WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Aug 2, 2023 – 06:20 AM EDT

PDB ID	:	1B35
Title	:	CRICKET PARALYSIS VIRUS (CRPV)
Authors	:	Tate, J.G.; Liljas, L.; Scotti, P.D.; Christian, P.D.; Lin, T.W.; Johnson, J.E.
Deposited on	:	1998-12-17
Resolution	:	2.40 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:

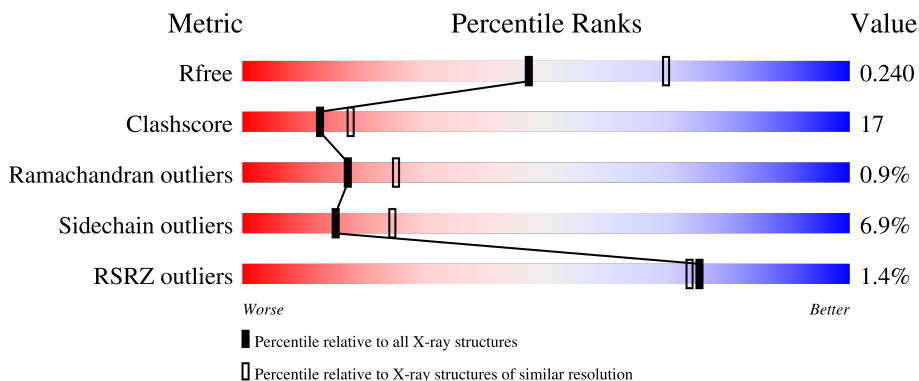|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.34
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
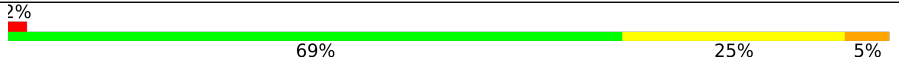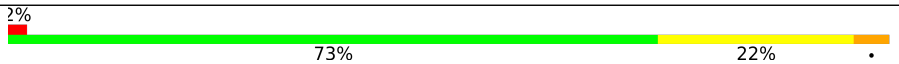*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	Percentile Ranks	Value
Rfree		0.240
Clashscore		17
Ramachandran outliers		0.9%
Sidechain outliers		6.9%
RSRZ outliers		1.4%

Worse ———— *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 <=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	260	74% 23% •
2	B	255	2% 69% 25% 5%
3	C	282	2% 73% 22% •
4	D	57	86% 12% •

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 6892 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 PROTEIN (CRICKET PARALYSIS VIRUS, VP1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	0	0
			2029	1288	340	390	11			

- Molecule 2 is a protein called PROTEIN (CRICKET PARALYSIS VIRUS, VP2).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	255	Total	C	N	O	S	0	0	0
			2024	1281	343	395	5			

- Molecule 3 is a protein called PROTEIN (CRICKET PARALYSIS VIRUS, VP3).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	282	Total	C	N	O	S	0	0	0
			2242	1418	380	430	14			

- Molecule 4 is a protein called PROTEIN (CRICKET PARALYSIS VIRUS, VP4).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	57	Total	C	N	O	0	0	0
			419	268	68	83			

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	70	Total	O	0	0
			70	70		
5	B	51	Total	O	0	0
			51	51		
5	C	56	Total	O	0	0
			56	56		
5	D	1	Total	O	0	0
			1	1		

