



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:49 PM GMT

PDB ID : 1CN3  
Title : INTERACTION OF POLYOMAVIRUS INTERNAL PROTEIN VP2 WITH  
MAJOR CAPSID PROTEIN VP1 AND IMPLICATIONS FOR PARTICIPA-  
TION OF VP2 IN VIRAL ENTRY  
Authors : Chen, X.; Stehle, T.; Harrison, S.C.  
Deposited on : 1999-05-24  
Resolution : 2.20 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

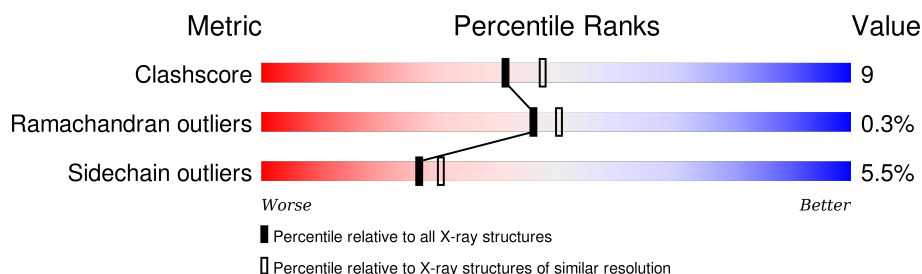
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	283	
1	B	283	
1	C	283	
1	D	283	
1	E	283	
2	F	29	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11261 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 COAT PROTEIN VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	283	Total	C	N	O	S	0	0	0
			2213	1400	371	431	11			
1	B	283	Total	C	N	O	S	0	0	0
			2213	1400	371	431	11			
1	C	283	Total	C	N	O	S	0	0	0
			2213	1400	371	431	11			
1	D	283	Total	C	N	O	S	0	0	0
			2213	1400	371	431	11			
1	E	283	Total	C	N	O	S	0	0	0
			2213	1400	371	431	11			

- Molecule 2 is a protein called FRAGMENT OF COAT PROTEIN VP2.

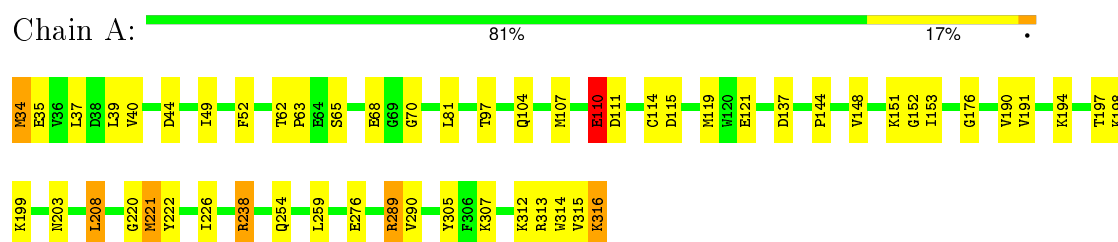
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	29	Total	C	N	O	S	0	0	0
			196	124	36	35	1			

### 3 Residue-property plots

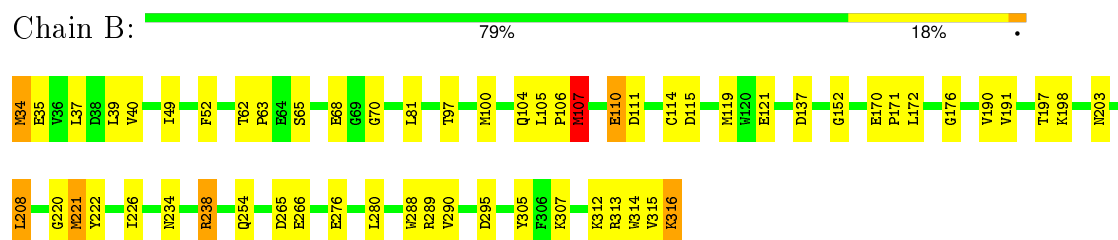
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

