



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 05:18 am BST

PDB ID : 6IXP
Title : Structure of Myo2-GTD in complex with Mmr1
Authors : Tang, K.; Wei, Z.
Deposited on : 2018-12-11
Resolution : 2.73 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

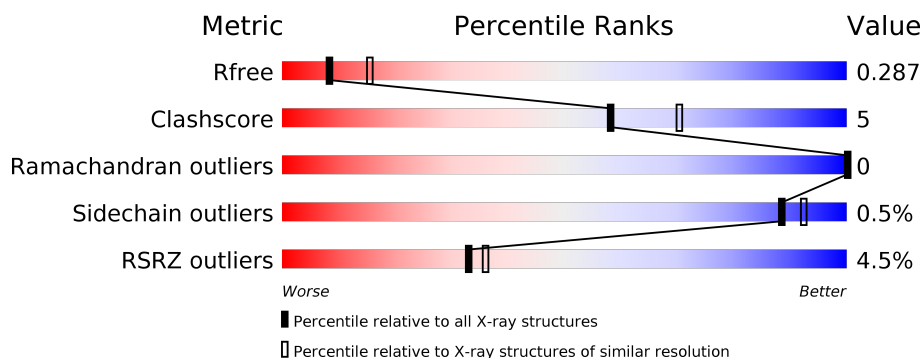
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.73 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	1271 (2.76-2.72)
Clashscore	141614	1322 (2.76-2.72)
Ramachandran outliers	138981	1297 (2.76-2.72)
Sidechain outliers	138945	1298 (2.76-2.72)
RSRZ outliers	127900	1243 (2.76-2.72)

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 on 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	421	<div> <div>4%</div> <div> <div></div> <div>80%</div> <div>12%</div> <div>7%</div> </div> </div>
1	D	421	<div> <div>3%</div> <div> <div></div> <div>80%</div> <div>11%</div> <div>8%</div> </div> </div>
2	B	39	<div> <div>5%</div> <div> <div></div> <div>31%</div> <div>10%</div> <div>59%</div> </div> </div>
2	C	39	<div> <div>3%</div> <div> <div></div> <div>33%</div> <div>13%</div> <div>54%</div> </div> </div>
2	E	39	<div> <div>8%</div> <div> <div></div> <div>41%</div> <div>59%</div> </div> </div>
2	F	39	<div> <div>3%</div> <div> <div></div> <div>33%</div> <div>13%</div> <div>54%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6796 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 Myosin-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	390	Total	C	N	O	S	0	1	0
			3149	2045	504	590	10			
1	D	386	Total	C	N	O	S	0	1	0
			3121	2027	499	585	10			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1148	GLY	-	expression tag	UNP P19524
A	1149	PRO	-	expression tag	UNP P19524
A	1150	GLY	-	expression tag	UNP P19524
A	1151	SER	-	expression tag	UNP P19524
A	?	-	PHE	deletion	UNP P19524
A	?	-	LEU	deletion	UNP P19524
A	?	-	ASN	deletion	UNP P19524
A	?	-	LYS	deletion	UNP P19524
A	?	-	ILE	deletion	UNP P19524
A	?	-	PHE	deletion	UNP P19524
D	1148	GLY	-	expression tag	UNP P19524
D	1149	PRO	-	expression tag	UNP P19524
D	1150	GLY	-	expression tag	UNP P19524
D	1151	SER	-	expression tag	UNP P19524
D	?	-	PHE	deletion	UNP P19524
D	?	-	LEU	deletion	UNP P19524
D	?	-	ASN	deletion	UNP P19524
D	?	-	LYS	deletion	UNP P19524
D	?	-	ILE	deletion	UNP P19524
D	?	-	PHE	deletion	UNP P19524

- Molecule 2 is a protein called Mitochondrial MYO2 receptor-related protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	16	Total	C	N	O	S	0	0	0
			120	76	23	20	1			
2	C	18	Total	C	N	O		0	0	0
			146	92	27	27				
2	E	16	Total	C	N	O	S	0	0	0
			110	69	22	18	1			
2	F	18	Total	C	N	O		0	0	0
			146	92	27	27				