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.
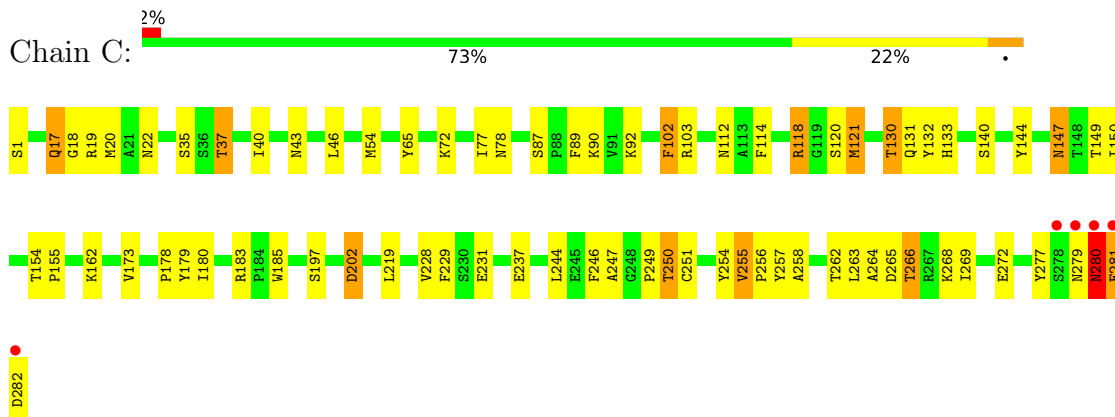
• Molecule 1: PROTEIN (CRICKET PARALYSIS VIRUS, VP1)
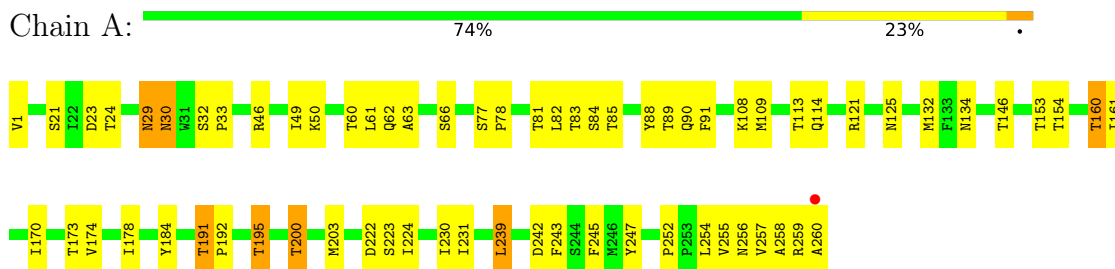
Chain A:

• Molecule 2: PROTEIN (CRICKET PARALYSIS VIRUS, VP2)
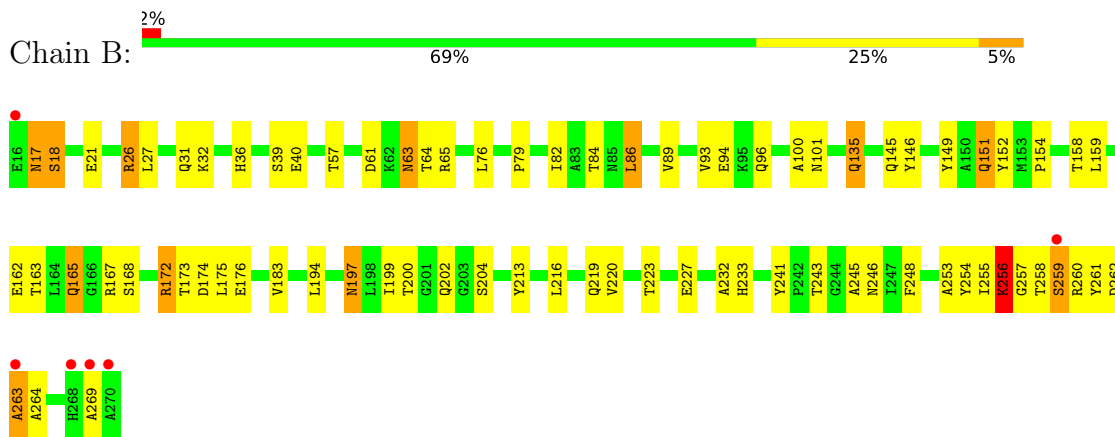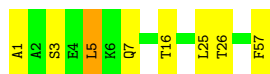
Chain B:

• Molecule 3: PROTEIN (CRICKET PARALYSIS VIRUS, VP3)

Chain C:

• Molecule 4: PROTEIN (CRICKET PARALYSIS VIRUS, VP4)

Chain D:

