



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:45 PM UTC

PDB ID : 5CDD / pdb_00005cdd
Title : Crystal Structure of Israel acute Paralysis Virus Pentamer
Authors : Mullapudi, E.; Plevka, P.
Deposited on : 2015-07-03
Resolution : 2.70 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
Xtrriage (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

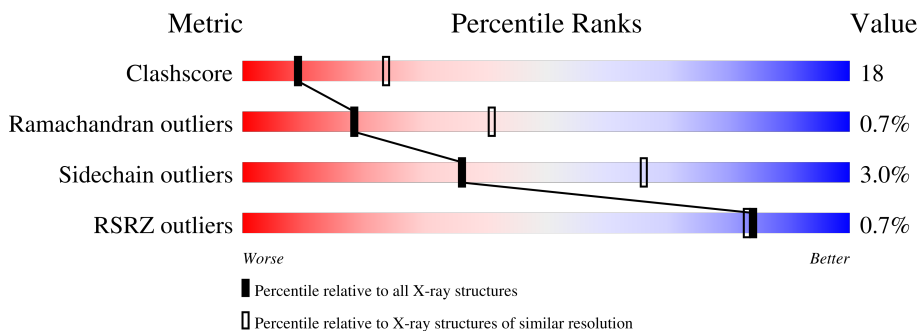
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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))
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	208	 68% 28% . .
2	B	301	 67% 30% .
3	C	200	 54% 41% 5%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5617 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 Structural polyprotein, VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	208	1682	1065	286	324	7	0	0	0

- Molecule 2 is a protein called Structural polyprotein, VP3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	301	2345	1500	386	446	13	0	0	0

- Molecule 3 is a protein called Structural polyprotein, VP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	200	1577	1012	257	303	5	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	87	ALA	ASN	conflict	UNP D1FK67

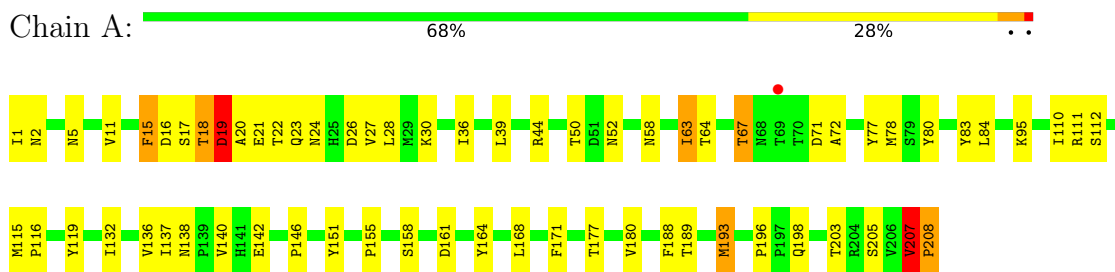
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	10	Total	O	0	0
			10	10		
4	B	1	Total	O	0	0
			1	1		
4	C	2	Total	O	0	0
			2	2		

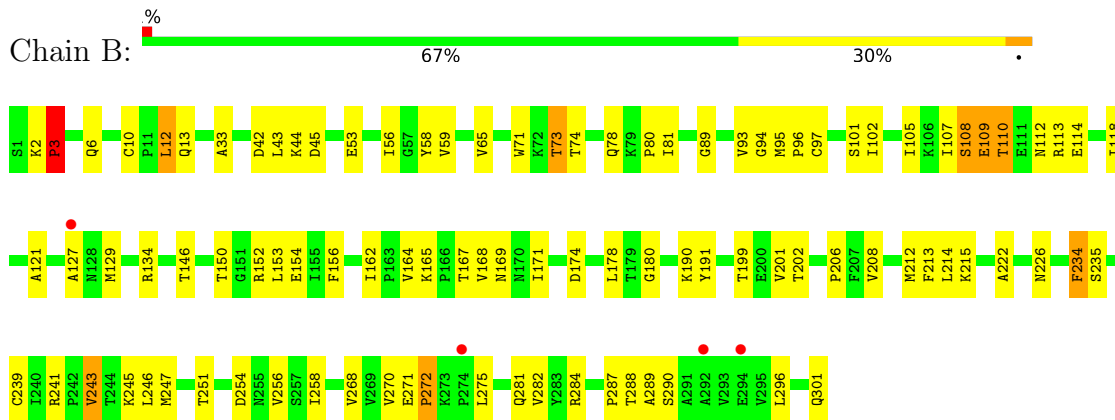
3 Residue-property plots

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.

