Full wwPDB X-ray Structure Validation Report ⓘ

Oct 31, 2021 – 10:06 AM EDT

PDB ID	:	2EFR
Title	:	Crystal structure of the c-terminal tropomyosin fragment with N- and C-terminal extensions of the leucine zipper at 1.8 angstroms resolution
Authors	:	Minakata, S.; Nitanai, Y.; Maeda, K.; Oda, N.; Wakabayashi, K.; Maeda, Y.
Deposited on	:	2007-02-23
Resolution	:	1.80 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 following versions of software and data (see references ⓘ) were used in the production of this report:

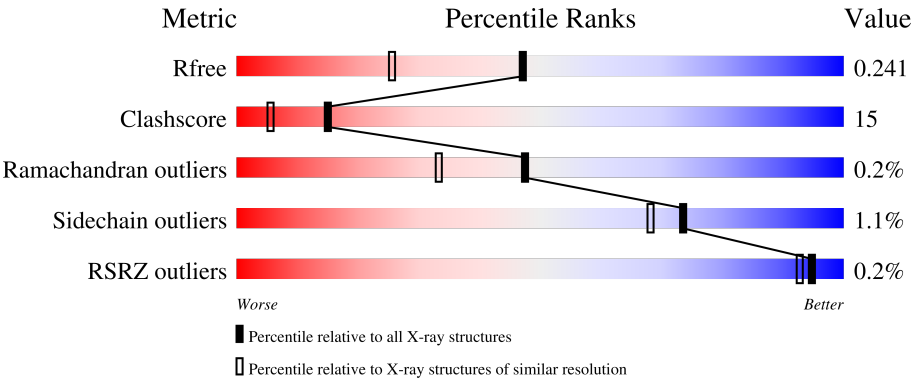
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 1.80 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}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 <=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	155	% 68% 32%
1	B	155	75% 24% .
1	C	155	76% 23% ..
1	D	155	76% 22% .

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6578 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 General control protein GCN4 and Tropomyosin 1 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	155	Total	C	N	O	S	0	0	0
			1285	799	215	269	2			
1	B	154	Total	C	N	O	S	0	0	0
			1274	793	211	268	2			
1	C	154	Total	C	N	O	S	0	0	0
			1274	793	211	268	2			
1	D	155	Total	C	N	O	S	0	0	0
			1285	799	215	269	2			

There are 116 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	190	SER	CYS	engineered mutation	UNP P58772
A	274	MET	-	expression tag	UNP P58772
A	275	LYS	-	expression tag	UNP P58772
A	276	GLN	-	expression tag	UNP P58772
A	277	LEU	-	expression tag	UNP P58772
A	278	GLU	-	expression tag	UNP P58772
A	279	ASP	-	expression tag	UNP P58772
A	280	LYS	-	expression tag	UNP P58772
A	281	VAL	-	expression tag	UNP P58772
A	282	GLU	-	expression tag	UNP P58772
A	283	GLU	-	expression tag	UNP P58772
A	284	LEU	-	expression tag	UNP P58772
A	285	LEU	-	expression tag	UNP P58772
A	286	SER	-	expression tag	UNP P58772
A	287	LYS	-	expression tag	UNP P58772
A	288	ASN	-	expression tag	UNP P58772
A	289	TYR	-	expression tag	UNP P58772
A	290	HIS	-	expression tag	UNP P58772
A	291	LEU	-	expression tag	UNP P58772
A	292	GLU	-	expression tag	UNP P58772
A	293	ASN	-	expression tag	UNP P58772

