Full wwPDB X-ray Structure Validation Report ⓘ

Jul 11, 2022 – 04:14 pm BST

PDB ID	:	7BDX
Title	:	Armadillo domain of HSF2BP in complex with BRCA2 peptide
Authors	:	Le Du, M.H.; Zinn-Justin, S.; Ghouil, R.; Miron, S.; Legrand, P.
Deposited on	:	2020-12-22
Resolution	:	2.60 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 types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

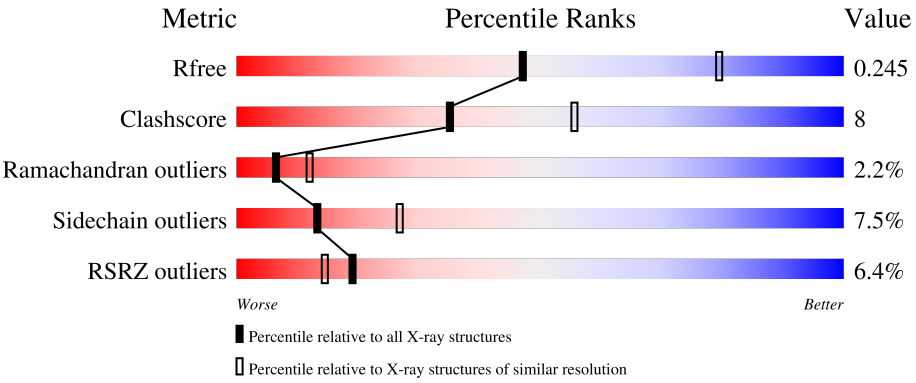
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	A	214	3% 83% 13%
1	B	214	5% 81% 16%
1	C	214	7% 71% 27%
1	D	214	8% 75% 22%
2	E	59	7% 51% 32% 7% 10%

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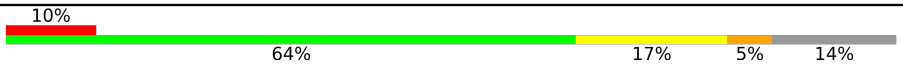
Mol	Chain	Length	Quality of chain
2	F	59	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7434 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 Heat shock factor 2-binding protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	211	Total	C	N	O	S	Se	0	0	0
			1614	1034	265	306	4	5			
1	B	212	Total	C	N	O	S	Se	4	0	0
			1628	1042	268	309	4	5			
1	C	213	Total	C	N	O	S	Se	7	0	0
			1612	1030	268	305	4	5			
1	D	211	Total	C	N	O	S	Se	43	0	0
			1581	1012	258	302	4	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	121	ALA	-	expression tag	UNP O75031
B	121	ALA	-	expression tag	UNP O75031
C	121	ALA	-	expression tag	UNP O75031
D	121	ALA	-	expression tag	UNP O75031

- Molecule 2 is a protein called Breast cancer type 2 susceptibility protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	53	Total	C	N	O	Se	0	0	0
			435	270	81	83	1			
2	F	51	Total	C	N	O	Se	5	0	0
			405	253	74	77	1			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	2332	THR	CYS	conflict	UNP P51587
E	2344	ASN	-	expression tag	UNP P51587
E	2345	LEU	-	expression tag	UNP P51587
E	2346	TYR	-	expression tag	UNP P51587

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Chain	Residue	Modelled	Actual	Comment	Reference
E	2347	PHE	-	expression tag	UNP P51587
E	2348	GLN	-	expression tag	UNP P51587
E	2349	GLY	-	expression tag	UNP P51587
F	2332	THR	CYS	conflict	UNP P51587
F	2344	ASN	-	expression tag	UNP P51587
F	2345	LEU	-	expression tag	UNP P51587
F	2346	TYR	-	expression tag	UNP P51587
F	2347	PHE	-	expression tag	UNP P51587
F	2348	GLN	-	expression tag	UNP P51587
F	2349	GLY	-	expression tag	UNP P51587

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0

- Molecule 4 is water.

