Full wwPDB X-ray Structure Validation Report (i)

Jun 24, 2024 – 05:41 PM EDT

PDB ID	:	6IKN
Title	:	Crystal structure of the GAS7 F-BAR domain
Authors	:	Hanawa-Suetsugu, K.; Itoh, Y.; Kohda, D.; Shimada, A.; Suetsugu, S.
Deposited on	:	2018-10-16
Resolution	:	3.00 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 (i) 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 (i)) were used in the production of this report:

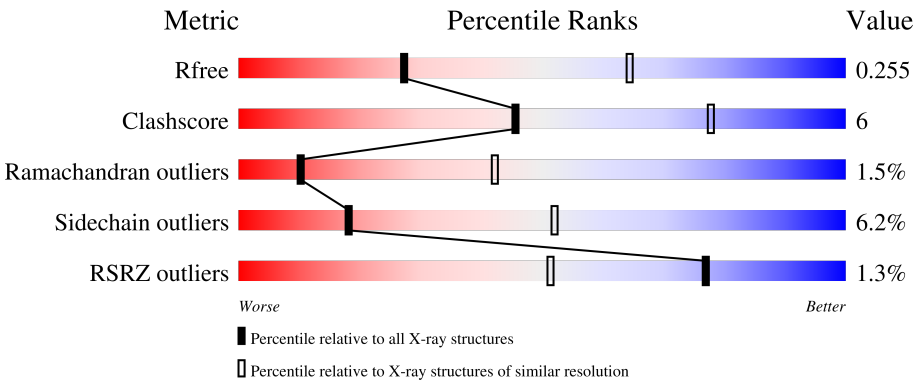
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	331	77% 12% • • 8%
1	B	331	76% 13% • 8%
1	C	331	76% 13% • 8%
1	D	331	4% 73% 15% • 8%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 10017 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 Growth arrest-specific protein 7.

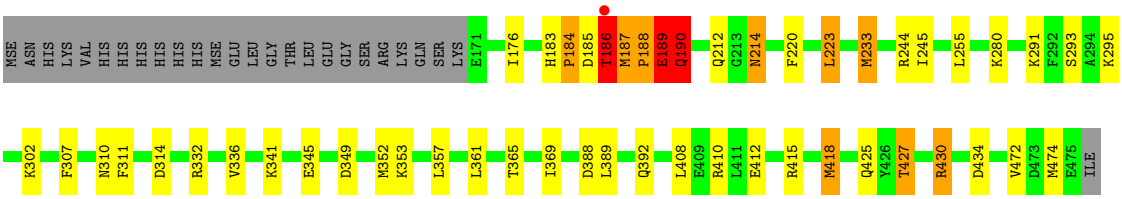
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	305	2511	1566	446	483	5	11	0	0	0
1	B	304	2502	1561	445	480	5	11	0	0	0
1	C	304	2502	1561	445	480	5	11	0	0	0
1	D	304	2502	1561	445	480	5	11	0	0	0

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.

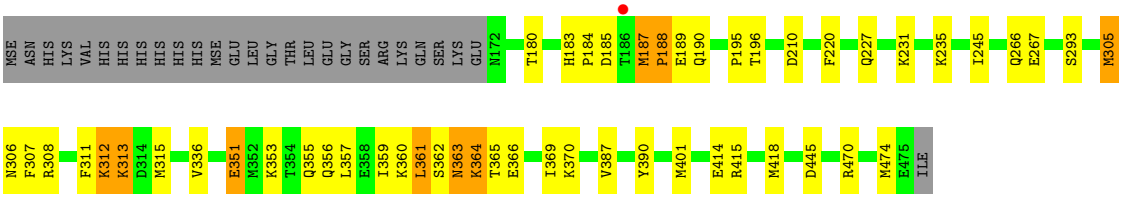
• Molecule 1: Growth arrest-specific protein 7

Chain A:



