Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:00 PM GMT

PDB ID	:	4GX9
Title	:	Crystal structure of a DNA polymerase III alpha-epsilon chimera
Authors	:	Li, N.; Horan, N.; Xu, Z.-Q.; Jacques, D.; Dixon, N.E.; Oakley, A.J.
Deposited on	:	2012-09-04
Resolution	:	2.15 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

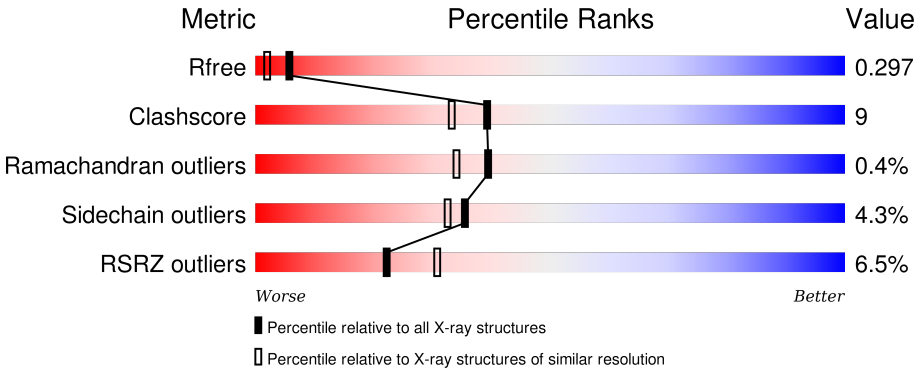
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.15 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}	91344	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

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	324	3% 79% 17%
1	B	324	8% 77% 17%
1	C	324	8% 82% 14%
1	D	324	5% 77% 18%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10076 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 DNA polymerase III subunit epsilon, DNA polymerase III subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	312	Total	C	N	O	S	0	6	0
			2438	1536	426	463	13			
1	B	313	Total	C	N	O	S	0	5	0
			2440	1537	428	462	13			
1	C	317	Total	C	N	O	S	0	6	0
			2480	1562	435	470	13			
1	D	312	Total	C	N	O	S	0	7	0
			2441	1540	423	465	13			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	MET	-	EXPRESSION TAG	UNP P03007
A	66	PRO	LEU	ENGINEERED MUTATION	UNP P10443
B	-8	MET	-	EXPRESSION TAG	UNP P03007
B	66	PRO	LEU	ENGINEERED MUTATION	UNP P10443
C	-8	MET	-	EXPRESSION TAG	UNP P03007
C	66	PRO	LEU	ENGINEERED MUTATION	UNP P10443
D	-8	MET	-	EXPRESSION TAG	UNP P03007
D	66	PRO	LEU	ENGINEERED MUTATION	UNP P10443

- Molecule 2 is water.

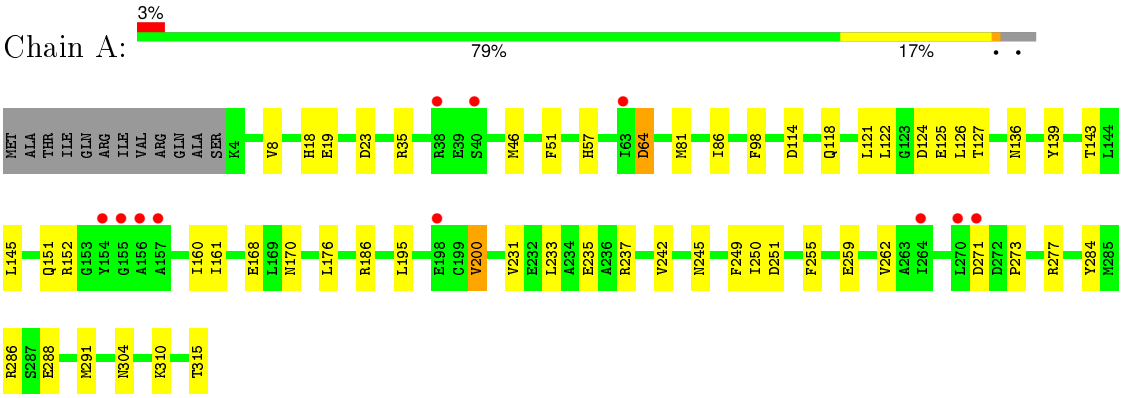
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	87	Total	O	0	0
			87	87		
2	B	45	Total	O	0	0
			45	45		
2	C	75	Total	O	0	0
			75	75		
2	D	70	Total	O	0	0
			70	70		

3 Residue-property plots (i)

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.

