

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	8V9O
Title	:	Imaging scaffold engineered to bind the therapeutic protein target BARD1
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Deposited on	:	2023-12-08
Resolution	:	3.81 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 (1)) were used in the production of this report:

MolProbity		4 09b 467
Mon robity	•	4.020-407
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
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)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 3.81 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.



Motria	Whole archive	Similar resolution		
Metric	$(\# {\rm Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$		
R _{free}	130704	1231 (4.04-3.60)		
Clashscore	141614	$1031 \ (4.02-3.62)$		
Ramachandran outliers	138981	$1261 \ (4.04-3.60)$		
Sidechain outliers	138945	1255 (4.04-3.60)		
RSRZ outliers	127900	1139 (4.04-3.60)		

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 -	3%		
	A	178	75%	14%	• 11%
	D	1 -	4%		
1	В	178	76%	13%	11%
	~		4%		
1	С	178	78%	9% •	12%
			.%		
2	D	322	74%	20%	7%
			3%		
2	E	322	71%	22%	7%



Mol	Chain	Length	Quality of chain		
			5%		
2	F	322	69%	24%	7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CA	А	401	-	-	-	Х



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10640 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Λ	150	Total	С	Ν	0	S	0	0	0
1	Л	109	1261	807	214	236	4	0	0	0
1	В	150	Total	С	Ν	0	S	0	0	0
	D	109	1261	807	214	236	4	0	0	0
1	C	156	Total	С	Ν	0	S	0	0	0
		100	1237	793	208	232	4			U

• Molecule 1 is a protein called Tetrahedral Nanocage Cage, Non-Fusion Component.

• Molecule 2 is a protein called Tetrahedral Nanocage Cage Component Fused to Anti-BARD1 Darpin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
	201	Total	С	Ν	Ο	S	0	0	0	
	D	501	2300	1443	401	450	6	0	0	0
0	F	200	Total	С	Ν	0	S	0	0	0
		299	2286	1436	399	445	6	0		
0	Б	300	Total	С	Ν	0	S	0	0	0
	Г		2294	1440	400	448	6	0	0	0

• Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	Total Ca 1 1	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: Tetrahedral Nanocage Cage, Non-Fusion Component



• Molecule 2: Tetrahedral Nanocage Cage Component Fused to Anti-BARD1 Darpin

Chain E	3%	71%	22%	7%
MET PHE THR ARG ARG GLY	CLN CLN CLY CLY CLY CLY CLY ASP ASP ASS ASS ASS ASS ASS ASS ASS ASS	823 139 145 145 145 145 145 165 165 171 171 171 171 171 171 171	100 184 184 187 187 187 187 187 187 110 110 1110	8112 8113 8114 115 115 136
N141 N147 1152 L153	H156 N161 2179 2179 2000 2200 2200 2200 2200	1226 1226 1230 1237 1235 1246 1246 1246 1246 1246 1246 1251 1255 1255 1255 1255 1255 1255 125	V250 V250 N260 N261 S262 D263 D263 T268	H271 1 1272 4 A273 4274 4275 4 A276 4275 5 E280
1281 V282 D283 V284 L285 L285	H288 4289 4290 4292 4293 4295 4295 4295 7300 1304 1304	L305 1307 1307 1307 1318 1318 1318 1318 1318 1318 1318 131		
• Molecu	le 2: Tetrahedral Na	nocage Cage Component Fuse	ed to Anti-B.	ARD1 Darpin
Chain F:	5%	69%	24%	7%
	CLV CLV CLV CLV CLV CLV ASP ASP ASP ASP ASP ASP ASP CLV CLV CLV CLV CLV CLV CLV CLV CLV CLV	V25 139 441 145 145 164 059 059 059 059 059 059 059 059 059 059	24%	M119 1129 V142 N147
Chain F: HISE HISE VIII HISE VIIII VIIII VIIII VIIII VIIII VIIII VIIII VIIII VIIIII VIIIII VIIII VIIII VIIIIIII VIIII VIIII VIIII VIIIIIIII	22%	M194 V25 A195 V25 A195 V25 A195 V25 P202 P202 P202 P203 P203 P203 P203 P203	1237 1238 1238 1248 1248 1248 1248 1248 1248 1248 124	L253 R264 W266 W269 N260 N142 N260 N147