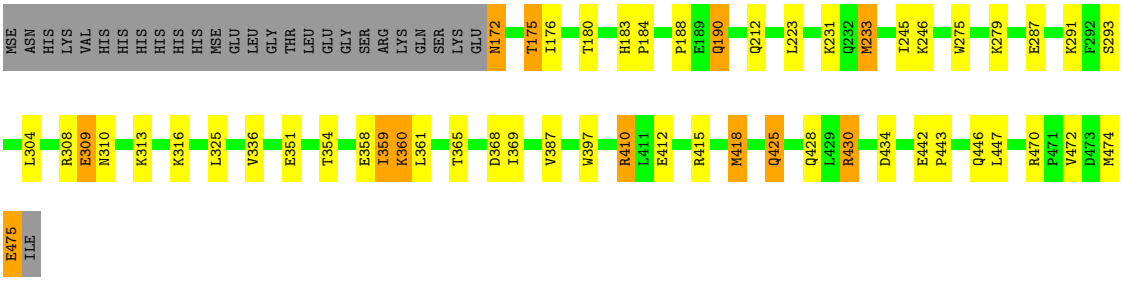
• Molecule 1: Growth arrest-specific protein 7

Chain B:



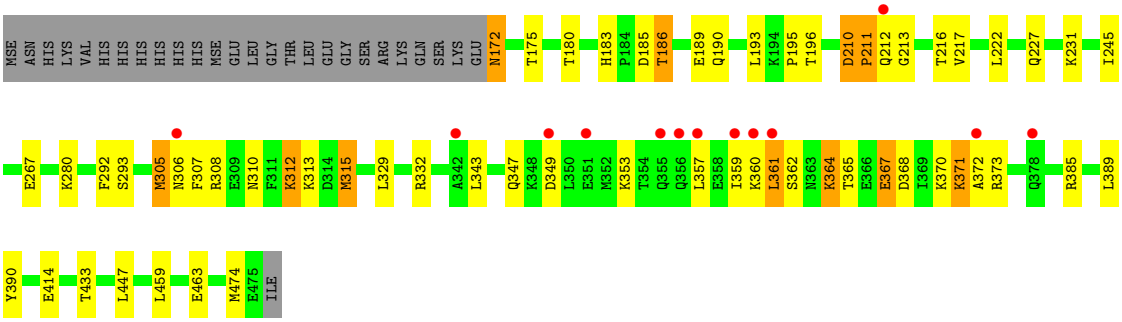
• Molecule 1: Growth arrest-specific protein 7

Chain C:



• Molecule 1: Growth arrest-specific protein 7

Chain D:


MSE
ASN
HIS
LYS
VAL
HIS
HIS
HIS
HIS
HIS
MSE
GLU
LEU
GLY
THR
LEU
GLU
GLY
SER
ARG
LYS
GLN
SER
LYS
GLU
N172
T175
T180
H183
P184
D185
T186
E189
Q190
L193
K194
P195
T196
D210
P211
Q212
G213
T216
V217
L222
Q227
K231
I245
E267
K280
F292
S293
M305
N306
F307
R308
E309
N310
F311
K312
K313
D314
M315
L329
R332
A342
L343
Q347
K348
D349
L350
E351
M352
K353
T354
Q355
Q356
L357
E358
I359
K360
L361
S362
N363
K364
T365
E366
E367
D368
I369
K370
K371
A372
R373
Q378
R385
L389
Y390
E414
T433
L447
L459
E463
M474
E475
ILE

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	53.26Å 87.28Å 88.79Å 80.98° 74.72° 79.73°	Depositor
Resolution (Å)	32.03 – 3.00 41.15 – 2.94	Depositor EDS
% Data completeness (in resolution range)	98.8 (32.03-3.00) 95.3 (41.15-2.94)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.61 (at 2.95Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.194 , 0.255 0.194 , 0.255	Depositor DCC
R_{free} test set	1533 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	53.8	Xtriage
Anisotropy	0.330	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 47.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10017	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.05% 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 (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	0.29	0/2541	0.49	0/3391
1	B	0.28	0/2532	0.49	0/3379
1	C	0.28	0/2532	0.48	0/3379
1	D	0.27	0/2532	0.47	0/3379
All	All	0.28	0/10137	0.48	0/13528

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	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	184	PRO	Peptide

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	2511	0	2508	33	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2502	0	2502	33	0
1	C	2502	0	2502	38	0
1	D	2502	0	2502	42	0
All	All	10017	0	10014	129	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 6.