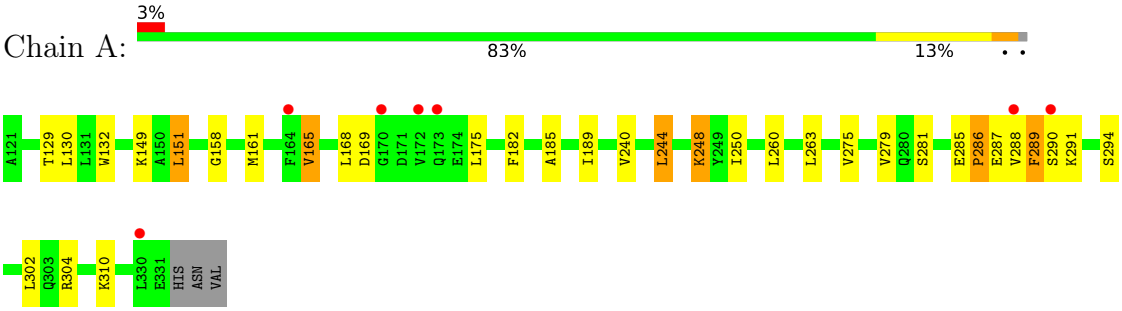
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	42	Total O 42 42	0	0
4	B	44	Total O 44 44	0	0
4	C	18	Total O 18 18	0	0
4	D	22	Total O 22 22	0	0
4	E	13	Total O 13 13	0	0
4	F	18	Total O 18 18	0	0

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.

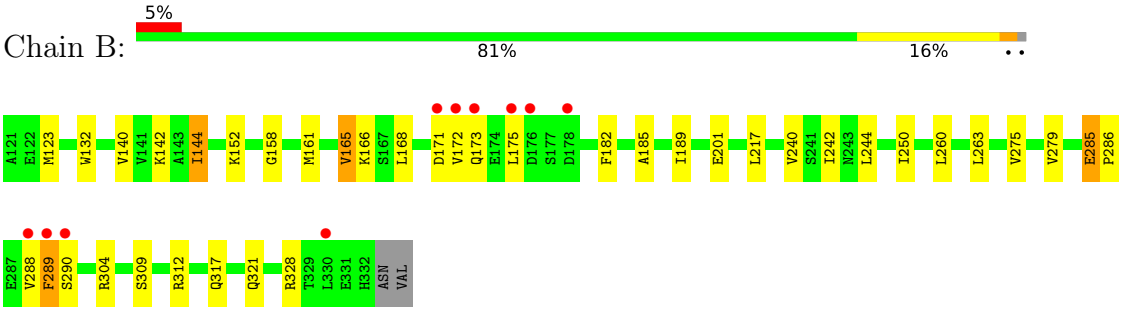
• Molecule 1: Heat shock factor 2-binding protein

Chain A:



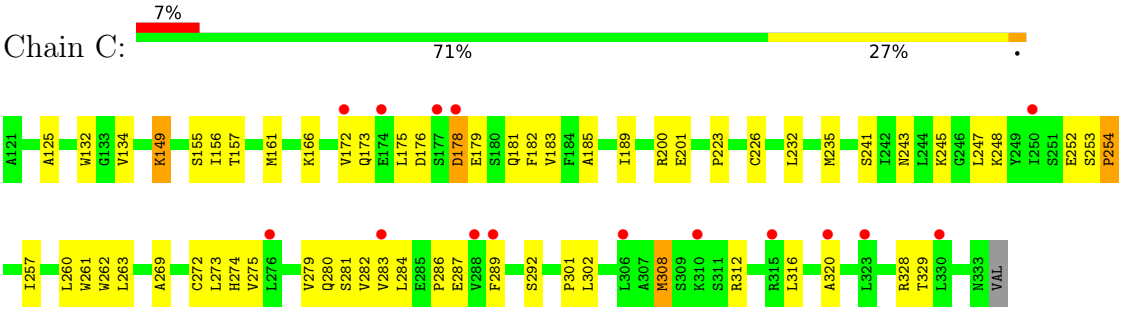
• Molecule 1: Heat shock factor 2-binding protein

Chain B:



