



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:32 AM UTC

PDB ID : 9PFO / pdb_00009pfo
Title : Structure of POU2F3 POU domains bound to coactivator OCA-T2 and DNA
(2.1 angstrom resolution)
Authors : Ipsaro, J.J.; Alpsoy, A.; Vakoc, C.R.; Joshua-Tor, L.
Deposited on : 2025-07-06
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:

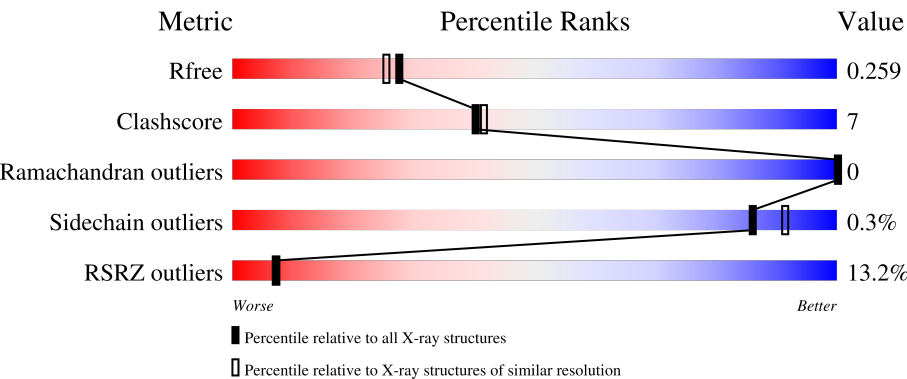
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

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	A	160	11% 74%15%11%
1	E	160	12% 75%9%16%
1	I	160	11% 78%9%13%
1	M	160	13% 79%9%11%
2	B	39	26% 54%13%33%

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Mol	Chain	Length	Quality of chain
2	F	39	
2	J	39	
2	N	39	
3	C	15	
3	G	15	
3	K	15	
3	O	15	
4	D	15	
4	H	15	
4	L	15	
4	P	15	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 15724 atoms, of which 7045 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 POU domain, class 2, transcription factor 3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	143	Total	C	H	N	O	S	0	0	0
			2368	733	1195	212	221	7			
1	E	134	Total	C	H	N	O	S	0	1	0
			2267	701	1152	203	204	7			
1	I	139	Total	C	H	N	O	S	0	0	0
			2326	720	1179	208	212	7			
1	M	142	Total	C	H	N	O	S	0	1	0
			2367	734	1199	211	216	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	182	GLY	-	expression tag	UNP Q9UKI9
E	182	GLY	-	expression tag	UNP Q9UKI9
I	182	GLY	-	expression tag	UNP Q9UKI9
M	182	GLY	-	expression tag	UNP Q9UKI9

- Molecule 2 is a protein called POU class 2 homeobox associating factor 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	26	Total	C	H	N	O	0	0	0
			445	134	233	44	34			
2	F	28	Total	C	H	N	O	0	0	0
			455	136	236	46	37			
2	J	25	Total	C	H	N	O	0	0	0
			430	129	225	43	33			
2	N	28	Total	C	H	N	O	0	0	0
			477	143	250	47	37			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	GLY	-	expression tag	UNP A8K830
F	0	GLY	-	expression tag	UNP A8K830
J	0	GLY	-	expression tag	UNP A8K830
N	0	GLY	-	expression tag	UNP A8K830

- Molecule 3 is a DNA chain called DNA containing POU domain recognition element octamer (sense strand).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	15	Total 481	C 149	H 171	N 61	O 86	P 14	0	0	0
3	G	15	Total 481	C 149	H 171	N 61	O 86	P 14	0	0	0
3	K	15	Total 481	C 149	H 171	N 61	O 86	P 14	0	0	0
3	O	15	Total 481	C 149	H 171	N 61	O 86	P 14	0	0	0

- Molecule 4 is a DNA chain called DNA containing POU domain recognition element octamer (antisense strand).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	15	Total 472	C 146	H 173	N 49	O 90	P 14	0	0	0
4	H	15	Total 472	C 146	H 173	N 49	O 90	P 14	0	0	0
4	L	15	Total 472	C 146	H 173	N 49	O 90	P 14	0	0	0
4	P	15	Total 472	C 146	H 173	N 49	O 90	P 14	0	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	86	Total 86	O 86	0	0
5	B	21	Total 21	O 21	0	0
5	C	40	Total 40	O 40	0	0
5	D	32	Total 32	O 32	0	0