All (129) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:475:GLU:HG2	1:D:172:ASN:HB2	1.67	0.77
1:B:308:ARG:NH1	1:B:414:GLU:OE1	2.18	0.76
1:B:361:LEU:HA	1:B:362:SER:HB3	1.67	0.75
1:D:227:GLN:HG2	1:D:315:MSE:HE2	1.69	0.72
1:B:353:LYS:HB3	1:B:369:ILE:HD12	1.72	0.71
1:D:359:ILE:O	1:D:361:LEU:N	2.23	0.70
1:B:185:ASP:HB3	1:B:187:MSE:HB3	1.75	0.68
1:A:186:THR:HG22	1:A:187:MSE:H	1.58	0.67
1:A:185:ASP:HB2	1:A:187:MSE:H	1.61	0.66
1:D:308:ARG:NH1	1:D:414:GLU:OE1	2.30	0.64
1:D:189:GLU:HB3	1:D:190:GLN:HB2	1.80	0.62
1:A:183:HIS:HB3	1:A:184:PRO:O	2.01	0.61
1:C:359:ILE:HD12	1:C:360:LYS:H	1.66	0.59
1:C:472:VAL:O	1:D:180:THR:OG1	2.20	0.59
1:C:415:ARG:NH2	1:D:267:GLU:OE1	2.36	0.58
1:A:185:ASP:HB2	1:A:187:MSE:N	2.19	0.58
1:C:365:THR:O	1:C:369:ILE:HG13	2.04	0.58
1:C:308:ARG:HH22	1:C:415:ARG:HB2	1.69	0.57
1:C:231:LYS:NZ	1:C:308:ARG:O	2.28	0.57
1:A:186:THR:CG2	1:A:187:MSE:H	2.18	0.57
1:C:430:ARG:NH2	1:C:434:ASP:OD2	2.38	0.56
1:B:187:MSE:HG2	1:B:188:PRO:O	2.06	0.56
1:C:304:LEU:HA	1:C:418:MSE:HE1	1.86	0.56
1:A:185:ASP:HB2	1:A:186:THR:HG22	1.87	0.55
1:D:332:ARG:HE	1:D:389:LEU:HB3	1.72	0.55
1:C:233:MSE:HG2	1:D:267:GLU:HB2	1.88	0.55
1:A:412:GLU:OE2	1:A:415:ARG:NH1	2.41	0.54
1:C:336:VAL:HG11	1:D:474:MSE:HE1	1.89	0.54
1:C:425:GLN:NE2	1:C:428:GLN:OE1	2.41	0.54
1:D:312:LYS:HG3	1:D:313:LYS:HG3	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:309:GLU:CD	1:C:309:GLU:H	2.10	0.54
1:B:245:ILE:HG23	1:B:293:SER:HB2	1.90	0.53
1:C:443:PRO:O	1:C:446:GLN:HG2	2.09	0.53
1:C:412:GLU:OE2	1:C:415:ARG:NH1	2.43	0.52
1:A:190:GLN:OE1	1:B:470:ARG:N	2.33	0.52
1:B:357:LEU:HD12	1:B:369:ILE:HG13	1.92	0.52
1:A:474:MSE:HE1	1:B:336:VAL:HG21	1.90	0.52
1:D:185:ASP:OD1	1:D:186:THR:N	2.43	0.51
1:A:430:ARG:NH2	1:A:434:ASP:OD2	2.43	0.51
1:D:292:PHE:CD1	1:D:433:THR:HG21	2.46	0.50
1:D:365:THR:O	1:D:368:ASP:HB2	2.10	0.50
1:C:245:ILE:HG23	1:C:293:SER:HB2	1.94	0.50
1:A:349:ASP:OD1	1:A:353:LYS:NZ	2.44	0.50
1:B:356:GLN:HA	1:B:359:ILE:HG12	1.94	0.49