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	294	GLU	-	expression tag	UNP P58772
A	295	VAL	-	expression tag	UNP P58772
A	296	ALA	-	expression tag	UNP P58772
A	297	ARG	-	expression tag	UNP P58772
A	298	LEU	-	expression tag	UNP P58772
A	299	LYS	-	expression tag	UNP P58772
A	300	LYS	-	expression tag	UNP P58772
A	301	LEU	-	expression tag	UNP P58772
B	190	SER	CYS	engineered mutation	UNP P58772
B	274	MET	-	expression tag	UNP P58772
B	275	LYS	-	expression tag	UNP P58772
B	276	GLN	-	expression tag	UNP P58772
B	277	LEU	-	expression tag	UNP P58772
B	278	GLU	-	expression tag	UNP P58772
B	279	ASP	-	expression tag	UNP P58772
B	280	LYS	-	expression tag	UNP P58772
B	281	VAL	-	expression tag	UNP P58772
B	282	GLU	-	expression tag	UNP P58772
B	283	GLU	-	expression tag	UNP P58772
B	284	LEU	-	expression tag	UNP P58772
B	285	LEU	-	expression tag	UNP P58772
B	286	SER	-	expression tag	UNP P58772
B	287	LYS	-	expression tag	UNP P58772
B	288	ASN	-	expression tag	UNP P58772
B	289	TYR	-	expression tag	UNP P58772
B	290	HIS	-	expression tag	UNP P58772
B	291	LEU	-	expression tag	UNP P58772
B	292	GLU	-	expression tag	UNP P58772
B	293	ASN	-	expression tag	UNP P58772
B	294	GLU	-	expression tag	UNP P58772
B	295	VAL	-	expression tag	UNP P58772
B	296	ALA	-	expression tag	UNP P58772
B	297	ARG	-	expression tag	UNP P58772
B	298	LEU	-	expression tag	UNP P58772
B	299	LYS	-	expression tag	UNP P58772
B	300	LYS	-	expression tag	UNP P58772
B	301	LEU	-	expression tag	UNP P58772
C	190	SER	CYS	engineered mutation	UNP P58772
C	274	MET	-	expression tag	UNP P58772
C	275	LYS	-	expression tag	UNP P58772
C	276	GLN	-	expression tag	UNP P58772
C	277	LEU	-	expression tag	UNP P58772

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	278	GLU	-	expression tag	UNP P58772
C	279	ASP	-	expression tag	UNP P58772
C	280	LYS	-	expression tag	UNP P58772
C	281	VAL	-	expression tag	UNP P58772
C	282	GLU	-	expression tag	UNP P58772
C	283	GLU	-	expression tag	UNP P58772
C	284	LEU	-	expression tag	UNP P58772
C	285	LEU	-	expression tag	UNP P58772
C	286	SER	-	expression tag	UNP P58772
C	287	LYS	-	expression tag	UNP P58772
C	288	ASN	-	expression tag	UNP P58772
C	289	TYR	-	expression tag	UNP P58772
C	290	HIS	-	expression tag	UNP P58772
C	291	LEU	-	expression tag	UNP P58772
C	292	GLU	-	expression tag	UNP P58772
C	293	ASN	-	expression tag	UNP P58772
C	294	GLU	-	expression tag	UNP P58772
C	295	VAL	-	expression tag	UNP P58772
C	296	ALA	-	expression tag	UNP P58772
C	297	ARG	-	expression tag	UNP P58772
C	298	LEU	-	expression tag	UNP P58772
C	299	LYS	-	expression tag	UNP P58772
C	300	LYS	-	expression tag	UNP P58772
C	301	LEU	-	expression tag	UNP P58772
D	190	SER	CYS	engineered mutation	UNP P58772
D	274	MET	-	expression tag	UNP P58772
D	275	LYS	-	expression tag	UNP P58772
D	276	GLN	-	expression tag	UNP P58772
D	277	LEU	-	expression tag	UNP P58772
D	278	GLU	-	expression tag	UNP P58772
D	279	ASP	-	expression tag	UNP P58772
D	280	LYS	-	expression tag	UNP P58772
D	281	VAL	-	expression tag	UNP P58772
D	282	GLU	-	expression tag	UNP P58772
D	283	GLU	-	expression tag	UNP P58772
D	284	LEU	-	expression tag	UNP P58772
D	285	LEU	-	expression tag	UNP P58772
D	286	SER	-	expression tag	UNP P58772
D	287	LYS	-	expression tag	UNP P58772
D	288	ASN	-	expression tag	UNP P58772
D	289	TYR	-	expression tag	UNP P58772
D	290	HIS	-	expression tag	UNP P58772

