



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 12:48 AM UTC

PDB ID : 4WIC / pdb_00004wic
Title : Immediate-early 1 protein (IE1) of rhesus macaque cytomegalovirus
Authors : Klingl, S.; Scherer, M.; Sevvana, M.; Muller, Y.A.; Stamminger, T.
Deposited on : 2014-09-25
Resolution : 2.85 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

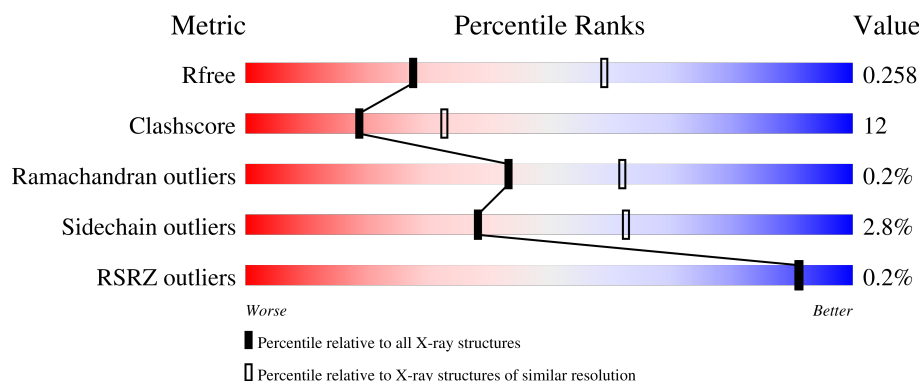
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	365	65% 29% • •
1	B	365	61% 30% • 7%
1	C	365	65% 30% • •
1	D	365	69% 24% • 7%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 11177 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 RhUL123.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	349	Total	C	N	O	S	0	0	0
			2829	1799	477	535	18			
1	B	341	Total	C	N	O	S	0	0	0
			2766	1761	468	519	18			
1	C	349	Total	C	N	O	S	0	0	0
			2829	1799	477	535	18			
1	D	340	Total	C	N	O	S	0	0	0
			2753	1755	464	516	18			

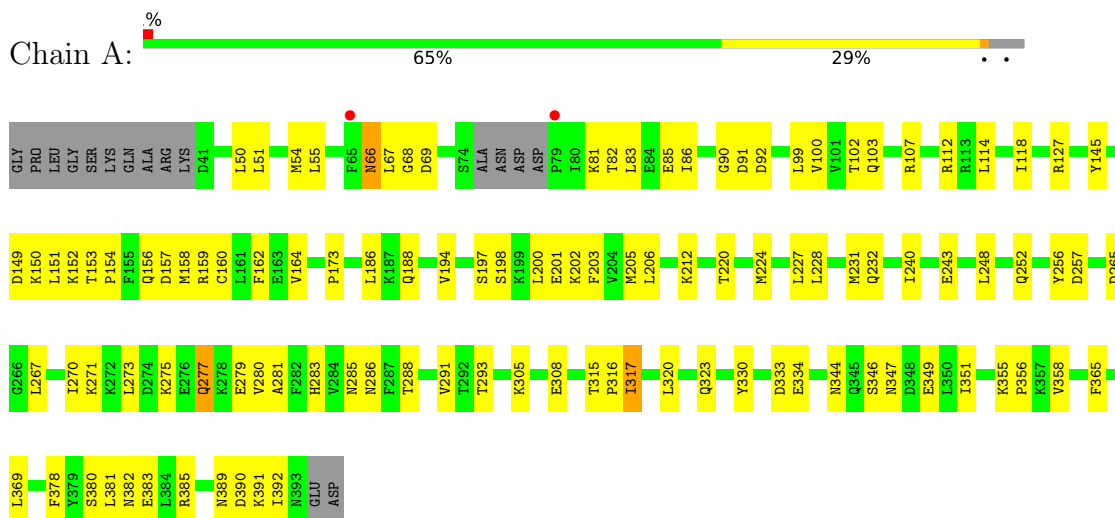
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	31	GLY	-	expression tag	UNP Q2FAE9
A	32	PRO	-	expression tag	UNP Q2FAE9
A	33	LEU	-	expression tag	UNP Q2FAE9
A	34	GLY	-	expression tag	UNP Q2FAE9
A	35	SER	-	expression tag	UNP Q2FAE9
B	31	GLY	-	expression tag	UNP Q2FAE9
B	32	PRO	-	expression tag	UNP Q2FAE9
B	33	LEU	-	expression tag	UNP Q2FAE9
B	34	GLY	-	expression tag	UNP Q2FAE9
B	35	SER	-	expression tag	UNP Q2FAE9
C	31	GLY	-	expression tag	UNP Q2FAE9
C	32	PRO	-	expression tag	UNP Q2FAE9
C	33	LEU	-	expression tag	UNP Q2FAE9
C	34	GLY	-	expression tag	UNP Q2FAE9
C	35	SER	-	expression tag	UNP Q2FAE9
D	31	GLY	-	expression tag	UNP Q2FAE9
D	32	PRO	-	expression tag	UNP Q2FAE9
D	33	LEU	-	expression tag	UNP Q2FAE9
D	34	GLY	-	expression tag	UNP Q2FAE9
D	35	SER	-	expression tag	UNP Q2FAE9