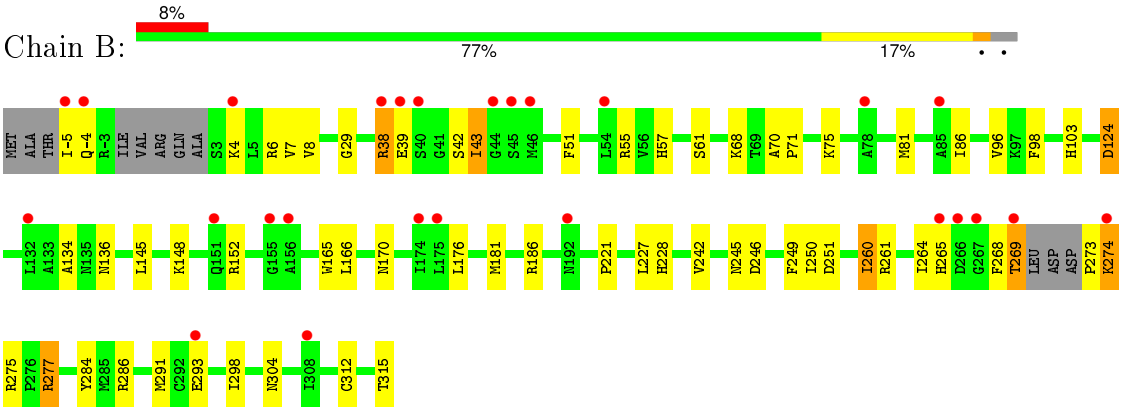
• Molecule 1: DNA polymerase III subunit epsilon, DNA polymerase III subunit alpha

Chain A:



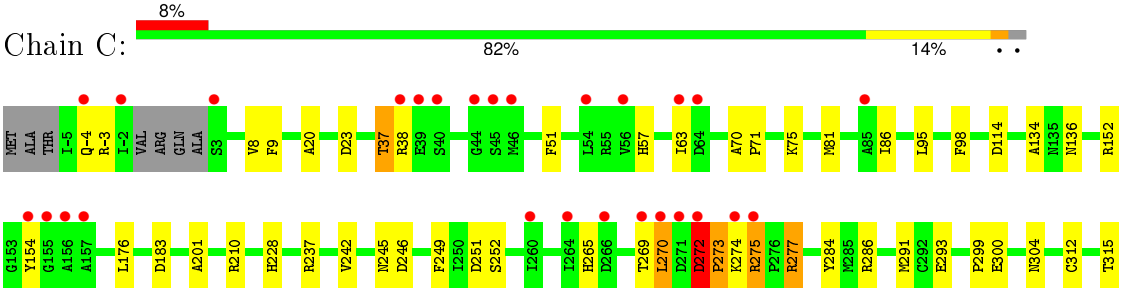
• Molecule 1: DNA polymerase III subunit epsilon, DNA polymerase III subunit alpha

Chain B:



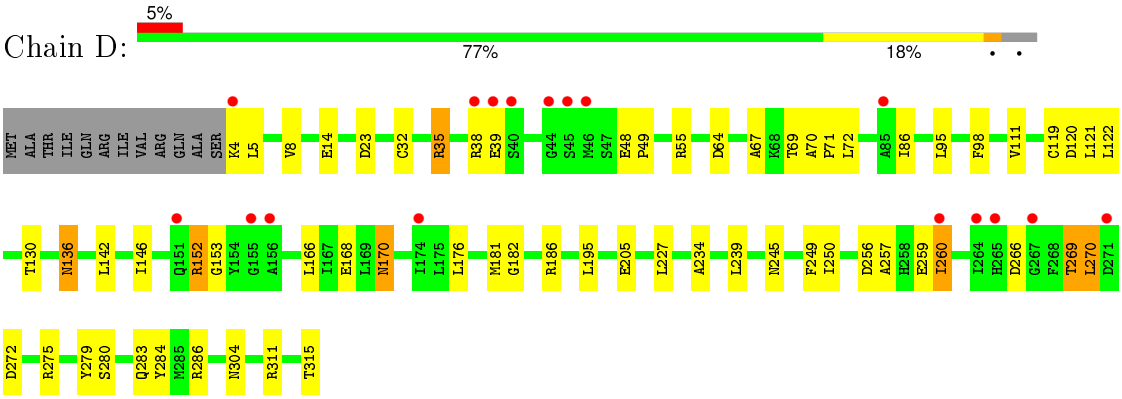
• Molecule 1: DNA polymerase III subunit epsilon, DNA polymerase III subunit alpha

Chain C:



• Molecule 1: DNA polymerase III subunit epsilon, DNA polymerase III subunit alpha

Chain D:


5%
77%
18%
MET ALA THR ILE GLN ARG ILE VAL ARG GLN ALA SER K4 L5 V8 E14 D23 C32 R35 R38 E39 S40 G44 S45 M46 S47 E48 P49 R55 D64 A67 K68 T69 A70 P71 L72 A85 I86 L95 F98 V111 C119 D120 L121 L122
T130 N136 L142 I146 Q151 R152 G153 Y154 G155 A156 L166 I167 E168 L169 N170 I174 L175 L176 M181 G182 R186 L195 E205 L227 A234 L239 N245 F249 I250 D256 A257 H258 E259 I260 I264 E265 D266 G267 F268 T269 L270 D271
D272 R275 Y279 S280 Q283 Y284 M285 R286 N304 R311 T315

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	83.02Å 56.98Å 135.07Å 90.00° 93.78° 90.00°	Depositor
Resolution (Å)	35.28 – 2.15 35.28 – 2.15	Depositor EDS
% Data completeness (in resolution range)	96.9 (35.28-2.15) 96.9 (35.28-2.15)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.19 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.226 , 0.291 0.231 , 0.297	Depositor DCC
R_{free} test set	3498 reflections (5.49%)	DCC
Wilson B-factor (Å^2)	31.4	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 42.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	14 of 67126 reflections (0.021%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10076	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 59.60 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.7219e-05.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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

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	0.94	1/2503 (0.0%)	0.88	1/3389 (0.0%)
1	B	0.89	0/2500	0.87	2/3380 (0.1%)
1	C	0.90	0/2544	0.89	3/3442 (0.1%)
1	D	0.97	0/2509	0.91	3/3399 (0.1%)
All	All	0.93	1/10056 (0.0%)	0.89	9/13610 (0.1%)

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	C	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	168	GLU	CB-CG	5.63	1.62	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	35	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	D	270	LEU	CA-CB-CG	6.59	130.45	115.30
1	D	35	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	B	124	ASP	CB-CG-OD1	5.43	123.18	118.30
1	C	210	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	A	81	MET	CG-SD-CE	-5.38	91.59	100.20
1	B	145	LEU	CA-CB-CG	5.19	127.24	115.30
1	C	183	ASP	CB-CG-OD1	5.12	122.91	118.30
1	C	81	MET	CG-SD-CE	-5.05	92.12	100.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	272	ASP	Peptide

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	2438	0	2419	41	0
1	B	2440	0	2426	40	0
1	C	2480	0	2469	40	0
1	D	2441	0	2423	60	0
2	A	87	0	0	3	0
2	B	45	0	0	5	0
2	C	75	0	0	4	0
2	D	70	0	0	5	0
All	All	10076	0	9737	174	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 9.