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	291	LEU	-	expression tag	UNP P58772
D	292	GLU	-	expression tag	UNP P58772
D	293	ASN	-	expression tag	UNP P58772
D	294	GLU	-	expression tag	UNP P58772
D	295	VAL	-	expression tag	UNP P58772
D	296	ALA	-	expression tag	UNP P58772
D	297	ARG	-	expression tag	UNP P58772
D	298	LEU	-	expression tag	UNP P58772
D	299	LYS	-	expression tag	UNP P58772
D	300	LYS	-	expression tag	UNP P58772
D	301	LEU	-	expression tag	UNP P58772

- Molecule 2 is water.

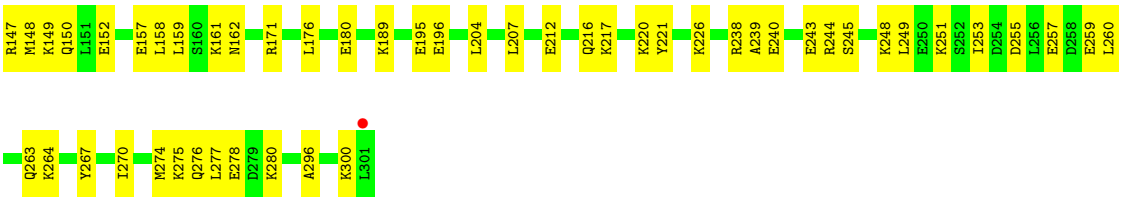
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	331	Total O 331 331	0	0
2	B	391	Total O 391 391	0	0
2	C	321	Total O 321 321	0	0
2	D	417	Total O 417 417	0	0

3 Residue-property plots (i)

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.

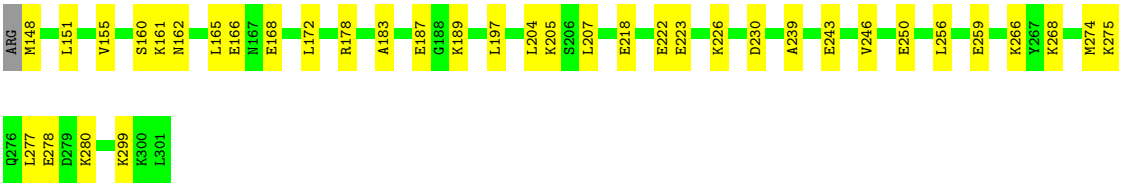
• Molecule 1: General control protein GCN4 and Tropomyosin 1 alpha chain

Chain A:



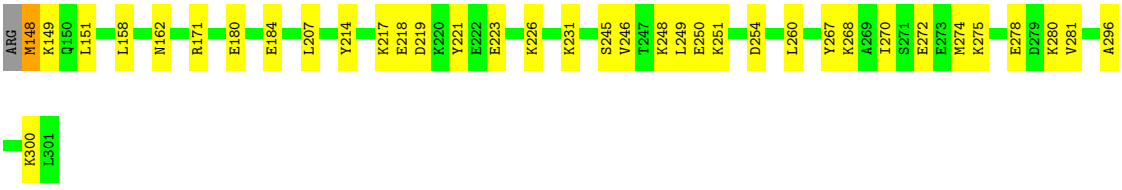
• Molecule 1: General control protein GCN4 and Tropomyosin 1 alpha chain

Chain B:



• Molecule 1: General control protein GCN4 and Tropomyosin 1 alpha chain

Chain C:



• Molecule 1: General control protein GCN4 and Tropomyosin 1 alpha chain

Chain D:


K300
L301

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	42.36Å 65.84Å 71.14Å 66.40° 89.93° 90.03°	Depositor
Resolution (Å)	19.80 – 1.80 19.80 – 1.80	Depositor EDS
% Data completeness (in resolution range)	96.0 (19.80-1.80) 95.7 (19.80-1.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.44 (at 1.80Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.237 , 0.316 0.240 , 0.241	Depositor DCC
R_{free} test set	3163 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	26.4	Xtriage
Anisotropy	0.497	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 74.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.467 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6578	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.91% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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	0.40	0/1293	0.54	0/1720
1	B	0.42	0/1282	0.54	0/1706
1	C	0.43	0/1282	0.54	0/1706
1	D	0.41	0/1293	0.55	0/1720
All	All	0.42	0/5150	0.54	0/6852

There are no bond length outliers.