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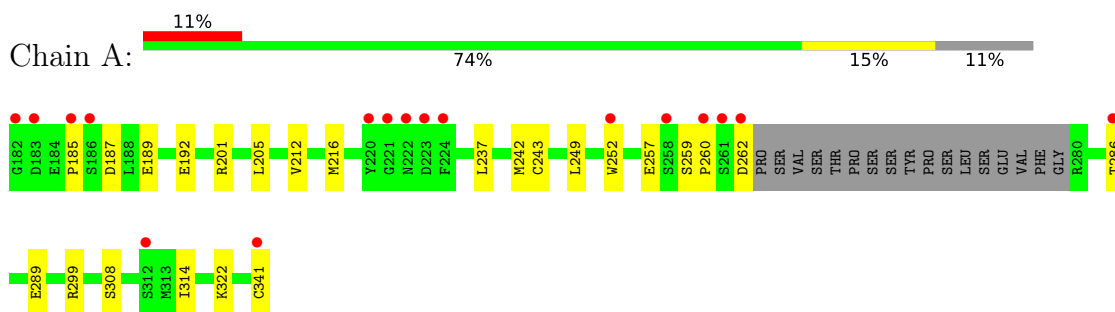
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	98	Total 98	O 98	0	0
5	F	17	Total 17	O 17	0	0
5	G	39	Total 39	O 39	0	0
5	H	33	Total 33	O 33	0	0
5	I	111	Total 111	O 111	0	0
5	J	11	Total 11	O 11	0	0
5	K	35	Total 35	O 35	0	0
5	L	38	Total 38	O 38	0	0
5	M	104	Total 104	O 104	0	0
5	N	24	Total 24	O 24	0	0
5	O	43	Total 43	O 43	0	0
5	P	45	Total 45	O 45	0	0

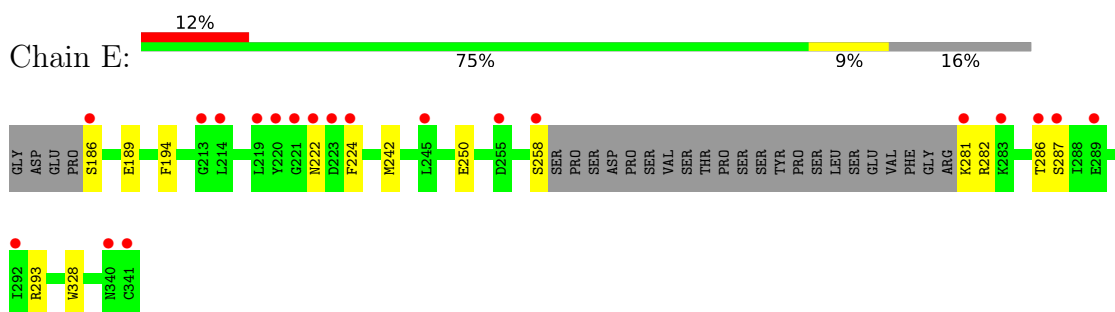
3 Residue-property plots [i](#)

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.

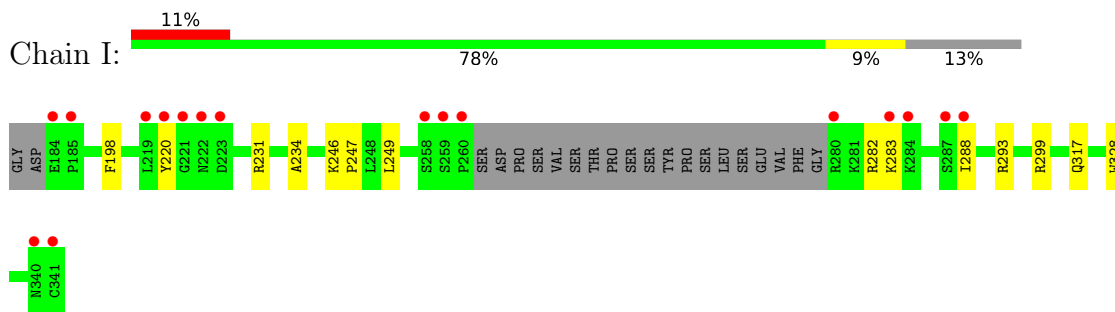
- Molecule 1: POU domain, class 2, transcription factor 3