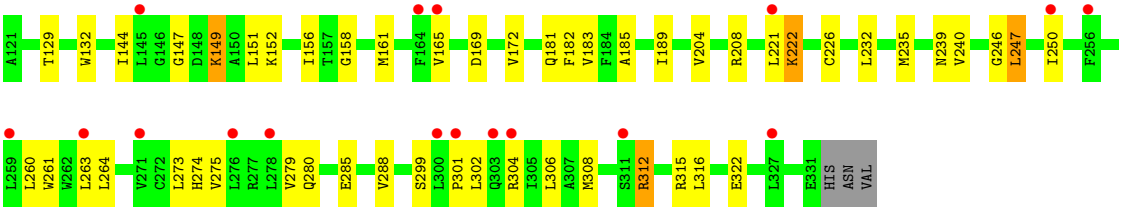
• Molecule 1: Heat shock factor 2-binding protein

Chain C:

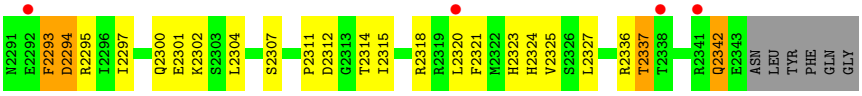


• Molecule 1: Heat shock factor 2-binding protein

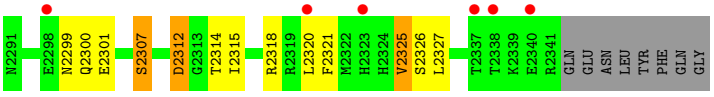
Chain D:



• Molecule 2: Breast cancer type 2 susceptibility protein



• Molecule 2: Breast cancer type 2 susceptibility protein



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	52.89Å 135.83Å 75.79Å 90.00° 110.38° 90.00°	Depositor
Resolution (Å)	49.58 – 2.60 49.58 – 2.60	Depositor EDS
% Data completeness (in resolution range)	83.9 (49.58-2.60) 83.8 (49.58-2.60)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.56 (at 2.61Å)	Xtriage
Refinement program	BUSTER 2.10.3 (19-MAR-2020)	Depositor
R, R_{free}	0.198 , 0.241 0.205 , 0.245	Depositor DCC
R_{free} test set	1226 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å^2)	69.0	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.178 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7434	wwPDB-VP
Average B, all atoms (Å^2)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.14% 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

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

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	0.43	0/1633	0.55	0/2202
1	B	0.43	0/1648	0.58	0/2222
1	C	0.40	0/1631	0.56	0/2201
1	D	0.38	0/1599	0.53	0/2160
2	E	0.45	0/441	0.69	0/590
2	F	0.42	0/411	0.63	0/552
All	All	0.41	0/7363	0.57	0/9927

