Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 07:46 PM GMT

PDB ID	:	4WIC
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)

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

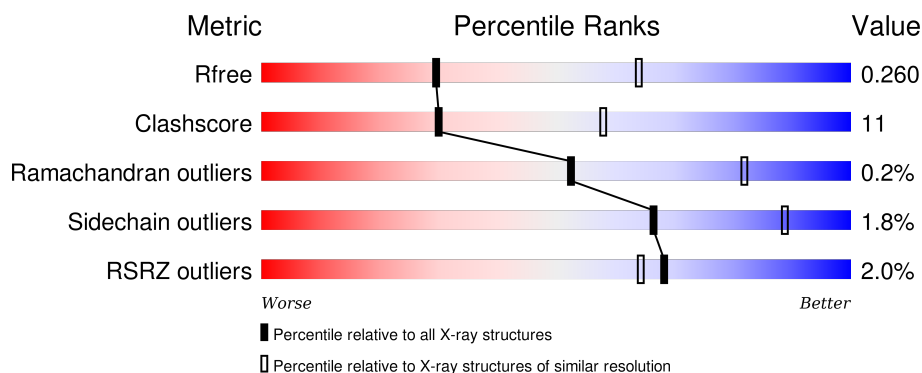|		
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

1 Overall quality at a glance (i)

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	Percentile Ranks	Value
Rfree		0.260
Clashscore		11
Ramachandran outliers		0.2%
Sidechain outliers		1.8%
RSRZ outliers		2.0%

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}	91344	2228 (2.90-2.82)
Clashscore	102246	2499 (2.90-2.82)
Ramachandran outliers	100387	2439 (2.90-2.82)
Sidechain outliers	100360	2442 (2.90-2.82)
RSRZ outliers	91569	2236 (2.90-2.82)

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 >=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 <=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	3% / 69% / 26% / · ·
1	B	365	2% / 64% / 28% / · 7%
1	C	365	% / 68% / 27% / · ·
1	D	365	2% / 71% / 22% / 7%

2 Entry composition (i)

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.

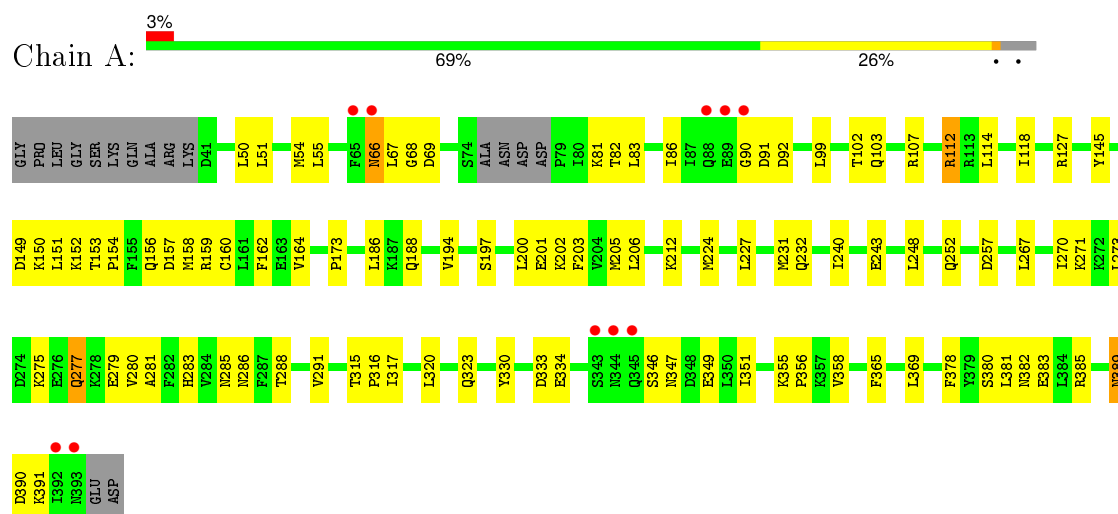| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	349	Total 2829	C 1799	N 477	O 535	S 18	0	0	0
1	B	341	Total 2766	C 1761	N 468	O 519	S 18	0	0	0
1	C	349	Total 2829	C 1799	N 477	O 535	S 18	0	0	0
1	D	340	Total 2753	C 1755	N 464	O 516	S 18	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