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants	128.01Å 195.57Å 228.37Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Bosolution(A)	19.99 - 3.81	Depositor
Resolution (A)	19.99 - 3.81	EDS
% Data completeness	99.5 (19.99-3.81)	Depositor
(in resolution range)	89.7 (19.99-3.81)	EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.00 (at 3.82 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
P. P.	0.197 , 0.231	Depositor
n, n_{free}	0.201 , 0.230	DCC
R_{free} test set	2816 reflections (10.00%)	wwPDB-VP
Wilson B-factor $(Å^2)$	147.2	Xtriage
Anisotropy	0.282	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.29, 114.9	EDS
L-test for $twinning^2$	$ < L >=0.47, < L^2>=0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10640	wwPDB-VP
Average B, all atoms $(Å^2)$	188.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.33% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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).

Mal	Chain	Bond	lengths	Bond angles		
		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.27	0/1276	0.53	0/1711	
1	В	0.26	0/1276	0.51	0/1711	
1	С	0.26	0/1252	0.50	0/1679	
2	D	0.25	0/2333	0.45	0/3160	
2	Е	0.27	0/2319	0.45	0/3142	
2	F	0.27	0/2327	0.47	0/3153	
All	All	0.26	0/10783	0.48	0/14556	

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 (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	А	1261	0	1314	20	0
1	В	1261	0	1314	14	0
1	С	1237	0	1287	16	0
2	D	2300	0	2297	36	0
2	Е	2286	0	2288	43	0
2	F	2294	0	2292	47	0
3	А	1	0	0	0	0
All	All	10640	0	10792	163	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 8.

All (163) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom_1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
2:D:253:LEU:HD11	2:D:285:LEU:HD23	1.74	0.69
2:F:292:VAL:HG13	2:F:318:LEU:HB3	1.75	0.68
2:F:275:GLN:HE21	2:F:305:LEU:HD13	1.60	0.66
2:F:226:ILE:HD13	2:F:255:TRP:HB3	1.76	0.66
2:D:213:LEU:HD11	2:D:251:LEU:HD12	1.79	0.65
2:F:260:ASN:HA	2:F:268:THR:HB	1.77	0.65
2:E:71:THR:HB	2:E:74:LYS:HB2	1.79	0.65
2:E:295:GLN:HG2	2:E:301:THR:HG22	1.77	0.64
2:E:286:LEU:HD11	2:E:318:LEU:HD23	1.79	0.64
2:E:286:LEU:HD23	2:E:290:ALA:HB3	1.80	0.64
2:D:187:LEU:HD11	2:D:219:LEU:HD23	1.80	0.63
2:E:109:SER:O	2:E:113:ALA:N	2.28	0.63
2:E:213:LEU:HD11	2:E:251:LEU:HD12	1.80	0.62
2:F:295:GLN:HG2	2:F:301:THR:HG22	1.82	0.62
2:F:300:LYS:HD3	2:F:308:ASP:OD2	2.00	0.62
2:F:253:LEU:HD11	2:F:285:LEU:HD23	1.81	0.61
2:D:174:ALA:HB1	2:D:179:GLN:HB2	1.82	0.60
2:F:166:GLU:HG3	2:F:170:LYS:HE3	1.84	0.60
2:E:253:LEU:HD11	2:E:285:LEU:HD23	1.83	0.59
1:B:43:GLU:OE2	1:C:114:LYS:NZ	2.25	0.59
2:F:258:ASP:HB3	2:F:261:ALA:HB2	1.83	0.58
2:F:286:LEU:HD23	2:F:290:ALA:HB3	1.85	0.58
2:E:226:ILE:HD13	2:E:255:TRP:HB3	1.85	0.57
1:A:143:ALA:HB1	1:C:22:TRP:CZ3	2.39	0.57
1:A:105:LEU:HD11	1:C:60:GLN:HB3	1.85	0.57
1:A:143:ALA:HB1	1:C:22:TRP:HZ3	1.69	0.57
1:B:65:LYS:HE3	1:B:79:ILE:HA	1.87	0.57
2:F:270:LEU:HD11	2:F:282:VAL:HG13	1.87	0.57
2:D:286:LEU:HD23	2:D:290:ALA:HB3	1.86	0.56
2:F:291:ASP:OD2	2:F:294:ALA:HB2	2.06	0.55
2:E:64:VAL:HG22	2:E:76:ARG:HD3	1.88	0.55
2:E:275:GLN:HE21	2:E:305:LEU:HD13	1.71	0.55
2:D:179:GLN:HB3	2:D:182:GLU:HB2	1.89	0.55
2:E:86:LEU:HD22	2:E:152:ILE:HG21	1.88	0.55
2:E:292:VAL:HG21	2:E:321:ALA:HB3	1.88	0.55
2:F:267:LYS:HD3	2:F:275:GLN:HE22	1.72	0.55
2:E:300:LYS:HD3	2:E:308:ASP:OD2	2.06	0.54



