



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 10:19 pm GMT

PDB ID : 5FLV
Title : Crystal structure of NKX2-5 and TBX5 bound to the Nppa promoter region
Authors : Stirnimann, C.U.; Glatt, S.; Mueller, C.W.
Deposited on : 2015-10-28
Resolution : 3.00 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

<http://wwpdb.org/validation/2016/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
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28683
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

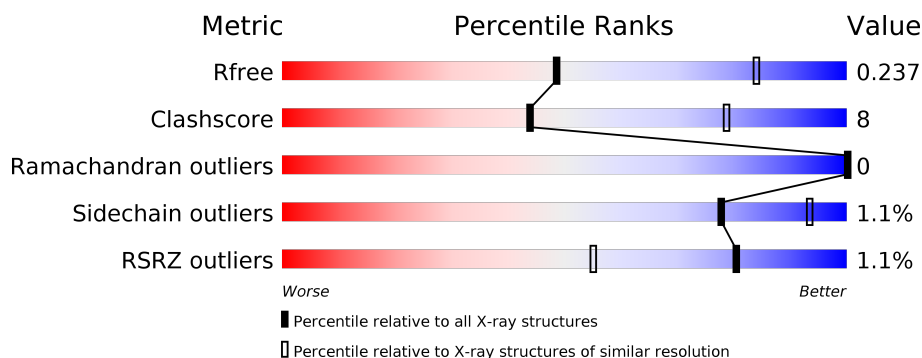
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	100719	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)

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. 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	285	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%; height: 10px; background-color: red;"></div> <div style="position: absolute; bottom: 0; left: 0; width: 100%; height: 10px; background-color: green;"></div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 10px; background-color: yellow;"></div> <div style="position: absolute; top: 0; left: 100%; width: 100%; height: 10px; background-color: grey;"></div> </div> <div> 67% 13% 21% </div> </div>
1	E	285	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; bottom: 0; left: 0; width: 100%; height: 10px; background-color: green;"></div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 10px; background-color: yellow;"></div> <div style="position: absolute; top: 0; left: 100%; width: 100%; height: 10px; background-color: grey;"></div> </div> <div> 62% 17% 20% </div> </div>
1	I	285	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%; height: 10px; background-color: red;"></div> <div style="position: absolute; bottom: 0; left: 0; width: 100%; height: 10px; background-color: green;"></div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 10px; background-color: yellow;"></div> <div style="position: absolute; top: 0; left: 100%; width: 100%; height: 10px; background-color: grey;"></div> </div> <div> 63% 16% 21% </div> </div>
1	M	285	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%; height: 10px; background-color: red;"></div> <div style="position: absolute; bottom: 0; left: 0; width: 100%; height: 10px; background-color: green;"></div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 10px; background-color: yellow;"></div> <div style="position: absolute; top: 0; left: 100%; width: 100%; height: 10px; background-color: grey;"></div> </div> <div> 64% 16% 20% </div> </div>
2	B	22	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; bottom: 0; left: 0; width: 100%; height: 10px; background-color: green;"></div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 10px; background-color: yellow;"></div> <div style="position: absolute; top: 0; left: 100%; width: 100%; height: 10px; background-color: grey;"></div> </div> <div> 59% 36% 5% </div> </div>
2	F	22	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; bottom: 0; left: 0; width: 100%; height: 10px; background-color: green;"></div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 10px; background-color: yellow;"></div> <div style="position: absolute; top: 0; left: 100%; width: 100%; height: 10px; background-color: grey;"></div> </div> <div> 77% 18% 5% </div> </div>