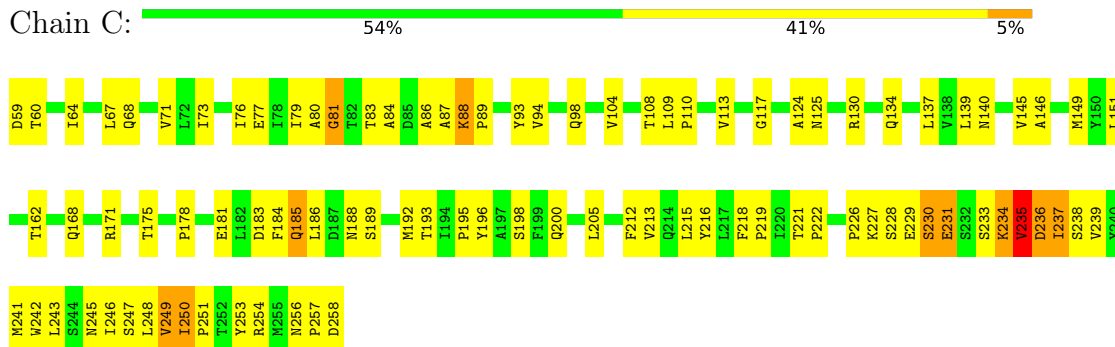
- Molecule 1: Structural polyprotein, VP1



- Molecule 2: Structural polyprotein, VP3



- Molecule 3: Structural polyprotein, VP2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	112.18Å 274.25Å 288.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.00 – 2.70 70.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.7 (70.00-2.70) 57.6 (70.00-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.05 (at 1.22Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.244 , 0.251 (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	1.6	Xtrriage
Anisotropy	1.986	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 508.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	0.012 for -h,l,k	Xtrriage
F_o, F_c correlation	0.40	EDS
Total number of atoms	5617	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.39% 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	0.48	4/1724 (0.2%)	0.99	13/2345 (0.6%)
2	B	0.37	1/2408 (0.0%)	0.92	9/3298 (0.3%)
3	C	1.48	26/1612 (1.6%)	1.10	22/2198 (1.0%)
All	All	0.86	31/5744 (0.5%)	1.00	44/7841 (0.6%)

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

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	249	VAL	C-O	-24.30	0.95	1.23
3	C	250	ILE	C-O	-17.87	1.01	1.24
3	C	229	GLU	CA-C	-15.99	1.31	1.52
3	C	229	GLU	C-O	-15.51	1.04	1.24
3	C	251	PRO	C-O	-15.42	1.03	1.24
3	C	231	GLU	C-O	-13.94	1.06	1.23
3	C	229	GLU	CA-CB	-12.92	1.35	1.54
3	C	251	PRO	CA-C	-12.06	1.35	1.52
3	C	249	VAL	N-CA	-12.01	1.32	1.46
3	C	230	SER	C-O	-11.56	1.08	1.24
3	C	249	VAL	CA-C	-9.72	1.40	1.52
3	C	231	GLU	CD-OE1	-9.47	1.07	1.25
3	C	251	PRO	CA-CB	-8.78	1.41	1.53
1	A	208	PRO	N-CD	7.92	1.58	1.47
3	C	249	VAL	CA-CB	-7.31	1.44	1.55
3	C	230	SER	C-N	-6.89	1.24	1.33
3	C	250	ILE	CA-CB	-6.65	1.45	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	208	PRO	CA-C	-6.57	1.39	1.52
3	C	235	VAL	C-N	-6.49	1.24	1.33
3	C	230	SER	CA-C	-6.09	1.44	1.52
2	B	3	PRO	N-CD	5.97	1.56	1.47
3	C	231	GLU	N-CA	-5.88	1.38	1.46
3	C	249	VAL	CB-CG1	-5.50	1.34	1.52
3	C	250	ILE	CB-CG1	-5.37	1.42	1.53
3	C	230	SER	CB-OG	-5.34	1.31	1.42
3	C	230	SER	CA-CB	-5.30	1.44	1.53
1	A	208	PRO	CA-CB	-5.25	1.43	1.53
3	C	251	PRO	CG-CD	-5.18	1.33	1.50
3	C	231	GLU	CD-OE2	-5.17	1.15	1.25
1	A	207	VAL	C-N	-5.04	1.26	1.34
3	C	251	PRO	C-N	-5.01	1.27	1.33