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:D:109:SER:O	2:D:113:ALA:N	2.32	0.54
2:F:174:ALA:HB1	2:F:179:GLN:HB2	1.91	0.53
2:D:86:LEU:HD22	2:D:152:ILE:HG21	1.91	0.52
2:F:251:LEU:HD23	2:F:254:ARG:HD2	1.91	0.52
1:B:119:ARG:HD3	1:B:154:PHE:HB2	1.90	0.52
1:C:17:GLY:HA2	2:E:80:MET:HB3	1.92	0.51
1:C:65:LYS:HE3	1:C:79:ILE:HA	1.92	0.51
2:D:47:ARG:NH1	2:D:190:GLY:HA3	2.26	0.51
2:D:83:ILE:O	2:D:87:ILE:HG13	2.11	0.51
2:D:246:LEU:HD22	2:D:280:GLU:HG3	1.92	0.50
1:A:119:ARG:HD3	1:A:154:PHE:HB2	1.92	0.50
2:D:32:ILE:HG12	2:D:125:LEU:HD21	1.92	0.50
2:E:45:LEU:HD12	2:E:114:SER:HB3	1.92	0.50
2:E:292:VAL:HG13	2:E:318:LEU:HB3	1.93	0.50
2:D:213:LEU:HD22	2:D:247:GLU:HB3	1.94	0.49
1:C:62:ASP:HA	1:C:65:LYS:HD3	1.95	0.49
1:A:65:LYS:HE3	1:A:79:ILE:HA	1.95	0.49
2:E:179:GLN:HB3	2:E:182:GLU:HB2	1.93	0.49
2:E:260:ASN:HA	2:E:268:THR:HB	1.95	0.49
2:E:46:SER:HA	2:E:111:GLU:HB3	1.94	0.48
1:C:91:ILE:HD11	1:C:148:LEU:O	2.13	0.48
2:D:71:THR:HB	2:D:74:LYS:HB2	1.94	0.48
2:E:301:THR:N	2:E:304:ASP:HB2	2.29	0.48
1:A:48:VAL:HG12	1:A:160:ILE:HD11	1.96	0.48
2:D:94:LYS:HG2	2:D:100:ILE:HD11	1.96	0.48
2:D:202:THR:O	2:D:206:VAL:HG23	2.14	0.47
2:E:270:LEU:HD11	2:E:282:VAL:HG13	1.95	0.47
1:A:114:LYS:NZ	1:C:43:GLU:OE2	2.37	0.47
2:F:83:ILE:O	2:F:87:ILE:HG13	2.15	0.47
2:E:200:GLY:HA3	2:E:230:ASP:HA	1.96	0.47
2:E:208:ALA:HA	2:E:248:ILE:HD13	1.97	0.47
2:F:208:ALA:HA	2:F:248:ILE:HD13	1.97	0.47
2:D:111:GLU:H	2:D:111:GLU:CD	2.18	0.47
2:F:129:ILE:HD13	2:F:142:VAL:HG12	1.97	0.47
1:C:47:TYR:CZ	1:C:114:LYS:HE3	2.50	0.47
2:E:270:LEU:HD11	2:E:318:LEU:HD21	1.97	0.46
2:F:45:LEU:HD12	2:F:114:SER:HB3	1.96	0.46
2:E:301:THR:H	2:E:304:ASP:HB2	1.80	0.46
1:A:164:LYS:HE2	1:A:164:LYS:HB2	1.80	0.46
2:F:271:HIS:NE2	2:F:302:PRO:HD3	2.30	0.46
1:C:105:LEU:HD12	1:C:106:PRO:HD2	1.97	0.46