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	392	GLY	-	expression tag	UNP Q06324
B	393	PRO	-	expression tag	UNP Q06324
B	394	GLY	-	expression tag	UNP Q06324
B	395	SER	-	expression tag	UNP Q06324
B	396	GLU	-	expression tag	UNP Q06324
B	397	PHE	-	expression tag	UNP Q06324
C	392	GLY	-	expression tag	UNP Q06324
C	393	PRO	-	expression tag	UNP Q06324
C	394	GLY	-	expression tag	UNP Q06324
C	395	SER	-	expression tag	UNP Q06324
C	396	GLU	-	expression tag	UNP Q06324
C	397	PHE	-	expression tag	UNP Q06324
E	392	GLY	-	expression tag	UNP Q06324
E	393	PRO	-	expression tag	UNP Q06324
E	394	GLY	-	expression tag	UNP Q06324
E	395	SER	-	expression tag	UNP Q06324
E	396	GLU	-	expression tag	UNP Q06324
E	397	PHE	-	expression tag	UNP Q06324
F	392	GLY	-	expression tag	UNP Q06324
F	393	PRO	-	expression tag	UNP Q06324
F	394	GLY	-	expression tag	UNP Q06324
F	395	SER	-	expression tag	UNP Q06324
F	396	GLU	-	expression tag	UNP Q06324
F	397	PHE	-	expression tag	UNP Q06324

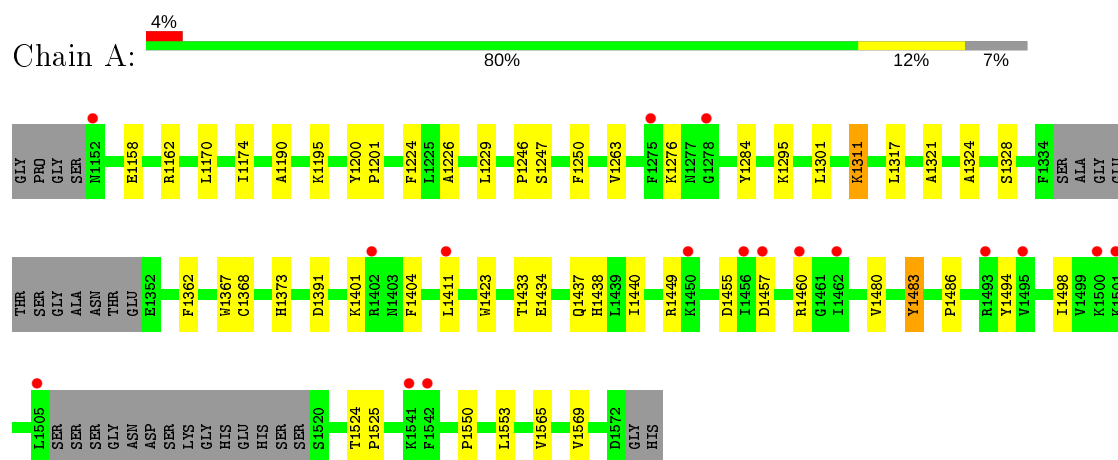
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	O	0	0
			4	4		

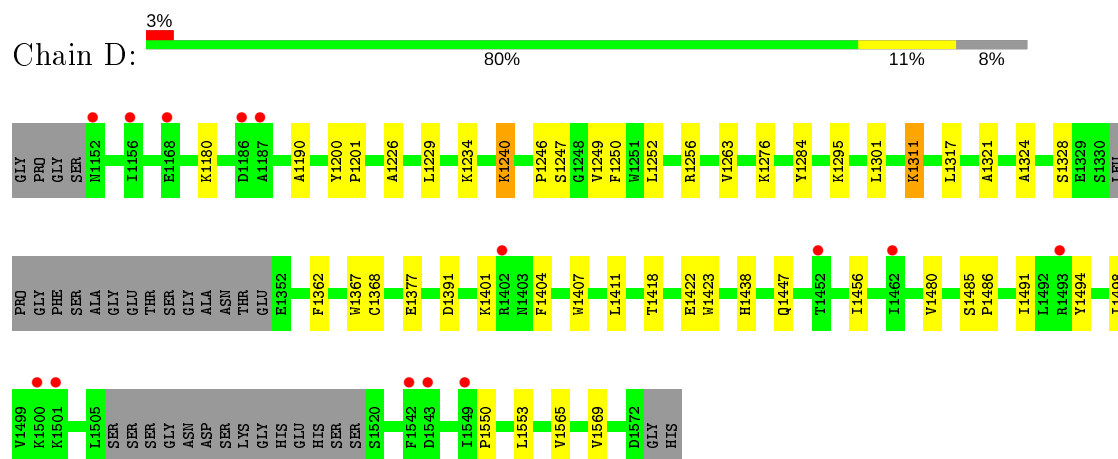
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

