



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:28 AM UTC

PDB ID : 3ES5 / pdb_00003es5
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

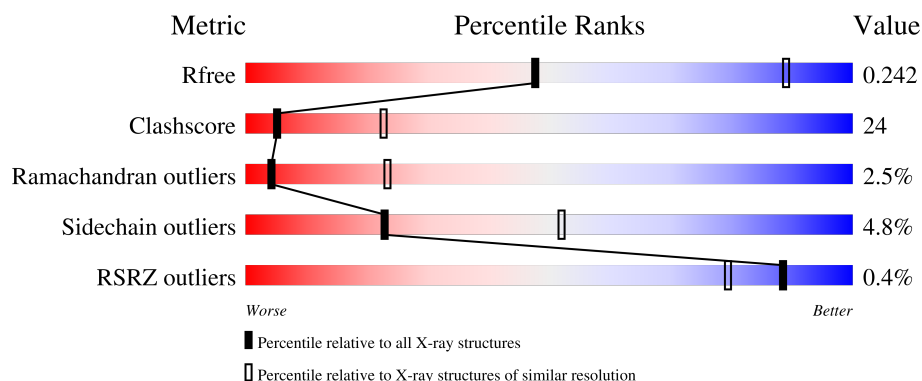
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

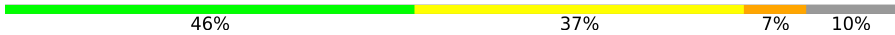
The reported resolution of this entry is 3.30 Å.

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}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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 of 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	
1	B	420	

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.

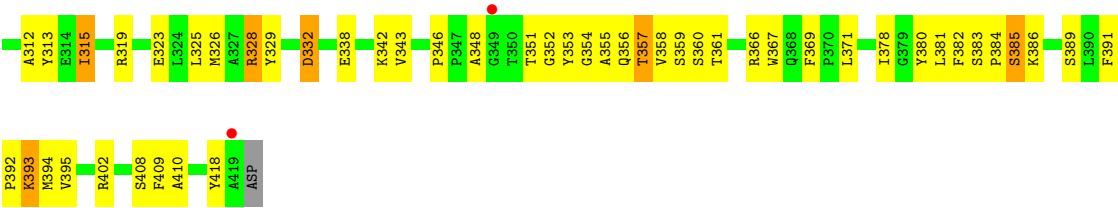
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Putative capsid protein.

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

- Molecule 1: Putative capsid protein





4 Data and refinement statistics

Property	Value	Source
Space group	F 2 3	Depositor
Cell constants a, b, c, α , β , γ	459.27 Å 459.27 Å 459.27 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.96 – 3.30 48.96 – 3.30	Depositor EDS
% Data completeness (in resolution range)	74.9 (48.96-3.30) 74.9 (48.96-3.30)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 3.33 Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.248 , 0.267 0.238 , 0.242	Depositor DCC
R_{free} test set	4540 reflections (3.80%)	wwPDB-VP
Wilson B-factor (Å ²)	61.6	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 91.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.020 for k,h,-l	Xtriage
F_o, F_c correlation	0.39	EDS
Total number of atoms	5919	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage'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

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	0.49	0/3032	1.03	19/4119 (0.5%)
1	B	0.50	0/3023	1.05	19/4108 (0.5%)
All	All	0.50	0/6055	1.04	38/8227 (0.5%)