86%   12%

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	330.00Å 334.00Å 395.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.40 48.47 – 2.40	Depositor EDS
% Data completeness (in resolution range)	25.1 (15.00-2.40) 25.2 (48.47-2.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.65 (at 2.39Å)	Xtriage
Refinement program	CNS 0.4	Depositor
R, R_{free}	0.228 , 0.242 0.226 , 0.240	Depositor DCC
R_{free} test set	11814 reflections (5.60%)	wwPDB-VP
Wilson B-factor (Å^2)	18.2	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 33.0	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.011 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	6892	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.00% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.39	0/2081	0.65	0/2837
2	B	0.36	0/2067	0.65	1/2812 (0.0%)
3	C	0.39	0/2296	0.67	0/3120
4	D	0.35	0/427	0.62	0/580
All	All	0.38	0/6871	0.66	1/9349 (0.0%)

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
3	C	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	256	LYS	N-CA-C	-5.48	96.20	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	144	TYR	Sidechain

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	2029	0	1985	73	0
2	B	2024	0	1984	82	0
3	C	2242	0	2184	79	0
4	D	419	0	425	4	0
5	A	70	0	0	2	0
5	B	51	0	0	2	0
5	C	56	0	0	0	0
5	D	1	0	0	0	0
All	All	6892	0	6578	220	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