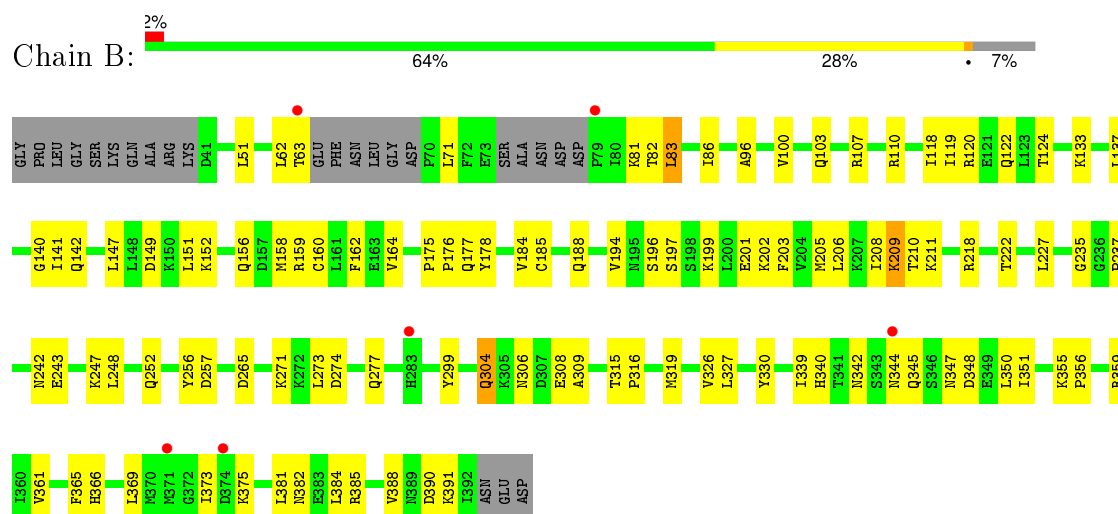| Chain	Residue	Modelled	Actual	Comment	Reference
A	31	GLY	-	expression tag	UNP Q2FAE9
A	32	PRO	-	expression tag	UNP Q2FAE9
A	33	LEU	-	expression tag	UNP Q2FAE9
A	34	GLY	-	expression tag	UNP Q2FAE9
A	35	SER	-	expression tag	UNP Q2FAE9
B	31	GLY	-	expression tag	UNP Q2FAE9
B	32	PRO	-	expression tag	UNP 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 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.
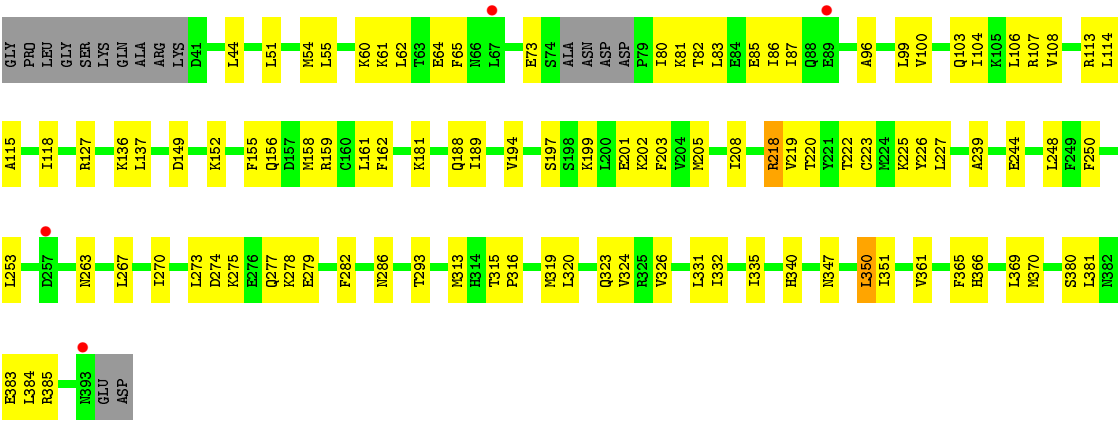
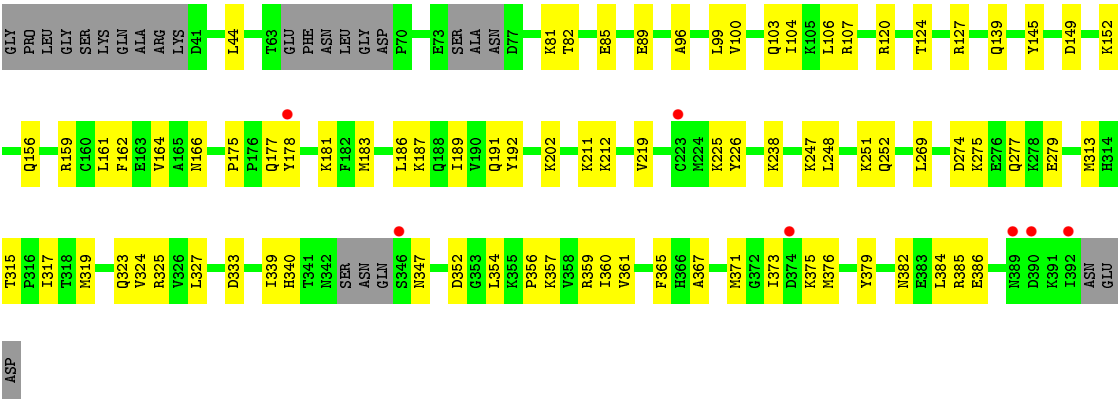- Molecule 1: RhUL123

