



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:25 PM UTC

PDB ID : 2QFJ / pdb_00002qfj
Title : Crystal Structure of First Two RRM Domains of FIR Bound to ssDNA from a Portion of FUSE
Authors : Crichlow, G.V.; Yang, Y.; Fan, C.; Lolis, E.; Braddock, D.
Deposited on : 2007-06-27
Resolution : 2.10 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
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

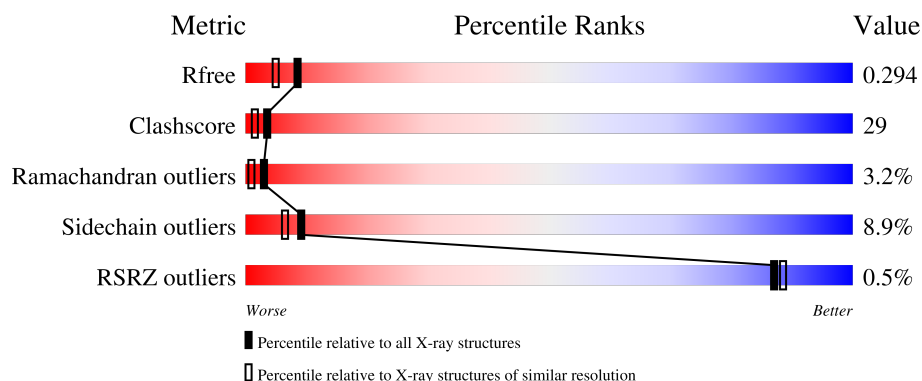
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	C	25	 8% 8% 84%
2	A	216	 % 44% 37% 7% • 11%
2	B	216	 48% 30% 12% 10%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3010 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 DNA chain called DNA (5'-D(*DTP*DCP*DGP*DGP*DGP*DAP*DTP*DTP*DTP*DTP*DTP*DAP*DTP*DTP*DTP*DTP*DGP*DTP*DGP*DTP*DTP*DAP*DTP*DT)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	4	Total	C	N	O	P	0	0	1
			41	19	8	12	2			

- Molecule 2 is a protein called FBP-interacting repressor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	193	Total	C	N	O	S	0	0	0
			1472	932	251	283	6			
2	B	194	Total	C	N	O	S	0	0	0
			1475	931	253	284	7			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	84	GLY	-	expression tag	UNP Q9NZA0
A	85	SER	-	expression tag	UNP Q9NZA0
A	86	HIS	-	expression tag	UNP Q9NZA0
A	87	MET	-	expression tag	UNP Q9NZA0
A	88	ALA	-	expression tag	UNP Q9NZA0
A	89	SER	-	expression tag	UNP Q9NZA0
A	90	MET	-	expression tag	UNP Q9NZA0
A	91	THR	-	expression tag	UNP Q9NZA0
A	92	GLY	-	expression tag	UNP Q9NZA0
A	93	GLY	-	expression tag	UNP Q9NZA0
A	94	GLN	-	expression tag	UNP Q9NZA0
A	95	GLN	-	expression tag	UNP Q9NZA0
A	96	MET	-	expression tag	UNP Q9NZA0
A	97	GLY	-	expression tag	UNP Q9NZA0
A	98	ARG	-	expression tag	UNP Q9NZA0
A	99	GLY	-	expression tag	UNP Q9NZA0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	100	SER	-	expression tag	UNP Q9NZA0
A	106	GLY	ARG	engineered mutation	UNP Q9NZA0
A	112	SER	CYS	engineered mutation	UNP Q9NZA0
A	238	ALA	CYS	engineered mutation	UNP Q9NZA0
B	84	GLY	-	expression tag	UNP Q9NZA0
B	85	SER	-	expression tag	UNP Q9NZA0
B	86	HIS	-	expression tag	UNP Q9NZA0
B	87	MET	-	expression tag	UNP Q9NZA0
B	88	ALA	-	expression tag	UNP Q9NZA0
B	89	SER	-	expression tag	UNP Q9NZA0
B	90	MET	-	expression tag	UNP Q9NZA0
B	91	THR	-	expression tag	UNP Q9NZA0
B	92	GLY	-	expression tag	UNP Q9NZA0
B	93	GLY	-	expression tag	UNP Q9NZA0
B	94	GLN	-	expression tag	UNP Q9NZA0
B	95	GLN	-	expression tag	UNP Q9NZA0
B	96	MET	-	expression tag	UNP Q9NZA0
B	97	GLY	-	expression tag	UNP Q9NZA0
B	98	ARG	-	expression tag	UNP Q9NZA0
B	99	GLY	-	expression tag	UNP Q9NZA0
B	100	SER	-	expression tag	UNP Q9NZA0
B	106	GLY	ARG	engineered mutation	UNP Q9NZA0
B	112	SER	CYS	engineered mutation	UNP Q9NZA0
B	238	ALA	CYS	engineered mutation	UNP Q9NZA0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	13	Total O 13 13	0	0
3	B	9	Total O 9 9	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	63.13Å 63.13Å 82.59Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.59 – 2.10 45.59 – 2.10	Depositor EDS
% Data completeness (in resolution range)	91.3 (45.59-2.10) 91.4 (45.59-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 2.10Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.258 , 0.295 0.260 , 0.294	Depositor DCC
R_{free} test set	953 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	47.2	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 72.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.038 for -h,-k,l 0.318 for h,-h-k,-l 0.046 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3010	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.97% 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