All (220) 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:239:LEU:HD12	1:A:239:LEU:H	1.08	1.11
2:B:63:ASN:HD22	2:B:64:THR:N	1.52	1.06
1:A:239:LEU:H	1:A:239:LEU:CD1	1.72	1.01
3:C:130:THR:HG22	3:C:132:TYR:H	1.20	1.00
1:A:239:LEU:HD12	1:A:239:LEU:N	1.76	0.98
1:A:49:ILE:HD12	1:A:239:LEU:HD22	1.45	0.97
1:A:81:THR:HG22	1:A:83:THR:H	1.31	0.96
2:B:151:GLN:H	2:B:151:GLN:HE21	1.05	0.96
3:C:255:VAL:HG22	3:C:256:PRO:HD2	1.48	0.95
2:B:199:ILE:HD11	2:B:243:THR:HG21	1.50	0.94
2:B:63:ASN:ND2	2:B:64:THR:H	1.66	0.91
3:C:262:THR:HG22	3:C:264:ALA:H	1.37	0.89
2:B:96:GLN:NE2	2:B:167:ARG:HH22	1.71	0.87
1:A:30:ASN:HD22	1:A:32:SER:H	1.20	0.86
1:A:88:TYR:CE2	3:C:255:VAL:HG21	2.10	0.86
2:B:96:GLN:HE21	2:B:167:ARG:HH22	0.92	0.85
1:A:60:THR:HG21	1:A:62:GLN:HE21	1.44	0.83
3:C:17:GLN:HG3	3:C:20:MET:HE2	1.61	0.83
3:C:280:ASN:N	3:C:280:ASN:HD22	1.76	0.82
1:A:91:PHE:HB2	1:A:239:LEU:HD11	1.63	0.80
2:B:255:ILE:HG21	3:C:277:TYR:HA	1.64	0.80
3:C:130:THR:CG2	3:C:132:TYR:H	1.95	0.78
1:A:89:THR:HG22	1:A:91:PHE:H	1.48	0.78
3:C:140:SER:HB3	3:C:162:LYS:HB3	1.64	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:255:VAL:HG22	3:C:256:PRO:CD	2.14	0.77
2:B:199:ILE:HD13	2:B:245:ALA:HB3	1.67	0.76
2:B:63:ASN:HD22	2:B:64:THR:H	0.81	0.73
2:B:162:GLU:OE1	3:C:269:ILE:HD11	1.88	0.73
1:A:49:ILE:HD12	1:A:239:LEU:CD2	2.16	0.73
2:B:165:GLN:NE2	3:C:103:ARG:HH11	1.86	0.73
3:C:280:ASN:ND2	3:C:281:GLU:H	1.86	0.73
2:B:96:GLN:HE21	2:B:167:ARG:NH2	1.77	0.73
1:A:81:THR:HG22	1:A:82:LEU:N	2.03	0.72
1:A:23:ASP:O	1:A:24:THR:HB	1.89	0.72
2:B:101:ASN:H	2:B:256:LYS:HE3	1.54	0.71
1:A:30:ASN:ND2	1:A:32:SER:H	1.88	0.71
3:C:77:ILE:HG22	3:C:219:LEU:O	1.90	0.70
1:A:239:LEU:HD23	1:A:243:PHE:CE1	2.26	0.70
3:C:118:ARG:HG3	3:C:185:TRP:CE3	2.27	0.70
2:B:258:THR:HG22	2:B:260:ARG:H	1.57	0.70
2:B:197:ASN:HD22	2:B:199:ILE:H	1.39	0.69
2:B:17:ASN:O	2:B:18:SER:HB2	1.91	0.69
1:A:160:THR:HG22	1:A:161:ILE:N	2.07	0.68
3:C:147:ASN:HD22	3:C:149:THR:H	1.41	0.68
1:A:239:LEU:HD23	1:A:243:PHE:CD1	2.28	0.68
2:B:151:GLN:H	2:B:151:GLN:NE2	1.88	0.68
2:B:31:GLN:NE2	2:B:36:HIS:HB2	2.08	0.68
2:B:31:GLN:HE21	2:B:36:HIS:CD2	2.12	0.68
2:B:260:ARG:HG2	2:B:263:ALA:HB3	1.74	0.67
3:C:112:ASN:HD21	3:C:254:TYR:H	1.41	0.67
3:C:268:LYS:O	3:C:272:GLU:HG3	1.94	0.67
2:B:255:ILE:O	2:B:256:LYS:HB2	1.93	0.67
1:A:230:ILE:HD12	5:A:321:HOH:O	1.94	0.66
2:B:145:GLN:HE22	2:B:167:ARG:HE	1.41	0.66