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GLY PRO LEU GLY SER LYS GLN ALA ARG LYS D41 L44 L51 M54 L55 K60 K61 L62 T63 E64 F65 N66 L67 E73 S74 ALA ASN ASP P79 I80 K81 T82 L83 E84 E85 I86 I87 Q88 E89 A96 L99 V100 Q103 I104 K105 L106 R107 V108 R113 L114

A115 I118 R127 K136 L137 D149 K152 F155 Q156 D157 M158 R159 C160 L161 F162 K181 Q188 I189 V194 S197 S198 K199 L200 E201 K202 F203 V204 M205 I208 R218 V219 T220 Y221 T222 C223 M224 K225 Y226 L227 A239 E244 L248 F249 F250

L253 D257 N263 L267 I270 L273 D274 K275 E276 Q277 K278 E279 F282 N286 T293 M313 H314 T315 P316 M319 L320 Q323 V324 R325 V326 L331 I332 I335 H340 N347 L350 I351 V361 F365 H366 L369 M370 S380 L381 N382

E383 L384 R385 N393 GLU ASP

● **Molecule 1: RhUL123**

Chain D:

2%
71% 22% 7%

GLY PRO LEU GLY SER LYS GLN ALA ARG LYS D41 L44 T63 GLU PHE ASN LEU GLY ASP P70 E73 SER ALA ASN D77 K81 T82 E85 E89 A96 L99 V100 Q103 I104 K105 L106 R107 R120 T124 R127 Q139 Y145 D149 K152

Q156 R159 C160 L161 F162 E163 V164 A165 N166 P175 P176 Q177 Y178 K181 F182 M183 L186 K187 Q188 I189 V190 Q191 Y192 K202 K211 K212 V219 C223 M224 K225 Y226 K238 K247 L248 K251 Q252 L269 D274 K275 E276 Q277 K278 E279 M313 H314

T315 P316 I317 T318 M319 Q323 V324 R325 V326 L327 D333 I339 H340 T341 N342 SER ASN GLN S346 N347 D352 G353 L354 K355 P356 K357 V358 R359 I360 V361 F365 H366 A367 M371 G372 I373 D374 K375 M376 Y379 N382 E383 L384 R385 E386 N389 D390 K391 I392 ASN GLU

ASP

4   Data and refinement statistics (i)

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) 99.8 (19.93-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.08 (at 2.83Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.212 , 0.259 0.212 , 0.260	Depositor DCC
R_{free} test set	2269 reflections (5.03%)	DCC
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 , 44.2	EDS
Estimated twinning fraction	0.044 for h,-k,-l	Xtriage
L-test for twinning[2]	$<|L|> = 0.48$, $<L^2> = 0.31$	Xtriage
Outliers	0 of 45137 reflections	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.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.49	0/2871	0.65	0/3859
1	B	0.51	0/2806	0.69	0/3769
1	C	0.54	0/2871	0.70	1/3859 (0.0%)
1	D	0.52	0/2792	0.71	0/3750
All	All	0.52	0/11340	0.69	1/15237 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	350	LEU	CA-CB-CG	5.20	127.25	115.30

There are no chirality outliers.