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	C	1.07	1/44 (2.3%)	1.56	1/66 (1.5%)
2	A	0.73	0/1500	1.26	19/2023 (0.9%)
2	B	0.77	1/1504 (0.1%)	1.26	18/2029 (0.9%)
All	All	0.76	2/3048 (0.1%)	1.26	38/4118 (0.9%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	148	VAL	C-O	-5.60	1.17	1.24
1	C	1	DT	O3'-P	-5.39	1.53	1.61

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	176	VAL	N-CA-C	10.75	123.39	107.80
2	B	176	VAL	N-CA-C	10.54	123.08	107.80
1	C	23	DA	C2'-C3'-O3'	-8.67	98.50	111.50
2	A	290	MET	CA-C-N	8.14	130.02	119.84
2	A	290	MET	C-N-CA	8.14	130.02	119.84
2	A	135	PHE	CA-CB-CG	-7.27	106.53	113.80
2	A	177	MET	CA-C-N	7.24	134.73	121.70
2	A	177	MET	C-N-CA	7.24	134.73	121.70
2	B	183	ILE	N-CA-C	6.16	118.84	109.12
2	A	183	ILE	N-CA-C	5.98	118.57	109.12
2	A	270	MET	N-CA-C	5.84	120.41	113.28
2	B	224	ASP	N-CA-C	-5.83	104.83	111.07
2	B	127	THR	N-CA-C	-5.83	104.84	111.14
2	A	224	ASP	N-CA-C	-5.82	104.85	111.14
2	B	162	VAL	N-CA-C	5.80	113.95	109.19
2	A	127	THR	N-CA-C	-5.71	104.97	111.14
2	B	270	MET	N-CA-C	5.67	120.19	113.28
2	A	246	THR	N-CA-C	5.65	118.64	111.69
2	B	246	THR	N-CA-C	5.64	118.63	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	135	PHE	CA-CB-CG	-5.58	108.22	113.80
2	B	121	TYR	N-CA-C	5.57	119.18	112.38
2	A	162	VAL	N-CA-C	5.55	113.74	109.19
2	A	189	SER	N-CA-C	5.45	119.65	112.89
2	B	189	SER	N-CA-C	5.40	119.58	112.89
2	B	276	GLY	N-CA-C	-5.28	100.66	113.18
2	A	276	GLY	N-CA-C	-5.24	100.77	113.18
2	B	290	MET	CA-C-N	5.19	126.32	119.84
2	B	290	MET	C-N-CA	5.19	126.32	119.84
2	B	146	ASP	N-CA-C	5.18	119.29	112.92
2	B	122	GLU	CA-C-O	5.17	125.33	119.18
2	A	198	ILE	CB-CA-C	-5.13	105.40	111.97
2	B	172	GLN	N-CA-C	5.13	120.39	113.72
2	A	172	GLN	N-CA-C	5.05	120.29	113.72
2	A	182	ASN	CA-C-N	-5.04	113.30	122.43
2	A	182	ASN	C-N-CA	-5.04	113.30	122.43
2	B	182	ASN	CA-C-N	-5.02	113.35	122.43
2	B	182	ASN	C-N-CA	-5.02	113.35	122.43
2	A	229	PHE	N-CA-C	5.00	117.62	111.82

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	C	41	0	21	0	0
2	A	1472	0	1426	84	0
2	B	1475	0	1438	95	0
3	A	13	0	0	0	0
3	B	9	0	0	1	0
All	All	3010	0	2885	173	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 29.