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	251	PRO	CA-N-CD	-9.95	98.07	112.00
3	C	229	GLU	CB-CA-C	-9.93	92.69	109.38
1	A	208	PRO	CA-N-CD	-9.81	98.26	112.00
1	A	16	ASP	N-CA-C	-9.77	95.30	109.96
3	C	249	VAL	N-CA-C	9.19	121.57	108.42
1	A	207	VAL	CB-CA-C	-9.10	94.80	111.36
1	A	207	VAL	C-N-CD	-8.55	89.94	125.00
3	C	229	GLU	CA-C-O	-8.29	109.78	118.90
2	B	89	GLY	N-CA-C	-8.18	102.30	112.77
1	A	208	PRO	N-CA-CB	7.83	111.62	103.00
1	A	17	SER	N-CA-C	7.54	120.02	109.31
2	B	234	PHE	N-CA-C	7.37	122.99	113.18
1	A	19	ASP	N-CA-C	-7.30	94.59	107.73
3	C	230	SER	CB-CA-C	-7.03	96.22	109.72
1	A	207	VAL	O-C-N	-6.64	113.53	121.10
3	C	83	THR	N-CA-C	6.53	121.29	113.12
1	A	208	PRO	N-CD-CG	-6.50	93.44	103.20
3	C	229	GLU	N-CA-CB	6.48	119.82	110.88
3	C	236	ASP	O-C-N	-6.27	114.25	122.59
3	C	81	GLY	N-CA-C	-6.17	98.54	113.18
2	B	121	ALA	N-CA-C	-6.07	102.45	110.40
3	C	249	VAL	CG1-CB-CG2	-5.99	97.63	110.80
3	C	237	ILE	CB-CA-C	-5.95	106.14	111.74
1	A	138	ASN	CA-C-N	5.92	125.60	119.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	138	ASN	C-N-CA	5.92	125.60	119.56
3	C	249	VAL	CB-CA-C	-5.88	100.59	111.18
2	B	199	THR	N-CA-C	-5.85	106.77	114.31
3	C	231	GLU	CA-C-N	5.58	131.02	122.93
3	C	231	GLU	C-N-CA	5.58	131.02	122.93
2	B	73	THR	N-CA-C	-5.54	106.37	113.01
3	C	230	SER	N-CA-C	5.49	119.97	113.28
3	C	249	VAL	CA-C-N	5.44	132.19	122.13
3	C	249	VAL	C-N-CA	5.44	132.19	122.13
1	A	44	ARG	N-CA-C	-5.42	107.22	113.88
3	C	188	ASN	N-CA-C	-5.36	106.90	113.50
3	C	237	ILE	N-CA-CB	5.30	116.83	109.84
1	A	193	MET	N-CA-C	5.29	117.75	110.35
2	B	243	VAL	N-CA-C	-5.25	106.01	111.58
2	B	109	GLU	N-CA-C	-5.22	106.75	113.02
3	C	231	GLU	CA-C-O	-5.08	114.29	120.54
2	B	6	GLN	N-CA-C	-5.08	105.87	113.89
2	B	108	SER	N-CA-C	-5.07	101.40	108.96
3	C	231	GLU	N-CA-CB	-5.06	101.97	111.13
3	C	251	PRO	CB-CA-C	-5.06	103.21	111.56

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	207	VAL	Mainchain

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	1682	0	1624	79	0
2	B	2345	0	2308	99	0
3	C	1577	0	1575	73	0
4	A	10	0	0	0	0
4	B	1	0	0	0	0
4	C	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5617	0	5507	203	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 18.