There are no planarity outliers.

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	2829	0	2880	61	0
1	B	2766	0	2830	75	0
1	C	2829	0	2880	68	0
1	D	2753	0	2811	57	0
All	All	11177	0	11401	251	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 11.

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All (251) 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:A:380:SER:OG	1:A:382:ASN:OD1	2.07	0.68
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:D:333:ASP:CG	1:D:385:ARG:HH11	2.00	0.64
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
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:D:152:LYS:HE3	1:D:156:GLN:HE21	1.65	0.61
1:C:44:LEU:HD21	1:C:219:VAL:HG12	1.83	0.61
1:B:103:GLN:O	1:B:107:ARG:HG3	2.00	0.60
1:A:82:THR:O	1:A:86:ILE:HG13	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: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:96:ALA:O	1:B:100:VAL:HG13	2.03	0.58
1:B:62:LEU:HD21	1:B:119:ILE:HG21	1.86	0.58
1:A:149:ASP:O	1:A:152:LYS:HG2	2.04	0.58
1:C:104:ILE:HD11	1:C:250:PHE:CZ	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:LYS:HG3	1:B:309:ALA:HB1	1.86	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:C:80:ILE:HG12	1:C:106:LEU:HD23	1.85	0.57
1:D:103:GLN:O	1:D:107:ARG:HG3	2.05	0.56
1:A:252:GLN:HG2	1:B:340:HIS:CE1	2.40	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
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: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:D:319:MET:HE2	1:D:376:MET:HG2	1.90	0.54
1:C:83:LEU:O	1:C:86:ILE:HG22	2.08	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:B:382:ASN:HA	1:B:385:ARG:HB3	1.90	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: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:B:162:PHE:CZ	1:B:194:VAL:HG21	2.45	0.51
1:A:378:PHE:CD2	1:B:237:PRO:HA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:ASP:O	1:C:152:LYS:HB2	2.10	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: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:A:275:LYS:O	1:A:279:GLU:HG3	2.12	0.49
1:B:345:GLN:OE1	1:B:350:LEU:HB2	2.11	0.49
1:D:178:TYR:HB3	1:D:339:ILE:HD13	1.94	0.49
1:C:158:MET:HG3	1:C:197:SER:OG	2.11	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:D:107:ARG:NH1	1:D:274:ASP:OD2	2.46	0.48
1:A:380:SER:OG	1:A:383:GLU:HG3	2.13	0.48
1:B:256:TYR:OH	1:B:265:ASP:OD2	2.30	0.48
1:B:347:ASN:OD1	1:B:348:ASP:N	2.47	0.48
1:A:99:LEU:O	1:A:102:THR:HG22	2.12	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:A:151:LEU:HD23	1:A:317:ILE:HD12	1.95	0.48
1:D:367:ALA:O	1:D:371:MET:HG2	2.14	0.48
1:C:263:ASN:O	1:C:267:LEU:HD13	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:D:183:MET:O	1:D:187:LYS:HG3	2.13	0.48
1:D:96:ALA:O	1:D:100:VAL:HG13	2.13	0.48
1:C:340:HIS:CD2	1:D:252:GLN:HG2	2.48	0.48
1:D:82:THR:CG2	1:D:85:GLU:HG3	2.44	0.47
1:A:390:ASP:OD1	1:A:391:LYS:N	2.47	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:107:ARG:CB	1:A:273:LEU:HD23	2.45	0.47
1:A:55:LEU:HD11	1:A:127:ARG:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:LYS:HD2	1:B:205:MET:SD	2.55	0.47
1:A:355:LYS:HB2	1:A:356:PRO:HD3	1.96	0.47
1:A:51:LEU:HD13	1:A:227:LEU:HD11	1.96	0.47
1:B:201:GLU:O	1:B:205:MET:HG2	2.14	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: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
1:D:247:LYS:O	1:D:251:LYS:HB2	2.15	0.47
1:D:159:ARG:HA	1:D:162:PHE:HD2	1.80	0.46
1:B:137:LEU:O	1:B:141:ILE:HG13	2.15	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:C:54:MET:HE1	1:C:227:LEU:HG	1.98	0.46
1:B:184:VAL:O	1:B:188:GLN:HG3	2.16	0.46
1:D:339:ILE:HG22	1:D:340:HIS:HD2	1.80	0.46
1:C:361:VAL:HG13	1:C:384:LEU:HD11	1.97	0.46
1:A:152:LYS:HB2	1:A:205:MET:SD	2.56	0.46
1:D:81:LYS:N	1:D:103:GLN:OE1	2.41	0.46