3:C:72:LYS:HG2	3:C:231:GLU:HG2	1.77	0.65
1:A:91:PHE:CD1	1:A:239:LEU:HD21	2.32	0.64
1:A:84:SER:O	1:A:257:VAL:HG13	1.98	0.63
3:C:130:THR:HG22	3:C:132:TYR:N	2.03	0.63
1:A:81:THR:HG22	1:A:82:LEU:H	1.61	0.63
2:B:163:THR:HB	2:B:165:GLN:HE21	1.63	0.63
2:B:31:GLN:HE21	2:B:36:HIS:HD2	1.47	0.63
2:B:200:THR:HG22	2:B:202:GLN:HG3	1.79	0.63
3:C:262:THR:O	3:C:266:THR:HG22	1.97	0.63
3:C:19:ARG:HA	3:C:22:ASN:HD22	1.65	0.62
1:A:29:ASN:C	1:A:29:ASN:HD22	2.02	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:32:LYS:HE2	2:B:32:LYS:HA	1.81	0.62
3:C:43:ASN:OD1	3:C:46:LEU:HD11	1.99	0.62
3:C:280:ASN:CG	3:C:281:GLU:H	2.03	0.62
3:C:130:THR:HB	3:C:133:HIS:CD2	2.34	0.62
2:B:199:ILE:CD1	2:B:243:THR:HG21	2.28	0.61
2:B:86:LEU:CD1	2:B:227:GLU:HG2	2.30	0.61
2:B:172:ARG:HG2	2:B:173:THR:N	2.14	0.61
1:A:146:THR:HA	1:A:200:THR:HG22	1.81	0.61
2:B:262:ASP:C	2:B:264:ALA:H	2.04	0.60
1:A:184:TYR:OH	1:A:191:THR:HG22	2.01	0.60
2:B:255:ILE:CG2	3:C:277:TYR:HA	2.30	0.60
1:A:49:ILE:O	1:A:239:LEU:HD13	2.01	0.60
2:B:26:ARG:HB2	2:B:26:ARG:HH11	1.66	0.60
2:B:135:GLN:HE22	2:B:219:GLN:HE21	1.49	0.60
2:B:165:GLN:HE22	3:C:103:ARG:HH11	1.50	0.59
2:B:89:VAL:HG23	2:B:216:LEU:O	2.02	0.59
2:B:197:ASN:ND2	2:B:199:ILE:H	2.00	0.59
1:A:77:SER:OG	1:A:195:THR:CG2	2.50	0.59
3:C:280:ASN:N	3:C:280:ASN:ND2	2.49	0.58
3:C:121:MET:CE	3:C:244:LEU:HD13	2.34	0.58
1:A:81:THR:HG22	1:A:83:THR:N	2.10	0.58
2:B:145:GLN:NE2	2:B:167:ARG:HE	2.01	0.58
1:A:255:VAL:HG21	3:C:257:TYR:CD1	2.39	0.57
1:A:160:THR:HG22	1:A:161:ILE:HG23	1.87	0.57
1:A:255:VAL:HG12	1:A:256:ASN:O	2.05	0.57
3:C:281:GLU:O	3:C:282:ASP:CB	2.53	0.56
1:A:132:MET:CE	1:A:134:ASN:HD21	2.18	0.56
1:A:81:THR:CG2	1:A:82:LEU:H	2.19	0.56
2:B:63:ASN:ND2	2:B:64:THR:N	2.37	0.56
3:C:262:THR:HG22	3:C:264:ALA:N	2.13	0.56
1:A:81:THR:CG2	1:A:82:LEU:N	2.68	0.55
3:C:17:GLN:HG2	3:C:18:GLY:N	2.21	0.55
3:C:121:MET:HE1	3:C:244:LEU:HD13	1.88	0.55
2:B:31:GLN:HE22	2:B:36:HIS:HB2	1.70	0.55
2:B:21:GLU:HB3	5:B:272:HOH:O	2.06	0.55
2:B:93:VAL:O	2:B:94:GLU:HB2	2.06	0.54
3:C:147:ASN:HD22	3:C:149:THR:N	2.06	0.54
3:C:19:ARG:HA	3:C:22:ASN:ND2	2.21	0.54
1:A:29:ASN:C	1:A:29:ASN:ND2	2.62	0.53
2:B:151:GLN:HE21	2:B:151:GLN:N	1.90	0.53
3:C:118:ARG:O	3:C:244:LEU:HD12	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:258:THR:HG22	2:B:260:ARG:N	2.24	0.52
1:A:146:THR:HG22	5:A:302:HOH:O	2.10	0.52