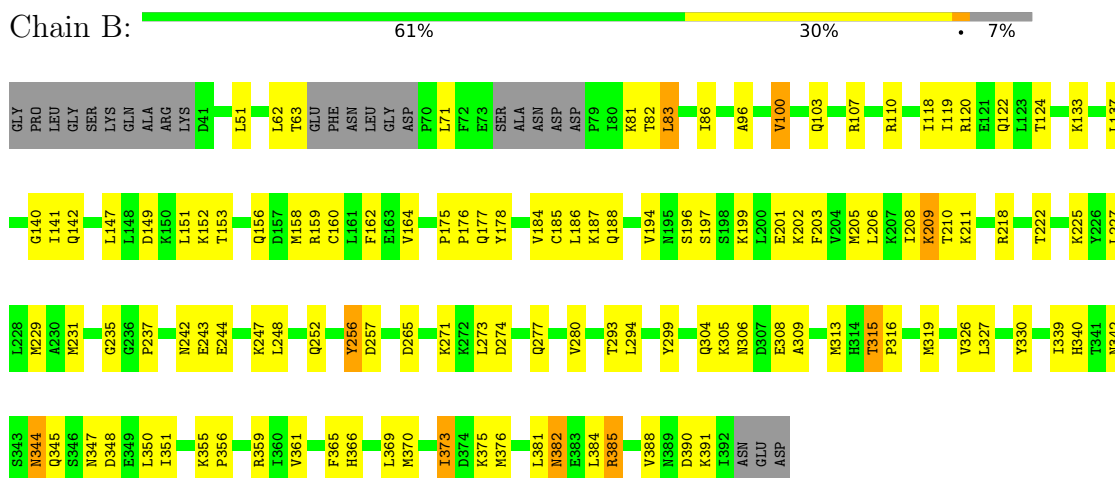
3 Residue-property plots

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: RhUL123

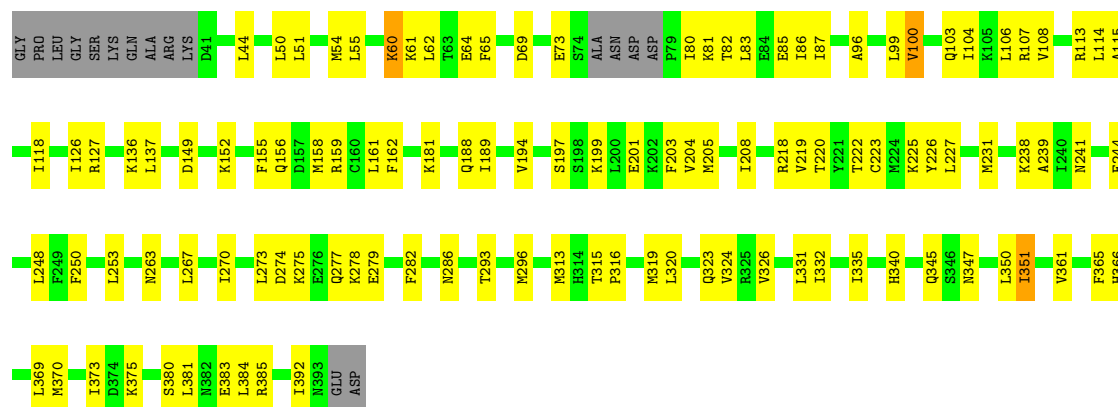


• Molecule 1: RhUL123



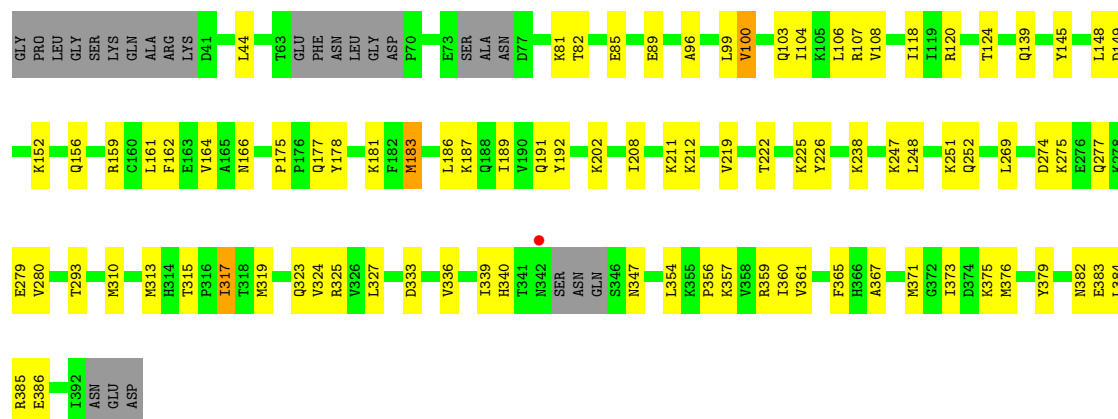
• Molecule 1: RhUL123





• Molecule 1: RhUL123

Chain D: 69% 24% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	57.95Å 278.55Å 61.62Å 90.00° 90.90° 90.00°	Depositor
Resolution (Å)	19.93 – 2.85 19.93 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.93-2.85) 99.5 (19.93-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 2.83Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.212 , 0.259 0.213 , 0.258	Depositor DCC
R_{free} test set	2270 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	70.1	Xtriage
Anisotropy	0.300	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 34.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.044 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11177	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.36% 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	0.66	0/2871	0.99	4/3859 (0.1%)
1	B	0.67	0/2806	1.01	8/3769 (0.2%)
1	C	0.71	1/2871 (0.0%)	1.02	7/3859 (0.2%)
1	D	0.68	0/2792	1.00	0/3750
All	All	0.68	1/11340 (0.0%)	1.00	19/15237 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	351	ILE	CA-CB	-5.19	1.48	1.54

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	69	ASP	CA-C-N	-9.17	111.33	120.31
1	C	69	ASP	C-N-CA	-9.17	111.33	120.31
1	C	392	ILE	N-CA-C	-6.88	106.60	113.20
1	A	305	LYS	N-CA-C	-6.67	104.08	111.82
1	B	305	LYS	N-CA-C	-6.47	104.64	112.54
1	A	392	ILE	N-CA-C	-6.21	107.08	113.10
1	B	344	ASN	N-CA-C	6.16	117.79	111.14
1	B	373	ILE	N-CA-C	-5.67	102.27	109.58
1	B	315	THR	CA-C-N	-5.56	113.19	118.97
1	B	315	THR	C-N-CA	-5.56	113.19	118.97
1	A	344	ASN	N-CA-C	5.53	117.39	111.36
1	A	198	SER	N-CA-C	-5.46	105.43	111.71
1	C	241	ASN	N-CA-C	5.45	116.91	110.97
1	B	256	TYR	N-CA-C	5.42	119.98	112.45
1	C	60	LYS	N-CA-C	-5.38	106.72	113.28
1	B	153	THR	CA-C-N	-5.33	113.42	119.28
1	B	153	THR	C-N-CA	-5.33	113.42	119.28
1	C	204	VAL	N-CA-C	5.05	115.27	110.42
1	C	345	GLN	N-CA-C	5.01	117.56	110.50

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	2829	0	2880	67	0
1	B	2766	0	2830	84	0
1	C	2829	0	2880	72	0
1	D	2753	0	2811	59	0
All	All	11177	0	11401	269	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 12.