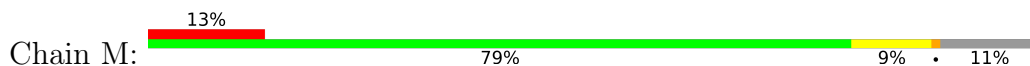
- Molecule 1: POU domain, class 2, transcription factor 3

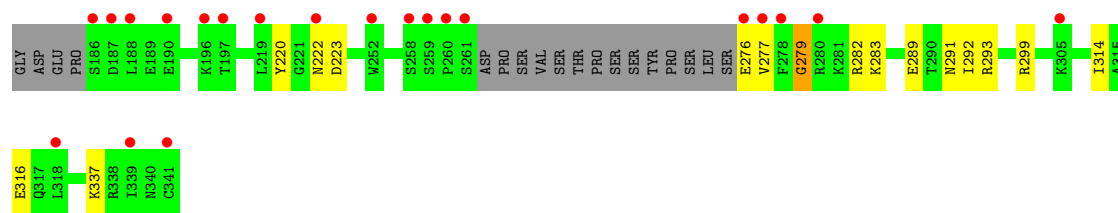


- Molecule 1: POU domain, class 2, transcription factor 3

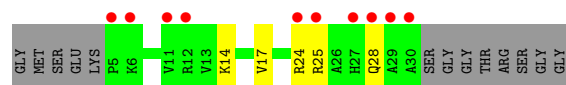


- Molecule 1: POU domain, class 2, transcription factor 3





- Molecule 2: POU class 2 homeobox associating factor 3



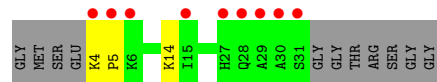
- Molecule 2: POU class 2 homeobox associating factor 3



- Molecule 2: POU class 2 homeobox associating factor 3



- Molecule 2: POU class 2 homeobox associating factor 3



- Molecule 3: DNA containing POU domain recognition element octamer (sense strand)

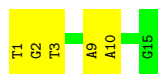


- Molecule 3: DNA containing POU domain recognition element octamer (sense strand)



- Molecule 3: DNA containing POU domain recognition element octamer (sense strand)

Chain K:  67% 33%



- Molecule 3: DNA containing POU domain recognition element octamer (sense strand)

Chain O:  93% 7%



- Molecule 4: DNA containing POU domain recognition element octamer (antisense strand)

Chain D:  7% 73% 27%



- Molecule 4: DNA containing POU domain recognition element octamer (antisense strand)

Chain H:  7% 73% 27%



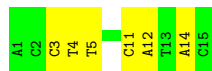
- Molecule 4: DNA containing POU domain recognition element octamer (antisense strand)

Chain L:  53% 47%



- Molecule 4: DNA containing POU domain recognition element octamer (antisense strand)

Chain P:  60% 40%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	79.02Å 95.80Å 85.64Å 90.00° 101.24° 90.00°	Depositor
Resolution (Å)	29.83 – 2.10 29.83 – 2.10	Depositor EDS
% Data completeness (in resolution range)	96.6 (29.83-2.10) 96.6 (29.83-2.10)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.95 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.219 , 0.259 0.220 , 0.259	Depositor DCC
R_{free} test set	3552 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	25.5	Xtriage
Anisotropy	0.831	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	15724	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.60% 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	A	0.26	0/1189	0.40	0/1584
1	E	0.43	0/1132	0.57	0/1505
1	I	0.34	0/1163	0.50	0/1549
1	M	0.34	0/1195	0.48	0/1590
2	B	0.30	0/214	0.56	0/285
2	F	0.47	0/220	0.76	0/292
2	J	0.31	0/206	0.50	0/274
2	N	0.28	0/229	0.50	0/305
3	C	0.38	0/349	0.64	0/538
3	G	0.38	0/349	0.61	0/538
3	K	0.42	0/349	0.65	0/538
3	O	0.38	0/349	0.62	0/538
4	D	0.48	0/333	0.70	0/511
4	H	0.38	0/333	0.69	0/511
4	L	0.41	0/333	0.65	0/511
4	P	0.53	0/333	0.74	0/511
All	All	0.37	0/8276	0.57	0/11580