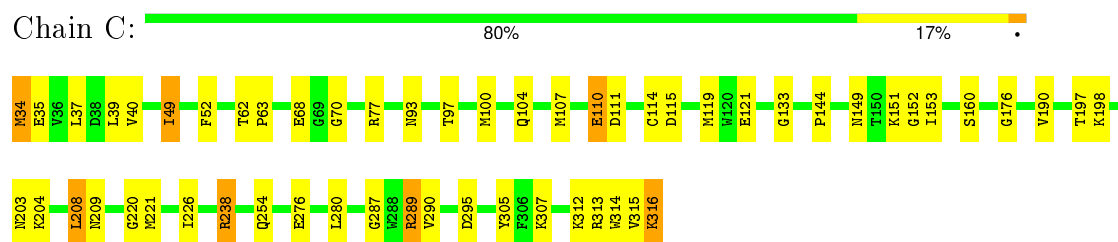
#### • Molecule 1: COAT PROTEIN VP1



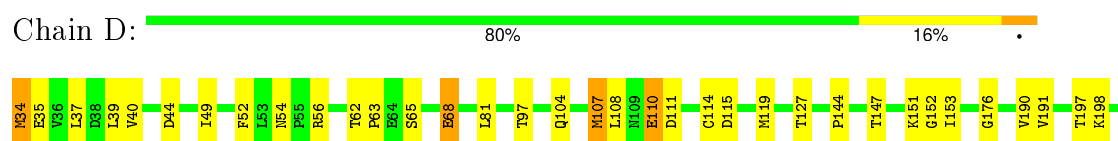
#### • Molecule 1: COAT PROTEIN VP1



#### • Molecule 1: COAT PROTEIN VP1

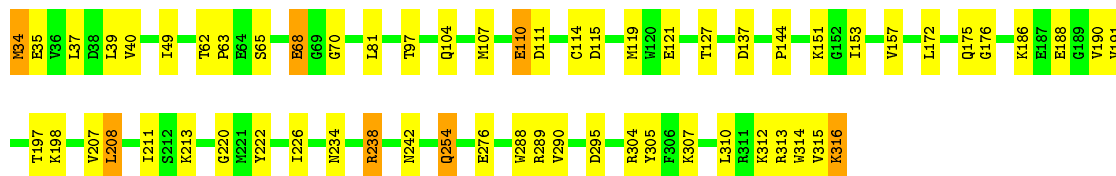
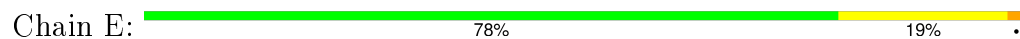


#### • Molecule 1: COAT PROTEIN VP1





• Molecule 1: COAT PROTEIN VP1



• Molecule 2: FRAGMENT OF COAT PROTEIN VP2



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	219.00 Å   219.00 Å   99.00 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	20.00 – 2.20	Depositor
% Data completeness (in resolution range)	95.0 (20.00-2.20)	Depositor
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.15	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.230 , 0.260	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11261	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

## 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	1.04	3/2266 (0.1%)	1.01	3/3088 (0.1%)
1	B	1.07	6/2266 (0.3%)	0.99	1/3088 (0.0%)
1	C	1.06	3/2266 (0.1%)	0.99	2/3088 (0.1%)
1	D	1.08	7/2266 (0.3%)	1.01	4/3088 (0.1%)
1	E	1.07	4/2266 (0.2%)	0.99	2/3088 (0.1%)
2	F	0.65	0/201	1.03	1/271 (0.4%)
All	All	1.06	23/11531 (0.2%)	1.00	13/15711 (0.1%)

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	221	MET	SD-CE	6.56	2.14	1.77
1	C	238	ARG	CZ-NH2	6.36	1.41	1.33
1	B	52	PHE	CE2-CZ	6.21	1.49	1.37
1	D	68	GLU	CD-OE2	6.17	1.32	1.25
1	C	68	GLU	CD-OE2	5.99	1.32	1.25
1	E	238	ARG	NE-CZ	5.92	1.40	1.33
1	D	221	MET	SD-CE	5.79	2.10	1.77
1	D	290	VAL	CB-CG2	-5.71	1.40	1.52
1	D	238	ARG	NE-CZ	5.67	1.40	1.33
1	B	288	TRP	CB-CG	-5.66	1.40	1.50
1	B	221	MET	SD-CE	5.55	2.08	1.77
1	A	52	PHE	CD2-CE2	5.54	1.50	1.39
1	D	52	PHE	CD1-CE1	5.34	1.50	1.39
1	B	238	ARG	CZ-NH2	5.27	1.39	1.33
1	B	107	MET	SD-CE	5.15	2.06	1.77
1	E	238	ARG	CZ-NH2	5.14	1.39	1.33
1	E	68	GLU	CD-OE2	5.09	1.31	1.25
1	B	238	ARG	NE-CZ	5.08	1.39	1.33
1	E	238	ARG	CZ-NH1	5.05	1.39	1.33
1	A	238	ARG	NE-CZ	5.04	1.39	1.33
1	C	52	PHE	CD1-CE1	5.03	1.49	1.39
1	D	68	GLU	CG-CD	5.03	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	238	ARG	CZ-NH1	5.03	1.39	1.33