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	332	ASP	N-CA-C	9.10	122.88	111.69
1	A	160	ILE	N-CA-C	8.43	119.24	110.05
1	A	238	ALA	N-CA-C	-8.36	102.18	112.38
1	A	54	ASP	N-CA-C	8.32	122.78	113.21
1	B	342	LYS	N-CA-C	-8.22	96.67	109.25
1	A	52	GLN	N-CA-C	7.31	120.28	109.24
1	B	402	ARG	N-CA-C	6.68	118.56	111.28
1	B	161	GLY	N-CA-C	6.48	118.72	111.85
1	A	342	LYS	N-CA-C	-6.37	99.50	109.25
1	B	385	SER	N-CA-C	6.34	120.03	109.95
1	A	384	PRO	N-CA-C	6.29	121.73	113.86
1	B	262	ILE	CA-C-N	6.07	126.28	119.90
1	B	262	ILE	C-N-CA	6.07	126.28	119.90
1	B	50	LEU	CA-C-N	5.95	127.28	119.84
1	B	50	LEU	C-N-CA	5.95	127.28	119.84
1	B	282	SER	N-CA-C	-5.91	100.27	109.72
1	A	57	PHE	N-CA-C	5.90	122.84	109.81
1	A	385	SER	N-CA-C	5.89	119.32	109.95
1	A	369	PHE	CA-C-N	5.83	127.12	119.84
1	A	369	PHE	C-N-CA	5.83	127.12	119.84
1	A	416	LYS	N-CA-C	5.81	118.08	111.11
1	A	254	ALA	N-CA-C	-5.75	100.30	109.96
1	B	386	LYS	N-CA-C	-5.72	105.97	113.12
1	A	383	SER	CA-C-N	5.71	125.33	119.56
1	A	383	SER	C-N-CA	5.71	125.33	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	352	GLY	N-CA-C	-5.57	104.06	112.41
1	A	55	THR	N-CA-C	-5.52	105.26	111.28
1	B	384	PRO	N-CA-C	5.45	120.67	113.86
1	B	369	PHE	CA-C-N	5.29	126.45	119.84
1	B	369	PHE	C-N-CA	5.29	126.45	119.84
1	B	137	GLN	CA-C-N	5.14	125.19	119.32
1	B	137	GLN	C-N-CA	5.14	125.19	119.32
1	B	153	MET	N-CA-C	-5.14	105.86	111.82
1	A	194	ASP	N-CA-C	-5.14	100.66	109.24
1	A	206	LEU	N-CA-C	5.09	117.61	110.23
1	B	54	ASP	N-CA-C	5.08	121.62	110.80
1	A	120	ALA	N-CA-C	-5.04	105.87	111.36
1	B	96	ASP	N-CA-C	5.01	116.44	111.07

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	2964	0	2908	150	1
1	B	2955	0	2904	160	2
All	All	5919	0	5812	287	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 24.