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	M	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	M	279	GLY	Mainchain

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	1173	1195	1195	22	0
1	E	1115	1152	1154	20	0
1	I	1147	1179	1179	13	0
1	M	1168	1199	1185	16	0
2	B	212	233	233	6	0
2	F	219	236	236	3	0
2	J	205	225	225	2	0
2	N	227	250	250	2	0
3	C	310	171	171	7	0
3	G	310	171	171	7	0
3	K	310	171	171	4	0
3	O	310	171	171	1	0
4	D	299	173	173	3	0
4	H	299	173	173	5	0
4	L	299	173	173	7	0
4	P	299	173	173	6	0
5	A	86	0	0	2	0
5	B	21	0	0	1	0
5	C	40	0	0	3	1
5	D	32	0	0	0	1
5	E	98	0	0	8	0
5	F	17	0	0	1	0
5	G	39	0	0	0	1
5	H	33	0	0	2	1
5	I	111	0	0	3	1
5	J	11	0	0	0	0
5	K	35	0	0	0	0
5	L	38	0	0	3	0
5	M	104	0	0	4	2
5	N	24	0	0	1	0
5	O	43	0	0	0	0
5	P	45	0	0	3	0
All	All	8679	7045	7033	99	4

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 7.

All (99) 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:289:GLU:OE1	5:A:401:HOH:O	1.83	0.96
1:I:288:ILE:O	5:I:401:HOH:O	1.87	0.92
1:M:316:GLU:OE1	5:M:401:HOH:O	1.89	0.90
3:C:15:DG:OP2	5:C:101:HOH:O	1.88	0.90
1:I:282:ARG:NH2	5:I:402:HOH:O	2.03	0.89
1:M:222:ASN:ND2	5:M:402:HOH:O	1.93	0.86
4:L:13:DT:OP2	5:L:101:HOH:O	2.00	0.79
1:E:293[A]:ARG:NE	5:E:401:HOH:O	2.04	0.77
4:H:1:DA:N6	5:H:101:HOH:O	2.17	0.76
4:P:11:DC:OP1	5:P:101:HOH:O	2.04	0.74
1:E:293[A]:ARG:NH2	3:G:9:DA:OP1	2.21	0.73
1:A:187:ASP:OD2	1:M:293:ARG:NH2	2.23	0.72
1:M:277:VAL:HG12	1:M:279:GLY:H	1.57	0.69
1:E:224:PHE:CD2	5:E:402:HOH:O	2.47	0.68
1:A:189:GLU:OE2	2:B:24:ARG:NH1	2.28	0.66
1:E:286:THR:HG22	3:G:9:DA:O3'	1.96	0.66
3:G:1:DT:H1'	3:G:2:DG:H5'	1.78	0.65
1:I:293:ARG:NH1	3:K:9:DA:OP1	2.30	0.64
4:P:12:DA:OP1	5:P:102:HOH:O	2.14	0.64
1:I:283:LYS:NZ	3:K:10:DA:OP1	2.31	0.63
2:N:14:LYS:HG3	5:N:103:HOH:O	2.01	0.61
2:B:24:ARG:NE	2:B:28:GLN:OE1	2.34	0.60
3:C:12:DA:OP1	5:C:102:HOH:O	2.16	0.60
1:A:286:THR:HG22	3:C:9:DA:O3'	2.02	0.59
1:E:286:THR:HG22	3:G:9:DA:C3'	2.32	0.59
4:L:4:DT:OP1	5:L:102:HOH:O	2.16	0.59
1:A:286:THR:HG22	3:C:10:DA:P	2.43	0.58
1:I:234:ALA:O	2:J:18:LYS:HE2	2.04	0.58
1:E:189:GLU:OE1	2:F:24:ARG:NH1	2.38	0.56
1:E:287:SER:HA	5:E:432:HOH:O	2.07	0.55
3:C:1:DT:H1'	3:C:2:DG:H5'	1.89	0.55
1:M:220:TYR:HA	1:M:277:VAL:HB	1.88	0.55
1:I:198:PHE:CZ	1:I:249:LEU:HD22	2.43	0.54
4:P:14:DA:O4'	5:P:103:HOH:O	2.19	0.54
1:M:277:VAL:HG12	1:M:279:GLY:N	2.22	0.53
4:D:1:DA:HO5'	4:D:1:DA:H8	1.54	0.53
1:A:341:CYS:SG	5:A:476:HOH:O	2.59	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:282:ARG:HD3	5:E:420:HOH:O	2.09	0.52
1:I:299:ARG:NH1	1:I:317:GLN:OE1	2.43	0.51
4:D:3:DC:H2'	4:D:4:DT:C6	2.46	0.51
1:E:258:SER:HA	1:M:316:GLU:HG3	1.93	0.51