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	208	LEU	CA-CB-CG	-6.63	100.04	115.30
1	D	208	LEU	CA-CB-CG	-6.61	100.10	115.30
1	E	208	LEU	CA-CB-CG	-6.57	100.18	115.30
1	A	208	LEU	CA-CB-CG	-6.50	100.36	115.30
1	C	208	LEU	CA-CB-CG	-6.09	101.29	115.30
1	D	289	ARG	NE-CZ-NH2	-5.91	117.35	120.30
2	F	11	SER	N-CA-C	5.87	126.84	111.00
1	E	238	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	A	289	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	A	238	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	D	56	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	C	289	ARG	NE-CZ-NH2	-5.47	117.57	120.30
1	D	238	ARG	NE-CZ-NH1	5.22	122.91	120.30

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	2213	0	2181	38	1
1	B	2213	0	2181	41	0
1	C	2213	0	2181	37	1
1	D	2213	0	2181	36	1
1	E	2213	0	2181	42	3
2	F	196	0	192	28	0
All	All	11261	0	11097	191	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 9.



All (191) 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:C:221:MET:SD	1:C:221:MET:CE	2.05	1.44
1:B:107:MET:CE	1:B:107:MET:SD	2.06	1.43
1:B:221:MET:SD	1:B:221:MET:CE	2.08	1.40
1:D:221:MET:SD	1:D:221:MET:CE	2.10	1.38
1:A:221:MET:SD	1:A:221:MET:CE	2.14	1.35
1:E:254:GLN:O	2:F:10:ALA:HB3	1.58	1.03
1:A:259:LEU:HD13	2:F:15:VAL:HG21	1.56	0.87
2:F:7:GLY:O	2:F:9:ALA:N	2.08	0.86
1:A:34:MET:HA	1:A:34:MET:CE	2.09	0.82
1:C:34:MET:HA	1:C:34:MET:CE	2.08	0.82
1:A:259:LEU:CD1	2:F:15:VAL:HG21	2.10	0.82
1:D:34:MET:HA	1:D:34:MET:CE	2.10	0.82
1:E:34:MET:CE	1:E:34:MET:HA	2.12	0.79
1:B:34:MET:CE	1:B:34:MET:HA	2.13	0.78
1:B:119:MET:HE3	1:B:315:VAL:HG21	1.67	0.77
2:F:23:LEU:HD23	2:F:27:LEU:HD21	1.68	0.76
1:D:119:MET:CE	1:D:315:VAL:HG21	2.18	0.74
1:B:119:MET:CE	1:B:315:VAL:HG21	2.18	0.73
1:D:119:MET:HE3	1:D:315:VAL:HG21	1.72	0.72
1:C:111:ASP:HB3	1:C:114:CYS:HB2	1.73	0.71
1:D:34:MET:HA	1:D:34:MET:HE2	1.71	0.71
1:B:266:GLU:HA	2:F:18:ASP:O	1.91	0.70
1:A:119:MET:CE	1:A:315:VAL:HG21	2.21	0.70
1:C:34:MET:HA	1:C:34:MET:HE3	1.74	0.69
2:F:13:GLN:HG2	2:F:14:ARG:N	2.07	0.69
1:C:119:MET:CE	1:C:315:VAL:HG21	2.23	0.69
1:B:111:ASP:HB3	1:B:114:CYS:HB2	1.75	0.68
1:E:119:MET:CE	1:E:315:VAL:HG21	2.24	0.67
1:C:119:MET:HE3	1:C:315:VAL:HG21	1.77	0.66
1:A:34:MET:HE3	1:A:34:MET:HA	1.78	0.66
1:A:34:MET:HE2	1:A:34:MET:HA	1.78	0.65
1:D:111:ASP:HB3	1:D:114:CYS:HB2	1.78	0.65