1:B:51:LEU:HA	1:B:227:LEU:HD21	1.98	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: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:B:175:PRO:HA	1:B:176:PRO:HD3	1.85	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:C:203:PHE:CZ	1:C:369:LEU:HB3	2.52	0.45
1:C:86:ILE:HG13	1:C:99:LEU:CD2	2.45	0.45
1:D:161:LEU:HA	1:D:161:LEU:HD23	1.85	0.45
1:C:60:LYS:O	1:C:64:GLU:HG2	2.15	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:B:277:GLN:HG2	1:B:277:GLN:O	2.16	0.45
1:A:315:THR:OG1	1:A:316:PRO:HD3	2.17	0.45
1:C:155:PHE:CE1	1:C:320:LEU:HD23	2.51	0.45
1:D:319:MET:HE1	1:D:376:MET:HA	1.98	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:A:54:MET:SD	1:A:231:MET:HG3	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:380:SER:OG	1:C:383:GLU:HG3	2.17	0.45
1:A:173:PRO:O	1:B:252:GLN:NE2	2.50	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
1:D:319:MET:CE	1:D:376:MET:HA	2.47	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:203:PHE:HD2	1:C:370:MET:HE2	1.82	0.44
1:C:61:LYS:O	1:C:65:PHE:HB3	2.17	0.44
1:B:83:LEU:HD13	1:B:271:LYS:HG2	1.99	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:C:199:LYS:HG2	1:C:366:HIS:ND1	2.32	0.44
1:B:202:LYS:HD3	1:B:202:LYS:HA	1.65	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:D:354:LEU:HD23	1:D:357:LYS:HD2	1.99	0.44
1:A:280:VAL:HG13	1:A:281:ALA:N	2.33	0.44
1:C:208:ILE:HA	1:C:313:MET:HE3	2.00	0.43
1:C:114:LEU:HD21	1:C:277:GLN:HG3	2.00	0.43
1:B:355:LYS:HB2	1:B:356:PRO:HD3	2.01	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: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:50:LEU:HD23	1:A:224:MET:HG2	2.01	0.42
1:D:354:LEU:O	1:D:357:LYS:N	2.52	0.42
1:B:256:TYR:O	1:B:257:ASP:HB2	2.19	0.42
1:A:55:LEU:CD1	1:A:127:ARG:HB2	2.49	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: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:B:356:PRO:HA	1:B:359:ARG:CZ	2.49	0.42
1:A:153:THR:OG1	1:A:154:PRO:HD3	2.19	0.42
1:D:44:LEU:HD21	1:D:219:VAL:HG12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:LEU:O	1:A:69:ASP:N	2.53	0.42
1:A:389:ASN:HD22	1:A:389:ASN:C	2.23	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:D:164:VAL:HG11	1:D:325:ARG:HA	2.02	0.42
1:D:161:LEU:HD23	1:D:324:VAL:HG13	2.01	0.42
1:A:346:SER:OG	1:A:349:GLU:HG3	2.20	0.42
1:A:381:LEU:HD23	1:A:381:LEU:HA	1.76	0.42
1:D:187:LYS:O	1:D:191:GLN:HB2	2.20	0.41
1:C:82:THR:OG1	1:C:83:LEU:N	2.54	0.41
1:C:62:LEU:HA	1:C:65:PHE:CD1	2.55	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:C:55:LEU:CD1	1:C:127:ARG:HB2	2.51	0.41
1:B:118:ILE:O	1:B:122:GLN:HG3	2.20	0.41
1:B:315:THR:OG1	1:B:316:PRO:HD3	2.21	0.41
1:D:99:LEU:HA	1:D:99:LEU:HD12	1.76	0.41
1:C:201:GLU:O	1:C:205:MET:HG2	2.20	0.41
1:C:323:GLN:HB3	1:C:365:PHE:CD2	2.56	0.41
1:B:326:VAL:HG12	1:B:384:LEU:HD22	2.03	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:B:140:GLY:C	1:B:306:ASN:HD21	2.24	0.41
1:B:156:GLN:O	1:B:159:ARG:NH1	2.54	0.41
1:A:83:LEU:HD12	1:A:267:LEU:HD22	2.03	0.41
1:B:83:LEU:CD1	1:B:271:LYS:HG2	2.51	0.41
1:C:208:ILE:HA	1:C:313:MET:CE	2.50	0.41
1:A:200:LEU:HD23	1:A:200:LEU:HA	1.78	0.41
1:B:177:GLN:HG2	1:B:178:TYR:CD1	2.56	0.41
1:A:66:ASN:OD1	1:A:66:ASN:N	2.51	0.41
1:C:220:THR:O	1:C:223:CYS:HB2	2.21	0.41
1:D:177:GLN:HG2	1:D:178:TYR:CD2	2.56	0.41
1:C:331:LEU:HD23	1:C:331:LEU:HA	1.86	0.41
1:B:327:LEU:CD1	1:B:361:VAL:HG21	2.51	0.40
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:HA	1:B:208:ILE:HD13	1.91	0.40
1:C:104:ILE:HD11	1:C:250:PHE:CE1	2.56	0.40
1:B:147:LEU:O	1:B:151:LEU:HD13	2.21	0.40
1:A:160:CYS:O	1:A:164:VAL:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:275:LYS:HA	1:C:278:LYS:NZ	2.36	0.40
1:D:275:LYS:O	1:D:279:GLU:HG3	2.21	0.40
1:C:100:VAL:HG11	1:C:267:LEU:HD11	2.02	0.40
1:A:347:ASN:O	1:A:351:ILE:HG13	2.22	0.40
1:D:248:LEU:HD12	1:D:248:LEU:HA	1.77	0.40
1:C:137:LEU:HD23	1:C:137:LEU:HA	1.92	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%)	21	52
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%)	52	82