1:A:114:GLN:HB2	1:A:121:ARG:HG2	1.92	0.52
1:A:170:ILE:CD1	1:A:178:ILE:HG23	2.39	0.52
2:B:135:GLN:HE22	2:B:219:GLN:NE2	2.08	0.51
1:A:61:LEU:HB3	1:A:224:ILE:HD13	1.93	0.51
3:C:268:LYS:HE2	3:C:272:GLU:OE2	2.11	0.51
2:B:154:PRO:HG3	3:C:277:TYR:CE2	2.45	0.51
3:C:17:GLN:CG	3:C:20:MET:HE2	2.37	0.51
3:C:130:THR:HB	3:C:133:HIS:HD2	1.73	0.51
3:C:281:GLU:O	3:C:282:ASP:HB2	2.11	0.51
2:B:82:ILE:HD11	2:B:232:ALA:CB	2.40	0.50
1:A:61:LEU:O	1:A:230:ILE:HG23	2.10	0.50
1:A:91:PHE:CB	1:A:239:LEU:HD11	2.37	0.50
2:B:145:GLN:HE22	2:B:167:ARG:NE	2.08	0.50
1:A:60:THR:HG22	1:A:62:GLN:HG2	1.94	0.50
1:A:259:ARG:O	1:A:260:ALA:HB2	2.11	0.50
2:B:101:ASN:HB2	2:B:256:LYS:HD2	1.93	0.50
2:B:86:LEU:HD12	2:B:227:GLU:HG2	1.92	0.50
3:C:247:ALA:O	3:C:249:PRO:HD3	2.11	0.50
3:C:197:SER:HB3	3:C:202:ASP:HA	1.93	0.49
2:B:197:ASN:HD22	2:B:197:ASN:C	2.13	0.49
2:B:165:GLN:HE22	3:C:103:ARG:NH1	2.09	0.49
2:B:168:SER:HA	2:B:172:ARG:HD2	1.93	0.49
4:D:1:ALA:O	4:D:5:LEU:HD22	2.13	0.49
1:A:170:ILE:HD13	1:A:178:ILE:HG23	1.94	0.49
2:B:89:VAL:HG11	2:B:223:THR:HA	1.94	0.49
3:C:65:TYR:HA	3:C:237:GLU:HG2	1.94	0.49
1:A:257:VAL:CG1	1:A:258:ALA:N	2.77	0.48
3:C:77:ILE:O	3:C:78:ASN:HB2	2.13	0.48
1:A:49:ILE:CD1	1:A:239:LEU:HD22	2.32	0.48
3:C:147:ASN:ND2	3:C:150:ILE:H	2.12	0.48
1:A:46:ARG:O	1:A:50:LYS:HE3	2.13	0.48
1:A:153:THR:O	1:A:154:THR:HG23	2.14	0.48
3:C:114:PHE:CD2	3:C:246:PHE:HB3	2.49	0.48
3:C:250:THR:HB	3:C:251:CYS:H	1.53	0.48
1:A:91:PHE:HD1	1:A:239:LEU:HD21	1.77	0.47
1:A:160:THR:CG2	1:A:161:ILE:N	2.77	0.47
1:A:257:VAL:HG12	1:A:258:ALA:N	2.30	0.47
3:C:147:ASN:ND2	3:C:149:THR:HB	2.28	0.47
3:C:102:PHE:CD1	3:C:102:PHE:N	2.83	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:152:TYR:CE2	2:B:253:ALA:HB2	2.50	0.47
2:B:200:THR:CG2	2:B:202:GLN:HG3	2.44	0.47
2:B:152:TYR:CE1	2:B:253:ALA:HB3	2.50	0.46
2:B:173:THR:HG22	2:B:174:ASP:H	1.79	0.46
3:C:280:ASN:HD22	3:C:280:ASN:H	1.59	0.46
1:A:49:ILE:HD11	3:C:54:MET:HE1	1.96	0.46
2:B:165:GLN:NE2	3:C:103:ARG:NH1	2.59	0.46
2:B:246:ASN:ND2	5:B:321:HOH:O	2.40	0.46
2:B:199:ILE:HD11	2:B:243:THR:CG2	2.31	0.46
3:C:179:TYR:O	3:C:180:ILE:HD13	2.16	0.46
1:A:108:LYS:HA	1:A:178:ILE:O	2.16	0.45
3:C:140:SER:HB3	3:C:162:LYS:CB	2.42	0.45
4:D:3:SER:O	4:D:7:GLN:HG3	2.16	0.45
1:A:88:TYR:CD2	3:C:255:VAL:HG21	2.49	0.45
2:B:152:TYR:CZ	2:B:253:ALA:HB3	2.51	0.45
2:B:158:THR:O	2:B:162:GLU:HG2	2.17	0.45