All (174) 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:260:ILE:HD12	1:C:201:ALA:HB2	1.46	0.95
1:B:268:PHE:HE1	1:B:274:LYS:HD2	1.34	0.93
1:C:269:THR:HG23	1:C:272:ASP:HB3	1.49	0.92
1:D:280:SER:H	1:D:283:GLN:HE21	1.20	0.85
1:D:72:LEU:HD12	1:D:86:ILE:CD1	2.08	0.83
1:C:70:ALA:HB3	1:C:71:PRO:HD3	1.60	0.83
1:D:245:ASN:HD21	1:D:286:ARG:HH11	1.25	0.83
1:B:70:ALA:HB3	1:B:71:PRO:HD3	1.60	0.82
1:A:136:ASN:HD21	1:A:315:THR:H	1.28	0.80
1:D:168:GLU:HG2	2:D:442:HOH:O	1.81	0.78
1:A:251:ASP:OD2	1:D:120:ASP:CB	2.32	0.78
1:B:43:ILE:HD13	1:B:43:ILE:H	1.49	0.77
1:A:127:THR:HG22	1:A:186:ARG:HH11	1.50	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:272:ASP:HB3	1:C:273:PRO:HD3	1.67	0.77
1:A:64:ASP:OD1	1:A:64:ASP:N	2.18	0.76
1:D:136:ASN:HD21	1:D:315:THR:H	1.30	0.76
1:B:136:ASN:HD21	1:B:315:THR:H	1.32	0.75
1:C:8:VAL:H	1:C:304:ASN:HD21	1.35	0.75
1:C:270:LEU:O	1:C:275:ARG:NH2	2.19	0.74
1:C:245:ASN:HD21	1:C:286:ARG:HH11	1.33	0.73
1:D:269:THR:HG23	1:D:272:ASP:HB2	1.69	0.73
1:A:251:ASP:OD2	1:D:120:ASP:HB3	1.89	0.73
1:A:118:GLN:HE21	1:A:124:ASP:HA	1.53	0.72
1:C:86:ILE:HG12	1:C:98:PHE:CZ	2.24	0.72
1:A:19:GLU:OE1	2:A:456:HOH:O	2.07	0.72
1:C:269:THR:HG23	1:C:272:ASP:CB	2.20	0.71
1:D:72:LEU:CD1	1:D:86:ILE:CD1	2.68	0.71
1:D:8:VAL:H	1:D:304:ASN:HD21	1.39	0.71
1:A:8:VAL:H	1:A:304:ASN:HD21	1.41	0.69
1:D:280:SER:H	1:D:283:GLN:NE2	1.91	0.68
1:A:251:ASP:OD2	1:D:120:ASP:HB2	1.94	0.68
1:D:257:ALA:HA	1:D:260:ILE:HD12	1.76	0.67
1:A:245:ASN:HD21	1:A:286:ARG:HH11	1.40	0.67
1:B:260:ILE:HD11	1:C:237:ARG:HH22	1.60	0.67
1:B:81:MET:HG2	2:B:409:HOH:O	1.95	0.66
1:D:152:ARG:HG2	1:D:153:GLY:O	1.96	0.66
1:C:37:THR:HG22	2:C:446:HOH:O	1.97	0.65
1:D:72:LEU:CD1	1:D:86:ILE:HD13	2.27	0.65
1:D:23:ASP:OD1	1:D:35:ARG:NH2	2.25	0.65
1:C:136:ASN:HD21	1:C:315:THR:H	1.46	0.64
1:B:8:VAL:H	1:B:304:ASN:HD21	1.45	0.64
1:D:181:MET:CE	1:D:186:ARG:NH2	2.60	0.64
1:A:288:GLU:OE1	2:A:415:HOH:O	2.15	0.64
1:B:43:ILE:CD1	1:B:43:ILE:H	2.10	0.63
1:B:260:ILE:HD11	1:C:237:ARG:NH2	2.14	0.63
1:A:231:VAL:O	1:A:235:GLU:HG3	1.98	0.63
1:B:96:VAL:HG23	2:B:424:HOH:O	2.00	0.62
1:A:127:THR:HA	1:A:186:ARG:HH12	1.64	0.61
1:D:72:LEU:HD13	1:D:86:ILE:HD13	1.81	0.61
1:B:265:HIS:HD2	2:B:411:HOH:O	1.84	0.61
1:A:86:ILE:HG12	1:A:98:PHE:CZ	2.35	0.61
1:C:154:TYR:HA	2:C:429:HOH:O	2.01	0.61
1:D:259:GLU:OE1	1:D:275:ARG:NH2	2.32	0.60
1:B:268:PHE:CE1	1:B:274:LYS:HD2	2.26	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:ILE:CD1	1:B:43:ILE:N	2.63	0.60
1:A:127:THR:HG22	1:A:186:ARG:NH1	2.17	0.58
1:B:86:ILE:HG12	1:B:98:PHE:CZ	2.39	0.58
1:A:176:LEU:HD22	1:A:242:VAL:HG11	1.85	0.58
1:D:86:ILE:HG13	1:D:98:PHE:CD1	2.39	0.57