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Mol	Chain	Length	Quality of chain
2	J	22	<div><div></div><div>64%32%5%</div></div>
2	N	22	<div><div></div><div>59%36%5%</div></div>
3	C	22	<div><div></div><div>64%27%9%</div></div>
3	G	22	<div><div></div><div>50%45%5%</div></div>
3	K	22	<div><div></div><div>64%36%</div></div>
3	O	22	<div><div></div><div>59%41%</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11035 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 HOMEBOX PROTEIN NKX-2.5, T-BOX TRANSCRIPTION FACTOR TBX5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	226	Total	C	N	O	S	0	0	0
			1872	1211	339	316	6			
1	E	227	Total	C	N	O	S	0	0	0
			1893	1223	346	318	6			
1	I	226	Total	C	N	O	S	0	0	0
			1884	1215	345	318	6			
1	M	229	Total	C	N	O	S	0	0	0
			1901	1230	344	321	6			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	130	GLY	-	EXPRESSION TAG	UNP P42582
A	131	ALA	-	EXPRESSION TAG	UNP P42582
A	132	MET	-	EXPRESSION TAG	UNP P42582
A	133	GLY	-	EXPRESSION TAG	UNP P42582
A	192	SER	CYS	ENGINEERED MUTATION	UNP P42582
A	198	SER	-	LINKER	UNP P42582
A	199	SER	-	LINKER	UNP P42582
A	200	SER	-	LINKER	UNP P42582
A	201	SER	-	LINKER	UNP P42582
A	202	SER	-	LINKER	UNP P42582
A	203	SER	-	LINKER	UNP P42582
A	204	SER	-	LINKER	UNP P42582
A	205	SER	-	LINKER	UNP P42582
A	206	SER	-	LINKER	UNP P42582
A	207	SER	-	LINKER	UNP P42582
A	208	SER	-	LINKER	UNP P42582
A	209	SER	-	LINKER	UNP P42582
A	210	SER	-	LINKER	UNP P42582
A	211	SER	-	LINKER	UNP P42582
A	212	SER	-	LINKER	UNP P42582

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Chain	Residue	Modelled	Actual	Comment	Reference
A	213	ALA	-	LINKER	UNP P42582
A	1202	SER	CYS	ENGINEERED MUTATION	UNP P70326
E	130	GLY	-	EXPRESSION TAG	UNP P42582
E	131	ALA	-	EXPRESSION TAG	UNP P42582
E	132	MET	-	EXPRESSION TAG	UNP P42582
E	133	GLY	-	EXPRESSION TAG	UNP P42582
E	192	SER	CYS	ENGINEERED MUTATION	UNP P42582
E	198	SER	-	LINKER	UNP P42582
E	199	SER	-	LINKER	UNP P42582
E	200	SER	-	LINKER	UNP P42582
E	201	SER	-	LINKER	UNP P42582
E	202	SER	-	LINKER	UNP P42582
E	203	SER	-	LINKER	UNP P42582
E	204	SER	-	LINKER	UNP P42582
E	205	SER	-	LINKER	UNP P42582
E	206	SER	-	LINKER	UNP P42582
E	207	SER	-	LINKER	UNP P42582
E	208	SER	-	LINKER	UNP P42582
E	209	SER	-	LINKER	UNP P42582
E	210	SER	-	LINKER	UNP P42582
E	211	SER	-	LINKER	UNP P42582
E	212	SER	-	LINKER	UNP P42582
E	213	ALA	-	LINKER	UNP P42582
E	1202	SER	CYS	ENGINEERED MUTATION	UNP P70326
I	130	GLY	-	EXPRESSION TAG	UNP P42582
I	131	ALA	-	EXPRESSION TAG	UNP P42582
I	132	MET	-	EXPRESSION TAG	UNP P42582
I	133	GLY	-	EXPRESSION TAG	UNP P42582
I	192	SER	CYS	ENGINEERED MUTATION	UNP P42582
I	198	SER	-	LINKER	UNP P42582
I	199	SER	-	LINKER	UNP P42582
I	200	SER	-	LINKER	UNP P42582
I	201	SER	-	LINKER	UNP P42582
I	202	SER	-	LINKER	UNP P42582
I	203	SER	-	LINKER	UNP P42582
I	204	SER	-	LINKER	UNP P42582
I	205	SER	-	LINKER	UNP P42582
I	206	SER	-	LINKER	UNP P42582
I	207	SER	-	LINKER	UNP P42582
I	208	SER	-	LINKER	UNP P42582
I	209	SER	-	LINKER	UNP P42582
I	210	SER	-	LINKER	UNP P42582