1:E:186:SER:HA	2:F:24:ARG:HH12	1.76	0.50
1:A:212:VAL:HG22	1:A:252:TRP:CH2	2.46	0.50
1:M:276:GLU:HG3	5:M:420:HOH:O	2.11	0.50
1:E:293[A]:ARG:CD	5:E:401:HOH:O	2.57	0.49
1:M:223:ASP:OD1	1:M:223:ASP:C	2.55	0.49
1:A:308:SER:O	1:A:322:LYS:NZ	2.45	0.49
1:E:293[A]:ARG:NH2	3:G:9:DA:P	2.85	0.49
1:M:276:GLU:CG	5:M:420:HOH:O	2.61	0.48
1:A:259:SER:N	1:A:260:PRO:CD	2.77	0.48
4:H:1:DA:H5'	4:H:1:DA:N3	2.28	0.48
3:K:1:DT:H1'	3:K:2:DG:H5''	1.96	0.48
1:I:246:LYS:HB3	1:I:247:PRO:HD3	1.96	0.48
4:H:3:DC:OP1	5:H:102:HOH:O	2.20	0.47
1:I:299:ARG:NH2	1:I:317:GLN:OE1	2.45	0.47
1:E:224:PHE:CE2	5:E:402:HOH:O	2.65	0.47
1:A:205:LEU:HD11	1:A:257:GLU:HG3	1.96	0.47
1:A:185:PRO:HB2	2:B:24:ARG:CZ	2.45	0.47
1:A:259:SER:N	1:A:260:PRO:HD3	2.31	0.46
1:E:258:SER:HA	1:M:316:GLU:CG	2.45	0.46
1:M:337:LYS:NZ	4:P:5:DT:OP1	2.44	0.46
4:P:3:DC:H2'	4:P:4:DT:C6	2.50	0.46
1:M:283:LYS:NZ	3:O:10:DA:OP1	2.49	0.46
4:D:4:DT:H2'	4:D:5:DT:C6	2.51	0.45
1:E:293[A]:ARG:NH2	1:E:328:TRP:HE1	2.14	0.45
1:A:237:LEU:HB2	1:A:242:MET:HG3	1.99	0.45
3:K:2:DG:H2'	3:K:3:DT:H71	1.99	0.45
4:H:3:DC:H2'	4:H:4:DT:C6	2.52	0.45
4:L:2:DC:H1'	4:L:3:DC:C6	2.52	0.45
5:F:104:HOH:O	3:G:7:DC:H6	2.00	0.44
1:A:212:VAL:HG12	1:A:216:MET:HE2	2.00	0.44
4:L:3:DC:H2'	4:L:4:DT:C6	2.52	0.44
1:A:243:CYS:O	1:M:291:ASN:ND2	2.43	0.44
2:B:14:LYS:HE2	5:B:119:HOH:O	2.17	0.44
1:I:220:TYR:O	1:I:220:TYR:CG	2.71	0.44
1:I:231:ARG:NH2	4:L:10:DG:O6	2.42	0.43
1:A:192:GLU:OE2	2:B:25:ARG:NH2	2.51	0.43
1:E:222:ASN:O	5:E:402:HOH:O	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:ARG:HD2	1:A:314:ILE:HD11	2.00	0.43
1:E:194:PHE:CE1	1:E:250:GLU:HG2	2.54	0.43
4:P:11:DC:H2'	4:P:12:DA:C8	2.54	0.43
1:I:293:ARG:HD2	5:I:401:HOH:O	2.19	0.42
1:A:201:ARG:NE	1:A:257:GLU:OE2	2.52	0.42
1:E:293[B]:ARG:NH1	5:E:415:HOH:O	2.52	0.42
2:J:29:ALA:O	2:J:30:ALA:HB3	2.19	0.42
1:I:293:ARG:NH1	1:I:328:TRP:HE1	2.18	0.41
4:L:4:DT:H2'	4:L:5:DT:C6	2.56	0.41
3:C:6:DG:H3'	5:C:128:HOH:O	2.20	0.41
1:A:262:ASP:O	1:E:281:LYS:NZ	2.50	0.41
1:A:205:LEU:HD11	1:A:257:GLU:CG	2.50	0.41
1:A:286:THR:HG22	3:C:9:DA:C3'	2.50	0.41
1:E:242:MET:HG3	2:F:17:VAL:HG21	2.03	0.41
1:M:299:ARG:NH1	1:M:314:ILE:HG12	2.35	0.41
4:H:4:DT:H2'	4:H:5:DT:C6	2.56	0.41
4:L:15:DC:O3'	5:L:103:HOH:O	2.22	0.41
3:G:12:DA:C6	3:G:13:DA:C6	3.09	0.40
1:M:289:GLU:HB3	1:M:292:ILE:HD12	2.03	0.40
2:N:4:LYS:HB3	2:N:5:PRO:HD2	2.03	0.40
1:A:242:MET:SD	2:B:17:VAL:HG21	2.61	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:413:HOH:O	5:M:468:HOH:O[1_554]	2.04	0.16
5:C:124:HOH:O	5:D:118:HOH:O[2_655]	2.13	0.07
5:G:118:HOH:O	5:H:128:HOH:O[2_746]	2.14	0.06
5:M:463:HOH:O	5:M:483:HOH:O[2_646]	2.18	0.02