1:D:69:THR:HG22	1:D:86:ILE:HD12	1.85	0.57
1:D:64:ASP:HA	2:D:416:HOH:O	2.05	0.56
1:C:-4:GLN:HG3	1:C:228:HIS:CE1	2.40	0.55
1:B:51:PHE:CE2	1:B:291:MET:HG3	2.41	0.55
1:C:299:PRO:HD2	1:C:300:GLU:OE1	2.05	0.55
1:C:75:LYS:NZ	1:C:251:ASP:OD1	2.29	0.55
1:D:257:ALA:HA	1:D:260:ILE:CD1	2.35	0.55
1:B:265:HIS:CD2	2:B:411:HOH:O	2.58	0.55
1:D:86:ILE:HG13	1:D:98:PHE:CG	2.42	0.55
1:C:272:ASP:HB3	1:C:273:PRO:CD	2.37	0.55
1:C:245:ASN:HD21	1:C:286:ARG:NH1	2.03	0.55
1:D:86:ILE:CG1	1:D:98:PHE:CE1	2.90	0.54
1:D:95[B]:LEU:HD23	2:D:436:HOH:O	2.06	0.54
1:D:152:ARG:HG3	1:D:152:ARG:O	2.06	0.54
1:B:245:ASN:HD21	1:B:286:ARG:HH11	1.56	0.54
1:B:275:ARG:HB3	1:B:277:ARG:NH2	2.23	0.53
1:D:182:GLY:O	1:D:186:ARG:HG3	2.09	0.52
1:B:227:LEU:HD21	1:B:298:ILE:HD11	1.92	0.52
1:D:86:ILE:HG12	1:D:98:PHE:CZ	2.44	0.52
1:C:51:PHE:CE2	1:C:291:MET:HG3	2.45	0.52
1:D:72:LEU:HD12	1:D:86:ILE:HD12	1.88	0.51
1:C:245:ASN:ND2	1:C:286:ARG:HH11	2.06	0.51
1:D:55:ARG:HD2	1:D:130:THR:OG1	2.10	0.51
1:D:256:ASP:O	1:D:260:ILE:HG13	2.11	0.51
1:A:121:LEU:HB3	1:A:195:LEU:HD11	1.93	0.51
1:B:136:ASN:HD21	1:B:315:THR:N	2.07	0.50
1:A:86:ILE:HD11	1:A:98:PHE:CE1	2.46	0.50
1:A:122[A]:LEU:HD23	1:A:195:LEU:HD21	1.94	0.50
1:D:166:LEU:O	1:D:170:ASN:HB3	2.11	0.50
1:D:48[B]:GLU:HG3	1:D:49:PRO:HD2	1.94	0.50
1:A:139:TYR:O	1:A:143[B]:THR:HG23	2.12	0.50
1:B:269:THR:OG1	1:B:273:PRO:HG2	2.12	0.50
1:D:95[A]:LEU:HD11	1:D:111:VAL:HG22	1.94	0.49
1:A:200:VAL:HG12	1:A:237[A]:ARG:NH2	2.27	0.49
1:B:29:GLY:HA3	1:B:103:HIS:O	2.13	0.49
1:A:86:ILE:HG13	1:A:98:PHE:CG	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:ASN:HD21	1:A:286:ARG:NH1	2.10	0.49
1:A:233:LEU:O	1:A:237[A]:ARG:HG2	2.12	0.49
1:D:181:MET:HE3	1:D:186:ARG:NH2	2.27	0.49
1:D:86:ILE:HG12	1:D:98:PHE:CE1	2.49	0.48
1:B:75:LYS:NZ	1:B:251:ASP:OD1	2.46	0.48
1:A:125:GLU:HG2	1:A:126:LEU:N	2.28	0.48
1:D:122[A]:LEU:HD23	1:D:195:LEU:HD21	1.95	0.48
1:D:260:ILE:H	1:D:260:ILE:HG13	1.44	0.48
1:A:245:ASN:ND2	1:A:286:ARG:HH11	2.10	0.48
1:D:142:LEU:O	1:D:146:ILE:HG13	2.14	0.47
1:D:181:MET:HE3	1:D:186:ARG:HH22	1.79	0.47
1:A:51:PHE:CE2	1:A:291:MET:HG3	2.49	0.47
1:C:269:THR:CG2	1:C:272:ASP:HB3	2.33	0.47
1:A:200:VAL:CG1	1:A:237[A]:ARG:NH2	2.78	0.47
1:A:23:ASP:OD1	1:A:35:ARG:NH1	2.39	0.47
1:B:136:ASN:ND2	1:B:315:THR:H	2.09	0.47
1:B:181:MET:CE	1:B:186:ARG:HH21	2.28	0.46
1:D:67:ALA:HA	2:D:413:HOH:O	2.15	0.46
1:B:261:ARG:NH2	2:B:443:HOH:O	2.48	0.46
1:D:181:MET:HE1	1:D:186:ARG:NH2	2.31	0.46
1:C:63:ILE:HG22	1:C:265:HIS:ND1	2.29	0.46
1:C:249:PHE:O	1:C:284:TYR:HA	2.15	0.46
1:D:168:GLU:HA	1:D:168:GLU:OE2	2.16	0.46
1:B:249:PHE:O	1:B:284:TYR:HA	2.15	0.46