1:E:119:MET:HE3	1:E:315:VAL:HG21	1.80	0.64
1:B:34:MET:HA	1:B:34:MET:HE3	1.79	0.64
1:E:34:MET:HA	1:E:34:MET:HE2	1.77	0.63
1:E:111:ASP:HB3	1:E:114:CYS:HB2	1.81	0.63
1:C:197:THR:O	1:C:198:LYS:HB2	1.99	0.63
1:C:34:MET:HA	1:C:34:MET:HE2	1.82	0.61
1:A:111:ASP:HB3	1:A:114:CYS:HB2	1.81	0.60
1:B:197:THR:O	1:B:198:LYS:HB2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:MET:HE3	1:A:315:VAL:HG21	1.83	0.59
1:E:34:MET:HA	1:E:34:MET:HE3	1.83	0.59
1:A:119:MET:HE2	1:A:315:VAL:HG21	1.85	0.58
1:E:197:THR:O	1:E:198:LYS:HB2	2.04	0.58
1:B:110:GLU:OE2	1:B:110:GLU:HA	2.05	0.57
1:E:242:ASN:ND2	2:F:7:GLY:C	2.59	0.56
1:A:259:LEU:HD13	2:F:15:VAL:HG11	1.87	0.56
1:D:197:THR:O	1:D:198:LYS:HB2	2.06	0.56
1:B:34:MET:HA	1:B:34:MET:HE2	1.86	0.56
1:E:254:GLN:O	2:F:10:ALA:CB	2.45	0.55
1:B:39:LEU:HD23	1:B:313:ARG:HD2	1.89	0.55
1:C:110:GLU:OE2	1:C:110:GLU:HA	2.06	0.55
1:C:153:ILE:HA	1:D:81:LEU:HD21	1.88	0.55
1:C:39:LEU:HD23	1:C:313:ARG:HD2	1.89	0.55
1:C:305:TYR:OH	1:C:307:LYS:HE2	2.07	0.54
1:B:37:LEU:HD11	1:B:316:LYS:HB2	1.90	0.54
1:E:305:TYR:OH	1:E:307:LYS:HE2	2.08	0.54
2:F:27:LEU:HD12	2:F:28:TYR:HE1	1.73	0.53
1:D:40:VAL:HB	1:D:312:LYS:HB2	1.89	0.53
1:A:37:LEU:HD11	1:A:316:LYS:HB2	1.90	0.53
1:C:40:VAL:HB	1:C:312:LYS:HB2	1.89	0.53
1:C:37:LEU:HD11	1:C:316:LYS:HB2	1.90	0.53
1:E:40:VAL:HB	1:E:312:LYS:HB2	1.91	0.53
1:A:259:LEU:HD22	2:F:15:VAL:CG2	2.39	0.53
1:D:34:MET:HA	1:D:34:MET:HE3	1.86	0.53
1:A:110:GLU:OE2	1:A:110:GLU:HA	2.09	0.53
1:B:70:GLY:O	1:C:203:ASN:HB2	2.09	0.53
1:E:304:ARG:NH2	2:F:8:GLY:O	2.36	0.53
1:A:197:THR:O	1:A:198:LYS:HB2	2.09	0.52
1:E:39:LEU:HD23	1:E:313:ARG:HD2	1.90	0.52
2:F:18:ASP:O	2:F:21:LEU:HB2	2.10	0.52
1:D:119:MET:HE2	1:D:315:VAL:HG21	1.90	0.52
1:A:40:VAL:HB	1:A:312:LYS:HB2	1.91	0.52
1:D:37:LEU:HD11	1:D:316:LYS:HB2	1.91	0.52
1:A:259:LEU:HD13	2:F:15:VAL:CG2	2.35	0.51
1:B:305:TYR:OH	1:B:307:LYS:HE2	2.10	0.51
1:E:242:ASN:HD22	2:F:7:GLY:C	2.12	0.51
1:D:110:GLU:HA	1:D:110:GLU:OE2	2.09	0.51
1:B:97:THR:OG1	1:B:220:GLY:HA2	2.11	0.51
1:A:81:LEU:HD21	1:E:153:ILE:HA	1.92	0.50
1:E:35:GLU:HB3	1:E:316:LYS:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:252:VAL:HG21	2:F:4:GLY:H	1.77	0.50
1:C:35:GLU:HB3	1:C:316:LYS:HB3	1.93	0.50
1:C:97:THR:OG1	1:C:220:GLY:HA2	2.11	0.50
1:D:39:LEU:HD23	1:D:313:ARG:HD2	1.94	0.50
1:C:40:VAL:HG22	1:C:314:TRP:CE2	2.47	0.50