All (203) 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:207:VAL:HB	1:A:208:PRO:CD	1.74	1.14
1:A:207:VAL:HB	1:A:208:PRO:HD3	1.18	1.11
2:B:65:VAL:H	3:C:175:THR:HG21	1.27	0.98
1:A:5:ASN:ND2	3:C:181:GLU:H	1.62	0.96
1:A:5:ASN:HD21	3:C:181:GLU:N	1.64	0.96
2:B:2:LYS:HB2	2:B:3:PRO:CD	1.98	0.94
1:A:27:VAL:CG1	2:B:212:MET:HB3	2.00	0.91
1:A:207:VAL:O	1:A:208:PRO:C	1.96	0.91
2:B:2:LYS:HB2	2:B:3:PRO:HD3	1.56	0.88
3:C:235:VAL:HG12	3:C:236:ASP:N	1.91	0.83
3:C:139:LEU:HD21	3:C:184:PHE:HA	1.61	0.82
2:B:107:ILE:HD11	2:B:113:ARG:HB2	1.62	0.82
2:B:165:LYS:HE3	2:B:174:ASP:HA	1.60	0.81
1:A:2:ASN:HD21	1:A:5:ASN:HD22	1.26	0.80
1:A:24:ASN:HD22	2:B:134:ARG:HE	1.29	0.79
1:A:207:VAL:CB	1:A:208:PRO:CD	2.57	0.79
1:A:27:VAL:HG13	2:B:212:MET:HB3	1.66	0.78
1:A:5:ASN:HD21	3:C:181:GLU:H	0.81	0.76
1:A:23:GLN:O	1:A:27:VAL:HG23	1.84	0.75
3:C:130:ARG:HB3	3:C:247:SER:HB3	1.67	0.75
3:C:77:GLU:CD	3:C:234:LYS:HD2	2.12	0.75
1:A:24:ASN:ND2	2:B:134:ARG:HE	1.85	0.74
2:B:12:LEU:HD22	2:B:13:GLN:H	1.50	0.74
1:A:1:ILE:HG23	3:C:178:PRO:HA	1.69	0.74
3:C:76:ILE:O	3:C:236:ASP:OD1	2.06	0.73
3:C:59:ASP:CG	3:C:60:THR:H	1.97	0.72
1:A:2:ASN:ND2	1:A:5:ASN:HD22	1.89	0.71
2:B:214:LEU:HD11	2:B:235:SER:HB3	1.73	0.71
3:C:104:VAL:HG21	3:C:149:MET:HE1	1.72	0.69
1:A:207:VAL:HG12	1:A:208:PRO:N	2.08	0.68
3:C:84:ALA:C	3:C:86:ALA:H	2.00	0.67
2:B:44:LYS:O	2:B:45:ASP:HB2	1.96	0.66
1:A:67:THR:HG23	1:A:71:ASP:OD2	1.95	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:ASN:HD21	1:A:5:ASN:ND2	1.94	0.64
2:B:71:TRP:HB3	2:B:256:VAL:HG23	1.80	0.64
1:A:11:VAL:HG22	2:B:202:THR:HB	1.80	0.63
1:A:27:VAL:HG11	2:B:212:MET:HB3	1.80	0.63
1:A:189:THR:HG21	2:B:43:LEU:HD21	1.79	0.63
1:A:198:GLN:HE22	3:C:94:VAL:H	1.47	0.63
2:B:150:THR:OG1	2:B:247:MET:HB2	1.98	0.63
1:A:136:VAL:HG13	1:A:137:ILE:HG23	1.81	0.63
1:A:155:PRO:HB2	1:A:158:SER:HB2	1.79	0.63
1:A:111:ARG:HD2	1:A:132:ILE:HB	1.81	0.62
3:C:77:GLU:HA	3:C:236:ASP:HA	1.81	0.62
2:B:134:ARG:HB3	2:B:268:VAL:CG2	2.29	0.62
3:C:235:VAL:CG1	3:C:236:ASP:N	2.59	0.61
2:B:154:GLU:HB2	2:B:243:VAL:HG23	1.83	0.60
2:B:65:VAL:H	3:C:175:THR:CG2	2.10	0.60
3:C:253:TYR:CE1	3:C:254:ARG:HG3	2.36	0.60
2:B:153:LEU:HD21	2:B:258:ILE:HD13	1.84	0.60