All (269) 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:B:81:LYS:O	1:B:107:ARG:NH2	2.10	0.84
1:A:157:ASP:N	1:A:201:GLU:OE2	2.14	0.79
1:D:81:LYS:NZ	1:D:89:GLU:OE2	2.16	0.79
1:A:333:ASP:OD2	1:A:385:ARG:NH1	2.16	0.78
1:C:73:GLU:HG2	1:C:113:ARG:HH22	1.50	0.77
1:D:81:LYS:O	1:D:107:ARG:NH2	2.20	0.74
1:A:240:ILE:HB	1:A:243:GLU:HB3	1.73	0.70
1:B:243:GLU:O	1:B:247:LYS:HG3	1.91	0.70
1:D:333:ASP:CG	1:D:385:ARG:HH11	2.00	0.68
1:D:319:MET:HE2	1:D:376:MET:HA	1.75	0.68
1:A:380:SER:OG	1:A:382:ASN:OD1	2.07	0.68
1:D:148:LEU:HG	1:D:310:MET:HE1	1.77	0.67
1:B:319:MET:HE2	1:B:376:MET:HA	1.76	0.66
1:C:161:LEU:HD23	1:C:324:VAL:HG13	1.77	0.66
1:A:81:LYS:O	1:A:107:ARG:NH2	2.29	0.66
1:B:107:ARG:HB2	1:B:273:LEU:HD23	1.77	0.65
1:A:69:ASP:OD1	1:A:112:ARG:NH2	2.29	0.65
1:A:107:ARG:HB2	1:A:273:LEU:HD23	1.79	0.63
1:D:361:VAL:HG22	1:D:384:LEU:HD22	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:152:LYS:HG2	1:C:205:MET:SD	2.39	0.63
1:A:90:GLY:O	1:A:92:ASP:N	2.32	0.63
1:D:373:ILE:HG13	1:D:375:LYS:H	1.63	0.63
1:B:218:ARG:NH1	1:B:308:GLU:OE1	2.31	0.62
1:C:51:LEU:HA	1:C:227:LEU:HD21	1.80	0.62
1:B:339:ILE:HG22	1:B:340:HIS:HD2	1.62	0.62
1:B:330:TYR:HA	1:B:381:LEU:HD11	1.81	0.61
1:B:304:GLN:O	1:B:308:GLU:HB2	1.99	0.61
1:D:181:LYS:HE3	1:D:347:ASN:OD1	2.00	0.61
1:B:342:ASN:HD22	1:B:345:GLN:HE21	1.48	0.61
1:C:44:LEU:HD21	1:C:219:VAL:HG12	1.83	0.61
1:D:152:LYS:HE3	1:D:156:GLN:HE21	1.65	0.61
1:A:82:THR:O	1:A:86:ILE:HG13	2.00	0.60
1:B:103:GLN:O	1:B:107:ARG:HG3	2.00	0.60
1:A:158:MET:HG3	1:A:197:SER:OG	2.02	0.60
1:D:327:LEU:HD13	1:D:361:VAL:HG11	1.82	0.60
1:B:330:TYR:OH	1:B:388:VAL:HG11	2.02	0.59
1:C:383:GLU:OE2	1:D:238:LYS:NZ	2.36	0.59
1:A:231:MET:HE2	1:A:231:MET:HA	1.85	0.59
1:A:114:LEU:O	1:A:118:ILE:HG23	2.03	0.59
1:A:103:GLN:O	1:A:107:ARG:HG3	2.03	0.58
1:B:62:LEU:HD21	1:B:119:ILE:HG21	1.86	0.58
1:B:96:ALA:O	1:B:100:VAL:HG13	2.03	0.58
1:A:149:ASP:O	1:A:152:LYS:HG2	2.04	0.58
1:B:211:LYS:HG3	1:B:309:ALA:HB1	1.86	0.57
1:C:104:ILE:HD11	1:C:250:PHE:CZ	2.39	0.57
1:B:203:PHE:CZ	1:B:369:LEU:HB3	2.38	0.57
1:B:110:ARG:NH2	1:B:277:GLN:OE1	2.29	0.57
1:A:156:GLN:HB3	1:A:159:ARG:NH1	2.19	0.57
1:B:208:ILE:HD13	1:B:313:MET:HE2	1.85	0.57
1:C:80:ILE:HG12	1:C:106:LEU:HD23	1.85	0.57
1:A:252:GLN:HG2	1:B:340:HIS:CE1	2.40	0.56
1:D:103:GLN:O	1:D:107:ARG:HG3	2.05	0.56
1:B:160:CYS:O	1:B:164:VAL:HG23	2.05	0.56
1:B:199:LYS:HB3	1:B:366:HIS:ND1	2.20	0.56