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Chain	Residue	Modelled	Actual	Comment	Reference
I	211	SER	-	LINKER	UNP P42582
I	212	SER	-	LINKER	UNP P42582
I	213	ALA	-	LINKER	UNP P42582
I	1202	SER	CYS	ENGINEERED MUTATION	UNP P70326
M	130	GLY	-	EXPRESSION TAG	UNP P42582
M	131	ALA	-	EXPRESSION TAG	UNP P42582
M	132	MET	-	EXPRESSION TAG	UNP P42582
M	133	GLY	-	EXPRESSION TAG	UNP P42582
M	192	SER	CYS	ENGINEERED MUTATION	UNP P42582
M	198	SER	-	LINKER	UNP P42582
M	199	SER	-	LINKER	UNP P42582
M	200	SER	-	LINKER	UNP P42582
M	201	SER	-	LINKER	UNP P42582
M	202	SER	-	LINKER	UNP P42582
M	203	SER	-	LINKER	UNP P42582
M	204	SER	-	LINKER	UNP P42582
M	205	SER	-	LINKER	UNP P42582
M	206	SER	-	LINKER	UNP P42582
M	207	SER	-	LINKER	UNP P42582
M	208	SER	-	LINKER	UNP P42582
M	209	SER	-	LINKER	UNP P42582
M	210	SER	-	LINKER	UNP P42582
M	211	SER	-	LINKER	UNP P42582
M	212	SER	-	LINKER	UNP P42582
M	213	ALA	-	LINKER	UNP P42582
M	1202	SER	CYS	ENGINEERED MUTATION	UNP P70326

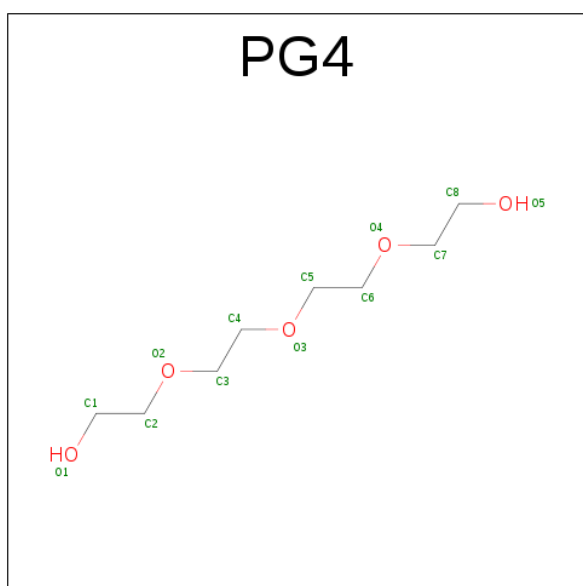
- Molecule 2 is a DNA chain called 5'-D(*TP*CP*TP*TP*CP*TP*CP*AP*CP*AP*CP*CP*TP*TP*TP*GP*AP*AP*GP*TP*GP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	21	Total	C	N	O	P	0	0	0
			426	204	72	129	21			
2	F	21	Total	C	N	O	P	0	0	0
			426	204	72	129	21			
2	J	21	Total	C	N	O	P	0	0	0
			425	203	72	129	21			
2	N	21	Total	C	N	O	P	0	0	0
			422	203	72	127	20			

- Molecule 3 is a DNA chain called 5'-D(*AP*CP*CP*AP*CP*TP*TP*CP*AP*AP*AP*GP*GP*TP*GP*TP*GP*AP*GP*AP*AP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	20	Total	C	N	O	P	0	0	0
			413	196	80	117	20			
3	G	21	Total	C	N	O	P	0	0	0
			435	206	85	123	21			
3	K	22	Total	C	N	O	P	0	0	0
			456	216	90	128	22			
3	O	22	Total	C	N	O	P	0	0	0
			456	216	90	128	22			

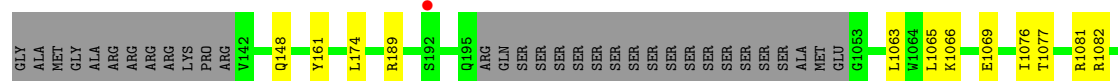
- Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	8	5		
4	C	1	Total	C	O	0	0
			13	8	5		