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:91:ILE:HD11	1:B:148:LEU:O	2.16	0.46
1:B:105:LEU:HD12	1:B:106:PRO:HD2	1.98	0.46
2:F:316:GLU:O	2:F:320:LYS:HG2	2.16	0.46
2:F:213:LEU:HD11	2:F:251:LEU:HD12	1.98	0.46
2:F:271:HIS:HE1	2:F:294:ALA:HB3	1.81	0.46
2:E:55:LEU:HD11	2:E:115:LEU:HD21	1.98	0.45
2:F:119:ARG:HD2	2:F:154:PHE:HB2	1.98	0.45
1:A:69:GLU:HB2	1:A:78:GLY:HA3	1.98	0.45
2:D:200:GLY:HA3	2:D:230:ASP:HA	1.99	0.45
2:E:258:ASP:HB3	2:E:261:ALA:HB2	1.98	0.45
1:A:111:GLU:OE1	1:A:164:LYS:HE3	2.17	0.45
1:A:18:GLY:HA3	1:B:151:ARG:HD3	1.99	0.45
2:D:286:LEU:HD11	2:D:318:LEU:HD23	1.98	0.45
2:D:226:ILE:HD13	2:D:255:TRP:HB3	1.99	0.45
2:E:199:LYS:O	2:E:231:SER:N	2.39	0.45
1:A:168:LYS:HG3	1:A:171:ARG:HH21	1.81	0.45
1:B:60:GLN:HB3	1:C:105:LEU:HD11	1.99	0.44
2:F:275:GLN:NE2	2:F:305:LEU:HD13	2.29	0.44
1:A:34:LEU:HD21	1:A:146:LEU:HD11	1.99	0.44
2:D:46:SER:HA	2:D:111:GLU:HB3	2.00	0.44
2:F:55:LEU:O	2:F:59:GLN:HG3	2.17	0.44
2:F:195:ALA:O	2:F:203:PRO:HD3	2.18	0.44
2:E:83:ILE:O	2:E:87:ILE:HG13	2.18	0.44
1:B:29:GLU:HB3	1:B:128:LYS:HD3	2.00	0.44
2:D:47:ARG:HH12	2:D:164:LYS:HE2	1.83	0.44
2:F:270:LEU:HB2	2:F:290:ALA:HB1	2.00	0.44
2:F:261:ALA:O	2:F:268:THR:HA	2.19	0.43
2:D:167:LEU:HB3	2:D:191:ALA:HB2	2.01	0.43
2:D:295:GLN:HG2	2:D:301:THR:HG22	2.01	0.43
2:D:222:ARG:HD3	2:D:222:ARG:HA	1.75	0.43
2:F:187:LEU:HD11	2:F:219:LEU:HD23	2.00	0.43
2:F:194:ASN:OD1	2:F:224:ALA:HA	2.19	0.43
2:E:283:ASP:OD1	2:E:317:VAL:HG11	2.19	0.43
2:D:41:TYR:O	2:D:44:VAL:HG12	2.19	0.43
2:D:216:VAL:HG21	2:D:248:ILE:HD13	2.01	0.43
2:F:202:THR:O	2:F:206:VAL:HG23	2.18	0.43
2:E:227:ASN:HA	2:E:236:PRO:HD2	2.01	0.42
2:E:251:LEU:HD23	2:E:254:ARG:HD2	2.00	0.42
2:F:109:SER:O	2:F:113:ALA:N	2.40	0.42
2:F:238:HIS:HE2	2:F:269:PRO:HD3	1.84	0.42
2:F:41:TYR:O	2:F:44:VAL:HG12	2.19	0.42