1:B:149:ASP:O	1:B:152:LYS:HG2	2.06	0.56
1:D:323:GLN:HB3	1:D:365:PHE:CE2	2.41	0.56
1:B:188:GLN:HB2	1:B:351:ILE:HD13	1.87	0.56
1:C:188:GLN:HB2	1:C:351:ILE:HD13	1.88	0.55
1:D:103:GLN:NE2	1:D:106:LEU:HD12	2.21	0.55
1:A:145:TYR:CD1	1:A:212:LYS:HG2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:ASN:HB3	1:B:273:LEU:HD11	1.87	0.55
1:D:104:ILE:HD13	1:D:269:LEU:HD23	1.88	0.55
1:D:192:TYR:OH	1:D:359:ARG:NH1	2.36	0.55
1:B:62:LEU:O	1:B:63:THR:HB	2.06	0.54
1:C:100:VAL:HA	1:C:103:GLN:HB2	1.89	0.54
1:A:54:MET:HE1	1:A:228:LEU:HD21	1.89	0.54
1:C:104:ILE:HG22	1:C:270:ILE:HG13	1.88	0.54
1:B:119:ILE:HG12	1:B:235:GLY:HA2	1.89	0.54
1:B:133:LYS:HG3	1:B:299:TYR:HB2	1.90	0.54
1:C:83:LEU:O	1:C:86:ILE:HG22	2.08	0.53
1:B:382:ASN:HA	1:B:385:ARG:HB3	1.90	0.53
1:C:96:ALA:O	1:C:100:VAL:HG13	2.09	0.53
1:D:315:THR:O	1:D:319:MET:HB2	2.08	0.53
1:C:239:ALA:O	1:D:325:ARG:NH2	2.35	0.53
1:B:248:LEU:O	1:B:252:GLN:HG2	2.09	0.52
1:C:50:LEU:HG	1:C:54:MET:HE2	1.90	0.52
1:C:86:ILE:HG13	1:C:99:LEU:HD23	1.89	0.52
1:C:162:PHE:CZ	1:C:194:VAL:HG21	2.44	0.52
1:A:201:GLU:O	1:A:205:MET:HG2	2.10	0.52
1:C:218:ARG:O	1:C:222:THR:HG23	2.09	0.52
1:A:252:GLN:HG2	1:B:340:HIS:HE1	1.73	0.52
1:B:185:CYS:SG	1:B:347:ASN:HB2	2.50	0.52
1:D:82:THR:HG23	1:D:85:GLU:H	1.74	0.51
1:A:378:PHE:CD2	1:B:237:PRO:HA	2.45	0.51
1:B:162:PHE:CZ	1:B:194:VAL:HG21	2.45	0.51
1:B:342:ASN:OD1	1:B:344:ASN:HB2	2.11	0.51
1:C:107:ARG:NH1	1:C:274:ASP:OD2	2.44	0.51
1:C:149:ASP:O	1:C:152:LYS:HB2	2.10	0.51
1:D:319:MET:HE2	1:D:376:MET:HG2	1.92	0.51
1:C:282:PHE:O	1:C:286:ASN:HB2	2.11	0.51
1:A:232:GLN:NE2	1:B:375:LYS:HA	2.26	0.51
1:A:323:GLN:HB3	1:A:365:PHE:CE2	2.46	0.50
1:A:188:GLN:HB2	1:A:351:ILE:HD13	1.93	0.50
1:C:244:GLU:O	1:C:248:LEU:HB2	2.11	0.50
1:C:115:ALA:O	1:C:118:ILE:HG12	2.11	0.50
1:D:357:LYS:O	1:D:361:VAL:HG23	2.11	0.50
1:A:267:LEU:O	1:A:271:LYS:HG3	2.11	0.49
1:A:275:LYS:O	1:A:279:GLU:HG3	2.12	0.49
1:B:152:LYS:HE3	1:B:156:GLN:HE21	1.78	0.49
1:C:225:LYS:HE2	1:C:226:TYR:CE2	2.47	0.49
1:B:345:GLN:OE1	1:B:350:LEU:HB2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:GLU:OE2	1:B:225:LYS:NZ	2.31	0.49
1:C:158:MET:HG3	1:C:197:SER:OG	2.11	0.49
1:D:178:TYR:HB3	1:D:339:ILE:HD13	1.94	0.49
1:C:323:GLN:HB3	1:C:365:PHE:CE2	2.48	0.49
1:D:356:PRO:O	1:D:360:ILE:HG13	2.12	0.49
1:D:186:LEU:HA	1:D:189:ILE:HG22	1.95	0.48
1:A:380:SER:OG	1:A:383:GLU:HG3	2.13	0.48
1:D:107:ARG:NH1	1:D:274:ASP:OD2	2.46	0.48