- Molecule 1: HOMEBOX PROTEIN NKX-2.5, T-BOX TRANSCRIPTION FACTOR TBX5



- Molecule 2: 5'-D(*TP*CP*TP*TP*CP*TP*CP*AP*CP*AP*CP*CP*TP*TP *TP*GP*AP*A P*GP*TP*GP*G)-3'



- Molecule 2: 5'-D(*TP*CP*TP*TP*CP*TP*CP*AP*CP*AP*CP*CP*TP*TP *TP*GP*AP*A P*GP*TP*GP*G)-3'



- Molecule 2: 5'-D(*TP*CP*TP*TP*CP*TP*CP*AP*CP*AP*CP*CP*TP*TP *TP*GP*AP*A P*GP*TP*GP*G)-3'

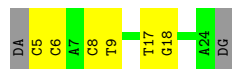


- Molecule 2: 5'-D(*TP*CP*TP*TP*CP*TP*CP*AP*CP*AP*CP*CP*TP*TP *TP*GP*AP*A P*GP*TP*GP*G)-3'



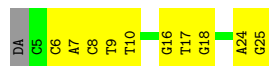
● Molecule 3: 5'-D(*AP*CP*CP*AP*CP*TP*TP*CP*AP*AP*AP*GP*GP*TP *GP*TP*GP*AP*GP*AP*AP*G)-3'

Chain C:  64% 27% 9%



● Molecule 3: 5'-D(*AP*CP*CP*AP*CP*TP*TP*CP*AP*AP*AP*GP*GP*TP *GP*TP*GP*AP*GP*AP*AP*G)-3'

Chain G:  50% 45% 5%



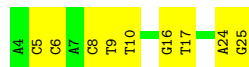
● Molecule 3: 5'-D(*AP*CP*CP*AP*CP*TP*TP*CP*AP*AP*AP*GP*GP*TP *GP*TP*GP*AP*GP*AP*AP*G)-3'

Chain K:  64% 36%



● Molecule 3: 5'-D(*AP*CP*CP*AP*CP*TP*TP*CP*AP*AP*AP*GP*GP*TP *GP*TP*GP*AP*GP*AP*AP*G)-3'

Chain O:  59% 41%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.08Å 158.62Å 87.86Å 90.00° 89.95° 90.00°	Depositor
Resolution (Å)	19.97 – 3.00 19.97 – 3.01	Depositor EDS
% Data completeness (in resolution range)	98.0 (19.97-3.00) 97.9 (19.97-3.01)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.97 (at 2.98Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.190 , 0.241 0.191 , 0.237	Depositor DCC
R_{free} test set	1076 reflections (3.48%)	DCC
Wilson B-factor (Å ²)	65.4	Xtriage
Anisotropy	0.705	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 37.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.397 for h,-k,-l	Xtriage
Reported twinning fraction	0.570 for H,-K,-L	Depositor
Outliers	1 of 30939 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11035	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PG4

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	0.23	0/1923	0.41	0/2593
1	E	0.23	0/1943	0.41	0/2618
1	I	0.23	0/1934	0.40	0/2606
1	M	0.22	0/1952	0.39	0/2631
2	B	0.58	0/475	1.06	0/730
2	F	0.57	0/475	1.08	0/730
2	J	0.59	0/474	1.06	0/728
2	N	0.61	0/470	1.06	0/720
3	C	0.60	0/464	0.95	0/714
3	G	0.57	0/489	0.95	0/753
3	K	0.55	0/513	0.95	0/790
3	O	0.57	0/513	0.96	0/790
All	All	0.38	0/11625	0.69	0/16403

