50:LEU:O	1:B:52:GLN:N	2.48	0.44
1:A:281:MET:HE2	1:A:300:LEU:CD2	2.48	0.43
1:B:181:ARG:HH22	1:B:216:MET:HE1	1.83	0.43
1:B:140:LYS:HG2	1:B:144:TYR:HE1	1.84	0.43
1:B:328:ARG:HG3	1:B:328:ARG:NH1	2.34	0.43
1:B:183:THR:O	1:B:187:VAL:HG23	2.18	0.43
1:A:187:VAL:HG13	1:A:321:GLN:HG3	2.01	0.43
1:A:271:GLN:N	1:A:271:GLN:CD	2.72	0.43
1:B:214:LEU:HD11	1:B:281:MET:HE3	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:ILE:HA	1:B:263:PRO:HD2	1.87	0.42
1:B:55:THR:CG2	1:B:56:ILE:H	2.26	0.42
1:A:119:LYS:HD2	1:A:346:PRO:CB	2.47	0.42
1:A:278:ALA:HB1	1:A:281:MET:HE2	2.01	0.42
1:B:96:ASP:O	1:B:98:ILE:O	2.37	0.42
1:A:228:LEU:C	1:A:230:LYS:H	2.22	0.42
1:A:56:ILE:HG13	1:A:57:PHE:N	2.34	0.42
1:B:360:SER:OG	1:B:380:TYR:HA	2.19	0.42
1:B:354:GLY:HA3	1:B:371:LEU:HD22	2.00	0.42
1:A:101:VAL:HG12	1:A:102:ASP:N	2.34	0.42
1:B:224:LYS:HB3	1:B:275:LEU:HD13	2.01	0.42
1:B:65:VAL:HG22	1:B:394:MET:CE	2.49	0.42
1:B:378:ILE:HD13	1:B:378:ILE:HA	1.85	0.42
1:A:346:PRO:HA	1:A:347:PRO:HD3	1.94	0.42
1:A:221:ALA:O	1:A:225:ILE:HG12	2.20	0.42
1:A:301:LEU:CD1	1:A:308:TYR:HB2	2.50	0.42
1:A:135:VAL:HG23	1:A:136:ASN:N	2.35	0.42
1:A:162:HIS:CE1	1:A:172:VAL:H	2.38	0.42
1:A:85:LYS:CB	1:A:86:PRO:HD3	2.49	0.42
1:B:332:ASP:N	1:B:332:ASP:OD1	2.51	0.42
1:A:147:THR:HG21	1:A:329:TYR:CE2	2.55	0.41
1:A:47:ILE:HG13	1:B:165:THR:HG22	2.02	0.41
1:B:156:ALA:O	1:B:159:ILE:HG12	2.19	0.41
1:A:255:LEU:HD23	1:A:255:LEU:HA	1.89	0.41
1:A:296:ASP:HB2	1:A:299:ASP:OD2	2.20	0.41
1:A:249:GLN:HE21	1:B:249:GLN:HE21	1.68	0.41
1:A:119:LYS:HA	1:A:119:LYS:HD3	1.62	0.41
1:A:174:ASP:OD2	1:A:216:MET:HB2	2.20	0.41
1:A:225:ILE:HD11	1:A:275:LEU:CB	2.50	0.41
1:B:319:ARG:HD3	1:B:323:GLU:OE2	2.20	0.41
1:A:235:VAL:O	1:A:235:VAL:HG12	2.20	0.41
1:A:82:THR:HG22	1:A:382:PHE:HD2	1.86	0.41
1:A:56:ILE:O	1:A:58:PRO:HD2	2.20	0.41
1:A:386:LYS:HA	1:A:386:LYS:HD3	1.84	0.41
1:A:242:VAL:O	1:A:242:VAL:HG23	2.20	0.41
1:A:245:VAL:CG2	1:A:246:SER:H	2.26	0.41
1:A:66:GLU:OE2	1:B:366:ARG:NH1	2.54	0.41
1:A:134:ALA:O	1:A:137:GLN:HB2	2.21	0.41
1:A:209:ALA:O	1:A:283:LEU:HD11	2.21	0.41
1:B:194:ASP:C	1:B:196:ASP:H	2.23	0.41
1:B:273:ARG:HG2	1:B:273:ARG:HH11	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:VAL:HG21	1:B:112:ILE:CD1	2.51	0.41
1:A:86:PRO:HB2	1:B:410:ALA:HB2	2.04	0.40
1:B:149:ILE:O	1:B:150:PRO:C	2.59	0.40
1:A:248:PRO:CB	1:B:232:ARG:HD3	2.51	0.40
1:B:274:VAL:O	1:B:277:ALA:HB3	2.21	0.40
1:A:137:GLN:N	1:A:138:PRO:CD	2.84	0.40
1:A:287:ARG:O	1:A:297:ARG:NH2	2.53	0.40
1:B:102:ASP:O	1:B:103:ASP:C	2.59	0.40
1:B:249:GLN:O	1:B:253:GLN:NE2	2.54	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)
1:B:236:THR:CG2	1:B:239:GLN:CG[32_555]	2.01	0.19
1:A:238:ALA:CB	1:A:238:ALA:CB[32_555]	2.10	0.10
1:B:236:THR:C	1:B:238:ALA:CB[32_555]	2.14	0.06