1:B:256:TYR:OH	1:B:265:ASP:OD2	2.30	0.48
1:A:99:LEU:O	1:A:102:THR:HG22	2.12	0.48
1:B:347:ASN:OD1	1:B:348:ASP:N	2.47	0.48
1:A:151:LEU:HD23	1:A:317:ILE:HD12	1.95	0.48
1:B:330:TYR:CA	1:B:381:LEU:HD11	2.44	0.48
1:D:82:THR:HG22	1:D:85:GLU:HG3	1.95	0.48
1:D:367:ALA:O	1:D:371:MET:HG2	2.14	0.48
1:B:120:ARG:O	1:B:124:THR:HG23	2.13	0.48
1:B:315:THR:O	1:B:319:MET:HB2	2.14	0.48
1:C:81:LYS:HB3	1:C:85:GLU:OE1	2.14	0.48
1:C:156:GLN:HB2	1:C:159:ARG:NH1	2.29	0.48
1:C:263:ASN:O	1:C:267:LEU:HD13	2.14	0.48
1:D:96:ALA:O	1:D:100:VAL:HG13	2.13	0.48
1:D:183:MET:O	1:D:187:LYS:HG3	2.13	0.48
1:C:340:HIS:CD2	1:D:252:GLN:HG2	2.48	0.48
1:A:390:ASP:OD1	1:A:391:LYS:N	2.47	0.47
1:D:82:THR:CG2	1:D:85:GLU:HG3	2.44	0.47
1:B:229:MET:HE2	1:B:294:LEU:HD21	1.97	0.47
1:B:390:ASP:OD1	1:B:391:LYS:N	2.47	0.47
1:C:326:VAL:HG12	1:C:384:LEU:HD22	1.96	0.47
1:A:55:LEU:HD11	1:A:127:ARG:HB2	1.96	0.47
1:A:107:ARG:CB	1:A:273:LEU:HD23	2.45	0.47
1:D:208:ILE:HG12	1:D:313:MET:HE2	1.97	0.47
1:A:355:LYS:HB2	1:A:356:PRO:HD3	1.96	0.47
1:B:152:LYS:HD2	1:B:205:MET:SD	2.55	0.47
1:C:203:PHE:HD2	1:C:370:MET:HE2	1.80	0.47
1:A:51:LEU:HD13	1:A:227:LEU:HD11	1.96	0.47
1:A:389:ASN:HD22	1:A:389:ASN:C	2.23	0.47
1:B:82:THR:O	1:B:86:ILE:HG13	2.15	0.47
1:B:158:MET:HG3	1:B:197:SER:OG	2.14	0.47
1:B:201:GLU:O	1:B:205:MET:HG2	2.14	0.47
1:B:218:ARG:O	1:B:222:THR:HG23	2.15	0.47
1:D:149:ASP:O	1:D:152:LYS:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:247:LYS:O	1:D:251:LYS:HB2	2.15	0.47
1:B:137:LEU:O	1:B:141:ILE:HG13	2.15	0.46
1:D:159:ARG:HA	1:D:162:PHE:HD2	1.80	0.46
1:C:315:THR:OG1	1:C:316:PRO:HD3	2.15	0.46
1:D:313:MET:O	1:D:317:ILE:HG22	2.15	0.46
1:D:365:PHE:HE1	1:D:379:TYR:CD2	2.32	0.46
1:B:184:VAL:O	1:B:188:GLN:HG3	2.16	0.46
1:C:361:VAL:HG13	1:C:384:LEU:HD11	1.97	0.46
1:D:339:ILE:HG22	1:D:340:HIS:HD2	1.80	0.46
1:A:152:LYS:HB2	1:A:205:MET:SD	2.56	0.46
1:B:51:LEU:HA	1:B:227:LEU:HD21	1.98	0.46
1:D:81:LYS:N	1:D:103:GLN:OE1	2.41	0.46
1:B:209:LYS:HG3	1:B:210:THR:N	2.28	0.46
1:C:275:LYS:O	1:C:279:GLU:HG3	2.16	0.46
1:B:175:PRO:HA	1:B:176:PRO:HD3	1.85	0.46
1:C:315:THR:O	1:C:319:MET:HB2	2.15	0.46
1:D:120:ARG:O	1:D:124:THR:HG23	2.15	0.46
1:A:267:LEU:O	1:A:270:ILE:HB	2.16	0.46
1:C:156:GLN:HB2	1:C:159:ARG:HH12	1.80	0.46
1:B:140:GLY:C	1:B:306:ASN:HD21	2.24	0.45
1:C:203:PHE:CZ	1:C:369:LEU:HB3	2.52	0.45
1:B:231:MET:HE2	1:B:231:MET:HA	1.97	0.45
1:C:60:LYS:O	1:C:64:GLU:HG2	2.15	0.45