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	1872	0	1901	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1893	0	1930	35	0
1	I	1884	0	1909	28	0
1	M	1901	0	1930	29	0
2	B	426	0	239	4	0
2	F	426	0	239	3	0
2	J	425	0	236	6	0
2	N	422	0	238	7	0
3	C	413	0	225	4	0
3	G	435	0	236	6	0
3	K	456	0	247	7	0
3	O	456	0	247	11	0
4	A	13	0	18	0	0
4	C	13	0	18	0	0
All	All	11035	0	9613	146	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 (146) 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:J:19:DG:H1	3:K:5:DC:H5	1.37	0.72
1:I:1087:TYR:HB3	1:I:1155:PHE:HB2	1.71	0.72
1:E:1084:PHE:O	1:E:1226:LYS:NZ	2.22	0.69
1:E:177:THR:H	1:E:180:GLN:HE21	1.44	0.65
1:A:1099:LYS:HA	1:A:1144:THR:HA	1.77	0.65
1:A:167:ARG:HD2	1:A:178:SER:HB3	1.81	0.63
1:I:1084:PHE:O	1:I:1226:LYS:NZ	2.31	0.62
1:M:148:GLN:NE2	1:M:174:LEU:O	2.32	0.62
1:E:1182:ARG:HG2	1:E:1205:VAL:HG22	1.82	0.61
2:N:19:DG:N2	3:O:6:DC:C2	2.69	0.61
1:I:1099:LYS:HA	1:I:1144:THR:HA	1.83	0.60
1:M:1099:LYS:HA	1:M:1144:THR:HA	1.84	0.60
1:E:1187:LYS:HG2	1:E:1188:ALA:H	1.66	0.60
1:M:1082:ARG:HH11	3:O:16:DG:H5''	1.66	0.59
1:E:1182:ARG:HH21	1:E:1184:HIS:HE1	1.49	0.59
1:E:1225:LEU:O	1:E:1229:ASN:ND2	2.31	0.58
3:G:9:DT:H2''	3:G:10:DT:H5''	1.85	0.58
1:A:1103:LEU:HD22	1:E:1135:LEU:HD11	1.87	0.57
1:I:1231:PRO:HA	1:I:1234:LYS:HE3	1.86	0.57
1:E:1099:LYS:HA	1:E:1144:THR:HA	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:9:DT:H2''	3:K:10:DT:H5''	1.87	0.56
1:M:1234:LYS:HB3	2:N:9:DC:H4'	1.87	0.56
2:B:18:DG:H2''	2:B:19:DG:O5'	2.05	0.56
1:A:150:TYR:OH	1:E:1164:HIS:ND1	2.33	0.56
2:J:18:DG:H2''	2:J:19:DG:H8	1.72	0.55
1:I:1182:ARG:HH21	1:I:1184:HIS:CE1	2.25	0.55
1:E:1075:ILE:HD13	1:E:1214:VAL:HG23	1.88	0.55
1:E:1164:HIS:HA	1:E:1172:ILE:HG21	1.89	0.55
1:M:1164:HIS:HA	1:M:1172:ILE:HG21	1.90	0.54
1:E:161:TYR:HA	1:E:189:ARG:HH21	1.73	0.54
1:E:192:SER:O	1:E:196:ARG:HG3	2.08	0.54
2:J:6:DC:H2''	2:J:7:DA:C8	2.43	0.54
1:M:1175:SER:O	1:M:1177:HIS:ND1	2.34	0.54
1:E:1182:ARG:HH21	1:E:1184:HIS:CE1	2.26	0.53
1:E:196:ARG:HE	1:E:1150:ARG:HH12	1.57	0.53
2:J:18:DG:H4'	2:J:19:DG:OP1	2.08	0.53
1:M:1182:ARG:HG2	1:M:1205:VAL:HG12	1.90	0.53
3:O:9:DT:H2''	3:O:10:DT:H5''	1.91	0.53
1:E:1134:ARG:NH2	1:E:1166:ASP:O	2.28	0.53
1:A:1182:ARG:HH21	1:A:1184:HIS:HE1	1.56	0.53
1:I:1113:ARG:O	1:I:1124:THR:N	2.40	0.53
1:M:1105:ASP:HB3	1:M:1135:LEU:HD22	1.90	0.53
1:E:1106:ILE:HG22	1:E:1179:TYR:HB3	1.91	0.52
1:M:1225:LEU:O	1:M:1229:ASN:ND2	2.33	0.51
3:K:24:DA:H2''	3:K:25:DG:O5'	2.10	0.51
1:M:1076:ILE:HD12	1:M:1162:ASN:HB3	1.93	0.51