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	1614	0	1664	22	0
1	B	1628	0	1675	23	0
1	C	1612	0	1647	39	0
1	D	1581	0	1604	31	0
2	E	435	0	437	20	0
2	F	405	0	396	15	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
4	A	42	0	0	0	0
4	B	44	0	0	0	0
4	C	18	0	0	1	0
4	D	22	0	0	0	0
4	E	13	0	0	1	0
4	F	18	0	0	0	0
All	All	7434	0	7423	119	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 (119) 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:291:LYS:HA	1:A:294:SER:HB2	1.40	1.01
1:A:244:LEU:HD22	2:E:2318:ARG:HG2	1.54	0.90
1:A:248:LYS:NZ	1:A:287:GLU:HG3	1.87	0.90
1:B:285:GLU:HG3	2:F:2318:ARG:HE	1.37	0.90
1:A:248:LYS:HZ1	1:A:287:GLU:HG3	1.44	0.81
1:D:147:GLY:HA3	1:D:149:LYS:NZ	1.96	0.80
2:E:2297:ILE:HD11	2:E:2304:LEU:HG	1.65	0.77
1:D:240:VAL:HG23	1:D:250:ILE:HD11	1.66	0.76
1:A:285:GLU:HG3	2:E:2318:ARG:HD2	1.71	0.72
1:C:157:THR:HG22	1:C:161:MSE:HE3	1.72	0.72
1:A:240:VAL:HG23	1:A:250:ILE:HD11	1.71	0.72
1:B:240:VAL:HG23	1:B:250:ILE:HD11	1.71	0.71
1:D:147:GLY:HA3	1:D:149:LYS:HZ2	1.55	0.71
1:C:157:THR:HG22	1:C:161:MSE:CE	2.24	0.68
1:A:129:THR:HG22	1:D:149:LYS:HG2	1.80	0.63
1:B:285:GLU:CG	2:F:2318:ARG:HE	2.11	0.61
1:C:176:ASP:HB3	1:C:179:GLU:HB3	1.82	0.61
1:A:248:LYS:HZ2	1:A:287:GLU:HG3	1.63	0.61
1:C:125:ALA:HA	1:C:182:PHE:HD1	1.66	0.61
1:D:240:VAL:CG2	1:D:250:ILE:HD11	2.31	0.59
1:D:264:LEU:HD22	1:D:308:MSE:HE1	1.83	0.59
2:E:2320:LEU:HD13	2:E:2327:LEU:HB2	1.83	0.59
2:F:2320:LEU:HD13	2:F:2327:LEU:HB2	1.83	0.59
1:D:247:LEU:HD13	1:D:288:VAL:HG21	1.86	0.58
1:A:165:VAL:HA	1:A:168:LEU:HD12	1.88	0.56
1:B:240:VAL:CG2	1:B:250:ILE:HD11	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:232:LEU:HD11	2:E:2314:THR:HG21	1.88	0.54
1:D:147:GLY:HA3	1:D:149:LYS:HZ1	1.70	0.54
1:A:240:VAL:CG2	1:A:250:ILE:HD11	2.38	0.54
1:B:285:GLU:HG3	2:F:2318:ARG:NE	2.16	0.53
1:B:140:VAL:HG13	1:C:134:VAL:HG11	1.91	0.53
1:C:248:LYS:O	1:C:252:GLU:HG2	2.08	0.53
1:A:129:THR:CG2	1:D:149:LYS:HG2	2.38	0.53
1:D:152:LYS:O	1:D:156:ILE:HG22	2.10	0.52
1:A:130:LEU:HD11	1:D:144:ILE:HG23	1.91	0.52
1:D:302:LEU:HD22	1:D:306:LEU:HD13	1.91	0.52
1:C:272:CYS:HA	1:C:275:VAL:HG22	1.93	0.51
2:E:2336:ARG:O	2:E:2337:THR:O	2.29	0.51
1:D:181:GLN:HG3	2:F:2315:ILE:HD13	1.93	0.51
1:D:239:ASN:HD21	2:F:2307:SER:H	1.57	0.51
1:A:285:GLU:HG3	2:E:2318:ARG:HH11	1.76	0.51
1:C:260:LEU:HD13	1:C:279:VAL:HG22	1.93	0.51
1:C:308:MSE:HB3	1:C:320:ALA:HB2	1.93	0.50
1:D:280:GLN:HE22	1:D:322:GLU:HB3	1.76	0.50
1:D:161:MSE:HG2	1:D:183:VAL:HG23	1.94	0.49
1:B:123:MSE:SE	1:C:156:ILE:HG13	2.61	0.49
1:D:260:LEU:HD13	1:D:279:VAL:HG22	1.94	0.49
1:D:304:ARG:O	1:D:308:MSE:HB2	2.13	0.49
1:B:286:PRO:HB3	1:B:289:PHE:HB2	1.95	0.49
1:C:286:PRO:HA	1:C:289:PHE:HB3	1.95	0.49
1:D:315:ARG:CB	2:F:2321:PHE:HE1	2.25	0.49
1:B:140:VAL:O	1:B:144:ILE:HG22	2.13	0.49
1:B:242:ILE:HG23	2:F:2320:LEU:HD12	1.95	0.49
2:E:2297:ILE:CD1	2:E:2304:LEU:HG	2.40	0.49
1:B:263:LEU:HB3	1:B:275:VAL:HG21	1.95	0.48
1:A:263:LEU:HB3	1:A:275:VAL:HG21	1.95	0.48
2:E:2323:HIS:HB3	4:E:2412:HOH:O	2.13	0.48
1:C:161:MSE:HG2	1:C:183:VAL:HG23	1.96	0.48
1:B:286:PRO:HA	1:B:289:PHE:CD1	2.48	0.48