All (287) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:GLN:HE21	1:A:253:GLN:N	1.73	0.87
1:B:65:VAL:HG22	1:B:394:MET:HE1	1.58	0.83
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:281:MET:HE1	1:A:300:LEU:HD21	1.64	0.79
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:181:ARG:HH22	1:B:216:MET:HE1	1.45	0.78
1:B:128:MET:HE1	1:B:136:ASN:HD22	1.47	0.78
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:A:47:ILE:CD1	1:B:163:MET:HE2	2.14	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:HB2	1:B:232:ARG:HH11	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:163:MET:HE3	1:B:353:TYR:C	2.21	0.64
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:PHE:HB3	1:A:325:LEU:HD22	1.79	0.63
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:271:GLN:CD	1:A:271:GLN:H	2.07	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:225:ILE:HD11	1:B:275:LEU:HB3	1.81	0.62
1:B:236:THR:HA	1:B:242:VAL:HA	1.82	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:A:56:ILE:C	1:A:58:PRO:HD2	2.26	0.60
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:278:ALA:HB1	1:A:281:MET:HE2	1.85	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:A:112:ILE:CG2	1:A:153:MET:HE1	2.33	0.58
1:B:299:ASP:HA	1:B:302:THR:CG2	2.34	0.58
1:B:180:LYS:CD	1:B:315:ILE:HD11	2.33	0.57
1:A:194:ASP:C	1:A:196:ASP:H	2.12	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:HH11	1:A:273:ARG:HG2	1.71	0.56
1:A:281:MET:HE1	1:A:300:LEU:CD2	2.34	0.56
1:A:237:ASP:HA	1:B:237:ASP:OD2	2.06	0.56
1:A:278:ALA:CB	1:A:281:MET:HE2	2.36	0.56
1:A:247:MET:HE2	1:A:272:LEU:HD13	1.87	0.56
1:B:75:LEU:HD21	1:B:356:GLN:HG2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:382:PHE:O	1:A:383:SER:C	2.51	0.54
1:B:129:LEU:HB2	1:B:132:GLU:HG3	1.90	0.54
1:B:181:ARG:NH2	1:B:216:MET:HE1	2.19	0.54
1:B:260:ASP:O	1:B:262:ILE:N	2.39	0.54
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:A:181:ARG:NH2	1:A:216:MET:HE1	2.23	0.53
1:B:260:ASP:C	1:B:262:ILE:H	2.17	0.53
1:A:163:MET:HE2	1:A:356:GLN:NE2	2.24	0.53
1:A:112:ILE:HG23	1:A:153:MET:HE1	1.89	0.53
1:B:107:ASN:HB3	1:B:193:ILE:HD12	1.90	0.53
1:A:165:THR:C	1:A:167:VAL:H	2.17	0.53
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:382:PHE:O	1:B:383:SER:C	2.53	0.52
1:B:354:GLY:O	1:B:357:THR:HB	2.10	0.52
1:A:47:ILE:HG12	1:A:48:ASP:N	2.25	0.52
1:A:164:LYS:O	1:A:164:LYS:HG3	2.09	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:A:243:TYR:O	1:A:244:SER:C	2.53	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:HE3	1:B:119:LYS:HA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:278:ALA:HA	1:A:281:MET:HE2	1.94	0.49
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:216:MET:HE2	1:B:220:LEU:HD11	1.95	0.49
1:B:255:LEU:HB2	1:B:256:PRO:HD3	1.93	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:163:MET:HE3	1:B:353:TYR:O	2.13	0.49
1:B:225:ILE:C	1:B:227:GLN:H	2.21	0.48
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:B:86:PRO:O	1:B:90:THR:HG23	2.14	0.48
1:B:147:THR:HG21	1:B:329:TYR:CE2	2.49	0.48
1:A:271:GLN:CD	1:A:271:GLN:N	2.72	0.47
1:A:278:ALA:CA	1:A:281:MET:HE2	2.44	0.47
1:B:201:LEU:HD12	1:B:313:TYR:CD1	2.49	0.47
1:A:63:PRO:HB3	1:B:367:TRP:HZ2	1.78	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: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:A:326:MET:HE2	1:A:326:MET:HA	1.95	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:A:181:ARG:HH21	1:A:216:MET:HE1	1.80	0.47
1:A:228:LEU:C	1:A:230:LYS:H	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:GLU:HB2	1:B:395:VAL:HG23	1.97	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: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:47:ILE:HD11	1:B:163:MET:HE2	1.97	0.46
1:B:50:LEU:HD12	1:B:51:PRO:CD	2.44	0.46
1:B:296:ASP:HB2	1:B:299:ASP:OD2	2.16	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:56:ILE:HG13	1:A:57:PHE:H	1.81	0.46
1:A:203:CYS:HA	1:A:206:LEU:HG	1.98	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:HG2	1:A:273:ARG:NH1	2.31	0.45
1:B:42:MET:O	1:B:166:LYS:NZ	2.49	0.45
1:B:149:ILE:O	1:B:150:PRO:C	2.59	0.45
1:B:194:ASP:C	1:B:196:ASP:H	2.23	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:O	1:A:229:VAL:CG1	2.63	0.45
1:B:102:ASP:O	1:B:103:ASP:C	2.59	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:69:PRO:HB3	1:B:171:LEU:CD1	2.47	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:ALA:CB	1:B:381:LEU:HD21	2.47	0.44
1:B:161:GLY:N	1:B:356:GLN:OE1	2.48	0.44
1:B:269:SER:O	1:B:273:ARG:HG3	2.18	0.44
1:A:221:ALA:HA	1:A:275:LEU:HD22	1.99	0.44
1:A:249:GLN:NE2	1:B:249:GLN:HE21	2.16	0.44
1:B:57:PHE:CB	1:B:58:PRO:HD2	2.46	0.44
1:B:240:GLY:O	1:B:241:HIS:O	2.35	0.44
1:B:50:LEU:O	1:B:52:GLN:N	2.48	0.44
1:A:260:ASP:C	1:A:262:ILE:H	2.25	0.43
1:B:282:SER:O	1:B:283:LEU:C	2.60	0.43
1:B:125:TYR:CD1	1:B:128:MET:HE2	2.53	0.43
1:B:408:SER:O	1:B:409:PHE:C	2.60	0.43
1:A:237:ASP:C	1:A:239:GLN:N	2.75	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:237:ASP:HA	1:B:237:ASP:CG	2.44	0.43
1:B:46:TRP:CD1	1:B:46:TRP:C	2.97	0.43
1:B:55:THR:CG2	1:B:56:ILE:H	2.26	0.42
1:B:262:ILE:HA	1:B:263:PRO:HD2	1.87	0.42
1:A:119:LYS:HD2	1:A:346:PRO:CB	2.47	0.42
1:B:96:ASP:O	1:B:98:ILE:O	2.37	0.42
1:A:56:ILE:HG13	1:A:57:PHE:N	2.34	0.42
1:A:191:SER:HG	1:A:199:TRP:CD1	2.37	0.42
1:B:354:GLY:HA3	1:B:371:LEU:HD22	2.00	0.42
1:B:360:SER:OG	1:B:380:TYR:HA	2.19	0.42
1:A:101:VAL:HG12	1:A:102:ASP:N	2.34	0.42
1:A:194:ASP:C	1:A:196:ASP:N	2.76	0.42
1:B:224:LYS:HB3	1:B:275:LEU:HD13	2.01	0.42
1:B:326:MET:HA	1:B:326:MET:HE2	2.00	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:B:225:ILE:C	1:B:227:GLN:N	2.78	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:B:65:VAL:HA	1:B:394:MET:HE2	2.01	0.42
1:A:85:LYS:CB	1:A:86:PRO:HD3	2.49	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:B:214:LEU:HD11	1:B:281:MET:HE3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:ASP:OD1	1:B:332:ASP:N	2.51	0.42
1:A:47:ILE:HG13	1:B:165:THR:HG22	2.02	0.41
1:A:147:THR:HG21	1:A:329:TYR:CE2	2.55	0.41
1:B:156:ALA:O	1:B:159:ILE:HG12	2.19	0.41
1:A:165:THR:C	1:A:167:VAL:N	2.78	0.41
1:A:249:GLN:HE21	1:B:249:GLN:HE21	1.68	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:B:355:ALA:C	1:B:357:THR:H	2.28	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:314:GLU:O	1:A:315:ILE:C	2.64	0.41
1:A:56:ILE:O	1:A:58:PRO:HD2	2.20	0.41
1:A:82:THR:HG22	1:A:382:PHE:HD2	1.86	0.41
1:A:235:VAL:O	1:A:235:VAL:HG12	2.20	0.41
1:A:386:LYS:HD3	1:A:386:LYS:HA	1.84	0.41
1:A:66:GLU:OE2	1:B:366:ARG:NH1	2.54	0.41
1:A:242:VAL:HG23	1:A:242:VAL:O	2.20	0.41
1:A:245:VAL:CG2	1:A:246:SER:H	2.26	0.41
1:A:61:LEU:HD23	1:A:397:TYR:C	2.46	0.41
1:A:78:ASN:O	1:A:79:LEU:C	2.63	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:91:VAL:HG21	1:B:112:ILE:CD1	2.51	0.41
1:B:273:ARG:HG2	1:B:273:ARG:HH11	1.86	0.41
1:A:86:PRO:HB2	1:B:410:ALA:HB2	2.04	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:291:LEU:O	1:A:292:PRO:C	2.65	0.40
1:B:194:ASP:C	1:B:196:ASP:N	2.79	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:249:GLN:O	1:B:253:GLN:NE2	2.54	0.40
1:B:304:LEU:O	1:B:305:ASP:C	2.65	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%)	4	24
1	B	376/420 (90%)	327 (87%)	39 (10%)	10 (3%)	4	22
All	All	753/840 (90%)	648 (86%)	86 (11%)	19 (2%)	4	23