All (173) 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)
2:B:175:SER:HA	2:B:181:ARG:NH1	1.59	1.15
2:B:135:PHE:HZ	2:B:173:MET:HE3	1.06	1.12
2:B:175:SER:CA	2:B:181:ARG:HH12	1.70	1.04
2:A:294:THR:H	2:A:295:PRO:HD2	1.24	1.01
2:A:176:VAL:HB	2:A:180:GLY:O	1.58	1.01
2:A:176:VAL:HB	2:A:180:GLY:C	1.86	1.01
2:B:135:PHE:CZ	2:B:173:MET:HE3	1.96	1.00
2:B:176:VAL:HB	2:B:180:GLY:C	1.88	0.99
2:A:164:GLU:OE2	2:A:286:VAL:HG22	1.68	0.93
2:B:176:VAL:HB	2:B:180:GLY:O	1.70	0.90
2:A:294:THR:N	2:A:295:PRO:HD2	1.90	0.86
2:B:104:ARG:HH11	2:B:291:PRO:CA	1.89	0.86
2:B:104:ARG:HH11	2:B:291:PRO:HA	1.42	0.85
2:B:175:SER:HA	2:B:181:ARG:HH12	0.75	0.83
2:A:291:PRO:O	2:A:292:LEU:HB3	1.76	0.83
2:B:104:ARG:HH11	2:B:291:PRO:C	1.88	0.82
2:A:146:ASP:HA	2:A:153:LYS:HE2	1.62	0.81
2:A:122:GLU:O	2:A:122:GLU:HG2	1.79	0.81
2:B:146:ASP:O	2:B:148:VAL:N	2.13	0.80
2:B:143:MET:HG2	2:B:156:ALA:HB2	1.63	0.80
2:A:104:ARG:O	2:A:108:LEU:HG	1.83	0.79
2:B:174:ASN:C	2:B:181:ARG:HH22	1.91	0.79
2:A:135:PHE:CE2	2:A:173:MET:HE3	2.18	0.79
2:B:234:LYS:HD2	2:B:258:GLU:OE1	1.82	0.78
2:A:167:GLN:HE22	2:A:187:ARG:HH22	1.31	0.77
2:B:286:VAL:O	2:B:286:VAL:HG12	1.85	0.75
2:A:292:LEU:O	2:A:292:LEU:HD12	1.86	0.75
2:B:104:ARG:NE	2:B:291:PRO:O	2.21	0.72
2:A:152:HIS:CD2	2:A:154:GLY:H	2.08	0.71
2:A:135:PHE:CZ	2:A:173:MET:HE3	2.27	0.70
2:A:167:GLN:HE22	2:A:187:ARG:NH2	1.89	0.70
2:B:184:LYS:HZ2	2:B:184:LYS:HB3	1.58	0.69
2:A:246:THR:OG1	2:A:248:LYS:HG2	1.92	0.69
2:A:152:HIS:HD2	2:A:154:GLY:H	1.41	0.68
2:A:236:LYS:HE3	2:A:258:GLU:HA	1.77	0.67
2:B:286:VAL:O	2:B:286:VAL:CG1	2.42	0.66
2:A:107:ALA:O	2:A:111:MET:HG3	1.96	0.66
2:A:294:THR:H	2:A:295:PRO:CD	2.06	0.66
2:A:217:HIS:HB3	2:A:220:LEU:HD22	1.77	0.66
2:B:148:VAL:O	2:B:149:THR:C	2.34	0.65
2:B:119:ILE:HD13	2:B:143:MET:HE3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:227:SER:O	2:B:230:GLU:HG2	1.97	0.64
2:A:119:ILE:HD13	2:A:143:MET:HE3	1.81	0.63
2:B:104:ARG:NH1	2:B:291:PRO:HA	2.12	0.63
2:B:184:LYS:HB3	2:B:184:LYS:NZ	2.15	0.62
2:B:139:LYS:HD3	2:B:161:GLU:HG2	1.81	0.62
2:A:143:MET:HG2	2:A:156:ALA:HB2	1.82	0.62
2:B:210:ARG:HD3	3:B:308:HOH:O	1.99	0.61
2:B:107:ALA:O	2:B:111:MET:HG3	2.00	0.61
2:A:131:ALA:HB1	2:A:177:MET:HE3	1.82	0.60
2:B:237:SER:HB3	2:B:256:GLU:HG3	1.82	0.60
2:B:242:ARG:HH11	2:B:242:ARG:HG2	1.65	0.60
2:A:221:SER:O	2:A:225:ILE:HG12	2.02	0.59
2:A:152:HIS:HD2	2:A:154:GLY:N	2.02	0.58
2:B:139:LYS:HB3	2:B:159:GLU:OE1	2.04	0.58
2:B:227:SER:HA	2:B:230:GLU:CD	2.29	0.58
2:A:131:ALA:CB	2:A:177:MET:HE3	2.34	0.58
2:B:139:LYS:HB3	2:B:159:GLU:CD	2.29	0.58
2:B:241:ALA:C	2:B:242:ARG:HG3	2.29	0.57