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%)	312 (98%)	7 (2%)	60	86
1	B	312/332 (94%)	307 (98%)	5 (2%)	70	90
1	C	319/332 (96%)	314 (98%)	5 (2%)	70	90
1	D	309/332 (93%)	303 (98%)	6 (2%)	65	88
All	All	1259/1328 (95%)	1236 (98%)	23 (2%)	66	89

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	ASN
1	A	112	ARG
1	A	150	LYS
1	A	202	LYS
1	A	277	GLN
1	A	358	VAL
1	A	389	ASN
1	B	83	LEU
1	B	142	GLN
1	B	209	LYS
1	B	304	GLN
1	B	373	ILE
1	C	87	ILE
1	C	202	LYS
1	C	218	ARG
1	C	293	THR
1	C	350	LEU
1	D	127	ARG
1	D	139	GLN
1	D	202	LYS
1	D	211	LYS
1	D	277	GLN
1	D	352	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	252	GLN
1	B	340	HIS

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Mol	Chain	Res	Type
1	B	345	GLN
1	D	156	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 (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%)	-0.10	10 (2%)	55	49	43, 74, 114, 137	0
1	B	341/365 (93%)	-0.07	6 (1%)	71	68	45, 77, 108, 131	0
1	C	349/365 (95%)	-0.18	4 (1%)	82	80	33, 64, 120, 137	0
1	D	340/365 (93%)	-0.09	7 (2%)	67	62	35, 74, 119, 133	0
All	All	1379/1460 (94%)	-0.11	27 (1%)	68	64	33, 72, 117, 137	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	344	ASN	3.8
1	A	343	SER	3.8
1	D	389	ASN	3.4
1	C	89	GLU	3.3
1	A	89	GLU	3.2
1	C	393	ASN	3.1
1	A	66	ASN	2.9
1	D	346	SER	2.7
1	A	65	PHE	2.6
1	A	392	ILE	2.5
1	B	283	HIS	2.5
1	C	67	LEU	2.4
1	A	345	GLN	2.3
1	D	374	ASP	2.2
1	D	390	ASP	2.1
1	B	344	ASN	2.1
1	D	223	CYS	2.1
1	D	392	ILE	2.1
1	C	257	ASP	2.1
1	A	90	GLY	2.1
1	B	63	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	88	GLN	2.1
1	A	393	ASN	2.1
1	D	178	TYR	2.0
1	B	371	MET	2.0
1	B	79	PRO	2.0
1	B	374	ASP	2.0

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 carbohydrates 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.