1:C:221:MET:CG	1:C:221:MET:CE	2.90	0.50
1:A:115:ASP:OD2	1:A:316:LYS:HD2	2.12	0.50
1:B:266:GLU:HA	2:F:19:TRP:HA	1.92	0.49
1:D:35:GLU:HB3	1:D:316:LYS:HB3	1.92	0.49
1:E:110:GLU:HA	1:E:110:GLU:OE2	2.11	0.49
1:A:191:VAL:HG11	1:A:222:TYR:CE1	2.47	0.49
1:B:35:GLU:HB3	1:B:316:LYS:HB3	1.94	0.49
1:D:144:PRO:HB2	1:D:151:LYS:O	2.13	0.49
1:A:203:ASN:HB2	1:E:70:GLY:O	2.12	0.49
1:E:37:LEU:HD11	1:E:316:LYS:HB2	1.94	0.49
1:C:119:MET:HE2	1:C:315:VAL:HG21	1.95	0.49
1:A:35:GLU:HB3	1:A:316:LYS:HB3	1.93	0.49
1:B:40:VAL:HB	1:B:312:LYS:HB2	1.94	0.49
1:A:39:LEU:HD23	1:A:313:ARG:HD2	1.95	0.48
1:D:305:TYR:OH	1:D:307:LYS:HE2	2.12	0.48
1:E:119:MET:HE2	1:E:315:VAL:HG21	1.95	0.48
1:D:97:THR:OG1	1:D:220:GLY:HA2	2.14	0.48
1:B:40:VAL:HG22	1:B:314:TRP:CE2	2.49	0.48
1:B:137:ASP:OD1	1:B:137:ASP:C	2.51	0.48
1:A:305:TYR:OH	1:A:307:LYS:HE2	2.15	0.47
1:B:121:GLU:OE2	1:B:313:ARG:HD3	2.15	0.47
1:D:40:VAL:HG22	1:D:314:TRP:CE2	2.49	0.47
1:E:115:ASP:OD2	1:E:316:LYS:HD2	2.15	0.47
1:E:137:ASP:C	1:E:137:ASP:OD1	2.53	0.47
1:A:97:THR:OG1	1:A:220:GLY:HA2	2.15	0.47
1:E:176:GLY:HA2	1:E:226:ILE:O	2.15	0.47
1:B:115:ASP:OD2	1:B:316:LYS:HD2	2.15	0.47
2:F:27:LEU:HD12	2:F:28:TYR:CE1	2.50	0.46
1:B:266:GLU:CA	2:F:18:ASP:O	2.62	0.46
1:B:265:ASP:O	2:F:19:TRP:HA	2.15	0.46
1:B:100:MET:HA	1:B:280:LEU:O	2.15	0.46
1:E:40:VAL:HG22	1:E:314:TRP:CE2	2.51	0.46
1:E:144:PRO:HB2	1:E:151:LYS:O	2.16	0.45
1:D:221:MET:CE	1:D:221:MET:CG	2.93	0.45
1:C:110:GLU:OE2	1:C:110:GLU:CA	2.65	0.45
1:C:70:GLY:O	1:D:203:ASN:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:VAL:HG11	1:B:222:TYR:CE1	2.52	0.45
2:F:21:LEU:N	2:F:22:PRO:HD2	2.32	0.45
1:D:127:THR:HA	1:D:305:TYR:O	2.17	0.45
1:C:176:GLY:HA2	1:C:226:ILE:O	2.17	0.45
1:A:121:GLU:OE2	1:A:313:ARG:HD3	2.16	0.45
1:D:153:ILE:HA	1:E:81:LEU:HD21	1.99	0.45
1:B:119:MET:HE2	1:B:315:VAL:HG21	1.97	0.45
1:A:40:VAL:HG22	1:A:314:TRP:CE2	2.52	0.45
1:A:62:THR:HA	1:A:63:PRO:C	2.37	0.45
1:B:110:GLU:OE2	1:B:110:GLU:CA	2.65	0.44
1:B:176:GLY:HA2	1:B:226:ILE:O	2.17	0.44
1:C:144:PRO:HB2	1:C:151:LYS:O	2.18	0.44
1:A:194:LYS:HG3	1:A:199:LYS:O	2.18	0.44
1:D:115:ASP:OD2	1:D:316:LYS:HD2	2.17	0.44
1:A:153:ILE:HA	1:B:81:LEU:HD21	1.99	0.44
1:D:54:ASN:OD1	1:E:207:VAL:HB	2.18	0.44
1:B:65:SER:HB3	1:B:68:GLU:HB2	1.99	0.44
1:D:65:SER:HB3	1:D:68:GLU:HB2	1.99	0.44