1:E:1221:LYS:O	1:E:1224:GLN:HG2	2.11	0.50
1:I:1075:ILE:HD13	1:I:1214:VAL:HG23	1.93	0.49
1:A:1182:ARG:HG2	1:A:1205:VAL:HG22	1.95	0.49
1:A:1181:PRO:HG3	1:A:1211:PHE:HE2	1.77	0.49
1:I:1116:PHE:CD2	1:I:1218:GLN:HB3	2.48	0.49
1:I:1225:LEU:O	1:I:1229:ASN:ND2	2.31	0.49
3:C:8:DC:H2'	3:C:9:DT:C6	2.47	0.49
1:A:1135:LEU:HD12	1:E:1135:LEU:HD12	1.94	0.49
2:N:6:DC:H2''	2:N:7:DA:C8	2.47	0.49
1:M:1134:ARG:NH2	1:M:1166:ASP:O	2.31	0.49
1:M:1114:TYR:HE2	1:M:1178:LYS:HD2	1.78	0.49
1:A:1101:ILE:HG12	1:A:1142:PRO:HB3	1.95	0.48
1:E:177:THR:H	1:E:180:GLN:NE2	2.11	0.48
1:I:1082:ARG:HD2	3:K:16:DG:H5''	1.94	0.48
1:A:1135:LEU:HD11	1:E:1103:LEU:HD22	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:1063:LEU:HD12	1:I:1066:LYS:HD3	1.95	0.48
2:N:19:DG:H1	3:O:5:DC:H42	1.60	0.48
1:A:1075:ILE:HD13	1:A:1214:VAL:HG23	1.96	0.48
2:F:18:DG:H2''	2:F:19:DG:O5'	2.14	0.48
1:I:1235:GLY:HA2	2:J:9:DC:H5'	1.95	0.48
1:E:196:ARG:NE	1:E:1150:ARG:HH12	2.11	0.47
3:G:24:DA:H2''	3:G:25:DG:O5'	2.14	0.47
3:G:7:DA:H2''	3:G:8:DC:C6	2.48	0.47
1:I:1182:ARG:HH21	1:I:1184:HIS:HE1	1.60	0.47
1:I:160:ARG:NH2	1:I:196:ARG:HH22	2.13	0.47
1:E:189:ARG:O	1:E:193:LYS:HG2	2.15	0.47
2:N:10:DT:H1'	2:N:11:DT:H5'	1.95	0.47
1:I:1182:ARG:HG2	1:I:1205:VAL:HG22	1.97	0.47
1:I:161:TYR:HD2	3:K:5:DC:OP1	1.98	0.46
1:E:1227:ILE:O	1:E:1237:ARG:NE	2.45	0.46
1:E:1076:ILE:HG22	1:E:1160:LEU:HB3	1.98	0.45
1:E:1112:HIS:HB3	1:E:1123:VAL:HG13	1.99	0.45
1:I:1116:PHE:CZ	1:I:1119:ASN:HA	2.50	0.45
1:A:185:PHE:O	1:A:189:ARG:HG3	2.16	0.45
1:A:1095:ASN:HB3	1:A:1098:THR:HB	1.98	0.45
1:I:1106:ILE:HG22	1:I:1179:TYR:HB3	1.98	0.45
3:O:24:DA:H2''	3:O:25:DG:O5'	2.17	0.45
1:A:1106:ILE:HG22	1:A:1179:TYR:HB3	1.99	0.44
1:I:1110:ASP:OD2	1:I:1114:TYR:OH	2.26	0.44
1:M:1181:PRO:HG3	1:M:1211:PHE:HE1	1.82	0.44
2:B:10:DT:H1'	2:B:11:DT:H5'	1.98	0.44
2:J:10:DT:H1'	2:J:11:DT:H5'	1.99	0.44
1:A:1107:VAL:HG11	1:A:1182:ARG:NH1	2.31	0.44
1:M:161:TYR:HD2	3:O:5:DC:OP1	2.01	0.44
1:E:1081:ARG:NH2	3:G:18:DG:OP2	2.45	0.44
1:I:1175:SER:O	1:I:1177:HIS:ND1	2.39	0.44
1:M:1077:THR:HG23	1:M:1081:ARG:HB2	2.00	0.44
1:I:1176:MET:N	1:I:1213:ALA:O	2.48	0.44
1:A:1208:GLU:OE1	1:A:1208:GLU:N	2.47	0.44
1:M:1063:LEU:HD12	1:M:1066:LYS:HE3	1.99	0.44
1:A:1105:ASP:OD1	1:A:1184:HIS:NE2	2.48	0.43
1:A:1076:ILE:HD13	1:A:1213:ALA:HB1	2.00	0.43
2:F:10:DT:H1'	2:F:11:DT:H5'	2.00	0.43
2:B:6:DC:H2''	2:B:7:DA:C8	2.54	0.43
1:M:1208:GLU:OE1	1:M:1208:GLU:N	2.44	0.43
1:A:1062:GLU:O	1:A:1066:LYS:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1095:ASN:HB3	1:E:1098:THR:HB	1.99	0.43