There are no bond angle outliers.

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	1285	0	1306	56	0
1	B	1274	0	1293	52	0
1	C	1274	0	1293	36	0
1	D	1285	0	1306	40	0
2	A	331	0	0	20	0
2	B	391	0	0	14	0
2	C	321	0	0	8	0
2	D	417	0	0	15	0
All	All	6578	0	5198	156	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 15.

All (156) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:ALA:O	1:A:300:LYS:HD3	1.65	0.95
1:A:162:ASN:HD21	1:B:161:LYS:HD3	1.38	0.88
1:D:162:ASN:HB3	2:D:395:HOH:O	1.75	0.87
1:B:274:MET:HA	1:B:274:MET:HE3	1.56	0.86
2:A:454:HOH:O	1:B:189:LYS:HG2	1.75	0.85
1:A:207:LEU:HD22	2:A:523:HOH:O	1.78	0.83
1:A:204:LEU:CD1	1:B:207:LEU:HD12	2.13	0.78
1:A:162:ASN:ND2	1:B:161:LYS:HD3	1.98	0.77
1:B:268:LYS:HD3	2:B:404:HOH:O	1.86	0.75
1:A:267:TYR:CZ	1:B:266:LYS:HE2	2.21	0.75
2:C:416:HOH:O	1:D:161:LYS:HD3	1.86	0.74
1:D:183:ALA:O	1:D:187:GLU:HG3	1.87	0.74
1:A:207:LEU:HD12	1:B:204:LEU:HD12	1.72	0.72
1:B:230:ASP:HB3	2:B:604:HOH:O	1.90	0.71
1:A:277:LEU:HD12	1:B:274:MET:HE1	1.71	0.71
1:A:162:ASN:HD21	1:B:161:LYS:CD	2.03	0.70
1:B:205:LYS:HB3	1:B:205:LYS:NZ	2.06	0.70
1:A:204:LEU:HD11	1:B:207:LEU:HD12	1.73	0.69
1:B:275:LYS:HE2	2:B:565:HOH:O	1.92	0.69
1:C:180:GLU:O	1:C:184:GLU:HG3	1.93	0.68
1:A:249:LEU:HD11	2:A:391:HOH:O	1.92	0.68
1:B:274:MET:HA	1:B:274:MET:CE	2.24	0.68
1:D:227:VAL:O	1:D:231:LYS:HG3	1.93	0.67
1:A:149:LYS:HD2	1:A:149:LYS:H	1.60	0.66
1:A:217:LYS:HE2	1:A:221:TYR:OH	1.95	0.66
1:C:151:LEU:HD22	1:D:151:LEU:HB3	1.76	0.66
1:B:178:ARG:HG2	2:B:587:HOH:O	1.97	0.65
1:C:245:SER:O	1:C:248:LYS:HG2	1.97	0.64
1:A:300:LYS:HE2	2:A:380:HOH:O	1.97	0.64
1:A:204:LEU:HD12	1:B:207:LEU:HD12	1.79	0.64
1:A:259:GLU:HG3	2:A:339:HOH:O	1.99	0.63
1:C:171:ARG:HD2	2:C:382:HOH:O	1.98	0.63
1:B:274:MET:HE1	1:B:277:LEU:HD23	1.80	0.63
1:C:219:ASP:O	1:C:223:GLU:HG3	1.99	0.62
1:A:148:MET:O	1:A:152:GLU:HG3	2.00	0.62
1:C:207:LEU:HD12	1:D:204:LEU:HD12	1.82	0.62
1:D:275:LYS:HD2	2:D:591:HOH:O	2.01	0.61
1:A:189:LYS:HE2	2:B:621:HOH:O	2.01	0.60
1:A:196:GLU:OE2	1:B:197:LEU:HD21	2.00	0.60
1:A:277:LEU:CD1	1:B:274:MET:HE1	2.31	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:ALA:O	1:B:187:GLU:HG3	2.02	0.60