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	139/160 (87%)	135 (97%)	4 (3%)	0	100	100
1	E	131/160 (82%)	129 (98%)	2 (2%)	0	100	100
1	I	135/160 (84%)	132 (98%)	3 (2%)	0	100	100
1	M	139/160 (87%)	136 (98%)	3 (2%)	0	100	100
2	B	24/39 (62%)	24 (100%)	0	0	100	100
2	F	26/39 (67%)	24 (92%)	2 (8%)	0	100	100
2	J	23/39 (59%)	22 (96%)	1 (4%)	0	100	100
2	N	26/39 (67%)	26 (100%)	0	0	100	100
All	All	643/796 (81%)	628 (98%)	15 (2%)	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	132/148 (89%)	131 (99%)	1 (1%)	73	81
1	E	125/148 (84%)	125 (100%)	0	100	100
1	I	129/148 (87%)	129 (100%)	0	100	100
1	M	132/148 (89%)	131 (99%)	1 (1%)	73	81
2	B	22/30 (73%)	22 (100%)	0	100	100
2	F	22/30 (73%)	22 (100%)	0	100	100
2	J	21/30 (70%)	21 (100%)	0	100	100
2	N	24/30 (80%)	24 (100%)	0	100	100
All	All	607/712 (85%)	605 (100%)	2 (0%)	86	91

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	249	LEU
1	M	282	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	340	ASN
1	E	241	ASN
1	I	236	ASN
1	M	222	ASN

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 [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	143/160 (89%)	1.00	17 (11%) 9 9	19, 37, 76, 126	0
1	E	134/160 (83%)	0.97	20 (14%) 5 5	18, 36, 67, 98	1 (0%)
1	I	139/160 (86%)	0.87	17 (12%) 8 8	19, 31, 71, 94	0
1	M	142/160 (88%)	1.05	21 (14%) 5 6	16, 37, 59, 99	0
2	B	26/39 (66%)	1.66	10 (38%) 1 1	22, 38, 91, 104	0
2	F	28/39 (71%)	1.57	6 (21%) 2 2	33, 50, 96, 104	0
2	J	25/39 (64%)	0.95	2 (8%) 18 19	24, 41, 84, 102	0
2	N	28/39 (71%)	1.32	9 (32%) 1 1	20, 39, 92, 111	0
3	C	15/15 (100%)	0.63	0 100 100	21, 27, 43, 47	0
3	G	15/15 (100%)	0.45	0 100 100	28, 35, 53, 57	0
3	K	15/15 (100%)	0.14	0 100 100	22, 27, 39, 46	0
3	O	15/15 (100%)	0.05	0 100 100	18, 21, 41, 42	0
4	D	15/15 (100%)	0.49	1 (6%) 24 25	21, 26, 48, 61	0
4	H	15/15 (100%)	0.51	1 (6%) 24 25	30, 35, 52, 69	0
4	L	15/15 (100%)	0.42	0 100 100	23, 30, 50, 56	0
4	P	15/15 (100%)	0.42	0 100 100	20, 27, 42, 50	0
All	All	785/916 (85%)	0.94	104 (13%) 7 7	16, 35, 79, 126	1 (0%)