1:D:210:ASP:HB3	1:D:217:VAL:HG22	1.93	0.49
1:D:353:LYS:HD3	1:D:368:ASP:HB3	1.93	0.49
1:A:186:THR:CG2	1:A:187:MSE:N	2.75	0.49
1:A:415:ARG:NH2	1:B:267:GLU:OE1	2.45	0.49
1:C:425:GLN:HE21	1:C:425:GLN:HA	1.78	0.49
1:A:332:ARG:HE	1:A:389:LEU:HB3	1.77	0.48
1:B:195:PRO:HA	1:B:196:THR:HA	1.50	0.48
1:C:313:LYS:HG3	1:C:316:LYS:HE2	1.96	0.48
1:B:189:GLU:HB3	1:B:190:GLN:CA	2.43	0.47
1:A:341:LYS:NZ	1:A:345:GLU:OE2	2.45	0.47
1:C:275:TRP:NE1	1:C:279:LYS:HE3	2.29	0.47
1:C:387:VAL:HG13	1:D:474:MSE:HE2	1.95	0.47
1:A:474:MSE:HE3	1:B:387:VAL:HG22	1.97	0.47
1:B:362:SER:OG	1:B:363:ASN:N	2.47	0.47
1:A:185:ASP:H	1:A:186:THR:C	2.18	0.46
1:C:309:GLU:HB2	1:C:310:ASN:OD1	2.15	0.46
1:C:183:HIS:ND1	1:C:184:PRO:HD2	2.30	0.46
1:D:343:LEU:O	1:D:347:GLN:HG2	2.16	0.46
1:A:233:MSE:HG2	1:B:267:GLU:HB2	1.98	0.46
1:D:189:GLU:HB3	1:D:190:GLN:CB	2.45	0.46
1:D:385:ARG:HH21	1:D:389:LEU:HD11	1.81	0.46
1:D:175:THR:OG1	1:D:180:THR:HG22	2.17	0.45
1:D:305:MSE:O	1:D:307:PHE:N	2.48	0.45
1:C:359:ILE:CD1	1:C:360:LYS:H	2.29	0.45
1:D:371:LYS:HG3	1:D:372:ALA:N	2.32	0.45
1:C:175:THR:HG22	1:C:180:THR:HG23	1.99	0.45
1:B:235:LYS:HG3	1:B:305:MSE:HE3	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:LYS:H	1:B:313:LYS:HG3	1.58	0.45
1:C:359:ILE:HD12	1:C:360:LYS:N	2.31	0.45
1:C:183:HIS:CG	1:C:184:PRO:HD2	2.52	0.45
1:D:310:ASN:HA	1:D:312:LYS:HE3	1.98	0.45
1:A:220:PHE:HA	1:A:223:LEU:HD22	1.99	0.45
1:D:195:PRO:HA	1:D:196:THR:HA	1.50	0.45
1:D:332:ARG:HB3	1:D:390:TYR:HA	1.99	0.45
1:A:472:VAL:O	1:B:180:THR:OG1	2.35	0.44
1:D:183:HIS:ND1	1:D:185:ASP:OD1	2.50	0.44
1:A:233:MSE:SE	1:B:266:GLN:HG3	2.67	0.44
1:A:245:ILE:HG23	1:A:293:SER:HB2	2.00	0.44
1:C:360:LYS:NZ	1:C:360:LYS:HB2	2.32	0.44
1:D:180:THR:HG23	1:D:390:TYR:OH	2.16	0.44
1:B:189:GLU:HB3	1:B:190:GLN:HA	1.98	0.43
1:C:291:LYS:HE2	1:C:291:LYS:HB3	1.83	0.43
1:D:305:MSE:C	1:D:307:PHE:H	2.21	0.43
1:A:388:ASP:O	1:A:392:GLN:HG3	2.18	0.43
1:B:227:GLN:HG2	1:B:315:MSE:HE2	2.00	0.43
1:D:212:GLN:HB3	1:D:213:GLY:H	1.49	0.43