3:C:130:THR:H	3:C:133:HIS:HD2	1.64	0.45
2:B:194:LEU:HD23	2:B:194:LEU:N	2.32	0.45
1:A:60:THR:HG21	1:A:62:GLN:NE2	2.24	0.45
1:A:78:PRO:HG2	2:B:159:LEU:HD11	1.97	0.45
1:A:91:PHE:CG	1:A:239:LEU:HD11	2.52	0.45
3:C:154:THR:HG23	3:C:155:PRO:HD2	1.99	0.45
2:B:197:ASN:HD22	2:B:199:ILE:N	2.13	0.45
3:C:280:ASN:CG	3:C:281:GLU:N	2.69	0.44
2:B:145:GLN:HG2	2:B:146:TYR:N	2.33	0.44
3:C:130:THR:HG21	3:C:228:VAL:HG11	2.00	0.44
1:A:32:SER:N	1:A:33:PRO:CD	2.81	0.44
1:A:63:ALA:O	1:A:66:SER:HB2	2.18	0.44
2:B:257:GLY:O	2:B:258:THR:HB	2.16	0.44
3:C:130:THR:HG23	3:C:132:TYR:HD1	1.82	0.44
3:C:280:ASN:ND2	3:C:281:GLU:N	2.60	0.44
1:A:60:THR:HG22	1:A:61:LEU:N	2.32	0.44
1:A:222:ASP:OD1	1:A:223:SER:N	2.51	0.44
2:B:255:ILE:O	2:B:256:LYS:CB	2.62	0.43
2:B:26:ARG:O	2:B:40:GLU:HA	2.18	0.43
2:B:262:ASP:C	2:B:264:ALA:N	2.72	0.43
1:A:1:VAL:O	3:C:173:VAL:HA	2.18	0.43
1:A:230:ILE:HG22	1:A:231:ILE:N	2.34	0.43
1:A:255:VAL:HG23	3:C:257:TYR:HB2	2.00	0.43
2:B:159:LEU:HD21	3:C:258:ALA:HB2	2.01	0.43
1:A:21:SER:C	1:A:23:ASP:N	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1:SER:HB3	4:D:57:PHE:C	2.39	0.43
3:C:87:SER:O	3:C:90:LYS:HE2	2.19	0.43
3:C:133:HIS:HE1	3:C:229:PHE:O	2.02	0.43
2:B:79:PRO:HA	2:B:233:HIS:HB3	2.01	0.43
2:B:61:ASP:HA	2:B:65:ARG:HB3	2.01	0.42
1:A:89:THR:HG22	1:A:90:GLN:N	2.33	0.42
3:C:92:LYS:O	3:C:102:PHE:HB3	2.19	0.42
3:C:118:ARG:O	3:C:244:LEU:HA	2.20	0.42
1:A:160:THR:HG22	1:A:161:ILE:H	1.85	0.42
2:B:27:LEU:HA	2:B:39:SER:O	2.20	0.42
3:C:120:SER:HB3	3:C:178:PRO:HA	2.02	0.42
2:B:100:ALA:HA	2:B:256:LYS:HE3	2.02	0.42
2:B:93:VAL:HG12	2:B:94:GLU:HG3	2.02	0.42
2:B:165:GLN:NE2	2:B:165:GLN:H	2.17	0.41
2:B:258:THR:C	2:B:260:ARG:H	2.24	0.41
3:C:130:THR:CG2	3:C:131:GLN:N	2.83	0.41
1:A:23:ASP:O	1:A:24:THR:CB	2.65	0.41
1:A:125:ASN:HD22	1:A:173:THR:HG21	1.85	0.41
1:A:242:ASP:OD2	3:C:40:ILE:HG12	2.20	0.41
1:A:254:LEU:O	1:A:255:VAL:HG23	2.20	0.41
4:D:16:THR:O	4:D:16:THR:HG22	2.20	0.41
3:C:37:THR:O	3:C:37:THR:CG2	2.67	0.41
1:A:191:THR:HA	1:A:192:PRO:HD3	1.92	0.41
1:A:21:SER:C	1:A:23:ASP:H	2.24	0.41
3:C:35:SER:C	3:C:37:THR:H	2.23	0.41
1:A:255:VAL:HG12	1:A:256:ASN:N	2.36	0.40
2:B:84:THR:HG22	2:B:227:GLU:OE1	2.21	0.40
2:B:259:SER:HB2	2:B:261:TYR:CD2	2.57	0.40
2:B:248:PHE:HE2	2:B:254:TYR:CB	2.34	0.40
3:C:130:THR:H	3:C:133:HIS:CD2	2.39	0.40
2:B:82:ILE:HD11	2:B:232:ALA:HB3	2.03	0.40
3:C:263:LEU:O	3:C:266:THR:HG23	2.21	0.40