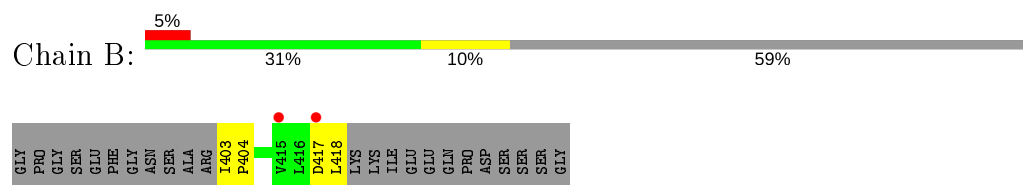
• Molecule 1: Myosin-2



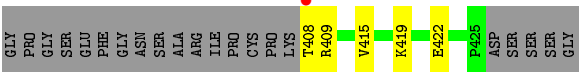
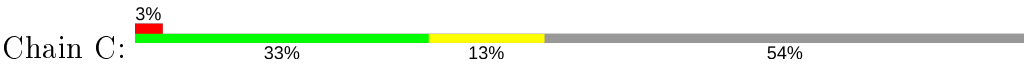
• Molecule 1: Myosin-2



• Molecule 2: Mitochondrial MYO2 receptor-related protein 1



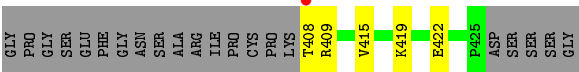
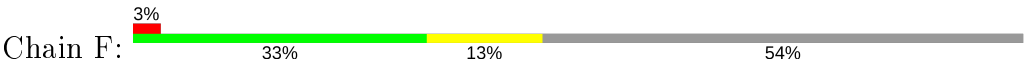
• Molecule 2: Mitochondrial MYO2 receptor-related protein 1



• Molecule 2: Mitochondrial MYO2 receptor-related protein 1



• Molecule 2: Mitochondrial MYO2 receptor-related protein 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	110.39 Å 63.46 Å 169.08 Å 90.00° 104.72° 90.00°	Depositor
Resolution (Å)	53.38 – 2.73 54.55 – 2.73	Depositor EDS
% Data completeness (in resolution range)	92.7 (53.38-2.73) 83.2 (54.55-2.73)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 2.73 Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.242 , 0.284 0.246 , 0.287	Depositor DCC
R_{free} test set	1326 reflections (4.69%)	wwPDB-VP
Wilson B-factor (Å ²)	67.5	Xtriage
Anisotropy	0.377	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 71.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for 1/2*h-3/2*k,-1/2*h-1/2*k,-1/2*h +1/2*k-l 0.000 for 1/2*h+3/2*k,1/2*h-1/2*k,-1/2*h- 1/2*k-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6796	wwPDB-VP
Average B, all atoms (Å ²)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.74 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.0360e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [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	0.26	0/3215	0.42	0/4371
1	D	0.26	0/3186	0.42	0/4331
2	B	0.17	0/121	0.43	0/164
2	C	0.20	0/146	0.39	0/195
2	E	0.17	0/111	0.43	0/152
2	F	0.19	0/146	0.39	0/195
All	All	0.26	0/6925	0.42	0/9408

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	A	3149	0	3158	31	0
1	D	3121	0	3129	30	0
2	B	120	0	131	2	0
2	C	146	0	161	4	0
2	E	110	0	109	0	0
2	F	146	0	161	4	0
3	A	4	0	0	0	0
All	All	6796	0	6849	65	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 5.