1:C:86:ILE:HG13	1:C:99:LEU:CD2	2.45	0.45
1:D:161:LEU:HD23	1:D:161:LEU:HA	1.85	0.45
1:C:108:VAL:HG12	1:C:273:LEU:HD21	1.98	0.45
1:D:361:VAL:HG13	1:D:384:LEU:HD21	1.98	0.45
1:A:315:THR:OG1	1:A:316:PRO:HD3	2.17	0.45
1:B:277:GLN:O	1:B:277:GLN:HG2	2.16	0.45
1:C:155:PHE:CE1	1:C:320:LEU:HD23	2.51	0.45
1:A:54:MET:SD	1:A:231:MET:HG3	2.57	0.45
1:A:281:ALA:O	1:A:285:ASN:ND2	2.42	0.45
1:B:327:LEU:HD13	1:B:361:VAL:HG21	1.98	0.45
1:D:382:ASN:O	1:D:386:GLU:HG2	2.16	0.45
1:A:330:TYR:O	1:A:334:GLU:HG2	2.16	0.45
1:D:145:TYR:CD1	1:D:212:LYS:HG2	2.52	0.45
1:A:173:PRO:O	1:B:252:GLN:NE2	2.50	0.45
1:B:203:PHE:HD1	1:B:370:MET:HE3	1.82	0.45
1:C:380:SER:OG	1:C:383:GLU:HG3	2.17	0.45
1:C:107:ARG:NH1	1:C:270:ILE:HG23	2.32	0.44
1:C:181:LYS:HE3	1:C:347:ASN:OD1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:LEU:HD13	1:B:271:LYS:HG2	1.99	0.44
1:B:107:ARG:NH1	1:B:274:ASP:OD1	2.50	0.44
1:B:339:ILE:HG22	1:B:340:HIS:CD2	2.48	0.44
1:B:365:PHE:O	1:B:369:LEU:HD13	2.18	0.44
1:C:61:LYS:O	1:C:65:PHE:HB3	2.17	0.44
1:A:381:LEU:HD12	1:B:244:GLU:CD	2.42	0.44
1:B:206:LEU:HD22	1:B:209:LYS:HG2	1.99	0.44
1:C:189:ILE:HD12	1:C:189:ILE:HA	1.82	0.44
1:B:202:LYS:HA	1:B:202:LYS:HD3	1.65	0.44
1:C:199:LYS:HG2	1:C:366:HIS:ND1	2.32	0.44
1:A:277:GLN:O	1:A:280:VAL:HG12	2.18	0.44
1:A:320:LEU:HD13	1:A:369:LEU:HD11	2.00	0.44
1:B:196:SER:O	1:B:196:SER:OG	2.34	0.44
1:A:280:VAL:HG13	1:A:281:ALA:N	2.33	0.44
1:D:354:LEU:HD23	1:D:357:LYS:HD2	1.99	0.44
1:A:82:THR:HG22	1:A:85:GLU:CD	2.43	0.43
1:C:114:LEU:HD21	1:C:277:GLN:HG3	2.00	0.43
1:A:256:TYR:OH	1:A:265:ASP:OD2	2.31	0.43
1:B:355:LYS:HB2	1:B:356:PRO:HD3	2.01	0.43
1:C:373:ILE:C	1:C:375:LYS:H	2.26	0.43
1:D:175:PRO:HG2	1:D:178:TYR:HD2	1.83	0.43
1:D:225:LYS:HE2	1:D:226:TYR:CE1	2.53	0.43
1:A:50:LEU:HD23	1:A:224:MET:HG2	2.01	0.42
1:A:162:PHE:CZ	1:A:194:VAL:HG21	2.54	0.42
1:A:206:LEU:HA	1:A:206:LEU:HD12	1.81	0.42
1:A:55:LEU:CD1	1:A:127:ARG:HB2	2.49	0.42
1:B:256:TYR:O	1:B:257:ASP:HB2	2.19	0.42
1:C:320:LEU:HD13	1:C:369:LEU:HD11	2.01	0.42
1:C:381:LEU:O	1:C:385:ARG:N	2.49	0.42
1:D:354:LEU:O	1:D:357:LYS:N	2.52	0.42
1:A:186:LEU:HD12	1:A:186:LEU:HA	1.86	0.42
1:B:71:LEU:HB3	1:D:166:ASN:OD1	2.19	0.42
1:A:153:THR:OG1	1:A:154:PRO:HD3	2.19	0.42
1:B:356:PRO:HA	1:B:359:ARG:CZ	2.49	0.42
1:D:44:LEU:HD21	1:D:219:VAL:HG12	2.00	0.42
1:A:67:LEU:O	1:A:69:ASP:N	2.53	0.42
1:C:253:LEU:HD23	1:C:253:LEU:HA	1.88	0.42
1:C:136:LYS:HB2	1:C:136:LYS:HE3	1.78	0.42