1:B:197:THR:O	1:B:198:LYS:CB	2.66	0.44
1:B:221:MET:CG	1:B:221:MET:CE	2.96	0.43
1:C:160:SER:O	1:C:287:GLY:HA2	2.18	0.43
1:E:191:VAL:HG11	1:E:222:TYR:CE1	2.53	0.43
1:C:121:GLU:OE2	1:C:313:ARG:HD3	2.17	0.43
1:C:62:THR:HA	1:C:63:PRO:C	2.38	0.43
1:A:144:PRO:HB2	1:A:151:LYS:O	2.19	0.43
1:E:121:GLU:OE2	1:E:313:ARG:HD3	2.18	0.43
2:F:25:LEU:HA	2:F:25:LEU:HD23	1.89	0.43
1:E:127:THR:HA	1:E:305:TYR:O	2.19	0.43
1:C:115:ASP:OD2	1:C:316:LYS:HD2	2.19	0.43
1:A:70:GLY:O	1:B:203:ASN:HB2	2.18	0.43
1:D:191:VAL:HG11	1:D:222:TYR:CE1	2.54	0.43
1:E:62:THR:HA	1:E:63:PRO:C	2.39	0.43
1:A:137:ASP:OD1	1:A:137:ASP:C	2.55	0.42
1:A:176:GLY:HA2	1:A:226:ILE:O	2.19	0.42
1:A:152:GLY:HA2	1:B:295:ASP:O	2.19	0.42
1:D:62:THR:HA	1:D:63:PRO:C	2.40	0.42
1:C:152:GLY:HA2	1:D:295:ASP:O	2.20	0.42
1:B:62:THR:HA	1:B:63:PRO:C	2.39	0.42
1:B:152:GLY:HA2	1:C:295:ASP:O	2.19	0.42
1:C:204:LYS:HB3	1:C:209:ASN:HB2	2.02	0.41
1:C:100:MET:HA	1:C:280:LEU:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:GLU:CA	1:A:110:GLU:OE2	2.67	0.41
2:F:16:THR:HG21	2:F:24:ILE:HG13	2.02	0.41
1:E:157:VAL:HA	1:E:288:TRP:O	2.20	0.41
1:A:44:ASP:O	1:A:312:LYS:HE3	2.21	0.41
1:E:97:THR:OG1	1:E:220:GLY:HA2	2.20	0.41
1:E:254:GLN:HE22	2:F:12:HIS:CG	2.39	0.41
2:F:21:LEU:O	2:F:25:LEU:HB2	2.20	0.41
1:C:77:ARG:HA	1:C:77:ARG:HD2	1.86	0.41
1:C:77:ARG:HG3	1:C:93:ASN:ND2	2.36	0.41
1:D:152:GLY:HA2	1:E:295:ASP:O	2.20	0.41
1:E:172:LEU:HD12	1:E:234:ASN:OD1	2.20	0.41
1:E:198:LYS:HD3	1:E:198:LYS:HA	1.72	0.41
1:D:44:ASP:O	1:D:312:LYS:HE3	2.21	0.41
1:E:121:GLU:O	1:E:310:LEU:HA	2.21	0.41
1:E:65:SER:HB3	1:E:68:GLU:HB2	2.03	0.41
1:D:107:MET:O	1:D:108:LEU:HD23	2.21	0.40
1:B:170:GLU:HB2	1:B:171:PRO:HD2	2.04	0.40
1:C:198:LYS:HD3	1:C:198:LYS:HA	1.69	0.40
1:D:110:GLU:CA	1:D:110:GLU:OE2	2.69	0.40
1:C:49:ILE:HG23	1:C:49:ILE:HD12	1.74	0.40
1:D:176:GLY:HA2	1:D:226:ILE:O	2.20	0.40
1:A:65:SER:HB3	1:A:68:GLU:HB2	2.02	0.40
1:E:242:ASN:HD22	2:F:7:GLY:CA	2.34	0.40
1:B:105:LEU:HB3	1:B:106:PRO:HD2	2.03	0.40
1:B:172:LEU:HD12	1:B:234:ASN:OD1	2.21	0.40
2:F:21:LEU:HD12	2:F:21:LEU:HA	1.85	0.40
1:C:133:GLY:O	1:D:225:GLU:HA	2.21	0.40
1:E:175:GLN:OE1	1:E:213:LYS:HE2	2.21	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:C:149:ASN:OD1	1:E:186:LYS:NZ[3_564]	2.03	0.17
1:D:147:THR:CG2	1:E:188:GLU:OE2[3_564]	2.07	0.13
1:A:148:VAL:CG2	1:E:211:ILE:CD1[3_564]	2.15	0.05