All (65) 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:1401:LYS:HB3	1:A:1404:PHE:HB3	1.75	0.67
1:D:1401:LYS:HB3	1:D:1404:PHE:HB3	1.78	0.66
1:A:1480:VAL:HG11	1:A:1486:PRO:HA	1.84	0.59
1:A:1483:TYR:HB2	1:D:1422:GLU:OE1	2.06	0.55
1:D:1391:ASP:OD2	1:D:1438:HIS:ND1	2.30	0.53
1:D:1190:ALA:HA	1:D:1367:TRP:HB3	1.91	0.53
1:D:1480:VAL:HG11	1:D:1486:PRO:HA	1.90	0.53
1:A:1433:THR:HG22	1:A:1437:GLN:NE2	2.24	0.52
2:F:415:VAL:HG12	2:F:419:LYS:HE3	1.90	0.52
1:D:1229:LEU:HD23	1:D:1301:LEU:HD22	1.91	0.52
2:B:417:ASP:OD1	2:B:418:LEU:N	2.42	0.51
1:D:1418:THR:O	1:D:1422:GLU:HG2	2.10	0.51
2:C:415:VAL:HG12	2:C:419:LYS:HE3	1.93	0.51
1:A:1411:LEU:HD21	1:D:1411:LEU:HD11	1.93	0.50
1:A:1449:ARG:O	1:A:1455:ASP:HB3	2.12	0.50
1:A:1247:SER:O	1:A:1250:PHE:HB3	2.12	0.49
1:A:1324:ALA:O	1:A:1328:SER:HB2	2.12	0.49
1:A:1229:LEU:HD23	1:A:1301:LEU:HD22	1.95	0.49
1:A:1457:ASP:HA	1:A:1460:ARG:HD3	1.94	0.49
1:D:1565:VAL:O	1:D:1569:VAL:HG23	2.13	0.49
1:D:1247:SER:O	1:D:1250:PHE:HB3	2.13	0.48
1:A:1190:ALA:HA	1:A:1367:TRP:HB3	1.96	0.48
2:F:408:THR:OG1	2:F:409:ARG:N	2.47	0.48
1:D:1362:PHE:HB3	1:D:1423:TRP:CZ2	2.49	0.47
1:D:1276:LYS:HE3	1:D:1284:TYR:CZ	2.49	0.47
2:C:408:THR:OG1	2:C:409:ARG:N	2.46	0.47
1:A:1565:VAL:O	1:A:1569:VAL:HG23	2.16	0.46
1:D:1494:TYR:CE2	1:D:1498:ILE:HD11	2.51	0.45
1:A:1317:LEU:HD22	1:A:1321:ALA:HB2	1.99	0.45
1:A:1200:TYR:CG	1:A:1201:PRO:HD3	2.52	0.45
1:A:1433:THR:HG23	1:A:1440:ILE:HD13	1.98	0.45
1:D:1256:ARG:HD2	1:D:1256:ARG:HA	1.70	0.45
1:D:1550:PRO:HD2	1:D:1553:LEU:HD12	1.98	0.45
1:A:1311:LYS:NZ	2:C:422:GLU:OE2	2.50	0.45
1:A:1362:PHE:HB3	1:A:1423:TRP:CZ2	2.52	0.44
1:D:1494:TYR:CZ	1:D:1498:ILE:HD11	2.52	0.44
1:A:1263:VAL:HG22	1:A:1295:LYS:HE2	2.00	0.44
1:A:1494:TYR:CZ	1:A:1498:ILE:HD11	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1391:ASP:OD2	1:A:1438:HIS:ND1	2.40	0.44
1:A:1550:PRO:HD2	1:A:1553:LEU:HD12	2.00	0.44
1:D:1246:PRO:HA	1:D:1368:CYS:SG	2.58	0.43
1:A:1195:LYS:HG2	1:A:1373:HIS:CD2	2.54	0.43
1:D:1180:LYS:HE2	1:D:1234:LYS:HE3	1.99	0.43
1:D:1200:TYR:CG	1:D:1201:PRO:HD3	2.53	0.43
1:D:1407:TRP:HD1	1:D:1447:GLN:HA	1.84	0.43
1:A:1158:GLU:O	1:A:1162:ARG:HG3	2.17	0.43
1:A:1246:PRO:HA	1:A:1368:CYS:SG	2.58	0.43
1:A:1226:ALA:HA	2:C:408:THR:HG22	2.00	0.43
1:A:1170:LEU:HA	1:A:1170:LEU:HD12	1.85	0.42
1:D:1263:VAL:HG22	1:D:1295:LYS:HE2	2.01	0.42
1:D:1311:LYS:HD3	2:F:422:GLU:HG3	2.01	0.42
1:D:1324:ALA:O	1:D:1328:SER:HB2	2.20	0.42
1:A:1524:THR:HA	1:A:1525:PRO:HD3	1.86	0.42
1:A:1158:GLU:HG2	1:A:1162:ARG:HE	1.86	0.41
1:A:1434:GLU:HA	1:A:1437:GLN:HG2	2.01	0.41
1:D:1456:ILE:HG13	1:D:1491:ILE:HG23	2.01	0.41
1:D:1226:ALA:HA	2:F:408:THR:HG22	2.02	0.41
1:D:1485:SER:HA	1:D:1486:PRO:HD3	1.90	0.41
1:A:1174:ILE:HG13	1:A:1224:PHE:HE1	1.86	0.41
1:D:1249:VAL:HA	1:D:1252:LEU:HD12	2.03	0.41
1:D:1317:LEU:HD22	1:D:1321:ALA:HB2	2.03	0.41
1:D:1240:LYS:HB3	1:D:1240:LYS:HE3	1.89	0.41
2:B:403:ILE:HA	2:B:404:PRO:HD3	1.84	0.40
1:D:1377:GLU:N	1:D:1377:GLU:OE1	2.49	0.40
1:A:1276:LYS:HE3	1:A:1284:TYR:CZ	2.57	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	385/421 (91%)	372 (97%)	13 (3%)	0	100	100
1	D	381/421 (90%)	369 (97%)	12 (3%)	0	100	100
2	B	14/39 (36%)	14 (100%)	0	0	100	100
2	C	16/39 (41%)	16 (100%)	0	0	100	100
2	E	14/39 (36%)	14 (100%)	0	0	100	100
2	F	16/39 (41%)	16 (100%)	0	0	100	100
All	All	826/998 (83%)	801 (97%)	25 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	349/378 (92%)	347 (99%)	2 (1%)	86	91
1	D	346/378 (92%)	344 (99%)	2 (1%)	86	91
2	B	14/33 (42%)	14 (100%)	0	100	100
2	C	17/33 (52%)	17 (100%)	0	100	100
2	E	11/33 (33%)	11 (100%)	0	100	100
2	F	17/33 (52%)	17 (100%)	0	100	100
All	All	754/888 (85%)	750 (100%)	4 (0%)	88	92