1:D:204:VAL:HG11	1:D:246:GLY:CA	2.44	0.48
1:A:158:GLY:HA2	1:A:161:MSE:HE2	1.96	0.47
1:C:284:LEU:HD23	2:E:2297:ILE:HD13	1.96	0.47
1:D:273:LEU:HD22	2:F:2321:PHE:CZ	2.50	0.47
1:C:261:TRP:CE3	1:C:301:PRO:HD3	2.49	0.47
1:D:235:MSE:HE3	1:D:274:HIS:CE1	2.50	0.47
1:C:308:MSE:HB3	1:C:320:ALA:CB	2.46	0.46
1:B:309:SER:O	1:B:317:GLN:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:181:GLN:HB2	4:C:416:HOH:O	2.15	0.46
1:C:185:ALA:O	1:C:189:ILE:HG13	2.16	0.46
1:D:232:LEU:HD11	2:F:2314:THR:HG21	1.97	0.46
1:A:185:ALA:O	1:A:189:ILE:HG13	2.16	0.46
1:C:257:ILE:HD11	1:C:292:SER:HB2	1.98	0.45
1:C:281:SER:OG	2:E:2295:ARG:NH2	2.48	0.45
1:D:185:ALA:O	1:D:189:ILE:HG13	2.16	0.45
1:C:312:ARG:HB3	2:E:2324:HIS:O	2.17	0.45
1:C:273:LEU:HD22	2:E:2321:PHE:CZ	2.51	0.45
2:E:2293:PHE:O	2:E:2294:ASP:O	2.34	0.45
1:C:157:THR:CG2	1:C:161:MSE:HE2	2.47	0.45
1:C:269:ALA:HB2	2:E:2323:HIS:CD2	2.52	0.44
1:B:185:ALA:O	1:B:189:ILE:HG13	2.18	0.44
1:A:281:SER:OG	2:E:2318:ARG:NH2	2.50	0.44
1:B:158:GLY:HA2	1:B:161:MSE:HE2	1.99	0.44
1:A:260:LEU:HD13	1:A:279:VAL:HG22	2.00	0.44
1:C:263:LEU:HB3	1:C:275:VAL:HG11	2.00	0.44
1:C:223:PRO:HD3	1:C:262:TRP:CZ2	2.53	0.44
1:C:257:ILE:CG2	1:C:261:TRP:NE1	2.81	0.43
1:C:247:LEU:HD22	2:E:2295:ARG:CZ	2.49	0.43
1:B:123:MSE:HG3	1:C:182:PHE:HZ	1.83	0.43
1:D:263:LEU:HB3	1:D:275:VAL:HG21	2.01	0.43
1:C:263:LEU:CB	1:C:275:VAL:HG11	2.49	0.43
1:D:132:TRP:CE3	1:D:185:ALA:HA	2.54	0.43
1:B:260:LEU:HD13	1:B:279:VAL:HG22	2.01	0.43
1:D:222:LYS:HB2	1:D:222:LYS:HE2	1.83	0.43
1:B:165:VAL:CG2	1:B:217:LEU:HD22	2.49	0.42
1:D:158:GLY:HA2	1:D:161:MSE:HE2	2.00	0.42
1:C:200:ARG:HD2	1:C:243:ASN:HB2	2.00	0.42
1:C:132:TRP:CE3	1:C:185:ALA:HA	2.54	0.42
1:C:223:PRO:HD3	1:C:262:TRP:HZ2	1.85	0.42
1:C:245:LYS:HE2	2:E:2293:PHE:CD1	2.55	0.42
2:E:2320:LEU:HD22	2:E:2327:LEU:HD12	2.01	0.42
1:B:244:LEU:HG	2:F:2318:ARG:HG3	2.01	0.42
1:B:285:GLU:HB2	2:F:2318:ARG:HH21	1.85	0.42
1:D:165:VAL:HG22	1:D:221:LEU:HD21	2.01	0.42
1:A:248:LYS:HA	1:A:248:LYS:HD3	1.83	0.41
1:C:308:MSE:HG2	1:C:316:LEU:HD11	2.01	0.41
1:D:261:TRP:CD2	1:D:301:PRO:HD3	2.56	0.41
1:B:132:TRP:CE3	1:B:185:ALA:HA	2.56	0.41
1:C:201:GLU:CD	1:C:245:LYS:HZ1	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:253:SER:O	1:C:254:PRO:O	2.38	0.41
2:F:2299:ASN:OD1	2:F:2301:GLU:OE1	2.39	0.41
2:F:2325:VAL:HG22	2:F:2326:SER:H	1.86	0.40
1:A:132:TRP:CE3	1:A:185:ALA:HA	2.56	0.40
1:A:286:PRO:HA	1:A:289:PHE:CD1	2.56	0.40
1:B:201:GLU:HG2	2:F:2312:ASP:OD1	2.21	0.40
1:C:261:TRP:CD2	1:C:301:PRO:HD3	2.56	0.40
1:B:142:LYS:HB3	1:B:142:LYS:HE3	1.95	0.40
1:A:151:LEU:HD21	1:D:129:THR:HG21	2.04	0.40
1:C:235:MSE:HE3	1:C:274:HIS:NE2	2.36	0.40
2:E:2311:PRO:O	2:E:2315:ILE:HB	2.22	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	209/214 (98%)	194 (93%)	11 (5%)	4 (2%)	8 15
1	B	210/214 (98%)	200 (95%)	6 (3%)	4 (2%)	8 15
1	C	211/214 (99%)	197 (93%)	9 (4%)	5 (2%)	6 10
1	D	209/214 (98%)	191 (91%)	16 (8%)	2 (1%)	15 32
2	E	51/59 (86%)	39 (76%)	7 (14%)	5 (10%)	0 0
2	F	49/59 (83%)	41 (84%)	7 (14%)	1 (2%)	7 14
All	All	939/974 (96%)	862 (92%)	56 (6%)	21 (2%)	6 12