1:D:130:THR:HB	1:D:176:LEU:HB2	1.97	0.46
1:C:277:ARG:HB2	1:C:277:ARG:HE	1.55	0.46
1:A:122[A]:LEU:CD2	1:A:195:LEU:HD21	2.46	0.46
1:D:181:MET:CE	1:D:186:ARG:HH22	2.28	0.46
1:C:269:THR:HG23	1:C:273:PRO:HD3	1.98	0.45
1:C:134:ALA:HA	1:C:312:CYS:HA	1.98	0.45
1:A:126:LEU:HD22	1:A:160:ILE:HD12	1.97	0.45
1:A:273:PRO:O	1:A:277:ARG:NH1	2.50	0.45
1:D:14:GLU:CD	1:D:311:ARG:HG2	2.36	0.45
1:C:176:LEU:HD22	1:C:242:VAL:HG11	1.98	0.45
1:C:273:PRO:HB2	1:C:274:LYS:HG3	1.98	0.45
1:B:176:LEU:HD22	1:B:242:VAL:HG11	1.99	0.45
1:C:57:HIS:HE1	1:C:114:ASP:OD2	1.99	0.45
1:D:205:GLU:O	1:D:205:GLU:HG3	2.14	0.45
1:D:86:ILE:CG1	1:D:98:PHE:CD1	3.00	0.44
1:A:200:VAL:HG11	1:A:237[A]:ARG:CZ	2.47	0.44
1:D:234:ALA:HA	1:D:239:LEU:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:GLU:HG2	2:A:451:HOH:O	2.16	0.44
1:C:86:ILE:CG1	1:C:98:PHE:CE1	3.00	0.44
1:A:18:HIS:HB2	1:A:310:LYS:O	2.17	0.44
1:D:227:LEU:HD23	1:D:227:LEU:C	2.38	0.44
1:A:255:PHE:CZ	1:A:259:GLU:HG3	2.53	0.44
1:D:71:PRO:HB2	1:D:250:ILE:HD11	2.00	0.44
1:D:5:LEU:HB3	2:D:440:HOH:O	2.18	0.43
1:C:86:ILE:HG13	1:C:98:PHE:CD1	2.53	0.43
1:C:20:ALA:O	1:C:23:ASP:HB2	2.19	0.43
1:C:57:HIS:CE1	1:C:114:ASP:OD2	2.72	0.43
1:B:-4:GLN:HB3	1:B:228:HIS:NE2	2.33	0.43
1:B:166:LEU:O	1:B:170:ASN:HB3	2.19	0.43
1:B:57:HIS:HD2	1:B:61:SER:OG	2.02	0.43
1:C:70:ALA:CB	1:C:71:PRO:HD3	2.38	0.42
1:B:148:LYS:HE3	1:B:165:TRP:CE2	2.55	0.42
1:C:37:THR:CG2	2:C:446:HOH:O	2.61	0.42
1:D:70:ALA:HB3	1:D:71:PRO:HD3	2.02	0.42
1:C:9:PHE:HD2	2:C:401:HOH:O	2.02	0.42
1:A:249:PHE:O	1:A:284:TYR:HA	2.19	0.42
1:D:249:PHE:O	1:D:284:TYR:HA	2.19	0.42
1:D:8:VAL:H	1:D:304:ASN:ND2	2.13	0.42
1:B:277:ARG:HB2	1:B:277:ARG:HE	1.77	0.42
1:A:35:ARG:HA	1:A:46:MET:HE1	2.02	0.42
1:B:55:ARG:HG2	1:B:246:ASP:HA	2.02	0.42
1:C:95:LEU:O	1:C:95:LEU:HD12	2.19	0.42
1:A:145:LEU:HG	1:A:161:ILE:HG21	2.01	0.41
1:C:245:ASN:O	1:C:246:ASP:C	2.58	0.41
1:B:134:ALA:HA	1:B:312:CYS:HA	2.02	0.41
1:D:279:TYR:HA	1:D:283:GLN:HE22	1.85	0.41
1:D:136:ASN:HD22	1:D:136:ASN:N	2.18	0.41
1:D:119[B]:CYS:SG	1:D:121:LEU:HB2	2.59	0.41
1:D:32:CYS:SG	1:D:35:ARG:HG3	2.61	0.41
1:A:118:GLN:HE21	1:A:124:ASP:CA	2.28	0.41
1:B:260:ILE:CD1	1:C:237:ARG:HH22	2.32	0.40
1:B:7:VAL:HA	1:B:304:ASN:HD21	1.85	0.40
1:B:8:VAL:H	1:B:304:ASN:ND2	2.14	0.40
1:B:227:LEU:HD21	1:B:298:ILE:CD1	2.51	0.40
1:A:57:HIS:CE1	1:A:114:ASP:OD2	2.75	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	316/324 (98%)	305 (96%)	11 (4%)	0	100	100
1	B	312/324 (96%)	294 (94%)	15 (5%)	3 (1%)	19	11
1	C	319/324 (98%)	303 (95%)	14 (4%)	2 (1%)	30	21
1	D	317/324 (98%)	302 (95%)	15 (5%)	0	100	100
All	All	1264/1296 (98%)	1204 (95%)	55 (4%)	5 (0%)	39	34