3:C:140:ASN:O	3:C:235:VAL:O	2.21	0.59
1:A:193:MET:CE	2:B:59:VAL:HG22	2.32	0.59
1:A:63:ILE:HG12	1:A:168:LEU:HB3	1.85	0.59
2:B:247:MET:HA	2:B:247:MET:HE2	1.84	0.58
3:C:237:ILE:HG22	3:C:238:SER:N	2.18	0.58
2:B:167:THR:HG22	2:B:168:VAL:N	2.19	0.58
1:A:95:LYS:HG2	1:A:142:GLU:HG2	1.86	0.58
3:C:145:VAL:CG2	3:C:233:SER:HB3	2.34	0.58
1:A:77:TYR:CD1	2:B:129:MET:HE2	2.39	0.58
2:B:95:MET:HE2	2:B:127:ALA:HB2	1.86	0.58
1:A:146:PRO:HG2	2:B:33:ALA:HB2	1.86	0.58
3:C:64:ILE:HG23	3:C:246:ILE:HD12	1.86	0.58
1:A:36:ILE:HG22	2:B:56:ILE:HD11	1.86	0.58
2:B:154:GLU:HB2	2:B:243:VAL:CG2	2.34	0.57
1:A:161:ASP:HA	1:A:164:TYR:CD2	2.40	0.57
3:C:64:ILE:O	3:C:68:GLN:HG3	2.04	0.57
1:A:19:ASP:C	1:A:21:GLU:N	2.60	0.57
1:A:27:VAL:HG12	2:B:213:PHE:CE2	2.40	0.57
3:C:87:ALA:O	3:C:88:LYS:C	2.48	0.56
3:C:139:LEU:CD2	3:C:184:PHE:HA	2.35	0.56
1:A:207:VAL:CG1	1:A:208:PRO:N	2.63	0.56
3:C:73:ILE:HG13	3:C:241:MET:HB2	1.88	0.55
2:B:73:THR:HA	2:B:246:LEU:HB3	1.87	0.55
2:B:42:ASP:OD1	2:B:44:LYS:HB3	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:71:TRP:HB3	2:B:256:VAL:CG2	2.36	0.55
1:A:110:ILE:O	1:A:132:ILE:HA	2.08	0.54
3:C:227:LYS:O	3:C:228:SER:HB2	2.08	0.54
3:C:234:LYS:HB3	3:C:234:LYS:NZ	2.23	0.54
1:A:18:THR:HG22	1:A:19:ASP:OD1	2.07	0.53
3:C:109:LEU:HB2	3:C:213:VAL:HG13	1.90	0.53
3:C:87:ALA:O	3:C:89:PRO:HD3	2.09	0.53
3:C:235:VAL:HG12	3:C:236:ASP:H	1.69	0.53
1:A:50:THR:HG22	1:A:180:VAL:HB	1.91	0.53
1:A:193:MET:HE1	2:B:59:VAL:HA	1.91	0.53
3:C:198:SER:HB2	3:C:212:PHE:CD2	2.43	0.53
1:A:52:ASN:HB2	2:B:301:GLN:HG3	1.91	0.52
3:C:196:TYR:CZ	3:C:198:SER:HB3	2.44	0.52
1:A:19:ASP:OD1	1:A:19:ASP:N	2.42	0.52
1:A:27:VAL:HG12	2:B:213:PHE:CZ	2.43	0.52
2:B:97:CYS:SG	2:B:118:ILE:HG22	2.49	0.52
2:B:288:THR:HG22	2:B:290:SER:H	1.73	0.52
1:A:27:VAL:HG13	2:B:212:MET:HE2	1.91	0.52
1:A:116:PRO:HB2	1:A:119:TYR:CD1	2.44	0.52
3:C:108:THR:O	3:C:108:THR:HG23	2.10	0.52
3:C:84:ALA:C	3:C:86:ALA:N	2.69	0.51
1:A:161:ASP:HA	1:A:164:TYR:CE2	2.45	0.51
3:C:124:ALA:O	3:C:125:ASN:HB2	2.09	0.51
3:C:248:LEU:C	3:C:249:VAL:HG13	2.34	0.51
1:A:30:LYS:HB2	2:B:212:MET:HE1	1.92	0.51
1:A:58:ASN:HA	1:A:171:PHE:CE1	2.46	0.51
2:B:80:PRO:HD3	2:B:178:LEU:O	2.11	0.51