1:B:189:GLU:HB3	1:B:190:GLN:HB2	2.00	0.43
1:C:410:ARG:HE	1:C:410:ARG:HB2	1.67	0.43
1:D:313:LYS:NZ	1:D:313:LYS:HB2	2.34	0.43
1:B:366:GLU:HA	1:B:369:ILE:HG12	2.01	0.42
1:C:447:LEU:HD23	1:C:447:LEU:HA	1.91	0.42
1:D:211:PRO:HB2	1:D:212:GLN:H	1.68	0.42
1:A:214:ASN:O	1:A:214:ASN:ND2	2.46	0.42
1:A:255:LEU:HD12	1:A:255:LEU:HA	1.93	0.42
1:A:307:PHE:CD2	1:A:418:MSE:HE2	2.54	0.42
1:A:311:PHE:HA	1:A:314:ASP:HB2	2.01	0.42
1:B:364:LYS:O	1:B:364:LYS:HD3	2.19	0.42
1:B:307:PHE:CG	1:B:418:MSE:HE3	2.54	0.42
1:C:172:ASN:N	1:C:172:ASN:ND2	2.67	0.42
1:D:245:ILE:HG23	1:D:293:SER:HB2	2.02	0.42
1:D:364:LYS:HE2	1:D:364:LYS:HB3	1.73	0.42
1:D:459:LEU:O	1:D:463:GLU:HG2	2.19	0.42
1:C:304:LEU:HD23	1:C:418:MSE:HE1	2.02	0.42
1:A:188:PRO:HB2	1:A:189:GLU:H	1.55	0.42
1:A:357:LEU:HD12	1:A:361:LEU:HA	2.02	0.42
1:D:364:LYS:O	1:D:367:GLU:HG3	2.20	0.42
1:A:336:VAL:HG21	1:B:474:MSE:HE1	2.01	0.42
1:C:351:GLU:O	1:C:354:THR:OG1	2.32	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:PHE:HB2	1:B:401:MSE:HE1	2.02	0.41
1:A:427:THR:HG21	1:B:445:ASP:OD1	2.20	0.41
1:C:246:LYS:HD3	1:C:246:LYS:HA	1.79	0.41
1:C:325:LEU:HD13	1:C:397:TRP:HA	2.02	0.41
1:A:291:LYS:HE2	1:A:295:LYS:NZ	2.36	0.41
1:D:353:LYS:HE2	1:D:371:LYS:HE2	2.03	0.41
1:D:367:GLU:O	1:D:370:LYS:HB3	2.21	0.41
1:A:365:THR:O	1:A:369:ILE:HG13	2.21	0.41
1:B:188:PRO:O	1:B:189:GLU:HB2	2.21	0.41
1:C:442:GLU:HB2	1:C:443:PRO:HD3	2.02	0.41
1:D:447:LEU:HD23	1:D:447:LEU:HA	1.86	0.41
1:C:470:ARG:HD3	1:D:193:LEU:HG	2.02	0.41
1:C:474:MSE:HG3	1:D:180:THR:HG21	2.02	0.41
1:D:292:PHE:HB2	1:D:433:THR:HG21	2.03	0.41
1:B:180:THR:HG23	1:B:390:TYR:OH	2.20	0.40
1:B:351:GLU:O	1:B:355:GLN:HG2	2.21	0.40
1:B:415:ARG:O	1:B:418:MSE:HG3	2.21	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	303/331 (92%)	290 (96%)	7 (2%)	6 (2%)	7 34
1	B	302/331 (91%)	287 (95%)	12 (4%)	3 (1%)	15 53
1	C	302/331 (91%)	289 (96%)	8 (3%)	5 (2%)	9 39
1	D	302/331 (91%)	289 (96%)	9 (3%)	4 (1%)	12 45
All	All	1209/1324 (91%)	1155 (96%)	36 (3%)	18 (2%)	10 42