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	272	ASP
1	C	273	PRO
1	B	264	ILE
1	B	42	SER
1	B	38	ARG

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	259/263 (98%)	251 (97%)	8 (3%)	47	47
1	B	259/263 (98%)	243 (94%)	16 (6%)	23	17
1	C	264/263 (100%)	254 (96%)	10 (4%)	40	37
1	D	260/263 (99%)	250 (96%)	10 (4%)	40	37
All	All	1042/1052 (99%)	998 (96%)	44 (4%)	35	34

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	ASP
1	A	151	GLN
1	A	152	ARG
1	A	170	ASN
1	A	200	VAL
1	A	250	ILE
1	A	262	VAL
1	A	271	ASP
1	B	-5	ILE
1	B	4	LYS
1	B	6	ARG
1	B	38	ARG
1	B	39	GLU
1	B	43	ILE
1	B	68	LYS
1	B	124	ASP
1	B	152	ARG
1	B	221	PRO
1	B	250	ILE
1	B	260	ILE
1	B	269	THR
1	B	274	LYS
1	B	277	ARG
1	B	293	GLU
1	C	-3	ARG
1	C	37	THR
1	C	38	ARG
1	C	152	ARG
1	C	252	SER
1	C	270	LEU
1	C	272	ASP
1	C	275	ARG
1	C	277	ARG
1	C	293	GLU
1	D	4	LYS
1	D	38	ARG
1	D	39	GLU
1	D	136	ASN
1	D	152	ARG
1	D	170	ASN
1	D	260	ILE
1	D	266	ASP

