



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:28 PM UTC

PDB ID : 7BDX / pdb_00007bdx
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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

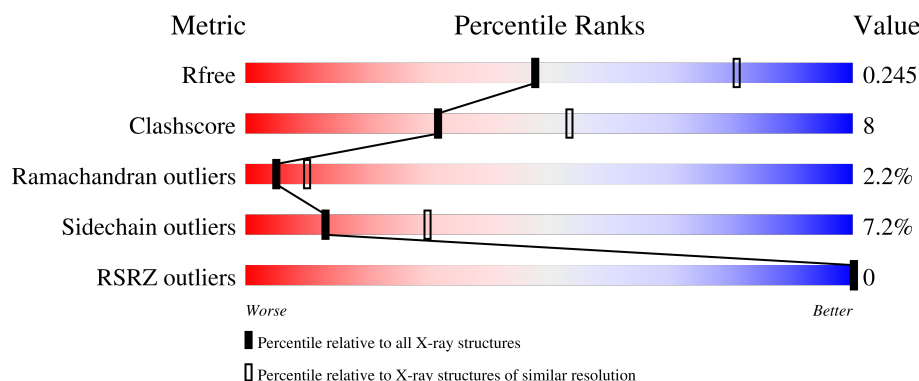
1 Overall quality at a glance

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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 $\leq 5\%$. 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	 82% 13% ..
1	B	214	 80% 16% ..
1	C	214	 71% 27% .
1	D	214	 75% 21% ..
2	E	59	 53% 29% 8% 10%

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Mol	Chain	Length	Quality of chain
2	F	59	 A horizontal bar chart showing the quality of chain F. The bar is divided into four segments: green (61%), yellow (20%), orange (5%), and grey (14%).

2 Entry composition

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 (CCD ID: 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

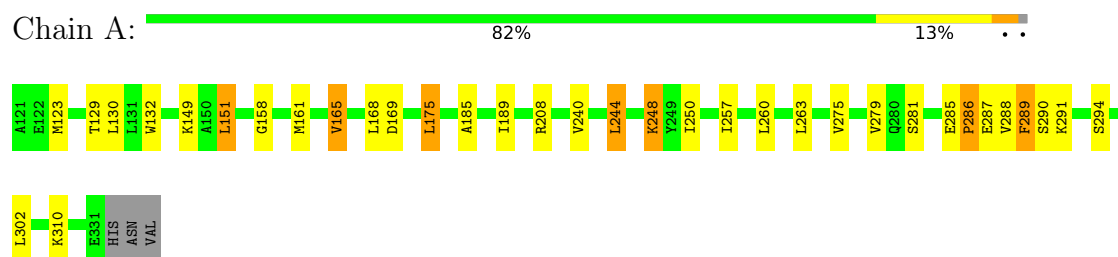
- Molecule 4 is water.

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

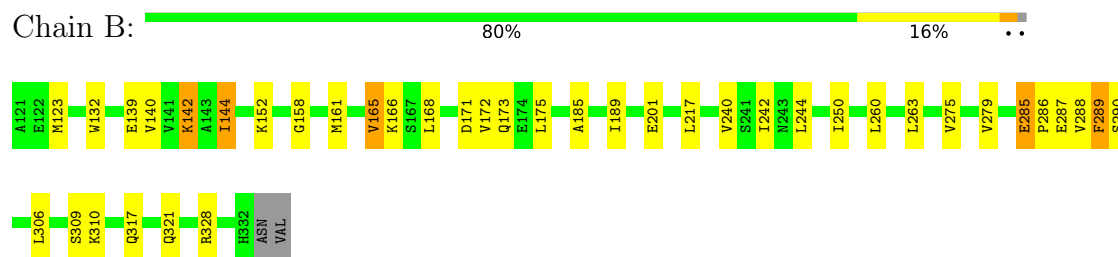
3 Residue-property plots

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.

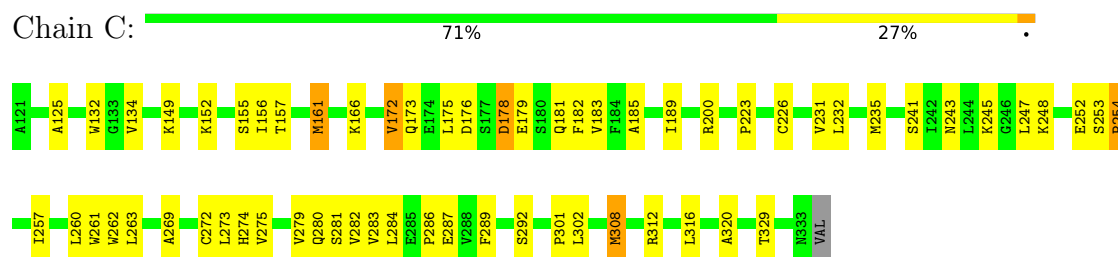
- Molecule 1: Heat shock factor 2-binding protein



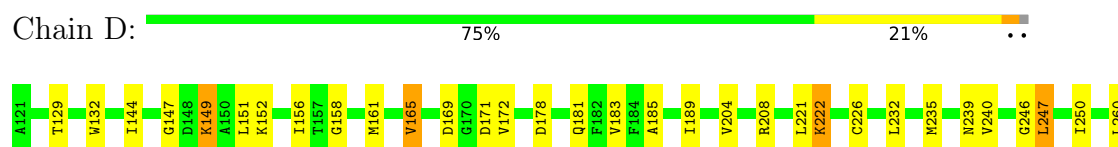
- Molecule 1: Heat shock factor 2-binding protein



- Molecule 1: Heat shock factor 2-binding protein

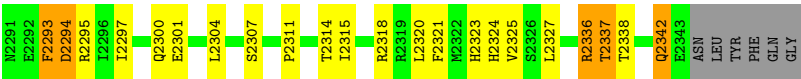


- Molecule 1: Heat shock factor 2-binding protein

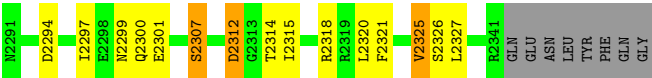




• Molecule 2: Breast cancer type 2 susceptibility protein



• Molecule 2: Breast cancer type 2 susceptibility protein



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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 (3.97%)	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)	0.33 , 69.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.178 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.97	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.*

¹Intensities estimated from amplitudes.