2:B:12:LEU:CD2	2:B:13:GLN:H	2.23	0.50
2:B:93:VAL:O	2:B:234:PHE:O	2.30	0.50
1:A:78:MET:HE3	1:A:188:PHE:CE2	2.47	0.49
2:B:97:CYS:SG	2:B:118:ILE:CG2	3.01	0.49
3:C:237:ILE:HG22	3:C:238:SER:H	1.76	0.49
3:C:76:ILE:O	3:C:236:ASP:HA	2.12	0.49
1:A:64:THR:HA	1:A:67:THR:HB	1.95	0.49
1:A:151:TYR:CE1	3:C:200:GLN:HG2	2.47	0.49
2:B:171:ILE:HD12	2:B:222:ALA:HB1	1.94	0.49
3:C:257:PRO:O	3:C:258:ASP:OD1	2.30	0.49
1:A:19:ASP:C	1:A:21:GLU:H	2.21	0.49
3:C:134:GLN:NE2	3:C:193:THR:OG1	2.46	0.49
3:C:137:LEU:O	3:C:189:SER:HA	2.12	0.49
2:B:162:ILE:O	2:B:164:VAL:HG13	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:183:ASP:HB3	3:C:186:LEU:HB2	1.94	0.48
2:B:2:LYS:CB	2:B:3:PRO:CD	2.81	0.48
2:B:102:ILE:HD11	2:B:169:ASN:O	2.13	0.48
3:C:236:ASP:C	3:C:237:ILE:HG13	2.39	0.48
2:B:2:LYS:HB2	2:B:3:PRO:HD2	1.92	0.47
2:B:2:LYS:CB	2:B:3:PRO:HD3	2.37	0.47
2:B:78:GLN:HB3	2:B:180:GLY:HA3	1.96	0.47
3:C:192:MET:HE1	3:C:215:LEU:CD1	2.45	0.47
1:A:24:ASN:HB3	2:B:268:VAL:HG11	1.95	0.47
1:A:177:THR:HG23	1:A:177:THR:O	2.14	0.47
1:A:111:ARG:HD3	1:A:132:ILE:HD12	1.97	0.47
1:A:205:SER:HA	2:B:112:ASN:O	2.14	0.47
3:C:234:LYS:HB3	3:C:234:LYS:HZ2	1.80	0.47
1:A:24:ASN:ND2	2:B:134:ARG:NE	2.60	0.47
2:B:288:THR:HG22	2:B:289:ALA:N	2.29	0.47
1:A:83:TYR:CD2	2:B:282:VAL:HG21	2.50	0.47
2:B:222:ALA:HA	2:B:226:ASN:O	2.14	0.47
1:A:193:MET:HE1	2:B:59:VAL:HG22	1.97	0.47
3:C:110:PRO:O	3:C:113:VAL:HG12	2.15	0.47
2:B:146:THR:HA	3:C:185:GLN:HG2	1.97	0.46
1:A:39:LEU:HD12	2:B:59:VAL:HG21	1.97	0.46
2:B:234:PHE:O	2:B:235:SER:CB	2.64	0.46
3:C:248:LEU:C	3:C:249:VAL:CG1	2.87	0.46
3:C:64:ILE:HG23	3:C:246:ILE:HB	1.98	0.46
2:B:156:PHE:CE2	2:B:239:CYS:HB3	2.51	0.46
2:B:95:MET:N	2:B:96:PRO:CD	2.79	0.46
3:C:59:ASP:CG	3:C:60:THR:N	2.67	0.45
1:A:63:ILE:CG1	1:A:168:LEU:HB3	2.46	0.45
3:C:67:LEU:HB2	3:C:246:ILE:HD13	1.98	0.45
1:A:72:ALA:HB1	2:B:284:ARG:CZ	2.46	0.45
1:A:28:LEU:HD12	2:B:213:PHE:HZ	1.82	0.45
1:A:140:VAL:HG12	1:A:142:GLU:HG3	1.99	0.45
2:B:270:VAL:O	2:B:271:GLU:HB3	2.17	0.45
1:A:112:SER:HB2	1:A:168:LEU:HD11	1.99	0.45
1:A:80:TYR:HD2	2:B:129:MET:HE3	1.83	0.44
2:B:156:PHE:CB	2:B:190:LYS:HB3	2.47	0.44
2:B:251:THR:O	3:C:226:PRO:HB3	2.18	0.44
1:A:1:ILE:HG23	1:A:1:ILE:O	2.17	0.44