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	377/420 (90%)	321 (85%)	47 (12%)	9 (2%)	6	28
1	B	376/420 (90%)	327 (87%)	39 (10%)	10 (3%)	5	26
All	All	753/840 (90%)	648 (86%)	86 (11%)	19 (2%)	5	27

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	PHE
1	A	195	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	261	SER
1	A	292	PRO
1	A	315	ILE
1	B	54	ASP
1	B	56	ILE
1	B	241	HIS
1	B	261	SER
1	A	61	LEU
1	A	244	SER
1	A	348	ALA
1	B	166	LYS
1	B	315	ILE
1	B	418	TYR
1	A	240	GLY
1	B	281	MET
1	B	52	GLN
1	B	51	PRO

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	323/359 (90%)	311 (96%)	12 (4%)	34 63
1	B	322/359 (90%)	304 (94%)	18 (6%)	21 52
All	All	645/718 (90%)	615 (95%)	30 (5%)	26 57

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	TRP
1	A	94	VAL
1	A	115	LEU
1	A	153	MET
1	A	234	ARG
1	A	247	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	253	GLN
1	A	288	ASN
1	A	292	PRO
1	A	359	SER
1	A	361	THR
1	A	391	PHE
1	B	46	TRP
1	B	54	ASP
1	B	57	PHE
1	B	62	GLU
1	B	100	LEU
1	B	119	LYS
1	B	232	ARG
1	B	239	GLN
1	B	247	MET
1	B	264	ASP
1	B	316	SER
1	B	319	ARG
1	B	328	ARG
1	B	357	THR
1	B	361	THR
1	B	389	SER
1	B	391	PHE
1	B	393	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	GLN
1	A	137	GLN
1	A	231	GLN
1	A	249	GLN
1	A	253	GLN
1	A	268	ASN
1	A	288	ASN
1	A	377	ASN
1	B	231	GLN
1	B	239	GLN
1	B	249	GLN
1	B	253	GLN
1	B	271	GLN
1	B	280	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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	379/420 (90%)	0.32	23 (6%) 21 20	25, 45, 90, 121	0
1	B	378/420 (90%)	0.27	22 (5%) 23 22	27, 44, 85, 113	0
All	All	757/840 (90%)	0.29	45 (5%) 22 22	25, 44, 87, 121	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	235	VAL	10.3
1	B	241	HIS	7.2
1	B	242	VAL	5.3
1	A	266	ALA	5.1
1	B	234	ARG	4.6
1	B	243	TYR	4.4
1	A	238	ALA	4.4
1	B	419	ALA	4.4
1	B	244	SER	4.3
1	B	235	VAL	4.1
1	A	243	TYR	4.1
1	B	238	ALA	3.9
1	A	269	SER	3.8
1	A	237	ASP	3.7
1	A	233	TYR	3.7
1	A	54	ASP	3.3
1	B	233	TYR	3.3
1	B	237	ASP	3.3
1	B	240	GLY	3.2
1	B	267	PRO	3.2
1	A	292	PRO	3.2
1	B	247	MET	2.9
1	A	236	THR	2.9
1	B	265	VAL	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	261	SER	2.6
1	B	236	THR	2.5
1	B	260	ASP	2.5
1	A	267	PRO	2.4
1	A	245	VAL	2.4
1	A	265	VAL	2.4
1	A	42	MET	2.4
1	B	55	THR	2.4
1	A	241	HIS	2.4
1	A	294	ASP	2.4
1	A	263	PRO	2.2
1	A	309	ALA	2.1
1	B	286	PHE	2.1
1	A	257	ASP	2.1
1	A	258	TYR	2.1
1	B	293	HIS	2.1
1	A	231	GLN	2.1
1	B	294	ASP	2.1
1	B	232	ARG	2.0
1	B	292	PRO	2.0
1	A	248	PRO	2.0

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.