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1311	LYS
1	A	1483	TYR
1	D	1240	LYS
1	D	1311	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 carbohydrates 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

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, 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	390/421 (92%)	0.41	17 (4%) 34 37	56, 99, 177, 213	2 (0%)
1	D	386/421 (91%)	0.34	14 (3%) 42 47	62, 99, 152, 190	2 (0%)
2	B	16/39 (41%)	0.87	2 (12%) 3 4	87, 116, 150, 155	0
2	C	18/39 (46%)	0.41	1 (5%) 24 27	86, 122, 148, 151	0
2	E	16/39 (41%)	0.70	3 (18%) 1 1	95, 134, 153, 160	0
2	F	18/39 (46%)	0.45	1 (5%) 24 27	87, 121, 148, 158	0
All	All	844/998 (84%)	0.39	38 (4%) 33 36	56, 101, 165, 213	4 (0%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1460	ARG	4.5
1	D	1152	ASN	4.4
1	A	1402	ARG	3.9
1	A	1505	LEU	3.8
1	A	1500	LYS	3.8
2	C	408	THR	3.7
1	D	1402	ARG	3.5
1	A	1462	ILE	3.5
1	A	1152	ASN	3.2
1	D	1187	ALA	2.8
1	A	1456	ILE	2.8
1	A	1411	LEU	2.8
1	A	1493	ARG	2.7
1	A	1495	VAL	2.7
1	A	1541	LYS	2.7
1	D	1493	ARG	2.7
2	F	408	THR	2.7
1	A	1501	LYS	2.5
2	B	415	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	1156	ILE	2.4
2	E	417	ASP	2.4
1	D	1186	ASP	2.4
1	A	1278	GLY	2.4
1	A	1450	LYS	2.4
1	A	1275	PHE	2.4
1	A	1542	PHE	2.4
1	D	1500	LYS	2.3
1	D	1452	THR	2.3
2	B	417	ASP	2.3
1	D	1542	PHE	2.3
1	D	1549	ILE	2.3
1	D	1501	LYS	2.3
2	E	416	LEU	2.2
1	D	1462	ILE	2.2
1	D	1168	GLU	2.1
2	E	418	LEU	2.1
1	A	1457	ASP	2.0
1	D	1543	ASP	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 carbohydrates 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.