## 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	281/283 (99%)	271 (96%)	9 (3%)	1 (0%)	39	42
1	B	281/283 (99%)	270 (96%)	11 (4%)	0	100	100
1	C	281/283 (99%)	272 (97%)	9 (3%)	0	100	100
1	D	281/283 (99%)	269 (96%)	12 (4%)	0	100	100
1	E	281/283 (99%)	270 (96%)	11 (4%)	0	100	100
2	F	27/29 (93%)	18 (67%)	5 (18%)	4 (15%)	0	0
All	All	1432/1444 (99%)	1370 (96%)	57 (4%)	5 (0%)	46	50

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	8	GLY
2	F	11	SER
2	F	10	ALA
2	F	23	LEU
1	A	110	GLU

### 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	249/249 (100%)	236 (95%)	13 (5%)	29	33
1	B	249/249 (100%)	236 (95%)	13 (5%)	29	33
1	C	249/249 (100%)	236 (95%)	13 (5%)	29	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	249/249 (100%)	236 (95%)	13 (5%)	29	33
1	E	249/249 (100%)	236 (95%)	13 (5%)	29	33
2	F	17/17 (100%)	13 (76%)	4 (24%)	1	0
All	All	1262/1262 (100%)	1193 (94%)	69 (6%)	27	30

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	MET
1	A	49	ILE
1	A	104	GLN
1	A	107	MET
1	A	110	GLU
1	A	190	VAL
1	A	208	LEU
1	A	238	ARG
1	A	254	GLN
1	A	276	GLU
1	A	289	ARG
1	A	290	VAL
1	A	316	LYS
1	B	34	MET
1	B	49	ILE
1	B	104	GLN
1	B	107	MET
1	B	110	GLU
1	B	190	VAL
1	B	208	LEU
1	B	238	ARG
1	B	254	GLN
1	B	276	GLU
1	B	289	ARG
1	B	290	VAL
1	B	316	LYS
1	C	34	MET
1	C	49	ILE
1	C	104	GLN
1	C	107	MET
1	C	110	GLU
1	C	190	VAL
1	C	208	LEU

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Mol	Chain	Res	Type
1	C	238	ARG
1	C	254	GLN
1	C	276	GLU
1	C	289	ARG
1	C	290	VAL
1	C	316	LYS
1	D	34	MET
1	D	49	ILE
1	D	104	GLN
1	D	107	MET
1	D	110	GLU
1	D	190	VAL
1	D	208	LEU
1	D	238	ARG
1	D	254	GLN
1	D	276	GLU
1	D	289	ARG
1	D	290	VAL
1	D	316	LYS
1	E	34	MET
1	E	49	ILE
1	E	104	GLN
1	E	107	MET
1	E	110	GLU
1	E	190	VAL
1	E	208	LEU
1	E	238	ARG
1	E	254	GLN
1	E	276	GLU
1	E	289	ARG
1	E	290	VAL
1	E	316	LYS
2	F	13	GLN
2	F	14	ARG
2	F	25	LEU
2	F	27	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	242	ASN
1	E	254	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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.