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Mol	Chain	Res	Type
1	D	269	THR
1	D	270	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	HIS
1	A	118	GLN
1	A	136	ASN
1	A	245	ASN
1	A	265	HIS
1	A	304	ASN
1	B	-4	GLN
1	B	57	HIS
1	B	136	ASN
1	B	245	ASN
1	B	258	HIS
1	B	265	HIS
1	B	304	ASN
1	C	-4	GLN
1	C	57	HIS
1	C	136	ASN
1	C	245	ASN
1	C	304	ASN
1	D	57	HIS
1	D	118	GLN
1	D	136	ASN
1	D	245	ASN
1	D	283	GLN
1	D	304	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	312/324 (96%)	0.19	11 (3%)	48	58	8, 20, 31, 47	0
1	B	313/324 (96%)	0.38	26 (8%)	14	20	14, 20, 42, 62	0
1	C	317/324 (97%)	0.49	27 (8%)	13	19	13, 20, 41, 59	0
1	D	312/324 (96%)	0.25	17 (5%)	29	40	13, 20, 33, 48	0
All	All	1254/1296 (96%)	0.33	81 (6%)	22	31	8, 20, 36, 62	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	45	SER	11.3
1	C	40	SER	9.2
1	C	-2	ILE	9.0
1	C	271	ASP	7.3
1	B	39	GLU	6.6
1	C	156	ALA	6.3
1	C	270	LEU	6.2
1	D	156	ALA	6.0
1	B	40	SER	5.8
1	A	40	SER	5.5
1	B	46	MET	5.5
1	B	266	ASP	5.3
1	B	156	ALA	5.2
1	C	39	GLU	5.2
1	D	45	SER	4.6
1	D	271	ASP	4.5
1	C	260	ILE	4.3
1	B	45	SER	4.3
1	D	40	SER	4.2
1	C	272	ASP	4.1
1	C	155	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	156	ALA	3.9
1	C	38	ARG	3.9
1	D	155	GLY	3.8
1	D	38	ARG	3.7
1	D	44	GLY	3.7
1	C	46	MET	3.7
1	A	155	GLY	3.6
1	B	38	ARG	3.6
1	C	264	ILE	3.5
1	A	271	ASP	3.4
1	C	266	ASP	3.3
1	A	264	ILE	3.3
1	D	39	GLU	3.2
1	B	54	LEU	3.2
1	C	154	TYR	3.1
1	C	157	ALA	3.1
1	A	38	ARG	3.1
1	C	269	THR	3.0
1	C	56	VAL	2.9
1	B	4	LYS	2.9
1	A	154	TYR	2.9
1	B	155	GLY	2.8
1	D	46	MET	2.8
1	B	265	HIS	2.7
1	C	63	ILE	2.7
1	B	274	LYS	2.6
1	C	64	ASP	2.6
1	B	-4	GLN	2.6
1	C	-4	GLN	2.6
1	D	264	ILE	2.5
1	C	3	SER	2.5
1	C	44	GLY	2.5
1	D	4	LYS	2.5
1	D	267	GLY	2.4
1	B	44	GLY	2.4
1	C	85	ALA	2.4
1	A	198	GLU	2.3
1	B	293	GLU	2.3
1	B	78	ALA	2.3
1	B	-5	ILE	2.3
1	B	192	ASN	2.3
1	B	267	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	308	ILE	2.3
1	D	260	ILE	2.3
1	C	274	LYS	2.2
1	A	63	ILE	2.2
1	C	275	ARG	2.2
1	D	151	GLN	2.2
1	D	85	ALA	2.2
1	B	132	LEU	2.2
1	C	54	LEU	2.2
1	B	269	THR	2.2
1	B	151	GLN	2.2
1	A	270	LEU	2.2
1	D	174	ILE	2.1
1	B	85	ALA	2.1
1	B	175	LEU	2.0
1	A	157	ALA	2.0
1	D	265	HIS	2.0
1	B	174	ILE	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.