2:B:243:ASP:OD2	2:B:245:THR:HB	2.04	0.57
2:B:242:ARG:HG2	2:B:242:ARG:NH1	2.18	0.57
2:B:271:ASN:ND2	2:B:272:LEU:HG	2.19	0.57
2:A:164:GLU:OE2	2:A:286:VAL:CG2	2.50	0.57
2:B:100:SER:OG	2:B:103:GLN:HG3	2.04	0.57
2:A:190:ASN:OD1	2:A:193:GLN:NE2	2.38	0.57
2:A:117:GLY:O	2:A:118:SER:HB2	2.05	0.56
2:B:120:TYR:HB3	2:B:123:LEU:CD1	2.35	0.56
2:B:234:LYS:HE3	2:B:258:GLU:CD	2.30	0.56
2:A:135:PHE:HE2	2:A:173:MET:HE3	1.70	0.56
2:A:199:ASP:O	2:A:203:GLU:HG3	2.06	0.56
2:B:126:ASP:OD2	2:B:127:THR:N	2.39	0.56
2:A:167:GLN:NE2	2:A:187:ARG:NH2	2.52	0.56
2:A:172:GLN:OE1	2:A:281:ARG:NH1	2.39	0.55
2:A:180:GLY:HA3	2:B:191:ILE:HD11	1.88	0.55
2:A:291:PRO:O	2:A:292:LEU:CB	2.50	0.55
2:A:173:MET:O	2:A:175:SER:N	2.40	0.55
2:B:173:MET:O	2:B:175:SER:N	2.40	0.55
2:B:208:PHE:CE2	2:B:289:PRO:HD2	2.42	0.55
2:A:294:THR:N	2:A:295:PRO:CD	2.68	0.55
2:A:164:GLU:CD	2:A:286:VAL:HG22	2.32	0.54
2:B:104:ARG:NH1	2:B:291:PRO:CA	2.66	0.54
2:B:200:GLN:O	2:B:204:GLU:HG3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:174:ASN:OD1	2:B:174:ASN:ND2	2.40	0.54
2:A:246:THR:HG21	2:A:248:LYS:HE3	1.90	0.54
2:B:218:GLN:HA	2:B:249:HIS:NE2	2.23	0.54
2:A:133:ALA:N	2:A:134:PRO:HD2	2.23	0.54
2:B:170:LEU:HD12	2:B:185:VAL:HG12	1.89	0.54
2:B:234:LYS:CE	2:B:258:GLU:CD	2.82	0.53
2:B:144:SER:OG	2:B:153:LYS:HB2	2.09	0.53
2:B:172:GLN:O	2:B:173:MET:HE2	2.09	0.53
2:A:229:PHE:C	2:A:231:ALA:H	2.17	0.51
2:A:167:GLN:OE1	2:A:187:ARG:NH2	2.36	0.51
2:B:229:PHE:C	2:B:231:ALA:H	2.17	0.51
2:A:193:GLN:H	2:A:193:GLN:CD	2.16	0.50
2:A:226:LYS:O	2:A:230:GLU:HG2	2.11	0.50
2:B:210:ARG:HG2	2:B:285:ALA:HB2	1.94	0.50
2:B:104:ARG:O	2:B:108:LEU:HG	2.11	0.50
2:B:146:ASP:C	2:B:148:VAL:H	2.16	0.50
2:A:178:LEU:O	2:A:182:ASN:ND2	2.44	0.49
2:B:284:LYS:HB3	2:B:284:LYS:HE2	1.48	0.48
2:A:227:SER:HA	2:A:230:GLU:HG2	1.94	0.48
2:A:272:LEU:HD21	2:A:281:ARG:NH1	2.28	0.48
2:A:242:ARG:HG2	2:A:249:HIS:HA	1.96	0.48
2:A:243:ASP:HB3	2:A:246:THR:OG1	2.12	0.48
2:A:118:SER:CB	2:A:182:ASN:O	2.62	0.48
2:A:209:ASN:ND2	2:A:260:ALA:N	2.62	0.48
2:B:229:PHE:C	2:B:231:ALA:N	2.72	0.48
2:B:150:MET:O	2:B:151:LYS:HG2	2.13	0.47
2:B:176:VAL:HG21	2:B:180:GLY:HA2	1.96	0.47
2:A:229:PHE:C	2:A:231:ALA:N	2.72	0.47
2:A:105:GLN:OE1	2:A:292:LEU:CD2	2.62	0.47
2:A:164:GLU:HB3	2:A:212:TYR:CD2	2.49	0.47
2:A:186:GLY:HA3	2:B:184:LYS:HE3	1.97	0.47
2:A:187:ARG:O	2:B:181:ARG:HD3	2.14	0.47
2:B:275:LEU:C	2:B:275:LEU:HD12	2.40	0.47
2:A:286:VAL:HG23	2:A:287:THR:HG23	1.96	0.47
2:B:220:LEU:HD21	2:B:275:LEU:HD21	1.97	0.47
2:B:188:PRO:O	2:B:191:ILE:HG23	2.15	0.46
2:A:168:LEU:HD21	2:A:283:GLY:HA3	1.97	0.46