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	175	LEU

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Mol	Chain	Res	Type
1	C	254	PRO
1	D	312	ARG
2	E	2294	ASP
2	E	2337	THR
1	A	169	ASP
1	B	171	ASP
1	B	288	VAL
1	C	172	VAL
1	C	173	GLN
1	B	285	GLU
1	B	290	SER
1	C	149	LYS
2	E	2293	PHE
2	E	2342	GLN
1	C	178	ASP
1	D	299	SER
1	A	288	VAL
2	F	2325	VAL
2	E	2325	VAL
1	A	286	PRO

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	182/181 (101%)	171 (94%)	11 (6%)	19 39
1	B	184/181 (102%)	170 (92%)	14 (8%)	13 26
1	C	179/181 (99%)	164 (92%)	15 (8%)	11 21
1	D	174/181 (96%)	162 (93%)	12 (7%)	15 31
2	E	50/55 (91%)	44 (88%)	6 (12%)	5 9
2	F	45/55 (82%)	42 (93%)	3 (7%)	16 33
All	All	814/834 (98%)	753 (92%)	61 (8%)	13 27

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	149	LYS
1	A	151	LEU
1	A	165	VAL
1	A	182	PHE
1	A	244	LEU
1	A	248	LYS
1	A	289	PHE
1	A	290	SER
1	A	302	LEU
1	A	304	ARG
1	A	310	LYS
1	B	144	ILE
1	B	152	LYS
1	B	165	VAL
1	B	166	LYS
1	B	168	LEU
1	B	172	VAL
1	B	173	GLN
1	B	175	LEU
1	B	182	PHE
1	B	289	PHE
1	B	304	ARG
1	B	312	ARG
1	B	321	GLN
1	B	328	ARG
1	C	149	LYS
1	C	155	SER
1	C	166	LYS
1	C	175	LEU
1	C	178	ASP
1	C	226	CYS
1	C	241	SER
1	C	280	GLN
1	C	282	VAL
1	C	283	VAL
1	C	287	GLU
1	C	302	LEU
1	C	308	MSE
1	C	328	ARG
1	C	329	THR
1	D	149	LYS
1	D	151	LEU
1	D	169	ASP