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:168:LYS:O	1:B:171:ARG:HG2	2.20	0.42
2:F:185:ALA:HB1	2:F:189:LYS:NZ	2.34	0.42
1:A:95:SER:HB3	1:C:15:LEU:HD22	2.01	0.42
1:A:101:LEU:HD13	1:A:104:VAL:HG21	2.01	0.42
2:D:129:ILE:HD13	2:D:142:VAL:HG12	2.01	0.42
2:F:39:ILE:HD11	2:F:153:LEU:HD11	2.02	0.42
1:A:24:ASP:OD1	1:B:127:ARG:NH1	2.53	0.42
1:A:95:SER:HB2	1:C:15:LEU:HD13	2.00	0.42
2:D:108:GLY:HA3	2:D:161:ASN:HD21	1.85	0.42
1:C:17:GLY:CA	2:E:80:MET:HB3	2.50	0.42
2:E:80:MET:HG3	2:E:84:ILE:HD13	2.02	0.42
2:E:108:GLY:HA3	2:E:161:ASN:HD21	1.85	0.42
2:E:246:LEU:HD22	2:E:280:GLU:HG3	2.01	0.42
2:F:220:LEU:HD23	2:F:224:ALA:HB3	2.02	0.42
2:F:260:ASN:HD21	2:F:290:ALA:HA	1.84	0.42
2:E:246:LEU:HD11	2:E:284:VAL:HG21	2.02	0.41
1:B:135:GLU:HB3	1:B:136:PHE:CD2	2.54	0.41
1:A:27:ILE:HD13	1:A:73:LYS:HG2	2.03	0.41
1:B:72:SER:OG	1:B:75:LYS:HB3	2.20	0.41
2:F:167:LEU:HA	2:F:170:LYS:HD2	2.02	0.41
2:F:81:ASP:HA	2:F:84:ILE:HB	2.03	0.41
2:F:213:LEU:HD22	2:F:247:GLU:HB3	2.02	0.41
2:D:270:LEU:HD23	2:D:302:PRO:HG2	2.01	0.41
2:E:227:ASN:HD22	2:E:235:THR:HB	1.86	0.41
2:E:55:LEU:O	2:E:59:GLN:HG3	2.20	0.41
2:F:286:LEU:HD11	2:F:318:LEU:HD23	2.03	0.41
1:A:22:TRP:HZ3	1:B:143:ALA:HB1	1.86	0.41
1:B:151:ARG:NH2	1:B:155:LEU:HD21	2.36	0.41
2:D:271:HIS:NE2	2:D:302:PRO:HD3	2.34	0.41
2:E:141:ASN:N	2:E:141:ASN:OD1	2.54	0.41
1:A:69:GLU:HB2	1:A:78:GLY:CA	2.51	0.41
2:D:50:ASP:OD1	2:D:50:ASP:N	2.54	0.41
2:D:55:LEU:HD11	2:D:115:LEU:HD21	2.03	0.41
2:E:237:LEU:HD11	2:E:249:VAL:HG13	2.02	0.41
1:C:29:GLU:HB3	1:C:128:LYS:HD3	2.02	0.40
2:F:226:ILE:H	2:F:226:ILE:HG13	1.73	0.40
2:F:115:LEU:HD13	2:F:156:HIS:HB3	2.02	0.40
2:F:249:VAL:HG11	2:F:281:ILE:HG23	2.02	0.40
2:D:39:ILE:HD11	2:D:153:LEU:HD11	2.04	0.40
2:E:39:ILE:HD11	2:E:153:LEU:HD11	2.02	0.40
2:D:163:ARG:HA	2:D:166:GLU:HB2	2.03	0.40