2:A:234:LYS:HE3	2:A:258:GLU:OE2	2.15	0.46
2:A:138:ILE:HD12	2:A:158:VAL:CG1	2.44	0.46
2:B:176:VAL:HG21	2:B:180:GLY:CA	2.45	0.46
2:B:176:VAL:CG2	2:B:180:GLY:N	2.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:292:LEU:O	2:B:292:LEU:HD12	2.15	0.46
2:A:294:THR:O	2:A:295:PRO:C	2.59	0.45
2:B:234:LYS:HE3	2:B:258:GLU:CG	2.46	0.45
2:B:149:THR:O	2:B:150:MET:HB2	2.16	0.45
2:B:123:LEU:N	2:B:123:LEU:HD23	2.31	0.45
2:B:291:PRO:O	2:B:292:LEU:HB3	2.16	0.45
2:B:249:HIS:CE1	2:B:251:GLY:HA2	2.51	0.45
2:A:152:HIS:HD2	2:A:154:GLY:CA	2.30	0.44
2:B:146:ASP:O	2:B:146:ASP:CG	2.60	0.44
2:B:133:ALA:N	2:B:134:PRO:CD	2.80	0.44
2:A:105:GLN:OE1	2:A:292:LEU:HD22	2.18	0.44
2:B:234:LYS:HE2	2:B:234:LYS:HB3	1.71	0.44
2:B:119:ILE:CD1	2:B:143:MET:HE3	2.47	0.44
2:B:271:ASN:HA	2:B:282:VAL:HG23	2.00	0.44
2:B:140:SER:OG	2:B:159:GLU:OE1	2.24	0.44
2:B:176:VAL:HG21	2:B:180:GLY:N	2.33	0.44
2:A:128:ILE:O	2:A:132:PHE:HD2	1.99	0.44
2:A:242:ARG:HG2	2:A:249:HIS:CA	2.48	0.44
2:B:234:LYS:HE3	2:B:258:GLU:HB2	2.00	0.44
2:B:135:PHE:HE1	2:B:172:GLN:OE1	2.01	0.43
2:A:290:MET:HA	2:A:291:PRO:HD2	1.81	0.43
2:A:194:ALA:O	2:A:198:ILE:HG13	2.18	0.43
2:A:167:GLN:CD	2:A:187:ARG:NH2	2.77	0.43
2:A:132:PHE:C	2:A:134:PRO:HD2	2.44	0.43
2:B:106:GLY:O	2:B:110:ILE:HG13	2.19	0.43
2:B:276:GLY:C	2:B:278:GLN:H	2.27	0.43
2:B:290:MET:HE2	2:B:290:MET:HB3	1.88	0.43
2:A:276:GLY:C	2:A:278:GLN:H	2.27	0.42
2:B:178:LEU:O	2:B:182:ASN:ND2	2.52	0.42
2:B:234:LYS:HE3	2:B:258:GLU:CB	2.49	0.42
2:A:118:SER:OG	2:A:184:LYS:NZ	2.38	0.42
2:A:244:PRO:HG2	2:A:245:THR:H	1.85	0.42
2:A:174:ASN:ND2	2:B:185:VAL:O	2.52	0.42
2:A:210:ARG:HD2	2:A:256:GLU:OE1	2.19	0.42
2:B:210:ARG:HH11	2:B:285:ALA:HB1	1.85	0.42
2:A:119:ILE:CD1	2:A:143:MET:HE3	2.47	0.42
2:B:143:MET:HG2	2:B:156:ALA:CB	2.43	0.42
2:B:225:ILE:CG2	2:B:255:ILE:HD11	2.50	0.41
2:B:241:ALA:O	2:B:249:HIS:HA	2.20	0.41
2:B:275:LEU:HD23	2:B:280:LEU:HD11	2.02	0.41
2:A:115:TYR:HD1	2:A:157:PHE:CZ	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:167:GLN:CD	2:A:187:ARG:HH21	2.26	0.41
2:B:290:MET:HA	2:B:291:PRO:HD2	1.88	0.41
2:A:187:ARG:N	2:B:181:ARG:HD3	2.36	0.41
2:A:197:ILE:O	2:A:200:GLN:HB3	2.21	0.41
2:A:241:ALA:O	2:A:249:HIS:HA	2.21	0.41
2:B:292:LEU:O	2:B:292:LEU:CG	2.69	0.41
2:A:176:VAL:HA	2:A:182:ASN:OD1	2.20	0.40
2:A:134:PRO:HG2	2:A:135:PHE:CE2	2.57	0.40
2:B:208:PHE:CE1	2:B:289:PRO:HG2	2.56	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	
2	A	185/216 (86%)	164 (89%)	16 (9%)	5 (3%)	4	1
2	B	192/216 (89%)	167 (87%)	18 (9%)	7 (4%)	2	1
All	All	377/432 (87%)	331 (88%)	34 (9%)	12 (3%)	3	1