All (19) Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
1	B	51	PRO

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	323/359 (90%)	308 (95%)	15 (5%)	24	53
1	B	322/359 (90%)	306 (95%)	16 (5%)	22	50
All	All	645/718 (90%)	614 (95%)	31 (5%)	23	52

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	TRP
1	A	90	THR
1	A	94	VAL
1	A	115	LEU
1	A	153	MET
1	A	160	ILE
1	A	234	ARG
1	A	235	VAL
1	A	247	MET
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	57	PHE
1	B	62	GLU
1	B	100	LEU
1	B	101	VAL
1	B	119	LYS
1	B	163	MET

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Mol	Chain	Res	Type
1	B	232	ARG
1	B	239	GLN
1	B	247	MET
1	B	264	ASP
1	B	328	ARG
1	B	357	THR
1	B	361	THR
1	B	389	SER
1	B	393	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	HIS
1	A	137	GLN
1	A	211	HIS
1	A	231	GLN
1	A	249	GLN
1	A	253	GLN
1	A	268	ASN
1	A	288	ASN
1	A	363	ASN
1	A	377	ASN
1	B	231	GLN
1	B	239	GLN
1	B	249	GLN
1	B	253	GLN
1	B	268	ASN
1	B	271	GLN
1	B	280	GLN
1	B	288	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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 [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	379/420 (90%)	-0.39	1 (0%) 90 82	25, 45, 90, 121	0
1	B	378/420 (90%)	-0.41	2 (0%) 87 76	27, 44, 85, 113	0
All	All	757/840 (90%)	-0.40	3 (0%) 88 79	25, 44, 87, 121	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	55	THR	5.5
1	B	349	GLY	5.0
1	B	419	ALA	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 oligosaccharides 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.