1:A:19:ASP:O	1:A:21:GLU:N	2.51	0.44
1:A:50:THR:O	1:A:50:THR:HG23	2.17	0.44
2:B:108:SER:OG	2:B:110:THR:HG23	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:80:ALA:O	3:C:81:GLY:C	2.60	0.44
2:B:156:PHE:HB3	2:B:190:LYS:HB3	2.00	0.43
2:B:287:PRO:O	3:C:98:GLN:HG3	2.18	0.43
3:C:205:LEU:O	3:C:256:ASN:HB2	2.18	0.43
3:C:195:PRO:O	3:C:196:TYR:C	2.61	0.43
3:C:171:ARG:O	3:C:175:THR:HG22	2.18	0.43
2:B:81:ILE:HD11	2:B:153:LEU:HD11	2.01	0.43
2:B:191:TYR:CD2	2:B:201:VAL:HG21	2.53	0.43
3:C:151:LEU:HD12	3:C:216:TYR:O	2.19	0.43
3:C:113:VAL:HG11	3:C:243:LEU:HD21	1.99	0.42
1:A:1:ILE:HG23	3:C:178:PRO:CA	2.46	0.42
1:A:19:ASP:O	1:A:20:ALA:C	2.61	0.42
1:A:84:LEU:CD2	1:A:196:PRO:HB3	2.48	0.42
1:A:208:PRO:HB2	2:B:112:ASN:HD21	1.85	0.42
3:C:162:THR:HG22	3:C:168:GLN:HG3	2.00	0.42
3:C:221:THR:HB	3:C:222:PRO:HD2	2.01	0.42
2:B:167:THR:CG2	2:B:168:VAL:N	2.82	0.42
3:C:79:ILE:HG22	3:C:81:GLY:H	1.83	0.42
2:B:154:GLU:HB3	2:B:241:ARG:O	2.19	0.42
2:B:208:VAL:HG23	2:B:208:VAL:O	2.19	0.42
2:B:101:SER:HB2	3:C:93:TYR:CE2	2.54	0.42
3:C:71:VAL:HG11	3:C:117:GLY:HA3	2.00	0.42
1:A:28:LEU:HD12	2:B:213:PHE:CZ	2.55	0.42
2:B:281:GLN:NE2	2:B:296:LEU:HG	2.34	0.42
1:A:27:VAL:HA	2:B:212:MET:HE2	2.02	0.42
2:B:80:PRO:HA	2:B:241:ARG:HG2	2.01	0.42
3:C:134:GLN:HB3	3:C:242:TRP:CE2	2.55	0.42
2:B:254:ASP:OD1	3:C:227:LYS:HE3	2.20	0.42
3:C:218:PHE:HA	3:C:219:PRO:HD3	1.83	0.41
1:A:15:PHE:CD2	2:B:206:PRO:HD2	2.55	0.41
2:B:73:THR:O	2:B:245:LYS:HE2	2.20	0.41
2:B:81:ILE:HD13	2:B:258:ILE:HD12	2.02	0.41
2:B:105:ILE:CG1	2:B:113:ARG:HB3	2.51	0.41
2:B:53:GLU:HA	2:B:58:TYR:CD2	2.56	0.41
2:B:146:THR:CG2	3:C:146:ALA:HB2	2.51	0.41
2:B:94:GLY:HA3	2:B:234:PHE:HD1	1.86	0.41
2:B:152:ARG:HH11	2:B:152:ARG:HG2	1.86	0.41
2:B:271:GLU:HG3	2:B:272:PRO:CD	2.51	0.41
1:A:203:THR:HA	2:B:114:GLU:O	2.21	0.41
2:B:12:LEU:HA	2:B:12:LEU:HD23	1.81	0.41
1:A:19:ASP:O	1:A:22:THR:N	2.53	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:137:LEU:HD22	3:C:239:VAL:HG22	2.04	0.40
3:C:236:ASP:OD1	3:C:237:ILE:N	2.51	0.40
1:A:27:VAL:CG1	2:B:213:PHE:CZ	3.04	0.40
1:A:146:PRO:CG	2:B:33:ALA:HB2	2.51	0.40
2:B:215:LYS:HB3	2:B:275:LEU:CD2	2.51	0.40
2:B:95:MET:CE	2:B:127:ALA:HB2	2.51	0.40