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	292	LEU
2	A	293	LEU
2	B	147	SER
2	B	150	MET
2	B	178	LEU
2	A	174	ASN
2	B	174	ASN
2	B	292	LEU
2	A	289	PRO

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Mol	Chain	Res	Type
2	A	294	THR
2	B	180	GLY
2	B	291	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	
2	A	151/171 (88%)	136 (90%)	15 (10%)	7	5
2	B	151/171 (88%)	139 (92%)	12 (8%)	11	9
All	All	302/342 (88%)	275 (91%)	27 (9%)	9	6

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	105	GLN
2	A	129	ARG
2	A	140	SER
2	A	143	MET
2	A	174	ASN
2	A	182	ASN
2	A	183	ILE
2	A	184	LYS
2	A	193	GLN
2	A	195	GLN
2	A	220	LEU
2	A	237	SER
2	A	263	SER
2	A	275	LEU
2	A	290	MET
2	B	105	GLN
2	B	143	MET
2	B	147	SER
2	B	159	GLU
2	B	181	ARG

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Mol	Chain	Res	Type
2	B	184	LYS
2	B	220	LEU
2	B	239	THR
2	B	249	HIS
2	B	256	GLU
2	B	275	LEU
2	B	289	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	130	GLN
2	A	152	HIS
2	A	278	GLN
2	B	182	ASN
2	B	278	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](#)

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 ⓘ

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	C	4/25 (16%)	-0.77	0 100 100	91, 92, 97, 99	0
2	A	193/216 (89%)	-0.81	2 (1%) 79 81	34, 51, 74, 87	4 (2%)
2	B	194/216 (89%)	-0.91	0 100 100	39, 51, 78, 85	0
All	All	391/457 (85%)	-0.86	2 (0%) 87 88	34, 51, 78, 99	4 (1%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	148	VAL	3.4
2	A	149	THR	2.1

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.