2:A:386:HOH:O	1:B:256:LEU:HD21	2.01	0.60
1:A:274:MET:O	1:A:278:GLU:HG3	2.03	0.59
1:B:268:LYS:HD2	2:B:505:HOH:O	2.03	0.59
1:C:149:LYS:NZ	1:C:149:LYS:HB3	2.17	0.59
1:C:231:LYS:HD2	2:C:402:HOH:O	2.02	0.59
1:B:223:GLU:OE2	1:B:223:GLU:HA	2.02	0.59
1:B:205:LYS:HB3	1:B:205:LYS:HZ3	1.68	0.58
1:C:217:LYS:HD3	1:D:218:GLU:OE1	2.04	0.58
1:D:198:LYS:HE3	2:D:363:HOH:O	2.04	0.57
1:B:226:LYS:HD2	2:B:646:HOH:O	2.04	0.56
1:B:274:MET:O	1:B:278:GLU:HG3	2.06	0.56
1:C:218:GLU:HG3	1:D:221:TYR:CE2	2.40	0.56
1:A:238:ARG:HD2	2:A:407:HOH:O	2.06	0.55
1:D:177:GLU:HG3	1:D:178:ARG:N	2.21	0.55
1:A:149:LYS:HD2	1:A:149:LYS:N	2.22	0.55
1:A:277:LEU:HD12	1:B:274:MET:CE	2.36	0.55
1:B:275:LYS:NZ	2:B:548:HOH:O	2.40	0.55
1:B:274:MET:CE	1:B:277:LEU:HD23	2.37	0.54
1:A:253:ILE:O	1:A:257:GLU:HG3	2.08	0.54
1:A:162:ASN:HD21	1:B:161:LYS:CE	2.20	0.54
1:A:300:LYS:NZ	2:A:344:HOH:O	2.41	0.53
1:C:217:LYS:HE2	1:C:221:TYR:OH	2.08	0.53
1:C:260:LEU:HD21	1:D:260:LEU:HA	1.91	0.53
1:A:157:GLU:HG3	1:A:161:LYS:HE2	1.90	0.53
1:D:174:LYS:O	1:D:177:GLU:HG2	2.10	0.52
1:A:264:LYS:HD2	2:A:428:HOH:O	2.10	0.52
1:D:239:ALA:O	1:D:243:GLU:HG3	2.10	0.51
1:B:160:SER:HB2	2:B:602:HOH:O	2.08	0.51
1:A:217:LYS:HE2	1:A:221:TYR:CZ	2.45	0.51
1:A:275:LYS:HE2	2:A:477:HOH:O	2.11	0.51
1:B:246:VAL:O	1:B:250:GLU:HG3	2.11	0.50
1:D:233:LYS:HD3	1:D:233:LYS:C	2.30	0.50
1:B:205:LYS:NZ	2:B:622:HOH:O	2.44	0.50
1:B:151:LEU:O	1:B:155:VAL:HG23	2.12	0.50
1:D:226:LYS:HD2	2:D:618:HOH:O	2.12	0.50
1:A:300:LYS:N	1:A:300:LYS:HD2	2.27	0.49
1:B:218:GLU:O	1:B:222:GLU:HG2	2.11	0.49
1:B:162:ASN:HB3	2:B:455:HOH:O	2.13	0.49
1:B:280:LYS:HE3	2:B:438:HOH:O	2.12	0.49
1:C:274:MET:O	1:C:278:GLU:HG3	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:161:LYS:HG3	2:D:556:HOH:O	2.12	0.49
1:A:276:GLN:HG2	2:A:362:HOH:O	2.12	0.49
1:C:158:LEU:HD22	1:D:162:ASN:HD22	1.77	0.49
1:D:147:ARG:NH1	1:D:150:GLN:OE1	2.46	0.48
1:C:246:VAL:O	1:C:250:GLU:HG3	2.13	0.48
1:A:248:LYS:HG3	1:A:249:LEU:N	2.29	0.47
1:A:280:LYS:NZ	2:A:401:HOH:O	2.47	0.47
1:D:178:ARG:HG2	2:D:459:HOH:O	2.13	0.47