There are no symmetry-related clashes.

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	258/260 (99%)	237 (92%)	21 (8%)	0	100	100
2	B	251/255 (98%)	225 (90%)	19 (8%)	7 (3%)	5	4
3	C	280/282 (99%)	256 (91%)	23 (8%)	1 (0%)	34	48
4	D	55/57 (96%)	51 (93%)	4 (7%)	0	100	100
All	All	844/854 (99%)	769 (91%)	67 (8%)	8 (1%)	17	25

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	17	ASN
2	B	256	LYS
2	B	18	SER
2	B	241	TYR
2	B	269	ALA
3	C	280	ASN
2	B	263	ALA
2	B	259	SER

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	230/230 (100%)	215 (94%)	15 (6%)	17	27
2	B	226/226 (100%)	209 (92%)	17 (8%)	13	21
3	C	250/250 (100%)	233 (93%)	17 (7%)	16	25
4	D	45/45 (100%)	42 (93%)	3 (7%)	16	26
All	All	751/751 (100%)	699 (93%)	52 (7%)	15	25

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

Mol	Chain	Res	Type
1	A	29	ASN
1	A	30	ASN
1	A	85	THR
1	A	109	MET
1	A	113	THR
1	A	160	THR
1	A	174	VAL
1	A	191	THR
1	A	195	THR
1	A	200	THR
1	A	203	MET
1	A	239	LEU
1	A	245	PHE
1	A	247	TYR
1	A	252	PRO
2	B	26	ARG
2	B	57	THR
2	B	63	ASN
2	B	76	LEU
2	B	86	LEU
2	B	135	GLN
2	B	149	TYR
2	B	151	GLN
2	B	165	GLN
2	B	172	ARG
2	B	175	LEU
2	B	176	GLU
2	B	183	VAL
2	B	197	ASN
2	B	204	SER
2	B	213	TYR
2	B	220	VAL
3	C	17	GLN
3	C	37	THR
3	C	89	PHE
3	C	102	PHE
3	C	118	ARG
3	C	121	MET
3	C	130	THR
3	C	147	ASN
3	C	183	ARG
3	C	202	ASP
3	C	250	THR

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Mol	Chain	Res	Type
3	C	255	VAL
3	C	265	ASP
3	C	266	THR
3	C	279	ASN
3	C	280	ASN
3	C	281	GLU
4	D	5	LEU
4	D	25	LEU
4	D	26	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	29	ASN
1	A	30	ASN
1	A	62	GLN
1	A	90	GLN
1	A	125	ASN
1	A	134	ASN
1	A	186	ASN
2	B	31	GLN
2	B	36	HIS
2	B	63	ASN
2	B	96	GLN
2	B	113	GLN
2	B	139	GLN
2	B	145	GLN
2	B	151	GLN
2	B	165	GLN
2	B	197	ASN
2	B	202	GLN
2	B	219	GLN
3	C	17	GLN
3	C	22	ASN
3	C	112	ASN
3	C	133	HIS
3	C	147	ASN
3	C	280	ASN
4	D	36	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 ⓘ

There are no monosaccharides 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 ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	251:ASN	C	252:GLU	N	13.40

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(Å²)	Q<0.9
1	A	260/260 (100%)	-0.89	1 (0%)	92	91	7, 14, 27, 35	0
2	B	255/255 (100%)	-0.90	6 (2%)	59	57	6, 13, 55, 67	0
3	C	282/282 (100%)	-0.94	5 (1%)	68	66	6, 13, 34, 71	0
4	D	57/57 (100%)	-0.52	0	100	100	11, 22, 41, 46	0
All	All	854/854 (100%)	-0.89	12 (1%)	75	73	6, 14, 35, 71	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	282	ASP	4.5
1	A	260	ALA	3.6
3	C	281	GLU	3.5
3	C	280	ASN	3.3
2	B	270	ALA	3.3
2	B	16	GLU	2.6
3	C	278	SER	2.4
3	C	279	ASN	2.3
2	B	259	SER	2.3
2	B	269	ALA	2.3
2	B	268	HIS	2.3
2	B	263	ALA	2.1

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.