There are no symmetry-related clashes.

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	206/208 (99%)	185 (90%)	19 (9%)	2 (1%)	12	32
2	B	299/301 (99%)	268 (90%)	29 (10%)	2 (1%)	18	41
3	C	198/200 (99%)	180 (91%)	17 (9%)	1 (0%)	24	48
All	All	703/709 (99%)	633 (90%)	65 (9%)	5 (1%)	18	41

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	272	PRO
1	A	207	VAL
3	C	250	ILE
1	A	15	PHE
2	B	3	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	189/189 (100%)	182 (96%)	7 (4%)	30	59
2	B	263/263 (100%)	258 (98%)	5 (2%)	50	77
3	C	177/177 (100%)	170 (96%)	7 (4%)	28	56
All	All	629/629 (100%)	610 (97%)	19 (3%)	36	66

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	THR
1	A	19	ASP
1	A	26	ASP
1	A	63	ILE
1	A	67	THR
1	A	115	MET
1	A	207	VAL
2	B	10	CYS
2	B	12	LEU
2	B	74	THR
2	B	109	GLU
2	B	110	THR
3	C	88	LYS
3	C	185	GLN
3	C	230	SER
3	C	231	GLU
3	C	234	LYS
3	C	235	VAL
3	C	245	ASN

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

Mol	Chain	Res	Type
1	A	5	ASN
1	A	8	ASN
1	A	24	ASN
1	A	106	GLN
1	A	131	HIS
1	A	141	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	198	GLN
2	B	13	GLN
2	B	37	ASN
2	B	187	ASN
2	B	231	HIS
2	B	255	ASN
2	B	281	GLN
3	C	97	GLN
3	C	134	GLN
3	C	188	ASN

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 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	208/208 (100%)	-0.51	1 (0%) 87 86	20, 34, 62, 80	0
2	B	301/301 (100%)	-0.28	4 (1%) 75 73	24, 39, 69, 92	0
3	C	200/200 (100%)	-0.32	0 100 100	27, 42, 89, 102	0
All	All	709/709 (100%)	-0.36	5 (0%) 84 83	20, 39, 72, 102	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	294	GLU	3.1
2	B	292	ALA	3.1
2	B	274	PRO	2.7
1	A	69	THR	2.2
2	B	127	ALA	2.2

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.