1:B:205:LYS:NZ	1:B:205:LYS:CB	2.76	0.47
1:C:248:LYS:NZ	2:C:537:HOH:O	2.47	0.47
1:A:216:GLN:HB3	2:A:596:HOH:O	2.13	0.47
1:D:182:ARG:NH1	2:D:432:HOH:O	2.47	0.47
1:B:274:MET:CE	1:B:277:LEU:HB3	2.45	0.47
1:B:162:ASN:O	1:B:166:GLU:HG3	2.15	0.47
1:C:162:ASN:ND2	1:D:161:LYS:HG2	2.30	0.47
1:A:239:ALA:O	1:A:243:GLU:HG3	2.14	0.47
1:A:226:LYS:HD3	2:A:524:HOH:O	2.15	0.46
1:D:147:ARG:N	2:D:703:HOH:O	2.47	0.46
1:A:220:LYS:HD2	2:A:573:HOH:O	2.14	0.46
1:B:168:GLU:O	1:B:172:LEU:HG	2.16	0.46
1:A:195:GLU:HG2	2:A:317:HOH:O	2.15	0.46
1:A:217:LYS:HD3	1:B:218:GLU:OE1	2.16	0.46
1:D:267:TYR:O	1:D:270:ILE:HG22	2.15	0.46
1:B:239:ALA:O	1:B:243:GLU:HG3	2.16	0.46
1:A:176:LEU:O	1:A:180:GLU:HG3	2.15	0.46
1:D:233:LYS:NZ	2:D:486:HOH:O	2.49	0.45
1:C:267:TYR:O	1:C:270:ILE:HG22	2.16	0.45
1:A:277:LEU:CD1	1:B:274:MET:CE	2.94	0.45
1:A:260:LEU:HD21	1:B:259:GLU:CD	2.37	0.45
1:C:149:LYS:HB3	1:C:149:LYS:HZ3	1.80	0.45
1:D:147:ARG:N	2:D:704:HOH:O	2.50	0.45
1:C:223:GLU:HB2	2:C:383:HOH:O	2.16	0.45
1:A:245:SER:O	1:A:248:LYS:HG2	2.18	0.44
1:B:266:LYS:NZ	2:B:409:HOH:O	2.49	0.44
1:C:221:TYR:CE2	1:D:218:GLU:HG3	2.52	0.44
1:C:245:SER:HA	1:C:248:LYS:HG2	2.00	0.44
1:A:158:LEU:HD23	1:A:161:LYS:HE3	2.00	0.43
1:C:248:LYS:HG3	1:C:249:LEU:N	2.33	0.43
1:B:161:LYS:HE2	1:B:165:LEU:HD11	2.00	0.43
1:B:205:LYS:HD3	2:B:656:HOH:O	2.18	0.43
1:A:240:GLU:HG2	1:A:244:ARG:NH2	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:MET:HG3	1:B:151:LEU:HD12	2.01	0.43
1:C:218:GLU:HG3	1:D:221:TYR:HE2	1.81	0.43
1:D:205:LYS:HE3	1:D:205:LYS:HB2	1.77	0.43
1:A:251:LYS:NZ	1:A:255:ASP:OD1	2.52	0.42
1:A:267:TYR:O	1:A:270:ILE:HG22	2.19	0.42
1:D:203:ASN:O	1:D:207:LEU:HD23	2.18	0.42
1:A:171:ARG:HD2	2:A:315:HOH:O	2.18	0.42
1:C:268:LYS:O	1:C:272:GLU:HG3	2.19	0.42
1:D:161:LYS:NZ	2:D:635:HOH:O	2.48	0.42
1:C:254:ASP:HB3	2:C:581:HOH:O	2.20	0.42
1:A:212:GLU:O	1:A:216:GLN:HG3	2.20	0.42
1:C:280:LYS:CE	2:C:582:HOH:O	2.67	0.42
1:D:274:MET:O	1:D:278:GLU:HG3	2.19	0.42
1:A:159:LEU:HB3	2:A:614:HOH:O	2.20	0.42
2:A:372:HOH:O	1:B:299:LYS:HE2	2.19	0.42
1:D:148:MET:O	1:D:152:GLU:HG2	2.20	0.42
1:A:157:GLU:O	1:A:161:LYS:HE2	2.20	0.41