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	221	GLY	6.2
1	M	186	SER	5.6
1	M	277	VAL	5.1
1	I	341	CYS	5.0
1	A	183	ASP	4.9

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Mol	Chain	Res	Type	RSRZ
1	I	185	PRO	4.8
1	M	261	SER	4.8
1	E	341	CYS	4.6
1	I	220	TYR	4.4
2	F	33	GLY	4.4
1	E	220	TYR	4.3
1	A	286	THR	4.3
1	E	255	ASP	4.1
1	I	260	PRO	4.0
1	M	260	PRO	4.0
2	B	5	PRO	4.0
2	B	30	ALA	3.9
2	N	30	ALA	3.8
1	I	259	SER	3.8
2	B	28	GLN	3.7
1	M	259	SER	3.6
1	M	318	LEU	3.5
2	F	21	LEU	3.5
1	A	182	GLY	3.5
2	N	5	PRO	3.4
1	E	219	LEU	3.4
1	E	286	THR	3.4
2	B	29	ALA	3.3
1	M	276	GLU	3.3
2	J	30	ALA	3.3
2	B	27	HIS	3.3
1	E	222	ASN	3.3
1	E	213	GLY	3.2
2	B	25	ARG	3.2
1	A	185	PRO	3.2
1	E	340	ASN	3.1
2	N	6	LYS	3.1
1	A	260	PRO	3.1
1	I	280	ARG	3.0
1	M	280[A]	ARG	3.0
2	N	4	LYS	3.0
1	M	341	CYS	3.0
1	E	258	SER	3.0
1	I	219	LEU	3.0
1	E	214	LEU	2.9
1	M	187	ASP	2.9
2	N	31	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	I	184	GLU	2.8
2	J	7	VAL	2.8
2	F	26	ALA	2.8
2	B	11	VAL	2.8
1	E	224	PHE	2.8
2	N	27	HIS	2.7
1	M	188	LEU	2.7
1	A	261	SER	2.7
1	A	223	ASP	2.7
2	N	29	ALA	2.7
1	E	287	SER	2.7
1	M	305	LYS	2.6
1	M	190	GLU	2.6
1	M	278	PHE	2.6
2	F	32	GLY	2.6
1	A	262	ASP	2.5
1	M	197	THR	2.5
1	I	283	LYS	2.5
1	E	292	ILE	2.5
1	M	222	ASN	2.5
4	D	15	DC	2.4
1	A	220	TYR	2.4
1	A	186	SER	2.4
1	A	258	SER	2.4
1	A	224	PHE	2.4
1	A	341	CYS	2.4
1	I	284	LYS	2.4
1	E	186	SER	2.4
1	M	196	LYS	2.4
1	A	252	TRP	2.4
1	I	222	ASN	2.3
1	I	340	ASN	2.3
1	E	221	GLY	2.3
1	I	258	SER	2.3
1	A	221	GLY	2.3
1	M	258	SER	2.3
2	N	28	GLN	2.3
1	M	252	TRP	2.3
1	I	288	ILE	2.2
2	F	17	VAL	2.2
2	B	24	ARG	2.2
2	F	15	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	M	339	ILE	2.2
1	E	245	LEU	2.2
2	N	15	ILE	2.1
1	E	283	LYS	2.1
1	A	222	ASN	2.1
1	I	287	SER	2.1
1	M	219	LEU	2.1
1	E	289	GLU	2.1
1	E	223	ASP	2.1
1	E	281	LYS	2.1
2	B	6	LYS	2.1
1	I	223	ASP	2.0
1	A	312	SER	2.0
2	B	12	ARG	2.0
4	H	15	DC	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 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.