1:A:1112:HIS:HD2	1:A:1123:VAL:HG11	1.84	0.43
2:F:18:DG:H1	3:G:6:DC:H42	1.67	0.43
1:A:189:ARG:NH1	3:C:6:DC:OP2	2.48	0.43
1:M:189:ARG:HD2	3:O:6:DC:OP2	2.19	0.43
3:K:16:DG:H2''	3:K:17:DT:H5'	2.01	0.42
1:E:1062:GLU:H	1:E:1062:GLU:CD	2.23	0.42
1:I:1208:GLU:N	1:I:1208:GLU:OE1	2.47	0.42
2:B:13:DG:H2''	2:B:14:DA:C8	2.54	0.42
1:E:1065:LEU:O	1:E:1069:GLU:HG2	2.20	0.42
2:N:13:DG:H2''	2:N:14:DA:C8	2.54	0.42
1:M:1116:PHE:CD2	1:M:1218:GLN:HB3	2.54	0.42
1:M:1182:ARG:HH21	1:M:1184:HIS:CE1	2.37	0.42
1:A:1084:PHE:O	1:A:1226:LYS:NZ	2.37	0.42
3:C:17:DT:H2''	3:C:18:DG:C8	2.54	0.42
1:I:1110:ASP:N	1:I:1110:ASP:OD1	2.53	0.42
1:M:1105:ASP:OD1	1:M:1184:HIS:NE2	2.49	0.42
3:C:5:DC:H2'	3:C:6:DC:C6	2.55	0.42
1:E:1058:LEU:HB2	1:E:1206:PHE:CE2	2.54	0.42
3:K:5:DC:H2'	3:K:6:DC:C6	2.55	0.42
3:O:8:DC:H2'	3:O:9:DT:C6	2.55	0.41
1:A:1110:ASP:OD1	1:A:1110:ASP:N	2.53	0.41
1:A:1182:ARG:HH21	1:A:1184:HIS:CE1	2.37	0.41
1:E:1062:GLU:O	1:E:1066:LYS:HG3	2.20	0.41
1:I:185:PHE:O	1:I:189:ARG:HG3	2.20	0.41
1:M:1105:ASP:OD1	1:M:1182:ARG:HB2	2.19	0.41
1:I:140:PRO:N	1:I:141:ARG:HA	2.35	0.41
1:M:1065:LEU:O	1:M:1069:GLU:HG2	2.20	0.41
1:I:1077:THR:HG23	1:I:1081:ARG:HB2	2.03	0.41
1:M:1110:ASP:N	1:M:1110:ASP:OD1	2.53	0.41
1:M:1166:ASP:HA	1:M:1167:PRO:HD3	1.88	0.41
2:N:19:DG:N2	3:O:5:DC:N3	2.63	0.41
1:I:1106:ILE:CG2	1:I:1179:TYR:HB3	2.51	0.41
1:I:1073:GLU:HB2	1:I:1222:ILE:HG21	2.02	0.41
1:M:1101:ILE:HG12	1:M:1142:PRO:HB3	2.02	0.41
1:M:1091:VAL:HG13	1:M:1149:MET:HG2	2.03	0.41
1:M:1082:ARG:HD2	3:O:16:DG:H5''	2.03	0.41
1:E:1164:HIS:HA	1:E:1172:ILE:HD13	2.03	0.41
3:G:16:DG:H2''	3:G:17:DT:H5'	2.03	0.41
3:O:16:DG:H2''	3:O:17:DT:H5'	2.03	0.40
1:E:1099:LYS:HG2	1:E:1144:THR:HG22	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1110:ASP:OD1	1:E:1110:ASP:N	2.53	0.40
1:M:1186:VAL:HG12	1:M:1187:LYS:H	1.87	0.40
1:A:1076:ILE:HD12	1:A:1162:ASN:HB3	2.03	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	220/285 (77%)	214 (97%)	6 (3%)	0	100	100
1	E	221/285 (78%)	215 (97%)	6 (3%)	0	100	100
1	I	218/285 (76%)	209 (96%)	9 (4%)	0	100	100
1	M	223/285 (78%)	215 (96%)	8 (4%)	0	100	100
All	All	882/1140 (77%)	853 (97%)	29 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	202/253 (80%)	201 (100%)	1 (0%)	91	97
1	E	205/253 (81%)	202 (98%)	3 (2%)	70	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	204/253 (81%)	201 (98%)	3 (2%)	70	91
1	M	205/253 (81%)	203 (99%)	2 (1%)	80	94
All	All	816/1012 (81%)	807 (99%)	9 (1%)	78	93