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:115:LEU:HD13	2:E:156:HIS:HB3	2.04	0.40
2:F:96:GLU:HG2	2:F:162:LYS:HE2	2.03	0.40
2:D:216:VAL:HG11	2:D:248:ILE:HG23	2.02	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	Perce	ntiles
1	А	157/178~(88%)	154 (98%)	3 (2%)	0	100	100
1	В	157/178~(88%)	154 (98%)	3 (2%)	0	100	100
1	С	154/178~(86%)	151 (98%)	3 (2%)	0	100	100
2	D	299/322~(93%)	293~(98%)	6 (2%)	0	100	100
2	Е	297/322~(92%)	290 (98%)	7 (2%)	0	100	100
2	F	298/322~(92%)	291 (98%)	7 (2%)	0	100	100
All	All	1362/1500~(91%)	1333 (98%)	29 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	Perce	ntiles
1	А	134/151~(89%)	132~(98%)	2(2%)	65	80
1	В	134/151~(89%)	132~(98%)	2~(2%)	65	80
1	С	131/151 (87%)	129~(98%)	2(2%)	65	80
2	D	243/259~(94%)	241~(99%)	2(1%)	81	89
2	Ε	242/259~(93%)	238~(98%)	4 (2%)	60	78
2	F	243/259~(94%)	239~(98%)	4(2%)	62	79
All	All	1127/1230~(92%)	1111 (99%)	16 (1%)	67	81

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	15	LEU
1	А	22	TRP
1	В	15	LEU
1	В	22	TRP
1	С	20	GLU
1	С	22	TRP
2	D	84	ILE
2	D	147	ASN
2	Е	84	ILE
2	Е	136	THR
2	Е	147	ASN
2	Е	263	ASP
2	F	25	VAL
2	F	84	ILE
2	F	147	ASN
2	F	263	ASP

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such side chains are listed below:

Mol	Chain	Res	Type
1	А	60	GLN
2	D	156	HIS
2	F	275	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)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 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	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	159/178~(89%)	-0.20	6 (3%) 40 33	120, 159, 237, 264	0
1	В	159/178~(89%)	-0.14	7 (4%) 34 29	119, 162, 247, 299	0
1	С	156/178~(87%)	-0.01	8 (5%) 28 24	121, 159, 236, 307	0
2	D	301/322~(93%)	-0.34	2 (0%) 87 83	121, 176, 227, 265	0
2	Е	299/322~(92%)	-0.02	10 (3%) 46 37	122, 193, 330, 393	0
2	F	300/322~(93%)	0.03	17 (5%) 23 19	121, 200, 333, 418	0
All	All	1374/1500~(91%)	-0.11	50 (3%) 42 35	119, 172, 304, 418	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	С	18	GLY	4.9
1	С	19	GLU	4.6
1	В	18	GLY	3.9
2	Е	288	HIS	3.6
2	F	22	ASP	3.6
2	F	297	LYS	3.5
2	F	259	VAL	3.5
1	В	23	LYS	3.5
2	F	205	HIS	3.2
2	Е	293	ASN	3.1
2	F	260	ASN	3.1
1	С	21	VAL	3.1
1	В	19	GLU	3.0
2	F	309	ASN	3.0
1	А	18	GLY	3.0
1	С	23	LYS	2.9
1	В	24	ASP	2.9
1	С	24	ASP	2.9
1	А	17	GLY	2.8



Mol	Mol Chain Re		Type	RSRZ	
1	А	102	SER	2.8	
2	Е	297	LYS	2.8	
2	F	271	HIS	2.8	
2	Е	273	ALA	2.8	
2	Е	268	THR	2.8	
2	Е	307	ILE	2.8	
2	F	307	ILE	2.7	
1	В	21	VAL	2.7	
2	Е	271	HIS	2.7	
1	А	23	LYS	2.7	
2	F	293	ASN	2.6	
1	С	20	GLU	2.6	
2	F	264	SER	2.5	
1	В	20	GLU	2.5	
2	D	22	ASP	2.4	
2	F	296	ASP	2.3	
1	С	167	LEU	2.3	
1	А	103	PHE	2.2	
2	Е	321	ALA	2.2	
1	С	17	GLY	2.2	
2	Е	313	ASP	2.2	
2	F	268	THR	2.2	
2	Е	320	LYS	2.2	
2	F	203	PRO	2.1	
2	F	76	ARG	2.1	
2	D	269	PRO	2.0	
1	В	171	ARG	2.0	
1	А	14	ARG	2.0	
2	F	236	PRO	2.0	
2	F	265	SER	2.0	
2	F	269	PRO	2.0	

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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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(A^2)$	Q<0.9
3	CA	А	401	1/1	0.71	0.76	158,158,158,158	0

6.5 Other polymers (i)

There are no such residues in this entry.