1:D:147:ARG:HD3	2:D:391:HOH:O	2.20	0.41
1:C:251:LYS:HD2	1:C:251:LYS:HA	1.79	0.41
1:D:236:GLU:O	1:D:240:GLU:HG3	2.20	0.41
1:C:158:LEU:HD22	1:D:162:ASN:ND2	2.36	0.41
1:C:249:LEU:HD11	2:D:394:HOH:O	2.20	0.41
1:D:189:LYS:HE3	2:D:335:HOH:O	2.20	0.41
1:A:245:SER:HA	1:A:248:LYS:HG2	2.02	0.41
1:C:148:MET:O	1:C:151:LEU:HB2	2.21	0.41
1:C:226:LYS:HG3	2:C:412:HOH:O	2.20	0.41
1:A:147:ARG:HA	1:A:150:GLN:NE2	2.36	0.41
1:C:245:SER:O	1:C:249:LEU:HG	2.21	0.41
1:C:281:VAL:HG21	1:D:280:LYS:HD2	2.03	0.40
1:D:300:LYS:NZ	2:D:647:HOH:O	2.53	0.40
1:A:226:LYS:NZ	2:A:316:HOH:O	2.55	0.40
1:C:296:ALA:O	1:C:300:LYS:HD2	2.21	0.40
1:B:148:MET:O	1:B:148:MET:HG2	2.21	0.40
1:C:207:LEU:HD12	1:D:204:LEU:CD1	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	153/155 (99%)	152 (99%)	1 (1%)	0	100	100
1	B	152/155 (98%)	152 (100%)	0	0	100	100
1	C	152/155 (98%)	152 (100%)	0	0	100	100
1	D	153/155 (99%)	152 (99%)	0	1 (1%)	22	10
All	All	610/620 (98%)	608 (100%)	1 (0%)	1 (0%)	47	33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	148	MET

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	142/142 (100%)	141 (99%)	1 (1%)	84	81
1	B	141/142 (99%)	141 (100%)	0	100	100
1	C	141/142 (99%)	138 (98%)	3 (2%)	53	42
1	D	142/142 (100%)	140 (99%)	2 (1%)	67	59
All	All	566/568 (100%)	560 (99%)	6 (1%)	73	68

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	263	GLN
1	C	148	MET
1	C	214	TYR
1	C	275	LYS
1	D	274	MET
1	D	275	LYS

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

Mol	Chain	Res	Type
1	A	150	GLN
1	A	263	GLN
1	A	276	GLN
1	C	263	GLN

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 monosaccharides 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	155/155 (100%)	-0.23	1 (0%) 89 87	26, 40, 54, 63	0
1	B	154/155 (99%)	-0.35	0 100 100	26, 37, 52, 63	0
1	C	154/155 (99%)	-0.25	0 100 100	26, 40, 53, 64	0
1	D	155/155 (100%)	-0.34	0 100 100	25, 37, 52, 64	0
All	All	618/620 (99%)	-0.29	1 (0%) 95 93	25, 38, 53, 64	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	301	LEU	2.9

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.