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1059	HIS
1	E	146	GLN
1	E	1061	ARG
1	E	1062	GLU
1	I	141	ARG
1	I	143	LEU
1	I	1204	HIS
1	M	1150	ARG
1	M	1220	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	180	GLN
1	E	1156	GLN
1	I	1156	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	PG4	A	2239	-	12,12,12	0.68	0	11,11,11	1.49	0
4	PG4	C	2025	-	12,12,12	0.68	0	11,11,11	1.46	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PG4	A	2239	-	-	0/10/10/10	0/0/0/0
4	PG4	C	2025	-	-	0/10/10/10	0/0/0/0

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, 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	226/285 (79%)	-0.01	3 (1%) 77 51	41, 63, 84, 105	0
1	E	227/285 (79%)	0.08	1 (0%) 92 77	44, 66, 98, 117	0
1	I	226/285 (79%)	0.26	4 (1%) 69 40	47, 79, 103, 119	0
1	M	229/285 (80%)	0.15	4 (1%) 70 42	49, 74, 99, 117	0
2	B	21/22 (95%)	-0.36	0 100 100	68, 77, 92, 101	0
2	F	21/22 (95%)	-0.31	0 100 100	65, 77, 88, 108	0
2	J	21/22 (95%)	-0.25	0 100 100	70, 81, 92, 120	0
2	N	21/22 (95%)	-0.32	0 100 100	48, 70, 85, 94	0
3	C	20/22 (90%)	-0.23	0 100 100	64, 86, 98, 101	0
3	G	21/22 (95%)	-0.28	0 100 100	65, 76, 102, 111	0
3	K	22/22 (100%)	-0.12	0 100 100	67, 80, 108, 116	0
3	O	22/22 (100%)	-0.16	0 100 100	63, 69, 98, 117	0
All	All	1077/1316 (81%)	0.06	12 (1%) 80 55	41, 72, 100, 120	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	1201	PHE	3.2
1	A	1118	ASP	3.1
1	A	1128	GLU	2.8
1	I	172	SER	2.8
1	I	1062	GLU	2.7
1	M	192	SER	2.7
1	I	1119	ASN	2.5
1	A	1130	ALA	2.5
1	M	1202	SER	2.5
1	I	1091	VAL	2.4
1	M	1220	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	197	GLN	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
4	PG4	C	2025	13/13	0.78	0.28	-0.12	75,91,106,107	0
4	PG4	A	2239	13/13	0.83	0.23	-0.60	61,68,83,85	0

6.5 Other polymers [i](#)

There are no such residues in this entry.