1:A:346:SER:OG	1:A:349:GLU:HG3	2.20	0.42
1:D:161:LEU:HD23	1:D:324:VAL:HG13	2.01	0.42
1:D:164:VAL:HG11	1:D:325:ARG:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:LEU:HD23	1:A:381:LEU:HA	1.76	0.42
1:C:107:ARG:NH1	1:C:274:ASP:CG	2.78	0.42
1:C:126:ILE:HG21	1:C:231:MET:HE2	2.00	0.42
1:D:187:LYS:O	1:D:191:GLN:HB2	2.20	0.41
1:B:186:LEU:O	1:B:187:LYS:C	2.63	0.41
1:C:62:LEU:HA	1:C:65:PHE:CD1	2.55	0.41
1:C:82:THR:OG1	1:C:83:LEU:N	2.54	0.41
1:C:189:ILE:HG21	1:C:335:ILE:HD11	2.01	0.41
1:C:332:ILE:HG22	1:D:248:LEU:HD21	2.02	0.41
1:A:203:PHE:CE2	1:A:369:LEU:HB3	2.55	0.41
1:B:118:ILE:O	1:B:122:GLN:HG3	2.20	0.41
1:C:55:LEU:CD1	1:C:127:ARG:HB2	2.51	0.41
1:B:315:THR:OG1	1:B:316:PRO:HD3	2.21	0.41
1:D:99:LEU:HD12	1:D:99:LEU:HA	1.76	0.41
1:C:201:GLU:O	1:C:205:MET:HG2	2.20	0.41
1:B:326:VAL:HG12	1:B:384:LEU:HD22	2.03	0.41
1:C:323:GLN:HB3	1:C:365:PHE:CD2	2.56	0.41
1:B:381:LEU:HD12	1:B:381:LEU:HA	1.74	0.41
1:A:248:LEU:HD12	1:A:248:LEU:HA	1.84	0.41
1:A:66:ASN:OD1	1:A:66:ASN:N	2.51	0.41
1:A:83:LEU:HD12	1:A:267:LEU:HD22	2.03	0.41
1:A:200:LEU:HA	1:A:200:LEU:HD23	1.78	0.41
1:B:83:LEU:CD1	1:B:271:LYS:HG2	2.51	0.41
1:B:156:GLN:O	1:B:159:ARG:NH1	2.54	0.41
1:B:177:GLN:HG2	1:B:178:TYR:CD1	2.56	0.41
1:B:208:ILE:CD1	1:B:313:MET:HE2	2.50	0.41
1:C:208:ILE:HA	1:C:313:MET:CE	2.50	0.41
1:C:220:THR:O	1:C:223:CYS:HB2	2.21	0.41
1:C:238:LYS:NZ	1:D:383:GLU:OE2	2.53	0.41
1:C:331:LEU:HA	1:C:331:LEU:HD23	1.86	0.41
1:D:177:GLN:HG2	1:D:178:TYR:CD2	2.56	0.41
1:A:283:HIS:HA	1:A:286:ASN:HB2	2.03	0.40
1:A:288:THR:HA	1:A:291:VAL:HG12	2.03	0.40
1:B:208:ILE:HD13	1:B:208:ILE:HA	1.91	0.40
1:B:327:LEU:CD1	1:B:361:VAL:HG21	2.51	0.40
1:C:104:ILE:HD11	1:C:250:PHE:CE1	2.56	0.40
1:A:160:CYS:O	1:A:164:VAL:HG23	2.21	0.40
1:B:147:LEU:O	1:B:151:LEU:HD13	2.21	0.40
1:C:275:LYS:HA	1:C:278:LYS:NZ	2.36	0.40
1:C:296:MET:HE2	1:C:296:MET:HB2	1.92	0.40
1:D:275:LYS:O	1:D:279:GLU:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:ASN:O	1:A:351:ILE:HG13	2.22	0.40
1:C:100:VAL:HG11	1:C:267:LEU:HD11	2.02	0.40
1:C:137:LEU:HD23	1:C:137:LEU:HA	1.92	0.40
1:D:248:LEU:HD12	1:D:248:LEU:HA	1.77	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	345/365 (94%)	339 (98%)	3 (1%)	3 (1%)	14	28
1	B	335/365 (92%)	330 (98%)	5 (2%)	0	100	100
1	C	345/365 (94%)	338 (98%)	7 (2%)	0	100	100
1	D	332/365 (91%)	327 (98%)	5 (2%)	0	100	100
All	All	1357/1460 (93%)	1334 (98%)	20 (2%)	3 (0%)	43	62