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.

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	0.77	1/1633 (0.1%)	1.13	1/2202 (0.0%)
1	B	0.77	0/1648	1.16	2/2222 (0.1%)
1	C	0.71	1/1631 (0.1%)	1.14	1/2201 (0.0%)
1	D	0.69	0/1599	1.11	2/2160 (0.1%)
2	E	0.80	0/441	1.18	4/590 (0.7%)
2	F	0.78	0/411	1.15	1/552 (0.2%)
All	All	0.74	2/7363 (0.0%)	1.14	11/9927 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	161	MSE	SE-CE	-6.19	1.76	1.95
1	A	123	MSE	SE-CE	-5.54	1.78	1.95

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	287	GLU	N-CA-C	-7.65	101.00	110.65
1	B	139	GLU	CB-CG-CD	6.94	124.40	112.60
1	D	178	ASP	CA-CB-CG	6.60	119.20	112.60
2	E	2338	THR	CA-C-N	5.84	132.69	121.54
2	E	2338	THR	C-N-CA	5.84	132.69	121.54
1	D	171	ASP	CB-CA-C	-5.43	110.29	116.54
2	E	2336	ARG	CA-C-N	5.43	131.92	121.54
2	E	2336	ARG	C-N-CA	5.43	131.92	121.54
1	A	257	ILE	N-CA-CB	5.39	114.65	110.45
1	C	178	ASP	CA-CB-CG	5.18	117.78	112.60
2	F	2294	ASP	CA-CB-CG	5.11	117.71	112.60

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	38	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
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	118	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 (118) 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:248:LYS:HZ1	1:A:287:GLU:HG3	1.33	0.92
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:248:LYS:HZ2	1:A:287:GLU:HG3	1.75	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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

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	209/214 (98%)	194 (93%)	11 (5%)	4 (2%)	6	13
1	B	210/214 (98%)	200 (95%)	6 (3%)	4 (2%)	6	13
1	C	211/214 (99%)	197 (93%)	9 (4%)	5 (2%)	4	9
1	D	209/214 (98%)	191 (91%)	16 (8%)	2 (1%)	12	28
2	E	51/59 (86%)	39 (76%)	7 (14%)	5 (10%)	0	0
2	F	49/59 (83%)	41 (84%)	7 (14%)	1 (2%)	6	12
All	All	939/974 (96%)	862 (92%)	56 (6%)	21 (2%)	5	10

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	175	LEU
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 ⓘ

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%)	17	37
1	B	184/181 (102%)	170 (92%)	14 (8%)	12	27
1	C	179/181 (99%)	164 (92%)	15 (8%)	10	23
1	D	174/181 (96%)	163 (94%)	11 (6%)	16	36
2	E	50/55 (91%)	46 (92%)	4 (8%)	11	25
2	F	45/55 (82%)	41 (91%)	4 (9%)	9	20
All	All	814/834 (98%)	755 (93%)	59 (7%)	13	30

All (59) 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	175	LEU
1	A	208	ARG
1	A	244	LEU
1	A	248	LYS
1	A	289	PHE
1	A	290	SER
1	A	302	LEU
1	A	310	LYS
1	B	142	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	289	PHE
1	B	306	LEU
1	B	310	LYS
1	B	321	GLN
1	B	328	ARG
1	C	152	LYS
1	C	155	SER
1	C	166	LYS
1	C	172	VAL
1	C	175	LEU

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Mol	Chain	Res	Type
1	C	226	CYS
1	C	231	VAL
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	329	THR
1	D	149	LYS
1	D	151	LEU
1	D	165	VAL
1	D	169	ASP
1	D	172	VAL
1	D	208	ARG
1	D	222	LYS
1	D	226	CYS
1	D	247	LEU
1	D	306	LEU
1	D	316	LEU
2	E	2300	GLN
2	E	2301	GLU
2	E	2307	SER
2	E	2342	GLN
2	F	2297	ILE
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 (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	181	GLN
1	A	216	GLN
1	A	280	GLN
1	B	173	GLN
1	B	216	GLN
1	C	216	GLN
1	C	321	GLN
1	D	216	GLN
1	D	239	ASN

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Mol	Chain	Res	Type
1	D	280	GLN
1	D	317	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [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	206/214 (96%)	-1.40	0 100 100	48, 69, 115, 122	0
1	B	207/214 (96%)	-1.45	0 100 100	48, 66, 114, 130	2 (0%)
1	C	207/214 (96%)	-1.35	0 100 100	50, 92, 127, 136	1 (0%)
1	D	201/214 (93%)	-1.26	0 100 100	56, 101, 150, 175	3 (1%)
2	E	52/59 (88%)	-1.39	0 100 100	52, 83, 131, 135	0
2	F	50/59 (84%)	-1.34	0 100 100	51, 89, 129, 133	1 (2%)
All	All	923/974 (94%)	-1.36	0 100 100	48, 83, 133, 175	7 (0%)

There are no RSRZ outliers to report.

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 oligosaccharides 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, 95th 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	0.99	0.10	70,70,70,70	0
3	MG	B	401	1/1	0.99	0.06	56,56,56,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.