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	184	PRO
1	C	190	GLN
1	C	358	GLU
1	C	359	ILE
1	D	306	ASN
1	D	360	LYS
1	A	186	THR
1	A	188	PRO
1	D	211	PRO
1	A	189	GLU
1	A	190	GLN
1	B	188	PRO
1	C	361	LEU
1	A	187	MSE
1	B	312	LYS
1	C	188	PRO
1	D	362	SER
1	B	306	ASN

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	277/288 (96%)	258 (93%)	19 (7%)	15	48
1	B	276/288 (96%)	261 (95%)	15 (5%)	22	57
1	C	276/288 (96%)	260 (94%)	16 (6%)	20	55
1	D	276/288 (96%)	258 (94%)	18 (6%)	17	50
All	All	1105/1152 (96%)	1037 (94%)	68 (6%)	18	52

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	176	ILE
1	A	186	THR
1	A	189	GLU
1	A	190	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	212	GLN
1	A	214	ASN
1	A	223	LEU
1	A	233	MSE
1	A	244	ARG
1	A	280	LYS
1	A	302	LYS
1	A	310	ASN
1	A	352	MSE
1	A	408	LEU
1	A	410	ARG
1	A	418	MSE
1	A	425	GLN
1	A	427	THR
1	A	430	ARG
1	B	183	HIS
1	B	187	MSE
1	B	210	ASP
1	B	231	LYS
1	B	305	MSE
1	B	311	PHE
1	B	312	LYS
1	B	313	LYS
1	B	351	GLU
1	B	360	LYS
1	B	361	LEU
1	B	363	ASN
1	B	364	LYS
1	B	365	THR
1	B	370	LYS
1	C	172	ASN
1	C	175	THR
1	C	176	ILE
1	C	190	GLN
1	C	212	GLN
1	C	223	LEU
1	C	233	MSE
1	C	287	GLU
1	C	309	GLU
1	C	360	LYS
1	C	368	ASP
1	C	410	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	418	MSE
1	C	425	GLN
1	C	430	ARG
1	C	475	GLU
1	D	172	ASN
1	D	186	THR
1	D	210	ASP
1	D	216	THR
1	D	222	LEU
1	D	231	LYS
1	D	280	LYS
1	D	305	MSE
1	D	312	LYS
1	D	315	MSE
1	D	329	LEU
1	D	349	ASP
1	D	357	LEU
1	D	361	LEU
1	D	364	LYS
1	D	367	GLU
1	D	371	LYS
1	D	373	ARG

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

Mol	Chain	Res	Type
1	C	172	ASN
1	C	425	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 monosaccharides 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	294/331 (88%)	-0.48	1 (0%)	94	84	35, 59, 106, 139	0
1	B	293/331 (88%)	-0.35	1 (0%)	94	84	30, 62, 132, 187	0
1	C	293/331 (88%)	-0.46	0	100	100	40, 66, 125, 174	0
1	D	293/331 (88%)	-0.06	13 (4%)	34	13	32, 75, 164, 211	0
All	All	1173/1324 (88%)	-0.34	15 (1%)	77	51	30, 65, 135, 211	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	212	GLN	4.7
1	D	349	ASP	3.8
1	D	356	GLN	3.4
1	D	378	GLN	3.2
1	B	186	THR	3.0
1	D	342	ALA	3.0
1	D	372	ALA	2.9
1	D	355	GLN	2.7
1	A	186	THR	2.4
1	D	361	LEU	2.4
1	D	359	ILE	2.4
1	D	360	LYS	2.3
1	D	306	ASN	2.2
1	D	357	LEU	2.0
1	D	351	GLU	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 monosaccharides 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.