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	68	GLY
1	A	91	ASP
1	A	257	ASP

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	319/332 (96%)	310 (97%)	9 (3%)	38	62
1	B	312/332 (94%)	303 (97%)	9 (3%)	37	61
1	C	319/332 (96%)	315 (99%)	4 (1%)	61	79
1	D	309/332 (93%)	296 (96%)	13 (4%)	26	51
All	All	1259/1328 (95%)	1224 (97%)	35 (3%)	38	62

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	ASN
1	A	100	VAL
1	A	150	LYS
1	A	202	LYS
1	A	220	THR
1	A	277	GLN
1	A	293	THR
1	A	317	ILE
1	A	358	VAL
1	B	83	LEU
1	B	100	VAL
1	B	142	GLN
1	B	209	LYS
1	B	280	VAL
1	B	293	THR
1	B	373	ILE
1	B	382	ASN
1	B	385	ARG
1	C	87	ILE
1	C	100	VAL
1	C	293	THR
1	C	350	LEU
1	D	100	VAL
1	D	108	VAL
1	D	118	ILE
1	D	139	GLN
1	D	183	MET
1	D	202	LYS
1	D	211	LYS
1	D	222	THR
1	D	277	GLN

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Mol	Chain	Res	Type
1	D	280	VAL
1	D	293	THR
1	D	317	ILE
1	D	336	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	232	GLN
1	A	286	ASN
1	A	337	HIS
1	A	344	ASN
1	B	156	GLN
1	B	306	ASN
1	B	340	HIS
1	B	344	ASN
1	B	345	GLN
1	C	103	GLN
1	D	156	GLN
1	D	337	HIS

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

There are no such residues in this entry.

5.8 Polymer linkage issues

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	349/365 (95%)	-0.36	2 (0%) 85 82	43, 74, 114, 137	0
1	B	341/365 (93%)	-0.34	0 100 100	45, 77, 108, 131	0
1	C	349/365 (95%)	-0.46	0 100 100	33, 64, 120, 137	0
1	D	340/365 (93%)	-0.35	1 (0%) 90 89	35, 74, 119, 133	0
All	All	1379/1460 (94%)	-0.38	3 (0%) 91 91	33, 72, 117, 137	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	65	PHE	2.7
1	A	79	PRO	2.3
1	D	342	ASN	2.1

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.