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Mol	Chain	Res	Type
1	D	172	VAL
1	D	182	PHE
1	D	208	ARG
1	D	222	LYS
1	D	226	CYS
1	D	247	LEU
1	D	285	GLU
1	D	312	ARG
1	D	316	LEU
2	E	2300	GLN
2	E	2301	GLU
2	E	2302	LYS
2	E	2307	SER
2	E	2312	ASP
2	E	2342	GLN
2	F	2300	GLN
2	F	2307	SER
2	F	2312	ASP

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

Mol	Chain	Res	Type
1	D	239	ASN
1	D	280	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

Of 2 ligands modelled in this entry, 2 are 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

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	206/214 (96%)	0.11	7 (3%) 45 38	48, 69, 115, 122	0
1	B	207/214 (96%)	0.19	10 (4%) 30 24	48, 66, 117, 130	2 (0%)
1	C	207/214 (96%)	0.46	15 (7%) 15 11	50, 92, 128, 136	1 (0%)
1	D	201/214 (93%)	0.60	17 (8%) 10 7	56, 101, 152, 175	3 (1%)
2	E	52/59 (88%)	0.30	4 (7%) 13 10	52, 83, 131, 135	0
2	F	50/59 (84%)	0.59	6 (12%) 4 2	60, 93, 129, 133	1 (2%)
All	All	923/974 (94%)	0.35	59 (6%) 19 14	48, 83, 134, 175	7 (0%)

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	288	VAL	4.7
2	F	2337	THR	4.5
1	B	173	GLN	4.2
1	B	288	VAL	4.2
1	D	303	GLN	4.0
2	F	2338	THR	3.9
1	B	175	LEU	3.9
1	C	306	LEU	3.8
1	B	178	ASP	3.7
1	A	290	SER	3.6
2	F	2323	HIS	3.5
1	C	250	ILE	3.4
1	D	276	LEU	3.4
1	D	165	VAL	3.4
1	D	250	ILE	3.3
1	D	221	LEU	3.3
1	C	288	VAL	3.3
1	C	178	ASP	3.3
1	D	263	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	170	GLY	3.2
1	D	304	ARG	3.2
1	C	310	LYS	3.2
2	E	2341	ARG	3.1
1	C	289	PHE	3.1
1	B	171	ASP	3.1
1	D	164	PHE	3.0
1	C	323	LEU	3.0
1	C	172	VAL	2.9
1	D	300	LEU	2.9
1	B	290	SER	2.9
1	C	320	ALA	2.9
1	C	177	SER	2.9
1	A	164	PHE	2.8
1	B	172	VAL	2.8
1	D	256	PHE	2.8
1	D	278	LEU	2.8
1	D	327	LEU	2.8
1	D	311	SER	2.7
1	A	330	LEU	2.7
1	A	172	VAL	2.6
2	F	2340	GLU	2.6
2	E	2320	LEU	2.6
1	C	283	VAL	2.6
1	D	259	LEU	2.5
2	E	2292	GLU	2.5
2	F	2320	LEU	2.4
1	B	289	PHE	2.4
1	C	174	GLU	2.4
2	E	2338	THR	2.4
1	A	173	GLN	2.3
1	B	176	ASP	2.3
1	C	330	LEU	2.3
1	B	330	LEU	2.3
1	D	301	PRO	2.3
2	F	2298	GLU	2.2
1	D	145	LEU	2.2
1	C	315	ARG	2.2
1	C	276	LEU	2.1
1	D	271	VAL	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)

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(Å^2)	Q<0.9
3	MG	A	401	1/1	0.93	0.28	70,70,70,70	0
3	MG	B	401	1/1	0.97	0.20	56,56,56,56	0

6.5 Other polymers (i)

There are no such residues in this entry.